Type: Renewal
Title: "Ab Initio Simulations of Carrier Transports in Organic and Inorganic Nanosystems"

Principal Investigator: Lin-Wang Wang, Lawrence Berkeley National Laboratory
Co-Investigators: Emily Carter, Princeton University

Scientific Discipline: Materials Science: Nanoscience

INCITE Allocation: **25,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (25,000,000 processor hours)

Research Summary:
Carrier transports in organic and inorganic nanosystems are poorly understood, but they are extremely important for electronic applications of these systems. Organic systems—either disordered polymers or molecular crystals—have found broad applications from solar cells and large area displays to cheap electronic devices. However, compared to bulk semiconductor systems, our understanding of their carrier transport properties is still in its infancy.

We propose to study three types of problems: the electronic structure and carrier transport in organic systems; the effect of surface passivation on the electronic structure and carrier transport of inorganic nanocrystals with organic molecule attachments; and the defect and dislocation structures and their dynamics in aluminum alloys.

This project uses two methods developed in previous INCITE projects: One is an *ab initio* non-adiabatic molecular dynamics (NA-MD) method, and the other is a linear scaling three-dimensional fragment code (LS3DF) to study how the electron moves in organic systems and nanosystems. The methods will reveal the underlying mechanisms of electron transports in different types of organic and nanosystems.

While there have been many theoretical studies for these problems, our INCITE supported project will have the following distinguishing characteristics: (1) *ab initio* non-adiabatic molecular dynamics will be used for the first time to study the carrier transport of thousand atom organic systems, with the potential to reveal underlying transport mechanisms; (2) a realistic atomic surface passivation model will be used to describe the nanocrystal surface, which enables the study of surface defect states and surface dipole moments, as well as their influence on carrier dynamics and charge transports; and (3) direct million atom simulations at a level higher than the classical force field or embedded atom model to study aluminum alloy defects and dislocations.

Besides revealing the fundamental mechanisms in carrier transport and surface effects, our simulations will open up new areas of research and elevate the large-scale material simulations in these fields to new levels.

Type: New
Title: "Accelerated Climate Modeling for Energy"

Principal Investigator: Mark Taylor, Sandia National Laboratories
Co-Investigators: Valentine Anantharaj, Oak Ridge National Laboratory
David Bader, Lawrence Livermore National Laboratory
William Collins, Lawrence Berkley National Laboratory
Katherine Evans, Oak Ridge National Laboratory
Robert Jacob, Argonne National Laboratory
Philip Jones, Los Alamos National Laboratory
Matthew Norman, Oak Ridge National Laboratory
Philip Rasch, Pacific Northwest National Laboratory

Scientific Discipline: Earth Science: Climate Research

INCITE Allocation: **190,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (140,000,000 processor hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (50,000,000 processor hours)

Research Summary:
The Accelerated Climate Modeling for Energy (ACME) project seeks to develop the simulation capability needed to answer "grand challenge" science questions. Two of these science questions—concerning the water cycle and cryosphere systems—will be pursued in the first three years of the project while researchers also seek to quantify the benefits of high resolution on the simulated climate. Through ACME, researchers can assist the U.S. Department of Energy in preparing for the coming paradigm shift to exascale computing.

With regard to water cycles, researchers hypothesize that over the next 40 years, changes to fresh water supplies such as river flow will have signatures dominated more by greenhouse gas emissions than by other "forcing" agents, such as land management, water management, and aerosols. Changes in the hydrological cycle will be simulated, with a specific focus on precipitation and surface water in orographically complex regions. For the cryosphere, the objective is to examine whether a near-term risk exists of initiating the dynamic instability and onset of the collapse of the Antarctic Ice Sheet due to rapid melting by warming waters adjacent to the ice sheet grounding lines. ACME capstone simulations will include a 100-year pre-industrial control followed by an ensemble of five to six 80-year (1970–2050) simulations.

Type: New
Title: "Accelerator Modeling for Discovery"

Principal Investigator: James Amundson, Fermilab
Co-Investigators: Qiming Lu, Fermilab
Alexandru Macridin, Fermilab
Chong Shik Park, Fermilab
Panagiotis Spentzouris, Fermilab
Eric Stern, Fermilab

Scientific Discipline: Physics: Accelerator Physics

INCITE Allocation: **60,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (60,000,000 processor hours)

Research Summary:
This INCITE project aims to advance the priorities of the U.S. particle physics community by optimizing the output of the world's two largest accelerator facilities: Fermilab and CERN. Researchers from Fermilab will combine large-scale multi-bunch simulations of wakefield effects with space charge for a computational approach that is unique in the field. The simulations will significantly advance the understanding of wakefields in accelerators, while also providing the most detailed comparisons of experimental results with high-fidelity simulations of space charge effects to date. Together, these results will advance particle physics and accelerator science.

Over the past year, the Particle Physics Project Prioritization Panel (P5) worked to put together a unified plan for the future of the U.S. high energy physics program. In their report, the panel identified three scientific drivers that require accelerator-based experiments (using the Higgs boson as a new tool for discovery, pursuing the physics associated with neutrino mass, and exploring the unknown through new particles and interactions). This INCITE project will support the P5 recommendations by simulating the physics of high-intensity beams in Fermilab and CERN accelerators.

In the U.S., the P5 report recommends that Fermilab direct its efforts to the newly christened Proton Improvement Plan-II, which will help researchers to better explore the properties of neutrinos. At CERN, the highest-priority accelerator-based project identified by the P5 report is the high-luminosity upgrade to the Large Hadron Collider, which will enable new experiments to explore the physics of the Higgs boson as well as search for new particles and interactions.

Type: New
Title: "Adaptive Detached Eddy Simulation of a High Lift Wing with Active Flow Control"

Principal Investigator: Kenneth Jansen, University of Colorado Boulder
Co-Investigators: Michel Rasquin, Argonne National Laboratory
Onkar Sahni, Rensselaer Polytechnic Institute
Mark Shephard, Rensselaer Polytechnic Institute

Scientific Discipline: Engineering: Aerodynamics

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

Research Summary:
Active flow control can alter a natural flow field into a more desirable state when synthetic jet actuators are placed at key locations along an aircraft wing to improve efficiency and performance. Researchers plan a series of simulations focused on active flow control on a realistic high lift wing configuration, which includes a leading edge slat, a main wing, and a trailing edge flap along with their respective supports.

This project applies more advanced turbulence models which resolve, rather than model, the energetic turbulent eddies that accompany very complicated high lift, aerodynamic geometries, such as multi-element wings. Specifically, researchers will model an array of synthetic jets that have been vectored to augment the streamwise momentum near the flap suction peak. This can prevent or reduce flow separation, which limits flap effectiveness for high-deflection angles.

It is anticipated that synthetic jet flow control may prove effective in increasing or decreasing the lift on time scales rapid enough to offset the unsteady wind environment in which wind turbines are forced to operate. This would directly reduce the unsteady loads that prove detrimental both to wind turbine blades and the gearboxes used to convert wind energy into electric power. Understanding the fundamental flow physics of these synthetic jets is essential to these and many other applications.

The computational approach used for these simulations is the finite-element based flow solver, PHASTA, employed with anisotropic adaptive meshing and partitioning procedures. An excellent match to the active flow control simulations of complex and realistic wing configurations, these tools are applicable to flow problems that involve complicated geometries or complex physics.

Type: Renewal
Title: "Advancing Models for Multiphase Flow and Transport in Porous Medium System"

Principal Investigator: James McClure, Virginia Tech
Co-Investigators: Casey Miller, University of North Carolina at Chapel Hill
Jan Prins, University of North Carolina at Chapel Hill

Scientific Discipline: Earth Science: Geological Science

INCITE Allocation: **60,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (60,000,000 processor hours)

Research Summary:
Multiphase porous medium systems arise routinely in natural and engineered systems. Some example applications from natural systems include land–atmosphere interaction, infiltration and drainage, contaminant remediation of subsurface systems, petroleum reservoir simulation, carbon sequestration, and fluid flow and contaminant transport resulting from hydraulic fracturing of shale formations. Collectively, understanding and describing multiphase porous medium systems are of significant importance to society.

We consider model development work to advance the description of multiphase flow processes in porous media, including land–water interactions, carbon sequestration, and fuel cell development.

The overall goal of this work is to advance a recently developed thermodynamically constrained averaging theory (TCAT) model of multiphase flow and transport phenomena in porous medium systems. The specific objectives of this work are to: determine a lower bound on the size at which a macroscale model can be applied for a specified allowable error; perform a dense set of microscale simulations needed to elucidate the relationship among fluid pressures and saturations as well as interfacial areas and curvatures between phases; determine the relationship among volume fractions, interfacial areas, and fluid viscosities that determine the resistance tensors for fluid flow; investigate factors affecting the mobility of entrapped non-wetting phase fluids; extend the analysis of TCAT models to compositional two-fluid-phase flow systems; and extend the analysis to TCAT models for three-fluid-phase flow.

The proposed simulations will establish the scale of the system needed for the TCAT theory to be valid, produce the detailed simulations needed to produce specific closure relations, test the hypothesis that states that properly framed closure relations are non-hysteretic, elucidate typically ignored dynamic aspects of two-phase flow, and provide an overall validation of the latest theoretical advances in this important area of multiphase transport phenomena. Work in years two and three will extend the microscale simulations to include species transport and three-fluid-phase flow.

Type: New
Title: "Approaching Exascale Models of Astrophysical Explosions"

Principal Investigator: Michael Zingale, Stony Brook University
Co-Investigators: Ann Almgren, Lawrence Berkeley National Laboratory
John Bell, Lawrence Berkeley National Laboratory
Alan Calder, Stony Brook University
Adam Jacobs, Stony Brook University
Daniel Kasen, University of California, Berkeley
Max Katz, Stony Brook University
Christopher Malone, Los Alamos National Laboratory
Stan Woosley, University of California, Santa Cruz

Scientific Discipline: Physics: Astrophysics

INCITE Allocation: **50,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (50,000,000 processor hours)

Research Summary:
We will explore two classes of stellar explosions: Type Ia supernovae (SNe Ia) and x-ray bursts (XRBs) through high-resolution, multiphysics hydrodynamics simulations. Our simulation codes, Maestro and Castro, are well tuned to Titan, using a hybrid approach to parallelism and beginning to offload time-consuming microphysics calculations to the GPUs.

A fundamental uncertainty in our understanding of SNe Ia is the nature of the progenitor—a single white dwarf accreting from a normal companion star (single degenerate scenario) or two white dwarfs that inspiral (or violently collide) and merge (the double degenerate scenario). No progenitor system of an SN Ia has ever been identified, so astronomers must look for indirect clues. Regardless of the progenitor system, in every case the majority of the carbon and oxygen in the white dwarf(s) is converted into iron/nickel and intermediate-mass elements like silicon, and this nuclear energy release unbinds the star.

We propose to carry out a comprehensive study of two classes of thermonuclear-powered stellar explosions involving compact objects, Type SNe Ia and XRBs, using the state-of-the-art multiphysics simulation codes Maestro and Castro. This work builds upon the successes of our current INCITE campaign while shifting the focus to exciting new problems.

Maestro and Castro—which were designed specifically for the efficient modeling of astrophysical explosions—make excellent use of the multi-core architecture by using a hybrid approach to parallelism (MPI and OpenMP), and we have made considerable progress in targeting the effective use of GPUs.

Type: New
Title: "Catalyst Support Interactions"

Principal Investigator: Frank Abild-Pedersen, Stanford University

Scientific Discipline: Chemistry: Catalytic

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

Research Summary:

Platinum is a widely used catalyst in industrial-scale reactions due to its high activity and stability. But platinum is scarce and the extraction methods are costly and time consuming, making it one of the most expensive elemental metals on Earth. This has spurred research into new catalytic materials and methods, including the use of nanoparticles as a means to reduce the quantity of materials needed.

In catalysis, the surface of the support material is where bonds in reactants are made and broken. Therefore, decreasing the particle size to increase the surface-to-volume ratio of the catalyst is an important avenue to explore for lower cost options. However, this area of research opens up a new set of challenges both experimentally and theoretically.

For this INCITE project, researchers from the SLAC National Accelerator Laboratory will carry out density functional theory simulations on Mira to develop models that can predict the structure and size of supported platinum and gold nanoparticles, and then correlate that data with catalytic functionality. Building on previous research efforts, the simulations will advance the understanding of catalysis by accounting for the support's impact on the reactivity of metal catalyst particles.

The research team will also study the adhesion properties by simulating the interactions between metal particles of different sizes and a metal oxide support. These extremely computationally demanding tasks are only possible with access to supercomputers like Mira. The calculations will be performed with the highly scalable GPAW code, which will allow the researchers to use hundreds of thousands of cores on Mira.

Type: Renewal
Title: "CESM Century-Scale Climate Experiments with a High-Resolution Atmosphere"

Principal Investigator: Warren Washington, UCAR
Co-Investigators: Susan Bates, UCAR
John Dennis, UCAR
Jim Edwards, UCAR
Gerald Meehl, UCAR
Joseph Tribbia, UCAR
Mariana Vertenstein, UCAR

Scientific Discipline: Earth Science: Climate Science

INCITE Allocation: **200,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (200,000,000 processor hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (0 processor hours)

Research Summary:
Researchers in the Climate Change Prediction group at the National Center for Atmospheric Research (NCAR) will carry out various sets of climate change simulations using the latest release of the Community Earth System Model (CESM). This INCITE research builds upon NCAR's previous and collaborative work on how weather and climate extremes could change in a climate that is warmer in the future by obtaining data from simulations totaling 500 years' worth of climate change modeling under various scenarios.

Time-slice simulations are suitable for investigating climate and weather extremes by removing the long-term model bias and providing improved statistics. These simulations will be performed for the present-day climate from 1979–2012 (34 years) and a future scenario for 2070–2099 (30 years) in the mesoscale range (~200–2,000 km). Once the control or near-equilibrium 1850 initial dataset becomes available in early 2015, the researchers will also complete one historical (1850–2005) simulation followed by two 100-year future scenarios, as follows: (1) a business-as-usual case with increasing greenhouse gases (GHGs), and (2) a scenario incorporating the most aggressively low GHG emissions possible. The project will also address spread in the climate model's sensitivity—a major factor that contributes to ranges in climate change projections—via two other simulations. One will increase carbon dioxide (CO_2) in the atmosphere at regular intervals until it is four times current levels, whereas another quadruple CO_2 levels instantaneously then integrate until the model reaches equilibrium (approximately 100 years).

Type: New
Title: "Characterizing Large-Scale Structural Transitions in Membrane Transporters"

Principal Investigator: Emad Tajkhorshid, University of Illinois at Urbana-Champaign

Scientific Discipline: Biological Sciences: Biophysics

INCITE Allocation: **96,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (96,000,000 processor hours)

Research Summary:
One of the most fundamental processes in all living cells is active exchange of materials across the cellular membrane, a task primarily performed by membrane transporters. The fundamental role of membrane transporters in diverse biological and physiological processes and their biomedical significance as key drug targets have further stimulated widespread interest in their mechanistic studies at a molecular level. The main goal of the project is to describe, for the first time, at a full atomic scale, the large-scale conformational changes involved in the mechanism of active membrane transporters, which are at the heart of the mechanism of function of this highly biomedically and biophysically relevant class of membrane proteins.

Capitalizing on a recently developed and tested computational methodology in our lab, we propose to study the transition between structural intermediates of a number of transporters using a novel combination of several replica-based techniques coupling a massive array of all-atom molecular dynamics (MD) simulations, which are exclusively possible on extensive resources available at the leadership computational facilities. Our novel approach is based on an extensive sampling in a multi-dimensional reaction coordinate space to identify the most relevant structural transition pathway(s), and then use these complex pathways to accurately calculate the associated free energies, as the ultimate quantitative metric of the quality and relevance of the transition pathway(s). The replica-based algorithms proposed here include bias-exchange umbrella sampling as well as a parallel variation of string method with swarms of trajectories.

These calculations will be performed using the NAnoscale Molecular Dynamics program (NAMD), a highly parallelized and widely used code for MD simulations of biomolecular systems at supercomputing centers. The replica-based simulations performed by NAMD have been extensively optimized over the past two years, primarily in connection with the usage of the program on leadership computing facilities machines (Mira and Titan). The code and the particular type of calculations and systems described in this project show excellent performance on the platforms for which allocation is requested.

Type: Renewal
Title: "Computational Actinide Chemistry: Reliable Predictions and New Concepts"

Principal Investigator: David Dixon, University of Alabama
Co-Investigators: Jochen Autschbach, University at Buffalo
Enrique Batista, Los Alamos National Laboratory
Aurora Clark, Washington State University
Wibe de Jong, Lawrence Berkeley National Laboratory
Laura Gagliardi, University of Minnesota
Richard Martin, Los Alamos National Laboratory
Kirk Peterson, Washington State University
Gustavo Scuseria, Rice University
Alvaro Vazquez-Mayagoitia, Argonne National Laboratory

Scientific Discipline: Chemistry: Physical

INCITE Allocation: **150,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (150,000,000 processor hours)

Research Summary:
There is substantial interest in the development of new nuclear reactors with advanced fuel cycles offering the appropriate safety and nonproliferation constraints to meet the nation's and world's energy needs. In addition, there are ongoing critical issues with respect to the environmental cleanup of US Department of Energy nuclear weapons production sites as well as the safety and reliability of the nation's nuclear weapons stockpile.

These studies will provide unique insights into the solvation of actinides and how to treat collective weak interactions.

To reliably predict actinide behavior and develop new concepts for the proper treatment of heavy elements relevant to the US nuclear energy and environmental remediation portfolio, a three-pronged approach is needed. We must: (1) be able to calculate structural, spectroscopic, and thermodynamic properties with a high amount of accuracy; (2) investigate chemical reactions that are of practical importance and be able to realistically account for the experimental conditions; and (3) study the solid-state chemistry of heavy elements so that we can not only predict new materials with technological relevance but also overcome the long-standing problem imposed by strong correlation.

Our use of computational resources will have a broad and sustained impact on the field of actinide chemistry and will provide the basis upon which to build the science underpinning future cost-effective nuclear energy technologies and DOE's environmental cleanup efforts.

Type: New
Title: "Computational Spectroscopy of Heterogeneous Interfaces"

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

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation: **180,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (180,000,000 processor hours)

Research Summary:
The interfaces between solids, nanoparticles, and liquids play a fundamental role in determining the properties of materials. With an understanding of the microscopic structure of heterogeneous interfaces, researchers can predict the properties of optimal materials for many applications, including photoelectrochemical water splitting, solar cells, clean fuel production, and energy storage.

However, the properties of interfaces are seldom explicitly included in *ab initio* models, due to the complexity and cost of the associated calculations. With this INCITE project, researchers from the University of Chicago and the University of California, Davis, aim to tackle the characterization and control of heterogeneous interfaces at the atomic and molecular scale from a computational standpoint.

The research team will use the Qbox and WEST codes, which have been optimized for Mira, to investigate the properties of interfaces present in materials of interest to solar energy conversion processes. This includes performing *ab initio* calculations of electronic and vibrational spectra, integrated with large-scale *ab initio* molecular dynamics simulations, to study realistic interfaces that can be compared directly to experimental results.

The main objective of the project is to calculate the physical properties of aqueous interfaces with solid oxides and semiconductors, and of inorganic interfaces at the nanoscale. The results can be used to interpret experiments and to optimize materials properties to improve solar energy applications, including photoeletrochemical water splitting and third-generation solar cells. This work will help establish a robust strategy to enable the comparison of *ab initio* data with experiments carried out at light sources, such as Argonne's Advanced Photon Source. Ultimately, the results could lead to analysis tools for spectroscopic data that can be used by theorists and experimentalists alike.

Type: New
Title: "Cosmic Reionization On Computers"

Principal Investigator: Nickolay Gnedin, Fermilab

Scientific Discipline: Physics: Astrophysics

INCITE Allocation: **74,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (74,000,000 processor hours)

Research Summary:

Cosmic reionization, one of major phase changes in the universe, was the process in which neutral cosmic gas was ionized by high-energy radiation from early galaxies. In the National Research Council's most recent Astronomy and Astrophysics Decadal Survey (Astro2010), cosmic reionization was highlighted as one of the most promising areas of research. With a better understanding of this process, researchers will be able to shed light on other aspects of modern cosmology, including cosmic microwave background observations and the physical state of intergalactic gas in front of high redshift quasars.

Because the observational constraints on reionization are limited, theoretical modeling and numerical simulations play a critical role in reionization studies. The emergence of modern petascale supercomputers, like Mira, is enabling potential breakthroughs in the field that were impossible to pursue in the past.

Taking advantage of this technological progress, the Fermilab research team started the Cosmic Reionization On Computers project to carry out simulations that model all relevant physics, from radiative transfer to gas dynamics and star formation. The simulations will be performed in volumes of over 100 comoving megaparsecs and with spatial resolution approaching 100 parsecs to cover the full range of spatial, temporal, and mass scales needed to study reionization.

Results from this project will be instrumental in achieving a wide range of scientific goals, from understanding the detailed physics of the reionization process, to providing theoretical predictions of the spatial distribution and internal properties of early galaxies for future observations with the James Webb Space Telescope. This work will also help researchers to explore other recent observational campaigns, including the residuals of reionization in the absorption spectra of distant quasars that were discovered by the Sloan Digital Sky Survey.

Type: Renewal
Title: "Cosmological Simulations for Large-Scale Sky Surveys"

Principal Investigator: Salman Habib, Argonne National Laboratory

Scientific Discipline: Physics: High Energy Physics

INCITE Allocation: **160,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (80,000,000 processor hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (80,000,000 processor hours)

Research Summary:
The focus of cosmology today revolves around two mysterious pillars, dark matter and dark energy. Large-scale sky surveys are the current drivers of precision cosmology and have been instrumental in making fundamental discoveries, with cosmic acceleration being the most recent. The next generation of surveys aims to establish a new regime of cosmic discovery by making fundamental measurements of the geometry of the universe and the growth of structure and by accurately characterizing key quantities such as the dark energy equation of state, the sum of neutrino masses, and the spatial statistics of the distribution of mass.

This project will provide a matching computational effort by running very large cosmological simulations—some of the most challenging to be undertaken worldwide.

We will use the hardware accelerated cosmology codes (HACC) computational cosmology framework to run two sets of simulations—one to build precision emulators to attack the problem of inference, the other to generate realistic synthetic sky catalogs and simulated observations—to help constrain a host of systematic uncertainties, by working closely with a number of leading surveys.

The HACC code can be tuned for performance and scaling on all HPC systems. In particular, on the IBM BG/Q system, HACC has reached very high levels of performance—almost 14 petaflops (the highest ever recorded by a science code) with scaling verified to about 1.5 M cores. Recently, excellent scaling of HACC on Titan has been demonstrated on more than 90 percent of the full machine at similar levels of performance.

In addition to HACC, the project rests on two other computational platforms: the Cosmic Calibration Framework, used to build precision prediction tools (or emulators) for survey observables; and pipelines to generate synthetic galaxy catalogs using halo occupation distribution models and semi-analytic models.

Type: Renewal
Title: "Designing O_2 Tolerant Hydrogenases"

Principal Investigator: Vijay Pande, Stanford University

Scientific Discipline: Biology: Biophysics

INCITE Allocation: **13,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (13,000,000 processor hours)

Research Summary:

Molecular hydrogen has been promoted as an ultimate clean fuel and energy carrier. Yet conventional approaches for its production rely on inefficient catalytic turnovers through rare metals (i.e., platinum). Hydrogenases offer an increasingly viable biochemical alternative. They are known to catalyze both the H_2 oxidation and its production by using iron and nickel cofactors in their reactive centers. These enzymes have been studied for their potential uses in electrochemical devices, for developing biomimetic H_2-production catalysts and genetically engineered hydrogenases for photo-biological H_2-production. A limiting aspect of hydrogenases is their susceptibility to inhibition by molecular oxygen and carbon monoxide. Those that can resist inhibition are typically less catalytically active than the oxygen-sensitive enzymes. One strategy to limit inhibition is to reduce the diffusion rate of the inhibitors to the active site, which is buried deep inside the protein and is accessible only via diffusion through the protein matrix.

We propose to perform extensive simulations of wild type (WT) hydrogenases and mutants, with the intent of mapping out the complete network of diffusion pathways in hydrogenases to engineer robust enzyme variants for H_2 production and oxidation. We will perform these in the presence of O_2, CO, and H_2 to gain a quantitative understanding of the diffusion process. Based on these observations, we will identify a set of residues that can be mutated to counter the influx of molecular O_2 and CO. The goal is to produce hydrogenase variants that operate at WT levels of activity without suffering from the typical inhibition patterns.

The design of O_2 tolerant hydrogenases can provide critical insight toward the development of future H_2 based energy technologies. Because we still do not have a complete picture of the complex network of diffusion pathways and of the protein conformations around the metallocenters, we believe that our work could make significant contributions to the field.

The approach that we propose to employ here for the first time at this scale holds the promise to be of broad utility for the rapid conformational sampling of large protein systems that have thus far eluded statistically sound studies at the atomistic level. If we succeed, thorough future studies of large protein systems will move one step closer to becoming routine.

Type: New
Title: "Direct Numerical Simulations and Robust Predictions of Cloud Cavitation Collapse"

Principal Investigator: Petros Koumoutsakos, Swiss Federal Institute of Technology Zurich, Switzerland

Scientific Discipline: Engineering: Fluids and Turbulence

INCITE Allocation: **88,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (88,000,000 processor hours)

Research Summary:

Cloud cavitation collapse is detrimental to the lifetime of high-pressure injection engines as well as instrumental to kidney lithotripsy and ultrasonic drug delivery. Despite its importance, we have limited understanding of its governing mechanisms so as to design informed strategies for preventing and controlling it.

The study of cloud cavitation collapse presents a formidable challenge to experimental and computational studies owing to its geometric complexity and the wide range of its characteristic spatiotemporal scales. Its simulation requires two-phase flow solvers capable of capturing interactions between multiple deforming bubbles, pressure waves, formation of shocks, and their interaction with boundaries and turbulent vortical flows.

The goal of this project is to perform simulations that capture the collapse of more than 50,000 bubbles interacting with a turbulent flow field at unprecedented resolution and performance. Direct numerical simulations will provide databases for turbulent cavitation bubble clouds that can be used to extract relevant models for large eddy simulations. Moreover, the researchers will perform multilevel uncertainty quantification (UQ) on quantities of using the nonintrusive multi-level Monte Carlo method coupled with the present finite volume solver. The UQ studies will enable robust predictions for uncertainties in input parameters that will assist the development of engineering models. The researchers envision that the proposed simulations will drastically improve understanding of cloud cavitation collapse in turbulent flows and will revolutionize the development of engineering models for the prediction of the cavitation damage potential.

Type: Renewal
Title: "DNS of Turbulent Combustion Towards Fuel-Flexible Gas Turbines and IC Engines"

Principal Investigator: Jacqueline Chen, Sandia National Laboratories
Co-Investigators: Alex Aiken, Stanford University
John Bell, Lawrence Berkeley National Laboratory
Ankit Bhagatwala, Sandia National Laboratories
Marc Day, Lawrence Berkeley National Laboratory
Ray Grout, National Renewable Energy Laboratory
Andrea Gruber, The Foundation for Scientific and Industrial Research
Hemanth Kolla, Sandia National Laboratories
Sgouria Lyra, Sandia National Laboratories
Yuki Minamoto, Sandia National Laboratories
Ramanan Sankaran, Oak Ridge National Laboratory

Scientific Discipline: Chemistry: Combustion

INCITE Allocation: **106,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (106,000,000 processor hours)

Research Summary:
First principles direct numerical simulation (DNS) of turbulent combustion sheds light on underlying turbulence–chemistry interactions relevant to the design of next-generation fuel-flexible stationary gas turbines and fuel-efficient, clean internal combustion engines using biofuels. A proposed suite of DNS benchmarks will enable the development of predictive models for lifted diesel flame stabilization, discerning flame and ignition propagation in reactivity controlled compression ignition combustion, and ensuring intrinsic flashback safety in fuel injection systems for fuel-flexible gas turbines.

Projections of global energy use ensure that combustion will continue to be the predominant mode of energy conversion for transportation, power generation, and industrial thermal processes for the next half-century. Considerations of energy and environmental security and sustainability, as well as economic competiveness, demand accelerated development of advanced combustion technologies that combine high efficiency, low emissions, and the ability to reliably operate on an increasingly diverse range of fuels, including bio-derived and synthetic fuels, as well as evolving fossil fuels. First-principles petascale DNSs of underlying turbulence-chemistry interactions in gas-phase combustion are a powerful tool for creating the underlying science foundation that will enable predictive modeling in the design of future engines for transportation and power generation.

Type: New
Title: "DNS/LES of Complex Turbulent Flows"

Principal Investigator: Krishnan Mahesh, University of Minnesota

Scientific Discipline: Engineering: Fluids and Turbulence

INCITE Allocation: **100,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (100,000,000 processor hours)

Research Summary:

This project will study two fluid dynamical problems with high-fidelity, finite volume flow simulations using petascale resources: (1) direct numerical simulation (DNS) of autoignition in a vitiated coflow burner and (2) large eddy simulation (LES) of propeller crashback. Its three broad aims include developing numerical algorithms for turbulence simulation, performing high–fidelity simulations of important flows, and using the simulation results to develop simpler scaling laws and engineering models.

Regarding the first fluid dynamics problem, the autoignition of fuels is crucial to the design and understanding of the next generation of internal combustion engines using homogeneous charge compression ignition, as these engines can achieve higher thermal efficiencies with lower nitrogen oxide emissions. The DNS will provide data that will assist in understanding the influence of turbulent mixing on ignition-delay times and flame stability, as well as in analyzing existing combustion models and developing novel models.

Crashback occurs when a forward-moving marine vessel is decelerated by rotating the propeller in the reverse direction, thereby yielding negative thrust. The reverse flow interacts with the incoming freestream, generating unsteady forces that are transmitted to the vessel body, adversely affecting its maneuverability and potentially causing damage to and reducing performance of the propeller blades. Understanding crashback will enable better designs of marine propellers and the determination of safe operating envelopes. The researchers will focus on developing and demonstrating the capability of using LES to simulate highly turbulent flows on propelled bodies in crashback; to their knowledge, this is the first time detailed simulations will be performed of such complicated flow.

Type: New
Title: "Dynamic and Adaptive Parallel Programming for Exascale Research"

Principal Investigator: Robert Harrison, Brookhaven National Laboratory
Co-Investigators: George Fann, Oak Ridge National Laboratory
Laura Ratcliff, Argonne National Laboratory
Saday Sadayappan, Ohio State University
Edward Valeev, Virginia Tech

Scientific Discipline: Computer Science

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

Research Summary:
Many challenges await along the path from petascale to exascale and beyond for hardware architectures, as well as for system software developers and application programmers; however, three concepts in particular have been identified as critical: algorithmic concurrency, reduction in data movement, and asynchrony. There is a need to move beyond bulk-synchronous programming models and to address both data and computation in a nonlocal fashion (e.g., via partitioned global address space models). However, programming models alone are insufficient for enabling exascale application programming because they do not—and by design can not—take into account the mathematical properties of numerical computations that are essential to addressing the concurrency problem.

This project will support research and development activities on the design, development, deployment, and demonstration of a novel programming environment that addresses both the programming model and algorithmic challenges of exascale computing within multiple domains. The experiment apparatus will be the MADNESS (Multiresolution ADaptive NumErical Scientific Simulation) framework, which encapsulates a dynamic active-message runtime system, a global data model based upon distributed containers, a multi-resolution analysis toolkit, and scalable numerical solvers. The application domains targeted for demonstration include nuclear physics, density-functional theory of materials, quantum many-body methods for chemistry, and the MADNESS general purpose numerical environment for the solution of integral and differential equations.

The researchers seek to illuminate a path toward exascale application programming in the mission-critical scientific domains of the U.S. Department of Energy. The computer science and math research will bring a broad suite of science applications closer to exascale readiness.

Type: Renewal
Title: "First-Principles Simulations of High-Speed Combustion and Detonation"

Principal Investigator: Alexei Khokhlov, University of Chicago
Co-Investigators: Joanna Austin, University of Illinois at Urbana–Champaign
Marta Garcia, Argonne National Laboratory

Scientific Discipline: Chemistry: Combustion

INCITE Allocation: **150,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (150,000,000 processor hours)

Research Summary:
This research seeks to understand the mechanisms responsible for deflagration-to-detonation transition (DDT) to help determine safety measures in settings as varied as industrial sites and nuclear production facilities. Because detonation occurs quickly and on a very small spatial scale compared to the size of the system, high-resolution, multidimensional simulations are the most feasible method by which to investigate the detailed physics of a DDT.
This study requires first-principles, compressible, reactive flow Navier-Stokes direct numerical simulations, which take into account and explicitly resolve physical processes on spatial scales ranging from meters to microns, as well as attendant shocks, discontinuities, and physical variables.

Initial studies will focus on hydrogen-oxygen mixtures, which have relatively simple chemical kinetics. The research will then extend to hydrogen-air; syngas, a synthetic mixture of H_2 and CO used as a clean fuel for increasing energy efficiency, and; ethylene, among the most used hydrocarbons in chemical industries.
Where such simulations were not practical in the past, the supercomputing power of ALCF's Mira will allow for the spatial and temporal resolutions necessary to accurately investigate such processes. Researchers will perform these simulations using a reactive flow Navier-Stokes high-speed combustion and simulation code. The code incorporates detailed physics and chemistry suitable for hydrogen combustion and high-resolution treatment of shock waves, and it supplies a uniform grid as well as static and dynamic adaptive mesh refinement capabilities.

By better understanding the complex mechanisms involved in these reactions, researchers and engineers will be able to better predict the onset of detonation and develop safety mechanisms for real-world applications.

Type: New
Title: "Frontiers in Planetary and Stellar Magnetism through High-Performance Computing"

Principal Investigator: Jonathan Aurnou, University of California, Los Angeles
Co-Investigators: Benjamin Brown, University of Colorado Boulder
Bruce Buffett, University of California, Berkeley
Nicholas Featherstone, University of Colorado Boulder
Gary Glatzmaier, University of California, Santa Cruz
Lorraine Hwang, University of California, Davis
Louise Kellogg, University of California, Davis
Hiroaki Matsui, University of California, Davis
Peter Olson, Johns Hopkins University
Sabine Stanley, University of Toronto

Scientific Discipline: Earth Science: Geological Sciences

INCITE Allocation: **83,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (83,000,000 processor hours)

Research Summary:
Astronomical bodies ubiquitously generate self-sustaining, large-scale magnetic fields that are maintained through the turbulent motions of electrically-conducting fluids. These dynamo processes are now known to operate within diverse cosmologic entities throughout the universe. The existence of a large-scale magnetic field is essential to our understanding of the present dynamical state of a given body, as well as its evolutionary path.

However, dynamo models of both planets and stars, to date, have been unable to resolve strongly turbulent dynamo action in fluids with properties similar to liquid metals and plasmas. Instead, these models simulate dynamo action driven by rotating, convective flows that are nearly laminar. In order for these modest, laminar flows to generate efficient dynamo action, highly electrically-conductive fluids must be employed. To address these limitations, the National Science Foundation's Computational Infrastructure for Geodynamics (CIG) has developed *Rayleigh,* an open source, community dynamo code. This code simulates convection driven dynamo action in rotating spherical shells, such as those at the cores of planets and stars.

Researchers propose three dynamo models. The Liquid Metal Geodynamo Model will focus on magnetic-field generation as influenced by the physical properties of liquid metal under high pressure at the cores of terrestrial planets, like the Earth. The Jovian Interior Dynamics Model will help determine where the dynamo process occurs in gaseous planets. And the Extreme Solar Dynamo Model will address the hydrodynamics of sub-surface convection that drives the dynamo responsible for sunspots and magnetic active regions at the solar surface.

Type: New
Title: "Global Adjoint Tomography"

Principal Investigator: Jeroen Tromp, Princeton University
Co-Investigators: Ebru Bozdag, University of Nice Sophia Antipolis
Dimitri Komatitsch, The French National Centre for Scientific Research
Matthieu Lefebvre, Princeton University
Daniel Peter, Swiss Federal Institute of Technology Zurich, Switzerland

Scientific Discipline: Earth Science: Geological Sciences

INCITE Allocation: **50,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (50,000,000 processor hours)

Research Summary:
The goal of the proposed research is to further image Earth's global interior based on full waveform inversion by taking into account anelasticity and anisotropy. By assimilating all available data from more than 6,000 earthquakes, we can facilitate a deeper understanding of Earth's physics and chemistry. In recent years, we have begun to harness spectral-element and adjoint methods to address seismic inverse problems. We propose to build on our experiences in imaging the crustal structure of Southern California and the crustal and upper-mantle structure of Europe, as well as the global inversion being performed on Titan.

Seismic imaging based on spectral-element and adjoint methods has enabled the assimilation of this information into three-dimensional models of elastic and anelastic heterogeneity. These methods fully account for the physics of wave excitation and propagation by numerically solving the equations of motion for a heterogeneous anelastic solid. Such methods require the execution of complex computational procedures that challenge the most advanced high-performance computing systems.

Building on our research experiences and advances on Titan, our goals for the requested allocation are: to complete higher resolution simulations, reducing the shortest period first to 17 s and then to 9 s, and increasing the record length for 27 s simulations to 200 min (thereby capturing short-period body waves up to the microseismic noise band and major-arc surfaces waves); to exploit and further develop the Adaptable Seismic Data Format to grow the earthquake database; to incorporate azimuthal anisotropy, which is essential for understanding lithospheric and mantle dynamics; and, as the elastic structure improves, to move toward full waveform inversion by incorporating amplitude information and simultaneously inverting for elastic and anelastic heterogeneity (thereby placing constraints on, for example, water content in the crust and mantle).

Type: New
Title: "High Frequency Ground Motion Simulation for Seismic Hazard Analysis"

Principal Investigator: Thomas Jordan, Southern California Earthquake Center
Co-Investigators: Jacobo Bielak, Carnegie Mellon University
Po Chen, University of Wyoming
Yifeng Cui, San Diego Supercomputer Center
Philip Maechling, Southern California Earthquake Center
Kim Olsen, San Diego State University
Ricardo Taborda, University of Memphis

Scientific Discipline: Earth Sciences: Geological Sciences

INCITE Allocation: **167,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (48,000,000 processor hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (119,000,000 processor hours)

Research Summary:
Economic exposure to earthquake devastation in seismically active regions has increased significantly over the last few decades because of massive growth of urban areas. To understand risk and improve resilience, we need to quantify earthquake hazards at higher levels of fidelity. Physics-based modeling and simulation provide a path to a more accurate representation of earthquake systems—from the rupture at the fault to the response of the built environment. This approach relies on numerical simulation of rupture dynamics and seismic wave propagation in realistic three-dimensional models of the crust's heterogeneous structure to represent the ground motion during strong earthquakes.

Our goal is to produce simulations at a level of resolution valid for engineering applications (that is, at frequencies higher than previously used). Higher frequency earthquake system modeling needs to be coupled to engineering models of infrastructure systems such as buildings, bridges, and other critical distributed systems (e.g., lifeline and medical networks) that depend strongly on how complex earthquake wavefields interact with the mechanical heterogeneities of the ground and the built landscape, including both off-fault and near-surface plasticity and other site effects such as surface topography.

This project also will provide a framework for evaluating alternative ground motion simulation methods, such as existing hybrid deterministic and nondeterministic methods, and for investigating the threshold frequency at which both of these approaches provide a viable tradeoff for hybrid simulation, leading to the production of more physically realistic synthetic seismograms for use in earthquake engineering.

Type: Renewal
Title: "High-fidelity Simulation of Tokamak Edge Plasma Transport"

Principal Investigator: Choong-Seock Chang, Princeton Plasma Physics Laboratory
Co-Investigators: Scott Klasky, Oak Ridge National Laboratory
Seung-Hoe Ku, Princeton Plasma Physics Laboratory
Scott Parker, University of Colorado Boulder

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation: **270,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (100,000,000 processor hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (170,000,000 processor hours)

Research Summary:
It is a common prediction that the world's oil resources will run out in less than 50 years if the oil production rate should increase to meet the rise in world energy demand. In the extraterrestrial world, thermonuclear fusion energy has been stably powering the sun and the stars for billions of years. Its energy source is virtually inexhaustible and intrinsically safe.

This project is to study tokamak edge plasma physics and transport, which are known to have a critical impact on the performance of a tokamak fusion reactor. Extreme scale computing is required because of the nonlinear multiscale, multiphysics nature of the problem in complex magnetic and wall geometry.

We propose a comprehensive electromagnetic turbulence study. There is a vast amount of physics phenomena to study. The majority of the important turbulence modes will be included in the simulation, such as the ion temperature gradient and trapped electron mode (ITG-TEM), drift-Alfvenic, resistive ballooning, intermediate wavelength kink-peeling, short wavelength kinetic ballooning, intermediate to short wavelength tearing, and other modes. These modes are expected to self-organize, not only among themselves, but also with the background neoclassical dynamics, radial electric field, edge plasma flows, impurity particles, and neutral particles. Many of the important experimental observables will be attacked in collaboration with the experimental participants in Edge Physics Simulation (EPSI). The three-dimensional magnetic perturbation edge physics, which has been successfully conducted in the neoclassical guiding center particle code, XGC0, with a limited capability without turbulence, will be upgraded to XGC1 in the EPSI project.

Successfully solving and understanding a few of the above problems cannot be done outside of the INCITE program; XGC1 is currently the only working edge gyrokinetic code in realistic diverted geometry in the world fusion program.

Type: New
Title: "High-Fidelity Simulations of Gas Turbine Stages with GPU Acceleration"

Principal Investigator: Vittorio Michelassi, General Electric Company
Co-Investigators: Richard Sandberg, University of Southampton

Scientific Discipline: Engineering: Fluids and Turbulence

INCITE Allocation: **40,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (40,000,000 processor hours)

Research Summary:
Because of the migration from coal to natural gas-fueled gas turbines (GTs) over the last 20 years, CO_2 emissions from the electric power generation industry have been reduced; in 2012, natural gas-fueled GTs accounted for 30 percent of US electrical power generation. This technology platform offers a high degree of operating flexibility and is compatible with intermittent renewable power generation. With GE gas turbines making up more than 50 percent of the world's installed base, any GT efficiency increase has significant potential to reduce fuel burn and global environmental impact.

Although GT performance has improved considerably over the last decade, it is becoming increasingly difficult to make further advances based on the current state-of-the-art analytical tools used in design. High-fidelity computational fluid dynamics, coupled with appropriate validation, offers an opportunity to resolve the physics with an unprecedented level of detail.

The purpose of this program is to leverage recent advances in direct numerical simulation (DNS) and large eddy simulation (LES) to improve our understanding of the unsteady physics that occur between stationary and rotating components in the high-turbulence environment of a GT and to improve the accuracy of turbulence models in the design of GTs. Using the HiPSTAR code that our team optimized for HPC under previous programs, we will increase our understanding of the physics of a highly turbulent flow superimposed to discrete wakes and shocks. This will enable us to identify opportunities to increase turbine aero-thermal efficiency by 2 to 4%, which will translate into combined cycle efficiency gains of 0.4 to 0.8%.

We will conduct a careful comparison between DNS and LES at realistic turbine operating conditions to assess the validity of some of the previous LES assumptions. Such an approach will lead to the generation of gold-standard datasets that can be employed by the broader research community to improve its understanding of unsteady flow physics in GTs.

Type: Renewal
Title: "Innovative Simulations of High-Temperature Superconductors"

Principal Investigator: Thomas Maier, Oak Ridge National Laboratory
Co-Investigators: Thomas Schulthess, Swiss Federal Institute of Technology Zurich, Switzerland
Peter Staar, Swiss Federal Institute of Technology Zurich, Switzerland

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation: **60,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (60,000,000 processor hours)

Research Summary:
Since its discovery in 1986, high-temperature superconductivity has fascinated countless physicists and materials scientists and continues to captivate researchers as new materials in this class are discovered. But despite one of the most intensive attacks on a problem in the history of condensed matter physics, the mystery of the underlying physics that drives superconductivity at temperatures as high as 150 K in these systems has yet to be resolved.

Superconducting materials are key components to developing new energy-related technologies but require optimization to unleash their full potential. This project will perform high-end simulations of cuprate high-temperature superconductors to understand, predict, and optimize their complex behavior and, thus, help accelerate development in this area.

Researchers will conduct the first-ever controlled and reliable simulations of the Hubbard model of copper-oxide high-temperature superconductors using a new quantum cluster Monte Carlo method, the DCA+, which has been implemented for hybrid multicore, leadership-class architectures. The DCA+ algorithm is designed to cure the problems of current state-of-the-art techniques and thus will allow researchers to compute the superconducting transition temperature, Tc, in the Hubbard model. Understanding the mechanism that leads to superconductivity in these systems and the nature of the enigmatic pseudogap phase from which it emerges, as well as the factors that determine the variation of Tc between different materials, are among the grand challenges of condensed matter physics.

As active users of ORNL's computing platforms for almost a decade, the proposal team members have strong experience with leadership-class computing to solve high-impact problems. The proposed computations use a code that is proven to run and scale efficiently on ORNL's Titan, allowing us to transform petascale cycles into high-impact science.

Type: Renewal
Title: "Large Eddy Simulations of Combustor Liner Flows"

Principal Investigator: Anne Dord, GE Global Research
Co-Investigators: Frank Ham, Cascade Technologies
Lee Shunn, Cascade Technologies

Scientific Discipline: Engineering: Fluids and Turbulence

INCITE Allocation: **89,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (89,000,000 processor hours)

Research Summary:

In 2012, the commercial aviation industry spent an estimated $207 billion on fuel, or about 33 percent of their operating costs. That amounts to approximately 5 million barrels of oil per day, or about 6 percent of the world's total oil usage. Aviation gas turbine engines are also significant producers of CO2 and other harmful greenhouse gas emissions. As the aviation industry continues to grow, the cost and environmental impacts of operating gas turbine engines will continue to increase as well.

In the second year of this multiyear INCITE project, researchers will continue their studies of the complex near-wall physics of combustor liner flows with a focus on aircraft engine applications. Understanding and predicting the aero-thermal flow field is key to designing and optimizing combustors for better fuel efficiency, lower emissions, and improved performance. The proposed calculations require significantly greater computational resources than those traditionally used in industry, necessitating the use of DOE's leadership-class supercomputers.

The calculations use large eddy simulations to model the behavior of an idealized configuration representative of combustor liners. This will enable modelers to generate high-fidelity datasets that will be used to improve the low-fidelity models currently available to designers. The same approach will be applied to a more complex configuration, involving a larger domain, and more realistic flow characteristics, representative of large-scale flow unsteadiness present in aircraft engines. Ultimately, the findings will be applied to an actual multi-cup General Electric rig, providing a vehicle to test the improved models developed in the first two phases of the program. This will give designers a better understanding of the complex unsteady processes governing the aero-thermal field around combustor liners.

Type: New
Title: "Large-Eddy Simulation of the Bachalo-Johnson Flow, with Shock-Induced Separation"

Principal Investigator: Philippe Spalart, Boeing

Scientific Discipline: Engineering: Fluids and Turbulence

INCITE Allocation: **135,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (135,000,000 processor hours)

Research Summary:

Turbulence strongly controls many flows. Shock–boundary layer interactions (SBLIs) are of particular interest to aerospace companies and the gas-turbine industry, and some proposals for carbon capture and sequestration also involve supersonic flows in the compressors. This project will focus on the upper surface of a transport aircraft wing, especially in off-design conditions, such as an increased Mach number or an angle of attack. It takes as its reference Bachalo and Johnson's 1981 experiment at the National Aeronautics and Space Administration (NASA), which has been a very useful test case for computational fluid mechanics (CFD), and Reynolds-Averaged Navier-Stokes (RANS) turbulence models. However, although the experiment featured fairly detailed measurements, there was no independent confirmation, and it yielded much less information compared to what a simulation can provide, for instance, in terms of skin friction.

Therefore, as researchers continue a worldwide effort to improve RANS models and to enhance the general understanding of complex turbulent flows, it will be very valuable to have a large eddy simulation (LES) of this 1981 experiment's flow. The simulation will be very large because of the extended separated region and the high Reynolds ($Re/m=13.6 \times 10^6$) number. It will be conducted at the correct Mach number (M=0.875) as well, with converged turbulence statistics and in good agreement with the experiment. The overall objective is to reach the state of the art for simulations of SBLIs for grids up to two billion points and to thoroughly extract findings pertaining to physics and numerical resolution.

Type: Renewal
Title: "Large-scale Coupled-Cluster Calculations of Supramolecular Wires"

Principal Investigator: Poul Jørgensen, Aarhus University
Co-Investigators: Jacek Jakowski, Oak Ridge National Laboratory
Kasper Kristensen, Aarhus University
Bobby Sumpter, Oak Ridge National Laboratory

Scientific Discipline: Chemistry: Physical

INCITE Allocation: **48,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (48,000,000 processor hours)

Research Summary:

Electronic structure calculations of a wide range of molecular properties today are an integrated part of many branches of molecular sciences. The coupled-cluster (CC) model is the state-of-the-art wave function method, and, for small molecular systems, various molecular properties have been computed to an accuracy challenging experimental results. However, the application range of CC methods so far has been limited to small molecular systems because of their computational scaling with system size. For this reason, density functional theory (DFT) has developed into a workhorse for large-scale applications. The major drawback of DFT calculations is that they generally do not possess the accuracy and the predictive power of the CC methods.

We are developing non-commercial open source software for electronic structure calculations by extending the application range of coupled-cluster wave function methods to large molecular systems. Applications will be performed on a new class of organogelators generated from self-assembly of 1-aza-adamantanetriones (AATs) into one-dimensional molecular wires.

The goal of this project is twofold: we wish to develop a stable, massively parallel CC program to make available free to the general user, and we want to apply it to the AAT class of supramolecular wires. The computational method for achieving these goals is the divide–expand–consolidate (DEC) scheme—where the inherent locality of electron correlation effects is used to formulate CC calculations in a linear-scaling and massively parallel manner.

The outlook for the proposed development is immense. Today, quantum mechanical calculations on large molecular systems are routinely carried out using DFT. The reliability of these calculations is severely limited. With the DEC development, CC methods may also be applied to large molecular systems with the same rigorous error control as for small molecules. This proposal is a huge step in this direction, which, in a larger perspective, will transform the field of electronic structure calculations for large molecules from being largely a tool for rationalizing observed phenomena to becoming truly predictive.

Type: Renewal
Title: "Lattice QCD"

Principal Investigator: Paul Mackenzie, Fermilab
Co-Investigator: Richard Brower, Boston University
Norman Christ, Columbia University
Frithjof Karsch, Brookhaven National Laboratory
Julius Kuti, University of California, San Diego
John Negele, Massachusetts Institute of Technology
David Richards, Thomas Jefferson National Accelerator Facility
Martin Savage, University of Washington
Robert Sugar, University of California, Santa Barbara

Scientific Discipline: Physics: Particle Physics

INCITE Allocation: **280,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (180,000,000 processor hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (100,000,000 processor hours)

Research Summary:
For this INCITE project, researchers from the U.S. Quantum Chromodynamics (USQCD) Collaboration will advance exploration in lattice QCD and other strongly coupled field theories. The research team will use DOE leadership computing resources to generate gauge configurations with up, down, strange, and, in some cases, charmed quarks on lattices that are sufficiently fine grained to enable full control of systematic errors for a number of key quantities. These gauge configurations will be used to address fundamental questions in high energy and nuclear physics, and are directly related to several major experimental programs in these fields (e.g., the Large Hadron Collider at CERN in Switzerland and the Gluex experiment at the Thomas Jefferson National Accelerator Facility).

In high energy physics, precise lattice QCD calculations are required to investigate and pin down the properties of the Standard Model of particle physics and to search for new physics beyond the Standard Model. A central goal of the nuclear physics research program is to utilize QCD as a predictive tool for nuclear systems and their constituents. In particular, the next five years will be a critical period for the application of lattice QCD to cold nuclear physics, as the calculations will be performed routinely at the physical value of the pion mass, allowing for direct comparisons with experiment. Results from this project are essential for meeting milestones set by DOE's Office of Science.

Type: Renewal
Title: "Linkages Between Turbulence and Reconnection in Kinetic Plasmas"

Principal Investigator: William Daughton, Los Alamos National Laboratory
Co-Investigators: Kai Germaschewski, University of New Hampshire
Homa Karimabadi, University of California, San Diego
Vadim Roytershteyn, SciberQuest, Inc.

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation: **60,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (60,000,000 processor hours)

Research Summary:

We will explore the relationship between turbulence and magnetic reconnection in high-temperature plasmas. These two basic processes occur in a wide range of applications, including laboratory experiments, the solar wind, and the Earth's magnetosphere.

Historically, much of the research on these two subjects has been carried within separate research communities that had only minimal interactions. However, it has become increasingly clear in recent years that these two subjects may be intimately connected.

This project will explore both the formation and break-up of these current sheets using fully kinetic simulations, which rigorously describe the plasma physics. The two primary focus areas of our research include simulations of decaying turbulence to examine the statistics of current sheet formation and their relative contribution to the dissipation. These simulations are highly anticipated by the solar wind turbulence community and will be compared against spacecraft data. The exact parameters for these record runs will be chosen in part based on the input from a wider community of turbulence experts and data will be appropriately disseminated for multi-institutional collaborations.

Our second focus area is on the development of reconnection in ion-scale current sheets in close collaboration with three experimental groups at UCLA, Madison and Princeton. Each experiment targets a different aspect of the physics of current sheet dissipation and breakup. We will employ parameters and boundary conditions relevant to three laboratory experiments, thus allowing us to perform validation studies on some key aspects of this physics.

We anticipate these results will lead to major advancements in our understanding of both turbulence and reconnection, which will have impact in a variety of fields including space physics, solar physics, laboratory plasmas, and astrophysics.

Type: Renewal
Title: "Multiscale Simulations of Human Pathologies"

Principal Investigator: George Karniadakis, Brown University

Scientific Discipline: Biological Sciences: Biophysics

INCITE Allocation: **70,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (45,000,000 processor hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (25,000,000 processor hours)

Research Summary:

Thoracic aortic aneurysm and dissection (TAAD) is a serious health condition in which an aneurysm in the aorta expands and causes a tear in the artery wall. TAADs are estimated to be responsible for around 30,000 deaths per year in the U.S. alone, and the condition is still not well understood. However, recent advances in genetics and medical imaging have resulted in a significant increase in the number of diagnosed TAADs and an increased appreciation of roles played by thrombus (i.e., blood clots) in aortic dissections.

Building on extensive computational expertise and past INCITE awards, the Brown University research group is using DOE leadership computing resources to develop the first data-driven, multiscale, multiphysics model of the biomechanics of thrombus in aortic dissection. Specifically, they are examining the hemodynamical conditions under which an intramural thrombus forms in aortic dissections and the biomechanical consequences of thrombus on the remnant wall. In the second year of this INCITE allocation, the team plans to study the interplay between blood flow and intramural thrombus remodeling, which is believed to play a prominent role in the development and evolution of TAAD.

With a better understanding of the roles of thrombus in aortic dissection, this research has the promise to lead to an improved prognostic capability and interventional planning. Although the project is focused on aortic dissection, the findings will be equally applicable to understanding the biomechanics of other artery dissections and diverse aneurysms. Therefore, insight gained in this study will have important implications for a host of other vascular conditions, providing information that could contribute to improved treatments for a broad class of clinical problems.

Type: Renewal
Title: "Non-covalent Bonding in Complex Molecular Systems with Quantum Monte Carlo"

Principal Investigator: Dario Alfe, University College London
Co-Investigators: Mike Gillan, University College London
Ken Jordan, University of Pittsburgh
Angelos Michaelides, University College London
Alexandre Tkatchenko, Fritz Haber Institute
Mike Towler, University College London
Anatole von Lilienfeld, Argonne National Laboratory

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation: **148,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (68,000,000 processor hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (80,000,000 processor hours)

Research Summary:
Given the key role of hydrogen bonding and other non-covalent interactions in the cohesion of the molecular materials that are so important for our world, it is unfortunate that the widely used computational science techniques of density functional theory (DFT) give an inadequate account of these interactions.

A full quantitative understanding of hydrogen bonding is crucial for all systems involving water, including the pure liquid and the many forms of ice, water nanoparticles, low-dimensional aggregates such as adsorbed water layers, aqueous solutions, hydrated biomolecules, biological structures stabilized by hydrophobicity, gas hydrates, and many others.

We will use highly accurate quantum Monte Carlo (QMC) techniques to provide benchmark energies for these systems to create improved simulation methods, as well as an extensive database of energy benchmarks for molecular systems bound by non-covalent forces, particularly hydrogen bonding and van der Waals dispersion. The benchmarks will be used to develop improved versions of DFT and to assess and improve parameterized force fields for molecular systems.

The main outcomes of the project will be: (1) a greatly improved understanding of water systems in many different aggregation states, embodied in improved versions of DFT and force fields; (2) more accurate energetics of industrially and environmentally important gas hydrates; (3) better predictive power of computational techniques for designing important supramolecular systems; and (4) the establishment of QMC on petascale platforms as a routine, generally usable technique for investigating non-covalent bonding in complex molecular systems.

Type: Renewal
Title: "Nuclear Structure and Nuclear Reactions"

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

Scientific Discipline: Physics: Nuclear Physics

INCITE Allocation: **204,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (100,000,000 processor hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (104,000,000 processor hours)

Research Summary:

Predictions for the structures and reactions of nuclei, with assessed uncertainties, are important for the future of U.S. energy and security needs. The development of a robust and precise nuclear theory, based on the underlying theory of the Standard Model of elementary particles, incorporating both the strong and electroweak sectors, represents a "holy grail" for physics, with many applications in both basic science and applied science. However, developing a comprehensive description of all nuclei and their reactions requires investigations of exotic isotopes that are difficult or impossible to study experimentally.

For this multiyear INCITE project, researchers will continue to use DOE supercomputers to provide needed predictions where direct experiments are not possible or are subject to large uncertainties. Such calculations are relevant to applications in nuclear energy, nuclear security, and nuclear astrophysics, since rare nuclei lie at the heart of nucleosynthesis and energy generation in stars. In regard to nuclear energy, a fundamental description of nuclear structure and nuclear reactions that retains predictive power and carries quantified uncertainties is vital for the future development of advanced fission reactors and fusion energy. The INCITE team's research agenda is focused on basic nuclear physics that is relevant to DOE's current and planned user experimental facilities, such as Jefferson Lab and the Facility for Rare Isotope Beams, where new phenomena and precision tests of the theory are anticipated.

Type: New
Title: "Nucleation and Growth of Colloidal Crystals Using Highly Scalable Monte Carlo"

Principal Investigator: Sharon Glotzer, University of Michigan

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

INCITE Allocation: **55,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (55,000,000 processor hours)

Research Summary:

The use of nanoparticles as building blocks for self-assembly is enabling new approaches to materials designed and synthesized with target applications in mind. This project will discover the mechanisms by which complex crystals assemble for a large library of particle shapes, yielding insights for design and development of new nanomaterials.

Monte Carlo normally is an inherently serial algorithm. We have developed the first and only massively parallel Hard Particle Monte Carlo (HPMC) simulation tool necessary to complete a study of this scale, and it is production ready. We combine Monte Carlo simulations with umbrella sampling, transition interface sampling, and other free methods to determine the energy barrier for nucleation, properties of the critical cluster, growth rates, and yield.

A single simulation to characterize nucleation and growth for a particular shape requires tens of thousands of core-hours. To design materials and understand how behaviors change as the underlying structures are varied, we will simulate thousands of different shapes at system sizes much larger than previously studied. Only a supercomputer on the scale of Titan is big enough to complete this task.

We will use our open source package HOOMD-blue with our HPMC plug-in to carry out detailed studies of nucleation and growth of entropically-stabilized complex crystals not previously possible. We will demonstrate HOOMD-blue's effectiveness on this problem in the context of hard particle (colloidal) systems where complexity of structure arises solely from particle shape, as is the case for many real colloidal materials.

Our findings will be of immediate interest to the nanoparticle and colloidal assembly communities, and our approaches and tools are transferable and will be of immediate and broad interest to the materials, engineering, and chemistry communities interested in crystallization of atoms, molecules, and proteins.

Type: Renewal
Title: "Parameter Studies of Boussinesq Flows"

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

Scientific Discipline: Engineering: Fluids and Turbulence

INCITE Allocation: **44,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (44,000,000 processor hours)

Research Summary:
The dynamics of rotating, stratified fluids include the complex interaction of waves and turbulence, and are the basis for understanding the behavior of many physical systems in astrophysical, geophysical, and engineering applications. On long time scales, coupling between waves and slow motions is likely responsible, in part, for the behavior of large-scale astrophysical and geophysical phenomena. This work focuses on quantifying the structures generated by such coupling, ranging from layers in strongly stratified flows to columnar structures in strongly rotating flows.

This project will also improve the current understanding of turbulence by computing statistical patterns gleaned after "seeding" a turbulent fluid with a large number of particles to be conveyed by the flow. The researchers, motivated by the presence of both upscale and downscale transfer of energy in strongly rotating stratified flows, are implementing Lagrangian particle tracking to the Geophysical High Order Suite for Turbulence (GHOST) code application. Such particle-tracking capabilities form a natural route to understanding the fluxes and mixing properties of the flows.

Tall aspect-ratio simulations remain under-explored in the field of rotating and stratified flows, particularly in those regimes that are relevant to geophysical flows. Parts of the ocean that are closer to the poles (e.g., the abyssal Southern Ocean) are more strongly affected by rotation, where such deep water flows are of particular interest. Researchers will perform a parameter scan with the largest tall aspect-ratio simulation of its type (2048 × 2048 × 16384 grid points) to study how the developing structure scales are related to the characteristic scales of mixing.

Type: Renewal
Title: "Particle Acceleration in Shocks: From Astrophysics to Laboratory In Silico"

Principal Investigator: Frederico Fiuza, Lawrence Livermore National Laboratory
Co-Investigators: Bruce Cohen, Lawrence Livermore National Laboratory
Ricardo Fonseca, Instituto Superior Técnico
Warren Mori, University of California, Los Angeles
Dmitri Ryutov, Lawrence Livermore National Laboratory
Michail Tzoufras, University of California, Los Angeles

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation: **110,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (110,000,000 processor hours)

Research Summary:
Particle acceleration in astrophysical shocks is believed to be one of the most important sources of energetic cosmic rays. This project aims to answer two important science questions recently highlighted by the U.S. National Academy of Sciences: What are the acceleration mechanisms for cosmic rays? Can we generate relativistic shocks in the laboratory and mimic these extreme cosmic accelerators?

Computational modeling is critical in addressing these questions to gain an understanding of the physical mechanisms behind shock formation and particle acceleration and to establish the conditions whereby these shock waves can be excited in the laboratory and explored for different applications. To this end, the research team has already produced results demonstrating that laser-driven shock waves can accelerate proton beams with the potential—when augmented by moderate laser intensities—to reach energies relevant for cancer therapy.

The researchers are employing the state-of-the-art, relativistic, and massively parallel particle-in-cell code OSIRIS (and its recently incorporated hybrid model) to develop massively parallel and fully kinetic first-principles simulations. Project goals include (1) understanding the conditions that are needed for the formation of collisionless shocks; (2) understanding the dominant particle acceleration mechanisms in shocks; and (3) identifying the setups to probe this physics for the first time in the laboratory. These efforts will trigger unique scientific results and open new avenues for research on the fundamental processes associated with shock formation, propagation, and particle acceleration, enabling reproduction in the laboratory of conditions found in gamma-ray bursts, supernovae, and other extreme astrophysical events.

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

Principal Investigator: Leonid Oliker, Lawrence Berkeley National Laboratory
Co-Investigators: Peter Beckman, Argonne National Laboratory
Laura Carrington, San Diego Supercomputer Center
James Demmel, University of California, Berkeley
Bronis de Supinski, Lawrence Livermore National Laboratory
Jack Dongarra, University of Tennessee, Knoxville, and ORNL
Todd Gamblin, Lawrence Livermore National Laboratory
William Gropp, University of Illinois at Urbana–Champaign
Mary Hall, University of Utah
Jeffrey Hollingsworth, University of Maryland
Darren Kerbyson, Pacific Northwest National Laboratory
Robert Lucas, Information Sciences Institute at USC
Allen Malony, University of Oregon
John Mellor-Crummey, Rice University
Barton Miller, University of Wisconsin–Madison
Philip Roth, Oak Ridge National Laboratory
Patrick Worley, Oak Ridge National Laboratory
Katherine Yelick, Lawrence Berkeley National Laboratory

Scientific Discipline: Computer Science

INCITE Allocation: **90,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (45,000,000 processor hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (45,000,000 processor hours)

Research Summary:
To facilitate further understanding of Leadership Class systems, this proposal focuses on five goals: (1) develop new programming models and runtime systems for emerging and future generation leadership computing platforms that exploit thread-level parallelism and potential architectural heterogeneity; (2) update and extend performance evaluation of all systems using suites of standard and custom micro, kernel, and application benchmarks; (3) continue to port performance tools and performance middleware to the BG/Q and XK7, make them available to high-end computing users, and further develop the tools and middleware to support the scale and unique modes of parallelism of the Leadership Class systems; (4) validate and modify performance prediction technologies to improve utility for production runs on the Leadership Class systems; and (5) analyze and help optimize current or candidate Leadership Class application codes and potentially develop new parallel algorithms.

Type: New
Title: "Petascale Simulation of Magnetorotational Core-Collapse Supernovae"

Principal Investigator: Sean Couch, California Institute of Technology
Co-Investigators: Almudena Arcones, Technische Universitat Darmstadt
Emmanouil Chatzopoulos, University of Chicago
Carla Frohlich, North Carolina State University
Dongwook Lee, University of Chicago
Evan O'Connor, North Carolina State University
Petros Tzeferacos, University of Chicago
J. Craig Wheeler, University of Texas at Austin
Daan van Rossum, University of Chicago

Scientific Discipline: Physics: Astrophysics

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

Research Summary:
Core-collapse supernovae (CCSNe) are the luminous explosions that herald the death of massive stars and serve as the source of origin for cosmic anomalies, such as neutron stars, pulsars, stellar-mass black holes, and, possibly, certain types of gamma-ray bursts. CCSNe produce many elements throughout the universe, especially those heavier than iron, thus, their importance in galactic chemical evolution cannot be underestimated.

Despite the importance of CCSNe to our understanding of many aspects of the universe, the mechanism that reverses stellar core collapse and drives supernova explosions is not fully understood, making it one of the most important challenges of computational astrophysics.

Project researchers propose a comprehensive study of the impact of rotation and magnetic fields on CCSNe using the FLASH multi-physics, adaptive mesh refinement (AMR) simulation framework run on Mira. A series of 3D magnetohydrodynamics (MHD) simulations of the collapse of rotating, magnetic stellar cores will include realistic treatments for neutrino physics, progenitor rotation, and magnetic fields. And, ALCF's leadership class resources will allow, for the first time, sufficient resolution to capture the growth of the magnetorotational instability.

Simulations will quantify how much rotational energy of the progenitor cores can be tapped to aid neutrinos in driving successful and robust explosions. They also will help predict the spins, kicks, magnetic-field strengths and alignments of newly-formed neutron stars, pulsars, and magnetars, as well as the dependence of these parameters on progenitor conditions.

Type: New
Title: "Petascale Simulations of Laser Plasma Interaction Relevant to IFE"

Principal Investigator: Frank Tsung, University of California, Los Angeles
Co-Investigators: Warren Mori, University of California, Los Angeles

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation: **90,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (90,000,000 processor hours)

Research Summary:
Inertial (laser-initiated) fusion energy (IFE) holds incredible promise as a source of clean and sustainable energy for powering devices. However, significant obstacles to obtaining and harnessing IFE in a controllable manner remain, including the fact that self-sustained ignition has not yet been achieved in IFE experiments. This inability is attributed in large part to excessive laser-plasma instabilities (LPIs) encountered by the laser beams.

LPIs such as two-plasmon decay and stimulated Raman scattering can absorb, deflect, or reflect laser light, disrupting the fusion drive, and can also generate energetic electrons that threaten to preheat the target. Nevertheless, IFE schemes like shock ignition (where a high-intensity laser is introduced toward the end of the compression pulse) could potentially take advantage of LPIs to generate energetic particles to create a useful shock that drives fusion. Therefore, developing an understanding of LPIs will be crucial to the success of any IFE scheme.

The physics involved in LPI processes is complex and highly nonlinear, involving both wave-wave and wave-particle interactions and necessitating the use of fully nonlinear kinetic computer models, such as fully explicit particle-in-cell (PIC) simulations that are computationally intensive and thus limit how many spatial and temporal scales can be modeled.

By using highly optimized PIC codes, however, researchers will focus on using fully kinetic simulations to study the key basic high energy density science directly relevant to IFE. The ultimate goal is to develop a hierarchy of kinetic, fluid, and other reduced-description approaches that can model the full space and time scales, and close the gap between particle-based simulations and current experiments.

Type: Renewal
Title: "Petascale Simulations of Self-Healing Nanomaterials"

Principal Investigator: Rajiv Kalia, University of Southern California
Co-Investigator: Aiichiro Nakano, University of Southern California

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation: **180,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (180,000,000 processor hours)

Research Summary:
Novel self-healing nanomaterials will play a vital role in the design of components for high-temperature turbines, wind and solar energy technologies, and lighting applications. These materials can significantly enhance the reliability and lifetime of such products while reducing manufacturing and maintenance costs.

For this multiyear INCITE project, researchers from the University of Southern California (USC) are examining self-healing nanomaterial systems capable of sensing and repairing damage in harsh chemical environments and in high-temperature/high-pressure operating conditions. Specifically, they are looking at anticorrosion coatings for metals and ceramic nanocomposites consisting of silicon carbide nanoparticles embedded in alumina and silicon nitride.

To study the materials in great detail, the USC research team is using Mira to carry out petascale quantum molecular dynamics (QMD), reactive molecular dynamics (RMD), and mesoscale reactive dissipative particle dynamics (R-DPD) simulations. In the second year of this INCITE award, they will perform billion-atom RMD simulations to determine the mechanical properties of aluminum sponges using nanoindentation. They will also perform RMD/R-DPD simulations to study the encapsulation and release of anticorrosion agents from silica nanocontainers in SiO_x-ZrO_x coating.

Ultimately, computational results from this project will be integrated with data from experiments conducted at DOE facilities, such as the Advanced Photon Source at Argonne, the Spallation Neutron Source at Oak Ridge, and the X-ray Laser Source at Stanford, to provide a comprehensive and efficient validation of the simulations. This synergy is key to enabling a fundamental understanding of self-healing processes and to the discovery of new materials for extreme conditions.

Type: Renewal
Title: "Predictive and Insightful Calculations of Energy Materials"

Principal Investigator: Paul Kent, Oak Ridge National Laboratory
Co-Investigators: Panchapakesan Ganesh, Oak Ridge National Laboratory
Jaron Krogel, Oak Ridge National Laboratory
Fernando Reboredo, 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 XK7 (50,000,000 processor hours)

Research Summary:
The project will use advanced *ab initio* quantum Monte Carlo methods to solve key problems in the modeling of titanium-based metals and metal oxides. Researchers aim to understand metal oxides that have wide applications in energy storage, catalysis, and energy production and metals that are widely used as structural materials. The project could have significant scientific impact and also a longer-standing effect in the materials modeling community.

The titanium "problem" is very large and cannot be solved overnight. Therefore, researchers have chosen to initially focus on fundamental properties such as the equations of state and then proceed to studying the most pertinent properties for applications and current research: defect properties of the metals and the surface properties of the oxide. Researchers hope to obtain fully converged results that can be compared with experiments, but should this be impossible (e.g., due to computational cost in testing all parameters), the project will address density functional theory accuracy by setting up model calculations.

Type: Renewal
Title: "Predictive Materials Modeling for Li-Air Battery Systems"

Principal Investigator: Larry Curtiss, Argonne National Laboratory
Co-Investigator: Ray Bair, Argonne National Laboratory
Alessandro Curioni, IBM
Teodoro Laino, IBM
Kah Lau, Argonne National Laboratory
Winfried Wilcke, IBM
Peter Zapol, Argonne National Laboratory

Scientific Discipline: Materials Science: Condensed Matter and Materials

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

Research Summary:
A rechargeable lithium-air (Li-air) battery can potentially store five to ten times the energy of a lithium-ion (Li-ion) battery of the same weight. Realizing this enormous potential presents a challenging scientific problem that requires the development of new electrode materials and electrolytes. Researchers continue to conduct *ab initio* density functional theory and classical molecular dynamics simulations to help address this problem by providing insight, not possible to glean from experiment, into electrochemical nucleation and growth processes.

A portion of this INCITE allocation will go toward the study of novel solid-state electrolytes with the goal of developing a material that potentially could replace liquid electrolytes. Solid-state electrolytes are extremely stable to chemical oxidation, have a Li-ion mobility comparable to liquid electrolytes, and produce almost zero electronic conductivity. The most promising solid-state conductor thus far is the zirconium-containing, garnet-like lithium-lanthanum-oxide.

Current project milestones are connected to the modeling of the crystallization process. Understanding the formation origins, or nucleation, of these structures is crucial to the development of Li-air batteries. Researchers will address the debated problem of lithium peroxide nucleation by combining large-scale molecular dynamics simulations with an optimized classical force field to understand the driving force behind its formation.

The Li-air project is also considering metal nanoparticles, such as silver, as catalysts for electrodes. Studies have shown that the small clusters easily activate, or break up, oxygen to boost chemical reactions. Metal nanoparticles have been shown to significantly affect the morphology of the discharge product and reduce the charge over-potential of Li-air batteries.

Type: Renewal
Title: "QMC Simulations DataBase for Predictive Theory and Modeling"

Principal Investigator: David Ceperley, University of Illinois at Urbana–Champaign
Co-Investigators: Jeffrey Greeley, Purdue University
Burkhard Militzer, University of California, Berkeley
Miguel Morales, Lawrence Livermore National Laboratory
Fernando Reboredo, Oak Ridge National Laboratory
Luke Shulenburger, Sandia National Laboratories

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation: **185,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (100,000,000 processor hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (85,000,000 processor hours)

Research Summary:
For many classes of materials and molecular systems, existing theoretical methods based on quantum mechanics offer a predictive capability: properties and performance can be calculated, to a meaningful accuracy, without empirical tuning parameters. For other classes of materials, as well as combinations of solid and molecular systems, a predictive capability is still lacking.

Recent theoretical and algorithmic developments of the continuum quantum Monte Carlo (QMC) method—accomplished from previous INCITE projects—offer a path toward high accuracy calculations for a broad range of electronic systems from molecules to solids. These developments also are opening up realistic opportunities to compute materials properties of high quality, in substantial quantity.

The project will involve QMC studies in heterogeneous catalysis of transition metal nanoparticles, phase transitions, properties of materials under pressure, and strongly correlated materials. These research directions share a common need for predictive simulations where the relevant energy scales are small enough to be beyond the reach of other methods and where correlations, van der Walls interactions, or localization of d or f states play critical roles. These systems have significant scientific and community impact by providing accurate predictions for energy-related materials and predictions of fundamental material properties that other methods are unable to reliably provide.

The project will both provide direct answers to fundamental materials science questions and establish benchmark levels of accuracy that will, in turn, provide targets for future developments in related electronic structure approaches.

Type: Renewal
Title: "Quantum Monte Carlo Simulations of Hydrogen and Water Ice"

Principal Investigator: Richard Needs, University of Cambridge
Co-Investigators: Neil Drummond, Lancaster University
Pablo Lopez Rios, University of Cambridge

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation: **80,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (80,000,000 processor hours)

Research Summary:
Water ice is the most widely known example of a hydrogen-bonded molecular solid. Achieving accurate descriptions of hydrogen-bonded molecular solids at the atomic level is an important research goal. Life on Earth depends on water and hydrogen bonds, DNA and proteins are held together primarily by hydrogen bonds, and hydrogen bonding is crucial in drug design. Determining the solid structures that drug molecules may adopt is important in the pharmaceutical industry because different polymorphs can show important differences in physical properties such as solubility. Water is an important, complicated, and interesting material with many anomalies, including several related to nuclear vibrations. For example, water ice expands if the hydrogen is replaced by deuterium, although intuition suggests that it should contract because the vibrational motion of deuterium is smaller. Advances in describing water ice will be influential over a broad range of activities.

Powerful but computationally demanding quantum Monte Carlo (QMC) methods will be used to determine the structural properties and phase behavior of two iconic materials: hydrogen and water ice. We will treat the quantum motion of nuclei as well as electrons in our calculations to achieve unprecedented accuracy.

The goals of our project are to obtain the most accurate description of water ice at the atomic level achieved so far and to perform simulations of hydrogen at high pressures that will provide reliable predictions of the thermodynamically stable phases and their properties. We will use the variational and diffusion QMC methods, which are wave-function-based approaches for solving many-particle quantum problems. QMC is the most accurate method known for computing the energies of large assemblies of interacting quantum particles. A crucial aspect of our project is that we will treat the nuclei as quantum particles.

The proposed research is expected to lead to new understanding of hydrogen at high pressures as well as to further improvements in QMC methods for tackling systems of quantum particles with widely differing masses.

Type: New
Title: "Quark Flavors and Conserved Charges at Finite Density in the QCD Phase Diagram"

Principal Investigator: Rene Bellwied, University of Houston
Co-Investigators: Sandor Katz, Eotvos University Budapest
Claudia Ratti, University of Houston

Scientific Discipline: Physics: Nuclear Physics

INCITE Allocation: **150,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (150,000,000 processor hours)

Research Summary:
Ordinary hadronic matter is expected to undergo a phase transition to the Quark-Gluon Plasma (QGP) or deconfined phase of matter in extreme conditions of temperature or density. This transition, predicted by the fundamental theory of strong interactions (quantum chromodynamics, or QCD), is now being realized in heavy ion collisions at the Relativistic Hadron Collider (RHIC) at Brookhaven National Laboratory and at the Large Hadron Collider (LHC) at CERN near Geneva, Switzerland.

This project is pursuing a microscopic understanding of the QGP properties near the QCD transition, that is, an understanding of the properties of primordial deconfined matter near the transition to ordinary nuclear matter. The researchers, as part of another ongoing INCITE project, have already made fundamental contributions to the field by extracting from first principles the temperature at which hadrons (protons, pions, kaons, etc.) are formed. They have also simulated several observables, which can be compared directly to the experimental measurement to determine details of particle formation during the transition. In fact, these comparisons can be made today for the first time because of the precision reached in their continuum-extrapolated calculations. This new project extends the previous analysis to larger chemical potentials (i.e., larger densities).

The researchers seek to obtain a precise, continuum-limit determination of high-order fluctuations of light, strange, and charm quark flavors, or equivalently of electric charge, baryon number, and strangeness. Doing so will help them determine the microscopic description necessary to understanding the underlying physics principles of the QCD transition.

Type: Renewal
Title: "Reactive MD Simulations of Electrochemical Oxide Interfaces at Mesoscale"

Principal Investigator: Subramanian Sankaranarayanan, Argonne National Laboratory
Co-Investigators: Sanket Deshmukh, Argonne National Laboratory
Ganesh Kamath, Argonne National Laboratory
Badri Narayanan, Argonne National Laboratory
Shriram Ramanathan, Harvard University
Ram Subbaraman, Argonne National Laboratory
Masako Yamada, GE Global Research

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

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

Research Summary:
Electrochemical oxide interfaces are at the center of a broad spectrum of physico-chemical systems relevant to energy security and environmental protection, ranging from electrochemical energy conversion/storage systems to corrosion surfaces. The goal of this project is to understand the growth mechanisms and transport phenomena occurring at and across these electrochemical interfaces at the atomistic and molecular levels.

The dynamic processes in such oxide interfaces combine the remarkable complexity of numerous interfacial reactions, transport phenomena, and interface structural evolution with the formidable subtleties of material defect chemistry. Breakthroughs in the fundamental understanding of mesoscale, or intermediate, electrochemical oxide interfaces will spur the design and development of novel functional oxide materials for emerging energy applications and biomedical technologies.

Simulations from the project's first year provided new perspective on the long-standing problem of corrosion initiation. This year, the researchers seek to perform atomistic simulations of the electric field effects on nanoscale oxide synthesis; develop simulation models to discover athermal synthesis routes; decouple thermal and electric field effects during nanoscale oxide sintering; perform atomistic simulations of nanoscale corrosion at electrochemical oxide interfaces; and probe sulphur's effects on nanoscale corrosion and oxide breakdown. They will use the highly scalable molecular dynamics (MD) simulation codes, LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) and nanoscale MD (NAMD) software.

Type: Renewal
Title: "Scalable First Principles Calculations for Materials at Finite Temperature"

Principal Investigator: Markus Eisenbach, Oak Ridge National Laboratory
Co-Investigators: G. Malcolm Stocks, Oak Ridge National Laboratory

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation: **150,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (150,000,000 processor hours)

Research Summary:
Magnetic materials represent an important class of materials for technological applications and are also of basic science interest. Petaflop computers enable the calculation of finite temperature properties from first principles in materials important for energy applications such as magnets and steel.

The goal of this project is to address the need for accurate calculation for magnetic systems at finite temperature by applying first principles methods in conjunction with statistical physics methods. The code to be employed—first principles Wang-Landau (WL)—shares as common features a high level stochastic part and a compute intensive deterministic kernel that will ultimately allow the exposure of multiple levels of parallelism and fault tolerant scaling toward the exascale.

First principles density functional theory (DFT) calculations have proven to be useful tools for ground state studies of many materials, but there also are many applications where results at finite temperature are required. The work proposed here will address the shortcomings of conventional applications of DFT by using new computational capabilities to investigate first principles based thermodynamics of materials that are of significant importance for various aspects of DOE's mission. The enabling of first principles based finite temperature treatment will contribute to the grand challenges in nanomaterials design by providing insight beyond the ground state properties usually accessible with DFT.

Finite temperature effects will be modeled by sampling the energy landscape with the WL statistical approach. The value of the energy at the sampled points will be determined by the locally self-consistent multiple scattering (LSMS) method. The efficiency of WL sampling, the speed of LSMS, and the computing power of will Titan combine to allow a truly first principles thermodynamic description of magnetism. The combined WL sampling and LSMS will lead to a realistic treatment of magnetic materials that will ultimately include dynamic and temperature effects associated with spin and atomic position.

Type: Renewal
Title: "Scalable System Software for Parallel Programming"

Principal Investigator: Robert Latham, Argonne National Laboratory
Co-Investigators: Pavan Balaji, Argonne National Laboratory
Tom Peterka, Argonne National Laboratory
Rajeev Thakur, Argonne National Laboratory

Scientific Discipline: Computer Science

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

Research Summary:

The Scalable Systems Software for Parallel Programs (SSSPP) project aims to improve the software environment for leadership-class applications through programming models, high-performance I/O, and analysis. In all three areas, researchers are exploring ways to make the existing software environment more productive for computational scientists.

For example, researchers deployed the Darshan lightweight trace tool on IBM Blue Gene/Q computers Vesta and Mira, to collect I/O statistics for significant fractions of the machines. The resultant logs will help generate and validate models of typical leadership-class I/O workloads.

While current work has focused on applications for petascale systems, initial evaluations have begun on future exascale designs through the performance of million-node simulations of network topologies. The massively parallel ROSS event simulator scales to significant fractions of Mira, and allows for the evaluation of future designs by using current hardware. Exascale designs will require fault tolerance, resilience, and power-aware approaches in system software. This research will explore that design space with projects like fault tolerant message passing interface MPI (MPIXFT), multi-level checkpointing (FTI), and power-aware monitoring (MonEQ).

Working with IBM, SSSPP collaborators identified areas for improvement in the MPI library that was installed on Blue Gene/Q computers. The development of a "community edition" of the MPI library, while not officially supported by IBM, will provide MPI-3 features, improved I/O performance, and better scalability for several important MPI routines.

Analysis and visualization efforts helped to develop a new parallel algorithm for computing Delaunay and Voronoi tessellations, which convert discrete point data into a continuous field. Demonstrating both correctness and scalability, the approach suggests that answers can be more readily accessed, and computing resources can produce more science.

Type: New
Title: "Shutdown and Recovery of the Barrier Function of Human Skin"

Principal Investigator: Michael Klein, Temple University
Co-Investigators: Russell DeVane, Procter & Gamble, Inc.
Giacomo Fiorin, Temple University

Scientific Discipline: Biology: Biophysics

INCITE Allocation: **92,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (92,000,000 processor hours)

Research Summary:

This project is designed to discover how surfactants, such as detergents or emulsifiers, control the permeation of chemical compounds into human skin. Do surfactants only change the stability of the molecules of the outer layer, or do they also form larger objects capable of carrying other chemicals?

Harmful chemicals in solid or liquid form, as well as pathogens such as viruses or bacteria, are usually stopped at the stratum corneum from entering the human body. However, some molecules can cross this barrier fairly unhindered and be found within the bloodstream hours after their first contact with human skin. The small molecules best known to possess this ability can be as diverse as steroid hormones, nicotine, certain analgesics, and even chemical warfare agents (Sarin, VX). To safely develop more advanced materials, it is also necessary to reveal the hidden pathways used by these molecules, either individually or with assistance from surfactants.

We intend to study the permeation into skin of vesicles and micelles made by lipids and surfactant molecules, along and across the layers of the stratum corneum's lipid matrix.

Our strategy is twofold: (1) we will quantify, both in solution and within the stratum corneum, the relative equilibria among phospholipids, added surfactants such as polysorbate, and cofactors such as testosterone; and (2) we will compare the rates of permeation of individual lipids and surfactants under the two alternative hypotheses that a molecule can either travel while embedded in a vesicle or micelle, or individually by migrating into the stratum corneum lipid matrix.

This study is likely to transform several years of fundamental research into novel predictive tools, allowing one to manipulate the skin's barrier function in ways that preserve and even promote the health of individuals that come in contact with new materials or formulations.

Type: New
Title: "Simulation of Correlated Electrons for Superconducting Materials"

Principal Investigator: Lucas Wagner, University of Illinois at Urbana–Champaign

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation: **106,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (106,000,000 processor hours)

Research Summary:

The study of emergent physics, that is, how unique properties emerge from fundamental physics, is a major frontier in condensed matter physics. In particular, electronic systems are a fundamental part of modern technology and offer great promise for enabling the development of new materials. The understanding of quantum mechanics has advanced to the point that many new electronic systems can be designed for targeted objectives.

However, this understanding is primarily based on a critical assumption—that the interactions between electrons are small. When this assumption is not valid, a challenge and an opportunity arise. The challenge is that the equations used to calculate the electronic structure become very hard to solve. The opportunity is that new and exciting effects, like high-temperature superconductivity, can occur.

For this INCITE project, researchers from the University of Illinois at Urbana–Champaign will use the computing power of Mira to solve the Schrödinger equation with unprecedented accuracy for high-temperature superconductors. Their objective is to completely characterize, for the first time, the electronic structure of unconventional superconductors. The simulations will serve a dual purpose. First, the researchers aim to uncover new microscopic physics in materials that exhibit high-temperature superconductivity. Second, they will use the high-fidelity simulations to predict materials with unique properties. Their findings will help to improve the fundamental understanding of electronic matter, which will aid scientists in the development of novel materials with new and exotic properties, including unconventional superconducting materials.

Type: New
Title: "Simulation of Fundamental Energy Conversion Processes in the Cell"

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

Scientific Discipline: Biology: Biophysics

INCITE Allocation: **150,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (150,000,000 processor hours)

Research Summary:
Using petascale resources, this project will investigate two related bioenergetic processes relevant to green energy technologies: harvesting of solar energy in a photosynthetic organelle and energy conversion in adenosine triphosphate (ATP) synthase. The proposed research will also aid in the development of new anti-cancer therapies.

The process will be twofold. The first objective proposes to perform atomic-level molecular dynamics (MD) simulations of an entire photosynthetic organelle, called a chromatophore, 100 million atoms in size. The chromatophore simulations will provide insight into how requirements for structural stability, assembly, supramolecular organization, and efficient light-harvesting are balanced by photosynthetic systems and how competing functional constraints are met at the organelle scale. The second objective will use the string method with a swarm of conventional MD simulations to find the minimum free energy pathway connecting the various adenosine diphosphate/ATP bound ATP synthase conformations and will study how that pathway changes in well-studied ATP synthase mutants.

Energy harvesting and conversion are processes essential to all life forms. The energy needs of most life on Earth are sustained by sunlight harvested by photosynthetic organisms with an efficiency and resilience that surpass manmade solar energy solutions. The molecular architecture of the energy harvesting systems is now known in atomic detail all the way to the supramolecular organization at the organelle level, enabling the study of how complex energy conversion processes are integrated across hundreds of cooperating proteins, such as in a bacterial light harvesting organelle (the so-called chromatophore). Biomolecular simulations of an entire photosynthetic apparatus, such as the chromatophore, require petascale computing resources to reveal, on the one hand, how the function of hundreds of proteins is integrated across an entire organelle, and, on the other hand, how efficient energy harvesting is achieved in nature.

Type: Renewal
Title: "SiO2 Fracture: Chemomechanics with a Machine Learning Hybrid QM/MM Scheme"

Principal Investigator: James Kermode, King's College London
Co-Investigators: Alessandro De Vita, King's College London
Anatole von Lilienfeld, University of Basel

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation: **125,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (125,000,000 processor hours)

Research Summary:

According to the World Business Council for Sustainable Development, about five percent of total human energy consumption is currently expended by crushing and grinding rocks. Doing this more efficiently would eliminate millions of tons of carbon dioxide emissions per year. However, the underlying "stress corrosion" fracture processes in rocks are poorly understood.

This INCITE project is pioneering simulation methodologies for predictive modelling in these kinds of systems with the goal of modelling failure processes in oxides, which is relevant not only for the mining industry, but for structural glasses, photovoltaic devices, and biomedical implants, as well. Insights garnered from these studies could help rationalize and guide future materials design and processing developments.

Until recently, the theoretical study of these processes has been difficult because of the high cost of experiments and the tight chemo-mechanical coupling of the chemistry and elastic fields, which creates an inextricably multiscale problem.

To solve this, the research team is applying a hybrid multiscale simulation program that combines various levels of theories to help describe the fracturing of silicon dioxide in a wet environment. In this quantum mechanical/molecular mechanical (QM/MM) scheme, higher level theories account for the breaking of chemical bonds; the less expensive levels enable the inclusion of thermal fluctuations that link the microscopic behavior of these breaking bonds to the macroscopic stress that drives crack propagation.

As the INCITE project develops, the QM/MM approach will be coupled with a machine learning method, Learn on the Fly, that allows for quantum mechanical accuracy on a large model system.

Type: New
Title: "State-of-the Art Simulations of Liquid Phenomena"

Principal Investigator: Mark Gordon, Iowa State University
Co-Investigators: Spencer Pruitt, Argonne National Laboratory
Gregory Voth, University of Chicago
Theresa Windus, Iowa State University

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation: **200,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (200,000,000 processor hours)

Research Summary:
This project will study liquid behaviors: both of the liquids themselves and of the behaviors of solutes in the liquids. Such studies are of paramount importance given that most chemical and biological processes occur in the liquid phase. Thus, high-quality quantum mechanics methods will be used to study water and ionic liquids and the important processes that occur in these liquids.

This project will examine the solvated proton, halides, NO_3^-, HSO_4^-, ClO_4^-, and SO_4^{-2} because of their importance in many different aqueous chemical reactions. Researchers will perform high-level correlated *ab initio* calculations to address the key issues of water structure and bonding, and the nature of solvation of electrolytes that contain the aforementioned ions. Combined with molecular dynamics simulations, including periodic boundary conditions, these calculations will provide—for the first time—a systematic and highly accurate description and interpretation of these processes.

Ionic liquids are of particular interest for their potential abilities to improve the mass and/or charge transport in dye-sensitized solar cells and to be used as extractants, or with extractants, to separate complexes of the lanthanide elements. This is an important first step in the recovery of heavy elements that have been identified as "critical materials"—essential components in cellphones, computers, tablets, and household electronic devices. High-level electronic structure theory methods will be used—again for the first time—to study the properties of the relevant ionic liquids.

Type: Renewal
Title: "Studies of Large Conformational Changes in Biomolecular Machines"

Principal Investigator: Benoît Roux, University of Chicago

Scientific Discipline: Biological Sciences: Biophysics

INCITE Allocation: **120,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (120,000,000 processor hours)

Research Summary:

In biology, proteins, nucleic acids, and carbohydrates can be considered complex "molecular machines" that consume energy in order to perform specific biological functions. Their concerted actions trigger many of the critical activities that occur in living cells. In particular, membrane-associated proteins play essential roles in controlling the bidirectional flow of material and information. These vital proteins change shape and go through many conformational states to perform their functions. However, malfunctioning proteins can result in various diseases such as cancer, epilepsy, or cardiac arrhythmia.

To understand how membrane proteins operate and how they are affected by disease, researchers need detailed knowledge about all of the relevant conformational states, as well as the free energy changes that connect them. This INCITE project aims to gain a deep mechanistic perspective on membrane protein function, linking structure to dynamics by characterizing the free energy landscape that governs functional motions.

Within the unified computational perspective provided by free energy landscapes, two membrane proteins of increasing complexity and size were considered. In its third year, the project is focusing on the four remaining critical conformational transition pathways needed to describe the transport cycle of a P-type calcium pump called SERCA (pathways for two transitions have been described in the prior two years). To determine these conformational transition pathways, researchers leverage the NAMD/Charm++ with MPI-level, multiple-copy algorithms with the String Method — a computational methodology that achieves extreme scalability on leadership-class supercomputers and is at the forefront in the field of biomolecular simulations. The researchers, by studying experimentally well-characterized systems of increasing size and complexity within a unified theoretical framework based on free energy landscapes, are advancing theory-modeling-simulation (TMS) technology, which offers a virtual route for addressing fundamental biological questions such as rational protein design. Computations performed for this study are serving as a roadmap for simulating, visualizing, and elucidating how biomolecular nano-machines work.

Type: New
Title: "Targeting Cancer with High Power Lasers"

Principal Investigator: Michael Bussmann, Helmholtz-Zentrum Dresden-Rossendorf

Scientific Discipline: Physics: Accelerator Physics

INCITE Allocation: **57,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (57,000,000 processor hours)

Research Summary:
Compared with photon or electron beam radiotherapy, radiotherapy of cancer with ion beams has proven to be less harmful to healthy tissue surrounding deep-seated tumors because the dose can be applied with high spatial precision.

Unfortunately, conventional ion beam accelerators and beam lines have a large spatial and financial footprint. Laser-driven ion acceleration has the potential to deliver ion beams requiring much less space for the overall radiation facility. In turn, radiotherapy of cancer with ion beams could be made available to more patients.

Until now, laser-driven ion energy fell short both in beam quality and energy in delivering ion beams suitable for irradiation of deep-seated tumors. With new high power and high contrast lasers, this could change.

However, development on new targets is necessary to optimize the acceleration process. Recently, it has become possible to levitate ultra-small, mass-limited targets in vacuum, reaching an experimental situation that can be realistically simulated using the most advanced three-dimensional particle-in-cell simulations available today.

We plan to simulate laser-driven ion acceleration using levitating mass-limited targets. Laser-driven ion acceleration has the potential to provide sources for radiotherapy of cancer, replacing large-scale facilities with more compact structures that reduce the cost of ion radiotherapy.

We propose to simulate levitating mass-limited targets and compare the results with experimental results using the particle-in-cell code PIConGPU, which holds the record for peak performance for particle-in-cell codes of 7.1 PFLOP/s (double precision) and 1.4 PFLOP/s (single precision) on Titan to advance our understanding of laser-driven ion acceleration towards its application in radiotherapy.

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

Principal Investigator: David Baker, University of Washington

Scientific Discipline: Chemistry: Biochemistry

INCITE Allocation: **80,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (80,000,000 processor hours)

Research Summary:

Proteins are the major functional macromolecules in living cells. With the emergence of protein structure modeling capabilities, researchers have a tool that can be used to design biomolecules with targeted applications, such as treating diseases and catalyzing medically and industrially useful reactions. While progress is continually being made to protein modeling applications, the ability to sufficiently sample conformational space remains a limiting factor for such tools.

Led by principal investigator David Baker, this INCITE project aims to develop and apply new computational methods to address this issue and other emerging challenges in protein structure calculation and design. The researchers will use Mira to enhance the capabilities of Rosetta, a simulation software suite developed by the Baker group for modeling and designing biomolecular structures. This includes making improvements to the Rosetta energy function and further developing homology model refinement methods.

The researchers also aim to apply an established multistate design protocol to design therapeutic peptides that bind to targets of interest, including influenza and other pathogens. Additionally, the team will use this INCITE award to develop a massively parallel enzyme design protocol for the *de novo* design of novel enzymes and catalytic sites. The broader impacts of this research will address challenges in medicine, energy, and technology, including the development of protein therapeutics for a number of diseases and the design of protein reagents to capture and destroy various bioterror agents.