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INCITE
Advancing America's Science
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Type: New

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

Proposal Title: “Computational Protein Structure Prediction and Protein Design”
Scientific Discipline: Computational Proteomics

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

Research Summary:

Prediction of high-resolution protein structures from their amino acid sequences and the refinement of low-resolution models to high resolution are long standing 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.

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Type: New

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

Proposal Title: “Interaction of Turbulence and Chemistry in Lean Premixed Laboratory Flames”
Scientific Discipline: Combustion

INCITE allocation: 3,384,615 Processor Hours
Site: Lawrence Berkeley National Laboratory
Machine: NERSC HPC
Allocation: 3,384,615 processor hours (22,000,000 MPP Units)

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.

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Type: New

Principal Investigator: Paola Cessi
Affiliation: University of California, San Diego
Co-Investigators:

Proposal Title: "The Role of Eddies in the Meridional Overturning Circulation"
Scientific Discipline: Climate Research

INCITE allocation: 486,000 Processor Hours
Site: Oak Ridge National Laboratory
Machine: Cray X1E
Allocation: 486,000 processor hours

Research Summary:

This project will study the processes that maintain the abyssal circulation of the ocean to understand its response to altered atmospheric composition. Meridional overturning circulation (MOC), sometimes called the ocean conveyer belt, is an essential component of the ocean-atmosphere heat budget and a major player in sequestering CO2 into the deep ocean. The MOC creates mixing between different ocean basins, transporting energy and matter around the globe. High resolution models of the ocean component of the climate system will be analyzed 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. This research will contribute to establishing the fundamental dynamics of thermohaline circulation.

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Type: New

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

Proposal Title: “High-Fidelity Simulations for Clean and Efficient Combustion of Alternative Fuels”
Scientific Discipline: Combustion

INCITE allocation: 18,000,000 Processor Hours
Site: Oak Ridge National Laboratory
Machine: Cray XT4
Allocation: 18,000,000 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, and pollutant and green-house gas emissions. This project will use Direct Numerical Simulation (DNS) and Large Eddy Simulation (LES) approaches in high-fidelity simulations that capture complex aero-thermo-chemical interactions, and in particular, the effects of fuel variability – interactions that are currently not understood even at a fundamental level. These studies will provide the foundational science required to develop a validated, predictive combustion modeling capability to optimize the design and operation of evolving fuels in advanced engines for transportation applications. This will enable transportation technology breakthroughs, assuring American competetiveness, U.S. energy security, and minimizing emissions.

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Type: New

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

Proposal Title: "Computational Nuclear Structure"
Scientific Discipline: Nuclear Physics

INCITE allocation: 17,500,000 Processor Hours
Site: Argonne National Laboratory
Machine: IBM Blue Gene/P
Allocation: 10,000,000 processor hours

Site: Oak Ridge National Laboratory
Machine: Cray XT4
Allocation: 7,500,000 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.

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Type: New

Principal Investigator: Patrick Diamond
Affiliation: 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

Proposal Title: “Verification and validation of petascale simulation of turbulent transport in fusion plasmas”
Scientific Discipline: Fusion Energy (Plasma Physics)

INCITE allocation: 8,000,000 Processor Hours
Site: Oak Ridge National Laboratory
Machine: Cray XT4
Allocation: 8,000,000 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, require multi-scale, non-local processes of turbulence self-organization, and address problems which are highly relevant to ITER. 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.

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Type: New

Principal Investigator: William Dorland
Affiliation: University of Maryland
Co-Investigators: Gregory Howes, University of California, Berkeley

Proposal Title: "Fluctuation Spectra and Anomalous Heating in Magnetized Plasma Turbulence"
Scientific Discipline: Solar/Space Physics

INCITE allocation: 4,000,000 Processor Hours
Site: Oak Ridge National Laboratory
Machine: Cray XT4
Allocation: 4,000,000 processor hours

Research Summary:
Plasma is a ubiquitous form of matter in the universe. It is nearly always found to be magnetized and turbulent. If we can understand the turbulence in the solar wind streaming past the Earth, then we can understand similar turbulence in the distant universe, such as is found between the stars and swirling around supermassive black holes. To understand X-ray observational data from Chandra, one must characterize the small-scale, kinetic plasma turbulence. In the solar wind and in the interstellar medium, there are similar unsolved, interesting problems. However, in these cases, there are also direct observations of the small-scale fluctuations, presenting concrete opportunities for testing the insights gained from theory and simulation. Comprehensive, in situ satellite measurements of all aspects of the electromagnetic fluctuations in the solar wind offer particularly exciting possibilities for confronting and testing our understanding of plasma turbulence. This project will investigate the properties of magnetized plasma turbulence, a key problem in space physics and astrophysics. This will be the first program to pursue ab initio simulations of kinetic, low-frequency turbulence in astrophysical plasmas, with the goal of carrying out direct quantitative comparisons with observations.

Type: New

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

Proposal Title: "Landmark Direct Numerical Simulations of Separation and Transition for Aerospace-Relevant Wall-Bounded Shear Flows"
Scientific Discipline: Fluid Turbulence

INCITE allocation: 400,000 Processor Hours
Site: Oak Ridge National Laboratory
Machine: Cray X1E
Allocation: 400,000 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.

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Type: New

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

Proposal Title: “Large-scale simulations of cardiac electrical activity”
Scientific Discipline: Life Sciences

INCITE allocation: 846,720 Processor Hours
Site: Argonne National Laboratory
Machine: IBM Blue Gene/P
Allocation: 846,720 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 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.

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Type: New

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

Proposal Title: “Modeling the Rheological Properties of Concrete”
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.

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Type: New

Principal Investigator: Robert Harrison
Affiliation: 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 Tech
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
David Dixon, University of Alabama

Proposal Title: "An Integrated Approach to the Rational Design of Chemical Catalysts"
Scientific Discipline: Chemical Sciences

INCITE allocation: 10,000,000 Processor Hours
Site: Oak Ridge National Laboratory
Machine: Cray XT4
Allocation: 10,000,000 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. 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.

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Type: New

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

Proposal Title: “Understanding the electronic structure of novel electronic materials using many-body perturbation theory”
Scientific Discipline: Materials Sciences

INCITE allocation: 124,615 Processor Hours
Site: Lawrence Berkeley National Laboratory
Machine: NERSC HPC
Allocation: 124,615 processor hours (810,000 MPP Units)

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.

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Type: New

Principal Investigator: Don Lamb
Affiliation: ASC/Alliance Flash Center, University of Chicago
Co-Investigators:

Proposal Title: “Study of Buoyancy-Driven Turbulent Nuclear Burning and Validation of Type Ia Supernova Models”
Scientific Discipline: Astrophysics

INCITE allocation: 21,000,000 Processor Hours
Site: Argonne National Laboratory
Machine: IBM Blue Gene/P
Allocation: 21,000,000 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. This project will provide definitive answers to the questions: “Does R-T driven turbulent nuclear burning occur primarily at large scales or at small scales?” and “At what physical conditions does the transition from the flamelet burning regime to the distributed burning regime take place?” This will be the first rigorous, systematic validation of the four current models of SNe Ia. 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 the data from JDEM.

Type: New

Principal Investigator: Lie-Quan Lee
Affiliation: Stanford Linear Accelerator Center
Co-Investigators: Zenghai Li, Stanford Linear Accelerator Center
Kwok Ko, Stanford Linear Accelerator Center
Andreas Kabel, Stanford Linear Accelerator Center
Cho Ng, Stanford Linear Accelerator Center

Proposal Title: "Petascale Computing for Terascale Particle Accelerator: International Linear Collider Design and Modeling"
Scientific Discipline: Accelerator Physics

INCITE allocation: 4,500,000 Processor Hours
Site: Oak Ridge National Laboratory
Machine: Cray XT4
Allocation: 4,500,000 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 to 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: New

Principal Investigator: Anthony Mezzacappa
Affiliation: 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

Proposal Title: “Multidimensional Simulations of Core Collapse Supernovae”
Scientific Discipline: Astrophysics

INCITE allocation: 16,000,000 Processor Hours
Site: Oak Ridge National Laboratory
Machine: Cray XT4
Allocation: 16,000,000 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: New

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

Proposal Title: "BG/P Plan 9 measurements on large scale systems"
Scientific Discipline: Computer 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:
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.

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Type: New

Principal Investigator: Christopher Mundy
Affiliation: 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

Proposal Title: “Molecular simulation of complex chemical systems”
Scientific Discipline: Chemical Sciences

INCITE allocation: 1,500,000 Processor Hours
Site: Argonne National Laboratory
Machine: IBM Blue Gene/P
Allocation: 750,000 processor hours

Site: Oak Ridge National Laboratory
Machine: Cray XT4
Allocation: 750,000 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.

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Type: New

Principal Investigator: Nikolai Pogorelov
Affiliation: University of California, Riverside
Co-Investigators: Jacob Heerikhuisen, Institute of Geophysics and Planetary, University of California, Riverside

Proposal Title: "Modeling heliospheric phenomena with an adaptive, MHD-Boltzmann code"
Scientific Discipline: Solar/Space Physics

INCITE allocation: 850,000 Processor Hours
Site: Oak Ridge National Laboratory
Machine: Cray XT4
Allocation: 850,000 processor hours

Research Summary:
This project will use INCITE resources to model physical processes in the outer heliosphere that occur during solar wind (SW) interaction with local interstellar medium (LISM). A unique program package (MS-FLUKSS, Multi-Scale Fluid-Kinetic Simulation Suite), which implements an efficient coupling of the MHD and kinetic (or multi-neutral fluid) codes, is used to determine the distribution of plasma, neutrals, and magnetic fields in the 3D heliosphere starting from the Earth's orbit out to the boundary of the solar system. The scientific problems to be addressed include (i) effects of 11-year period of solar activity on the SW-LISM interaction pattern; (ii) analysis of Galactic cosmic ray (GCR) transport through the heliosphere; (iii) effect on the SW-LISM interaction of pick-up-ions (PUI's) originating in the SW due to charge exchange with the LISM neutral atoms (such as, hydrogen, oxygen, and heavier elements. The results of our calculations will be compared with observations from the NASA spacecraft fleet. Understanding the dependence of heavy GCR ion fluxes on the SW conditions in the heliosphere is key to planning future manned space missions to other planets.

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Type: New

Principal Investigator: Thierry Poinsot
Affiliation: European Center for Research and Advanced Training in Scientific Computation (CERFACS)
Co-Investigators: Gabriel Staffelbach, CERFACS

Proposal Title: “Massively Parallel Simulation of Combustion in Gas turbines”
Scientific Discipline: Combustion

INCITE allocation: 4,000,000 Processor Hours
Site: Argonne National Laboratory
Machine: IBM Blue Gene/P
Allocation: 4,000,000 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) 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.

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Type: New

Principal Investigator: Ji Qiang
Affiliation: 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
Ilya Pogorelov, Northern Illinois University

Proposal Title: "Beam Delivery System Optimization for X-Ray Free Electron Lasers"
Scientific Discipline: Accelerator Physics

INCITE allocation: 769,231 Processor Hours
Site: Lawrence Berkeley National Laboratory
Machine: NERSC HPC
Allocation: 769,231 processor hours (5,000,000 MPP Units)

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.

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Type: New

Principal Investigator: David Randall
Affiliation: 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

Proposal Title: “Simulation of Global Cloudiness”
Scientific Discipline: Climate Research

INCITE allocation: 153,846 Processor Hours
Site: Lawrence Berkeley National Laboratory
Machine: NERSC HPC
Allocation: 153,846 processor hours (1,000,000 MPP Units)

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: New

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

Proposal Title: "Three-Dimensional Particle-in-Cell Simulations of Fast Ignition"
Scientific Discipline: Fusion Energy (Plasma Physics)

INCITE allocation: 307,692 Processor Hours
Site: Lawrence Berkeley National Laboratory
Machine: NERSC HPC
Allocation: 307,692 processor hours (2,000,000 MPP Units)

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. This project will contribute toward the realization of fusion as a controllable energy source, solving the energy crisis facing the world today.

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Type: New

Principal Investigator: Thomas Schulthess
Affiliation: 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

Proposal Title: "Predictive and accurate Monte Carlo based simulations for Mott insulators, cuprate superconductors, and nanoscale systems."
Scientific Discipline: Materials Sciences

INCITE allocation: 10,000,000 Processor Hours
Site: Oak Ridge National Laboratory
Machine: Cray XT4
Allocation: 10,000,000 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.

Type: New

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

Proposal Title: “Predictions of thermal striping in sodium cooled reactors”
Scientific Discipline: Nuclear Energy

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 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.

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Type: New

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

Proposal Title: "Cellulosic Ethanol: Physical Basis of Recalcitrance to Hydrolysis of Lignocellulosic Biomass"
Scientific Discipline: Biophysics

INCITE allocation: 3,500,000 Processor Hours
Site: Oak Ridge National Laboratory
Machine: Cray XT4
Allocation: 3,500,000 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 computering 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.

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Type: New

Principal Investigator: Robert Sugar
Affiliation: 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

Proposal Title: "Lattice QCD"
Scientific Discipline: Lattice Gauge Theory

INCITE allocation: 26,700,000 Processor Hours
Site: Argonne National Laboratory
Machine: IBM Blue Gene/P
Allocation: 19,600,000 processor hours

Site: Oak Ridge National Laboratory
Machine: Cray XT4
Allocation: 7,100,000 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. The gauge configurations will be used to determine a wide range of physical quantities of importance in high energy and nuclear physics.

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Type: New

Principal Investigator: Madhava Syamlal
Affiliation: National Energy Technology Laboratory
Co-Investigators: Aytekin Gel, Aeolus Research Inc
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

Proposal Title: "Clean and Efficient Coal Gasifier Designs using Large-Scale Simulations"
Scientific Discipline: Combustion

INCITE allocation: 3,000,000 Processor Hours
Site: Oak Ridge National Laboratory
Machine: Cray XT4
Allocation: 3,000,000 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.

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Type: New

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

Proposal Title: “High Resolution Global Simulation of Plasma Microturbulence”
Scientific Discipline: Fusion Energy (Plasma Physics)

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

Principal Investigator: Warren Washington
Affiliation: National Center for Atmospheric Research
Co-Investigators: John Drake, Oak Ridge National Lab
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 Tech University
David Erickson, Oak Ridge National Laboratory
James Hack, National Center for Atmospheric Research
Lawrence Buja, National Center for Atmospheric Research

Proposal Title: "Climate-Science Computational End Station Development and Grand Challenge Team"
Scientific Discipline: Climate Research

INCITE allocation: 18,026,000 Processor Hours
Site: Argonne National Laboratory
Machine: IBM Blue Gene/P
Allocation: 1,000,000 processor hours

Site: Lawrence Berkeley National Laboratory
Machine: NERSC HPC
Allocation: 1,308,000 processor hours (8,502,000 MPP Units)

Site: Oak Ridge National Laboratory
Machine: Cray XT4
Allocation: 15,718,000 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.

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Type: New

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

Proposal Title: "Kinetics and Thermodynamics of Metal and Complex Hydride Nanoparticles"
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.

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Type: New

Principal Investigator: Jihui Yang
Affiliation: GM R&D Center
Co-Investigators: Changfeng Chen, University of Nevada, Las Vegas

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

INCITE allocation: 10,000,000 Processor Hours
Site: Oak Ridge National Laboratory
Machine: Cray XT4
Allocation: 10,000,000 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 on an annual basis. This project will address a key issue in the study of superior thermoelectric materials, the role of nanostructural features in the electronic, lattice, and mechanical properties of nanostructured bulk materials. (PbTe)1-x(AgSbTe2)x, one of the best intermediate temperature thermoelectric materials, will be used as a model material system for this study. Lattice dynamics and stress-strain calculations will produce 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.

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Type: Renewal

Principal Investigator: Kelly Anderson
Affiliation: 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

Proposal Title: “Molecular simulations of surfactant assisted aqueous foam formation”
Scientific Discipline: Chemical Sciences

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

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Type: Renewal

Principal Investigator: Paul Bemis
Affiliation: Fluent Inc.
Co-Investigators: James Johnson, General Motors
Sharan Kalwani, General Motors

Proposal Title: “CAE Simulation of full vehicle Windnoise and other CFD phenomena”
Scientific Discipline: Computer Sciences

INCITE allocation: 153,846 Processor Hours
Site: Lawrence Berkeley National Laboratory
Machine: NERSC HPC
Allocation: 153,846 processor hours (1,000,000 MPP Units)

Research Summary:

The proposed project is to use high performance computing resources together with an off the shelf engineering simulation software product in use at GM today (FLUENT) to illustrate the competitive benefits of large scale engineering simulation early in the design phase of automotive production. This project will explore the use of FLUENT software to perform emerging computational fluid dynamics (CFD) and thermal calculations on high-end parallel-processing computers in order to determine the hardware resources and software system behavior required to deliver results in time frames that significantly impact General Motors’ Global Vehicle Development Process (GVDP). Five specific application areas will be investigated: (1) Full-vehicle open-sunroof wind buffeting calculations. (2) Full-vehicle transient thermal calculations. (3) Simulations of semi-trucks passing stationary vehicles with raised hoods. (4) Vehicle underhood buoyancy convection airflow and thermal simulations. (5) Vehicle component and sub-assembly fluid immersion and drainage calculations.

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Type: Renewal

Principal Investigator: Peter Bradley
Affiliation: Pratt & Whitney
Co-Investigators:

Proposal Title: "High Fidelity LES Simluations of an Aircraft Engine Combustor to Improve Emissions and Operability"
Scientific Discipline: Engineering Physics

INCITE allocation: 1,377,000 Processor Hours
Site: Argonne National Laboratory
Machine: IBM Blue Gene/P
Allocation: 1,377,000 processor hours

Research Summary:
Future combustor design must rely more on computational fluid dynamics (CFD) modeling for emissions and operability. The goal of this study is to perform CFD simulations of gas-turbine engines to understand the impact of properly resolving turbulence scales on combustor swirler aerodynamics and to study its impact on the combusting simulation. The calculation will be extended to the full annulus to investigate asymmetric fueling effects on operability.

Type: Renewal

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

Proposal Title: "Gyrokinetic steady state transport simulations"
Scientific Discipline: Fusion Energy (Plasma Physics)

INCITE allocation: 1,500,000 Processor Hours
Site: Oak Ridge National Laboratory
Machine: Cray XT4
Allocation: 1,500,000 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.

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Type: Renewal

Principal Investigator: Joan Centrella
Affiliation: NASA/ Goddard Space Flight Center
Co-Investigators: John Baker, National Aeronautics and Space Administration/ Goddard Space Flight Center
James van Meter, National Aeronautics and Space Administration/ Goddard Space Flight Center

Proposal Title: "Numerical relativity simulations of binary black holes and gravitational radiation"
Scientific Discipline: Astrophysics

INCITE allocation: 1,000,000 Processor Hours
Site: Oak Ridge National Laboratory
Machine: Cray XT4
Allocation: 1,000,000 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

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

Proposal Title: "Computational Rheology of Dense Suspensions"
Scientific Discipline: Materials Sciences

INCITE allocation: 750,000 Processor Hours
Site: Pacific Northwest National Laboratory
Machine: HP-MPP
Allocation: 750,000 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 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

Principal Investigator: Gilbert Compo
Affiliation: University of Colorado Cooperative Institute for Research in the Environmental Sciences Climate Diagnostics Center and NOAA Earth System Research Laboratory
Co-Investigators: Prashant Sardeshmukh, University of Colorado Cooperative Institute for Research in the Environmental Sciences Climate Diagnostics Center and NOAA Earth System Research Laboratory
Jeffrey Whitaker, National Oceanic and Atmospheric Administration

Proposal Title: "The 20th Century Reanalysis Project"
Scientific Discipline: Climate Research

INCITE allocation: 2,861,538 Processor Hours
Site: Lawrence Berkeley National Laboratory
Machine: NERSC HPC
Allocation: 2,861,538 processor hours (18,600,000 MPP Units)

Research Summary:

The goal of this proposal is to use a newly developed Kalman filter-based technique to produce a global tropospheric circulation dataset at four-times daily resolution back to 1892. The only dataset available for the early 20th century consists of error-ridden hand-drawn analyses of the mean sea level pressure field over the Northern Hemisphere. Modern data assimilation systems have the potential to improve upon these maps, but prior to 1948, few digitized upper-air sounding observations are available for such a reanalysis. The timely production of the proposed global tropospheric circulation dataset will provide an important validation check on the climate models being used to make 21st century climate projections in the Fourth Assessment Report of the Intergovernmental Panel on Climate Change (IPCC) released in 2007.

Type: Renewal

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

Proposal Title: “Reactor Core Hydrodynamics”
Scientific Discipline: Applied Mathematics

INCITE allocation: 14,000,000 Processor Hours
Site: Argonne National Laboratory
Machine: IBM Blue Gene/P
Allocation: 14,000,000 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.

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Type: Renewal

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

Proposal Title: “Water in confined states.”
Scientific Discipline: Physical Chemistry

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

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Type: Renewal

Principal Investigator: Moeljo Hong
Affiliation: The Boeing Company
Co-Investigators:

Proposal Title: "Development and Correlations of Large Scale Computational Tools for Flight Vehicles"
Scientific Discipline: Engineering Physics

INCITE allocation: 400,000 Processor Hours
Site: Oak Ridge National Laboratory
Machine: Cray XT4
Allocation: 100,000 processor hours

Machine: Cray X1E
Allocation: 300,000 processor hours

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

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Type: Renewal

Principal Investigator: Hong Im
Affiliation: University of Michigan
Co-Investigators: Christopher Rutland, University of Wisconsin
Arnaud Trouve, University of Maryland

Proposal Title: “Direct Numerical Simulation of Turbulent Flame Quenching by Fine Water Droplets”
Scientific Discipline: Chemical Sciences

INCITE allocation: 307,692 Processor Hours
Site: Lawrence Berkeley National Laboratory
Machine: NERSC HPC
Allocation: 307,692 processor hours (2,000,0 MPP Units)

Research Summary:

The primary goal of the project is to undertake three-dimensional simulations of turbulent nonpremixed flames in the presence of a mean flow strain and fine water droplets. The proposed study aims at bringing the state-of-the-art high-fidelity simulation capability to the next level by incorporating various advanced physical models that have been developed under the university collaborative project supported by the DOE Scientific Discovery through Advanced Computing (SciDAC) Program. The canonical nature of the problem configuration and the high quality simulation data will serve as an opportunity for cross-validation against laser diagnostic measurements via worldwide collaborative activities in addressing important issues concerning energy and environmental research.

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Type: Renewal

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

Proposal Title: “High Power Electromagnetic Wave Heating in the ITER Burning Plasma”
Scientific Discipline: Fusion Energy (Plasma Physics)

INCITE allocation: 1,000,000 Processor Hours
Site: Oak Ridge National Laboratory
Machine: Cray XT4
Allocation: 1,000,000 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

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

Proposal Title: "Modeling Reactive Flows in Porous Media"
Scientific Discipline: Geosciences

INCITE allocation: 2,000,000 Processor Hours
Site: Oak Ridge National Laboratory
Machine: Cray XT4
Allocation: 1,800,000 processor hours

Site: Pacific Northwest National Laboratory
Machine: HP-MPP
Allocation: 200,000 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.

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INCITE
Advancing America's Science
and Industrial Competitiveness

Type: Renewal

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

Proposal Title: “Assessing Global Climate Response of the NCAR-CCSM3: CO2 Sensitivity and Abrupt Climate Change”
Scientific Discipline: Climate Research

INCITE allocation: 420,000 Processor Hours
Site: Oak Ridge National Laboratory
Machine: Cray X1E
Allocation: 420,000 processor hours

Research Summary:
The primary goal of this project is to perform the first synchronously coupled transient ocean/atmosphere/dynamic vegetation general circulation model simulation of the past 21,000 years using the NCAR Community Climate System Model (CCSM3). This experiment will addresses two fundamental questions on future climate changes: "What is the sensitivity of the climate system to the change of greenhouse gases, notably CO2?" and "How does the climate system exhibit abrupt changes on decadal-centennial time scales?"

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and Industrial Competitiveness

Type: Renewal

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

Proposal Title: "Petascale Particle-in-Cell Simulations of Plasma Based Accelerators"
Scientific Discipline: Accelerator Physics

INCITE allocation: 923,077 Processor Hours
Site: Lawrence Berkeley National Laboratory
Machine: NERSC HPC
Allocation: 923,077 processor hours (6,000,000 MPP Units)

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.

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Type: Renewal

Principal Investigator: Synte Peacock
Affiliation: ASC/Alliance Flash Center, University of Chicago
Co-Investigators: Frank Bryan, National Center for Atmospheric Research
Steven Jayne, Woods Hole Oceanographic Institute
Mathew Maltrud, Los Alamos National Laboratory
Julie McClean, Scripps Institute of Oceanography
Norikazu Nakashiki, CRIEPI, Japan
Kelvin Richards, University of Hawaii
Luanne Thompson, University of Washington
Darryn Waugh, Johns Hopkins University

Proposal Title: “Eulerian and Lagrangian Studies of Turbulent Transport in the Global Ocean”
Scientific Discipline: Climate Research

INCITE allocation: 3,163,000 Processor Hours
Site: Oak Ridge National Laboratory
Machine: Cray XT4
Allocation: 3,163,000 processor hours

Research Summary:

The goal of this project is to complete the first-ever centennial-scale eddy-resolving global ocean simulation, incorporating a suite of tracer experiments designed to yield fundamental information on timescales and mechanisms of transport in the ocean. This experiment will be followed by an ensemble of simulations spanning the period of intensive measurements over the last 20 years. Results of these simulations will be used to answer the following questions: At what rate and by which pathways will material entering the ocean at its surface be distributed throughout its interior? What are the relative roles of the broad-scale time-mean flow, small-scale structures in the mean flow, and turbulent eddies in transporting material through the ocean interior? Are current estimates of ocean uptake of radiatively important anthropogenic trace gases (such as carbon dioxide) biased by an incomplete representation of ocean eddy transports? What level of variability in observed ocean tracer distributions can be expected from intrinsic variations of the flow due to instability processes and from inter-annual to decadal variability in the atmospheric forcing of the ocean?

Type: Renewal

Principal Investigator: Michael Pindzola
Affiliation: Auburn University
Co-Investigators: Bill McCurdy, Lawrence Berkeley National Laboratory
David Schultz, Oak Ridge National Laboratory
Don Griffin, Rollins College
Francis Robicheaux, Auburn University
James Colgan, Los Alamos National Laboratory
Nigel Badnell, University of Strathclyde
Predrag Krstic, Oak Ridge National Laboratory
Tom Rescigno, Lawrence Berkeley National Laboratory

Proposal Title: “Computational Atomic and Molecular Physics for Advances in Astrophysics, Chemical Sciences and Fusion Energy Sciences”
Scientific Discipline: Other

INCITE allocation: 2,000,000 Processor Hours
Site: Oak Ridge National Laboratory
Machine: Cray X1E
Allocation: 2,000,000 processor hours

Research Summary:
This research team will apply state-of-the-art atomic and molecular collision codes to implement time-dependent simulations relevant for numerous applications, including ultra-short laser interactions with matter, plasma diagnostics in controlled fusion experiments, X-ray astronomy, synchrotron light sources, and free-electron lasers.

Type: Renewal

Principal Investigator: Lawrence Pratt
Affiliation: Fisk University
Co-Investigators:

Proposal Title: “Reactions of lithium carbenoids, lithium enolates, and mixed aggregates”
Scientific Discipline: Chemical Sciences

INCITE allocation: 138,462 Processor Hours
Site: Lawrence Berkeley National Laboratory
Machine: NERSC HPC
Allocation: 138,462 processor hours (900.000 MPP Units)

Research Summary:
This chemical science project will use ab initio and density functional theory methods to investigate the structure and reactions of some important organolithium compounds. These include lithium enolates, which are among the most important reagents for forming carbon-carbon bonds in organic synthesis. Detailed reaction mechanisms for these compounds remain unknown, and may involve several reactive species. This will lead to a better understanding of the reaction pathways and to alter the reactions by way of mixed aggregates with other lithium compounds.

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Type: Renewal

Principal Investigator: Tommaso Roscilde
Affiliation: Max-Planck Gesellschaft
Co-Investigators: Stephan Haas, University of Southern California

Proposal Title: “Bose-Einstein condensation vs. quantum localization in quantum magnets”
Scientific Discipline: Materials Sciences

INCITE allocation: 1,200,000 Processor Hours
Site: Oak Ridge National Laboratory
Machine: Cray XT4
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.

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Type: Renewal

Principal Investigator: Benoit Roux
Affiliation: Argonne Nat Lab & The University of Chicago
Co-Investigators: Klaus Schulten, University of Illinois, Urbana-Champaign
Emad Tajkhorshid, University of Illinois, Urbana-Champaign

Proposal Title: "Gating Mechanism of Membrane Proteins"
Scientific Discipline: Life Sciences

INCITE allocation: 5,000,000 Processor Hours
Site: Argonne National Laboratory
Machine: IBM Blue Gene/P
Allocation: 1,500,000 processor hours

Site: Oak Ridge National Laboratory
Machine: Cray XT4
Allocation: 3,500,000 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

Principal Investigator: Igor Tsigelny
Affiliation: University of California-- San Diego / SDSC
Co-Investigators: Eliezer Masliah, University of California, San Diego
Stanley Opella, University of California, San Diego

Proposal Title: “Simulation and modeling of synuclein-based 'protofibril structures' as a means of understanding the molecular basis of Parkinson's Disease”
Scientific Discipline: Life Sciences

INCITE allocation: 1,200,000 Processor Hours
Site: Argonne National Laboratory
Machine: IBM Blue Gene/P
Allocation: 1,200,000 processor hours

Research Summary:

Parkinson's disease progression is characterized by a decrease in limb mobility over time. The loss of movement is caused by the death of dopamine-producing cells in the brain, thought to be associated with defects that cause increased aggregation of alpha synucleins (aS). A key issue in treating Parkinson’s disease is thus the illumination of the factors that trigger aS aggregation and the development of strategies to prevent this phenomenon. This study will combine high-end computation with biochemical and NMR experiments to model the molecular basis for aS aggregation and to test hypotheses generated by our simulations using NMR and other biochemical techniques. By combining the theoretical findings with experimental validation, we hope to identify key amino acid interactions that favor amyloid pore formation, and to use this information to discover new drugs. The work described here will not only be informative in addressing the underlying molecular basis for Parkinson’s disease, but will likely be instructive in identifying risk factors for a large body of other diseases that are equally prevalent in human populations.

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Type: Renewal

Principal Investigator: Lin-Wang Wang
Affiliation: Lawrence Berkeley National Laboratory
Co-Investigators: Juan Meza, Lawrence Berkeley National Laboratory
Zhengji Zhao, Lawrence Berkeley National Laboratory

Proposal Title: "Linear Scale Electronic Structure Calculations for Nanostructures"
Scientific Discipline: Materials Sciences

INCITE allocation: 2,100,000 Processor Hours
Site: Oak Ridge National Laboratory
Machine: Cray XT4
Allocation: 2,100,000 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.

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Type: Renewal

Principal Investigator: Stan Woosley
Affiliation: University of Californ, 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

Proposal Title: "First Principles Models of Type Ia Supernovae"
Scientific Discipline: Astrophysics

INCITE allocation: 3,500,000 Processor Hours
Site: Oak Ridge National Laboratory
Machine: Cray XT4
Allocation: 3,500,000 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.

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Type: Renewal

Principal Investigator: Patrick H. Worley
Affiliation: Oak Ridge National Laboratory
Co-Investigators:
David H. Bailey, Lawrence Berkeley National Laboratory
Jack Dongarra, University of Tennessee
William D. Gropp, Argonne National Laboratory
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 at San Diego
Jeffrey S. Vetter, Oak Ridge National Laboratory
Katherine Yelick, University of California at Berkeley
Bronis R. de Supinski, Lawrence Livermore National Laboratory

Proposal Title: "Performance Evaluation and Analysis Consortium End Station"
Scientific Discipline: Computer Sciences

INCITE allocation: 8,000,000 Processor Hours
Site: Argonne National Laboratory
Machine: IBM Blue Gene/P
Allocation: 4,000,000 processor hours

Site: Oak Ridge National Laboratory
Machine: Cray XT4
Allocation: 4,000,000 processor hours

Research Summary:
To maximize the utility of Leadership Class systems, such as the Cray X1E, Cray XT3, and IBM BlueGene/L (BG/L), 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/L, X1E, and XT3, 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.