Type: New

Title: "CHiMES: Coupled High-resolution Modeling of the Earth System"

Principal Investigator: Venkatramani Balaji, NOAA/Geophysical Fluid Dynamics Laboratory (GFDL)

Co-Investigators: Christopher Kerr, University Corporation for Atmospheric Research
Tom Delworth, NOAA/GFDL
Tony Rosati, NOAA/GFDL
Isaac Held, NOAA/GFDL
S.-J. Lin, NOAA/GFDL

Scientific Discipline: Climate Research

INCITE allocation: 24,000,000 Processor Hours
  Site: Oak Ridge National Laboratory
    Machine: Cray XTs
    Allocation: 24,000,000 processor hours

Research Summary:
Current resolutions of IPCC-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: at 25 km resolution or so, we begin to see the influence of both ocean eddies and organized atmospheric storm systems.

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 statistically robust answers to key questions about the response of modeled tropical storm frequencies and intensity to climate change.

Type: New

Title: "Integrated Simulations of Energetic Particles Driven by High Power Electromagnetic Waves in Fusion Plasmas"

Principal Investigator: Paul Bonoli, Plasma Science and Fusion Center
Co-Investigators: Donald Batchelor, Oak Ridge National Laboratory

Scientific Discipline: Plasma Physics

INCITE allocation: 5,000,000 Processor Hours
   Site: Lawrence Berkeley National Laboratory
   Machine: NERSC HPC
   Allocation: 5,000,000 processor hours

Research Summary:
High-power electromagnetic waves in the radio frequency (RF) range have been widely used in fusion experiments to heat plasmas into the burning regime and to control plasma behavior through localized energy deposition, driven current, driven plasma flows and production of highly non-thermal, energetic particle populations. These processes can influence energy and particle transport in fusion devices, thereby affecting the efficiency of the magnetic confinement, and can also influence plasma stability—sometimes producing instability and sometimes reducing or eliminating instability. ITER will make use of waves at the tens of megawatt level in several frequency regimes. The capability to understand and predict the effects of RF waves on plasma behavior would be of significant scientific and economic benefit for fusion energy.

We propose to investigate two important aspects of interaction between RF waves and energetic plasma particles in tokamaks: 1) The interaction of waves in the ion cyclotron range of frequencies (ICRF) with energetic particles—specifically the dynamics of energetic particle production due to ICRF heating of minority plasma species and their effect on plasma evolution and stability. 2) The interaction of waves in the lower hybrid range of frequencies (LHRF) with nonthermal electrons produced by the lower hybrid waves themselves – specifically self-consistent studies of the "spectral gap" problem in lower hybrid current drive with a full, 3-dimensional antenna spectrum, and coming to an understanding of the discrepancy seen between full wave calculations of lower hybrid wave propagation compared to the results of geometrical optics.

Type: New

Title: "The Role of Eddies in the Meridional Overturning Circulation"

Principal Investigator: Paola Cessi, Scripps Institution of Oceanography/University of California, San Diego

Co-Investigators: Christopher Wolfe, Scripps Institution of Oceanography/ University of California, San Diego

Scientific Discipline: Climate Research

INCITE allocation: 5,000,000 Processor Hours
   Site: Argonne National Laboratory
   Machine: IBM Blue Gene/P
   Allocation: 5,000,000 processor hours

Research Summary:
Our goal is to study the processes that maintain the abyssal circulation of the ocean and to understand its response to altered atmospheric composition. Our approach is to analyze high resolution models of the ocean component of the climate system in domains of moderate size, but for a wide range of the external parameters, such as the wind speed, the surface temperature and the abyssal mixing. The proposed research will contribute to establishing the fundamental dynamics of the thermohaline circulation, an essential component of the ocean-atmosphere heat budget and a major player in sequestering CO_2 into the deep ocean.

Type: New

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: Plasma Physics

INCITE allocation: 20,000,000 Processor Hours
 Site: Oak Ridge National Laboratory
  Machine: Cray XTs
  Allocation: 20,000,000 processor hours

Research Summary:
It has been commonly predicted that the world oil resources will run out in approximately 30 years if the oil production is increased to meet the rise in the energy consumption, arousing serious concern over the possible political and economical instabilities. At the same time, avoidance of environmental disasters from the greenhouse effect requires that at least 90% of the additional energy supply must be from the CO_2 free resources by the year 2100. Even an optimistic estimate of the various renewable energy sources is far from solving these problems. Plasma fusion in a magnetically confinement reactor is one of very few possible options which can ease these problems. Commercialization of the magnetic fusion (and the success of ITER tokamak device) requires good confinement of plasma energy at the plasma edge to form an energy pedestal significantly above the cold, wall-interacting plasma energy in the "scrape-off" layer. Edge confinement is conjectured to be governed by the kinetic micro-scale turbulent transport and the kinetic macro-scale equilibrium transport in a mutually self-organizing manner. When the micro-scale turbulence is suppressed and a steep edge gradient forms above a critical level, the large scale edge localized mode (ELM) instabilities break out to destroy the steep edge pedestal.

This INCITE project will simulate the kinetic edge plasma properties and dynamics in realistic tokamak geometry, without spatial scale separation, through large scale simulations on HPC. The simulation results will be validated in the existing tokamaks, and applied to predict the edge pedestal shape and height in the future ITER plasmas.

Type: New

Title: "Surface Input Reanalysis for Climate Applications (SIRCA) 1850-2011"

Principal Investigator: Gilbert Compo, University of Colorado/CIRES/Climate Diagnostics Center and NOAA Earth System Research Laboratory/PSD

Co-Investigators: Jeffrey Whitaker, NOAA Earth System Research Laboratory

Prashant Sardeshmukh, University of Colorado/CIRES/Climate Diagnostics Center and NOAA Earth System Research Laboratory

Scientific Discipline: Climate Research

INCITE allocation: 1,100,000 Processor Hours
  Site: Oak Ridge National Laboratory
    Machine: Cray XTs
    Allocation: 1,100,000 processor hours

Research Summary:
High-quality six-hourly tropospheric circulation datasets for the period 1850 to present are urgently needed to validate the climate models now being used to predict anthropogenic climate change. High performance computing resources are required to generate such datasets. In this INCITE project, we will use the Ensemble Kalman Filter, developed at the University of Colorado and NOAA's Earth System Research Laboratory, and newly gathered surface pressure observations to produce the first-ever reanalysis dataset for the period 1850-2011 at a resolution of 100 km. This will more than double the record of 6-hourly tropospheric gridded global fields from 60 years to 162, spanning a period for which no gridded upper-air analyses are currently available. These tropospheric circulation fields will also be the first to have objective uncertainty estimates for every analyzed variable. In addition to validating and improving climate models, our dataset will be used to study climatic variations that could not previously be addressed observationally, such as the 1877 El Nino and Indian famine, the 1930s U.S. Dust Bowl and the 1920s to 1940s Arctic warming. The timely production of such as dataset will provide an important check on the climate models that were used to make 21st century climate projections in the Fourth Assessment Report of the Intergovernmental Panel on Climate Change (IPCC) and help improve the climate models that will contribute to the IPCC's Fifth Assessment Report.

Type: New

Title: "Large scale condensed matter and fluid dynamics simulations"

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

Scientific Discipline: Materials Sciences

INCITE allocation: 40,000,000 Processor Hours
  Site: Argonne National Laboratory
   Machine: IBM Blue Gene/P
   Allocation: 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 behaviour plays a crucial role in the understanding, diagnosis and treatment of cardiovascular disease; problems are often due to anomalous blood flow behaviour in the neighbourhood 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 clay-polymer 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: New

Title: "Massively parallel simulation of pump-probe time-resolved photoemission"

Principal Investigator: James Freericks, Georgetown University
Co-Investigators: Brian Moritz, SLAC National Accelerator Laboratory
Thomas Devereaux, SLAC National Accelerator Laboratory

Scientific Discipline: Materials Sciences

INCITE allocation: 2,250,000 Processor Hours
  Site: Lawrence Berkeley National Laboratory
   Machine: NERSC HPC
   Allocation: 2,250,000 processor hours

Research Summary:
New facilities and recent developments in experimental techniques open the door to studying, in real-time, the evolution of a system irradiated with intense pulses of light that excite the system into a nonequilibrium state with the aim of unlocking the nature of the processes that govern the physical and chemical properties of the material. Many of these new techniques utilize a pump-probe scheme that synchronizes the photoexcitation pulse with the probe pulse providing short time-scale information with femtosecond resolution of the excitation and relaxation processes at work. A key ingredient to the success of these endeavors will be developments in theory that shed light on the physics uncovered by these experiments and chart a new path forward for understanding systems out-of-equilibrium.

The general theoretical interpretation of pump-probe experiments has been that the pump pulse creates "hot electrons" in quasi-equilibrium at a higher effective temperature than the phonons in the material. Such a point of view is valid for situations where the nonequilibrium state is not being probed directly at the shortest time scales, and the electronic system rapidly relaxes to a quasi-equilibrium distribution. But this approach fails to address two important issues in these experiments: (1) the true nonequilibrium dynamics of the system and (2) the effects associated with the finite probe pulse width. These theoretical issues are fully addressed by the methods we propose to employ in our INCITE project.

Type: New

Title: "High fidelity computations for complex biological membranes"

Principal Investigator: Michael Heroux, Sandia National Laboratories
Co-Investigators: Laura Frink, Sandia National Laboratories

Scientific Discipline: Atomic/Molecular Physics

INCITE allocation: 1,000,000 Processor Hours
   Site: Oak Ridge National Laboratory
      Machine: Cray XTs
      Allocation: 1,000,000 processor hours

Research Summary:
Membranes, such as lipid bilayers, are fundamental entities in biological systems. Our goal is to provide insight into the detailed workings of the biophysics of these membranes, enabling breakthroughs in disease mechanisms and new treatments. Recent modeling advances in classical density functional theories (DFT), along with advanced scalable solution algorithms make high-fidelity simulations possible for the first time. Antimicrobial peptides (AMPs) are part of the innate immune systems of higher organisms, and can be lethal to bacteria. While AMPs are quite important, their mechanism of action (which may be varied among several families) is not yet completely understood. It is most likely that a direct (not receptor mediated) interaction between the AMPs and the cell outer membrane leads to increased cell permeability. However, in certain proline-rich AMPs, bacteria can be killed without significant membrane perturbation suggesting intracellular targets. Our research program seeks to elucidate the differences in membrane-AMP interactions. Specifically, we seek to calculate membrane perturbations in the presence of AMPs or AMP assemblies, and compute insertion energies associated with those AMPs and their assemblies.

We will extend existing results by considering AMPs of different geometry and chemistry, AMPs derived more explicitly from a molecular description of the peptide, and by performing comparative studies of different types of AMPs (for example cyclic and non-pore forming peptides). We will also consider insertion pathways and compute free energy of a single peptide or peptide assembly as a function of the position of the peptide relative to the center of the membrane. Finally, we will consider increasing the fidelity of the models with explicit charge groups and electrolyte components.

Type: New

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

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

Scientific Discipline: Engineering

INCITE allocation: 1,000,000 Processor Hours
   Site: Oak Ridge National Laboratory
      Machine: Cray XTs
      Allocation: 1,000,000 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 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, as well as more simulations to be included in the computation-result databases.

Several aspects of airplane aerodynamics of interest will be our focus areas. The list includes (but is 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 unstructured-grid Navier-Stokes solver for both transonic and high-lift (landing and take off) 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: New

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, The Scripps Research Institute and Lawrence Berkeley National Laboratory
Xiaolin Cheng, Oak Ridge National Laboratory
J. Andrew McCammon, University of California, San Diego and Howard Hughes Medical Institute

Scientific Discipline: Biological Sciences

INCITE allocation: 2,600,000 Processor Hours
  Site: Oak Ridge National Laboratory
    Machine: Cray XTs
    Allocation: 2,600,000 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 reseach 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, oxydative stress are of direct relevance to the mission of DOE.

Type: New

Title: "Petascale Adaptive CFD for Anisotropic Flows"

Principal Investigator: Kenneth Jansen, Rensselaer Polytechnic Institute

Co-Investigators: Onkar Sahni, Rensselaer Polytechnic Institute
Christopher Carothers, Rensselaer Polytechnic Institute
Mark Shephard, Rensselaer Polytechnic Institute

Scientific Discipline: Engineering

INCITE allocation: 5,000,000 Processor Hours
  Site: Argonne National Laboratory
   Machine: IBM Blue Gene/P
   Allocation: 5,000,000 processor hours

Research Summary:
This project will involve large-scale adaptive simulations including aerodynamic and multi-phase flows. These simulations will be performed in complement to existing and ongoing experimental investigations. The aerodynamic simulations involve modeling of synthetic jets that have been shown experimentally to produce large scale flow changes (e.g., re-attachment of separated flow) from micro-scale input (e.g., a 0.1 W piezoelectric disk resonating in a cavity); a process that has yet to be explained fundamentally. This active flow control offers the prospect of increasing or decreasing lift on wind turbine blades in dynamic response to gust loads, thereby reducing unsteady loads on blades and therefore on gearboxes which are currently the prime failure point. The two-phase simulation work is critical to nuclear reactor modeling where a variety of accident scenarios currently lack adequate modeling capability (e.g., classical burnout conditions in heat exchanger tubes or core breach in Generation IV reactors). Such high-fidelity simulations will result in better understanding of the complex flow physics leading to improved models in respective areas and also provide scientific insights that will be the first of their kind. This effort will also reinforce and advance the parallel computational tools like unstructured, anisotropic mesh adaptivity and iterative, implicit equation solvers, that are useful to other complex applications.

Type: New

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
Kim Bak Olsen, California State University San Diego

Scientific Discipline: Environmental Sciences

INCITE allocation: 5,000,000 Processor Hours
  Site: Argonne National Laboratory
   Machine: IBM Blue Gene/P
   Allocation: 5,000,000 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 (Mw7.0+) scenario earthquakes at frequencies above 1Hz on a regional scale. These simulations will utilize a realistic 3D 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 due to the scientific and societal information these simulations will produce. The two primary goals for this work are: (G1) Investigate the upper frequency limits of deterministic ground motion simulations, and (G2) Better quantify how high frequency seismic waves from large earthquakes contribute to the seismic hazard in Southern California and other regions.

Type: New

Title: "Petascale Simulations of Nano-electronic Devices"

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

Scientific Discipline: Engineering

INCITE allocation: 5,000,000 Processor Hours
   Site: Oak Ridge National Laboratory
      Machine: Cray XTs
      Allocation: 5,000,000 processor hours

Research Summary:
With the advent of nanoscale fabrication, a new generation of nano-electronic devices is expected to produce enormous advances not only in computing and information technologies, but in other fields such as medicine. The new generation of device models are atomistic, and need to account for strain, surface roughness, impurities that can affect properties and performance of nano-electronic devices. Whereas classical physics was used to build very successful semi-conductor device models in the past, nanoscale devices require a quantum mechanical description to capture 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 3D quantum transport in nano-devices. We also compute the electronic structure of nano-devices using an empirical tight-binding basis, for tens of millions of atoms. With a quantum mechanical description of a device comes a significantly greater modeling and computing challenge.

This work will enable discovery of new technologies for faster switching, smaller feature size, and reduced heat generation. The creation of a new switch 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: "Intermittency and Star Formation in Turbulent Molecular Clouds"

Principal Investigator: Alexei Kritsuk, UC, San Diego
Co-Investigators: Paolo Padoan, University of California, San Diego
Michael Norman, University of California, San Diego

Scientific Discipline: Astrophysics

INCITE allocation: 5,000,000 Processor Hours
  Site: Oak Ridge National Laboratory
   Machine: Cray XTs
   Allocation: 5,000,000 processor hours

Research Summary:
Supersonic turbulence within molecular clouds scattered around in the spiral arms of the Milky Way is believed to control the ongoing star formation processes. Shock waves traveling a few kilometers per second through the 10 Kelvin molecular gas tend to tear the clouds into smaller pieces and trigger the collapse of the most over-dense fragments. Understanding the statistics of supersonic turbulence is a key to a general theory of star formation. Our simulations will model this process in unprecedented detail. First, we will be able to study scaling relations and develop intermittency models for highly compressible MHD turbulence at large Reynolds numbers. Second, the simulations will help to validate modern theories for the origin of stars that aim to explain the stellar initial mass function (IMF). The origin of the IMF is a very basic aspect of any successful statistical theory of star formation.

Type: New

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: Climate Research

INCITE allocation: 25,000,000 Processor Hours
  Site: Argonne National Laboratory
   Machine: IBM Blue Gene/P
   Allocation: 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, a good approximation for quasi-geostrophic flows such as
large-scale, vortical 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: "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: Klaus Weide, University of Chicago ASC FLASH Center
George Jordan, University of Chicago ASC FLASH Center
Dean Townsley, University of Chicago ASC FLASH Center
Anshu Dubey, University of Chicago ASC FLASH Center
Robert Fisher, University of Chicago ASC FLASH Center
Katherine Riley, University of Chicago ASC FLASH Center
Michael Papka, University of Chicago ASC Flash Center
Nathan Hearn, University of Chicago ASC FLASH Center

Scientific Discipline: Astrophysics

INCITE allocation: 70,000,000 Processor Hours
  Site: Argonne National Laboratory
    Machine: IBM Blue Gene/P
    Allocation: 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: "Fundamental study of shock/turbulence interaction"

Principal Investigator: Sanjiva Lele, Stanford University
Co-Investigators: Johan Larsson, Stanford University
Parviz Moin, Stanford University
Eric Johnsen, Stanford University

Scientific Discipline: Engineering

INCITE allocation: 8,000,000 Processor Hours
  Site: Argonne National Laboratory
   Machine: IBM Blue Gene/P
   Allocation: 8,000,000 processor hours

Research Summary:
On supersonic aircraft, up to 10% of the mass flow into the inlet system is bled through various slots to maintain shock stability and controlled flow. The impact on the performance is thus considerable (up to 20% in range, 10% in gross take-off weight). Current turbulence models in use for predicting interactions between shock waves and turbulence are woefully inadequate because of a lack of basic understanding of shock/turbulence interaction. High quality direct numerical simulations (DNS) data of this problem will enable the development of a new class of lower-fidelity physics-based models for use in engineering design and analysis; these new models of turbulence behavior in supersonic and hypersonic flow may revolutionize the design and analysis of high-speed propulsion systems.

We propose to conduct unprecedented direct numerical simulation of canonical shock/turbulence interactions. These calculations will be the first in which the viscous dissipation behind the shock is fully resolved and in which truly broadband turbulence interacts with a shock wave. The INCITE allocation will allow us to study the fundamental physics governing this phenomenon, thus advancing the scientific knowledge in this field, and to develop physics-based turbulence models that will allow for exploration of new design ideas for supersonic aircrafts with greater confidence.

Type: New

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: Bette Otto-Bliesner, The National Center for Atmospheric Research
David Erickson III, Oak Ridge National Laboratory
Robert Jacob, Argonne National Laboratory

Scientific Discipline: Climate Research

INCITE allocation: 4,000,000 Processor Hours
  Site: Oak Ridge National Laboratory
   Machine: Cray XTs
   Allocation: 4,000,000 processor hours

Research Summary:
We propose to complete the first set of synchronously coupled transient ocean-atmosphere dynamic vegetation GCM simulations of the past 21,000 years. In comparison with proxy climate records of the last 21,000, these experiments will will significantly enhance our understanding of the transient response of the earth system to different climate forcings. Our 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: New

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: Marcel Zemp, 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
Juerg Diemand, University of California, Santa Cruz

Scientific Discipline: Astrophysics

INCITE allocation: 5,000,000 Processor Hours
  Site: Oak Ridge National Laboratory
   Machine: Cray XTs
   Allocation: 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 towards 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 abundance 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?

Type: New

Title: "Propulsor Analyses for a Greener, High Bypass Ratio, Aircraft Gas Turbine Engine"

Principal Investigator: Robert Malecki, Pratt & Whitney
Co-Investigators: Pete Bradley, Pratt & Whitney

Scientific Discipline: Engineering

INCITE allocation: 1,500,000 Processor Hours
   Site: Oak Ridge National Laboratory
     Machine: Cray XTs
     Allocation: 1,500,000 processor hours

Research Summary:
As world events have resulted in the end of "cheap" jet fuel, jet fuel has become a greater proportion (30-50%) of airline operating costs than it was in the first part of this decade. In addition, worldwide recognition of the threat of global warming has spurred interest in reducing CO_2 emissions of aircraft jet engines, which in turn is also driving future aircraft engines to become more fuel efficient. Concurrently, engine noise regulations continue to become more stringent, driving aircraft engine manufacturers to reduce community engine noise. One means to simultaneously achieve fuel burn, CO_2 emissions, and engine noise reduction is to increase the bypass ratio (BPR) of the turbofan aircraft gas turbine engine. As BPR increases, the aerodynamic performance of the fan stream becomes increasingly important.

Proposed is a two-year program which analytically investigates aerodynamic performance of the fully detailed fan stream along with acoustics generation and propagation within the fan stream. All analyses will model the Pratt & Whitney Geared Turbofan™ Demonstrator geometry and flow conditions, and will utilize the FLUENT® commercial CFD analysis solver. In the first year, aerodynamic performance analyses of the entire fan stream static structure, including the fan-exit-guide-vanes (FEGVs) and all details of the fan duct (intakes, offtakes, vents,heat-exchanger systems, etc.) will be conducted. In the second year, the entire propulsor stream, including the inlet, fan, FEGVs, fan duct and exhaust nozzle, will be simulated for aerodynamic performance at various condition, including in-flight windmilling, and also for fan/FEGV acoustic source generation and propagation through the fan duct.

Type: New

Title: "Structural and dynamical studies of hydronium and hydroxide ions in bulk water and at the water/air interface using ab initio path integral simulations"

Principal Investigator: Thomas Miller, California Institute of Technology

Co-Investigators: Douglas Tobias, University of California, Irvine
Mark Tuckerman, New York University

Scientific Discipline: Chemical Sciences

INCITE allocation: 12,000,000 Processor Hours
   Site: Oak Ridge National Laboratory
   Machine: Cray XTs
   Allocation: 12,000,000 processor hours

Research Summary:
Ab initio molecular dynamics calculations of the solvation and transport of hydroxide in bulk water have inspired a variety of recent experiments ranging from vibrational spectroscopy, neutron scattering, and X-ray studies. Here, we propose to employ ab initio path integral (AIPI) simulation methods to study the structural and dynamical properties of hydroxide and hydronium ions in bulk water and at the air/water interface. The subtle interactions that govern these systems demand simulations that account for quantization of the nuclear motion and that are fully converged with respect to system size and the electronic structure basis set. Using recently developed methodology, we will meet these demands and obtain results that will guide both experimental studies and more approximate modeling efforts. Key questions that will be investigated include: the relative affinity of hydroxide and hydronium ions for the air/water interface; the degree to which nuclear quantization affects the structure and diffusion of hydroxide ions in the interfacial region; and the degree to which temperature changes alter the diffusion and reorientation of hydroxide ions in bulk water. Understanding these ions is essential because of their important role in biological processes and in the basic chemistry of solar energy conversion.

Type: New

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

Principal Investigator: William Nevins, Lawrence Livermore National Laboratory

Co-Investigators: Scott Parker, University of Colorado
Christopher Holland, Univ of California at San Diego
Darin Ernst, Massachusetts Institute of Technology
Jeff Candy, General Atomics
David Mikkelsen, Princeton Plasma Physics Laboratory
William Dorland, University of Maryland

Scientific Discipline: Plasma Physics

INCITE allocation: 20,000,000 Processor Hours
   Site: Oak Ridge National Laboratory
   Machine: Cray XTs
   Allocation: 20,000,000 processor hours

Research Summary:
Plasma microturbulence, the dominant mechanism for the loss of heat from tokamaks, will determine the fusion gain that can be achieved in ITER (see http://www.iter.org/). 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 US fusion program,and achieving it requires the validation of high-fidelity plasma microturbulence codes. This proposal is to validate the three most advanced plasma microturublence codes in the US program (GYRO, GS2, and GEM) against transport and fluctuation data from the three large US 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 US 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: New

Title: "Dynamically tunable ferroelectric surface catalysts"

Principal Investigator: Andrew Rappe, University of Pennsylvania
Co-Investigators:

Scientific Discipline: Chemical Sciences

INCITE allocation: 2,283,200 Processor Hours
  Site: Oak Ridge National Laboratory
    Machine: Cray XTs
    Allocation: 2,283,200 processor hours

Research Summary:
The main objective of the proposed research program is a computational demonstration of feasible dynamically tunable heterogeneous catalysts. Many surface catalysts with valuable properties have been developed, but once a catalyst is fabricated, its ability to adapt to changing reaction conditions is limited. Tunable catalysts would bring significant advantages, enhancing reactivity in harsh environments where control of conditions is difficult, making new chemical transformations feasible, and reducing the process requirements for others. We propose to use density functional theory (DFT) to investigate the ferroelectric ABO_3 oxide surfaces, bare and metal-covered, as candidate tunable catalyst systems. This work builds on a wealth of recent theoretical and experimental research illustrating the importance of electric polarization for surface reactivity, as well as recent advances in understanding how to change the magnitude and direction of electric polarization reversibly in ferroelectric oxides.

Our work will illuminate how the polarization of a ferroelectric material can affect surface reactivity, and also identify lead candidate systems for experimental study and future industrial applications. Our extensive experience studying molecule-surface interactions and ferroelectrics enhances our ability to explore the range of phenomena exhibited by ferroelectric substrate catalysts. Our previous results strongly suggest that ferroelectric polarization can significantly change surface reactivity, and the proposed research program will help explain this promising finding and harness it for practical applications.

Type: New

Title: "Sculpting Biological Membranes by Proteins"

Principal Investigator: Klaus Schulten, University of Illinois
Co-Investigators:

Scientific Discipline: Biological Sciences

INCITE allocation: 9,240,000 Processor Hours
  Site: Argonne National Laboratory
   Machine: IBM Blue Gene/P
   Allocation: 9,240,000 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 multi-scale 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: "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

INCITE allocation: 3,000,000 Processor Hours
   Site: Argonne National Laboratory
   Machine: IBM Blue Gene/P
   Allocation: 3,000,000 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: Renewal

Title: "Molecular simulations of surfactant assisted aqueous foam formation"

Principal Investigator: Kelly Anderson, Procter and Gamble
Co-Investigators: Michael Klein, University of Pennsylvania
Bill Laidig, Procter and Gamble
Chris Stoltz, Procter and Gamble
Pierre Verstraete, Procter and Gamble

Scientific Discipline: Chemical Sciences

INCITE allocation: 6,000,000 Processor Hours
  Site: Argonne National Laboratory
   Machine: IBM Blue Gene/P
   Allocation: 6,000,000 processor hours

Research Summary:
Bubbles and suds (aqueous foams) are ubiquitous in personal and home care products. However, our only knowledge of surfactant-assisted aqueous foam generation, growth and stability is empirical. Understanding the molecular mechanisms of bubble formation, dynamics and stability are important for transforming our knowledge (i.e., beyond incremental improvement) of sudsing detergents, but are also of interest for developing better fire control chemicals, chemicals for hazardous cleanup/remediation, as well as designing environmentally friendly consumer products. The objective of this proposal is to gain insight into aqueous foam through large scale atomistic molecular dynamics simulations of cavitational and plateau regions of foams, and resultant coarse grained simulations of multiple dynamic, interacting bubbles.

Type: Renewal

Title: "Computational Protein Structure Prediction and Protein Design"

Principal Investigator: David Baker, University of Washington
Co-Investigators:

Scientific Discipline: Biological Sciences

INCITE allocation: 12,000,000 Processor Hours
  Site: Argonne National Laboratory
   Machine: IBM Blue Gene/P
   Allocation: 12,000,000 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: 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: Combustion

INCITE allocation: 3,000,000 Processor Hours
   Site: Lawrence Berkeley National Laboratory
      Machine: NERSC HPC
      Allocation: 3,000,000 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 ultra-lean 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 experimental data interpretation 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: "Gyrokinetic steady state transport simulations"

Principal Investigator: Jeff Candy, General Atomics
Co-Investigators: Mark Fahey, Oak Ridge National Laboratory
                              Ronald E. Waltz, General Atomics

Scientific Discipline: Plasma Physics

INCITE allocation: 2,000,000 Processor Hours
  Site: Oak Ridge National Laboratory
    Machine: Cray XTs
    Allocation: 2,000,000 processor hours

Research Summary:
The fundamental scientific advance targeted in this project is the multi-scale simulation of a burning plasma core for the International Thermonuclear Experimental Reactor (ITER) in particular. This multi-scale simulation will be used to predict the performance given the temperature and density, which is critical to the design of diagnostics and the selection of operating points for the ITER project.

Type: Renewal

Title: "Numerical relativity simulations of binary black holes and gravitational radiation"

Principal Investigator: Joan Centrella, National Aeronautics and Space Administration (NASA) Goddard Space Flight Center (GSFC)

Co-Investigators: John Baker, NASA GSFC
James van Meter, NASA GSFC

Scientific Discipline: Astrophysics

INCITE allocation: 500,000 Processor Hours
  Site: Oak Ridge National Laboratory
    Machine: Cray XTs
    Allocation: 500,000 processor hours

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

Type: Renewal

Title: "Computational Rheology of Dense Suspensions"

Principal Investigator: Athonu Chatterjee, Corning Inc.
Co-Investigators: David Heine, Corning Inc.

Scientific Discipline: Materials Sciences

INCITE allocation: 1,600,000 Processor Hours
  Site: Pacific Northwest National Laboratory
    Machine: HP-MPP
    Allocation: 1,600,000 processor hours

Research Summary:
Rheology deals with flow and deformation of materials. Rheology of dense suspensions is a complex phenomenon encompassing multiple length and time scales, and diverse physics ranging from hydrodynamics to electrostatics. Dense suspensions have applications in many industrial processes ranging from ceramics to polymers, from the food industry to pharmaceuticals. This proposal will use the requested INCITE resources to extend the development and validation of the generalized Dissipative Particle Dynamics (DPD) code, and then use the code to analyze realistic suspensions under conditions that prevail in real operations.

Type: Renewal

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

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

Scientific Discipline: Combustion

INCITE allocation: 30,000,000 Processor Hours
  Site: Oak Ridge National Laboratory
    Machine: Cray XTs
    Allocation: 30,000,000 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 U.S. 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 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 (IC) engines. Emphasis will be placed on fuel variability. Chen et al. will use DNS to understand how a lifted autoignitive flame is stabilized, and how thermal and composition stratification effects in kinetically-controlled compression ignition combustion can be used to control the rate of combustion. Oefelein et al. will use LES to to investigate turbulent reacting flow processes in an actual IC engine geometry at the actual operating conditions. 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. The combination of LES and DNS can potentially provide a near complete picture of IC engine processes well beyond the current state of the art.

Type: Renewal

Title: "Computational Nuclear Structure"

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

Scientific Discipline: Nuclear Physics

INCITE allocation: 25,000,000 Processor Hours
  Site: Argonne National Laboratory
   Machine: IBM Blue Gene/P
   Allocation: 10,000,000 processor hours

   Site: Oak Ridge National Laboratory
   Machine: Cray XTs
   Allocation: 15,000,000 processor hours

Research Summary:
This project will use complementary techniques, including Green's Function
Monte Carlo, Hamiltonian Diagonalization (the No Core Shell Model) and
Coupled-Cluster methods to perform ab initio calculations of both structural
and reaction properties of light and medium mass nuclei and of the three-
nucleon force. This could provide an ab initio understanding of triple-alpha
burning that is essential to life on earth. So far, ab initio investigations of the
role of three-nucleon forces have been limited to light nuclei up to mass 12.

This project will explore, for the first time, the role of the three-nucleon
force in substantially heavier nuclei like 16O, 40Ca, and 56Ni. This project
will also perform structure and nuclear reaction calculations for the entire
nuclear mass table to improve our understanding of the nuclear energy
density functional and to calculate nuclear properties relevant for the
description of nuclear reactions, in particular neutron-nucleus reaction cross
sections, and fission. Studies will include various scattering processes in light
nuclei of astrophysical interest, and bulk properties (masses, radii,
deformations, and neutron separation energies, giant resonance spectra) for
nuclei across the entire mass table. Such calculations are relevant to many
applications in nuclear energy and in nuclear astrophysics.

Type: Renewal

Title: "Verification and validation of petascale simulation of turbulent transport in fusion plasmas"

Principal Investigator: Patrick Diamond, University of California, San Diego

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: 30,000,000 Processor Hours
  Site: Oak Ridge National Laboratory
    Machine: Cray XTs
    Allocation: 30,000,000 processor hours

Research Summary:
Predicting and controlling turbulent transport are among the most important and challenging scientific issues facing the International Thermonuclear Experimental Reactor (ITER) project. Three topics that address the need to understand nonlinear plasma dynamics and self-organization in complex tokamak geometry are: 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, and require multi-scale, non-local processes of turbulence self-organization. All three topics address problems which 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 another 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 U.S. (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: "Landmark Direct Numerical Simulations of Separation and Transition for Aerospace-Relevant Wall-Bounded Shear Flows"

Principal Investigator: Hermann Fasel, University of Arizona
Co-Investigators: Stefan Wernz, University of Arizona

Scientific Discipline: Fluid Turbulence

INCITE allocation: 500,000 Processor Hours
  Site: Oak Ridge National Laboratory
   Machine: Cray XTs
   Allocation: 500,000 processor hours

Research Summary:
This project will perform landmark Direct Numerical Simulations (DNS) of two challenging flow problems of high technical relevance for aerospace applications. Problem I is the flow separation from the upper surface of a low-pressure turbine blade. The understanding of the complex physical mechanisms acting in this process is necessary for migrating pulsed vortex generator jet (VGJ) technology from the laboratory to production jet engines. Problem II concerns the development and separation of a turbulent Coanda wall jet from a curved surface. A profound physical understanding of the dynamics of these coherent structures will be crucial for the development of effective and efficient Coanda flow devices. The improved physical understanding and CFD modeling capabilities for flow transition in complex shear flows resulting from the proposed high-fidelity DNS data base will lead to aerospace design improvements and increased accuracy of CFD codes with major potential of cost-savings for the design and operation (fuel consumption) of flight vehicles.

Type: Renewal

Title: "Reactor Core Hydrodynamics"

Principal Investigator: Paul Fischer, Argonne National Laboratory
Co-Investigators: Carlos Pantano, University of Illinois
Andrew Siegel, Argonne National Laboratory

Scientific Discipline: Applied Mathematics

INCITE allocation: 30,000,000 Processor Hours
  Site: Argonne National Laboratory
    Machine: IBM Blue Gene/P
    Allocation: 30,000,000 processor hours

Research Summary:
Liquid-metal-cooled fast reactors are expected to provide a critical element in the Global Nuclear Energy Partnership (GNEP, www.gnep.energy.gov) that is being led by the Department of Energy. These advanced burner reactors (ABRs) will be used to recycle spent nuclear fuel and thereby reduce the loading demands, by up to a factor of 100, in geological repositories. In addition to reducing waste products by effectively closing the fuel cycle, the ABRs are expected to be economical sources of power. GNEP is expected to be an economically viable approach to addressing the issues of energy security, carbon management, and minimal nuclear waste. INCITE resources will be used in this project to carry out large-scale numerical simulations of turbulent thermal transport in sodium cooled reactor cores to gain an understanding of the fundamental thermal mixing phenomena within ABR cores that can lead to improved safety and economy of these pivotal designs.

Type: Renewal

Title: "Large-scale simulations of cardiac electrical activity"

Principal Investigator: Jeffrey Fox, Gene Network Sciences
Co-Investigators: Robert Miller, Gene Network Sciences
Gregery Buzzard, Gene Network Sciences
Fernando Siso-Nadal, Gene Network Sciences

Scientific Discipline: Biological Sciences

INCITE allocation: 21,405,500 Processor Hours
  Site: Argonne National Laboratory
   Machine: IBM Blue Gene/P
   Allocation: 21,405,500 processor hours

Research Summary:
Catastrophic rhythm disturbances of the heart are a leading cause of death in the United States. Treatment and prevention of cardiac rhythm disorders remains difficult because the electrical signal that controls the heart 's rhythm is determined by complex, multi-scale biological processes. Recent advances in experimental technologies have allowed for more detailed characterizations of normal and abnormal cardiac electrical activity. This project will use INCITE resources for rapid testing of hypotheses for the initiation and maintenance of rhythm disorders. These large-scale computer simulations represent a promising tool to help identify the underlying electrical mechanisms for dangerous arrhythmias and to determine the effects of interventions, such as drugs, that may prevent or exacerbate these arrhythmias. The first is an investigation of a deadly arrhythmia called ventricular fibrillation. The second is a study of how drug-induced modifications of molecular properties of heart cells can cause changes in tissue properties that might lead to a dangerous rhythm disorder called Torsades de Pointes. The results of these simulations may help elucidate mechanisms of heart rhythm disorders that pose a significant health risk to the general public. An improved understanding of these disorders will help lead to safer and better treatments for patients.

Type: Renewal

Title: "Water in confined states."

Principal Investigator: Giulia Galli, University of California, Davis
Co-Investigators: Jeffrey Grossman, University of California, Berkeley
Francois Gygi, University of California, Davis
Eric Schwegler, Lawrence Livermore National Laboratory

Scientific Discipline: Chemical Sciences

INCITE allocation: 2,000,000 Processor Hours
  Site: Argonne National Laboratory
   Machine: IBM Blue Gene/P
   Allocation: 2,000,000 processor hours

Research Summary:
Understanding the structure of water in its many phases is fundamental to research in fields as diverse as biochemistry, cellular biology, atmospheric chemistry and planetary physics. While the properties of the bulk fluid are relatively well characterized, much less is know about water confined at the nanometer scale, where conventional experimental probes (neutron diffraction and X-ray scattering) are difficult to use. This proposal will investigate water in confined states by (1) carrying out ab initio simulations for water confined between hydrophilic and hydrophobic surfaces and (2) studying the influence of dimensionality reduction and surface chemistry on the properties of the confined fluid. The grand challenge is to define a computational paradigm to simulate water flow and transport at the nanoscale which can be applied to both materials science problems (e.g., water in zeolites) and problems of biological interest (e.g., water in contact with amino acids and proteins).

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 Sciences

INCITE allocation: 750,000 Processor Hours
  Site: Argonne National Laboratory
    Machine: IBM Blue Gene/P
    Allocation: 750,000 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: "An Integrated Approach to the Rational Design of Chemical Catalysts"

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

Scientific Discipline: Chemical Sciences

INCITE allocation: 30,000,000 Processor Hours
  Site: Oak Ridge National Laboratory
    Machine: Cray XTs
    Allocation: 30,000,000 processor hours

Research Summary:
Leadership-scale simulation using advanced theory in close collaboration with experiment is the only path towards 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 100-1000x increase in effective simulation power required to make significant progress with our scientific objectives of improved activity and selectivity.

Type: Renewal

Title: "High Power Electromagnetic Wave Heating in the ITER Burning Plasma"

Principal Investigator: E. Fred Jaeger, Oak Ridge National Laboratory
Co-Investigators:

Scientific Discipline: Plasma Physics

INCITE allocation: 2,000,000 Processor Hours
  Site: Oak Ridge National Laboratory
    Machine: Cray XTs
    Allocation: 2,000,000 processor hours

Research Summary:
The next step toward fusion as a practical energy source is to develop a device capable of producing and controlling the high performance plasma required for self-sustaining fusion reactions, i.e., "burning" plasma. High-power electromagnetic waves in the radio frequency (RF) range have great potential to heat fusion plasmas into the burning regime, and to control plasma behavior through localized energy deposition, driven current, and driven plasma flows. Efforts in this proposal will extend wave-plasma interaction research conducted in the Scientific Discovery through Advanced Computing (SciDAC) program to the burning plasma regime of the International Tokamak Experimental Reactor (ITER). The extension to ITER is difficult because the physical size of ITER and the high plasma density require an order of magnitude increase in resolution over previous calculations.

Type: Renewal

Title: "Understanding the electronic structure of novel electronic materials using many-body perturbation theory"

Principal Investigator: Leeor Kronik, Weizmann Institute of Science
Co-Investigators: Sohrab Ismail-Beigi, Yale University

Scientific Discipline: Materials Sciences

INCITE allocation: 810,000 Processor Hours
  Site: Lawrence Berkeley National Laboratory
   Machine: NERSC HPC
   Allocation: 810,000 processor hours

Research Summary:
Two important, and at first glance disparate, theoretical challenges in the understanding of modern electronic materials are: (1) the electronic structure of the interface between an organic material and an inorganic conductor or semiconductor and its relation to transport phenomena across the interface, and (2) the electronic structure of novel magnetic materials and its relation to the mechanisms of magnetic interaction in such materials. Unfortunately, further theoretical progress based on the density functional theory (DFT) framework is hampered by two limitations of currently available DFT: the need to describe localized and delocalized electronic orbitals on the same footing, and the need to consider filled and empty electronic states equally. This project will overcome these difficulties by turning to many-body perturbation theory, specifically to using the GW approximation for computing quasi-particle excitation energies. The results will significantly help to elucidate pressing issues in the understanding of the electronic structure of organic/inorganic interfaces, novel magnetic materials, and their relations to transport phenomena and magnetic coupling mechanisms, respectively.

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: Accelerator Physics

INCITE allocation: 8,000,000 Processor Hours
  Site: Oak Ridge National Laboratory
   Machine: Cray XTs
   Allocation: 8,000,000 processor hours

Research Summary:
The International Linear Collider (ILC), a proposed electron-positron accelerator with an estimated cost of 6.75 billion dollars, will be one of the 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 linear accelerators (main linacs), each of which is 14 km in length for accelerating electron and positron beams to the energy of 250 GeV. The main linacs constitute a substantial portion of the overall cost of the ILC project. Thus it is important to optimize the designs of the essential components of the linac to achieve prescribed operational requirements. This project will combine the 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 multi-physics analysis. These large-scale simulations will make a significant impact on the ILC design that will provide improved performance, increased reliability and lower cost.

Type: Renewal

Title: "Modeling Reactive Flows in Porous Media"

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

Scientific Discipline: Geosciences

INCITE allocation: 10,500,000 Processor Hours
  Site: Oak Ridge National Laboratory
    Machine: Cray XTs
    Allocation: 10,000,000 processor hours

  Site: Pacific Northwest National Laboratory
    Machine: HP-MPP
    Allocation: 500,000 processor hours

Research Summary:
The goal of the project is to capture the observed slow leaching of uranium from the Hanford sediment and model the behavior of the uranium plume over time, taking into account variations in the Columbia River stage.

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: Astrophysics

INCITE allocation: 75,000,000 Processor Hours
  Site: Oak Ridge National Laboratory
    Machine: Cray XTs
    Allocation: 75,000,000 processor hours

Research Summary:
This project will perform 3-D simulations to understand how stars more than ten times the mass of our sun die in catastrophic stellar explosions known as core collapse supernovae. 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 presently there are 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 only be modeled 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: Renewal

Title: "BG/P Plan 9 measurements on large scale systems"

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

Scientific Discipline: Computer Sciences

INCITE allocation: 8,000,000 Processor Hours
   Site: Argonne National Laboratory
       Machine: IBM Blue Gene/P
       Allocation: 8,000,000 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 machne, in preparation for future systems with 10 million CPUs.

Type: Renewal

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

Principal Investigator: Warren Mori, UCLA
Co-Investigators: Cheng Kun Huang, University of California, Los Angeles
Tom Katsouleas, University of Southern California
Frank Tsung, University of California, Los Angeles

Scientific Discipline: Accelerator Physics

INCITE allocation: 4,600,000 Processor Hours
  Site: Lawrence Berkeley National Laboratory
    Machine: NERSC HPC
    Allocation: 4,600,000 processor hours

Research Summary:
The long-term future of experimental high-energy physics research using accelerators depends on the successful development of novel ultra high-gradient acceleration methods. New acceleration techniques using lasers and plasmas have already been shown to exhibit gradients and focusing forces more than 1000 times greater than conventional technology, raising the possibility of ultra-compact accelerators for applications in science, industry, and medicine. In the past few years, parallel simulation tools for plasma based acceleration have been verified against each other, against experiment, and against theory. The goal of this proposal is to use these tools for studying parameters that are in regimes that will not be accessible for experiments for years to come. This study will provide an environment to test key concepts under ideal conditions before tens to hundreds of millions of dollars are spent on the required facilities.

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
Alessandro Curioni, IBM Research-Zurich
Greg Schenter, Pacific Northwest National Laboratory
Shawn Kathmann, Pacific Northwest National Laboratory

Scientific Discipline: Chemical Sciences

INCITE allocation: 4,000,000 Processor Hours
  Site: Argonne National Laboratory
    Machine: IBM Blue Gene/P
    Allocation: 2,000,000 processor hours

  Site: Oak Ridge National Laboratory
    Machine: Cray XTs
    Allocation: 2,000,000 processor hours

Research Summary:
Moving the field of molecular simulation foward 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 U.S. competive in delivering future technologies.

Type: Renewal

Title: "Massively Parallel Simulation of Combustion in Gas turbines"

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

Scientific Discipline: Combustion

INCITE allocation: 8,000,000 Processor Hours
   Site: Argonne National Laboratory
      Machine: IBM Blue Gene/P
      Allocation: 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. This project will develop and apply the LES CFD approach to the simulation of unsteady reacting flows, focusing on technically challenging issues in real gas turbines, and thereby demonstrating the usefulness of LES in the design process. These issues, which are beyond the capacities of currently used CFD tools, include ignition, re-ignition, flame quenching and instabilities. The main applications of the study are energy production (industrial gas turbines) and propulsion (helicopter and aircraft engines). MaSiGaT, Massively Parallel Simulation of combustion in Gas Turbines, will use the AVBP CFD code (co-developed by CERFACS and IFP), to simulate ten different combustion cases. The geometries will correspond to real gas turbines, using the full geometry and not one sector only as is done today. Most of these questions relate to interactions between multiple burners and flames in the same cavity. Most academic set-ups include only one burner. In a real gas turbine, the interaction between the 15 to 20 burners placed in the annular chamber leads to a variety of new and unsolved physical questions: How do burners interact ? How do they generate azimutal acoustic modes which are seen in most gas turbines ? How does a burner ignite its neighbour ? How does quenching propagate from one burner to another one ?… Combining LES and massively parallel machines will allow investigation of these important physical mechanisms.

Type: Renewal

Title: "Beam Delivery System Optimization for X-Ray Free Electron Lasers"

Principal Investigator: Ji Qiang, Lawrence Berkeley National Laboratory

Co-Investigators: John Corlett, Lawrence Berkeley National Laboratory
Steve Lidia, Lawrence Berkeley National Laboratory
Robert Ryne, Lawrence Berkeley National Laboratory
Alexander Zholents, Lawrence Berkeley National Laboratory

Scientific Discipline: Accelerator Physics

INCITE allocation: 800,000 Processor Hours
  Site: Lawrence Berkeley National Laboratory
   Machine: NERSC HPC
   Allocation: 800,000 processor hours

Research Summary:
Next generation X-ray free electron lasers (FELs) present great opportunities for scientific discovery and applications in physics, material science, chemical science and bioscience. This project will use the INCITE computer resources to optimize the design and improvement of beam delivery systems including injector, laser heater, rf linac, bunch compressor, and beam switchyard for X-ray FELs being designed at LBNL. Optimizing beam delivery systems to produce and preserve high intensity and good quality electron beams will not only lower the cost of design and operation of FELs, but also improve the performance of X-ray light output.

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: Climate Research

INCITE allocation: 2,000,000 Processor Hours
  Site: Oak Ridge National Laboratory
   Machine: Cray XTs
   Allocation: 2,000,000 processor hours

Research Summary:
Understanding the role of clouds in the global atmosphere is key to development of more accurate climate models. This project will numerically simulate global circulation of the atmosphere on a grid with roughly a 2 km grid spacing. This entails very large computations (e.g., a sustained Teraflop for 10 wall-clock days) and very large model output files (e.g., several petabytes). The models are based on the solution of partial differential equations on a geodesic grid. The impact of this research will be improved understanding of the role of clouds in the global atmosphere, and an improved capability for both weather prediction and the simulation of climate change.

Type: Renewal

Title: "Three-Dimensional Particle-in-Cell Simulations of Fast Ignition"

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

Scientific Discipline: Plasma Physics

INCITE allocation: 2,500,000 Processor Hours
  Site: Argonne National Laboratory
    Machine: IBM Blue Gene/P
    Allocation: 1,500,000 processor hours

  Site: Lawrence Berkeley National Laboratory
    Machine: NERSC HPC
    Allocation: 1,000,000 processor hours

Research Summary:
Energy is the ultimate driver for economic growth and social development. Fusion energy is regarded as the true long-term energy solution for humanity that is environment-friendly and safe. Fast ignition (FI) is one of the most promising new schemes to improve the viability of inertial confinement fusion (ICF) as a practical energy source. FI uses an approach that separates the compression of the fusion fuel from the ignition step. First, a laser compresses a spherical shell of deuterium-tritium ice to high density at low temperature. Then, a second very high-intensity laser delivers a pulse of energy that ignites the compressed fuel. This concept promises much higher gain for the same driver energy and possible reduction of the energy needed for ignition. There is worldwide interest in FI and its associated science, with major "proof of principle" experimental facilities being constructed, most notably at the OMEGA-EP facility in the USA and the FIREX facility in Japan. INCITE resources will be used to carry out large-scale Particle-in-Cell (PIC) simulations of the ignition phase in FI. The ignition phase determines the coupling of the ignition laser to the target core and thus the viability of FI, but it is also the least understood phase in FI. Simulations will cover physics such as channeling, laser absorption, and electron transport up to moderate densities to answer key questions: (1) What is the minimum energy required to create a channel so that the ignition pulse can arrive at the critical surface without significant energy loss? (2) What are the amount and spectrum of the laser-generated energetic electrons? (3) What is the energetic electron transport process beyond the laser-plasma interface in a plasma with densities up to 100 times the critical density? This project will contribute toward the realization of fusion as a controllable energy source, solving the energy crisis facing the world today.

Type: Renewal

Title: "Bose-Einstein condensation vs. quantum localization in quantum magnets"

Principal Investigator: Tommaso Roscilde, Ecole Normale Superieure de Lyon

Co-Investigators: Stephan Haas, University of Southern California

Scientific Discipline: Materials Sciences

INCITE allocation: 1,200,000 Processor Hours
   Site: Oak Ridge National Laboratory
   Machine: Cray XTs
   Allocation: 1,200,000 processor hours

Research Summary:
This project focuses on the study of novel quantum phases and quantum phase transitions in disordered quantum antiferromagnets subject to a magnetic field. In absence of disorder, a strong magnetic field can drive quantum antiferromagnets with a spin gap through a quantum phase transition characterized by the Bose-Einstein condensation (BEC) of triplet quasiparticles. The presence of disorder is expected to induce a novel quantum-disordered phase dominated by quantum localization (Bose glass) before condensation occurs. The proposed project is framed within a collaboration with the National High Magnetic Field Laboratories at Los Alamos, aimed at the observation of boson localization in quantum magnetic systems, which would then represent the first experimental realization of a Bose glass.

Type: Renewal

Title: "Gating Mechanism of Membrane Proteins"

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

Co-Investigators: Klaus Schulten, University of Illinois, Urbana-Champaign
Emad Tajkhorshid, University of Illinois, Urbana-Champaign

Scientific Discipline: Biological Sciences

INCITE allocation: 45,000,000 Processor Hours
  Site: Argonne National Laboratory
    Machine: IBM Blue Gene/P
    Allocation: 30,000,000 processor hours

  Site: Oak Ridge National Laboratory
    Machine: Cray XTs
    Allocation: 15,000,000 processor hours

Research Summary:
The cell membrane represents the physical and functional boundary between living organisms and their environment. Membrane-associated proteins play an essential role in controlling the bidirectional flow of material and information, and as such, they are truly "molecular machines" able to accomplish complex tasks. Large-scale gating motions, occurring on a relatively slow time-scale, are essential for the function of many important membrane proteins such as transporters and channels. Many biological processes of interest to the Office of Science are mediated by membrane-associated proteins, ranging from biocatalysis of potential fuel stocks to the production and pumping of rare and unique compounds to the detoxification of organic waste products. The long-term goal of this study is to understand how the membrane-associated molecular protein-machines are able to carry out their function.

Type: Renewal

Title: "Predictive and accurate Monte Carlo based simulations for Mott insulators, cuprate superconductors, and nanoscale systems."

Principal Investigator: Thomas Schulthess, Oak Ridge National Laboratory

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

Scientific Discipline: Materials Sciences

INCITE allocation: 45,000,000 Processor Hours
   Site: Oak Ridge National Laboratory
   Machine: Cray XTs
   Allocation: 45,000,000 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 (QMC) based ab initio molecular dynamics (AIMD) simulations will provide new benchmarks for the development of empirical models, help validate choice of functionals in Density Functional Theory (DFT) based simulations, and in the distant future, might even be directly integrated with the Wang-Landau scheme.

Type: Renewal

Title: "Predictions of thermal striping in sodium cooled reactors"

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

Scientific Discipline: Nuclear Energy

INCITE allocation: 7,500,000 Processor Hours
  Site: Argonne National Laboratory
    Machine: IBM Blue Gene/P
    Allocation: 7,500,000 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: "Cellulosic Ethanol: Physical Basis of Recalcitrance to Hydrolysis of Lignocellulosic Biomass"

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

Scientific Discipline: Biological Sciences

INCITE allocation: 6,000,000 Processor Hours
  Site: Oak Ridge National Laboratory
    Machine: Cray XTs
    Allocation: 6,000,000 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 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: "Lattice QCD"

Principal Investigator: Robert Sugar, University of California, Santa Barbara

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
Paul Mackenzie, Fermi National Accelerator Laboratory
Norman Christ, Columbia University
Richard Brower, Boston University

Scientific Discipline: Lattice Gauge Theory

INCITE allocation: 87,000,000 Processor Hours

Site: Argonne National Laboratory
Machine: IBM Blue Gene/P
Allocation: 67,000,000 processor hours

Site: Oak Ridge National Laboratory
Machine: Cray XTs
Allocation: 20,000,000 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: Renewal

Title: "Clean and Efficient Coal Gasifier Designs using Large-Scale Simulations"

Principal Investigator: Madhava Syamlal, 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: Combustion

INCITE allocation: 13,000,000 Processor Hours
  Site: Oak Ridge National Laboratory
    Machine: Cray XTs
    Allocation: 13,000,000 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 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 like 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: "High Resolution Global Simulation of Plasma Microturbulence"

Principal Investigator: William Tang, Princeton Plasma Physics Laboratory

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

Scientific Discipline: Plasma Physics

INCITE allocation: 6,000,000 Processor Hours
  Site: Argonne National Laboratory
   Machine: IBM Blue Gene/P
   Allocation: 6,000,000 processor hours

Research Summary:
Turbulence is believed to be the primary mechanism by which particles and energy diffuse across the confining magnetic field in toroidal fusion systems. Understanding this process is of utmost importance for the design and operation of current and future fusion devices, such as the multi-billion dollar international burning plasma experiment known as ITER—currently the top priority in the Department of Energy (DOE) Office of Science. This project will use an advanced version of the Gyrokinetic Toroidal Code (GTC), the flagship code for studying plasma microturbulence in magnetically confined high-temperature plasmas, to enable a realistic examination of the influence of collisions on long time "steady-state" plasma transport behavior. 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: Renewal

Title: "Linear Scale Electronic Structure Calculations for Nanostructures"

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

Co-Investigators: Juan Meza, Lawrence Berkeley National Laboratory

Zhengji Zhao, Lawrence Berkeley National Laboratory

Scientific Discipline: Materials Sciences

INCITE allocation: 3,000,000 Processor Hours

Site:	Argonne National Laboratory
Machine:	IBM Blue Gene/P
Allocation:	1,000,000 processor hours
Site:	Oak Ridge National Laboratory
Machine:	Cray XTs
Allocation:	2,000,000 processor hours

Research Summary:
Nanostructures such as quantum dots and wires, composite quantum rods and core/shell structures have been proposed for electronic or optical devices like solar cells. For the successful design and deployment of such devices, however, a clear understanding of the electronic structure of such systems is essential. Yet, despite more than a decade of research, some critical issues regarding the electronic structure of even moderately complex nanostructures are still poorly understood. This proposal will use large scale density functional calculations to investigate nanostructures with different geometries and heterostructure composites; the effects of different surface passivations and surface layers, e.g, the cation (or anion) terminated (0001) bottom layer in a nanostructure; and the effect of a single dopant in a nanostructure. These theoretical calculations will help in the design of better solar cells using nanostructures, which could have a great impact on the solar cell field and thereby address several important energy issues.

Type: Renewal

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

Principal Investigator: Warren Washington, National Center for Atmospheric Research

Co-Investigators: John Drake, Oak Ridge National Laboratory
Peter Gent, National Center for Atmopsheric Research
Steven Ghan, Pacific Northwest National Laboratory
Donald Anderson, NASA Headquarters
Philip Jones, Los Alamos National Laboratory
Robert Jacobs, Argonne National Laboratory
David Bader, Lawrence Livermore National Laboratory
Robert Dickinson, Georgia Institute of Technology
David Erickson, Oak Ridge National Laboratory
James Hack, Oak Ridge National Laboratory
Lawrence Buja, National Center for Atmospheric Research

Scientific Discipline: Climate Research

INCITE allocation: 37,500,000 Processor Hours

Site:	Argonne National Laboratory
Machine:	IBM Blue Gene/P
Allocation:	7,500,000 processor hours

Site:	Oak Ridge National Laboratory
Machine:	Cray XTs
Allocation:	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 policies 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 interagency collaboration of NSF and DOE in developing the Community Climate System Model (CCSM), collaboration with NASA in carbon data assimilation, and university partners with expertise in computational climate research. Of particular importance is the correct 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: "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 Sciences

INCITE allocation: 1,000,000 Processor Hours
  Site: Argonne National Laboratory
    Machine: IBM Blue Gene/P
    Allocation: 1,000,000 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: Renewal

Title: "First Principles Models of Type Ia Supernovae"

Principal Investigator: Stan Woosley, University of California, Santa Cruz

Co-Investigators: Ann Almgren, Lawrence Berkeley National Laboratory
John Bell, Lawrence Berkeley National Laboratory
Marc Day, Lawrence Berkeley National Laboratory
L. Jonathan Dursi, University of Toronto
Dan Kasen, Johns Hopkins University
Fritz Röpke, University of California, Santa Cruz
Michael Zingale, State University of New York, Stony Brook

Scientific Discipline: Astrophysics

INCITE allocation: 3,000,000 Processor Hours
  Site: Oak Ridge National Laboratory
    Machine: Cray XTs
    Allocation: 3,000,000 processor hours

Research Summary:
The purpose of this proposal is to study four key stages of Type Ia supernovae: the long-time convection that leads to ignition of the first flames; the propagation of these resultant flame(s) through the star leading to the explosion itself; and finally, the radiation-dominated phase at the end of the explosion. This is an especially relevant problem in astrophysics today: by acting as standard candles, Type Ia supernovae have been at the forefront of a revolution in modern cosmology, leading to the discovery that the expansion rate of the Universe is accelerating. It is anticipated that the proposed set of calculations will produce the most detailed picture of Type Ia supernovae to date.

Type: Renewal

Title: "Performance Evaluation and Analysis Consortium End Station"

Principal Investigator: Patrick H. Worley, Oak Ridge National Laboratory

Co-Investigators: David H. Bailey, Lawrence Berkeley National Laboratory
Jack Dongarra, University of Tennessee
William D. Gropp, University of Illinois, Urbana-Champaign
Jeffrey K. Hollingsworth, University of Maryland
Allen Malony, University of Oregon
John Mellor-Crummey, Rice University
Barton P. Miller, University of Wisconsin
Leonid Oliker, Lawrence Berkeley National Laboratory
Daniel Reed, University of North Carolina
Allan Snavely, University of California, San Diego
Jeffrey S. Vetter, Oak Ridge National Laboratory
Katherine Yelick, University of California, Berkeley
Bronis R. de Supinski, Lawrence Livermore National Laboratory

Scientific Discipline: Computer Sciences

INCITE allocation: 16,000,000 Processor Hours
  Site: Argonne National Laboratory
    Machine: IBM Blue Gene/P
    Allocation: 8,000,000 processor hours

  Site: Oak Ridge National Laboratory
    Machine: Cray XTs
    Allocation: 8,000,000 processor hours

Research Summary:
To maximize the utility of Leadership Class systems such as the Cray XT4, Cray XT5, and IBM BlueGene/P (BG/P), the performance community (performance tool developers, system and appliation performance evaluators and performance optimization engineers) must understand how to use each system most efficiently. To further understanding of these high-end systems, this proposal is focusing 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 to the BG/P, XT4, and XT5, making these available to high-end computing users, and further develop the tools 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; (4) analyze and help optimize current or candidate Leadership Class application codes.

Type: Renewal

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

Principal Investigator: Jihui Yang, General Motors Reseach and Development Center

Co-Investigators: Changfeng Chen, University of Nevada, Las Vegas

Scientific Discipline: Materials Sciences

INCITE allocation: 15,000,000 Processor Hours
  Site: Oak Ridge National Laboratory
    Machine: Cray XTs
    Allocation: 15,000,000 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. $(PbTe)_{1-x}(AgSbTe_2)_x$, 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 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.