Type: New
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 core-hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 "Titan"(25,000,000 core-hours)

Research Summary:
The researchers will study three types of problems: (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; (3) and the defect and dislocation structures and their dynamics in aluminum alloys.

While there have been many theoretical studies for these problems, the INCITE-supported project will have the following distinguishing characteristics: (1) ab initio non-adiabatic molecular dynamics will be used for the first time to study the carrier transport of thousand atom organic systems, with the potential to reveal underlying transport mechanisms; (2) A realistic atomic surface passivation model will be used to describe the nanocrystal surface, which enables the study of surface defect states, surface dipole moments, and their influence on carrier dynamics and charge transports. (3) Direct million atom simulations will be at a level higher than the classical force field or embedded atom model to study aluminum alloy defects and dislocations. Besides revealing the fundamental mechanisms in carrier transport and surface effects, the simulations will open up new areas of research and elevate the large-scale material simulations in these fields to new levels. For example, currently, non-adiabatic molecular dynamics are mostly based on model Hamiltonians. The project will use ab initio type Hamiltonians for thousand-atom systems. Previously, most nanocrystal simulations relied on artificial model surface passivations (e.g., used pseudo-hydrogen atoms). The researchers in this project will use realistic organic ligand passivations. Previous million atom dislocation and defect dynamics might be based on classical force field, embedded atoms, or quantum mechanics/molecular mechanics (QM/MM) approaches, but the project will use a DFT level approach (based on orbital free DFT, OF-DFT method). The higher level simulations will provide the ability to study new physics, e.g., the interplay between polaron effects and dynamic disorder in organic system, the exact nature of surface state, the carrier transport between nanocrystals, and the interaction and crossing of dislocation lines. The deepened understanding and answering of these fundamental questions will be critical to the future applications of these systems.

Type: New
Title: "Accelerator Simulations for the Intensity Frontier of Particle Physics"

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: **80,000,000 core-hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q "Mira" (30,000,000 core-hours)
IBM Blue Gene/P "Intrepid" (50,000,000 core-hours)

Research Summary:
Particle accelerators are an enabling technology for both basic research and the applied sciences. This project will advance basic science in the form of particle physics by assisting Fermilab in developing world leadership in the production of high-intensity proton beams through the proposed Project X. These proton beams will, in turn, be used to create the world's best neutrino, kaon and muon beams, allowing particle physicists to dramatically expand our understanding of rare and hard-to-detect phenomena.

A broad course of simulations will be necessary to aid in the plans for upgrades to two existing accelerators crucial to Project X, Fermilab's Booster and Main Injector. These simulations will efficiently utilize petascale computing resources by addressing those problems that are too computationally demanding to be performed as part of the ongoing simulation efforts utilizing commodity Linux clusters. The proposed simulations include large multi-bunch simulations, ensembles of smaller single-bunch simulations, and scans in the spaces of magnet configurations and operating parameters.

The results of these simulations will advance both accelerator physics and basic science by enabling discoveries in particle physics.

Type: New
Title: "Advanced Modeling of the Human Skin Barrier"

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

Scientific Discipline: Biological Sciences: Biophysics

INCITE Allocation: **65,000,000 core-hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 "Titan" (65,000,000 core-hours)

Research Summary:
Understanding the structure of the stratum corneum (SC) is relevant to pharmaceutical research applications dealing with drug delivery and personal care. This project complements the ongoing effort at the Procter & Gamble labs to probe the microscopic structure of the human skin barrier and its response to an array of medical and personal care products using advanced techniques. The goal is to build a more credible model of the complex and not well-understood SC lipid structure. The proposed molecular dynamics (MD) simulations will provide much needed insights into the complex interactions occurring between the various lipid components. This requires exploration of multiple, long MD trajectories for an ensemble of large (million atom) heterogeneous subsystems, each comprising different concentrations of component ceramides, cholesterol, and fatty acid molecules.

The primary objective of this work is to refine a fully atomistic model of the SC lipid matrix to identify the arrangement of the component molecules (ceramides, cholesterol, and free fatty acids) within the structural motifs, which support the observed short and long-range order. A secondary objective is to lay the groundwork for the use of modeling to explore the consequences of variations in composition of the SC component lipids using MD simulations as a complement to relatively low-resolution structural experiments. To date, skin penetration models have brought some predictive capabilities to bear on the topic of safety. While these models are quite predictive for compounds of specific molecular characteristics, they do not provide a wide enough range of predictive capability to aid in safety evaluation. This suggests that the underlying penetration mechanisms are mostly unaccounted for. While an overarching model is still in the distant future, the proposed work lays the foundations to obtain it.

Type: New
Title: "Attributing Changes in the Risk of Extreme Weather and Climate"

Principal Investigator: Michael Wehner, Lawrence Berkeley National Laboratory

Scientific Discipline: Earth Science: Climate Research

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

Research Summary:
Extreme weather has substantial impacts on human livelihoods and on natural systems. Changes in it are expected to lead to the most significant impacts of human induced climate change. Variations in such extreme events due to climate change might have already impacted society and their effects are very likely to increase in the future. Existing studies using climate models with a resolution of 100-200 km suggests that changes in the occurrence of extreme events is already notable and will be larger in future. However, many of the most damaging extreme events occur at small spatial and temporal scales relative to the resolution of these models and damage from them occurs at smaller scales still. Hence, results from such models should be interpreted with great caution. We aim to make a significant advance in this field by generating and analyzing two large ensembles of a ~25km resolution global climate model.

This project's principal computational vehicle will be a very high-resolution version of the most recent publicly released version of the Community Atmospheric Model (CAM5.1). The first ensemble will emulate the "world that actually was," while the second ensemble will emulate "the world that might have been" had human activities not interfered with the climate system. The computational resources provided by INCITE will enable a significant leap forward in climate science's ability to understand causes of changes in the risk of localized extreme events, including severe weather and hurricanes.

Type: Renewal
Title: "Cellulosic Ethanol: Simulation of Multicomponent Biomass Systems"

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

Scientific Discipline: Biological Sciences: Biophysics

INCITE Allocation: **78,000,000 core-hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 "Titan"(78,000,000 core-hours)

Research Summary:
Lignocellulosic biomass is a complex material composed of cellulose microfibrils laminated with hemicellulose, pectin, and lignin polymers. Rational strategies for improving the efficiency of biofuel production from plant cell wall lignocellulosic biomass *via* cellulose hydrolysis require a detailed understanding of the structure and dynamics of the biomass. To reduce biomass recalcitrance, or resistance, to hydrolysis by the improvement of pretreatment and the design of improved feedstock plants, a detailed understanding of biomass structure, mechanics, and response to pretreatment regimes is needed. This project will extend the lengthscale of the systems under study to enable the simulation of full lignocellulosic biomass systems, consisting of cellulose, lignin and hemicelluloses, together in specific cases with hydrolyzing enzymes.

This project will provide simulation models of biomass and enzyme interactions that will help us understand the physical origins of biomass recalcitrance via the molecular dynamics (MD) method involving the stepwise integration of the equations of motion. The detailed multiscale structure revealed by these simulations will aid in understanding biomass recalcitrance to hydrolysis and in engineering efforts to improve second-generation biofuel yield.

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

Principal Investigator: Warren Washington, University Corporation for Atmospheric Research

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

Scientific Discipline: Earth Science: Climate Research

INCITE Allocation: **215,000,000 core-hours**
Site: Argonne National Laboratory
Oak Ridge National Laboratory
Machine (Allocation): IBM Blue Gene/Q "Mira" (130,000,000 core-hours)
IBM Blue Gene/P "Intrepid" (25,000,000 core-hours)
Cray XK7 "Titan"(60,000,000) core-hours)

Research Summary:
The Climate Science Computational End Station (CCES) will predict future climates using scenarios of anthropogenic emissions and other changes resulting from energy policy options. CCES will also improve the scientific basis, accuracy, and fidelity of climate models, delivering climate change simulations that directly inform national science policy, thereby contributing to the DOE, NSF and NASA science missions. Of particular importance is the improved simulation of the global carbon cycle and its feedbacks to the climate system, including its variability and modulation by ocean and land ecosystems. Continuing model development and extensive testing of the CCSM system to include recent new knowledge about such processes is at the cutting edge of climate science research.

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

Principal Investigator: Lorna Smith, University of Edinburgh

Scientific Discipline: Computer Science

INCITE Allocation: **21,000,000 core-hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 "Titan"(21,000,000 core-hours)

Research Summary:
The main goal of the €8.3M, three year CRESTA project is to develop techniques and solutions addressing the most difficult challenges facing exascale computing will provide. The project has two integrated strands; the first focused on enabling a set of key applications for exascale, or the *co-design applications*, the second focused on exploring and building appropriate *systemware* for exascale platforms.

The scale of today's leading HPC systems, operating at the petascale, has put a strain on many simulation codes, both scientific and commercial. The challenge addressed by CRESTA is to move simulation beyond the petascale to the exascale, as articulated by the International Exascale Software Project at the global level and the European Exascale Software Initiative in Europe. The co-design applications therefore lay at the heart of CRESTA. Together they represent an exceptional group of petascale applications used throughout academia and industry which have demonstrated a clear requirement for exascale performance to address key scientific challenges. CRESTA therefore requires access to the Cray XK7 at ORNL to facilitate its exascale research program around four applications—Biomolecular Simulations, Soft Matter Simulations, Global Numerical Weather Prediction, and Engineering—as a means of validating their performance at large-scale whilst also achieving key scientific results.

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

Principal Investigator: Lee Shunn, Cascade Technologies, Inc.
Co-Investigators: Shoreh Hajiloo, GE Global Research

Scientific Discipline: Engineering: Fluids and Turbulence

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

Research Summary:
Many industrial combustion systems are subject to instabilities that complicate operations and present cumbersome limitations to safety and efficiency. Since unstable combustion can lead to intense pressure fluctuations and increased heat transfer to combustor surfaces, the consequences are often problematic and in extreme cases can result in structural damage.

This project intends to numerically reproduce common combustion instabilities to better understand physical mechanisms behind their generation and to develop strategies to eliminate or control them.

The researchers will develop and validate a high-fidelity large eddy simulation (LES) combustion model for accurately predicting unsteady combustion problems based on the flamelet/progress-variable (FPV) approach of Pierce and Moin (2004). The LES results will contribute to a more thorough understanding of combustion physics in systems that are prone to instability-induced failures.

Steady and unsteady FPV models will be tested and compared and the effects of turbulent wall models and non-adiabatic conditions will be evaluated. Simulation results will be used to create a high-quality numerical database for assessment of industrial combustor performance and evaluation of lower-fidelity prediction tools.

Successful, high-fidelity simulations of these scenarios will help build the scientific insight and understanding necessary to engineer practical solutions to the ubiquitous challenges of combustion instabilities.

Type: New
Title: "Computational Prediction and Discovery of Magnet Materials"

Principal Investigator: Bruce Harmon, Ames Laboratory
Co-Investigators: Kai-Ming Ho, Ames Laboratory
Cai-Zhuang Wang, Ames Laboratory

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

INCITE Allocation: **45,000,000 core-hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 "Titan"(45,000,000 core-hours)

Research Summary:
Permanent magnetic materials are an essential component in electrical generators and motors. Permanent magnets are also essential in computer hard drives and other electro-mechanical devices, including levitators. Because of the role of such devices in new energy economies there is a greatly increased demand for strong permanent magnet materials. Currently, the most widely used permanent magnetic materials are Nd2Fe14B and SmCo5, both containing rare earth (RE) metals. Owing to limited RE mineral resources and further limited RE metal supplies, the price of Nd and Sm and all other rare earth metals increased dramatically in the past several years. Thus, there is a strategic national need to discover replacement magnet materials for Nd2Fe14B and SmCo5 to meet performance and cost goals for advanced electric drive motors and generators.

To meet performance and cost goals for advanced electric drive motors, it is essential to improve the alloy design and processing steps for permanent magnets. This computational project is an integrated part of a DOE team-project (including experimental synthesis and characterization) to develop the materials and processes needed to fabricate high performance permanent magnets (PM) that can be used for mass production of vehicle traction motors with an internal PM rotor design that meets the USA DRIVE targets for cost, volume, and weight. The project is driven both by the technical specifications that the fully developed PM materials must meet for operation at elevated temperature (180-200℃) with adequate magnetic flux and coercivity, and by the market factors of reduced cost and wide availability. While such magnetic material requirements may be achieved most readily using rare earth (RE)-based permanent magnets, the urgent concerns over elevated cost and foreign control of the current supply of rare earth resources have motivated the initiation of this major high risk thrust: development of non-RE based permanent magnets with performance metrics aligned with advanced motor requirements.

Type: New
Title: "Computational Studies of Nucleosome Stability"

Principal Investigator: George Schatz, Northwestern University
Co-Investigators: Yuri Alexeev, Argonne National Laboratory
Graham Fletcher, Argonne National Laboratory
Maricris Mayes, Argonne National Laboratory

Scientific Discipline: Biological Sciences: Biophysics

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

Research Summary:
This INCITE research project led by George Schatz is concerned with the molecular dynamics and electronic structure studies of the nucleosomes, which are complexes of DNA and proteins in chromatin and account for 75-90% of the packaging of the genomic DNA in mammalian cells. Nucleosomes consist of 147 base pair (bp) of DNA wrapped 1.7 times around a complex of proteins known as the histone octamer to give an overall nucleosome diameter of 11 nm, and a rather small DNA radius of curvature of 4.1 nm. Understanding the base-pair sequence dependence and propensities formation has long been a goal in cell biology as nucleosome stability is thought to be an important component of transcriptional regulation.

The research team will make a fundamental advance in computational modeling of nucleosome stability using the Argonne Leadership Computing Facility (ALCF). It is clear that there is now a significant opportunity for taking a major step forward in our understanding of nucleosome binding through the use of high performance computation (HPC). Empirical potential classical molecular dynamics calculations are now possible for whole nucleosome structures, and such calculations on an HPC system for a long enough time (~1 microsecond) to equilibrate structures that include explicit water and ions would enable us to determine useful information about nucleosome binding, including both sequence dependence effects and the effect of epigenetic markers. Electronic-structure studies of smaller models of the nucleosomes using the fragment molecular orbital (FMO) method will also be performed.

Type: New
Title: "Computing the Dark Universe"

Principal Investigator: Salman Habib, Argonne National Laboratory

Scientific Discipline: Physics: Astrophysics

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

Research Summary:
The scientific aim of the project led by Salman Habib is to establish a computation-based discovery capability for critical cosmological probes by exploiting next-generation high performance computing architectures.

The simulations will study the clustering of matter in the Universe and the evolution of the clustering as a multi-dimensional cosmological probe. They will provide access to studying different aspects of the 'Dark Universe', dominated by the mysterious duo of dark energy and dark matter. The project will bring together two next-generation high performance computation (HPC) codes, the HACC (Hardware/Hybrid, Accelerated Cosmology Codes) framework for N-body simulations, and NYX, a new cosmological hydrodynamics solver.

It is widely recognized that cosmology is entering one of its most scientifically exciting phases. Two decades of surveying the sky have culminated in a celebrated "Cosmological Standard Model". Yet, for two of its key pillars, dark energy and dark matter—together accounting for 95% of the mass-energy of the universe—remain mysterious. Key foundational questions demand answers: What is dark matter made of? Why is the Universe's expansion rate accelerating? Should general relativity be modified? What is the nature of primordial fluctuations? What is the exact geometry of the universe?

The ALCF's Mira, an IBM Blue Gene/Q, will enable the team's ultimate goal to compare the best telescope observations of the structure of the universe to the structure displayed in the computer model, to test the current cosmological theory and perhaps gain insights to some of these foundational questions.

Type: Renewal
Title: "CyberShake3.0: Physics-based Probabilistic Seismic Hazard Analysis"

Principal Investigator: Thomas Jordan, University of Southern California
Co-Investigators: Jacabo Bielak, Carnegie Mellon University
Yifeng Cui, San Diego Supercomputer Center
Geoffrey Ely, University of Southern California/Argonne National Laboratory
Philip Maechling, University of Southern California
Kim Olsen, San Diego State University
Ricardo Taborda, Carnegie Mellon University

Scientific Discipline: Earth Sciences: Geological Sciences

INCITE Allocation: **68,000,000 core-hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q "Mira" (16,000,000 core-hours)
Machine (Allocation): IBM Blue Gene/P "Intrepid" (7,000,000 core-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 "Titan"(45,000,000 core-hours)

Research Summary:
Recent destructive earthquakes including Haiti (2010), Chile (2010), New Zealand (2011), and Japan (2011) highlight the national and international need for improved seismic hazard information. What can be done to reduce the hazard from these inevitable natural events? INCITE high-performance computing resources can be used to reduce the hazards from these natural events. However, SCEC researchers need access to substantial HPC resources to apply recent computational improvements into standard seismic hazard forecasts.

SCEC will use INCITE resources to calculate an improved probabilistic seismic hazard forecast for California. The SCEC CyberShake 3.0 hazard model calculation will be based on a new USGS Unified California Earthquake Rupture Forecast 3.0 (UCERF3.0) scheduled for release by the USGS in June 2012. It will also produce a seismic hazard model for California that is directly comparable to the official USGS seismic hazard model and will show the seismic hazard community how HPC resources can improve official, broad-impact, USGS-regulated seismic hazard forecast data products. In the United States, the USGS has official regulatory authority to produce seismic hazard estimates. Official USGS seismic hazard estimates are used as inputs into state and national building code processes, thereby affecting billions of dollars in construction costs each year. Scientific improvements to seismic hazard forecasts must be accepted and adopted by the USGS before such improvements can have broad impact. SCEC, as a USGS- and NSF-funded research center, is in a unique position to pioneer, and accelerate, the application of HPC computational techniques into official, broad impact, seismic hazard forecast models.

Type: New
Title: "Developing and Testing Future Applications and Operating Systems for Exascale"

Principal Investigator: Maya Gokhale, Lawrence Livermore National Laboratory
Co-Investigators: Eric Van Hensbergen, IBM

Scientific Discipline: Computer Science: Computer Science

INCITE Allocation: **50,000,000 core-hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q "Mira" (30,000,000 core-hours)
IBM Blue Gene/P "Intrepid" (20,000,000 core-hours)

Research Summary:
The U.S. Department of Energy (DOE) has begun to determine the biggest problems likely to be seen on machines with 100 million cores (exascale systems). Two areas of concern are runtime systems, and adaptability.

Exascale computing systems will provide a thousand-fold increase in parallelism, challenging scalability and adaptability of software stacks and applications. Systems software for exascale machines must provide the infrastructure to support existing applications while simultaneously enabling efficient execution of new programming models that naturally express dynamic, adaptive, irregular computation; coupled simulations; and massive data analysis in an unreliable hardware environment with billions of threads of execution.

Project researchers will develop systems software and runtime support of a new approach to the data and work distribution based on task queues and dynamic adaptation for load balancing and fault mitigation. The project work includes adaptive, application tailored OS services optimized for multi-to-many core processors; advanced virtualization infrastructure; a distributed, fault tolerant key-value store that is the basis for task and data distribution; and fault tolerant load balancing schemes for massively task parallel applications.

Project researchers will test:

- Quantum chemistry kernel implementations using a work queue model (PNNL, Sandia, and OSU)
- An adaptive load balancing task distribution library (PNNL, OSU)
- Scalable implementations of a distributed data store (Boston University)
- New OS virtualization environments and runtime (Boston University)
- Asynchronous graph traversal algorithms based on a distributed work-queue model (LLNL)

Type: New
Title: "Direct Numerical Simulations of High Reynolds Number Turbulent Channel Flow"

Principal Investigator: Robert Moser, University of Texas

Scientific Discipline: Engineering: Fluids and Turbulence

INCITE Allocation: **175,000,000 core-hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q "Mira" (175,000,000 core-hours)

Research Summary:
Approximately 28% of U.S. energy resources are expended on transportation, in which vehicles move through air or water, or fluids are transported through pipes and ducts. The energy expenditure is due to turbulence and the energy it dissipates. Since much of the drag in these flows is due to the turbulent skin friction, much of this energy consumption is caused directly by wall-bounded turbulent shear layers. Further, the remainder of the energy is dissipated primarily in the wakes of vehicles; the characteristics of which are also controlled by the turbulent boundary layers on the vehicle surfaces. The engineering design of these fluid systems, particularly to manipulate turbulent wall layers, is hindered by our poor understanding of the physics of turbulence in these flows.

We propose to use the petascale computing power of Mira, an IBM Blue Gene/Q, to perform direct numerical simulations (DNS) of high Reynolds number turbulent wall-bounded flow in a channel. This DNS is aimed at developing a nearly complete understanding of the phenomena dominating wall-bounded turbulence, which is central to the energy losses inherent in transportation.

The central emphasis of this research is on reaching a sufficiently high Reynolds number to explore the physics that arise in the overlap region. The overlap region is where the viscous near-wall turbulence interacts with the outer-layer turbulences. This interaction is key to understanding high Reynolds number turbulent wall layers. To investigate this interaction, it is necessary that the Reynolds number be sufficiently high so that there is a substantial disparity in scale between the inner and outer layers. The results can then be extrapolated to arbitrary Reynolds numbers. Analysis of recent DNS of channel flow at $Re_\tau \approx 1000$ and 2000 indicate that $Re_\tau \approx 5000$ on a $16384 \times 1024 \times 12288$ grid should yield sufficient scale separation. This simulation will be performed using the supercomputing software that the proposing team has developed for Mira, an IBM Blue Gene/Q.

Type: New
Title: "Enabling Green Energy and Propulsion Systems via Direct Noise Computation"

Principal Investigator: Umesh Paliath, GE Global Research
Co-Investigators: Ramesh Balakrishnan, Argonne National Laboratory
Giridhar Jothiprasad, GE Global Research
Anupam Sharma, Iowa State University

Scientific Discipline: Engineering: Fluids and Turbulence

INCITE Allocation: **105,000,000 core-hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q "Mira" (45,000,000 core-hours)
IBM Blue Gene/P "Intrepid" (60,000,000 core-hours)

Research Summary: GE Global Research is using the Argonne Leadership Computing Facility (ALCF) to deliver significant improvements in efficiency, (renewable's) yield and lower emissions (noise) for advanced energy & propulsion systems. Understanding the fundamental physics of turbulent mixing has the potential to transform product design for components such as airfoils and jets to achieve improved performance, life and efficiency.

The GE team is leveraging the ALCF's increased high performance computational capability to now demonstrate the industrial impact of high-fidelity numerical methods. Large eddy simulations (LES) of turbulent wake and jet mixing phenomena will be conducted with a focus on realistic jet engine/wind turbine geometry and operating conditions.

Under previous INCITE awards, project researchers have utilized the ALCF facilities to demonstrate the applicability of the LES approach to predict free shear layer flow for complex jet nozzles, and turbulent boundary layer flow at high Reynolds number wind turbine airfoils. More recently, the team has applied the turbulent wake prediction capability to start evaluating broadband noise generation due to the wake interaction with an airfoil.

This research will enhance the understanding of the physics of turbulent noise generation mechanisms from industrial product, by coupling the LES approach with modern HPC facilities. GE's work will lead to the direct transfer of advanced simulation technology into the design of the next generation of green energy products.

Type: New
Title: "Evaluation of Mesoscale Atmospheric Model for Contrail Cirrus Simulations"

Principal Investigator: Roberto Paoli, CERFACS
Co-Investigators: Juan Escobar, Laboratoire d'Aérologie
Odile Thouron, CERFACS

Scientific Discipline: Earth Science: Environmental Sciences

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

Research Summary:
As the demand of air travel continues to grow, the environmental impact of aviation represents a source of increasing concern among scientists and policymakers. Because of long residence time, low background concentrations and large radiative sensitivity at cruise altitude, aircraft emissions can affect the chemical composition of the atmosphere and modify or create additional ice clouds in the upper-troposphere-lower stratosphere (UTLS) in the form of contrails and cirrus clouds.

These "contrail cirrus" have an important environmental significance because they artificially increase Earth's cloudiness, and become almost indistinguishable from natural cirrus.

This project will use large eddy simulations to analyze the three-dimensional structure and the ice particle distribution of a contrail generated from an airliner flying at cruise altitude. Simultaneously, this project will also provide a unique opportunity and insight into the physics of contrails cirrus in atmospheric situations found in typical commercial routes.

The project will be carried out in two main steps:

1. Researchers will select one flight of the campaign corresponding to a given set of ice microphysical properties (size distribution and shape) and spatial structure. Researchers will test two different turbulence-forcing parameters that reproduce the observed turbulence characteristics. This defines the initial time t0 of the LES.

2. Meso-NH will be run for an additional hour of physical time and the results contrasted with the observed data at t0+1h. Researchers will vary up to six sets of optical properties of the model in such a way to match the size and particle distributions of the experiment.

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

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

Scientific Discipline: Engineering: Fluid-Structure Interaction

INCITE Allocation: **45,000,000 core-hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 "Titan" (45,000,000 core-hours)

Research Summary:
This project will match the third year of an NSF PetaApps project for using simulation science to explore ways to minimize the damage caused by an unintentional detonation of a large array of explosive devices. Specifically, the project will examine different packing arrangements of the devices to prevent a transition from a low-violence deflagration (thermal combustion) to an extremely violent detonation reaction. The motivation for this work is illustrated by a 2005 semi-truck accident in which 36,000 pounds of seismic boosters ignited and detonated, destroying a section of a Utah state highway and adjacent railway.

This project uses the Uintah open-source software (developed initially at the University of Utah's DOE ASC C-SAFE Center) that has been used to study the violence of an explosion from a single exploding container. Uintah solves fluid-structure interaction problems using a combination of a multi-material fluid flow solver (ICE) and a particle-based algorithm for the solid materials (MPM). Uintah also uses a novel asynchronous task-based methodology that supports dynamic in order and out-of-order task execution and a hybrid MPI-Pthread model.

Resources such as Titan are needed because NSF platforms do not have sufficient resources to perform the full simulation. The physical mechanisms of a large scale DDT have never been investigated, and understanding them will lead to the increased safety of our roads and railways. Researchers hypothesize that hot combustion gases from a slow deflagration can damage the explosives, creating pockets of high pressure gas in the array leading to a detonation. Preventing these pockets from forming is of fundamental importance.

Type: New
Title: "From LES to DNS of Explosions in Semi-confined Domains"

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

Scientific Discipline: Chemistry: Combustion

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

Research Summary:
Accidents due to gas explosion in industrial buildings are a major safety issue. Understanding the mechanisms controlling explosions in buildings, typically in offshore platforms, is an economical and physical challenge.

Gas explosions are studied in confined or semi-confined vessels with obstacles where a premixed flame is ignited. The propagation of the flame and the resulting over-pressure are the key parameters that define safety concepts and guidelines for explosion protection. Codes based on the unsteady Reynolds averaged Navier-Stokes (URANS) approach are standard for gas explosion studies at industrial scales but they rely on crude parameterizations.

The recent emergence of large eddy simulation (LES) in the field of turbulent combustion opens new perspectives to make explosion simulations truly quantitative. Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique (CERFACS) recent LES of explosions has revealed the importance of the laminar phase which is often neglected or computed in approximate ways because the codes used in the literature are adapted to turbulent flames and not to laminar ones. A predictive solver must be able, with the same sub-models, to compute both a laminar flame and a turbulent one, something which is almost never done in combustion simulations.

This project aims to use the cutting-edge computational power of the IBM Blue Gene/P and Q systems at the ALCF to achieve this objective. It also suggests that a proper way to investigate the question is to begin by a fully resolved, DNS-type (Direct Numerical Simulation), simulation of the same flow to have a reference solution.

Type: New
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

Scientific Discipline: Earth Science: Geological Sciences

INCITE Allocation: **100,000,000 core-hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 "Titan"(100,000,000 core-hours)

Research Summary:
Precise information about the structure of the solid Earth comes from seismograms recorded at the surface of a highly heterogeneous lithosphere. 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. Such methods require the execution of complex computational procedures that challenge the most advanced high-performance computing systems. The researchers' ultimate goal is to move toward "adjoint tomography" of the entire planet.

Adjoint tomography provides new opportunities for improving images of the Earth's interior. Better resolution of tomographic images at all scales is essential for understanding mantle dynamics and related surface dynamics, 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.

Adjoint methods were introduced in the 1980s, but their application only became feasible recently with the availability of 3D wave propagation solvers and high-performance computing resources. This project addresses the long-standing challenge of imaging Earth's interior based on full waveform inversion on a global scale. The research will result in advances in seismology, such as iteratively updating and increasing the resolution of seismic images of the entire planet using adjoint techniques.

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

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

Scientific Discipline: Materials Science: Rheology

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

Research Summary:
Concrete is the most widely used building material in the world, representing a 100 billion dollar industry in the U.S. that is crucial to the nation's physical infrastructure. There is now a strong interest in making concrete a more sustainable material by finding new ways to recycle it, and by changing its ingredients in order to reduce the amount of greenhouse gas resulting from its production. As new mixture designs of concrete are developed to meet these needs, it is important to measure and control rheological properties, i.e. flow properties, to satisfy performance specifications.

Due to the complex nature of concrete, which is comprised of a suspension of rocks and sand embedded in cement paste, a non-Newtonian fluid whose properties change with time, it is a challenge to measure its rheological properties. Concrete rheometers are often utilized for such tasks but, at best, they make semi-empirical links between torque and angular velocity measurements and the concrete's true rheological properties. As a result, it is difficult to relate measurements made on different rheometers and, further, to understand how such measurements predict concrete performance in the field.

This project addresses the problem of relating measured quantities like torque and angular velocity within non-analytical rheometer and mixing geometries to fundamental rheological properties, like viscosity versus strain rate, by studying the flow of concrete in such rheometers and by the development of standard reference materials to calibrate rheometers. Results from this research will advance the science of dense suspensions while addressing the measurement science needs in the concrete industry through the development of standard reference materials.

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

Principal Investigator: Choong-Seock Chang, Princeton Plasma Physics Laboratory

Co-Investigators: Jan Hesthaven, Brown University
Scott Klasky, Oak Ridge National Laboratory
Scott Parker, University of Colorado

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation: **100,000,000 core-hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 "Titan"(100,000,000 core-hours)

Research Summary:
It is a common prediction that the world's oil resources will run out in less than 50 years if the oil production rate should increase to meet the rise in world energy demand. Thermonuclear fusion energy has been stably powering the sun and the stars for billions of years. Its energy source is virtually inexhaustible and intrinsically safe and will soon be tested in a prototype reactor known as ITER.

This projects proposes to perform a systematic multi-year study, based upon an extreme-scale, first-principles kinetic approach using the XGC1 global edge gyrokinetic code, to address the challenges associated with plasma transport physics in the edge region of magnetically confined plasmas. Success of ITER is critically dependent upon good edge plasma confinement. Despite their importance, neither the edge confinement physics nor the nonlocal core-edge interaction physics is well understood.

The proposed work is to attack this problem head-on using a first-principles code on the leadership-class computer Titan, representing the essential mission of the new SciDAC-3 Center for Edge Physics Simulation (EPSI). The proposed research integrates the most important physical processes on overlapping temporal and spatial scales to study: (a) the predictive understanding of edge pedestal formation, structure and dynamics; (b) the effect of the edge plasma on core confinement; (c) the heat load on the material wall; and (d) the transitions and thresholds for enhanced confinement regimes. Governing equations will be improved in association with the experimental validation activities and in collaboration with the analytic equation development efforts in EPSI and in the community.

Joint research in EPSI with the SciDAC-3 FASTMath, SUPER, QUEST, and SDAV Institutes will be utilized to increase the reliability and efficiency of the computational research in the extreme-scale, heterogeneous hardware/software and data production environment.

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

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

Scientific Discipline: Chemistry: Combustion

INCITE Allocation: **100,000,000 core-hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 "Titan"(100,000,000 core-hours)

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

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

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

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

Scientific Discipline: Physics: Plasma Physics

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

Research Summary:
To build the scientific foundations needed to develop fusion power as a clean and sustainable energy source, the timely development of a high-physics-fidelity predictive simulation capability for magnetically confined fusion plasmas is essential. The goal of this project is to harness the power of supercomputers to simulate the complex dynamics governing the magnetic confinement properties of fusion-grade plasmas, especially ITER, a multi-billion dollar international experiment under construction in France involving partnership of seven governments representing over half of the world's population.

An associated challenge is to better understand, predict, and control instabilities caused by the unavoidable spatial variations in such systems. One consequence is the occurrence of microturbulence, which can significantly increase the transport rate of heat, particles, and momentum across the confining magnetic field in tokamak devices. Understanding and possibly controlling the balance between these energy losses and the self-heating rates of the actual fusion reaction is key to achieving the efficiency needed to help ensure the practicality of future fusion power plants.

This project will use the Argonne Leadership Computing Facility resources to capture new physics insights into the key question of how turbulent transport and associated confinement characteristics scale from present generation laboratory plasmas to the much larger ITER-scale burning plasmas. The large-scale, high-resolution simulations will also provide the knowledge and experience necessary to help introduce more comprehensive gyrokinetic particle-in-cell (PIC) codes into the low memory per core path to exascale era of modern supercomputing applications.

Type: Renewal
Title: "Lattice QCD"

Principal Investigator: Paul Mackenzie, Fermilab
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, Thomas Jefferson National Accelerator Facility
Steven Sharpe, University of Washington
Robert Sugar, University of California, Santa Barbara

Scientific Discipline: Physics: Particle Physics

INCITE Allocation: **430,000,000 core-hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q "Mira" (250,000,000 core-hours)
IBM Blue Gene/P "Intrepid" (40,000,000 core-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 "Titan" (140,000,000 core-hours)

Research Summary:
Researchers are advancing exploration in lattice quantum chromodynamics and other strongly coupled field theories of importance to the study of high energy and nuclear physics. Leadership-class computers will be used to generate gauge configurations with up, down, strange, and, in one case, charmed quarks on lattices that are sufficiently fine grained and have sufficiently small up and down quark masses to enable full control of systematic errors for a number of key quantities. Four quark actions will be used in this work: domain wall, highly improved staggered, and isotropic and anisotropic clover. Each has advantages for different aspects of the work. In addition, they are creating new ensembles of configurations that will allow the study of the properties of the quark-gluon plasma and the behavior of new strongly coupled gauge theories that have been proposed to explain experiments at the Large Hadron Collider (LHC).

A major goal is to determine a number of underlying parameters of the standard model of subatomic physics, including the masses of the quarks, the strong coupling constant and elements of the Cabibbo-Kobayashi-Maskawa (CKM) matrix. Other goals are to determine the mass spectrum of strongly interacting particles; to calculate the electromagnetic properties of low-lying baryons and meson radiative transitions; to obtain a quantitative understanding of the internal structure of the nucleon; to predict the interactions among strongly interacting particles; and to investigate the properties of strongly interacting matter at high temperatures and densities. These goals are essential for meeting the milestones set out by the U.S. Department of Energy's Office of Science.

Type: Renewal
Title: "Magnetic Reconnection in High-Energy-Density Laser-Produced Plasmas"

Principal Investigator: Amitava Bhattacharjee, University of New Hampshire
Co-Investigators: Naoki Bessho, University of New Hampshire
William Fox, University of New Hampshire
Kai Germaschewski, University of New Hampshire
Yi-Min Huang, University of New Hampshire

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation: **35,000,000 core-hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 "Titan"(35,000,000 core-hours)

Research Summary:
Magnetic reconnection—the process by which the magnetic topology in plasmas is rearranged—is ubiquitous in fusion, space and astrophysical plasmas. It is widely believed to play a central role in phenomena as diverse as sawtooth crashes in fusion plasmas, magnetospheric substorms, and solar flares, which are among some of the most challenging problems in plasma physics. This project focuses on magnetic reconnection as observed in high-energy-density (HED), laser-produced plasmas in the presence of extremely high magnetic fields. The computations are central to the DOE Experimental Program to Stimulate Competitive Research's Center for Integrated Computation and Analysis of Reconnection and Turbulence. It is a main premise of the center that fundamental aspects of magnetic reconnection and turbulence in fusion devices, smaller-scale laboratory experiments, and space and astrophysical plasmas can be viewed from a common perspective, and that progress in understanding in any of these interconnected fields is likely to lead to progress in others.

Recent experiments on magnetic reconnection in HED laser-produced plasmas open up a new experimental regime, potentially of interest for plasma astrophysics as well as inertial fusion energy applications. This project seeks to improve our understanding of these experiments and this general regime of reconnection in large systems at the intersection of kinetic, collisional, and two-fluid effects, through a detailed comparison of computation (including both kinetic and fluid codes) with experiment, with the goal of bringing the two into quantitative agreement.

Type: New
Title: "Multibillion-atom MD Studies of the Mechanical Response of Nanocrystalline Ta"

Principal Investigator: Timothy Germann, Los Alamos National Laboratory
Co-Investigators: Ramesh Balakrishnan, Argonne National Laboratory
Eduardo Bringa, La Universidad Nacional de Cuyo
Virginie Rollin, Embry-Riddle Aeronautical University
Ramon Ravelo, The University of Texas at El Paso

Scientific Discipline: Materials Science: Nanomechanics

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

Research Summary:
Just over 50 years ago, British metallurgists E. O. Hall and N. J. Petch independently discovered a striking relationship between the strength of steel samples and their grain size; namely, that the yield stress σ_y increases with decreasing grain diameter d with an inverse square-root dependence: $\sigma_y = \sigma_0 + k\, d^{-1/2}$.

Since then, materials scientists have found that this empirically observed "Hall-Petch" relationship is surprisingly universal. The yield, flow, and fracture stresses for a wide variety of materials obey a similar relationship down to the smallest grain sizes typically encountered.

However, this dependence must eventually break down; materials cannot continue to become stronger as the grain sizes approach the atomic (sub-nm) scale, since then materials become amorphous rather than (poly-)crystalline. Where this breakdown occurs remains difficult to probe experimentally, due to the challenges in synthesizing samples with well-controlled nanoscale grain sizes.

This project will conduct Molecular Dynamics (MD) simulations of compression under uniaxial strain of Tantalum nanocrystalline samples. This project will model grain sizes between 70 nanometers and 0.4 micrometers, which is well above grain sizes ever modeled so far with 3D MD simulations and are the first step towards micron-size simulations, matching the length and time scales experimentally accessible at Argonne's Advanced Photon Source (APS) and SLAC's Linac Coherent Light Source (LCLS).

The results of this research will have a significant impact in the materials science community, both because of the scale of the simulations proposed, because of the grain sizes investigated and because of the physics insight that we can gain from such simulations.

Type: Renewal
Title: "Multiscale Blood Flow Simulations"

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

Scientific Discipline: Biological Sciences: Biophysics

INCITE Allocation: **71,000,000 core-hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P "Intrepid" (20,000,000 core-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 "Titan"(51,000,000 core-hours)

Research Summary:
This project will conduct physiologically correct multiscale simulations of the human vascular networks, focusing on multiscale modeling of devastating diseases such as malaria, sickle cell anemia, and cerebral aneurysms. The expected scientific result is the quantification of the biophysical features in both diseases at the mesoscopic and microscopic levels.
Researchers propose multiscale simulations for modeling blood flow in the human brain vasculature, the first of its kind, consisting of hundreds of large 3D arteries (Macrovascular Network, MaN), 10M arterioles (Mesovascular Network, MeN), and 1B capillaries (Microvascular Network, MiN). For MiN, the project will employ dissipative particle dynamics (DPD) simulations on representative capillary domains modeling explicitly (down to protein-level) the red blood cells.

The project has three phases. The first is to simulate the flow structure interaction (FSI) in patient-specific aneurysms to evaluate the effect of FSI on sounds produced by aneurysms—a possible diagnostic breakthrough for clinical practice. The second is to simulate the rupture of aneurysms using continuum-atomistic modeling that will shed light into this process and provide quantitative information on its genesis and hence possible clinical treatments. The third will consist of simulations applicable to the arterioles and capillary bed for red blood cell-related pathologies.

Type: Renewal
Title: "Multiscale Modeling of Energy Storage Materials"

Principal Investigator: Gregory A. Voth, University of Chicago

Scientific Discipline: Materials Science: Condensed Matter and Materials

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

Research Summary:
Reliance on fossil fuels is becoming increasingly recognized as a threat to national security and the climate patterns of the planet. In response to these crises, the U.S. Department of Energy (DOE) has listed the transformation of the energy system of the country as a central goal to achieving its mission of guaranteeing the future prosperity of the nation. In particular, fuel cells and lithium-ion batteries have been emphasized to replace the internal combustion engine in automobiles and already have applications in personal electronics.

The primary barrier remains the optimization of new materials, with current design efforts often relying on intuition-based "guess and check" approaches. In order to avoid these inefficient methods, the project team led by Gregory Voth will utilize the Argonne Leadership Computing Facility's resources to achieve truly transformative breakthroughs in battery and fuel cell engineering. It is anticipated that computational modeling will be essential to guide experimental efforts.

The leadership class computing resources provided by the INCITE program will be used for the multiscale modeling of charge transport processes in materials relevant to fuel cell and battery technologies. The primary goal of this work is the development of methods that are both systematic across several length scales and predictive for materials design. These efforts carry the potential for significant impact on both chemistry and material science communities through the development of multiscale methods, as well as provide tools for the design of next generation fuel cells and batteries for application to the looming energy crisis.

Type: New
Title: "Next-Generation Petascale Simulations of Type Ia Supernovae"

Principal Investigator: Don Lamb, University of Chicago
Co-Investigators: Alan Calder, Stony Brook University
Chris Daley, University of Chicago
Benedikt Diemer, University of Chicago
Anshu Dubey, University of Chicago
Carlo Graziani, University of Chicago
Aaron Jackson, U.S. Naval Research Laboratory
George Jordan, University of Chicago
Richard Kessler, University of Chicago
Dongwook Lee, University of Chicago
Min Long, University of Chicago
Vitali Morozov, Argonne National Laboratory
Michael Papka, Argonne National Laboratory
Katherine Riley, Argonne National Laboratory
Dean Townsley, University of Alabama
Daniel Van Rossum, University of Chicago
Venkatram Vishwanath, Argonne National Laboratory
Klaus Weide, University of Chicago

Scientific Discipline: Physics: Astrophysics

INCITE Allocation: **105,000,000 core-hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q "Mira" (75,000,000 core-hours)
IBM Blue Gene/P "Intrepid" (30,000,000 core-hours)

Research Summary:
Type Ia supernovae are among the brightest and most energetic events in the universe. They are important tools of cosmology. Lamb's will perform large-scale simulations of Type Ia supernovae with the goal of better understanding these explosions, enabling astronomers to improve the accuracy with which the explosions can be calibrated as "standard candles." The use of SNe Ia as "standard candles" showed that the expansion of the universe is accelerating and it led to the discovery of dark energy. An accurate "standard candle" will improve the understanding of dark energy, one of the most compelling problems in the physical sciences. Improving the use of SNe Ia as "standard candles" will make them better cosmic yardsticks for determining the properties of dark energy. FLASH code and petascale computing will be used to perform higher fidelity simulations of Type Ia supernovae. These higher fidelity simulations will explore the effect of different values of the parameters that specify the initial conditions for the simulation.

Type: New
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-Institut
Mike Towler, University College London
Anatole von Lilienfeld, Argonne National Laboratory

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation: **95,000,000 core-hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q "Mira" (40,000,000 core-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 "Titan" (55,000,000 core-hours)

Research Summary:
The work of Alfe's team is a major expansion of their previous QMC (quantum Monte Carlo) work to address practically important scientific problems concerning non-covalent bonding for a range of paradigm molecular materials, as well as QMC benchmarking for water clusters in thermal equilibrium. A full quantitative understanding of hydrogen bonding is crucial for all systems involving water and its many forms. Hydrogen bonding is also responsible for the cohesion of innumerable natural and synthetic materials. This project also focuses on dispersion as a binding force in its own right, both in biologically relevant systems and in artificial supramolecular structures.

This research on non-covalent bonding goes far beyond what has been attempted before and is designed to exploit the greatly increased power of Mira, an IBM Blue Gene/Q, and Titan, a Cray XK7. Alfe's project will cover a much wider range of water aggregation states, and calls for extensive QMC benchmarking of large thermal samples of clusters and liquid configurations of up to 64 molecules, as well as ambitious QMC work on the liquid surface and on defective crystal surfaces. Gas hydrate work will address the energetics of crystal structures having very large unit cells, and will use QMC to tackle the controversial problem of diffusion barriers and the properties of liquid gas-water systems. Supramolecular studies will be concerned with non-covalent bonding in large complexes and breaks completely new ground for QMC work.

The use of the QMC energy benchmarks to help create improved versions of DFT (density functional theory) and force fields is an integral part of the project. The accurate description of cooperative many-body effects in hydrogen bonding, and the inclusion of screening and many-body effects in dispersion corrected versions of DFT are important aspects of this work.

Type: New
Title: "Non-Perturbative QED Study for Matter and Anti-Matter Collisions"

Principal Investigator: Michael Pindzola, Auburn University
Co-Investigators: Connor Balance, Auburn University
Stuart Loch, Auburn University

Scientific Discipline: Physics: Atomic/Molecular Physics

INCITE Allocation: **30,000,000 core-hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 "Titan"(30,000,000 core-hours)

Research Summary:
The large-scale computational projects that this project will carry out are for direct application to several cutting-edge physics experiments that will be performed within the next year. These experiments are probing the fundamental dynamics of atoms and molecules, furthering our understanding of such systems. An accurate interpretation of these experiments requires computational modeling which can only be performed with access to massively parallel computing facilities.

The large scale computational resources will allow specific non-perturbative QED calculations to be performed in direct support of international experiments probing matter and antimatter collisions. The experiments that will be simulated can only be calculated with petascale computing resources. The impact that these calculations will have on the scientific community fall into two main areas. Firstly, they will improve our understanding of these fundamental processes. Included in this area is the grand challenge of the quantal four body Coulomb problem. Secondly, the calculations are expected to have benefits to the wider scientific community through the application of the data to a range of plasma environments. These applications include planetary nebulae, s-process nucleosynthesis, semi-conductor photo-lithography, and anti-matter experiments.

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

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

Scientific Discipline: Physics: Nuclear Physics

INCITE Allocation: **155,000,000 core-hours**
Site: Argonne National Laboratory
Oak Ridge National Laboratory
Machine (Allocation): IBM Blue Gene/Q "Mira" (66,000,000 core-hours)
IBM Blue Gene/P "Intrepid" (15,000,000 core-hours)
Cray XK7 "Titan"(74,000,000 core-hours)

Research Summary:
A team of researchers led by James Vary is conducting state-of-the-art simulations to provide needed predictions where direct experiment is not possible or is subject to large uncertainties. Such calculations are relevant to many applications such as nuclear energy, nuclear security, and nuclear astrophysics, where rare nuclei reside at the heart of nucleosynthesis and energy generation in the stars. This project uses complimentary methods applicable to different regions of the nuclear chart.

Among the goals, the team aims to provide an *ab initio* understanding of the triple-alpha burning that is essential to life on Earth. So far, *ab initio* investigations of the role of three-nucleon forces have been limited to light nuclei and to a few reactions. This project will investigate the role of the three-nucleon force in substantially heavier nuclei including the oxygen isotopes, ^{40}Ca, and ^{56}Ni and in an expanded range of nuclear reactions. The team will calculate nuclear properties relevant for the description of nuclear reactions, in particular neutron-nucleus reaction cross-sections, and fission. Studies will include various scattering processes in light nuclei and bulk properties for nuclei across the entire mass table.

A major key to achieving these goals is to deploy on leadership-class facilities the best available theoretical many-body physics tools coupled with current theory of the strong interactions, including three-nucleon potentials. The multi-institution team conducting this work has extensive experience developing the theory, the practical algorithms, and the codes to address several long-standing questions in nuclear theory.

Type: Renewal
Title: "Optimization of Complex Energy System Under Uncertainty"

Principal Investigator: Mihai Anitescu, Argonne National Laboratory
Co-Investigators: Cosmin Petra, Argonne National Laboratory

Scientific Discipline: Energy Technologies: Energy Grid

INCITE Allocation: **14,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/P "Intrepid" (14,000,000 processor hours)

Research Summary:
The electrical power system in the United States is at a crossroads between its mission to deliver cheap and safe electrical energy, a strategic aim to increase the penetration of renewable energy, an increased reliance on smart grid technology, and the critical need to maintain and increase the grid's reliability. As well, the operation and planning of the grid with these requirements involves an unprecedented amount of uncertainty in supply and demand brought on by the high variability of wind, solar, and other renewable power sources. This project will develop advanced optimization methods for optimal operation of the power grid under uncertainty. This will allow answering, at full resolution, important questions such as: Can 20% wind power penetration be achieved without compromise for reliability?

The ultimate goal of the researchers is to be able to solve power grid stochastic optimization problems in real time, and in the case of the unit commitment problems, real time means under one hour. However, the unit commitment formulations use binary (integer) variables and solving them in real time is a daunting task. The objectives and plans are to implement capabilities for solving problems involving binary (integer) decisions, and, in an effort to further improve the time to solution, to develop and implement asynchronous methods. The goal is to solve a full-resolution stochastic model set up for a vast geographical area (Midwest network) to assess the relationship between various facets of complex energy systems such as stochasticity, renewable energy, economic cost, and reliability.

High-performance computing will enable the researchers to incorporate larger geographical domains, longer forecast horizons, and higher temporal resolutions to maximize the power grid responsiveness. To tackle these challenges, the efforts will be focused primarily on improving time-to-solution and developing scalable capabilities for the solution of integer stochastic optimization problems. The description of this relationship will generate useful insights for policy-makers and players in the power grid and renewable energy industry.

Type: New
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, National Center for Atmospheric Research
Duane Rosenberg, National Center for Atmospheric Research
Leslie Smith, University of Wisconsin, Madison

Scientific Discipline: Engineering: Fluids and Turbulence

INCITE Allocation: **34,000,000 core-hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 "Titan"(34,000,000 core-hours)

Research Summary:
Fluid turbulence in critical applications such as geophysics, astrophysics, and many engineering problems is coupled to varying degrees with (frame) rotation, and stable or unstable stratification due to the presence of a scalar such as temperature, salinity, or mass density. There is limited quantitative understanding of the competing effects of rotation and stratification in the formation of structures ranging from columnar in shape to pancake-like. Further mediation by the aspect-ratio of the domain could enhance or suppress such structure formation depending on whether the domain is taller or smaller than it is wide. The goal of this research proposal is to parameterize such structure formation and the associated small, intermediate, and large-scale dynamics using statistical analysis of massive simulations.

Such a study combining careful parameter studies and massive simulations to address an extended parameter space is entirely unique and crucial for connecting the fundamental physics of fluid turbulence to applications in a wide variety of fields. The relevance to fundamental fluid dynamics of geophysical and astrophysical problems, and our close ties to related studies and experiments at LANL, provide the elements of urgency and validity to the proposed work.

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

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

Scientific Discipline: Computer Science

INCITE Allocation: **85,000,000 core-hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q "Mira" (30,000,000 core-hours)
IBM Blue Gene/P "Intrepid" (10,000,000 core-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 "Titan" (45,000,000 core-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 codes.

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

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

Scientific Discipline: Biological Sciences: Biophysics

INCITE Allocation: **110,000,000 core-hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK 7 "Titan" (110,000,000 core-hours)

Research Summary:
This project will study three biomolecular systems that can have a significant impact on addressing U.S. health and energy issues. These three systems include: the HIV capsid, the process of peptide bond formation in ribosomes, and the basic process of photosynthesis.

HIV is a global pandemic and has killed over 25 million people in the past three decades. The virus has the ability to acquire resistance to every currently administered treatment, which has prompted the need for new therapies. Recent data has shown that the stability and geometry of the HIV capsid is required for several key steps of the infection process and has a direct impact on both infectivity and viral load, so the capsid assembly process is viewed as an important unexploited therapeutic target that offers the best hope of generating drugs active against all of the HIV-1 variants. Using Titan, this project will construct and simulate a complete HIV capsid, which will shed light on the capsid assembly, helping to guide the development of new drugs to target the assembly process.

Ribosomes link hereditary information and cellular actions and are also fundamental in bacterial cells, offering binding sites for drugs, which makes them relevant for biomedical research. At the core of ribosomal function is the catalysis of peptide-bond formation, which adds one amino acid at a time to the nascent protein. This project will investigate this reaction to discover critical links between the structure and function of the ribosome that cannot be achieved by experimental means alone.

Photosynthetic organisms are able to convert sunlight into useable chemical energy with efficiency far beyond what current man-made devices can achieve. Mankind can learn from the examples set by nature by modeling photosynthetic chromatophores from purple bacteria in full atomic detail in order to characterize how the components of the chromatophore work together to perform photosynthesis. This will help mankind to harness solar power for future energy needs.

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

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

Scientific Discipline: Physics: Space Physics

INCITE Allocation: **53,000,000 core-hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q "Mira" (28,000,000 core-hours)
IBM Blue Gene/P "Intrepid" (25,000,000 core-hours)

Research Summary:
The origin of the solar wind and the heating of the solar corona stand as two of the most compelling problems in heliospheric physics. A number of observations suggest that Alfvén waves (AWs) and AW turbulence play a key role in the solution to both problems. These include optical observations of AWs in the chromosphere and near-infrared observations of AWs in the corona that carry an energy flux that is sufficient to power the solar wind. However, the scientific community remains divided about the viability of this scenario, in large part because we do not possess a detailed understanding of the properties of such turbulence in the highly inhomogeneous near-Sun region.

This project will promote large-scale numerical simulations of inhomogeneous Alfvén wave (AW) turbulence in the extended solar atmosphere and solar wind. The simulations will substantially extend previous (low-resolution) simulations to an unprecedented 35 billion-point mesh, in order to capture more realistic radial variations of the solar atmosphere, as well as the turbulent dynamics that are present in the solar-wind acceleration region. Researchers will use these simulations to test existing theories of MHD turbulence, develop new theoretical models, and investigate the viability of Alfvén-wave turbulence as a mechanism for generating the solar wind. The results from the simulations will answer a number of outstanding key questions that are the subject of strong debate in the heliophysics community. Researchers will also compare the simulation results to observations of coronal Faraday rotation fluctuations, in-situ measurements from the Helios spacecraft, and make detailed predictions of NASA's future Solar Probe Plus mission. The NASA spacecraft has an expected launch date in 2018, and it will be sent in to the region that the researchers will simulate numerically.

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

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

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation: **240,000,000 core-hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q "Mira" (200,000,000 core-hours)
IBM Blue Gene/P "Intrepid" (40,000,000 core-hours)

Research Summary:
The performance and lifetime of materials widely used in energy and nuclear technologies are often severely limited by corrosion under stress loads. Particularly important for the DOE are environmental degradations of nickel-based alloys in advanced nuclear reactors and in glass containers of nuclear waste.

This project performs petascale reactive molecular dynamics (MD) and quantum mechanical (QM) simulations to investigate fundamental mechanisms of stress corrosion cracking (SCC) and nanoindentation of silica glass in the presence of water as well as impurity segregation-induced embrittlement of nickel-aluminum alloys.

In order to prevent SCC and to predict the lifetime beyond which SCC may cause failure, the petascale hierarchical simulation approach is used to discover:
· The role of water in nanoindentation damage of silica glass;
· Fundamental mechanisms of SCC in silica glass in the presence of water; and
· Atomistic mechanisms of impurity (sulfur and boron)-segregation induced embrittlement in nickel-aluminum alloys.

In the first year of the project, the team performed a billion-atom reactive MD simulation to study silica-water chemistry at a nanoindent on a silica surface generated by the collapse of a cavitation nanobubble in water, thus revealing the role of water in nanoindentation damage.

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: **55,000,000 core-hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 "Titan"(55,000,000 core-hours)

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

This project proposes an "end to end," first principles simulation of a SN Ia using three codes that have been developed for this purpose with support from the DOE's SciDAC Program. Each code has been demonstrated to scale, for this particular problem, to over 100,000 CPUs on Jaguar. MAESTRO, a low-Mach-number AMR code, is unique in its ability to finely resolve the convective flow that precedes ignition. The nuclear burning is turbulent and must be resolved, initially at least, on sub-km scales in a star 2,000 km in radius. The integral scale of the turbulence is ~10 km and this must be resolved as the supernova expands to about 10,000 km. Finally, the 3D explosion will be post-processed using the Monte Carlo code SEDONA to obtain the light curve and spectra.

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 Drakauer, College of William and Mary
Gustavo Scuseria, Rice University
Cyrus Umrigar, Cornell University

Scientific Discipline: Chemistry: Physical

INCITE Allocation: **27,000,000 core-hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 "Titan"(27,000,000 core-hours)

Research Summary:
The project describes an ambitious set of calculations in two areas: quantum chemistry for energy-related and magnetic materials, and cold atoms in optical lattices in atomic, molecular, and optical (AMO) physics. If successful, the effort will lead to the solution of longstanding challenges in accurately predicting key properties of these systems. It will also provide significant benchmark results for future simulations, experimental studies, and technological applications.

The problems in these two areas have been chosen to create synergy. They have great commonality in the requirement of high accuracy to resolve small energy differences and quantum states. They are also complementary: the quantum chemistry calculations emphasize the ability to treat materials-specific characteristics reliably and precisely, 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 same simulation approach will be used and was made possible by recent advances in the auxiliary-field quantum Monte Carlo method. The two areas will provide a wider span in testing the capability for precision many-body quantum simulations. Accurate treatment of such systems is a grand challenge in modern science. The combination of methodological developments and the advent of petaflop computing (and beyond) presents a unique and outstanding opportunity now to make fundamental progress.

Type: New
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: **45,000,000 core-hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 "Titan"(45,000,000 core-hours)

Research Summary:
This project uses ab-initio many-body electronic structure calculations to unravel outstanding problems in the prediction of materials properties of interest to DOE. The researchers will use a state-of-the-art electronic structure method, Quantum Monte Carlo (QMC), implemented in QMCPACK. The project aims to understand metal oxides that have wide application, including energy storage, catalysis, and energy production, and metals that are widely used as structural materials. A careful "experimental design" is planned, with inter-related calculations in materials with very different electronic structure. The complementary nature of these calculations will improve confidence in the predicted results, and therefore the quality of science, compared to the unrelated "one off" calculations commonly performed. The researchers aim to solve some of the above scientific problems in these materials and also aim to identify the fundamental problems limiting accuracy with density functional approaches. Thus the project aims for significant scientific impact and a longer lasting impact in the materials modeling community.

The project will initially focus on titanium metals and titanium oxides. Titanium is a light transition metal element and is a natural next step in the direction of challenging correlated oxides. At the same time, titanium already presents significant obstacles to the approximate functionals used in the popular framework of density functional theory (e.g., the empirical choices employed in oxides worsen results in metals). The researchers aim to establish an accurate common methodology. The nature of the planned calculations will yield both important scientific results and a quantum leap in the confidence that can be placed in the theory, its accuracy and reliability. Titanium-based metals and oxides have very broad industrial uses yet remain a significant topic of research. In terms of materials modeling, both the metals and oxides are surprisingly and subtly problematic. Success in these materials will lead to a natural progression down the periodic table, examining zirconium/zirconia and eventually cerium/ceria materials. The latter are certainly exemplars of strong correlation physics but widely used in catalysts.

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

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

Scientific Discipline: Materials Science: Condensed Matter and Materials

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

Research Summary:
A rechargeable Lithium/Air battery can potentially store five to ten times the energy of a Lithium/Ion battery of the same weight and no other potential battery technology comes close. Realizing this enormous potential is a very challenging scientific problem both for experimental and computational investigations and will require development of new electrode materials and electrolytes. Utilization of petascale supercomputer simulations can help understand key scientific problems and advance solutions to them.

Over the last three years, several important goals have been achieved; the subtle chemical and physical properties have been revealed, the chemical discharge and re-charge process has been identified, and the establishment of the peta-scale simulations was used to understand the scientific problems associated with the Lithium/Air batteries. Despite much progress, a detailed molecular description of the electron transfer to oxygen during the discharge process and of the subsequent nucleation and growth process is still lacking.

This project will use large-scale simulations to understand and address key challenges of the physical and chemical mechanisms of Lithium/Air batteries. The goal of this research being carried out by Curtiss' team is to help discover breakthrough materials for Lithium/Air batteries that will be able to deliver more than 1000 Wh/kg, while sustaining many recharging cycles. Such batteries could enable widespread deployment of electric vehicles; greatly reducing the U.S. dependence on foreign oil, as 81% of imported oil is burned for road transportation uses (2007 data).

Type: New
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: **75,000,000 core-hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 "Titan"(75,000,000 core-hours)

Research Summary:
This project brings the powerful and computationally demanding quantum Monte Carlos (QMC) methods to bear on two materials of interest: hydrogen and pure water ice.

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

A crucial aspect of the project is that it will treat the nuclei as quantum particles. The zero-point energy arising from the quantum motion of a proton in a solid is usually more than 0.1 eV, and it gives rise to very important effects in water and hydrogen. The field of high-pressure studies of hydrogen has reached a very exciting stage. The recent observation of a new phase IV of hydrogen at room temperature by Eremets and Troyan has generated enormous excitement in the field and worldwide publicity. However, it has not proved possible to determine structures of hydrogen at high pressures experimentally, because protons scatter X-rays too weakly to permit high-resolution X-ray diffraction studies.

In water ice we know (more-or-less) where the atoms are, and the aim is to use QMC to calculate highly accurate data for structures and other properties which will improve our understanding of water ice and provide data for benchmarking different methods.

In both water ice and hydrogen the researchers will be able to isolate the contributions from the zero-point motion, because they can turn it on and off at will in the calculations. The project represents an exciting exploration of the properties of two iconic materials. Such an ambitious proposal could only be brought to fruition through a substantial allocation of resources on Titan.

Type: New
Title: "Safety in numbers: Discovery of new solid Li-ion electrolytes"

Principal Investigator: Boris Kozinsky, Robert Bosch LLC
Co-Investigators: Nicola Marzari, École Polytechnique Fédérale de Lausanne
Brandon Wood, Lawrence Livermore National Laboratory

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

INCITE Allocation: **48,000,000 core-hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 "Titan"(48,000,000 core-hours)

Research Summary:
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. As a result, existing lithium-ion batteries require safety devices and cooling systems, which both increase cost and reduce energy density on the system level. Solid inorganic non-combustible electrolytes are therefore ultimately the only path towards a truly safe battery.

The goal of this project is to discover and optimize new classes of solid inorganic Li-ion electrolytes with high ionic and low electronic conductivity, and good electrochemical stability. The researchers will accomplish their goal by applying state-of-the-art computational methodology which has been developed and validated with experimental synthesis and characterization. This project will follow a unique approach that will combine a large number of screening computations, performed in a massively parallelized high-throughput automated framework, with a series of in-depth ab-initio molecular dynamics investigations. Computational screening on ionic transport, electronic structure, and electrochemical properties will be automatically deployed on thousands of crystalline and amorphous structures in order to find candidates that are otherwise impossible to identify by intuition and experiments.

Type: Renewal
Title: "Scalable first principles calculations for materials at finite temperature"

Principal Investigator: Markus Eisenbach, Oak Ridge National Laboratory
Co-Investigators: Don Nicholson, Oak Ridge National Laboratory
Malcolm Stocks, Oak Ridge National Laboratory

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation: **105,000,000 core-hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 "Titan"(105,000,000 core-hours)

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

Magnetic materials represent an important class of materials for technological applications and are also of basic science interest. Applications of magnetic materials can be found in magnetic data storage where both the density and the stability of the recorded information are determined by material properties. Even more important for energy applications are permanent magnets. As all the currently used magnets that fulfill the physical requirements are rare earth-based, development of new materials is indicated to avoid a dependence on a scarce resource that is controlled by a very small number of suppliers. Magnetism also plays an important role in the atomic scale behavior in basic structural materials, such as steel, iron-nickel alloys, etc.

Improvements in the physical properties of these materials can lead to energy savings due to stronger, lighter materials in transportation applications as well as better predictions for structural materials in radiation environments, such as fission and fusion reactors.

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

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

Scientific Discipline: Computer Science: Computer Science

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

Research Summary:
The purpose of this project is to improve the performance and productivity of key system software components on leadership class platforms. High-end computing systems such as those being deployed at the Argonne Leadership Computing Facility consist of hundreds of thousands of processors, terabytes of memory, exotic high-speed networks, and petabytes of storage. While the capabilities of such machines have grown rapidly over the past several years, such growth comes at the cost of growing system complexity.

To keep individual component costs from overshadowing overall system cost, modern architectures are increasingly relying on hardware sharing that includes shared caches, shared memory and memory management devices, and shared network infrastructure. Multi-core architectures, simultaneous multi-threading capable processors, and flat torus-like network architectures are some examples of the hardware sharing that is becoming increasingly prevalent. As hardware complexity skyrockets in leadership class systems, it is not easy for applications to take complete advantage of the available system resources and avoid potential bottlenecks.

Specifically, the researchers propose studying four different classes of system software: Message Passing Libraries to increase productivity while achieving high performance; Parallel Input/Output (I/O) to manage the complexity of computational hardware for high performance and providing effective interfaces for scientific application data models; Data Analysis and Visualization to target the post-processing and co-processing of computed data in addition to simulation efficiency; and Operating System to more effectively manage the growing numbers of nodes on leadership platforms, especially for many task computing (MTC) and high throughput computing (HTC) jobs, which require more advanced caching of input and output data to offer adequate performance.

Type: New
Title: "Simulating Reionization of the Local Universe: Witnessing our own Cosmic Dawn"

Principal Investigator: Paul Shapiro, University of Texas
Co-Investigators: Kyungjin Ahn, Chosun University
Ilian Iliev, University of Sussex
Romain Teyssier, University of Zurich

Scientific Discipline: Physics: Astrophysics

INCITE Allocation: **40,000,000 core-hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 "Titan"(40,000,000 core-hours)

Research Summary:
When the first stars and galaxies formed in the dark universe, they released radiation that ripped apart the hydrogen atoms in the intergalactic medium and heated the gas there to 104 degrees Kelvin. This created a patchwork quilt of ionized zones that grew over the first billion years until they overlapped and the universe was fully reionized. This epoch of reionization is one of the last windows of cosmic time subject to direct detection and a critical missing link in the theory of galaxy formation. Reionization left an imprint on the smallest galaxies that formed almost 13 billion years ago that astronomers can still observe in the nearby universe when they study the dwarf galaxies bound to the Milky Way and Andromeda in our Local Group. The Local Group holds clues to the history of reionization. The theory of galaxy formation in the standard model of cosmology overpredicts the abundance of dwarf satellite galaxies in the Local Group, so reionization suppression is often invoked to explain the apparent discrepancy.

This project will simulate cosmic structure formation and reionization of the universe by starlight from the first galaxies in unprecedented detail. The project will push the envelope of size and mass resolution of Epoch of Reionization (EOR) simulation in three simulations: (1) The project will increase the mass resolution by orders of magnitude to resolve all halos of mass above 105*M*☐. This will require performing the largest cosmological N-body simulation ever attempted, with ☐ (11, 000)3, or 1.6 trillion particles. (2) The project will use C2-Ray radiative transfer simulation to model the reionization of this volume. This will allow the researchers to project forward in time to the present to see the "memory" of reionization in the Local Group, for comparison with observations. (3) The mass and length scales revealed by this advance to higher resolution are also those most susceptible to hydrodynamical back-reaction when radiation photoheats the atomic gas and raises its pressure. To study this back-reaction and its effect on the galaxy and star formation that drove reionization self-consistently, the project will use Titan to simulate the coupled radiation hydrodynamical evolution of the same Local Group volume, with the unprecedented resolution of 40963 particles and 40963 cells, resolving the formation of all galaxies above 5 × 107M☐ for the first time in such a volume, using our new RAMSES-CUDATON code, with GPU acceleration.

Type: New
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 core-hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q "Mira" (200,000,000 core-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, environmentally sustainable energy. Scientists have been working to achieve self-sustaining nuclear fusion and energy gain in the laboratory for more than half a century. The National Ignition Facility (NIF) laser is currently carrying out experiments whose goal is to compress a mixture of deuterium and tritium to temperatures and densities high enough that fusion ignition occurs.

The laser intensity at NIF is high enough that some of the laser energy backscatters off the target. Previous research quantified how overlapping quads (groups of 2 x 2 beams) impacted backscatter at NIF. Research demonstrated that overlapping quads can share a reflected light wave, thereby enhancing reflectivity. The simulations produced results similar to NIC experimental data and have allowed identification of several areas where the simulations need to be improved.

This project will perform a simulation of backscattered light generated from three overlapping quads (groups of 2 x 2 beams propagating in the same direction) over the full volume in which laser-plasma interactions (LPI) is expected to occur. The simulation will produce synthetic data that will be compared to experimental data from the National Ignition Facility (NIF). The simulation will provide detailed information about where LPI occurs and the interaction between stimulated Raman scattering and stimulated Brillouin scattering; the two main plasma instabilities acting in these experiments. This research will provide a better understanding of the conditions where overlapping quads generate more backscattered light than from the quads acting independently.

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

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

Scientific Discipline: Chemistry: Combustion

INCITE Allocation: **130,000,000 core-hours**

Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q "Mira" (100,000,000 core-hours)
IBM Blue Gene/P "Intrepid" (30,000,000 core-hours)

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

Plans for the second year include: (A) Simulation of hot spot formation and autoignition behind reflected shocks to study autoignition mechanisms and validate simulations against ignition delay simulations. (B) Study of initiation of detonation by individual hot spots. (C) DDT simulations behind reflected shock. This will be used to study disruption of the flame by turbulence, formation, and detonation of nonuniform areas of reactivity. (D) Propagation and acceleration of a flame ignited at the closed end of the tube. This will study flame instabilities and development of boundary layers ahead of and behind the flame, as well as formation of shock waves propagating ahead of the flame front.

Type: New
Title: "Simulations of Ribosome Biogenesis and Cellular Process"

Principal Investigator: Zaida Luthey-Schulten, University of Illinois

Scientific Discipline: Biological Sciences: Biophysics

INCITE Allocation: **51,410,000 core-hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 "Titan"(51,410,000 core-hours)

Research Summary:
Simulations on the fundamental and universal processes of ribosome biogenesis and other cellular processes will provide insight into the similarities and differences in all three domains of life. Researchers plan to conduct two projects. Aim 1: On the molecular level, classical molecular dynamics simulations of the folding/assembly landscape of the ribosomal small subunit will be carried out using NAMD 2.9. Aim 2: On the cellular level, stochastic simulations of cellular processes within models of whole methanogens, *E. coli,* and yeast cells will be carried out using GPU-based Lattice Microbe software.

The study will be guided by the positions of the rRNA and r-protein signatures and the assembly map to select initial conditions for the assembly process. To address Aim 1, researchers will systematically study the binding of ribosomal proteins onto the small subunits using molecular dynamics. To address Aim 2, collaborators will carry out stochastic simulations of kinetic models that have been developed for cell division in *E. coli* and *C. crescentus,* the methanogenesis energy pathway in *M. acetivorans,* and the galactose signaling network in yeast. A highly parallel, multiple-GPU version of Lattice Microbes will be used to simulate several systems under this proposal. Research will initially focus on expanding upon previous work on bacterial cell division. A simplified model of dividing *E. coli* has already proven capable of capturing the oscillatory behavior of MinD and MinE that is known to determine the locus of cell division. This model will be expanded to include more reactions involved in cell division and a more realistic model of the cell membrane and periplasm.

Type: New
Title: "Spectral Slope of MHD Turbulence"

Principal Investigator: Andrey Beresnyak, Los Alamos National Laboratory

Scientific Discipline: Physics: Astrophysics

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

Research Summary:
MHD turbulence has attracted attention of astronomers since mid 1960s. As most astrophysical media are ionized, plasmas are coupled to the magnetic fields. A simple one-fluid description known as magnetohydrodynamics (MHD) is broadly applicable to most astrophysical environments on macroscopic scales.

The Goldreich-Sridhar model uses a concept of critical balance, which maintains that turbulence will stay marginally strong down the cascade. In this model the spectrum was supposed to follow the -5/3 Kolmogorov scaling. However, shallower slopes were often reported by numerics. This prompted a number of suggestions to modify the standard theory, but the higher resolution studies confirmed -5/3 again. Another problem is that the standard theory only considers so-called balanced case, or the case with zero cross-helicity. As turbulence is a stochastic phenomenon, the average zero cross helicity does not preclude a fluctuations of this quantity in the turbulent volume. Thus, the special case of the balanced turbulence should be treated from the more general perspective. Furthermore, most of astrophysical turbulence is globally imbalanced due to being generated by a localized source. The Sun is one of such sources and the wealth of in-situ measurements in the solar wind confirms the imbalanced nature of heliospheric turbulence. Although several models for imbalanced turbulence has been reported in the literature, the full self-consistent analytical theory does not yet exist. In this situation observations and direct numerical simulations will provide necessary feedback to theorists.

This project seeks to unambiguously differentiate between -5/3 and -3/2 power spectral slopes of strong MHD turbulence and provide a deeper insight into the nature of imbalanced turbulence.

MHD turbulence is a ubiquitous basic physical phenomenon. The project findings will affect future theoretical and observational research in solar physics, heliospheric physics, plasma physics and astrophysics.

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

Principal Investigator: Benoit Roux, University of Chicago

Scientific Discipline: Biological Sciences: Biophysics

INCITE Allocation: **55,000,000 core-hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q "Mira" (35,000,000 core-hours)
Machine (Allocation): IBM Blue Gene/P "Intrepid" (20,000,000 core-hours)

Research Summary:
Proteins are extremely complex tiny "molecular machines". Their concerted action underlies many of the critical activities of living organisms. Membrane-associated proteins play an essential role in controlling the bi-directional flow of material and information. Malfunction of some critically important proteins can often lead to diseases such as cancer.

This project is aimed at gaining a deep mechanistic perspective of such protein function, linking structure to dynamics, by characterizing the free energy landscape that governs the key functional motions. Src tyrosine kinases and the ATP-driven ion pumps will be studied within a unified computational perspective provided by free energy landscapes. As a benchmark for quantifying the accuracy of the approach, the conformational propensity of small peptides in solution will also be studied.

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

Type: Renewal
Title: "The Solution of Three-Dimensional PWR Neutronics Benchmark Problems for CASL "

Principal Investigator: Thomas Evans, Oak Ridge National Laboratory
Co-Investigators: Greg Davidson, Oak Ridge National Laboratory
Josh Jarrell, Oak Ridge National Laboratory

Scientific Discipline: Physics: Nuclear Physics

INCITE Allocation: **21,000,000 core-hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 "Titan"(21,000,000 core-hours)

Research Summary:
The Consortium for Advanced Simulation of Light Water Reactors (CASL) is developing a virtual reactor simulation toolkit designed to use leadership-class computing resources.

CASL's primary modeling and simulation science driver is to enable nuclear reactor power uprates, life extensions, and higher fuel burnup. These objectives have been codified in 10 challenge problems, five of which are operational and five of which pertain to safety. In order to solve these problems, the Advanced Modeling Applications focus area in CASL has defined a series of test problems that each physics component in the virtual reactor toolkit must solve. These range from single fuel pins to whole cores and include varying levels of multiphysics coupling. Each of these problems requires a neutronics code capable of performing three-dimensional flux calculations with axial variations and sub-pin resolution depletion. Additionally, multigroup cross-section generation must be provided over a wide range of group structures in order to test the energy fidelity required to obtain accurate solutions to the test problems.

The project will use the Denovo transport system to solve the defined CASL neutronics problems in preparation for full-system simulations that will take place in years four and five of the CASL project.

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

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

Scientific Discipline: Energy Technologies: Nuclear Energy

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

Research Summary:
Generating clean, safe nuclear power is essential to meet the world's growing energy needs. Fischer's team is performing highly accurate computations that allow them to analyze, model, simulate, and predict complex thermo-fluid phenomena and, ultimately, produce economical, safe nuclear power.

Two critical safety parameters in nuclear power plants are maintaining the peak material temperature and monitoring pressure drops in coolant flow. Predicting peak temperature and pressure drop requires accurately computing thermal mixing governed by thermal conduction and convection in a coolant flow over a complex geometry. Higher-fidelity advanced thermal hydraulics (TH) codes help simulate nuclear systems with well-defined and validated prediction capabilities, allowing researchers to explore points in the parameter space outside the existing database. These simulations can also model the flow and heat transfer phenomena in next-generation nuclear reactors.

The Nuclear Energy Advanced Modeling and Simulation (NEAMS) program is developing simulation capabilities to leverage leadership class computing facilities in the design of advanced nuclear reactors. Its Advanced Fuel Cycle Initiative (AFCI) is examining a closed nuclear fuel cycle based on a new generation of fast neutron reactors designed to safely manage spent nuclear fuel. A central component of that project provides large eddy simulations (LES) and Reynolds-averaged Navier-Stokes (RANS) simulations to study turbulent coolant flow and associated heat transfer.

The TH behavior of multi-pin subassemblies with wire-wrap and grid spacers was identified by Argonne's reactor designers as a problem of primary interest that has most of the experimental data available for validation and therefore was chosen as a key areas for this multi-year effort.

Type: New
Title: "Thermodynamics of Binding Biomass to Cellulases for Renewable Fuel"

Principal Investigator: Michael Crowley, National Renewable Energy Laboratory (NREL)
Co-Investigators: Lintao Bu, National Renewable Energy Laboratory (NREL)
Wei Jiang, Argonne National Laboratory (ANL)

Scientific Discipline: Energy Technologies: Bioenergy

INCITE Allocation: **70,000,000 core-hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q "Mira" (30,000,000 core-hours)
IBM Blue Gene/P "Intrepid" (40,000,000 core-hours)

Research Summary:
The U.S. Department of Energy (DOE) has stipulated that 30% of the gasoline demand be displaced by renewable transportation fuels from non-food feedstock by 2030. The scientific community is pursuing many strategies to harness the vast available biomass resources.

A key component that crosscuts many technology options to realizing industrial scale biofuels production is the continued development of superior enzymatic catalysts to convert highly recalcitrant biomass into fermentable sugars.

Understanding the molecular-level steps in cellulose synthesis and conversion will enable experimental design approaches in a rational design paradigm both to develop superior enzymes and less recalcitrant plant-based feedstocks.

This project is aimed at using large-scale, high-performance computing to gain insights into the primary routes that nature uses to degrade plant cell walls. The overall goal is to enable rational design of superior biological catalysts for conversion of biomass to sugars for renewable liquid fuels. Project researchers will focus on the prevalent biological route to cellulose conversion: enzymatic hydrolysis by cellulases. This project will also enable an enhanced, fundamental understanding of how the energy-dense plant cell wall is degraded in the biosphere and how we can adapt cellulases to industrial environments. Advances enabled by this work will aid in the development of the U.S. renewable fuels industry.

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

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

Scientific Discipline: Physics: Astrophysics

INCITE Allocation: **65,000,000 core-hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q "Mira" (30,000,000 core-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 "Titan"(35,000,000 core-hours)

Research Summary:
Core collapse supernovae are the dominant source of elements in the Universe, dominating the origin of the elements between oxygen and iron and responsible for half the elements heavier than iron. They are complex, three-dimensional, multi-physics events, but presently there are no three-dimensional core collapse supernova models of sufficient realism, limiting our understanding of the explosion mechanism, and our ability to predict the element synthesis in these events, among other important observables.

The simulations proposed here are intended to begin to fill this void. Three-dimensional, multi-physics simulations with the CHIMERA code, which implements the ray-by-ray-plus (radial) approximation for neutrino (radiation) transport, will be performed. CHIMERA simulations are the first three-dimensional simulations performed with spectral neutrino transport, critical to realistic modeling of the neutrino shock reheating believed to be central to the supernova explosion mechanism. While the CHIMERA simulations will capture much of the realism in core collapse supernovae and advance the state of the art in three-dimensional supernova models significantly, they leave open additional outstanding questions that deal with physics or asymmetries ignored in CHIMERA. To address these this project is developing the GenASiS code. Initially tasked with investigations of the magnetic field development in the collapsed core in AY2011-12, GenASiS is acquiring the ability to perform full spectral neutrino transport including the effects of General Relativity. AY2013 will see the first full physics GenASiS simulation. Finally, advances in three-dimensional supernova modeling at macroscopic stellar scales must be matched by three-dimensional modeling at microscopic (nuclear) scales in the development of the input equation of state for core collapse supernova models.

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

Principal Investigator: David Baker, University of Washington

Scientific Discipline: Chemistry: Biochemistry

INCITE Allocation: **140,000,000 core-hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q "Mira" (100,000,000 core-hours)
IBM Blue Gene/P "Intrepid" (40,000,000 core-hours)

Research Summary:

Calculation of protein structure and design of novel proteins are two of the most important challenges in structural biology. Addressing these challenges will help researchers cure diseases and design proteins that can efficiently catalyze medically and industrially useful reactions. This project builds on earlier successes and increases the scope of research. In most cases, we will move from benchmarking to proof-of-concept applications.

A recent breakthrough in conformational sampling using highly parallel computations on the Blue Gene platform will allow us to compute highly accurate structures for proteins as large as 20 kDa while using very limited experimental data. The use of INCITE resources will facilitate advances in many challenging problems in computational structural biology, including the *ab initio* prediction of proteins larger than 15 kDa, the calculation of structures of proteins larger than 20 kDa using sparse nuclear magnetic resonance data, the determination of membrane protein structures, and the design of a novel enzyme system to fix carbon dioxide (CO_2) to produce biofuels.

We will use various models/methods to achieve success. For example, the use of *ab initio* structure prediction will help provide accurate models for biologists to suggest hypotheses relating to biological function and to afford phasing information for proteins for which X-ray diffraction experiments have been carried out, but phase information is not available. In addition, we will continue to develop and apply the Rosetta method to obtain accurate, fully automated predictions for proteins up to 20 kDa.

The major challenge in genomics is not in obtaining large amounts of sequence data, but in interpreting it. The broader impacts of this work will include pressing issues in the 21st century, including deciphering the structures and functions of the vast number of protein sequences generated in current high-throughput sequencing projects and reducing the levels of CO_2 in the atmosphere through enzymes designed to fixate CO_2 into industrially useful products.

Type: New
Title: "Transformative Advances in Plasma-based Acceleration"

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

Scientific Discipline: Physics: Accelerator Physics

INCITE Allocation: **30,000,000 core-hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 "Titan"(30,000,000 core-hours)

Research Summary:
The goal of this project is to use the UCLA particle-in-cell (PIC) code infrastructure to learn how to use plasma-based acceleration as the basis for extremely high-quality electron beams for use in a future collider and/or a next generation light source and for a new class of proton/ion accelerator used in cancer therapy.

The proposed research remains aimed at advancing the understanding of basic high-energy density science (HEDS) on the interactions of intense laser and particle beams with plasmas, and employing this understanding to aid in the development of plasma-based accelerator stages for use in high energy physics colliders, next-generation light sources, medicine, and homeland security, and to aid in the developing of compact proton/ion accelerators for using in medicine. This effort blends basic research with three-dimensional simulations, including full-scale PIC modeling of ongoing and planned experiments. The simulations provide a test bed for theoretical ideas and new concepts, as well as a method for guiding ongoing and future experiments. The research continues to include careful benchmarking of codes against well diagnosed experiments. Once codes are validated, concepts can be "tested" before building large and expensive experimental facilities.

Type: New
Title: "Transformative Simulation of Shock-Generated Magnetic Fields"

Principal Investigator: Milad Fatenejad, University of Chicago
Co-Investigators: Christopher Daley, University of Chicago
Anshu Dubey, University of Chicago
Norbert Flocke, University of Chicago
Carlo Graziani, University of Chicago
Don Lamb, University of Chicago
Dongwook Lee, University of Chicago
Michael Papka, Argonne National Laboratory
Katherine Riley, Argonne National Laboratory
Anthony Scopatz, University of Chicago
Petros Tzeferacos, University of Chicago
Venkat Vishwanath, Argonne National Laboratory
Klaus Weide, University of Chicago

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation: **40,000,000 core-hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q "Mira" (20,000,000 core-hours)
IBM Blue Gene/P "Intrepid" (20,000,000 core-hours)

Research Summary:
The study of magnetic fields requires an understanding the generation of the seed fields that magnetic dynamos require to operate, as well as the dynamo process itself. A promising mechanism for understanding the origin of such fields in the universe is the asymmetric shocks that occur in hierarchical structure formation when smaller halos merge to form galaxies and clusters of galaxies. These magnetic fields are generated by thermoionic currents that result from the asymmetry of the shock—the so-called the Biermann battery mechanism.

Researchers will perform high fidelity, end-to-end, two-dimensional (2D) and three-dimensional (3D) simulations of laser-driven experiments that measure shock-generated magnetic fields. Researchers will use FLASH, a highly capable community code with a large user base, to validate 2D hydrodynamic simulations and 3D magnetohydrodynamic simulations of shock-generated magnetic fields. These experiments will require laser illumination of a foil target, driving a shock into a gas-filled chamber, and an array of plasma and magnetic field diagnostics. The collaboration between simulators and experimentalists will produce the first validated 2D and 3D simulations of shock-generated magnetic fields.

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

Principal Investigator: William Daughton, Los Alamos National Laboratory
Co-Investigators: Vadim Roytershteyn, University of California-San Diego

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation: **55,000,000 core-hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 "Titan"(55,000,000 core-hours)

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

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

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

Principal Investigator: Giulia Galli, University of California, Davis
Co-Investigators: Francois Gygi, University of California, Davis
Detlef Hohl, Shell Corporation

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation: **100,000,000 core-hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q "Mira" (70,000,000 core-hours)
IBM Blue Gene/P "Intrepid" (30,000,000 core-hours)

Research Summary:
Understanding pure water is an essential prerequisite for grasping the behavior of aqueous solutions interacting with surfaces. The use of leadership class resources has been instrumental in assessing the accuracy of first principles theories for water. With earlier INCITE allocations, several accurate flavors of density functional theory (e.g., PBE0 and van der Waals functionals) were used to investigate water and ions in water with atomistic resolution. Specifically, researchers carried out *ab initio* molecular dynamics calculations using the Qbox code on Intrepid, an IBM Blue Gene/P, and determined the structural and vibrational properties of liquid water and simple anions in water for several temperatures. Findings suggest that through the use of high-performance computing, researchers can significantly improve their predictive power of aqueous environments.

The research team will continue to develop scalable software for first principles simulations using recursive bisection algorithms. Future work also includes expanding computational spectroscopy capabilities to study water at solid oxide interfaces and water/low Z mixtures at metal interfaces, including the calculation of infrared and Raman spectra.

This research is enabling the team to separate the effects responsible for observed phenomena that can't be easily probed experimentally, such as interface structure dependence of vibrational properties of liquids and liquid mixtures. Galli's ongoing work will play a key role in understanding the physical and chemical problem of processes involved in carbon-bearing fluids in the deep Earth, in particular, methane dissociation under upper mantle conditions, as well as in understanding structure and dissociation of water in contact with solid oxide surfaces.