Type: New

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
Site: Argonne National Laboratory
Machine: IBM Blue Gene/L
Allocation: 1,100,000 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: New

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

Proposal Title: "CAE Simulation of Full Vehicle Wind Noise and Other CFD Phenomena"
Scientific Discipline: Computer Sciences

INCITE allocation
Site: Lawrence Berkeley National Laboratory
Machine: NERSC HPC
Allocation: 166,000 processor hours

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.

January 8, 2007

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Type: New

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
Site: Oak Ridge National Laboratory
Machine: Cray XT3
Allocation: 1,000,000 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: New

Principal Investigator: Joan Centrella

Affiliation: National Aeronautics and Space Administration/ 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

Site: Oak Ridge National Laboratory

Machine: Cray XT3

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.

January 8, 2007

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Type: New

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

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

INCITE allocation
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: New

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, National Oceanic and Atmospheric Administration
Jeffrey Whitaker, National Oceanic and Atmospheric Administration

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

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

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) due in late 2007.

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Type: New

Principal Investigator: Robert Edwards
Affiliation: Jefferson Laboratory
Co-Investigators: David Richards, Thomas Jefferson Laboratory
Martin Savage, University of Washington
Robert Sugar, University of California, Santa Barbara

Proposal Title: "Lattice QCD for Hadronic and Nuclear Physics"
Scientific Discipline: Lattice Gauge Theory

INCITE allocation
Site: Oak Ridge National Laboratory
Machine: Cray XT3
Allocation: 10,000,000 processor hours

Research Summary:
This project will generate lattice gauge configurations for a broad program of study in high-energy and nuclear physics, but with an immediate emphasis on hadronic and nuclear physics. In particular, the computations will focus on the low-lying exotic meson resonance spectrum at pion masses down to 220 MeV, the photocouplings between some of these meson resonances, and the baryon resonance spectrum using newly developed group-theory methods. These calculations will be important steps on the road to the DOE's program in hadronic physics at Jefferson Laboratory. In addition, calculations of nucleon-nucleon and nucleon-hyperon scattering at pion masses sufficiently light to enable determinations of scattering lengths at the physical pion mass will be performed. This will be an important step toward achieving the DOE 2014 milestone in hadronic physics of obtaining a first-principles understanding of the nucleon-nucleon interaction.

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Type: New

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

Proposal Title: "Reactor Core Hydrodynamics"
Scientific Discipline: Applied Mathematics

INCITE allocation
Site: Argonne National Laboratory
Machine: IBM Blue Gene/L
Allocation: 1,000,000 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.

January 8, 2007

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Type: New

Principal Investigator: Giulia Galli
Affiliation: University of California, Davis
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
Site: Argonne National Laboratory
Machine: IBM Blue Gene/L
Allocation: 1,500,000 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: New

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

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.

Type: New

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
Site: Oak Ridge National Laboratory
Machine: Cray XT3
Allocation: 500,000 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: New

Principal Investigator: Don Lamb
Affiliation: ASC/Alliance Flash Center, University of Chicago
Co-Investigators: Alan Calder, ASC/Alliance Flash Center, University of Chicago
Anshu Dubey, ASC/Alliance Flash Center, University of Chicago
Tridivesh Jena, University of Chicago, Argonne National Laboratory
Dean Townsley, Argonne National Laboratory
James Truran, Argonne National Laboratory

Proposal Title: "Study of the Gravitationally Confined Detonation Mechanism for Type Ia Supernovae"
Scientific Discipline: Astrophysics

INCITE allocation
Site: Lawrence Berkeley National Laboratory
Machine: NERSC HPC
Allocation: 2,500,000 processor hours

Research Summary:
This INCITE allocation will be used to explore the gravitationally confined detonation (GCD) mechanism for incinerating a white dwarf in a stellar explosion known as a Type Ia supernova. The essential features of this mechanism have been confirmed in two-dimensional studies performed by other research groups, but confirmation of the mechanism with full three-dimensional whole-star simulations remains elusive. Through a series of simulations, the critical issue of the parameter space in which a detonation of the white dwarf star occurs (if such a parameter space exists) will be examined with three-dimensional whole-star simulations performed with the FLASH code. The most promising three of these simulations will be extended through the phases in which the hot nuclear ash spreads over the stellar surface and collides at the opposite point on the stellar surface — possibly producing a detonation.

Type: New

Principal Investigator: Peter Lichtner
Affiliation: Los Alamos National Laboratory
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
Site: Oak Ridge National Laboratory
Machine: Cray XT3
Allocation: 1,000,000 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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Type: New

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
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?"

Type: New

Principal Investigator: Piero Madau
Affiliation: University of California, Santa Cruz
Co-Investigators: Juerg Diemand, University of California, Santa Cruz
Michael Kuhlen, Institute for Advanced Studies, Princeton
Marcel Zemp, University of California, Santa Cruz

Proposal Title: "'Via Lactea': A Billion Particle Simulation of the Milky Way's Dark Matter Halo"
Scientific Discipline: Astrophysics

INCITE allocation
Site: Oak Ridge National Laboratory
Machine: Cray XT3
Allocation: 1,500,000 processor hours

Research Summary:
Revealing the nature of dark matter is fundamental to cosmology and particle physics. In the standard cosmological paradigm of structure formation (LambdaCDM), the universe is dominated by cold, collisionless dark matter (CDM), made flat by a cosmological constant (Lambda) and endowed with initial density perturbations via quantum fluctuations during inflation. In this model, galaxies form hierarchically, with low-mass objects ("halos") collapsing earlier and merging to form larger and larger systems over time. In this proposal, "Via Lactea," a new N-body cosmological simulation of unprecedented dynamic range, will be used to resolve the galaxy-forming region of a Milky-Way-size halo with one billion dark matter particles. This is two orders of magnitude more than typically used in previous simulations. "Via Lactea" will show whether surviving nearby subhalos are among the brightest sources of annihilation radiation and could be detectable by the forthcoming GLAST and VERITAS experiments.

Type: New

Principal Investigator: John Mauro
Affiliation: Corning Incorporated
Co-Investigators: Jitendra Balakrishnan, Corning Incorporated
Roger Loucks, Alfred University

Proposal Title: "Ab Initio Modeling of the Glass Transition"
Scientific Discipline: Materials Sciences

INCITE allocation
Site: Oak Ridge National Laboratory
Machine: Cray X1E
Allocation: 100,000 processor hours

Research Summary:
The properties of a glass depend strongly on both its composition and its thermal history. Prediction of glass properties from fundamental physics is especially difficult given the nonequilibrium nature of the glassy state and the slow relaxation times involved in the glass transition process. This proposal will use the INCITE resources to calculate the glass transition range behavior for silica and multicomponent silicate glasses. This project will enable the accurate computation of glass properties, accounting for both composition and thermal history, allowing for a significant savings in the research and development of new glass compositions and thermal processing cycles.

January 8, 2007

Type: New

Principal Investigator: Warren Mori
Affiliation: University of California, Los Angeles
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
Site: Lawrence Berkeley National Laboratory
Machine: NERSC HPC
Allocation: 1,000,000 processor hours

Research Summary:
The long-term future of experimental high-energy physics research using accelerators depends on the successful development of novel ultra high-gradient acceleration methods. New acceleration techniques using lasers and plasmas have already been shown to exhibit gradients and focusing forces more than 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: New

Principal Investigator: Phani Nukala
Affiliation: Oak Ridge National Laboratory
Co-Investigators: Srđjan Šimunović, Oak Ridge National Laboratory

Proposal Title: "Statistical Physics of Fracture: Scientific Discovery through High-Performance Computing"
Scientific Discipline: Materials Sciences

INCITE allocation
Site: Argonne National Laboratory
Machine: IBM Blue Gene/L
Allocation: 1,100,000 processor hours

Research Summary:
Fracture is an important issue for materials used in all energy technologies. The emphasis in this project is on obtaining quantitative agreement between simulation results (such as aniostropic roughness exponents) and experimental results. Investigations will focus on scaling laws of fracture, avalanche perecursors, universality of fracture strength distribution, size effect on the mean fracture strength, and finally the scaling and universality of crack surface roughness.

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Type: New

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
Site: Oak Ridge National Laboratory
Machine: Cray XT3
Allocation: 3,000,000 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: New

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

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

INCITE allocation
Site: Lawrence Berkeley National Laboratory
Machine: NERSC HPC
Allocation: 2,000,000 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 inertial confinement fusion (ICF) schemes to improve the viability of inertial fusion energy as a practical energy source. This proposal will carry out large-scale particle-in-cell (PIC) simulations of the ignition phase in FI. The proposed work covers almost all the physics in this phase (channeling, laser absorption, and electron transport up to moderate densities) with the goal of answering the following key questions: (1) Can a clean channel be created by a channeling pulse 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 10^{23} per cubic centimeter?

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Type: New

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
Site: Oak Ridge National Laboratory
Machine: Cray XT3
Allocation: 800,000 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: New

Principal Investigator: Benoit Roux
Affiliation: Argonne National Laboratory and 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
Site: Oak Ridge National Laboratory
Machine: Cray XT3
Allocation: 4,000,000 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.

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Type: New

Principal Investigator: Tamar Seideman
Affiliation: Northwestern University
Co-Investigators: Maxim Sukharev, Northwestern University

Proposal Title: "Coherent Control of Light in Nanoscale"
Scientific Discipline: Physical Chemistry

INCITE allocation
Site: Argonne National Laboratory
Machine: IBM Blue Gene/L
Allocation: 600,000 processor hours

Research Summary:
The goal of this project is to develop and apply a systematic tool for the design of plasmonic nanodevices which will contribute to the understanding, modeling, and manipulation of light propogation in the nanoscale, with potential applications in fields such as single molecule spectroscopy, nanoscale chemistry and solar energy.

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Type: New

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
Site: Oak Ridge National Laboratory
Machine: Cray XT3
Allocation: 1,500,000 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: New

Principal Investigator: Stan Woosley
Affiliation: 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

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

INCITE allocation
Site: Oak Ridge National Laboratory
Machine: Cray XT3
Allocation: 4,000,000 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.

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Type: New

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
Site: Oak Ridge National Laboratory
Machine: Cray XT3
Allocation: 1,000,000 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.

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INCITE
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Type: Renewal

Principal Investigator: Pratul Agarwal
Affiliation: Oak Ridge National Laboratory
Co-Investigators: Ed Uberbacher, Oak Ridge National Laboratory
Dean Myles, Oak Ridge National Laboratory
Jan Jensen, University of Iowa
Jeff Vetter, Oak Ridge National Laboratory
Sadaf Alam, Oak Ridge National Laboratory

Proposal Title: "Next Generation Simulations in Biology: Investigating Iomolecular Structure, Dynamics and Function through Multi-Scale Modeling"
Scientific Discipline: Life Sciences

INCITE allocation
Site: Oak Ridge National Laboratory
Machine: Cray XT3
Allocation: 1,000,000 processor hours

Research Summary:
Proteins are highly efficient machines working at the molecular level. The objective of this project is to simulate the atomistic level of a variety of protein complexes through multi-scale modeling using molecular dynamics simulations and mixed quantum classical modeling (QM/MM) to investigate several enzymes.

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INCITE

Advancing America's Science and Industrial Competitiveness

Type: Renewal

Principal Investigator: David Baker
Affiliation: University of Washington / Howard Hughes Medical Institute
Co-Investigators:

Proposal Title: "High-Resolution Protein Struction Prediction"
Scientific Discipline: Biology

INCITE allocation
Site: Argonne National Laboratory
Machine: IBM Blue Gene/L
Allocation: 3,000,000 processor hours

Research Summary:
Proteins are the workhorse molecules of all biological systems. A deep and predictive understanding of life thus requires functional portraits of all existing proteins, and these descriptions must necessarily include these molecules' high-resolution three-dimensional structures which, in turn, determine their functions. The goal of the proposed research is to compute structures for proteins of under 150 amino acids with atomic-level resolution. The alternative, experimental determination of protein structures is slow and expensive. In addition, the rate at which protein structures are obtained lags far behind the rate at which protein sequence information is being gathered by high-throughput genomic sequencing efforts.

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INCITE

Advancing America's Science and Industrial Competitiveness

Type: Renewal

Principal Investigator: Donald Batchelor

Affiliation: Oak Ridge National Laboratory

Co-Investigators:
S.C. Jardin, Princeton Plasma Physics Laboratory
L. A. Berry, Oak Ridge National Laboratory
D. Keyes, Columbia University
R. Bramley, Indiana University
S. P. Hirshman, Oak Ridge National Laboratory
D. E. Bernholdt, Oak Ridge National Laboratory
E. F. D'Azevedo, Oak Ridge National Laboratory
M. R. Fahey, Oak Ridge National Laboratory
W. Elwasif, Oak Ridge National Laboratory
E. F. Jaeger, Oak Ridge National Laboratory
D. A. Spong, Oak Ridge National Laboratory
R. Harvey, Comp-X
D. McCune, Princeton Plasma Physics Laboratory
G. Fu, Princeton Plasma Physics Laboratory
W. Park, Princeton Plasma Physics Laboratory
L. Sugiyama, Massachusetts Institute of Technology
D. Schnack, SAIC
H. Strauss, New York University
D. Schissel, General Atomics
P. Bonoli, Massachusetts Institute of Technology

Proposal Title: "Simulation of Wave-Plasma Interaction and Extended MHD in Fusion Systems"

Scientific Discipline: Fusion

INCITE allocation

Site: Oak Ridge National Laboratory

Machine: Cray XT3

Allocation: 2,000,000 processor hours

Research Summary:

Unstable plasma motions can degrade plasma containment or even terminate the plasma discharge, with the potential for damage to the containment device. These instabilities can be modeled using extended magnetohydrodynamics. High-power radio frequency (RF) electromagnetic waves can be used to influence plasma stability — sometimes producing instability, and sometimes reducing or eliminating instability. The purpose of this project is to advance understanding and predicting the effects of RF waves on plasma stability. This understanding is of significant scientific and economic benefit, with a direct benefit to the international ITER project in the prediction and control of the macroscopic stability of the ITER plasma and in the design and application of heating and current drive systems.

January 8, 2007

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INCITE

Advancing America's Science and Industrial Competitiveness

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
Site: Argonne National Laboratory
Machine: IBM Blue Gene/L
Allocation: 750,000 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.

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INCITE

Advancing America's Science and Industrial Competitiveness

Type: Renewal

Principal Investigator: Jackie Chen
Affiliation: Sandia National Laboratories
Co-Investigators: Ramanan Sankaran, Sandia National Laboratories
Evatt Hawkes, Sandia National Laboratories
Philip Smith, University of Utah
David Lignell, Sandia National Laboratories and University of Utah
Chun Sang Yoo, Sandia National Laboratories

Proposal Title: "High-Fidelity Numerical Simulations of Turbulent Combustion — Fundamental Science Towards Predictive Models"
Scientific Discipline: Combustion

INCITE allocation
Site: Oak Ridge National Laboratory
Machine: Cray X1E
Allocation: 50,000 processor hours

Site: Oak Ridge National Laboratory
Machine: Cray XT3
Allocation: 6,000,000 processor hours

Research Summary:

The objective of this INCITE project is to perform an array of direct numerical simulations that will provide fundamental understanding of key processes such as flame stabilization, flame structure, extinction, ignition, and soot formation, that underlie fuel-efficient low-temperature combustion engine designs for transportation and lean premixed combustion for stationary power generation. An increase in fuel efficiency from 30% to 45% would result in a savings of 3 million barrels of oil per day of the 20 million consumed for transportation with a simultaneous decrease in CO2 emissions.

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INCITE
Advancing America's Science and Industrial Competitiveness

Type: Renewal

Principal Investigator: David Dean
Affiliation: Oak Ridge National Laboratory
Co-Investigators: Thomas Papenbrock, Univeristy of Tennessee
Mario Stoitsov, Univeristy of Tennessee

Proposal Title: "Ab Initio Nuclear Structure Computations"
Scientific Discipline: Nuclear Physcis

INCITE allocation
Site: Oak Ridge National Laboratory
Machine: Cray XT3
Allocation: 5,000,000 processor hours

Research Summary:
Coupled-cluster theory is one of the most promising ab initio microscopic theories that can potentially provide a highly accurate description of a variety of many-body physical systems. In this project, codes specifically tailored for the nuclear many-body problem will be coupled with the significant developments of coupled-cluster theory that have occurred in quantum chemistry. With application of these techniques to the nuclear problem, the objective of this project is to calculate ground, excited, closed-shell and open-shell, non-degenerate and quasi-degenerate states of nuclei and certain nuclear properties.

Type: Renewal

Principal Investigator: Robert Harrison
Affiliation: Oak Ridge National Laboratory
Co-Investigators:
Jerzy Bernholc, North Carolina State University
A.C. Buchanan, Oak Ridge National Laboratory
Marco Buongiorno-Nardelli, North Carolina State University
James Caruthers, Purdue University
W. Nicholas Delgass, Purdue University
Dave Dixon, University of Alabama
Sharon Hammes-Schiffer, Pennsylvania State University
Duane Johnson, University of Illinois at Urbana Champaign
Manos Mavrikakis, University of Wisconsin - Madison
Djamaladdin Musaev, 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 G. Sumpter, Oak Ridge National Laboratory
Kendall Thomson, Purdue University
Ward Thompson, Kansas University

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

INCITE allocation
Site: Oak Ridge National Laboratory
Machine: Cray X1E
Allocation: 300,000 processor hours

Site: Oak Ridge National Laboratory
Machine: Cray XT3
Allocation: 3,000,000 processor hours

Research Summary:
This proposal focuses on the rational design of catalysts via the reliable and accurate prediction of the electronic structure of large molecules and surfaces. From such calculations can be derived the energetic, structural, kinetic and dynamical information necessary for a fundamental understanding of chemical transformation. The activities include three thrusts: catalytic transformation of hydrocarbons, clean energy including hydrogen production and storage, and the chemistry of transition metal clusters including metal oxide supports.

January 8, 2007

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INCITE

Advancing America's Science and Industrial Competitiveness

Type: Renewal

Principal Investigator: Moeljo Hong
Affiliation: The Boeing Company
Co-Investigators: Robert Narducci, The Boeing Company
Stephen LeDoux, The Boeing Company
Todd Michal, The Boeing Company

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

INCITE allocation
Site: Oak Ridge National Laboratory
Machine: Cray X1E
Allocation: 200,000 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 computationally what happens to a wing when a flap is suddenly deployed. Such "flutter analysis" has historically not included simulating both the structural wing response (the wing flaps) as well as the air flow around the wing. This requires coupling two complex codes together in a nonlinear fashion: one for the aerodynamics, and one for the structural response of the wing. Such work helps to guide control surface studies; learn aerodynamic time lags and how to account for them to better design control-laws; gain better confidence in control surface free play modeling; and help to prevent unnecessary maintenance through more aggressive designs.

Type: Renewal

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

Proposal Title: "Computational Design of the Low-loss Accelerating Cavity for the ILC"
Scientific Discipline: Accelerator Physics

INCITE allocation
Site: Oak Ridge National Laboratory
Machine: Cray X1E
Allocation: 400,000 processor hours

Research Summary:
The focus of this project is to address the Computational Grand Challenge proposed by the International Linear Collider (ILC) Global Design Effort Advisory Committee, which is stated as: "for a single three-cryomodule RF unit of the ILC Main Linac and by assuming realistic 3-D dimensions and misalignments, calculate multi-bunch beam dynamics effects, including wakefields and high-order-mode excitations." As a first step, the project will model a single ILC baseline 8-cavity cyromodule using similar techniques for modeling the Superconducting Testing Facility cryomodule which will be constructed at KEK, Japan. The modeling of a complete radio frequency (rf) unit comprised of three cyromodules requires a petascale computer to do a complete analysis.

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Type: Renewal

Principal Investigator: W. W. Lee
Affiliation: Princeton Plasma Physcis Laboratory
Co-Investigators: C.S. Chang, New York University
David Keyes, Columbia University

Proposal Title: "Gyrokinetic Plasma Simulation"
Scientific Discipline: Fusion

INCITE allocation
Site: Oak Ridge National Laboratory
Machine: Cray X1E
Allocation: 75,000 processor hours

Site: Oak Ridge National Laboratory
Machine: Cray XT3
Allocation: 6,000,000 processor hours

Research Summary:
The objective of this project is to understand the confinement and transport physics in the core and edge regions for the present generation of U.S. fusion experiments, (e.g., D3D and NSTX) with more realistic parameters. These are truly 3D (with two additional dimensions in the velocity space) simulations for understanding the meso-scale physics of turbulent transport in tokamaks. The goal is to have the capability to simulate ITER plasmas through the use of improved physics modules and linear solvers, as well as the implementation of multi-dimensional domain decompositions in these codes.

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Advancing America's Science and Industrial Competitiveness

Type: Renewal

Principal Investigator: David McGuire
Affiliation: University of Alaska, Fairbanks
Co-Investigators: Jeff McAllister, University of Alaska, Fairbanks

Proposal Title: "Modeling the Response of Terrestrial Ecosystems to Climate Change and Distrubance"
Scientific Discipline: Envirornmental Sciences

INCITE allocation
Site: Argonne National Laboratory
Machine: IBM Blue Gene/L
Allocation: 600,000 processor hours

Research Summary:
Simulations in this study will be performed using the Terrestrial Ecosystem Model (TEM), a framework for investigating fundamental aspects of terrestrial carbon cycle dynamics to obtain a better understanding of fundamental processes related to climate change and their dynamic interactions. These simulations provide an understanding of how anthropogenic disturbances interact with other disturbances and ecological dynamics.

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Type: Renewal

Principal Investigator: Anthony Mezzacappa
Affiliation: Oak Ridge National Laboratory
Co-Investigators: John Blondin, North Carolina State University
Steven Bruenn, Florida Atlantic University
Christian Cardall, Oak Ridge National Laboratory
David Dean, Oak Ridge National Laboratory
John Hayes, University of California, San Diego
Raphael Hix, Oak Ridge National Laboratory
Eric Myra, State University of New York at Stony Brook
Jirina Stone, Okford University, United Kingdom
Doug Swesty, State University of New York at Stony Brook

Proposal Title: "Multi-Dimensional Simulations of Core-Collapse Supernovae"
Scientific Discipline: Astrophysics

INCITE allocation
Site: Oak Ridge National Laboratory
Machine: Cray X1E
Allocation: 300,000 processor hours

Site: Oak Ridge National Laboratory
Machine: Cray XT3
Allocation: 7,000,000 processor hours

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

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
Site: Oak Ridge National Laboratory
Machine: Cray X1E
Allocation: 750,000 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
Site: Lawrence Berkeley National Laboratory
Machine: NERSC HPC
Allocation: 150,000 processor hours

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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INCITE

Advancing America's Science and Industrial Competitiveness

Type: Renewal

Principal Investigator: Thomas Schulthess
Affiliation: Oak Ridge National Laboratory
Co-Investigators:
Gonzalo Alverz, Oak Ridge National Laboratory
Jerzy Bernholc, North Carolina State University
Peter Cummings, Vanderbilt University
Elbio Dagotto, Oak Ridge National Laboratory
Markus Eisenbach, Oak Ridge National Laboratory
Mark Jarrell, University of Cincinnati
Paul Kent, Oak Ridge National Laboratory
Uzi Landman, Georgia Tech
Thomas Maier, Oak Ridge National Laboratory
Malcolm Stocks, Oak Ridge National Laboratory

Proposal Title: "Predictive Simulations in Strongly Correlated Electron Systems and Functional Nanostructures"
Scientific Discipline: Nano & Materials Science

INCITE allocation
Site: Oak Ridge National Laboratory
Machine: Cray X1E
Allocation: 500,000 processor hours

Site: Oak Ridge National Laboratory
Machine: Cray XT3
Allocation: 7,000,000 processor hours

Research Summary:
Recent discoveries in functional nanostructures and strongly correlated materials created extraordinarily promising materials that can revolutionize our way of life. Scientifically, the opportunities fall into two broad categories that will be studied in this project: strongly correlated electron systems that are studied with simplified models but have to be solved with computationally intensive quantum many-body calculations, and large-scale functional nanostructures that can be modeled with first principles electronic structure methods.

Type: Renewal

Principal Investigator: Evan Smyth
Affiliation: Dreamworks Animation
Co-Investigators:

Proposal Title: "Real-Time Ray-Tracing"
Scientific Discipline: Computer Science

INCITE allocation
Site: Oak Ridge National Laboratory
Machine: Cray XT3
Allocation: 900,000 processor hours

Research Summary:
Work in this proposal is focused on aggressively pushing the limits of high-quality real-time ray-tracing. The objective of this project is to develop a real-time ray-tracing system (instead of the current ~100 CPU hours required per image) that is designed to run on a distributed memory multi-computer comprised of a high number of multiprocessor nodes with vector processing capabilities. In addition to affecting the way films are produced, the proposed real-time, high-fidelity ray-tracing techniques have application in other fields requiring visualization of large complex datasets.

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
Site: Argonne National Laboratory
Machine: IBM Blue Gene/L
Allocation: 75,000 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.

Type: Renewal

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

Proposal Title: "Interaction of ITG/TEM and ETG Gyrokinetic Turbulence"
Scientific Discipline: Fusion

INCITE allocation
Site: Oak Ridge National Laboratory
Machine: Cray X1E
Allocation: 500,000 processor hours

Research Summary:
There is wide agreement in the Fusion community that prediction of the H-mode (good confinement) edge pedestal height is the key limitation in confidently predicting ITER performance. This requires an accurate knowledge of electron energy transport in the H-mode edge layer. The objective of this project is to increase understanding in this area. This project will use the GYRO gyrokinetic code to investigate the interaction of long-wavelength ion-temperature-gradient (ITG) turbulence with short-wavelength electron-temperature-gradient (ETG) turbulence. Existing GYRO simulations routinely include the interaction of ITG with trapped-electron modes (TEM) at long ion-scale wavelengths, but no attempt to couple ITG/TEM fluctuations to electron-scale ETG fluctuations has heretofore been made. Such simulations require unusually high equivalent Reynolds numbers due to the enormous disparity between ion (ITG/TEM) and electron (ETG) spatial and temporal scales.

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INCITE

Advancing America's Science and Industrial Competitiveness

Type: Renewal

Principal Investigator: Warren Washington
Affiliation: National Center for Atmospheric Research
Co-Investigators:
John Drake, Oak Ridge National Laboratory,
Donald Anderson, NASA Headquarters
David Bader, Lawrence Livermore National Laboratory
William Collins, National Center for Atmospheric Research
Robert Dickinson, Georgia Tech University
David Erickson, Oak Ridge National Laboratory
Peter Gent, National Center for Atmospheric Research
Steven Ghan, Pacific Northwest National Laboratory
Jim Hack, National Center for Atmospheric Research
Philip Jones, Los Alamos National Laboratory
Robert Malone, Los Alamos National Laboratory
William Schlesinger, Duke University

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

INCITE allocation
Site: Oak Ridge National Laboratory
Machine: Cray X1E
Allocation: 1,500,000 processor hours

Site: Oak Ridge National Laboratory
Machine: Cray XT3
Allocation: 4,000,000 processor hours

Research Summary:
A national challenge is to predict future climates based on scenarios of anthropogenic emissions and other changes resulting from options in energy policies. This proposal builds on the successful collaboration of the National Science Foundation (NSF) and Department of Energy (DOE) in developing the Community Climate System Model (CCSM3), and is expanded to include collaborations with the National Aeronautics and Space Administration (NASA) and additional university partners with expertise in high-end computational climate research.