Type: Renewal
Title: "Ab Initio Dynamical Simulations for the Prediction of Bulk Properties"

Principal Investigator: Theresa Windus, Iowa State University
Co-Investigators: Brett Bode, Iowa State University
Graham Fletcher, Argonne National Laboratory
Mark Gordon, Iowa State University
Monica Lamm, Iowa State University
Michael Schmidt, Iowa State University

Scientific Discipline: Chemistry: Physical

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

Research Summary:
This project uses high-quality electronic structure theory, statistical mechanical methods, and massively parallel computers to address the prediction of bulk properties of water systems that require high fidelity. These molecular-scale problems are of critical importance to national priority scientific issues such as global warming, the environment, and alternative fuels. Many critical problems in the chemical sciences are so computationally demanding that the only perceived option for addressing them is to employ low-level methods whose reliability is suspect. The electronic structure community already has well-established protocols for assessing the reliability of methods applied to small and medium systems, but this project will address extended systems whose sizes require the use of massive computational resources.

Driving the need for petascale computing in this community are a vast array of problems, ranging from simulations of liquids with unquestionable accuracy to studies of reaction mechanisms in the condensed phase to ground and excited state studies of polymers, biomolecules, and other extended systems. This work is focusing on understanding the molecular level dynamics of water, the formation of aerosols important in cloud formation, and the interactions of dendrimers with ligands of environmental importance. In each of these applications, the underlying research will set a new standard for the predictive computation of bulk properties. The two primary electronic structure codes to be used in these simulations are GAMESS and NWChem. Both codes are, without question, the most broadly scalable electronic structure systems, and both are available to all users at no cost. Therefore, the impact of this research will cut across a broad area of the chemical sciences and will forge a path for subsequent research by the community. In addition, the use of the computational resources for the science and engineering areas will aid in training the next generation of massively parallel-literate researchers.

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

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

Scientific Discipline: Energy Technologies: Nuclear Energy

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

Research Summary:
The DOE Nuclear Energy Advanced Modeling and Simulation (NEAMS) program is developing simulation capabilities to leverage U.S. leadership computing facilities in the design of next-generation reactors. One of the active areas of research is in the Advanced Fuel Cycle Initiative (AFCI), which is examining a closed nuclear fuel cycle based on a new generation of fast neutron reactors specifically designed for the transmutation of spent nuclear fuel to address nuclear waste management concerns. Partitioning and transmutation of transuranic elements from nuclear spent fuel is considered as a way of reducing the burden of geological disposal. Advanced simulation is viewed as critical in bringing fast reactor technology to fruition in an economic and timely manner, and the DOE has recently established area-specific campaigns to look at open questions in closing the fuel cycle. Analysis of fast reactor cores is one of the areas of interest, and the thermal-hydraulic performance—pressure drop and mixing induced by the coolant flow—figures prominently in design questions.

In accordance with the original proposal, the primary computations scheduled for 2011 are:
- Additional DNS (direct numerical simulation) studies in plane channel flow with a wire that will conjugate heat transfer under different loading conditions (Reynolds and Prandtl numbers).
- Very high-resolution LES (Large Eddy Simulation) of wire-wrapped fuel pin bundles at intermediate pin counts (for example, 37 or 61).
- POD-based (proper orthogonal decomposition) reduced-order model analysis for intermediate and high (217) pin counts.
- Conjugate heat transfer analysis for intermediate pin counts, using a newly developed multi-domain solver.
- Outlet plenum analysis looking at the coolant flow leaving the pin bundles.

Type: New
Title: "Advanced Simulations of Plasma Microturbulence at the Petascale and Beyond"

Principal Investigator: William M. Tang, Princeton University
Co-Investigators: Mark F. Adams, Columbia University
Stéphane Ethier, Princeton Plasma Physics Laboratory
Scott Klasky, Oak Ridge National Laboratory
Bruce Scott, Max-Planck Institute for Plasma Physics
Weixing Wang, Princeton University

Scientific Discipline: Physics: Plasma Physics

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

Research Summary:
Worldwide energy consumption has risen twenty-fold during the 20th century and shows no sign of abating. Nuclear fusion presents tantalizing potential, promising a safe, clean, and sustainable way to meet a large portion of the world's energy needs on a continuous basis. However, the scientific and engineering challenges in designing a fusion reactor are formidable. Therefore, the first commercial power plants are not expected before the middle of the century. Computations carried out at the extreme scale of key plasma physics and materials science processes in fusion devices will be key to helping design, run, and interpret expensive large-scale experiments and are expected to significantly speed up the realization of fusion power plants.

A major plasma physics problem on the road to a working fusion power plant involves significantly improving the understanding, prediction, and control of large- and small-scale instabilities caused by unavoidable plasma inhomogeneities. One consequence is the occurrence of turbulent fluctuations associated with the significant transport of heat, momentum, and particles across the confining magnetic field. Understanding and possibly controlling the balance between these energy losses and the self-heating rates of the actual fusion reaction is key to achieving the efficiency needed to help ensure the practicality of future fusion power plants. The present INCITE project on advanced Particle-in-Cell (PIC) global simulations of plasma microturbulence at the petascale and beyond is motivated by this FES grand challenge.

Engaging the power of modern high-performance computers will help scientists understand how to control the balance between energy losses caused by microturbulence and the self-heating rates of the actual fusion reaction. This is essential to achieving the efficiency needed to help ensure the practicality of future fusion power plants.

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

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

Scientific Discipline: Biological Sciences: Biophysics

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

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

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

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

Principal Investigator: Venkatramani Balaji, National Oceanic and Atmospheric Association (NOAA)

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

Scientific Discipline: Earth Science: Climate Research

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

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

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

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

Principal Investigator: Warren Washington, National Center for Atmospheric Research

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

Scientific Discipline: Earth Science: Climate Research

INCITE Allocation: **110,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (70,000,000 processor hours)
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (40,000,000 processor hours)

Research Summary:
The Climate Science Computational End Station (CCES) will project future climates using scenarios of anthropogenic emissions and other changes resulting from energy policy options. Climate change simulations and climate variability studies will directly inform national science policy, thereby contributing to the DOE, NSF and NASA science missions. Of particular importance are global high resolution simulations that will improve the scientific basis, accuracy, and fidelity of climate models. Continuing model development and extensive testing of the Community Earth System Model (CESM) to include recent new knowledge about ocean and land ecosystems is at the cutting edge of climate science research.

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

Principal Investigator: Michael Klein, Temple University
Co-Investigators: Kelly Anderson, Procter & Gamble
Russell DeVane, Temple University
Peter Koenig, Procter & Gamble
Axel Kohlmeyer, Temple University

Scientific Discipline: Chemistry: Physical

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

Research Summary:
Membrane fusion, the process in which two lipid bilayers merge to form a continuous structure, is a complex and fascinating phenomenon, influenced by many factors including membrane composition, hydration, electrostatics, and environmental conditions. Membrane fusion is essential for the life cycle of all living organisms. A molecular view of the role of fusion proteins in the membrane fusion process is largely lacking, and it is not likely that experiments alone can provide these details in the foreseeable future.

In industrial processes on the other hand, vesicle or membrane fusion is an undesirable event leading to product instabilities which limit shelf life. A number of formulated consumer products are made of dispersed vesicles which contain active components or are themselves active ingredients, and here a better understanding of how to stabilize such vesicles is needed.

To simulate these processes, accurate coarse-grain models, molecular dynamics software at the limit of its capabilities, as well as exceptionally capable computer hardware are required. In preparation for this project, enhancements to the LAMMPS molecular dynamics package have been implemented. Future improvements to overall performance and scaling to large node counts will be realized as indicated. The improvements are applicable to other projects using LAMMPS.

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

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

Scientific Discipline: Chemistry: Physical

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

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

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

Type: New
Title: "Detached-Eddy Simulations and Noise Predictions for Tandem Cylinders"

Principal Investigator: Philippe Spalart, The Boeing Company

Scientific Discipline: Engineering: Fluids and Turbulence

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

Research Summary:
To represent the flows created by aircraft landing gear, wind turbines, and bridges or buildings, this project simulates the turbulence and calculates the noise caused by two cylinders placed in tandem in an air stream, so that one is in the wake of the other. The project will lead to a better understanding of the numerical resolution needed and of the theory of noise generation.

The flow past tandem cylinders is a prime test case for detailed comparisons among computational fluid dynamics (CFD) approaches for studying the physics of massively separated flows, the impingement of turbulence on a solid body, and the aerodynamic noise that results from it.

The capabilities developed will contribute to the design of safe and quiet technologies. The result will be a set of simulations of flow past tandem cylinders that reflects the state-of-the-art of turbulence-resolving CFD approaches to massively separated flows.

The project will build on work accomplished in 2010 on the Blue Gene/P at Argonne National Laboratory and information gathered from fifteen other teams that participated in the AIAA Workshop on Benchmark Problems for Airframe Noise Computations (BANC-I) in June 2010. Completing this study will involve comparing the Delayed Detached-Eddy Simulation (DDES) and Improved Delayed Detached-Eddy Simulation (IDDES) approaches and the different domain and grid sizes.

Type: New
Title: "Deterministic Simulations of Large Regional Earthquakes at Frequencies up to 4Hz"

Principal Investigator: Thomas H. Jordan, University of Southern California
Co-Investigators: Jacobo Bielak, Carnegie Mellon University
Po Chen, University of Wyoming
Yifeng Cui, University of California, San Diego
Philip J. Maechling, University of Southern California
Kim Olsen, San Diego State University

Scientific Discipline: Earth Science: Geological Sciences

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

Research Summary:
An interdisciplinary research team from the Southern California Earthquake Center (SCEC) is conducting and analyzing deterministic earthquake-wave-propagation simulations of large-scenario (Mw7.0+) earthquakes at frequencies above 1Hz on a regional scale. Using a realistic 3-D structural model of Southern California, these simulations will help geoscientists better understand the earthquake-wave-propagation characteristics of large-magnitude events in this region, including the duration and distribution of strong ground motions at frequencies of interest to civil and structural engineers.

Scientific research into these issues is complicated by the fact that large earthquakes are rare events, and the strong-motion data from them are sparse. As a result, numerical simulations of large earthquakes in well-studied seismically active areas are important tools for basic earthquake science, because they provide a quantitative basis for comparing hypotheses about earthquake behavior with actual observations. Simulations are playing an increasingly crucial role in scientists' understanding of regional earthquake hazard and risk. SCEC researchers are developing the ability to conduct predictive, end-to-end simulations ("rupture to rafters"), which define the current understanding of earthquake processes and seismic hazards.

Simulations are of significant interest to members of California's seismological, engineering, and emergency management communities. The research has two primary goals: to investigate the upper frequency limits of deterministic ground motion simulations and to better quantify how high-frequency seismic waves from large earthquakes contribute to the seismic hazard in Southern California and other regions.

Type: Renewal
Title: "Electronic Structure Calculations for Nanostructures"

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

Scientific Discipline: Materials Science: Nanoscience

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

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

The goal is to understand the mechanisms of the critical steps inside a nano solar cell. These include: the photon absorption, exciton generation, exciton dissociation, exciton and carrier decays and recombinations, carrier transport, and carrier collection. In a thin film solar cell, if the carrier diffusion constant, the impurity trapping rate, and the exciton generation rates are known, the photovoltaic process and its efficiency can be simulated by Poisson drift-diffusion equation. However, some of the corresponding critical aspects of the nano systems are still not well understood. We plan to use ab initio level calculations to study the related problems in nano systems. All these studies are large scale simulations, which can only be carried out using INCITE allocations on the leadership facilities.

Type: New
Title: "Explosive Hazard Predictions with the Uintah Framework"

Principal Investigator: Martin Berzins, University of Utah
Co-Investigators: Todd Harman, University of Utah
John Schmidt, University of Utah
Chuck Wight, University of Utah

Scientific Discipline: Engineering: Fluid-Structure Interaction

INCITE Allocation: **15,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (15,000,000 processor hours)

Research Summary:
The safety of transporting and storing widely used commercial explosives is investigated by means of combustion and computational science. Large-scale simulations on some of the most powerful Department of Energy parallel computers will show how to avoid life-threatening accidents caused by fires and explosions.

Specifically, we will examine different packing arrangements of the devices to prevent a transition from a low violence deflagration (thermal combustion) to an extremely violent detonation reaction. The motivation for this work is a recent semi-truck accident in which 36,000 lbs of seismic boosters ignited and detonated, destroying a highway and railway.

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

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

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

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

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

The project will use two complementary global, nonlinear gyrokinetic codes: particle-in-cell GTC and continuum GYRO. Rigorous cross-code benchmarks between GTC and GYRO could provide verification of the gyrokinetic simulations. Comparisons with existing tokamak reactors, including the DIII-D tokamak dedicated experiments for energetic particle physics, will provide validations for the gyrokinetic simulations. The proposed gyrokinetic simulations using GTC and GYRO will comprehensively assess the confinement properties of fusion products in ITER experiments. These simulations require the full power of petascale computers, with the GTC and GYRO codes making full use of the petascale system and incorporating important physics elements.

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

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

Scientific Discipline: Chemistry: Combustion

INCITE Allocation: **60,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (60,000,000 processor hours)

Research Summary:

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

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

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

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

Scientific Discipline: Rheology

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

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

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

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

Scientific Discipline: Physics: Plasma Physics

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

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

Large scale simulations, pushing the limit of Jaguar, of tokamak plasma in realistic device geometries will be performed in this INCITE project. An extensive study of edge pedestal physics will be performed. In order to understand the nonlocal edge pedestal effect on the core plasma confinement, multiscale simulations of the whole volume plasma will also be performed. The whole volume includes the magnetic separatix, magnetic axis and the material wall boundary. Nonlocal turbulence propagation and the self-organization of the plasma profile to a critical global state will be simulated in H-mode plasmas. These simulations will hopefully shed light to the understanding of the edge pedestal physics and the tail-wagging-the-dog phenomenon, long awaited problems in magnetic fusion physics. As the edge plasma pedestal becomes steeper, a large scale instability called "edge localized modes" (ELMs) crashes the plasma pedestal, limiting the core confinement and damaging the material wall. Control of large scale ELMs is an essential condition to the success of the ITER program. This INCITE will study what the edge localized modes are and how to control them.

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

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

Scientific Discipline: Physics: Astrophysics

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

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

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

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

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

Scientific Discipline: Physics: Plasma Physics

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

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

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

Type: New
Title: "Large Eddy Simulation for Green Energy and Propulsion Systems"

Principal Investigator: Umesh Paliath, GE Global Research

Scientific Discipline: Energy Technologies: Energy Efficiency

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

Research Summary:
Advanced "green" energy and propulsion systems that deliver significant improvements in energy efficiency (e.g., fuel burn reductions) and yields from renewable sources (e.g., wind) have been a primary driver for the development of accurate, hi-fidelity simulation capabilities at GE. The inability of current computational fluid dynamics (CFD) methods to accurately and consistently characterize turbulent mixing processes in shear flows (wakes, jets from nozzles, and cooled blades) and boundary layer flows have slowed down the drive to higher efficiencies and lower emissions (noise, greenhouse gases, etc.). A simulation methodology that captures such phenomena accurately, and in conjunction with petascale computing, can create a design capability that has the potential to break through several barrier technologies.

Large Eddy Simulations (LES), when validated, are ideally suited to overcome these challenges. LES can provide a complete statistical description of the flow for the desired range of scales, providing a way of numerically analyzing the flow turbulent characteristics that would not be feasible experimentally. These numerical simulations, while providing insight into the science of boundary layers and wake mixing, also become computationally expensive especially as they move towards modeling full-scale designs. But when coupled with massively parallel computational capability, this approach provides a cost-efficient and excellent alternative to experimental test rigs for real-world industrial applications.

The 2010 INCITE award allowed the GE Global Research team to address fundamentals of wind and jet noise – direct airfoil noise computation at realistic Reynolds number, heated jet noise source characterization and Reynolds number scaling. In 2011, the team's research will focus on solving real-life challenges in wind and jet noise and initiate fundamental work in gas turbine heat transfer.

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

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

Scientific Discipline: Chemistry: Combustion

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

Research Summary:

With access to the INCITE program, CERFACS has been performing top-of-the-line, quality simulations on highly complex cases in the goal towards the fully numerical modeling of a real combustor. The overall framework of this project is focused on Large Eddy Simulation (LES) of these engines with the inclusion of the liquid phase phenomena. With this in mind, CERFACS has performed simulations and validation of two-phase flow experiments.

In parallel, taking advantage of the leadership class computers available through the INCITE program, CERFACS has performed the largest unstructured LES done so far on a real full combustion chamber (330 million elements). This simulation contributes to the validation of the LES approach when dealing with combustion instabilities, where the high unsteadiness of the flow makes the impact of the uncertainty behind the LES combustion model a highly critical point that needs to be addressed.

This validation allows CERFACS to focus on the challenges that await in 2011. First, can LES predict correctly ignition dynamics? This is a major step towards the visual design of a combustor since ignition is often the most critical step for an engine. This complex unsteady phase, that in reality lasts only a couple of milliseconds, can decide whether an engine is viable or not. Researchers will evaluate an experiment conducted at Cambridge where it was attempted to study the ignition via a spark of a fuel-air mixture. In parallel, injection studies will be continued with the fuel inclusion of a real turbine and no longer a simplified experimental setup. Additionally, the first steps towards the numerical study of biofuel combustion will be carried out with the inclusion of the complex granulometry and multi-composition of the liquid fuel used in an experimental setup. These characteristics are key to mimicking the behavior of biofuels, which are much more complex than current molecules. Along with these scientific challenges, new domain decomposition strategies will be implemented (coarse-mesh partitioning mapping, iso-tropic partitioned mesh refinement) and will be tested to increase the efficiency of the code and move closer to Peta or even Exascale computational fluid dynamics for combustion applications.

Type: New
Title: "Lattice QCD"

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

Scientific Discipline: Physics: Particle Physics

INCITE Allocation: **80,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (50,000,000 processor hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (30,000,000 processor hours)

Research Summary:
This project will deepen scientists' understanding of the interactions of quarks and gluons, the basic components of 99% of the visible matter in the universe, and will play an important role in ongoing efforts to develop a unified theory of the four fundamental forces of nature. These fundamental questions in high energy and nuclear physics are directly related to major experimental programs and milestones set out by the Office of Science.

The Leadership Computing Facility platforms are enabling the research team to dramatically advance research in lattice quantum chromodynamics and other strongly coupled field theories of importance to the study of high energy and nuclear physics.

Three quark actions will be used in this work: clover, domain wall, and improved staggered. The team is validating calculations that cannot be checked through direct comparison with experiment, by performing them with more than one action. Gauge configurations are being used to determine a wide range of physical quantities of importance in high energy and nuclear physics: underlying parameters of the Standard Model of subatomic physics, including the masses of the quarks and the strong coupling constant and the elements of the Cabibbo-Kobayashi-Maskawa (CKM) matrix; and the mass spectrum of strongly interacting particles, including the baryon spectrum and photo-transitions in the charmonium sector.

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

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

Scientific Discipline: Materials Science: Condensed Matter and Materials

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

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

Type: New
Title: "Multiscale Blood Flow Simulations"

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

Scientific Discipline: Biological Sciences: Biophysics

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

Research Summary:
Cerebral aneurysms (CAs) occur in up to 5% of the general population, leading to strokes for over 40,000 Americans each year. Sickle cell (SS) anemia – a chronic inflammatory disease – is the most common genetic diseases among African American, with an 8% incidence of the trait among this population; 50,000 individuals are suffering from sickle cell anemia in USA every year. Cerebral malaria (CM) is a related red blood cell (RBC) disease, with significant mortality of up to 20%, even when treatment is given. More than 1.5 million deaths each year have been reported – mostly in children. Currently, there are no quantitative tools to predict the rupture of aneurysms or the progression of RBC-related devastating pathologies such as SS and CM. Petaflop resources will allow for realistic simulations of these brain pathologies, quantifying, for the first time, their biophysical characteristics. This project will conduct multiscale simulations for modeling blood flow in the human brain vasculature, the first of its kind, consisting of hundreds of large 3-D arteries (Macrovascular Network, MaN), 10M arterioles (Mesovascular Network, MeN), and 1B capillaries (Microvascular Network, MiN).

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

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

Scientific Discipline: Physics: Nuclear Physics

INCITE Allocation: **43,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (28,000,000 processor hours)
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (15,000,000 processor hours)

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

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

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

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

Scientific Discipline: Earth Science: Climate Research

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

Research Summary:
A focal point in the traditional approach to modeling large-scale atmospheric and ocean flows is the assumption of hydrostatic balance between the gravitational force per unit volume and the vertical component of the pressure gradient. The hydrostatic balance assumes that vertical accelerations are small compared to vertical pressure gradients and vertical buoyancy forces, which is a good approximation for quasi-geostrophic flows such as large-scale vertical motions. However, the hydrostatic approximation is uncontrolled, valid only for variations in the horizontal direction that are large compared to the vertical height H of the domain.

While it is very accurate over a large part of the ocean, the approximation neglects vertical overturning processes, such as convection, and therefore hydrostatic models require parameterizations in areas where such processes occur. These climate scale models are being applied more frequently to high-resolution regional modeling studies such as those in the Gulf of Mexico and the Arctic basin. Regional models require very high resolution, on the order of a few kilometers or less, in order to resolve local topographic features. Therefore, they may violate the validity of the hydrostatic approximation so that the validity of the results and the extent of the inaccuracy involved is unknown.

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

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

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

Scientific Discipline: Computer Science

INCITE Allocation: **30,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (20,000,000 processor hours)
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (10,000,000 processor hours)

Research Summary:
To maximize the utility of Department of Energy leadership class systems such as the Cray XT4, Cray XT5, and IBM Blue Gene/P, we must understand how to use each system most efficiently. The performance community (performance tool developers, performance middleware developers, system and application performance evaluators, and performance optimization engineers) can provide the tools and studies to enable these insights, if they have adequate access to the systems. To provide further understanding of these high-end systems, this proposal focuses on four primary goals: (1) update and extend performance evaluation of all systems using suites of both standard and custom micro, kernel, and application benchmarks; (2) continue to port performance tools and performance middleware to the BG/P and XT4/5; (3) validate the effectiveness of performance prediction technologies, modifying them as necessary to improve their utility for predicting resource requirements for production runs on the leadership-class systems; and (4) analyze and help optimize current or leadership class application codes.

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

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

Scientific Discipline: Chemistry: Catalytic

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

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

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

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

Scientific Discipline: Materials Science: Nanoelectronics

INCITE Allocation: **15,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (15,000,000 processor hours)

Research Summary:

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

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

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

Principal Investigator: Warren Mori, UCLA
Co-Investigators: Frank Tsung, UCLA

Scientific Discipline: Physics: Accelerator Physics

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

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

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

Type: New
Title: "Petascale Simulations of Stress Corrosion Cracking"

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

Scientific Discipline: Materials Science: Condensed Matter and Materials

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

Research Summary:
Petascale quantum mechanical (QM)-molecular dynamics (MD) simulations that encompass large spatiotemporal scales (multibillion atoms for nanoseconds and multimillion atoms for microseconds) will be performed to determine atomistic mechanisms of stress corrosion cracking (SCC) in silica glass and nickel-based alloys.

Petascalable codes are in place: 218-billion-atom MD and 1.68-trillion electronic degrees-of-freedom QM simulations achieved parallel efficiency of well over 0.95 on 212,992 IBM Blue Gene/L processors at Lawrence Livermore National Laboratory, with similar performance on 131,072 IBM Blue Gene/P processors at Argonne National Laboratory. The performance is portable to Cell and GPU-accelerated platforms.

The project will build on the success of the largest-ever (48 million atoms), chemically reactive MD simulation on 65,536 Blue Gene/P processors at Argonne, answering a critical question for the design of the next-generation nuclear reactors to address the global energy problem—how a minute amount of impurities segregated to grain boundaries of metal essentially alters its fracture behavior. The project will carry over this success to the next level by determining fundamental mechanisms of SCC and nanoindentation of amorphous SiO_2 in the presence of water, as well as impurity segregation-induced embrittlement of NiAl alloys.

The project addresses a central problem for DOE's mission: Corrosion is an enormously complex technological and economic problem with an annual cost of about 3% of the U.S. gross domestic product. The performance and lifetime of materials widely used in energy and nuclear technologies are often severely limited by corrosion under stress loads. Particularly important for DOE are environmental degradation of nickel-based alloys in the advanced nuclear reactors and glass containers of nuclear waste. Safe and reliable operation is endangered by SCC, and petascale simulations will provide crucial understanding of the atomistic mechanisms underlying SCC to better prevent SCC and to predict the lifetime beyond which SCC may cause failure.

Type: New
Title: "Petascale Simulations of Type 1a Supernovae from Ignition to Observables"

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

Scientific Discipline: Physics: Astrophysics

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

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

We propose an "end to end", first principles, simulation of a SN Ia using three codes that have been developed for this purpose with support from the DOE SciDAC Program. Each code has been demonstrated to scale, for this particular problem, to over 100,000 CPU on Jaguar. MAESTRO, our low-Mach-number AMR code, is unique in its ability to finely resolve the convective flow that precedes ignition. The nuclear burning in this stage is turbulent and must be resolved, initially at least, on sub-km scales in a star 2000 km in radius. Subsequent burning and instabilities will be followed using the compressible AMR code, CASTRO. The integral scale of the turbulence is ~10 km and this must be resolved as the supernova expands to about 10,000 km. Observations suggest a late-time transition of the burning to a detonation. The fluid flow will be analyzed to determine the likely point(s) where this detonation occurs and the ensuing explosion will be followed to a coasting phase. Finally, the 3D explosion will be post-processed using our Monte Carlo code, SEDONA, to obtain the (angle-dependent) light curve and spectra.

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

Principal Investigator: Donald G. Truhlar, University of Minnesota

Scientific Discipline: Chemistry: Physical

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

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

The first class of problems is important for achieving a fundamental understanding of charge transfer and polarity in the context of molecular electronics and spintronics. The second class is important for understanding the cytoprotective effects of both natural agents and drugs or drug leads. The third class of problems is important for developing clean, efficient fuels and for understanding atmospheric chemistry. The project also explores density functional theory as applied to catalytic reactions at gas–solid and gas–nanoparticle–solid interfaces and to charge transfer at material interfaces.

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

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

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

Scientific Discipline: Materials Science: Nanoscience

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

Research Summary:
The project's work for 2011 will continue fundamental studies of the size-dependent properties of metal nanoparticles in the non-scalable nano regime. This size range, in which nanoparticles' properties change in a manner that cannot be extrapolated from less computationally demanding bulk or single-crystal surface calculations, is known to exhibit rapid, size-dependent property changes for a variety of applications. To understand variations in electronic and catalytic properties in this regime, it is essential to perform accurate first-principles calculations. These calculations, which will ultimately assist in the design of enhanced nanocatalysts, are the continuing focus of this proposal. Researchers will continue to make use of GPAW, their highly scalable, O(N3), real space, and grid-based Density Functional Theory (DFT) code, for nanocatalytic modeling efforts. To date, they have determined changes in key thermodynamic parameters relevant to the oxidation of carbon monoxide, a classic reaction in heterogeneous catalysis, on gold (Au) nanoparticles ranging in size from 13 to 1415 atoms. Building upon these results, and taking advantage of code improvements from the past year, the project will determine correlations between these thermodynamic properties and corresponding kinetic properties on Au nanoparticles; such relationships have been established on bulk-like single crystal metal surfaces, but never in the non-scalable nano regime. In addition, researchers intend to extend their analyses from Au, a noble metal with a full, 10-electron, d-band, to platinum (Pt) and rhodium (Rh), two catalytically relevant metals with partially filled d-bands which are known, in many cases, to exhibit properties substantially different from those of gold. The net result of these new studies will be a comprehensive, first principles-based picture of how the catalytic and electronic properties of a diverse array of metal nanoparticles, including Au, Pt, and Rh, evolve from those of molecular-like metal clusters to those of bulk-like metallic surfaces. Such understanding can only be obtained through a combination of accurate electronic structure calculations and the resources available through the INCITE program.

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

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

Scientific Discipline: Biological Sciences: Biophysics

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

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

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

In the next phase of the project, the team will use a production code to run protein-ligand interaction simulations on human pathogen targets of high biomedical value, such as *S. aureus* and *B. anthracis.*

Type: New
Title: "Quantum Monte Carlo Brings New Realism to Surface-Science Modeling"

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

Scientific Discipline: Materials Science: Condensed Matter and Materials

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

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

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

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

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

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation: **15,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (15,000,000 processor hours)

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

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

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

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

Scientific Discipline: Computer Science

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

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

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

Principal Investigator: Klaus Schulten, University of Illinois, Urbana-Champaign
Co-Investigators: Mike Gillan, University College London
Angelos Michaelides, University College London

Scientific Discipline: Biological Sciences: Biophysics

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

Research Summary:
The intrinsic disordered nature and malleability of cellular membranes severely limits the application of highly resolved experimental imaging methods that could otherwise identify the nature of membrane sculpting. However, there exist numerous observations at the smallest scale (e.g., crystallography) that identify molecular building blocks and at the cellular scale (e.g., light and electron microscopy) that identify membrane shapes resulting from various proteins under wide conditions of concentration, genetic knock-out, and mutation. Computer simulations are in principle an ideal substitute for furnishing the needed intermediate (1 - 100 nm) resolution images, but face methodological impediments due to the large size and long time scales to be covered.

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

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

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

Scientific Discipline: Engineering: Fluids and Turbulence

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

Research Summary:
This project is performing direct numerical simulations (DNS) of high Reynolds number turbulent flow in a boundary layer. Boundary layers are central to the energy losses inherent in transportation, which accounts for approximately 28% of U.S. energy consumption. This energy expenditure is due to the interaction between solid surfaces (of vehicles or pipes) and the fluid flowing past them, leading to drag and the dissipation of energy by turbulence. Since much of the drag in these flows is due to turbulent skin friction, much of this energy consumption is caused by turbulent shear layers. Engineering developments to reduce drag and energy consumption are greatly impeded by the lack of accurate models of the turbulence phenomena involved. DNS of the Reynolds numbers proposed in this project and the subsequent analysis of the resulting data can provide the insights needed to develop such models, as well as new concepts for improved vehicle design.

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

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

Scientific Discipline: Biological Sciences: Biophysics

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

Research Summary:

As the second most common neurological disorder in adults, the personal and economic impacts of Parkinson's disease are enormous. Currently, there are more than 2 million cases in the United States. In economic terms, the disease exacts an annual cost of $25 billion on the U.S. economy alone.

A research team from the University of California—San Diego leveraged the power of the Blue Gene/P supercomputer to learn more about the molecular basis of this disease and explore ways to treat it. Studying various mutations of a protein known as alpha-synuclein (aS), the team found that the clumping of aS in the brain can lead to harmful, pore-like structures in human membranes. In addition, the team found that specific patterns of cholesterol in human membranes can play a significant role in pore formation.

These findings provided a test bed for identifying possible therapeutic interventions through computational modeling. Understanding how the pore-like structures form and stopping their formation, scientists theorize, could halt the progression of Parkinson's disease as well as other similar conditions.

To date, researchers have found an encouraging correlation between their molecular dynamics modeling predictions and laboratory experimental results. As a result, the team expects to make continued steady progress, both with the computational model and the design of effective drugs based on modeling and simulations.

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

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

Scientific Discipline: Chemistry: Combustion

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

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

The study of fuels that are rich in hydrogen is problematic. The high diffusivity of hydrogen causes the flames to burn in cellular structures, which have a distinctly different character than the "thin flame" approach that forms the basis for standard premixed flame theory. This has significant ramifications for theoretical studies, engineering design models, and even for the processing of experimental diagnostics. High-fidelity simulations with detailed chemistry and transport provide the only viable mechanism for obtaining a more detailed characterization of the structure, dynamics and emissions characteristics of these types of flames. This is particularly true for high pressure flames where high-quality experimental measurements are very difficult to make. The simulations in this study will incorporate high fidelity models for the flame physics while still spanning the range of spatial scales needed to capture the range of turbulent scales characteristic of realistic flames, enabling us to capture the behavior of these types of flames.

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

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

Scientific Discipline: Chemistry: Combustion

INCITE Allocation: **18,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (18,000,000 processor hours)

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

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

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

Scientific Discipline: Physics: Plasma Physics

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

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

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

Type: New
Title: "Singularities and Multi-Scaling in MHD"

Principal Investigator: Annick Pouquet, National Center for Atmospheric Research
Co-Investigators: Marc-Etienne Brachet, École Normale Supérieure
Giorgio Krstulovic, École Normale Supérieure
Pablo Mininni, Ciudad Universitaria
Duane Rosenberg, National Center for Atmospheric Research

Scientific Discipline: Engineering: Fluids and Turbulence

INCITE Allocation: **15,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (15,000,000 processor hours)

Research Summary:
The class of problems that addresses the formation of singularities and the existence and structure of solutions of nonlinear equations for all times forms an important branch of mathematics, with wide application in numerous fields such as engineering, astro– and geophysics, and laboratory studies of plasmas and superfluids. The importance of this class of problems in meteorological research, in particular, and to society in general, cannot be overstated because of its profound connection to extreme events like tornadoes and hurricanes. Indeed, the Clay Mathematics Institute has recognized the importance of these problems by issuing a Millennium Prize for the Navier-Stokes equations for solutions with finite energy. Numerous studies have been devoted to the notion of existence and formation of singularities, asking, among other things: How fast do (potentially) singular structures form? What is their temporal evolution and geometry? What role do their interactions play and how might they lead to a modification of transport properties within complex flows, including those with magnetic fields? One thing seems clear: progress in tackling this class of problems must come from a combination of mathematics and experiments, in particular using computer codes with high accuracy to perform studies at the highest possible resolutions.

The purpose of this INCITE leadership-class proposal is to use direct numerical simulations to study several magnetohydrodynamic (MHD) flow configurations for their potential singular behavior. At lower resolutions, such flows have offered tantalizing hints that singularities may exist in MHD, in the form of current sheets and rotational (quasi)-discontinuities, but without clear conclusions. We will carry out our high accuracy simulations at the highest resolutions ever conducted, by up to a factor 4 in linear grid spacing, from 49 billion grid points for a flow with helical motions and fields, to the equivalent of 1 2 trillion points using a code that implements the inherent symmetries of the extension to MHD of Taylor-Green flows as used in several experiments in the US and in Europe.

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

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

Scientific Discipline: Physics: Astrophysics

INCITE Allocation: **80,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (80,000,000 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. Most scientists believe that using SNe Ia to determine the properties of dark energy will require a much better understanding of these events. Two major challenges face astrophysicists simulating SNe Ia: (1) buoyancy-driven turbulent nuclear combustion, which is a key physical process in SNe Ia, is not fully understood; and (2) very few simulations of the four current models of SNe Ia have been done, making it difficult to determine which model is favored by observations, and even more, what values of the many parameters specifying these models are consistent with observations. In our original INCITE proposal we described a three-year strategic plan that uses the FLASH code and computational resources of the INCITE program to address both challenges. We continue to execute the overall plan, but have made some changes in response to our results from our simulations. The insights gained from our simulations have led us to extend our study of buoyancy driven turbulent nuclear combustion to (i) flame bubbles in an open domain, which we simulate using a rectilinear computational domain having large lateral dimensions, and (ii) flame bubbles in a white dwarf star. We continued these studies in the latter half of 2010, and will culminate in 2011 with a capstone 1-km resolution 3-dimensional simulation of the buoyancy-driven turbulent nuclear combustion phase (the deflagration phase) of the gravitationally confined detonation (GCD) model of SNe Ia. Building on the results of this capstone simulation, we will carry out a very high resolution simulation of the in situ initiation of a detonation in the GCD model -- the first attempt to do so in 3D.

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

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

Scientific Discipline: Physics: Astrophysics

INCITE Allocation: **60,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (60,000,000 processor hours)

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

This project will perform three-dimensional simulations to understand how stars more than ten times the mass of our sun die in catastrophic stellar explosions known as core-collapse supernovae. Core-collapse supernovae are the dominant source of elements in the universe, including all the elements between oxygen and iron and half the elements heavier than iron; life would not exist without these elements. These supernovae are complex, three-dimensional, multi-physics events, but there are as yet no three-dimensional models of sufficient realism. This is a significant void in supernova theory. The simulations described here will begin to fill this void. These simulations will be the first three-dimensional simulations performed with multifrequency neutrino transport, critical to realistic modeling of the neutrino shock reheating that is believed to be central to the supernova explosion mechanism. A complete understanding of the core-collapse supernova mechanism requires parallel simulations in one, two, and three spatial dimensions. The nuclei in the stellar core undergo a transition through a series of complex shapes that can be modeled only in three spatial dimensions. These modeling efforts will extend to three dimensions both the macroscopic and microscopic models of stellar core phenomena in core-collapse supernovae.

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

Principal Investigator: David Baker, University of Washington

Scientific Discipline: Chemistry: Biochemistry

INCITE Allocation: **30,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (30,000,000 processor hours)

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

Researchers recently described a breakthrough in conformational sampling that utilized highly parallel computations on the Blue Gene platform. With this new methodology, they can compute accurate structures for proteins as large as 20 kDa, using very limited experimental data. INCITE resources will enable advances in many challenging problems in computational structural biology, including the *ab-initio* prediction of proteins larger than 15 kDa, the calculation of structures of proteins larger than 20 kDa using sparse NMR data, the calculation of structures using X-ray diffraction data without experimental phase information, the design of novel enzymes, including a system for fixing carbon dioxide to produce biofuels, and the design of proteins specifically targeting surfaces on pathogens and other targets of therapeutic and diagnostic interest.

The broader impacts of this project will include pressing issues in the 21st century, among them deciphering the structures and functions of the vast number of protein sequences generated in current high throughput sequencing projects, the creation of new enzymes fixing CO_2 into industrially useful products and catalyzing other reactions of current interest, and the design of new inhibitors of protein-protein interactions for fighting pathogens and treating disease.

Type: New
Title: "Trace Collection for Simulation-Driven Co-design of Exascale Platforms and Codes"

Principal Investigator: David Evensky, Sandia National Laboratories
Co-Investigators: Curtis Janssen, Sandia National Laboratories

Scientific Discipline: Computer Science

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

Research Summary:
The exascale machines that application developers are targeting will not be available for roughly another seven years. However, developers must begin adapting their codes now in order to be ready for these future machines. At the same time, due to the expense of building and operating an exascale machine, it will be necessary to apply tighter engineering margins to their design. Simple metrics such as the ratio of the floating point computation rate to communication rate will not be sufficient to specify machine requirements. Lower layers in the software stack will also have to adapt. Architecture simulation provides the tools that can bridge all of these areas and will be a key factor in enabling co-design of hardware, runtime components, and application code.

The Leadership Computing Facility platform is ideally suited for collecting exceptionally high-quality traces that have low OS noise and knowable/predictable node placement. This project is collecting data and cross-validating the results at very large scales. The thorough, large-scale validation will be essential to ensure the accuracy of simulated results and will give researchers confidence that they can successfully co-design applications, runtimes, and systems for exascale computing.

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

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

Scientific Discipline: Physics: Plasma Physics

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

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

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

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

Principal Investigator: Sanjiva Lele, Stanford University
Co-Investigators: Parviz Moin, Stanford University

Scientific Discipline: Engineering: Fluids and Turbulence

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

Research Summary:
Richtmyer-Meshkov instability (RMI) occurs when a shock wave interacts with a perturbed interface, separating fluids of different densities. After the shock refracts through the interface, perturbations grow; if the incoming shock is strong enough or if the interface is sufficiently perturbed, the instability evolves into a turbulent mixing region. Even though Richtmyer-Meshkov instability occurs in a wide range of flows (for example, in supernovae explosions, inertial confinement fusion, and hypersonic propulsion systems), the turbulent mixing is not well understood. Few investigations of this phenomenon have been carried out.

Leveraging the capabilities of the Blue Gene/P supercomputer, a research team is studying the fundamental physics governing this phenomenon, in particular the mechanisms at play in turbulent multi-material mixing in high-speed accelerated flows. The study employs a novel solution-adaptive numerical framework that scales well and that will enable science discovery through high-performance computing.

This study enables direct numerical simulations of the turbulent multi-material mixing generated after RMI. Capturing these turbulence statistics, researchers will be able to answer fundamental questions: Is the classical Kolmogorov theory for turbulence valid in a transient non-stationary flow? How anisotropic is the turbulence generated in such problems? Does it relax toward isotropy? What controls how long the flow depends on the initial conditions? Is the inertial scaling for the decay rate in the energy-cascade a central element of turbulence modeling, even valid in turbulent flows generated by the RMI?

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

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

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

Scientific Discipline: Earth Science: Environmental Sciences

INCITE Allocation: **15,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (15,000,000 processor hours)

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

High performance computing will be employed to better quantify parameter uncertainty and conduct sensitivity analyses for groundwater flow and uranium transport at the Hanford 300 Area. The project will leverage new data being produced by the Hanford 300 Area IFRC project (funded by DOE-SC BER SBR) that better defines hydrostratigraphy, physical heterogeneity, and geochemical process models for the Hanford 300 Area. PFLOTRAN is capable of launching thousands of simultaneous simulations, each simulation depicting large high-resolution problems domain with an independent set or realization of uncertain parameters. Results generated from these ensembles of simulations help to characterize parameter sensitivity and quantify uncertainty. Leadership class computing that provides tens to hundreds of thousands of processor cores is required to perform these large ensembles of simulations.

At the Oak Ridge IFRC site, we will work with members of the ORNL IFRC project in constructing a watershed scale groundwater model with refined resolution using high performance computing for a watershed scale model with refined resolution for the S-3 ponds and the Bear Creek Watershed on the DOE Oak Ridge Reservation. This model will integrate multiple processes at multiple scales to investigate the influence of process interactions at small scales on the fate and transport of contaminants in the field, and the scale dependence of the controlling parameters such as dispersivity, attenuation, mass transfer and reaction rates.

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

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

Scientific Discipline: Energy Technologies: Nuclear Energy

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

Research Summary:
The performance of nuclear fuel in boiling water reactors (BWRs) is strongly dependent on the power distribution within a nuclear fuel bundle. Vendor software, as is typical in the nuclear industry, provides pin-averaged power distribution data on a 6-inch axial grid, which is much too large to be able to determine the within-pin power distribution near the control blades, before and after withdrawal. However, the problem is not simply single-physics radiation transport. The effective macroscopic nuclear cross-sections, which are used in a radiation transport solver, are linearly dependent upon the density of the materials. Before we proceed to develop a coupled thermal-fluid-dynamics and radiation transport solver, it is necessary to evaluate the required fidelity of each. Evaluating the sensitivity of the radiation transport solution to the spatial resolution of the coolant density would guide the software development of a coupled physics solver by determining the "fidelity" requirements of the thermal-fluid-dynamics solver.

Recent work with the Denovo three-dimensional, discrete ordinates transport code has demonstrated the ability to model the power distribution for this problem on a ¼-inch axial grid with a 6 mil (0.006 inch) radial (*x, y*) mesh (using 60,000 cores on the Cray XT5 at ORNL). Therefore, it is clear that the solution is within reach. Uncertainty quantification is one of the most important, and least implemented, topics in computational science. As numerical algorithms and high-performance computing architectures have become more advanced and powerful, the ability to model complex physical phenomena has grown to the point where computer models are often used in place of experiment.

Type: New
Title: "Uncertainty Quantification for Turbulent Mixing"

Principal Investigator: James G. Glimm, State University of New York, Stony Brook

Scientific Discipline: Engineering: Fluids and Turbulence

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

Research Summary:
Hydrodynamic instabilities play a significant role in science and engineering, giving rise to intractable, chaotic, and complex flows. These flows are widespread in many applications, from climate studies to fusion energy to the design of targets for high-energy particle accelerators. Because it is not feasible to fully resolve the solution complexity, solution methods resort instead to models to describe important effects at scales below the grid level. Uncertainty quantification (UQ) for simulation models is a critical issue, as the models often constitute a primary source of uncertainty. This study addresses the UQ of simulations for turbulent mixing flows.

UQ issues can be characterized in terms of the length scales of the observations of the flow whose uncertainty is to be quantified. Macro UQ concerns the overall shape or location of the mixing zone, meso UQ concerns coherent structures within the mixing zone, and micro UQ concerns the probability distributions of the species, i.e., in effect, length scales close to laminar fluid scales or molecular scales. Recent progress using FronTier/LES, a powerful combination of Large Eddy Simulation (LES) and the mature front tracking code, FronTier, has addressed macro and meso scale validation for mixing. To date, the research team has solved a noted macro scale mixing problem (simulations in agreement with 14 different experiments for the Rayleigh-Taylor mixing rate) and an important meso scale mixing problem (mean droplet size in agreement with an experimental correlation for primary breakup of a high-speed jet). Findings also include meso scale validation for RT simulations in the bubble height to width simulation-experiment agreement. The code is based on the equations of compressible fluid flow, and is thus suitable for a wide range of DOE applications.

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

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

Scientific Discipline: Energy Technologies: Energy Storage

INCITE Allocation: **25,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P (15,000,000 processor hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (10,000,000 processor hours)

Research Summary:
Lithium-air cells consist of an anode (ideally lithium metal), an electrolyte - which can be either aprotic or aqueous - and the air cathode1-9. We will focus on aprotic systems, as these are known to be rechargeable and have the highest energy storage density. During the discharge process, Li-ions and atmospheric oxygen combine to form Li2O2 (and perhaps at higher currents some Li2O). The Li2O2 are solids and precipitate on the cathode. It has been demonstrated that it is possible, at least at low electrical current densities, to reverse this process and convert the Li2O2 back into lithium metal. This exciting proof-of-principle work still presents very big technical and engineering challenges before one can be confident that practical propulsion batteries can be based on the Li/Air system. The most important ones are to realize a high percentage of the theoretical energy density, to improve electrical efficiency of recharging, to increase the number of times the battery can be cycled, to limit the negative effects of moisture in the air, and to improve the power density. These five engineering goals depend critically on a deep understanding of four fundamental battery chemistry science issues. These are: (1) detailed mechanisms of the battery discharge and recharge, (2) role of catalysts, (3) solubility of lithium ions and solid lithium oxides and optimization of electrolyte, and (4) the role of the electrode-electrolyte interface in managing oxygen gas, liquid electrolyte, and solid lithium oxides in a nano-structured air-cathode.

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

Principal Investigator: William Daughton, Los Alamos National Laboratory
Co-Investigators: Vadim Roytershteyn, Los Alamos National Laboratory

Scientific Discipline: Physics: Plasma Physics

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

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

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

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

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

Scientific Discipline: Physics: Plasma Physics

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

Research Summary:
Plasma microturbulence, the dominant mechanism for the loss of heat from tokamak fusion reactors, will determine the fusion gain that can be achieved in the international ITER reactor. While plasma microturbulence has been studied since the 1960s, the magnetic fusion community has yet to develop a complete predictive understanding of the turbulent transport of heat, momentum, and particles across magnetic surfaces. The development of such a predictive understanding has been identified as a major goal for the U.S. fusion program, and achieving it requires the validation of high-fidelity plasma microturbulence codes.

This proposal is to validate the three most advanced plasma microturbulence codes in the U.S. program (GYRO, GS2, and GEM) against transport and fluctuation data from the three large U.S. tokamak experiments (DIII-D, C-MOD, and NSTX), and employ these codes to predict transport losses in ITER. This code validation effort directly addresses the U.S. fusion program goal of developing a predictive understanding of plasma transport, and supports the mission of the Center for the Study of Plasma Microturbulence.

Type: New
Title: "Vibrational Spectroscopy of Liquid Mixtures and Solid/Liquid Interfaces"

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

Scientific Discipline: Materials Science: Condensed Matter and Materials

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

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