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:
The project will use ab initio methods and large-scale computation to study how the electron moves in organic systems and nanosystems. It will reveal the underlying mechanisms of electron transports in different types of organic and nano systems, specifically (1) the electronic structure and carrier transport in organic systems; (2) the effect of surface passivation on the electronic structure and carrier transport of inorganic nanocrystals with organic molecule attachments; and (3) the defect and dislocation structures and their dynamics in aluminum alloys.

The project will reveal the fundamental mechanisms in carrier transport and surface effects, and it will open up new areas of research and elevate the large-scale material simulations in these fields to unprecedented levels. The higher-level simulations will provide the ability to study new physics, e.g., the interplay between polaron effects and dynamic disorder in organic systems, the exact nature of surface state, the carrier transport between nanocrystals, and the interaction and crossing of dislocation lines.

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

Principal Investigator: Kenneth Jansen, University of Colorado
Co-Investigators: Michael, Amitay, Rensselaer Polytechnic Institute
Michel Rasquin, University of Colorado
Onkar Sahni, Rensselaer Polytechnic Institute
Mark Shephard, Rensselaer Polytechnic Institute

Scientific Discipline: Engineering: Aerodynamics

INCITE Allocation: **66,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (66,000,000 processor hours)

Research Summary:

This project is focused on performing simulations of active flow control on a realistic, high-lift wing configuration that includes a leading-edge slat, a main wing, and a trailing-edge flap. Specifically, researchers propose to model an array of synthetic jets that have been vectored to enhance the streamwise momentum near the flap suction peak, limiting flap effectiveness for high angles of attack.

The selection of a high-lift wing assembly is based on a number of factors, including the dramatic energy savings a flow-control-based redesign of aeronautical control surfaces would provide. With active flow control, the required force can be created using a smaller and lighter control surface--which can include flaps, elevators, or even rudders--on a vertical tail.

The numerical simulations proposed will provide a complementary and detailed view of the flow interactions and, in turn, give the insight required to understand and exploit the underlying physical mechanisms related to active flow control. The proposed modeling approach was validated previously against coordinated, simultaneous experiments on a full 3D-wing geometry, which is a natural stepping stone for the high-lift wing. The numerical predictions were found to be in excellent agreement with the experimental measurements.

The computational approach used for these simulations is the finite-element-based flow solver, PHASTA, employed with anisotropic adaptive meshing and partitioning procedures. PHASTA will demonstrate that robust, open-source software, applicable to a very broad range of flow physics, can sustain high-petaflop performance. While it has been applied to active flow control on more fundamental aerodynamic configurations, this effort marks the most fundamental aerodynamic study yet attempted.

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
Jan Prins, University of North Carolina

Scientific Discipline: Earth Science: Geological Sciences

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

Research Summary:

The project aims to advance a recently developed thermodynamically constrained averaging theory (TCAT) model of multiphase flow and transport phenomena in porous medium systems. The specific objectives are to (1) determine a lower bound on the size at which a macroscale model can be applied for a specified allowable error; (2) perform a dense set of microscale simulations needed to elucidate the relationship among fluid pressures and saturations and interfacial areas and curvatures between phases; (3) determine the relationship among volume fractions, interfacial areas, and fluid viscosities that determine the resistance tensors for fluid flow; (4) investigate factors affecting the mobility of entrapped nonwetting phase fluids; (5) extend the analysis of TCAT models to compositional two-fluid-phase flow systems; and (6) extend the analysis to TCAT models for three-fluid-phase flow.

Collectively, understanding and describing multiphase porous medium systems are of significant importance to society. Mathematical modeling plays a central role in such understanding. Traditional models suffer from a lack of connection to the microscale, where the physics are better understood than at the macroscale, where the models are formulated and solved. It is essential to understand issues of scale in order to place the modeling challenges in proper perspective. While a significant amount of theoretical work has been advanced through the development of TCAT models, several open questions remain to be answered before these models can be reduced to application. The model development work will advance the description of multiphase flow processes in porous media, including land–water interactions, carbon sequestration, and fuel-cell development.

U.S. DEPARTMENT OF ENERGY
INCITE
LEADERSHIP COMPUTING

Type: New
Title: "Assembling and Sustaining the 'Acid Mantle' of the Human Skin Barrier"

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

Scientific Discipline: Biological Sciences: Biophysics

INCITE Allocation: **75,000,000 processor hours Site:**
Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (75,000,000 processor hours)

Research Summary:

The project builds on a long-time partnership between Temple University and Procter & Gamble to study the cohesive forces between the microscopic layers of human skin and thus build models to evaluate the impact of chemicals on one of the body's largest organs. The project's ultimate goal is to answer one fundamental question: What are the conditions under which certain chemical substances cross the stratum corneum into our body? The project's long-term target is the capability to predict either the permeability of a chemical substance or its harmful effects on skin cohesion using the same computational model. This capability will be of paramount importance to academic-based health research as well as to industry. Procter & Gamble, among others, aims to predict the safety of products accurately enough to meet the standards set by regulatory agencies.

The project will have ramifications in biophysics, materials science, and chemical safety. Researchers will quantitatively explain the cohesive forces that seal together the components of human skin and, in particular, of its relatively dry, acidic outer layer, the stratum corneum, which acts as the first line of defense of the human body against harmful agents such as toxic chemicals, viruses, and bacteria. Extensive effort has been devoted to resolve skin's intricate multilamellar structure at varying levels of resolution, with the ultimate goal of predicting how certain chemical substances can traverse it while others cannot. This information is vital to pharmaceutical research in applications dealing with drug delivery and to industry in general for evaluating the safety of personal care products.

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

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

Scientific Discipline: Earth Science: Climate Research

INCITE Allocation: **102,800,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (102,800,000 processor hours)

Research Summary: Researchers at the University Corporation for Atmospheric Research (UCAR) will carry out a specific set of climate change simulations using the Community Earth System Model (CESM) at the highest possible atmospheric resolutions. The proposed simulations represent a subset of those needed for control, historical, and future experiments.

This INCITE research will build upon UCAR's previous and collaborative work on how weather and climate extremes could change in a future warmer climate by analyzing century-scale climate simulations. Run with the latest release of CESM, they will accomplish these simulations using an atmosphere/land horizontal resolution of approximately 0.25°and an ocean/ice resolution of approximately 1.0°.

The proposed experiments are at the highest resolution currently feasible for century-scale climate simulations and represent a sweet spot in the simulation of extreme events. Leadership-class computers such as ALCF's Mira, an IBM Blue Gene/Q, provide the opportunity to jump over evolutionary improvements in climate modeling directly to groundbreaking levels of science. For example, current production simulations have the atmosphere and land at an approximate 1° resolution. Tests show, however, that 0.25° simulations are able to more realistically resolve important new dynamical features.

The simulations will supplement and complement control and historical simulations being performed at other facilities by the National Center for Atmospheric Research's CESM group. The overall plan begins with a 100-200-year control run with all forcing constituents, such as greenhouse gases, held constant at 1850 values; and a historical climate simulation, 1850 to 2005, with time-evolving forcing constituents, both natural and anthropogenic.

These simulations are useful in constraining future climate projections and in identifying future climate states, ranging from regional extreme events to global average temperature.

Type: New
Title: "Chombo-Crunch: Modeling Pore-Scale Reactive Transport in Carbon Sequestration"

Principal Investigator: David Trebotich, Lawrence Berkeley National Laboratory
Co-Investigator: Anshu Dubey, Lawrence Berkeley National Laboratory
Carl Steefel, Lawrence Berkeley National Laboratory
Brian Van Straalen, Lawrence Berkeley National Laboratory

Scientific Discipline: Earth Science: Geological Sciences

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

Research Summary:
Carbon sequestration, the process of capturing carbon dioxide (CO2) before it enters the atmosphere and transferring it into the earth, is a promising technique to help control greenhouse gas emissions. Researchers from the Nanoscale Control of Geologic CO2 (NCGC), a DOE Energy Frontier Research Center led by Lawrence Berkeley National Laboratory, will use supercomputers to advance the viability of carbon sequestration by gaining a better understanding of the flow and transport processes in porous rock materials. Specifically, NCGC's objectives are to build a next-generation understanding of molecular-to-pore-scale processes in rock systems, and to demonstrate the ability to control critical aspects of flow and transport in porous rock.

To help meet these goals, the researchers have developed a new tool, called Chombo-Crunch, to perform simulations of flow and transport in complex micro-scale geometries obtained from image data. Chombo-Crunch combines the team's multiscale, multiphysics simulation tools developed in the Chombo framework with the complex geochemistry module of CrunchFlow. This new combined approach delivers high-performance computational fluid dynamics with reactive transport modeling capabilities, enabling simulations at realistic time scales and at better-than-image data-grid resolution.

Researchers will run Chombo-Crunch to simulate reactive transport processes in realistic pore space obtained from image data of experiments. Simulation data will be used to inform X-ray synchrotron and neutron scattering experiments *a priori*, to help interpret the experimental results, and to generalize the results to the larger (porous-continuum) scales. Ultimately, this research effort aims to facilitate the safe storage of CO2 in subsurface reservoirs, which can help to reduce the threat of global warming by decreasing the amount of greenhouse gas emissions released in the atmosphere.

Type: Renewal
Title: "Collaborative Research into Exascale Systemware, Tools, and Applications (CRESTA)"

Principal Investigator: Lorna Smith, University of Edinburgh

Scientific Discipline: Computer Science

INCITE Allocation: **42,000,000 processor hours Site:** Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (42,000,000 processor hours)

Research Summary:
The CRESTA project involves research into the next generation of supercomputers, expected to carry out 1 quintillion (a million million million) calculations per second. It will enable scientific breakthroughs in areas as diverse as drug design, weather forecasting, and engineering. The project has two integrated strands. The first focuses on enabling a set of key applications for exascale—the codesign applications. The second focuses on exploring and building appropriate systemware for exascale platforms.

The CRESTA project will demonstrate techniques required to scale the current generation of petascale simulation codes toward the performance levels required for running on future exascale systems. The project will affect applications involving biomolecular systems, soft matter simulations, global numerical weather prediction, and engineering. GROMACS is a widely used molecular dynamics code that will use CRESTA developments to investigate viral infection mechanisms. The soft matter code Ludwig will be used to investigate the interaction of colloids with liquid crystals. IFS, a world-leading numerical weather prediction code, will be used to investigate the use of Fortran2008 coarrays as part of a hybrid programming model in a large-scale code. Similarly, Nek5000, an important code for computational fluid dynamics, will be used to investigate different models of hybrid CPU/GPU programming.

Type: Renewal
Title: "Combustion Stability in Complex Engineering Flows"

Principal Investigator: Lee Shunn, Cascade Technologies
CO-Investigator: Shoreh Hajiloo, GE Power & Water

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:
Combustion instabilities arise from complex interactions between chemical kinetics, turbulence, and acoustics. Analytical and empirical methods can be used to explain the growth and propagation of combustion instabilities, but the predictive capability of these theories remains extremely limited. The goal of this project is to develop efficient and scalable numerical methods to predict unsteady combustion in gas turbine engines and scramjets.

The researchers will use large eddy simulations (LES) with advanced multi-physics models to numerically reproduce combustion instabilities that are observed in industrial combustors. Two relevant configurations have been selected to highlight recurrent types of instabilities, namely a modern Dry Low-NOX (DLN) combustor used in land-based gas turbines, and a high-speed combustor inspired by the Hypersonic International Flight Research Experimentation program. The LES results will contribute to a more thorough understanding of combustion physics in these systems, help identify mechanisms that amplify unstable combustion modes, and test strategies to prevent or suppress self-excited dynamics.

The simulations will be performed on Mira, the ALCF's IBM Blue Gene/Q, using CharLES, the unstructured LES solver developed and licensed by Cascade Technologies. CharLES's unique low-dissipation numerics, dynamic turbulence models, and massive scalability enable these problems to be studied under realistic operating conditions in complex engineering geometries.

In addition to predicting engine-level stability, the simulations will be used to characterize operability limits, emission signatures, and reliability/durability requirements in the target applications. The results will be compiled in a high-quality numerical database that can be used to assess combustor performance and evaluate lower-fidelity prediction tools.

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

Principal Investigator: David Dixon, The University of Alabama & Argonne National Laboratory

Co-Investigators: Jochen Autschbach, University at Buffalo, State University of New York
Enrique Batista, Los Alamos National Laboratory
Aurora Clark, Washington State University
Wibe de Jong, Lawrence Berkeley National Laboratory
Laura Gagliardi, The University of Minnesota
Jeff Hammond, Argonne National Laboratory
Richard Martin, Los Alamos National Laboratory
Kirk Peterson, Washington State University
Gustavo Scuseria, Rice University

Scientific Discipline: Chemistry: Physical

INCITE Allocation: **250,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (150,000,000 processor hours)
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (100,000,000 processor hours)

Research Summary: The project will obtain some of the first highly accurate, extrapolated, complete basis set results for actinide compounds that can be used as benchmarks to test other methods, as well as to explain recent experimental results on the spectroscopy of small molecules. Calculations will be done at the coupled cluster and higher correlated levels including multi-reference configuration interaction and continue the development of new basis sets for the actinides. The project will carefully benchmark more approximate methods such as density functional theory, which will then be used to study much larger systems, including explicit solvation effects. It will develop new computational capabilities on advanced high-performance computing architectures and use them to study actinide complexes in various oxidation states in solution, at interfaces, and at the nanoscale.

The project will use high-performance computing to address critical issues in advanced nuclear technologies, including the processing of fuels and the behavior of actinide complexes in the environment. Modeling and simulation will be critical to the cost-effective development of next-generation nuclear reactor technologies, as well as to DOE's cleanup efforts. A team has been assembled with broad experience in computational actinide chemistry and high-performance computers to address the complex problem of predicting the properties of actinide complexes.

Type: New
Title: "Computational Design of Novel Multiscale Concrete Rheometers"

Principal Investigator: William George, NIST
Co-Investigator: Edward Garboczi, NIST
Pascal Hebraud, Institute of Physics and Chemistry of Materials of Strasbourg
Nicos Martys, NIST
Marc Olano, NIST
Judith Terrill, NIST

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:

Understanding the mechanisms of dispersion or agglomeration of particulate matter in complex fluids, such as suspensions, is of technological importance in many industries. A basic goal of this project is to advance the understanding of the flow properties of fresh concrete, which is a dense suspension composed of cement, water, sand, and rocks.

The National Institute of Standards and Technology (NIST) used a recent INCITE allocation to aid in the design and development of a Standard Reference Material (SRM), which is a mortar (a cement paste matrix fluid plus sand inclusions), used to calibrate rheometers in the field. Project researchers will now extend their modeling capability to more novel rheometer designs to resolve basic problems in rheological measurements of mortars and concrete, such as sedimentation, which results in an undesired heterogeneous mixture.

Utilizing the results of earlier project phases as a foundation, this current phase will run massively parallel computations to help design the actual rheometer blades themselves. Optimizing blade shape and rotational speed helps avoid problems of sedimentation and other artifacts that can occur in currently available rheometers.

Presently, there is interest in screw-like or double-helix rheometer blade designs that allow for the mixing of suspensions such that a more representative, homogeneous mixture is maintained. This work will model flow in single- and double-helical rheometers.

Also, the current project phase will finally unite the major length scales of concrete rheology—cement paste, mortar, and concrete—for traditional and novel rheometer designs. NIST has the capability to manufacture these new designs, and to perform experimental validation on the predicted rheological measurements produced by these novel blade designs. Results will prove useful in the many industries that make use of dense, complex suspensions.

Type: New
Title: "Correlated Electrons in Photoactive and Superconducting Materials"

Principal Investigator: Lucas Wagner, University of Illinois at Champaign-Urbana
Co-Investigators: So Hirata, University of Illinois at Champaign-Urbana

Scientific Discipline: Materials Science: Condensed Matter and Materials

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

Research Summary:
How materials behave is dependent on the behavior of interacting electrons, and since the equations governing quantum particles are computationally complex, predicting the properties of materials is often not a trivial matter.

Revolutionary advances in computer processing over the past few decades have made it possible to simulate the behavior of many interacting quantum particles. An important enabler of these advances is the existence of good approximate density functional theories. However, there are a number of important technological materials that evade description using a density functional theory.

This research aims to help push the computer simulation of electrons in materials to the next level by explicitly simulating the interactions between electrons. The two methods proposed leverage high performance computing and are directly based on the many-electron Schrödinger equation that describes the behavior of electrons with as few approximations as possible. These methods are based computationally on Monte Carlo integration of many-dimensional integrals that arise when solving the quantum problem. As such, they have the potential to take advantage of the resources available through INCITE to provide unprecedented detail of the emergent behavior of interacting electrons.

New materials and better control of existing materials can open the way for higher efficiency devices, energy conversion, and fundamentally new devices crucial for meeting our ongoing energy challenges.

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

Principal Investigator: Salman Habib, Argonne National Laboratory

Scientific Discipline: Physics: High Energy Physics

INCITE Allocation: **200,000,000 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 XT (100,000,000 processor hours)

Research Summary:
The next generation of large-scale sky surveys aims to establish a new regime of cosmic discovery through fundamental measurements of the universe's geometry and the growth of structure. The aim of this project is to accurately characterize key quantities, such as the spatial statistics of the distribution of mass, and the sum of neutrino masses and how they impact cosmic evolution and structure formation. By looking at the signatures of dynamical dark energy models on the large-scale structure of the universe, the project will also address fundamental questions at the junction of cosmology and particle physics.

This INCITE project will use the Hardware/Hybrid Accelerated Cosmology Code (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. Additionally, this project will rely on the Cosmic Calibration Framework to build precision prediction tools, or emulators, for survey observables; and pipelines to generate synthetic galaxy catalogs.

Emulators, which will span multiple cosmological probes, are now widely recognized as an essential component of next-generation cosmological analyses, and the synthetic sky catalogs are an invaluable resource for modeling the observation chain, testing the inference pipeline, and investigating sources of possible systematic errors. The desired improvements for simulations over the next decade are measured in orders of magnitude; high accuracy and robustness are central requirements that must be satisfied by this program.

The proposed simulation campaign will support a large number of follow-on projects. Therefore, to fully exploit its scientific power, the simulations and data products will be shared with the community at large.

Type: New
Title: "Designing O_2 Tolerant Hydrogenases"

Principal Investigator: Vijay Pande, Stanford University
Co-Investigators:

Scientific Discipline: Biological Sciences: Biophysics

INCITE Allocation: **16,000,000 processor hours Site:**
Oak Ridge National Laboratory **Machine**
(Allocation): Cray XK7 (16,000,000 processor hours)

Research Summary:
The project will involve mapping the conformational landscape of hydrogenases, enabling the design of novel enzymes to produce molecular hydrogen, and an ultimate clean fuel and energy carrier. By performing molecular dynamics simulations on [FeFe], [NiFe], and [NiFeSe] hydrogenases, scientists expect (1) to overcome the limitations of structural analyses, (2) to identify the elements that give rise to the differential sensitivity to O_2 inhibition between these three hydrogenases, and (3) to pour these insights into engineering efforts toward a highly active, yet oxygen-tolerant [FeFe] hydrogenase.

Hydrogenases are known to catalyze both oxidation of H_2 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 and for developing biomimetic H_2-production catalysts and genetically engineered hydrogenases for photobiological H_2 production. A limiting aspect of hydrogenases is their susceptibility to inhibition by molecular O_2 and CO. The project will help researchers identify a set of residues that can be mutated to counter the influx of molecular O_2 and CO.

Type: New
Title: "DNS of Forced- and Auto-Ignition in Spherical and Engine-Like Geometries"

Principal Investigator: Christos Frouzakis, Swiss Federal Institute of Technology Zurich, Switzerland
Co-Investigators: Paul Fischer, Argonne National Laboratory
Ananias Tomboulides, University of Western Macedonia, Greece

Scientific Discipline: Chemistry: Combustion

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

Research Summary:
The combustion of coal and petroleum-based fuels supply most of the energy needed to meet the world's transportation and power generation demands. To address the anticipated petroleum shortage, along with increasing energy demands and greenhouse gas emissions, new clean energy technologies, including advanced combustion strategies, must be developed.

Novel combustion regimes, such as low-temperature combustion for automobiles and lean premixed combustion for turbine power plants, have the potential to improve energy efficiency and reduce emissions. The development of these new combustion systems depends heavily on the availability of predictive models that incorporate the relevant physics and chemistry and account for the aero-thermo-chemical interactions in the regimes of interest.

For this INCITE project, researchers are using a highly accurate and scalable spectral element solver for low Mach number combustion to perform large-scale direct numerical simulations of forced and compression ignition in spherical and engine-like geometries. This will allow researchers to study the initiation, early flame evolution, and the long-term propagation of premixed flames. The conditions of interest (size, pressure, initial turbulence levels, etc.) will be of relevance primarily to internal combustion engines but also to gas turbines and other combustion devices. The simulation results will shed light on the complex flow and thermochemistry interactions of propagating premixed flame fronts and provide high-quality data for many important characteristics, including the turbulent burning velocity, flame surface density, and flame brush thickness. The findings will also help to identify the shortcomings of existing engineering models and foster the development of new models.

Type: New
Title: "DNS 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
Hemanth Kolla, Sandia National Laboratories
Sgouria Lyra, 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 suite of DNS benchmarks is proposed that 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 competitiveness, 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: "Dynamic and Adaptive Parallel Programming for Exascale Research"

Principal Investigator: Robert Harrison, Brookhaven National Laboratory
Co-Investigator: George Fann, Oak Ridge National Laboratory
Jeffrey Hammond, Argonne National Laboratory
Saday Sadayappan, Ohio State University
Eduard Valeev, Virginia Tech

Scientific Discipline: Computer Science

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

Research Summary:
The path from petascale to exascale computing poses many research and development challenges. In the area of application programming, three critical concepts have been identified: algorithmic concurrency, reduction in data movement, and asynchrony. To address these issues, there is a need to move beyond bulk-synchronous programming models and to approach data and computation in a nonlocal fashion.

Researchers will use this INCITE project to advance the design, development, and deployment of a novel programming environment that addresses both the programming model and algorithmic challenges of exascale computing within multiple domains. A major, but not exclusive, focus of this activity is the asynchronous, task-based, parallel runtime that sits under the open-source MADNESS computational environment. 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 solution of integral and differential equations.

This work will support the very active community developing and employing high-performance and high-productivity parallel programming paradigms that provide a natural and fully compatible extension of MPI to massively threaded, extreme-scale parallel systems. Expected research outcomes including a refined understanding of massively threaded, scalar-vector, programming models with experience at full system scale in complete and diverse science applications; preparation of the parallel runtime and associated science applications for the interim exascale systems; new science application functionality; the informed evolution of standards such as MPI; and greatly enhanced single node (vector and multi/many-core) and massively parallel performance.

Type: New
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
Charles Bacon, Argonne National Laboratory
Marta Garcia, Argonne National Laboratory
Venkatram Vishwanath, 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:
Explosions caused by the high-speed combustion and deflagration-to-detonation transition (DDT) in reactive gases present a significant hazard to a variety of industrial and energy-related applications. For example, hydrogen fuel, which used in fuel cells, internal combustion engines, and other devices, is particularly sensitive to detonation. A better understanding of DDT would help improve safety for hydrogen gas handling, storage, and transport. Nuclear reactors are another technology that is susceptible to catastrophic detonation events. Their extensive networks of long residual heat-removal pipes lend themselves to flame acceleration and DDT.

To date, a complete first-principles understanding of DDT is lacking. Researchers will address this issue by using the DOE's leadership-class supercomputers to perform a systematic numerical study of high-speed deflagration, DDT, and resulting detonation waves. This will help scientists understand the mechanisms responsible for DDT in various gaseous mixtures, including hydrogen-oxygen mixtures, syngas, and ethylene (one of the most widely used hydrocarbons in chemical industries).

The proposed study requires first-principles, reactive flow Navier-Stokes direct numerical simulations (DNS), which explicitly resolve physical processes on spatial scales ranging from the size of the combustion device to the micron scales associated with viscosity, heat conduction, and mass diffusion. The DNS also consider relevant chemical reactions, interaction of the flame with turbulence, sound and shock waves, boundary layers, and the development and auto-ignition of hot spots.

These simulations, which were not practical without the power of petascale computing, will produce findings that inform risk-reduction strategies and improve safety for hydrogen fuel use, nuclear reactors, and many other industrial settings.

Type: Renewal
Title: "Global Seismic Tomography Based on Spectral-Element and Adjoint Methods"

Principal Investigator: Jeroen Tromp, Princeton University
Co-Investigators: Olaf Schenk, Universita della Svizzera italina, Switzerland

Scientific Discipline: Earth Science: Geological Sciences

INCITE Allocation: **100,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (100,000,000 processor hours)

Research Summary:
The project aims to map Earth's interior based on seismic imaging. By harnessing data from thousands of earthquakes recorded by hundreds of seismographs, researchers will use iterative data assimilation techniques to image Earth's mantle, thereby improving understanding of the underlying physical and chemical processes. The project's ultimate goal is to move toward "adjoint tomography" of the entire planet.

A steady increase in the number of global seismographic stations combined with improvements in data quality have substantially grown the amount of data available for the construction of global Earth models. Seismic imaging based on spectral-element and adjoint methods can assimilate this information into three-dimensional models of elastic and anelastic structure. These methods fully account for the physics of wave excitation, propagation, and interaction by numerically solving the inhomogeneous equations of motion for a heterogeneous anelastic solid. Adjoint tomography ultimately leads to better resolution of tomographic images at all scales, which is essential for understanding mantle dynamics and related surface processes, such as the origin of hotspots and the forces behind plate motions and earthquakes. Higher-resolution wave-speed models are also important for accurately locating earthquakes and are required from an engineering point of view to assess seismic hazards in earthquake-prone regions and to detect nuclear explosions.

Type: New
Title: "High Frequency Physics-Based Earthquake System Simulations"

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

Scientific Discipline: Earth Science: Geological Sciences

INCITE Allocation: **112,200,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (64,200,000 processor hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (48,000,000 processor hours)

Research Summary:
Economic exposure to earthquake devastation in seismically active regions has increased significantly over the last few decades due to the massive growth of urban areas. To better understand risk and improve infrastructure resilience, earthquake hazards must be quantified at higher levels of fidelity. Physics-based modeling and simulation efforts provide a path to more accurate data on 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 3D models of the crust's heterogeneous structure to represent the ground motion during strong earthquakes.

For this INCITE project, researchers from the Southern California Earthquake Center (SCEC) will perform physics-based earthquake system research investigating high-frequency earthquake system simulations (High-F). Building on their work in past INCITE projects, the new SCEC High-F project will integrate scientific modeling and simulation efforts with the objective of reproducing earthquake physics and effects at high frequencies (up to 10 Hz) using deterministic approaches. Their goal is to produce simulations at higher frequencies than ever before, providing a level of resolution valid for engineering applications. The results will help to improve the earthquake resilience of buildings, bridges, and other critical distributed systems (e.g., lifeline and medical networks).

Type: New
Title: "High-resolution Simulation for Climate Means, Variability, and Extreme"

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

Scientific Discipline: Earth Science: Climate Research

INCITE Allocation: **150,000,000 processor hours**
Site: Oak Ridge National Laboratory **Machine**
(Allocation): Cray XK7 (100,000,000 processor hours)
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (50,000,000 processor hours)

Research Summary:
Although there is strong observational evidence for a global increase in climate extremes over the last century, it is much more difficult to characterize regional scale trends in extreme events. Climate science predicts that the frequency of extreme events is likely to increase as greenhouse gas concentrations increase, but the picture can be confusing. Climate models currently used in climate change studies only partially resolve many of the meteorological aspects important to the formation and representation of these climate features.

The project proposes to quantify the benefits of employing very-high-resolution global models with enhanced tracer transport to investigate these issues using the latest versions of the Community Earth System Model. In contrast to other investigations conducted over limited spatial domains or time periods, the project's scientific objectives require simulations spanning local to global scales of sufficient duration to quantify the interactions among fast and slow processes in the climate systems. An integral component of this project will be the deployment of new modeling configurations at high resolution to improve the simulation of regional scale hydrometeorological phenomena.

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

Principal Investigator: Choong-Seock Chang, Princeton Plasma Physics Laboratory
Co-Investigators: Stephane Ethier, Princeton Plasma Physics Laboratory
Scott Klasky, Oak Ridge National Laboratory
Robert Moser, The University of Texas at Austin
Scott Parker, University of Colorado
Mark Shephard, Rensselaer-Polytechnic Institute
Pat Worley, Oak Ridge National Laboratory

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation: **229,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (129,000,000 processor hours)
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (100,000,000 processor hours)

Research Summary:
The goals of this project are to perform a systematic multi-year study, based upon an extreme-scale, first-principles kinetic particle-in-cell approach using the XGC1 global edge gyrokinetic code, and to address the challenges associated with the non-equilibrium multiscale plasma transport physics in the edge region of magnetically confined plasmas. Success of ITER is critically dependent upon good edge plasma confinement. It has been over 30 years since experiments ubiquitously found that good edge plasma confinement, which leads to a steep edge plasma pedestal, has a crucial effect on core plasma performance through a stiff nonlocal core-edge interaction. This high-confinement mode of operation is called "H-mode". Despite their importance, neither the edge confinement physics nor the nonlocal core-edge interaction physics has been well understood yet. The proposed work represents the essential mission of the SciDAC-3 Center for Edge Physics Simulation (EPSI).

The plasma edge presents a set of multi-physics, multi-scale problems in the presence of the magnetic separatrix and material wall. Perhaps the greatest challenges are the lack of scale separation among the multi-physics processes: plasma turbulence, background plasma evolution, plasma flows, neutral particle transport and atomic physics, orbital motion of charged particles, and turbulence generated secondary flows. The plan here is to model these phenomena without scale separation within a comprehensive first-principles set of equations in XGC1, eliminating the need to address the very challenging issues of coupling multiple codes across either multiple physics phenomena or multiple spatial and temporal domains. As the computers become more powerful, the more important physics can be included at higher accuracy and fidelity.

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

Principal Investigator: Thomas Maier, Oak Ridge National Laboratory
Co-Investigators: Thomas Schulthess, ETH Zurich
Peter Staar, ETH Zurich

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:
Superconducting materials are key components to developing new energy-related technologies, but they require optimization to unleash their full potential. The 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.

U.S. DEPARTMENT OF ENERGY
INCITE
LEADERSHIP COMPUTING

Type: New
Title: "Intensity-Dependent Dynamics in Fermilab and CERN Accelerators"

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

Research Summary:

Particle accelerators are an enabling technology for both basic research and the applied sciences. In basic research, accelerator-based experiments are the primary tool for studying the fundamental constituents of matter and the structure of nuclei. In the applied sciences, particle accelerators are used to probe the structure of materials and study the transmutation of nuclear waste. This project focuses on simulating accelerators at the world's two largest accelerator facilities, Fermilab and CERN. Results will assist in upgrades at both facilities, enabling the next generation of particle accelerator research.

Upgrades for these facilities follow two paths. In the U.S., Fermilab is pursuing the Intensity Frontier, which will create intense proton beams for measurements of ultra-rare processes in nature and neutrino experiments, such as the Long Baseline Neutrino Experiment (LBNE). In Europe, CERN is pursuing the Energy Frontier by operating the Large Hadron Collider (LHC), the highest energy accelerator in the world. Although the LHC has only recently started operating, it has already facilitated an enormous impact on particle physics with the discovery of the Higgs boson.

Although the Fermilab and CERN accelerators support disparate areas of particle physics research, both upgrade efforts require an accurate understanding of intensity-dependent effects in their low- to medium-energy accelerators to move forward. Such understanding requires detailed numerical modeling that goes beyond the capabilities of desktop machines and simple clusters. This project combines state-of-the-art accelerator simulation software with petascale hardware to simulate the accelerators with unprecedented fidelity. The results will enable new discoveries in particle physics in both the Intensity and Energy Frontiers.

Type: Renewal
Title: "Kinetic Simulations of Fusion Energy Dynamics at the Extreme Scale"

Principal Investigator: William Tang, Princeton University
Co-Investigators: Mark Adams, Columbia University
Stephane Ethier, Princeton Plasma Physics Laboratory
Khaled Ibrahim, Lawrence Berkeley National Laboratory
Scott Klasky, Oak Ridge National Laboratory
Bruce Scott, Rechenzentrum Garching
Bei Wang, Princeton University
Weixing Wang, Princeton Plasma Physics Laboratory

Scientific Discipline: Physics: Plasma Physics

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

Research Summary:

The quest for alternatives to fossil fuels to meet the world's energy needs is generating increasing interest in nuclear fusion. In order to build the scientific foundations to develop fusion energy, a key need is the timely development of high-physics-fidelity predictive simulation capability for magnetically confined fusion plasmas. To do so in a timely way requires using the power of leadership-class supercomputers to simulate the complex dynamics governing fusion energy systems, including ITER, a multi-billion dollar international burning plasma experiment.

For this INCITE project, researchers will continue to use *ab initio* particle-in-cell global codes to solve the nonlinear equations underlying gyrokinetic theory. The goal is to gain new physics insights on magnetic confinement properties, while also answering the key question of how turbulent transport and associated confinement characteristics will scale from present generation devices to the much larger ITER-scale plasmas.

Researchers are also addressing another important physics challenge by studying the unavoidable spatial variations in such systems. The resulting microturbulence can significantly increase the transport rate of heat, particles, and momentum across the confining magnetic field in tokamak devices. The balance between these energy losses and the self-heating rates of fusion reactions ultimately determines the size and cost of an actual fusion reactor. Therefore, understanding and possibly controlling the underlying physical processes is key to achieving the efficiency needed to help ensure the practicality of future fusion reactors.

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

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

Scientific Discipline: Engineering: Fluids and Turbulence

INCITE Allocation: **75,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (75,000,000 processor hours)

Research Summary:
Aviation gas turbine engines are an essential part of the transportation industry. In 2012, the commercial aviation industry was estimated to spend $207 billion on fuel, or about 33% of their operating costs. That amounts to approximately 5 million barrels of oil per day, or about 6% of the world's total oil usage. Aviation gas turbine engines are also responsible for 2% of the world's CO2 production and 3% of the world's harmful greenhouse gas emissions. As the commercial aviation industry continues to grow and oil prices continue to rise, these impacts are forecasted to continue to increase for the foreseeable future.

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

The first group of calculations will 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 then 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. Finally, 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-Scale Coupled-Cluster Calculations of Supramolecular Wires"

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

Scientific Discipline: Chemistry: Physical

INCITE Allocation: **24,000,000 processor hours Site:**
Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (24,000,000 processor hours)

Research Summary:
Researchers are developing noncommercial 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 1D molecular wires.

Quantum mechanics is the key to understanding the molecular world of chemistry and other related molecular sciences. In particular, the electronic Schrödinger equation has to be solved to describe the electronic structure of a molecular system. Two different strategies have been used for obtaining approximate solutions to the Schrödinger equation: wave-function-based methods and density functional theory. The coupled-cluster model is the state-of-the-art wave function method and has been used to compute energy levels, structures, and various molecular properties for small molecular systems to an accuracy challenging that of experimental results. The proposed coupled-cluster scheme will extend the application range of accurate quantum chemical calculations into new territory. Researchers will use it to study a new class of molecules, the AATs, for which the use of coupled-cluster methods may turn out to be particularly useful. AATs efficiently self-assemble into ordered nanostructures, and their electronic and physical properties can be experimentally tuned. They are therefore promising model materials, and in their 1D self-assembled supramolecular wire form, they have potential applications in the fields of molecular electronics and optoelectronics.

Type: New
Title: "Lattice QCD"

Principal Investigator: Paul Mackenzie, Fermi National Accelerator Laboratory
Co-Investigators: 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, Jefferson National Laboratory
Martin Savage, University of Washington
Robert Sugar, University of California, Santa Barbara

Scientific Discipline: Physics: Particle Physics

INCITE Allocation: **340,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (240,000,000 processor hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XT (100,000,000 processor hours)

Research Summary:
For this multiyear project, scientists will continue tapping the DOE's leadership-class computers to advance quantum chromodynamics (QCD) research, the study of how quarks and gluons interact. Using a non-perturbative approach called Lattice QCD, the research team is calculating predictions of the Standard Model for quantities such as particle masses and decay rates, and to search for evidence of new physics beyond the standard model. The simulations will be used to generate new gauge configurations with up, down, strange, and, in some cases, charmed quarks at their physical mass values on lattices that are sufficiently fine grained to enable full control of systematic errors for a number of key quantities.

The new gauge configurations will be used to determine a wide range of physical quantities of importance to major experimental programs in high energy and nuclear physics. In high energy physics, for example, this project will help push the search for beyond-the-standard-model effects in particle physics to yet higher energies, and produce the new lattice calculations required for the DOE's Intensity Frontier program. In nuclear physics, Lattice QCD calculations have been critical in guiding the search for exotic states of matter at the GlueX experiment, and will be essential for interpreting the results. Findings from this project will also feed into nuclear physics experiments at the Facility for Rare Isotope Beams (FRIB), and at Los Alamos, Brookhaven, and Jefferson national laboratories, among others.

Type: New
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 Royterhsteyn, SciberQuest

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation: **86,000,000 processor hours Site:**
Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (86,000,000 processor hours)

Research Summary:
The project will explore the relationship between turbulence and magnetic reconnection in high-temperature plasmas. Researchers will investigate both the formation and breakup of electron-scale current sheets using fully kinetic simulations, which rigorously describe plasma physics. These two basic processes occur in a wide range of applications, including laboratory experiments, the solar wind, and the Earth's magnetosphere.

In theoretical plasma physics, turbulence and magnetic reconnection are two of the most outstanding basic problems, with widespread applications and daunting computational challenges. Historically, the research overlap between these topics has been rather minimal, but recent developments suggest these two areas may be intimately connected. The two primary focus areas include simulations of decaying turbulence to examine the statistics of current sheet formation and the areas' relative contributions to the dissipation. These simulations are highly anticipated by the solar wind turbulence community and will be compared to spacecraft data. The second focus area is on the development of reconnection in ion-scale current sheets in close collaboration with three experimental groups at the University of California-Los Angeles, Madison, and Princeton. Each experiment targets a different aspect of the physics of current sheet dissipation and breakup. The results could lead to major advances in our understanding of both turbulence and reconnection, which will have an impact on a variety of fields including space physics, solar physics, laboratory plasmas, and astrophysics.

Type: New
Title: "Molecular Engineering through Free Energy Mapping"

Principal Investigator: Juan de Pablo, University of Chicago
Co-Investigator: Chi-cheng Chiu, Argonne National Laboratory
Abelardo Ramirez-Hernandez, Argonne National Laboratory
Jonathan Whitmer, Argonne National Laboratory

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

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

Research Summary:
Block polymers (BP) are known to self-assemble into a wide variety of nanostructured morphologies, as do liquid crystals (LC) which similarly adopt ordered morphologies capable of interacting with light in distinct ways. These are examples of mesoscale assembly, where the behavior of a material over relatively long length-scales emerges from the subtle balance of disparate molecular-level interactions.

Yet, key questions for phenomena arising at the mesoscale remain unanswered, and can only be addressed by simulation over time and length scales that, until now, were inaccessible. This project seeks to demonstrate the predictive ability of powerful new models and methods that will utilize the large-scale computing power of ALCF's Mira, an IBM Blue Gene/Q. A team of researchers from the Institute for Molecular Engineering at the University of Chicago and Argonne National Laboratory, will use these tools to identify mesoscale assemblies in atomistic and coarse-grain simulations, and map their free energies with unprecedented accuracy through simulations of large ensembles.

Focusing on three platforms, this INCITE research will examine the dynamics of directed BP assembly, which is of considerable importance in the fabrication of next-generation integrated circuits and high-density storage media. The formation of polypeptide aggregates—which are implicated in several neurodegenerative diseases and known to be extremely toxic—will be examined, as will the formation of defects in LC systems, and the use of those systems in biosensors and programmed nanoparticle assembly.

Each of these platforms builds on the research group's expertise in novel free-energy calculations and is of considerable technological importance. The results could provide wide-ranging application in the design of microelectronics, self-assembly, and human health.

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

Principal Investigator: George Karniadakis, Brown University

Scientific Discipline: Biological Sciences: Biophysics

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

Research Summary:
The work proposed by researchers at Brown University involves both continuum-based as well as atomistic-based simulations. Specifically, this research projects aims to simulate blood flow and thrombus biomechanics in thoracic aortic aneurysms and dissections (TAADs).

Increasing clinical evidence suggests that a completely thrombosed false lumen (a diversionary passageway caused by a dissection of the aorta) results in an improved prognosis, whereas a partially thrombosed false lumen may render the wall more vulnerable to further dissection or rupture. Multiscale simulations of TAADs will lead to a better understanding of the mechanisms by which, and conditions under which, a false lumen is expected to develop either a partial or a full thrombus, and why the latter is beneficial.

The Brown University research group will take advantage of the ALCF's petascale resource Mira, an IBM Blue Gene/Q, to perform these simulations, as well as to advance understanding of the progression of red blood cell (RBC)-related pathologies. Specifically, they will examine *in silico*, for the first time, the hemodynamic conditions under which an intramural thrombus forms in aortic dissections, and the biomechanical consequences of thrombus on the remnant wall.

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: **126,000,000 processor hours**

Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (70,000,000 processor hours)
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (56,000,000 processor hours)

Research Summary:

Weak intermolecular bonds are ubiquitous in nature, including in water, gas hydrates, and supramolecular systems like DNA pairs, but they are poorly described with current computer simulation methods. The project will use quantum Monte Carlo calculations to create an extensive database of energy benchmarks for molecular systems bound by non-covalent forces, particularly hydrogen bonding and van der Waals dispersion forces. The benchmarks will be used to develop improved versions of density functional theory, whose current standard forms are inadequate for non-covalent forces; the benchmarks will also be used to assess and improve parameterized force fields for molecular systems. Three classes of paradigm molecular systems will be tackled: (a) water in a wide range of aggregation states, including solid, liquid, clusters, layers, and surfaces, (2) gas hydrates (clathrates) of importance for industry and the environment, and (3) supramolecular systems that are important for nanoscience and biology.

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 nano-particles, low-dimensional aggregates such as adsorbed water layers, aqueous solutions, hydrated biomolecules, biological structures stabilized by hydrophobicity, gas hydrates, and many others.

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

Principal Investigator: James Vary, Iowa State University
Co-Investigators: 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: Oak Ridge National Laboratory **Machine**
(Allocation): Cray XK7 (104,000,000 processor hours)
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (100,000,000 processor hours)

Research Summary:
Predictions for the structure and reactions of nuclei, with assessed uncertainties, are important for the future of the nation's energy and security needs. Developing a comprehensive description of all nuclei (stable and unstable) and their reactions requires investigations of rare and exotic isotopes with unusual proton-to-neutron ratios that are difficult to produce and study experimentally because of their short lifetimes. This project will result in state-of-the-art simulations that provide needed predictions where direct experiment is not possible or is subject to large uncertainties.

Such calculations are relevant to many applications in nuclear energy, nuclear security, and nuclear astrophysics, since rare nuclei lie at the heart of nucleosynthesis and energy generation in stars. A fundamental description of nuclear structure and nuclear reactions that retains predictive power and carries quantified uncertainties is vital for the future development of nuclear energy in the form of advanced fission reactors and fusion energy. This fundamental description also provides a foundation for interpreting experiments that test the basic laws of nature.

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

Principal Investigator: Susan Kurien, Los Alamos National Laboratory
Co-Investigators: Hussein Aluie, Los Alamos National Laboratory
Robert Ecke, Los Alamos National Laboratory
Annick Pouquet, University of Colorado
Duane Rosenberg, Oak Ridge National Laboratory
Leslie Smith, University of Wisconsin–Madison

Scientific Discipline: Engineering: Fluids and Turbulence

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

A secondary goal for this project is to improve the current understanding of turbulence by computing statistical patterns gleaned by seeding a turbulent fluid with a large number of particles to be conveyed by the flow. Motivated by the presence of both upscale and downscale transfer of energy in strongly rotating stratified flows, researchers have introduced Lagrangian particle tracking, a new computational and diagnostic capability, to the Geophysical High Order Suite for Turbulence (GHOST) code application used with previous allocations. Such particle tracking capabilities form a natural route to understanding the fluxes and mixing properties of the flows and will form a key component of future simulations and analysis.

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

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

Scientific Discipline: Physics: Plasma Physics

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

Research Summary:

This project focuses on longstanding scientific problems closely tied to extreme plasma physics processes, such as identifying the dominant acceleration mechanisms for cosmic rays, and determining whether it is possible to generate relativistic shocks in the laboratory and to mimic these extreme cosmic accelerators. Moreover, recent results produced by this research team have demonstrated that collisionless shock waves can accelerate monoenergetic proton beams with the potential—when augmented by moderate laser intensities—to reach energies relevant for cancer therapy.

Computational modeling is critical to understanding the physical mechanisms behind shock formation and particle acceleration, and to establishing the conditions whereby these shock waves can be excited in the laboratory. Researchers will perform, for the first time, realistic mass ratios in astrophysical- and laboratory- relevant conditions, and self-consistent *ab initio* massively parallel simulations to study the physics of shock waves.

The team will identify the physical processes and laboratory conditions that lead to the formation of electrostatic and electromagnetic collisionless shocks, and will study the self-consistent shock formation, propagation, and particle acceleration derived from the interaction of intense lasers with plasmas in realistic laboratory conditions. The generation of high-quality ion beams from electrostatic shocks driven by laser-plasma interactions will be examined, as well as the shock propagation in collisionless/collisional media in conditions relevant for inertial confinement fusion plasmas.

A combination of the team's technical expertise, their recent scientific results regarding plasma simulation, and the outstanding computational resources made available by INCITE will trigger unique scientific results and open new avenues for research on the fundamental processes associated with shock formation, propagation, and particle acceleration.

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

Principal Investigator: Leonid Oliker, Lawrence Berkeley National Laboratory
Co-Investigators: David Bailey, Lawrence Berkeley National Laboratory
Peter Beckman, Argonne National Laboratory
Laura Carrington, San Diego Supercomputer Center
James Demmel, University California Berkeley
Jack Dongarra, University of Tennessee and Oak Ridge National Laboratory
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 and University of Southern California
Allen Malony, University of Oregon
John Mellor-Crummey, Rice University
Barton Miller, University of Wisconsin
Philip Roth, Oak Ridge National Laboratory
Patrick Worley, Oak Ridge National Laboratory
Katherine Yelick, Lawrence Livermore National Laboratory
Bronis de Supinkski, Lawrence Livermore National Laboratory

Scientific Discipline: Computer Science

INCITE Allocation: **75,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (45,000,000 processor hours)
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (30,000,000 processor hours)

Research Summary: The performance research community needs to provide tools, runtimes, and methodologies to enable scientists to exploit leadership-class systems and how to use each system most efficiently.

This project will focus on five primary goals: (1) develop new programming models and runtime systems for emerging and future generation leadership computing platforms; (2) update and extend performance evaluation of all systems using suites of both standard and custom micro, (3) continue to port performance tools and performance middleware to the BG/Q and XK6, (4) validate and modify performance prediction technologies to improve their utility for production runs on the leadership-class systems; and (5) analyze and help optimize current or candidate leadership-class application code

Type: Renewal
Title: "Petascale Computing of Biomolecular Systems"

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

Scientific Discipline: Biological Sciences: Biophysics

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

Research Summary:
Researchers will use petascale resources to investigate three biomolecular systems: the assembly of the HIV capsid, the process of peptide bond formation in ribosomes, and the basic process of photosynthesis. The proposed research will aid in the development of new antibiotics, HIV therapies, and green-energy technologies.

Researchers will construct and simulate a complete HIV capsid, in full atomic detail, based on recently acquired experimental data. The simulation promises to uncover key insights about the capsid assembly, which will help guide the development of new drugs to interfere with the assembly process.

The details of the complex reactions that take place within the ribosome are fertile ground for future research and are only really accessible via large-scale simulations at atomic resolution and quantum-mechanical calculations.

Scientists will model photosynthetic chromatophores from purple bacteria, which are the simplest photosynthetic systems found in nature, also in full atomic detail, to characterize how the components of the chromatophore work together to perform photosynthesis.

Type: New
Title: "Petascale Simulations of Inhomogeneous Alfvén Turbulence in the Solar Wind"

Principal Investigator: Jean C. Perez, University of New Hampshire
Co-Investigator: Benjamin Chandran, University of New Hampshire

Scientific Discipline: Physics: Space Physics

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

Research Summary:

Evidence from spacecraft observations suggest that Alfvén wave (AW) turbulence, described by the model of incompressible magnetohydrodynamic (MHD), is important for heating the solar wind at large distances from the sun, though the precise role it plays in the origin of the solar wind is less clear. Reasons for this uncertainty include the lack of *in situ* measurements of solar wind closer to the Sun, in the region where most of the heating and acceleration occur, and the difficulty in modeling this problem theoretically.

This project's primary objective is to carry out large numerical simulations designed to advance our understanding of reduced MHD turbulence in an inhomogeneous background, which includes the physics of wave reflections that is present near the Sun. Because such reflections significantly increase the complexity of the turbulence dynamics, reflection-driven AW turbulence had remained beyond the realm of modern supercomputers. As such, researchers will investigate the fundamental properties of reflection-driven Alfvén wave turbulence and simulate it in realistic coronal conditions to assess its contribution toward coronal heating and the origin of the solar wind.

Researchers will also use the simulations to produce virtual *in situ* spacecraft measurements, similar to measurements obtained by spacecraft probing the solar wind. Understanding solar wind measurements will prove crucial for interpreting data derived from the upcoming Solar Probe Plus mission, which is scheduled to perform several fly-bys near the critical Alfvén point, precisely the region covered by the numerical simulations.

Type: New
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: **200,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (200,000,000 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 technologies while reducing manufacturing and maintenance costs.

For this INCITE project, researchers will focus on self-healing nanomaterial systems capable of sensing and repairing damage in harsh chemical environments and in high temperature/high pressure operating conditions. Specifically, they will be looking at anticorrosion coatings for metals and ceramic nanocomposites consisting of silicon carbide nanoparticles embedded in alumina and silicon nitride.

The research team will study the materials in great detail by performing petascale quantum molecular dynamics (QMD), reactive molecular dynamics (RMD), and mesoscale reactive dissipative particle dynamics (R-DPD) simulations. They will perform QMD simulations involving 10^4 atoms to shed light on the chemical and thermal aspects of self-healing processes. The team will also perform billion-atom RMD simulations to study: (1) how anticorrosion compounds in metal sponges and silica nanocontainers respond to changes in pH and temperature; and (2) how the size and spatial distributions of nanoparticles, temperature, and partial pressure of oxygen affect self-healing processes in ceramic nanocomposites.

Finally, the researchers will integrate these computational results with data from experiments at DOE facilities (Advanced Photon Source at Argonne, Spallation Neutron Source at Oak Ridge, and X-ray Laser Source at Stanford) to provide a comprehensive and efficient validation of 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: "Petascale Simulations of Type Ia Supernovae"

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

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:
Type Ia supernovas are among the brightest thermonuclear explosions in the modern universe. Because of their brilliance and nearly constant luminosity at peak, they are also a "standard candle" favored by cosmologists to measure the rate of cosmic expansion. Yet after 50 years of study, a first-principles understanding of how they operate is lacking. Researchers will use a suite of three highly scalable codes to model all aspects of the explosion of Type Ia supernovas, including ignition of the thermonuclear runaway, the explosion itself, and the light curves and spectra, all in three dimensions.

Type Ia supernovas have been of great interest to astronomers ever since it was recognized that they constitute a separate class of explosion from the hydrogen-rich Type IIs. More recently, a better understanding of these supernovas, achieved through computational simulation, was ranked as one of the principle goals of theoretical astrophysics for the next 10 years by the Decadal Survey of the National Academy. Type Ia supernovas are interesting, not only because they are bright lights of nearly constant luminosity and have made about two- thirds of the iron in our bodies, but also because they are unique laboratories for studying combustion in circumstances that cannot be achieved on Earth—a highly turbulent medium with large dimension and long duration.

Type: Renewal
Title: "Precision Many-Body Quantum Simulations of Functionalized Structures"

Principal Investigator: Shiwei Zhang, College of William and Mary
Co-Investigators: Joseph Carlson, Los Alamos National Laboratory
Henry Krakauer, College of William and Mary
Gustavo Scuseria, Rice University
Cyrus Umrigar, Cornell University

Scientific Discipline: Chemistry: Physical

INCITE Allocation: **30,000,000 processor hours Site:**
Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (30,000,000 processor hours)

Research Summary:

The project involves the application of a recently developed stochastic many-body method to a few targeted problems in two areas: quantum chemistry for energy-related and magnetic materials and cold atoms in optical lattices in atomic, molecular, and optical physics. The quantum chemistry calculations emphasize the ability to reliably and precisely treat materials-specific characteristics, while the optical lattice calculations allow model engineering in which the many-body effects can be magnified to generate exotic new physics and chemistry.

The study of systems in which there is a strong interplay between the quantum mechanical nature of particles and their interactions is one of the central themes in both physics and chemistry. Accurate treatment of such systems is a grand challenge in modern science. If successful, the project will lead to the solution of long-standing challenges in accurately predicting key properties of these systems. It will also provide significant benchmark results for future simulations and experiments. The combination of methodological developments and the advent of petaflop (and beyond) computing presents a unique and outstanding opportunity to now make fundamental progress in solving this problem. Harnessing the power of petaflop computing, these calculations aim to reliably predict candidate structures for energy storage and management, magnetic media, and new phases of matter formed by atoms in magnetic or laser traps.

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
Jeongnim Kim, 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-lasting 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 Research
Teodoro Laino, IBM Research
Kah Lau, Argonne National Laboratory
Winfried Wilcke, IBM Research
Peter Zapol, Argonne National Laboratory

Scientific Discipline: Materials Science: Condensed Matter and Materials

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

Research Summary:

A rechargeable lithium/air (Li/air) battery can potentially store five to ten times the energy of a lithium/ion 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 at Argonne and IBM continue to conduct *ab initio* density functional theory and classical molecular dynamics simulations to help address this problem. These simulations will provide insight into the electrochemical nucleation and growth processes involved, as well as provide predictions for new, more stable electrolytes.

Current project milestones are deeply connected to the modeling of the crystallization process. Understanding the formation origins of these macroscopic structures is crucial to the development of Li/air. Researchers will address the debated problem of nucleation of lithium peroxide (Li_2O_2) by combining large-scale molecular dynamics simulations utilizing an optimized classical force field to understand the driving force behind the formation of these structures.

A study of the oxygen-rich, core-shell-like nanoparticles based on stoichiometric nanoparticles will be conducted based on spin-polarized calculations. The relevant chemical reaction studies involving initial discharge species on Li_2O_2 and oxygen-rich Li_2O_2 nanoparticles obtained from previous simulations will help determine energetics and structures. The Argonne/IBM group will investigate these reactions at interfaces between metal nanoparticles and electrolyte interfaces.

Based on recent studies, researchers will begin to consider metal nanoparticles, such as palladium, instead of carbon surfaces with defects. Metal nanoparticles have been shown to significantly affect the morphology of the discharge product and reduce the charge over-potential, a key challenge for Li/air batteries. These calculations will help identify the role these metal catalysts play, and ultimately optimize them for improved performance of Li/air batteries.

Type: New
Title: "Probing Dark Matter at Extreme Scales"

Principal Investigator: Michael Warren, Los Alamos National Laboratory
Co-Investigators: Alexander Friedland, Los Alamos National Laboratory
Daniel Holz, University of Chicago
Samuel Skillman, Kavli Institute for Particle Astrophysics and Cosmology
Paul Sutter, Paris Institute of Astrophysics
Matthew Turk, Columbia University
Risa Wechsler, Kavli Institute for Particle Astrophysics and Cosmology

Scientific Discipline: Physics: Astrophysics

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

Research Summary:
Cosmological simulations are the cornerstone of theoretical analysis of structure in the universe from scales of kiloparsecs to gigaparsecs. Predictions from numerical models are critical to almost every aspect of the studies of dark matter and dark energy because of the intrinsically nonlinear gravitational evolution of matter. The project's researchers will perform precision tests of the standard cosmological model and produce trillion-particle simulations at scales of 8 Gpc and 1 Gpc, as well as a simulation of a statistical sample of 100 Milky Way halos with much higher resolution (but smaller particle count). The project could also advance the state of the art in domain decomposition and hierarchical tree-based computational techniques relevant to many simulation and data analysis problems.

Without computer simulations the current understanding of the large-scale universe would be little more than a rough theoretical approximation rather than the firmly established and spectacularly successful standard cosmological model we currently enjoy. The project will address a wide range of scientifically relevant tests of the standard cosmological model, including measurements of cluster abundance, void statistics, baryon acoustic oscillations, redshift-space distortions, velocity statistics, and gravitational lensing. At small scales researchers will test the abundance and central kinematics of the dwarf spheroidal galaxy satellites and related small-scale gravitational physics, which determine the expected signal for dark matter detection experiments. The simulations will produce an unprecedented suite of accurate and reliable halo, sub-halo, and mock galaxy catalogs.

Type: New
Title: "QMC Simulations Database for Predictive Modeling and Theory"

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

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation: **200,000,000 processor hours**
Site: Oak Ridge National Laboratory **Machine**
(Allocation): Cray XK7 (100,000,000 processor hours)
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (100,000,000 processor hours)

Research Summary:
The project will involve quantum Monte Carlo (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 Waals 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, University of Lancaster
Pablo Lopez Rios, University of Cambridge

Scientific Discipline: Materials Science: Condensed Matter and Materials

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

Research Summary:

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. To achieve unprecedented accuracy, calculations will treat the quantum motion of nuclei as well as electrons. The project will focus on the solid form—water ice—from zero pressure up to the pressures at which water ice may be found within planets and their icy satellites. It will also study pure hydrogen at pressures from about 100 GPa up to and somewhat beyond the highest pressures that can currently be achieved in diamond-anvil-cell experiments (over 300 GPa).

The goals of the project are to obtain the most accurate description achieved so far of water ice at the atomic level and to perform simulations of hydrogen at high pressures that will provide reliable predictions of the thermodynamically stable phases and their properties. Water ice is the most widely known example of a hydrogen-bonded molecular solid. Life on Earth depends on water and hydrogen bonds (they hold together DNA and proteins). Hydrogen bonding is also crucial in drug design.

As the simplest, most abundant, and ancient of the elements, hydrogen occupies a special place within both the periodic table and the minds of scientists. Gas-giant planets such as Saturn and Jupiter contain large amounts of metallic hydrogen at high pressures and temperatures. This research is expected to lead to new understanding of hydrogen at high pressures as well as further improvements in QMC methods for tackling systems of quantum particles with widely differing masses.

Type: New
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, University of Missouri-Columbia
Shriram Ramanathan, Harvard University
Ram Subbaraman, Argonne National Laboratory

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 lie 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 dynamical 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 are urgently needed for the design and development of novel functional oxide materials for energy applications.

Given the structural and compositional complexity of oxide materials and their interfaces, it is not surprising that both the passive state and functional properties of oxides and oxide interfaces are related to the defects, which in turn are dramatically influenced by the synthesis conditions. One approach to tuning oxide defect imbalances at room temperature involves the use of an electric field to stimulate oxide growth beyond what is possible through thermal diffusion.

The proposed computational research utilizing atomistic simulations such as classical molecular dynamics (MD) with ReaxFF—reactive force field—will demonstrate the potential of electrical field application for ceramics processing. This integrated simulation-experimental protocol will determine the way electrical field application affects the transport processes during oxidation, oxide growth, and sintering, and will establish methods for their exploitation in practical processes and applications.

This INCITE project could result in the development of a universal platform that harvests the unique advantages of electrical field application during ceramics sintering, benefiting the field of ceramics processing and industries that rely heavily on ceramics technologies, including energy-relevant industries.

Type: Renewal
Title: "Safety in Numbers: Discovery of New Solid Li-ion Electrolytes"

Principal Investigator: Boris Kozinsky, Bosch in the USA
Co-Investigators: Nicola Marzari, Ecole Polytechnique Fedrale de Lausanne
Brandon Wood, Lawrence Livermore National Laboratory

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

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

Research Summary:
Researchers will use high-throughput computational screening combined with in-depth ab initio dynamics simulations to discover and optimize new classes of Li-ion solid inorganic electrolytes to enable safe high-energy batteries. The project will advance the computational technology for predicting and analyzing new inorganic Li-ion conductors. By computationally screening a large subspace of inorganic materials, researchers will identify a list of promising candidates that will be synthesized and characterized by experimental partners. The effort will advance the state of the art of intensive computational discovery and understanding of new classes of electrolyte materials, with potential relevance to battery systems, fuel cells, and sensors.

Batteries are critical for enabling the widespread introduction of hybrid and electric vehicles, as well as compact stationary storage of energy from renewable source. There are several factors that prevent wide commercialization of large Li-ion batteries: their high cost, insufficient energy density, and poor safety. In the last few years significant interest has appeared in Li-sulfur and Li-air batteries, which promise far higher energy densities than Li-ion batteries, but also require Li metal anodes and consequently protection layers. There is great need for a solid layer to protect the Li metal surface to allow development of safe high-energy batteries, which is where new solid inorganic Li-ion conductors can have a tremendous impact on energy storage technology.

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

Principal Investigator: Markus Eisenbach, Oak Ridge National Laboratory
Co-Investigators: Donald Nicholson, Oak Ridge National Laboratory
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. 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 ones. While the ground-state properties of some pure compounds can be readily calculated, real materials with defects and impurities have to be considered. This makes the calculation of even the ground state for realistic models containing approximately 100,000 atoms a petascale problem. Petaflop computers can calculate the Curie temperature for simple materials from first principles. Realistic materials are significantly more complex than these idealized materials, requiring more computational resources.

Magnetism plays an important role in the atomic-scale behavior in basic structural materials, such as steel and iron-nickel alloys. Improvements in the physical properties of these materials can lead to energy savings as a result of stronger, lighter materials in transportation applications as well as better predictions for structural materials in radiation environments, such as fission and fusion reactors.

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

Principal Investigator: Robert Latham, Argonne National Laboratory
CO-Investigator: 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:
As hardware complexity in Leadership Class Facility systems skyrockets, it is not easy for applications to take complete advantage of available system resources and avoid potential bottlenecks. This project aims to improve the performance and productivity of key system software components on leadership-class platforms by studying four different classes of system software: message passing libraries, parallel I/O, data analysis and visualization, and operating systems.

While this work has pursued applications that make use of current 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, the ALCF's IBM Blue Gene/Q supercomputer, and allows for the evaluation of future designs by using current hardware.

The project's Parallel Models and Runtime Systems (PMRS) group is developing a large-scale, resilient data store to tolerate silent memory corruption. This is accomplished through a versioned data repository for applications that protects important memory regions and easily rolls back when necessary. PMRS also works on various runtimes that require large-scale testing to demonstrate their feasibility for production environments, and provides the basis upon which most production MPI libraries are developed. In addition, the group is extending research of the particular proprietary 5D torus topology of the system.

The techniques, algorithms, and performance-measuring methodologies used and developed at scale in this research can be applied to smaller platforms, as well. As a result, the improvements achieved can be immediately deployed throughout the high-performance computing community, improving the nation's capability for groundbreaking computational science and engineering.

Type: Renewal
Title: "Simulation of Laser-Plasma Interaction in National Ignition Facility Experiments"

Principal Investigator: Steven Langer, Lawrence Livermore National Laboratory
Co-Investigators: Denise Hinkel, Lawrence Livermore National Laboratory

Scientific Discipline: Physics: Plasma Physics

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

Research Summary:

Providing for the world's energy demands is one of the most urgent and difficult challenges facing our society. Inertial fusion energy provides an attractive solution to the demands for safe, secure, and environmentally sustainable energy. The National Ignition Facility (NIF) is currently carrying out experiments to compress a mixture of deuterium and tritium (DT) to temperatures and densities high enough to produce fusion ignition.

The laser intensity at NIF is high enough that some of the laser energy backscatters off the target. Previous research quantified how overlapping quads—a grouping of four laser beams propagating in the same direction—impacted backscatter at NIF.

pF3D, a massively parallel code that simulates LPI, is being optimized for Mira and should be ready to run efficiently using one third (or more) of Mira by early in CY14.

NIF has recently shot some experiments with high-density carbon capsules and with new hohlraum shapes. The backscattered light in these experiments differs in interesting ways from earlier experiments. Simulations produce synthetic data that can be compared to experimental data from NIF to gain insight into the generation of backscattered light.

The computational cost of a single quad simulation is much lower than a multi-quad simulation. Researchers plan to run several single-quad simulations to help identify the most interesting experiment. A three quad simulation of the chosen experiment is the key milestone for CY14.

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

Principal Investigator: James Kermode, King's College London
Co-Investigator: 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:

The fracture of silica is a problem that affects many diverse applications. In the mining industry, crushing and grinding mineral ores into fine power is an extremely energy-intensive process. In the biomedical realm, dental implants, for example, are made of silica-rich porcelain, which must survive years of tough mechanical work in the wet environment of the human body without breaking. A better understanding of the silica fracturing process could help address these issues, minimizing the energy cost required to fragment thousands of tons of rock and enabling the design of longer lasting prosthetic implants.

The underlying processes that cause silicates to crack in these applications are "chemomechanical"-- where stress fields and chemistry are tightly coupled. This is a very complex multiscale problem that can only be addressed with the computational power of the DOE's leadership-class supercomputers and highly efficient algorithms.

For this INCITE project, researchers will use DOE supercomputers to further the understanding of how silicate materials break in an oxidizing or wet environment, following stress corrosion patterns. To do so, they will use advanced multiscale atomistic computer simulations based on molecular dynamics (MD) and machine learning techniques. This includes applying the "Learn on the Fly" (LOTF) hybrid quantum mechanical/molecular mechanical (QM/MM) scheme to model fracture in silicone dioxide (SiO_2). LOTF is a nonuniform, precision MD scheme which augments MM force fields with QM information, only where and when this is necessary to ensure accurate MD trajectories.

The project aims to deliver the first series of efficient QM-accurate 3D simulations of catastrophic and stress-corrosion-induced fracture in crystalline and amorphous silica. The work will also demonstrate the power of a new general, predictive software tool to help other research projects achieve quantum mechanical accuracy when needed.

Type: New
Title: "Solving Petascale Public Health and Safety Problems Using Uintah"

Principal Investigator: Martin Berzins, University of Utah
Co-Investigator: Todd Harman, University of Utah
John Schmidt, University of Utah
Jennifer Spinti, University of Utah
Jeremy Thornock, University of Utah
Charles Wight, Weber State University

Scientific Discipline: Chemistry: Combustion

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

Research Summary:

Researchers at the University of Utah are addressing two separate public health and safety concerns with this project: (1) improving air quality in the San Joaquin Valley of California and (2) minimizing the damage caused by an unintentional detonation of a large array of explosive devices. The 2014 INCITE allocation matches the fourth year of a National Science Foundation PetaApps project aimed at solving health and safety problems with the Uintah Computational Framework (a set of software components and libraries that facilitate the solution of partial differential equations on structured adaptive mesh refinement grids).

The air quality issue within this project is focused on reducing nitrogen oxide (NOx) emissions from oilfield steam generators in the San Joaquin Valley. The researchers will use Mira to perform a petascale validation/uncertainty quantification study of NOx emissions from a full-scale generator. Simulations will also be carried out to predict the NOx emissions produced from steam generators with modified burner designs. This work addresses the impending change to the U.S. NOx emissions standard from 15 parts per million (ppm) to 5 ppm.

The portion of this research focused on explosives is motivated by a 2005 semi-truck accident in which 36,000 pounds of seismic boosters ignited and detonated, destroying a section of Utah state highway and adjacent railway. Researchers will use Mira to examine explosive devices to prevent the transition from a low-violence deflagration (thermal combustion) to an extremely violent detonation. Petascale simulations are required to investigate the different packing arrangements and storage techniques that can be used to stop such transitions. The results of this research will help improve the safe storage and transport of explosive devices.

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: **55,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (55,000,000 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 proteins change shape and go through many conformational states to perform their function. Malfunction of some vital proteins can lead to diseases such as cancer.

To understand how membrane proteins operate and how they are impacted by disease, researchers need detailed knowledge about all the relevant conformational states, as well as the free energy changes that connect them. This INCITE project is aimed at gaining a deep mechanistic perspective of 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 are considered (a Src kinase and a P-type ionic pump). For this project, researchers will leverage NAMD/Charm++ with MPI-level multiple copy algorithms, a computational methodology that achieves extreme scalability on leadership-class supercomputers and is at the forefront in the field of biomolecular simulations.

By studying experimentally well-characterized systems of increasing size and complexity within a unified theoretical framework based on free energy landscapes, the researchers will push the envelope and advance the theory-modeling-simulation (TMS) technology. TMS offers a virtual route to address fundamental biological questions and to help solve the problem of rational protein design. The computations planned for this study will serve as a roadmap for simulating, visualizing, and elucidating how biomolecular nano-machines work.

Type: Renewal
Title: "Thermal Hydraulic Modeling: Cross-Verification, Validation and Co-design"

Principal Investigator: Paul Fischer, Argonne National Laboratory
CO-Investigator: Katherine Heisey, Argonne National Laboratory
Elia Merzari, Argonne National Laboratory
Aleksandr Obabko, Argonne National Laboratory

Scientific Discipline: Physics: Nuclear Energy

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 continued INCITE project will push the boundaries of thermal hydraulic (TH) modeling in the spectral element code Nek5000 for co-design and validation, and serve as the focus of the current and future cross-verification activities for several international collaborations. As part of the Nuclear Energy Advanced Simulation (NEAMS) effort, Argonne researchers will conduct TH simulations to validate benchmarks for PANDA, the large-scale thermal hydraulics test facility in Switzerland, and continue computational fluid dynamics (CFD) simulations for Nuclear Reactor Safety workshops and their benchmarks.

In collaboration with Atomic Energy and Alternative Energies Commission (CEA), and Japan Atomic Energy Agency (JAEA), we will study the validation experiment PLAJEST. This triple-jet TH mixing experiment provides a unique opportunity to validate conjugate heat transfer simulation techniques for a variety of flow conditions in thermal stripping phenomena.

As a part of NEAMS' International Nuclear Energy Research Initiative (I-NERI), collaboration with the Nuclear Research Group (NRG) in Petten, Netherlands, calls for an exchange of high-fidelity CFD data between Argonne and NRG to verify the TH codes used by both institutions. This exchange of data will cover rod bundles previously simulated at Argonne, and pebble-bed reactors simulated by the NRG group. The immediate goal of this collaboration is to conduct a series of validation studies for simplified configurations currently designed at NRG that will require up to 200 million grid points and long time-averaging runs.

In collaboration with the U.S.-based, nuclear energy technology company TerraPower, the team will conduct numerical simulations of wire-wrapped rod bundles to quantify the effect of thermal expansion, which had not been considered previously. TerraPower will provide suitably deformed rod-bundle configurations based on its evaluation of thermal expansion. The effect and impact of the deformation due to thermal expansion will be evaluated using the Nek5000 code. Predicting thermal performance of such components is vital to the evaluation of overall reactor performance and safety, which could lead to a viable, carbon-free, energy production technology.

Type: New
Title: "Thermodynamics of Quark Flavors from Lattice QCD"

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

Scientific Discipline: Physics: Nuclear Physics

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

Research Summary:

Quantum Chromodynamics (QCD) is a fundamental particle physics theory that describes the interactions between quarks and gluons. At extreme temperatures and/or densities, QCD predicts that ordinary hadronic matter will undergo a phase transition to quark-gluon plasma (QGP). This prediction is now being tested in heavy ion collisions at the Relativistic Hadron Collider (RHIC) at Brookhaven National Laboratory and at the Large Hadron Collider (LHC) at CERN. The goal of this INCITE project is to achieve a fundamental microscopic understanding of the QGP properties near the transition by relating, for the first time, first-principle calculations to experimental measurements in a systematic way. This will provide theoretical background to the experimental efforts by numerically solving QCD on a discretized lattice, in the same conditions of temperature and density as those reached in heavy ion collisions, and for the same physical parameters.

The researchers will leverage DOE leadership-class supercomputers to determine the equation of state, which sets the relation between energy density, temperature and pressure in the hot matter. The research team will also study the QCD transition in great detail, matching computational results to the experiments to test whether there is a new, mixed phase of matter, in which hadrons and quarks can co-exist, and whether there is hierarchy due to flavor masses, which could lead to preferred formation of exotic states.

The project is very timely since the first measurements from the LHC have just recently concluded and the next experimental campaign will not start before 2015. The research aims to describe some of the obtained results, suggest new observables, and predict the necessary microscopic mechanisms to understand the underlying physics principles of the QCD transition. Findings will be applicable to RHIC and LHC measurements.

Type: New
Title: "Three-Dimensional Simulations of Core-Collapse Supernovae with Chimera"

Principal Investigator: Eric J. Lentz, University of Tennessee, Knoxville
Co-Investigators: John M. Blondin, North Carolina State University
Stephen W. Bruenn, Florida Atlantic University
W. Raphael Hix, Oak Ridge National Laboratory
Anthony Mezzacappa, Joint Institute for Computational Sciences and University of Tennessee, Knoxville
Konstantin N. Yakunin, University of Tennessee, Knoxville

Scientific Discipline: Physics: Astrophysics

INCITE Allocation: **85,000,000 processor hours Site:**
Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (85,000,000 processor hours)

Research Summary:
Core-collapse supernovas are the complex, dynamic, and inherently multidimensional explosions of massive stars. The proposed 3D supernova simulations will cover the range of massive stars from oxygen-neon-core stars on the lightest end (about 9 solar masses), through the range of iron-core stars (12–25 solar masses) seen to explode in axisymmetic simulations, to 40-solar-mass rotating progenitors on the upper extreme using the Chimera multiphysics supernova code. Chimera contains all of the relevant physics required for core-collapse supernova simulations including transport of energy by neutrinos and the required neutrino–matter interactions, general relativity and self-gravity, nuclear burning and nuclear equations of state, and 3D fluid dynamics.

The core-collapse supernova problem has been a computational challenge for several decades, but now we have entered an era in which well resolved, symmetry-free 3D simulations are now possible. From the simulations the project will examine the differences between the core-collapse supernova mechanism in these 3D simulations and in 2D (axisymmetric) simulations across the range of stellar progenitors. Researchers will also generate direct neutrino and gravitational wave signals, which directly probe the explosion mechanism. By including detailed nuclear reaction networks in the simulations, the project can generate detailed isotopic and elemental compositions of the material ejected by the supernova, which recent studies suggest will be quite different from current nucleosynthesis models that ignore the neutrino-driven, multidimensional nature of the explosion. These simulations will also be used to calibrate and correct larger sets of simpler models that are used to examine the detailed diversity of presupernova massive stars.

Type: New
Title: "Turbulent Rayleigh-Bénard Convection at High Rayleigh and Low Prandtl Numbers"

Principal Investigator: Janet Scheel, Occidental College
Co-Investigator: Joerg Schumacher, Imenau University of Technology

Scientific Discipline: Materials Science: Condensed Matter and Materials

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

Research Summary:
Rayleigh-Bénard convection (RBC) drives turbulent flows in nature and in many technologies, including chip-cooling devices, heat exchangers in power plants, and energy-efficient indoor ventilation via convection in the Earth's atmosphere, core, and oceans. Turbulent RBC also provides insight into the occasional, but extreme events that can occur in turbulent systems, such as the cessation of the large-scale circulation and the spontaneous emission of large, thermal plumes.

The RBC flow in cylindrical cells has been studied intensively over the last few years in several laboratory experiments all over the world. However, very few experiments or simulations have been performed for very low Prandtl numbers (the ratio of momentum diffusivity to thermal diffusivity). Low Prandtl numbers have direct application to convection in liquid metals, and can also shed light on the convection in the Earth's liquid metal core, in the sun, and in other stars.

With this INCITE project, researchers will use DOE supercomputers to investigate turbulent RBC at very high Rayleigh number and very low Prandtl number. For these studies, researchers will leverage the Nek5000 spectral element software package, which was developed for solving the flow equations on massively parallel supercomputers. The direct numerical simulations will help researchers to understand the global structure of the convective flow and the boundary layer dynamics for this new parameter regime. This will provide new insights into mysterious turbulent transport processes and the rare but potentially catastrophic events that can occur in turbulent systems.

Type: New
Title: "Upscaling Laws in Premixed Explosions"

Principal Investigator: Thierry Poinsot, CERFACS
Co-Investigator: Gabriel Stafflebach, CERFACS
Olivier Vermorel, CERFACS
Denis Veynante, Ecole Centrale Paris

Scientific Discipline: Chemistry: Combustion

INCITE Allocation: **86,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (86,000,000 processor hours)

Research Summary:
The advent of Computational Fluid Dynamics (CFD) as an alternative to expensive and dangerous experiments, and the recent emergence of Large Eddy Simulations (LES) in the field of turbulent combustion, have allowed for new perspectives on how to make explosion simulations truly quantitative.

This research, conducted by the European Centre for Research and Advanced Training in Scientific Computation (CERFACS) will study accidental gas explosions in buildings and develop models for turbulent pre-mixed flames. Using previous INCITE allocations, the team developed a unique experimental database created via LES. This database has led to a new experimental campaign which will allow researchers to check the validity of models over a range of scales previously not accessible.

The target configurations for the proposed research on gas explosions are the original small-scale configuration of 0.25 m long, and two larger configurations of 1.5 m and 6 m long. The experimental database includes several diagnostics—pressure signals, flame-front visualizations—for methane, propane and hydrogen. Databases for the medium- and large-scale configurations are more restrictive, considering only propane/air mixtures.

Based on these three experiments of increasing size, a unique set of data is available for validating and up-scaling LES models. In particular, this is a unique opportunity to highlight the limitations of constant-based models for flame wrinkling—the vorticity produced by various flame factors, such as stability and velocity—compared to the benefits that dynamic models may offer.

To perform these computations, CERFACS will rely on the AVBP code, one of the most advanced combustion solvers developed for parallel machines like the ALCF's Mira. AVBP has proven to be the proper tool to tackle explosion studies to achieve project objectives.

Type: New
Title: "Vibrational and Optical Spectroscopy of Electrolyte/Solid Interfaces"

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

Scientific Discipline: Chemistry: Physical

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

Research Summary:
Several federal funding agencies have adopted a strategy of sustained fundamental research to address the national energy problem. This project contributes to this strategy by tackling fundamental scientific issues underlying the key question of how best to take advantage of energy from the sun, e.g., through the formation of fuel from the oxidation and reduction of water.

Researchers from the University of California, Davis, and The University of Chicago will use large-scale quantum simulations to model, at the microscopic scale, the physical and chemical processes involved in photo-electrochemical (PEC) energy conversion. The project focuses on processes that occur at the interface between solid photo-electrodes and electrolytes (water with dissolved salts, acids, and bases). Although this project is focused on PEC, the methodologies and processes studied here from first principles are also relevant to other areas of interest to the energy problem, including electrical energy storage.

This project encompasses *ab initio* molecular dynamics simulations to obtain atomic trajectories, and compute ensemble averages of thermodynamic properties, and calculations, from first principles, of vibrational and electronic spectra. The simulations will rely on codes that have been optimized to take advantage of Mira's architecture, in particular the Qbox code, and that have shown to exhibit excellent parallel performance.

Researchers aim to provide the knowledge and computational tools necessary to interpret a large body of ongoing experiments on fuel production from water, and establish design rules to predict earth-abundant, non-toxic oxides with interfacial properties optimally suited to oxidize water.