**Type:** Renewal
**Title:** "Accelerated Climate Modeling for Energy"


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


**Scientific Discipline:** Earth Science

**INCITE Allocation:** **180,000,000 processor hours**
**Site:** Argonne National Laboratory
**Machine (Allocation):** IBM Blue Gene/Q (100,000,000 processor hours)
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** Cray XK7 (80,000,000 processor hours)


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

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

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


**Principal Investigator:** Kenneth Jansen, University of Colorado, Boulder
**Co-Investigators:** Jed Brown, University of Colorado, Boulder
Michel Rasquin, University of Colorado, Boulder
Onkar Sahni, Rensselaer Polytechnic Institute
Mark Shephard, Rensselaer Polytechnic Institute
Cameron Smith, Rensselaer Polytechnic Institute


**Scientific Discipline:** Engineering: Aerodynamics

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


**Research Summary:**
This project is economically motivated by the goal of redesigning control surfaces to reduce their size, thus reducing jet fuel usage at a cost-savings of approximately 0.3 billion dollars per year. With this INCITE award, researchers propose to develop adaptive detached eddy simulations of synthetic jet active flow control on a multi-component realistic high lift wing configuration. The simulations will provide fundamental insight into the interaction between synthetic jets and the main flow on a realistic geometry in aeronautics.

The team will model an array of synthetic jets that have been vectored to augment the stream-wise momentum near the flap suction peak, where separation is typically observed, to limit flap effectiveness for high-deflection angles and angles of attack. Simulations will allow for a fundamental study of flow control on a complex aeronautical control surface. The numerical simulations will provide a detailed view of the flow interactions as well as the insights required to understand and exploit the underlying physical mechanisms related to active flow control.

A secondary goal shows that the proposed baseline configuration is likely to become a reference for future simulations involving a lesser fidelity model, such as Reynolds-averaged Navier–Stokes (RANS) equations. Researchers will demonstrate that the recent developments in parallel adaptive meshing and parallel solver technology can yield fundamental insights into the complicated physics of flow control on real aircraft configurations.

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

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

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

**Scientific Discipline:** Earth Science: Geological Science

**INCITE Allocation:** **60,000,000 processor hours**
**Site:** Oak Ridge National Laboratory

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

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

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

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

**Type:** Renewal
**Title:** "Approaching Exascale Models of Astrophysical Explosions"


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


**Scientific Discipline:** Physics: Astrophysics

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


**Research Summary:**
For this multiyear project, the research team will continue to explore two classes of stellar explosions: Type Ia supernovae (SNe Ia) and X-ray bursts (XRBs) through high-resolution, multiphysics hydrodynamics simulations. The team's simulation codes, Maestro and Castro, are well tuned to Titan, using a hybrid approach to parallelism and beginning to offload time-consuming microphysics calculations to the GPUs. Both codes are freely available.

A fundamental uncertainty in the understanding of SNe Ia is the nature of the progenitor—a single white dwarf accreting from a normal companion star (single degenerate scenario) or two white dwarfs that inspiral (or violently collide) and merge (the double degenerate scenario). No progenitor system of an SN Ia has ever been identified, so astronomers must look for indirect clues. Regardless of the progenitor system, the majority of the carbon and oxygen in the white dwarf(s) is converted into iron/nickel and intermediate-mass elements like silicon, and this nuclear energy release unbinds the star. X-ray bursts are the explosive burning of a thin layer of hydrogen and helium on the surface of a neutron star. Models of XRBs help us understand the properties of neutron stars, and ultimately, how matter behaves at such extreme densities.

The team is carrying out a comprehensive study of SNe Ia and XRBs, using the state-of-the-art multiphysics simulation codes Maestro and Castro. Maestro and Castro were designed specifically for the efficient modeling of astrophysical explosions and make excellent use of Titan's multi-core architecture.

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

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

**Scientific Discipline:** Biological Sciences: Biophysics

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

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

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

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

**Type:** New
**Title:** "Charge Transport in Thin Film Ionomers"

**Principal Investigator:** Gregory Voth, University of Chicago
**Co-Investigators:** Christopher Knight, Argonne National Laboratory

**Scientific Discipline:** Materials Science: Condensed Matter and Materials

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

**Research Summary:**
One of the grand challenges for green energy (e.g., from solar and wind sources) is creating storage for excess electricity that can be inserted later into the power grid. Electrochemical energy-conversion devices, such as fuel cells, could, in theory, provide continuous power to a wide range of portable, residential, and transportation devices. But performance depends on fuel cell catalyst layers which, problematically, are a potential bottleneck for proton transport. This project extends the understanding of fundamental proton transport processes in thin film ionomers, which are critical components in electrochemical conversion devices.

Large-scale, reactive molecular dynamics (MD) simulations will be used to compute key physical properties relating to proton transport and solvation within thin film membranes and, most importantly, will account for the correlated motion of many excess protons. Researchers have teamed Mira with LAMMPS, an open-source molecular simulation code from Sandia National Laboratory, and their own reactive MD simulation code, RAPTOR, which incorporates accurate molecular interactions, chemical reactivity, and robust parallelization algorithms to enable sampling of required spatial and temporal scales.

The largest to date, these multistate simulations will enable detailed analysis of proton-membrane and proton-proton correlations within the membrane environment as a function of morphology, and comparison with ongoing experiments.

The successful development of low-cost, durable, multi-purpose electrochemical devices, such as high-performance fuel cells, demands collaborative science of an unparalleled nature. Working with the Functional Polymers Group at the National Institute of Standards and Technology (NIST), with its ability to perform a huge array of experimental measurements on systems studied through this project, will make this possible.

**Type:** New
**Title:** "Combining High Accuracy Electronic Structure Methods to Study Surface Reactions"

**Principal Investigator:** Maria Chan, Argonne National Laboratory
**Co-Investigators:** Anouar Benali, Argonne National Laboratory
Graham Fletcher, Argonne National Laboratory

**Scientific Discipline:** Materials Science: Condensed Matter and Materials

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

**Research Summary:**
The goals of this project are to push the accuracy and scalability frontiers on the quantum mechanical calculation of realistic materials, and advance renewable energy technologies by studying surface reactions on transition metal oxides. Molecular reactions on these surfaces are pertinent for high-capacity energy storage, as well as photocatalytic carbon dioxide reduction, which has the potential to turn sunlight directly into fuel.

Using highly accurate Quantum Monte Carlo (QMC) calculations with a new approach for scalable multi-configurational wave function determination—the variational subspace valence bond (VSVB) method—researchers aim to study energies relevant to key molecular reactions on the surfaces of several important systems for renewable energy applications. These systems include lithium-iron-oxides, lithium-manganese oxides, and cuprous oxide.

Both QMC and VSVB are highly parallel and well-suited to execution on the latest supercomputers. In this case, Mira is needed to expedite the investigation of cluster models for crystalline systems that are comprised of hundreds of atoms.

The results of this research will help evaluate approaches used to perform first-principles calculations and inform the choice of future techniques. The knowledge gained from these advanced approaches will deepen understanding of surface reactions on key materials that could lead to more efficient energy storage and energy conversion, and reduce dependency on fossil fuels for transportation and other energy needs.

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


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


**Scientific Discipline:** Chemistry: Physical

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


**Research Summary:**
The team will use its broad experience in computational actinide chemistry and high performance computers to address the complex problem of predicting the properties of actinide complexes. The team will obtain some of the first highly accurate, extrapolated complete basis set results for actinide compounds including high levels of correlation and relativistic effects, both scalar and spin-orbit, that can be used as benchmarks to test other methods as well as to explain recent experimental results on the spectroscopy of small molecules.

The team will develop new computational capabilities on advanced high performance architectures and use them to study actinide complexes in various oxidation states in solution, at interfaces, and at the nanoscale. Specific areas include hydrolysis and aggregation reactions, separation systems, spectroscopy and strong correlated solids. These calculations will involve complex spin-orbit coupled systems and will be extremely computationally demanding. This will lead to unprecedented new insights into the behavior of these important molecular systems in complex environments. The team will study how actinide nanoparticles are formed in hydrolysis reactions, which will be used in the development of new fuel particles. These studies will afford the team unique insights into the solvation of actinides and how to treat collective weak interactions. The project will have a broad and sustained impact on the field of actinide chemistry and provide the basis upon which to build the science underpinning future nuclear energy technologies.

**Type:** Renewal
**Title:** "Computational Spectroscopy of Heterogeneous Interfaces"

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

**Scientific Discipline:** Materials Science: Condensed Matter and Materials

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

**Research Summary:**

The interfaces between solids, nanoparticles and liquids play a fundamental role in determining the properties of materials. With an understanding of the microscopic structure of solid–water and solid–electrolyte interfaces, researchers can better predict the properties of photocathodes for water splitting in the production of clean fuels and energy conversion in solar cells. However, the properties of interfaces are seldom explicitly included in *ab initio* models, due to the complexity and cost of the associated calculations.

The main objective of the project is to calculate the physical properties of aqueous interfaces with solid oxides and semiconductors, and of inorganic interfaces at the nanoscale. Using Qbox and WEST codes optimized for Mira, researchers will perform *ab initio* calculations of electronic and vibrational spectra, integrated with large-scale *ab initio* molecular dynamics simulations, to study realistic interfaces. The Qbox code also includes new techniques for calculating sum frequency generation (SFG) spectra, which will help identify vibrational signatures of specific reaction pathways that occur at interfaces.

The results can be used to interpret experiments and to optimize materials properties to improve clean fuel production and solar energy applications. This work will help establish a robust strategy to enable the comparison of *ab initio* data with experiments carried out at light sources, such as Argonne's Advanced Photon Source. Ultimately, the results could lead to analysis tools for spectroscopic data that can be used by theorists and experimentalists alike.

**Type:** New
**Title:** "Convective Turbulence in Liquid Gallium and Sodium"

**Principal Investigator:** Janet Scheel, Occidental College
**Co-Investigators:** Joerg Schumacher, Technische Universitaet Ilmenau

**Scientific Discipline:** Engineering: Fluids and Turbulence

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

**Research Summary:**
Many turbulent flows found in nature and exploited for heat transfer in technology are driven by sustained temperature differences. Applications range from chip-cooling devices to the study of convection in the sun and Earth's atmosphere, core, and oceans. Turbulent Rayleigh-Bénard convection (RBC) is a type of heat transfer in which a fluid cell is kept at a constant temperature difference between top and bottom. Because the fluid is confined, thin boundary layers of the temperature and velocity fields form. To better understand whether heat transport is dominated by these boundary layers and their dynamics, researchers are using leadership-class computing to predict the transition to turbulence in the boundary layers of RBC.

A boundary layer transition to turbulence is expected at larger Rayleigh numbers, which characterize the driving of convective turbulence and is proportional to the temperature difference. However, this transition is also affected by a fluid's Prandtl number, which corresponds to the properties of that particular fluid. Most high-Rayleigh-number experiments have explored fluids with high or moderate Prandtl numbers, such as gases like helium or air. However, fluids with high Rayleigh numbers but very low Prandtl numbers are of interest for their applications in both nature and technology.

On Mira, researchers are using a highly efficient, parallel spectral element code, Nek5000, to simulate turbulent RBC in a regime with low Prandtl numbers and high Rayleigh numbers, relevant to liquid gallium and sodium. With resolutions on Mira of approximately 10 billion grid points and 100,000 time steps for each RBC simulation, researchers are characterizing the global structure of convective flow and the boundary layer dynamics for this new regime. Furthermore, this study is determining the exact relationship between heat transport and Rayleigh number for low Prandtl numbers. This information has not been obtained before and would be fundamentally useful for both theory and experiments.

**Type:** Renewal
**Title:** "Cosmic Reionization On Computers"

**Principal Investigator:** Nickolay Gnedin, Fermilab

**Scientific Discipline:** Physics: Astrophysics

**INCITE Allocation:** **65,000,000 processor hours**
**Site:** Argonne National Laboratory
**Machine (Allocation):** IBM Blue Gene/Q (65,000,000 processor hours)

**Research Summary:**

Cosmic reionization, the most recent phase transition in the history of the universe, is the process by which neutral cosmic gas was ionized by high-energy radiation from early galaxies. As the observational constraints on reionization are limited, theoretical modeling and numerical simulations play a critical role in reionization studies.

However, forthcoming observations from the soon-to-be-launched James Webb Space Telescope (JWST) and the currently-being-built Atacama Large Millimeter Array (ALMA) radio telescope will make all existing theoretical models of reionization obsolete. Hence, the theoretical community is now faced with the challenge of upgrading simulation technology to a qualitatively higher level to keep theory adequate for comparing with future observations.

Petascale supercomputers like Mira are enabling potential breakthroughs that were deemed impossible only a few years ago. Taking advantage of this technological progress, the Fermilab research team is carrying out simulations that model all relevant physics, from radiative transfer to gas dynamics and star formation, through its Cosmic Reionization On Computers (CROC) project, using the Adaptive Refinement Tree (ART) code as its main simulation tool.

An important objective of this research is to make predictions for future observations of the redshifted 21-cm line of neutral hydrogen. That line, coming unimpeded even from the most remote corners of the universe, will enable researchers to map the full 3D (2D sky plus redshift as the third dimension) distribution of neutral gas in the universe, once construction of the Hydrogen Epoch of Reionization Array (HERA) is completed.

With a better understanding of cosmic reionization, researchers will be able to shed light on other aspects of modern cosmology, from probing the nature of dark matter and dark energy through Cosmic Microwave Background observations, to observing the physical state of intergalactic gas in the absorption spectra of high redshift quasars.

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

**Principal Investigator:** Salman Habib, Argonne National Laboratory

**Scientific Discipline:** Physics: High Energy Physics

**INCITE Allocation:** **150,000,000 processor hours**
**Site:** Argonne National Laboratory
**Machine (Allocation):** IBM Blue Gene/Q (80,000,000 processor hours)
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** Cray XK7 (70,000,000 processor hours)

**Research Summary:**
The focus of cosmology today is on its two mysterious pillars, dark matter and dark energy. Large-scale sky surveys are the current drivers of precision cosmology and have been instrumental in making fundamental discoveries in these areas. This INCITE project focuses on two main areas in computational cosmology, both of which rely on the Hardware/Hybrid Accelerated Cosmology Code (HACC): the generation of Cosmic Emulators, precision prediction tools for different cosmological observables spanning a large range of cosmological parameters; and the construction of sophisticated synthetic sky maps from very large high-resolution cosmological simulations.

Members of this collaborative INCITE project carried out their first set of simulations for cosmological models that include neutrinos and dynamical dark energy, an important extension of the Cold Dark Matter cosmological model awaiting next-generation sky surveys. With more than 20 models developed to date, these simulations will be part of the complete Mira-Titan Universe suite that will provide high-accuracy emulators for a variety of cosmological summary statistics. Analysis, so far, is focused on the matter power spectrum, redshift space distortions, the halo mass function, and the halo concentration-mass relation.

In addition, researchers are using the simulations to generate Data Challenges for the Dark Energy Science Collaboration of the Large Synoptic Survey Telescope project, and have begun creating maps built around the Sunyaev-Zel'dovich effect—a distortion of the thermal Cosmic Microwave Background (CMB) photon spectrum—to aid the cross-correlation of CMB measurements from the South Pole Telescope and galaxy clusters from the Dark Energy Survey.

To enable sharing of these large-scale simulation data and analysis tools, the team continues to develop its Portal for Data Analysis services for Cosmological Simulations (PDACS). Deployed on Argonne's Magellan cloud computing platform, PDACS has enabled the sharing of processed data from the project's Outer Rim simulations which, when carried out on Mira, evolved more than one trillion particles describing the distribution of matter in the universe.

**Type:** New
**Title:** "Direct Numerical Simulation of Compressible, Turbulent Flow"

**Principal Investigator:** Jonathan Poggie, Purdue University
**Co-Investigators:** Nicholas Bisek, Air Force Research Laboratory
Ryan Gosse, Air Force Research Laboratory

**Scientific Discipline:** Engineering: Fluids and Turbulence

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

**Research Summary:**

During long-duration, supersonic or hypersonic flight in the atmosphere, the vehicle must withstand both intense heating and unsteady mechanical loads. A fundamental difficulty in this regime is the presence of long time-scale (1–100 ms), low-frequency (10–1000 Hz) pressure fluctuations under separated, turbulent boundary layers. These fluctuations lie in a regime near the typical resonant frequency of aircraft panels, and thus lead to severe structural fatigue loading. A key scientific question remains as to why such low-frequency oscillations exist.

The disparity of length and time scales between fine-grain turbulence and large-scale flow unsteadiness makes computational simulation of the thermal and mechanical loads on high-speed aircraft inherently challenging. Focusing on the basic science of unsteady separation in compressible, turbulence flow, the aim of this project is to investigate perturbed, supersonic turbulent boundary layers through massively-parallel, direct numerical simulations.

Using the high-order, finite-difference code HOPS (Higher Order Plasma Solver), the research team is employing a compression ramp configuration to generate flow separation—a configuration representative of aircraft structures. The main objective is to test the validity of the amplifier and oscillator models of separation unsteadiness by comparing the wall pressure spectra near separation for a turbulent incoming boundary layer and a laminar incoming boundary layer under the same flow conditions.

In this multi-year project, simulations will be carried out in four stages, with the first year focused on preliminary studies in preparation for production work. Coarse-grid simulations will determine grid resolution requirements and suitable flow conditions, such as ramp angle and Reynolds number. Eventually, this work will lead to fine-grid simulations of incoming turbulent flow meant to replicate published experimental data and explore the possibility of mitigating unsteadiness with flow control.

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

**Principal Investigator:** Petros Koumoutsakos, ETH Zurich

**Scientific Discipline:** Engineering: Fluids and Turbulence

**INCITE Allocation:** **72,000,000 processor hours**
**Site:** Argonne National Laboratory
**Machine (Allocation):** IBM Blue Gene/Q (72,000,000 processor hours)

**Research Summary:**

Cloud cavitation collapse—the evolution of clusters of vapor bubbles in high-pressure flow—is detrimental to the lifetime of high-pressure injection engines, yet beneficial to kidney lithotripsy and ultrasonic drug delivery. Despite its importance, researchers have limited understanding of the governing mechanisms necessary to design informed strategies for controlling it.

Cloud cavitation collapse presents a formidable challenge to experimental and computational studies. The latter requires two-phase flow solvers capable of capturing interactions between multiple deforming bubbles, pressure waves, formation of shocks, and their interactions with boundaries and turbulent vortical flows. Project researchers will use their award-winning, two-phase compressible flow code, CUBISM-MPCF, to capture the collapse of more than 50,000 bubbles interacting with a turbulent flow field at unprecedented resolution and performance.

During their first year, researchers used CUBISM-MPCF on Mira to successfully simulate a free-field collapsing cloud of 50,000 bubbles and a cloud of 20,000 bubbles in a homogenous turbulent flow. The 50,000-bubble simulation considered different geometrical arrangements (such as spherical or cylindrical), densities, and distributions (random or structured). These studies revealed that cavitation begins with the initiation of collapse at the bubble surface, followed by the formation of center-directed micro-jets that induce pressure up to 25 times higher than the ambient pressure.

Now, researchers are quantifying uncertainties in cloud peak pressures and collapse times under random initial conditions. Simulations of 5,000 to 10,000 bubbles permit 20,000 to 80,000 sources of randomness related to bubble radii, position, and vapor pressure. By exploiting the newly developed Multi-Level Monte Carlo method, a novel statistical sampling approach that is faster than its classical predecessor, researchers can simulate sources of randomness up to two orders of magnitude higher than similar state-of-the-art simulations.

Researchers predict that information gained from these simulations could revolutionize the development of engineering models for the prediction of the cavitation damage potential.

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


**Principal Investigator:** Jacqueline Chen, Sandia National Laboratories
**Co-Investigators:** Alex Aiken, Stanford University
John Bell, Lawrence Berkeley National Laboratory
Giulio Borghesi, Sandia National Laboratories
Marc Day, Lawrence Berkeley National Laboratory
Ray Grout, National Renewable Energy Laboratory
Andrea Gruber, SINTEF, Norway
Ramanan Sankaran, Oak Ridge National Laboratory


**Scientific Discipline:** Chemistry: Combustion

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


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

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

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


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


**Scientific Discipline:** Computer Science

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


**Research Summary:**
This project supports the very active community developing and employing high-performance and high-productivity parallel programming paradigms that provide a natural and fully compatible extension of the message passing interface (MPI) to massively threaded, extreme-scale parallel systems.

Research is centered around development activities for MADNESS (Multiresolution ADaptive NumErical Scientific Simulation), a general purpose numerical environment for deploying advanced scientific algorithms on petascale and post-petascale architecture. Research objectives involve a combination of lower-level optimizations and developments to the MADNESS runtime environment; general purpose numerical environment for the solution of integral and differential equations; and testing of higher-level applications and functionalities in different scientific domains, spanning multiple areas of chemistry and physics.

The team continues to build on its achievements from earlier INCITE awards. This included the implementation of task-based algorithms for dense and block-sparse tensor algebra in TiledArray, a block-sparse tensor toolkit based on the MADNESS runtime. These developments will lead to a new generation of many-body electronic structure capability necessary for combustion and catalysis.

The team will also improve strong scalability of the numerical density functional theory (DFT) code. The code's capability will be augmented to support pseudopotentials as well as frequency-dependent response properties, both key to practical application of the code to catalysis and energy storage systems.

The resources of this project are essential to support scientific users on IBM's Blue Gene petascale systems and other platforms, to develop new capabilities, and to ensure a strong path to exascale computing.

**Type:** New
**Title:** "Dynamics of Magnetic Fields in High-Energy-Density Plasmas"


**Principal Investigator:** Amitava Bhattacharjee, Princeton Physics Plasma Laboratory
**Co-Investigators:** William Fox, Princeton Physics Plasma Laboratory
Kai Germaschewski, University of New Hampshire
Yi-Min Huang, Princeton Physics Plasma Laboratory


**Scientific Discipline:** Physics: Plasma Physics

**INCITE Allocation:** **35,000,000 processor hours**
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** Cray XK7 (35,000,000 processor hours)


**Research Summary:**
The goal of this project is to understand and model the dynamics of magnetic fields in high-energy plasmas, including their generation, subsequent dynamics and destruction. These involve processes that play a role in both fusion and astrophysics, including magnetic field generation by processes such as the Biermann battery (thermoelectric) effect and Weibel instability, destruction of fields by magnetic reconnection, and the dynamics of the fields as dictated by the generalized Ohm's law.

The team will conduct both fully-kinetic particle-in-cell simulations (with our code PSC) and reduced (MHD and extended MHD), including detailed comparison of the two. Its work with HMHD will advance studies of magnetic reconnection in the large-system size, plasmoid-dominated regime. The team's kinetic simulations will study 3-D processes and particle-energization in laser-driven reconnection experiments including inertial-fusion-relevant effects such as magnetic field generation by the Biermann battery and heat-flux-driven plasma advection via the Nernst effect. The group has recently made the first experimental identification of the ion-driven Weibel instability, and the proposed leadership scale 3-D simulations will be used to benchmark this important astrophysical instability. Finally, a significant part of this project will also aim at direct contact between particle-in-cell simulation and experiment, through a collaboration with researchers at the Laboratory for Laser Energetics at the University of Rochester.

**Type:** New
**Title:** "Electronic Response to Particle Radiation in Condensed Matter"


**Principal Investigator:** Andre Schleife, University of Illinois at Urbana-Champaign
**Co-Investigators:** Alfredo Correa, Lawrence Livermore National Laboratory
Erik Draeger, Lawrence Livermore National Laboratory
Yosuke Kanai, University of North Carolina at Chapel Hill


**Scientific Discipline:** Materials Science: Condensed Matter and Materials

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


**Research Summary:**
This project will establish a predictive computational framework for quantum-mechanical, first-principles modeling of dynamical response of electrons to charged-particle radiation in semiconductors and water/DNA. Quantum dynamics simulations will uncover detailed mechanisms that are central to a wide range of applications, from aerospace electronics to proton beam therapy.

A fast, charged particle entering a target material produces complicated effects on a range of length and time scales. At the atomistic level, these begin on atto- to femto-second (one-quintillionth to one-quadrillionth of a second) time scales. Existing models for calculating electronic stopping power (transfer of energy from a charged particle into an electronic system) lack predictive capability and atomistic details. At the same time, first-principles electron dynamics simulations are very computationally demanding.

The team's implementation of Ehrenfest molecular dynamics into the Qbox/Qb@ll code, based on real-time time-dependent density functional theory, combines the quantum dynamics of electrons and the classical movement of ions for a quantitative understanding of these systems. The team focused its code development on strong scalability over many processors, allowing for accurate simulations of the dynamics of thousands of electrons on these ultrafast time scales.

On Mira, the team is modeling electronic stopping in three semiconductor materials with different band gaps, or degrees of electrical conductivity, and native defects. Preliminary studies have shown that both of these properties influence electronic stopping. They are also examining how highly energetic protons interact with DNA and water, as these protons can directly damage DNA or indirectly damage it through ionization of water. Detailed understanding of this interaction is of great importance for the semiconductor industry, for ensuring human health in space, and for advancing proton beam therapy for cancer treatment.

**Type:** New
**Title:** "Evaluation of a 1000 MW Commercial Ultra Super-Critical Coal Boiler"


**Principal Investigator:** Martin Berzins, University of Utah
**Co-Investigators:** Todd Harman, University of Utah
Ben Isaac, University of Utah
John Schmidt, University of Utah
Sean Smith, University of Utah
Jeremy Thornock, University of Utah


**Scientific Discipline:** Chemistry: Combustion

**INCITE Allocation:** **351,000,000 processor hours**
**Site:** Argonne National Laboratory
**Machine (Allocation):** IBM Blue Gene/Q (280,000,000 processor hours)
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** Cray XK7 (71,000,000 processor hours)


**Research Summary:**
Pulverized coal power plants in the United States currently account for 39 percent of the power on the grid. While environmental concerns over coal utilization are driving the industry to pursue change as quickly as possible, advances in clean-coal technologies are slow moving, requiring technological breakthroughs and full-scale demonstrations to inspire the accelerated adoption of new technologies across the coal industry. This INCITE initiative proposes to simulate and evaluate the design of cleaner, next-generation 1,000 megawatt (MW) Ultra Super-Critical (USC) coal boilers.

The model for the study is an Alstom's "twin-fireball" furnace, which is stoked when coal and air are injected from a main windbox, and over-fire air (OFA) is injected above it. The project aim is to run four large-eddy simulation (LES) test cases with different OFA configurations to validate and further improve the boiler design. The studies rely on LES-based codes in the Uintah open-source framework, which is comprised of computational components that simulate turbulent combustion and address fluid-structure interaction problems.

Preliminary indications suggest that these first-of-their-kind LES computations can provide greater accuracy in predicting temperature and velocity profiles in furnaces than steady-state computational fluid dynamics computations. In addition, design studies and benchmark solutions from this project will indicate the strengths and weaknesses of this approach with respect to research on present and future boilers, as well as on computer and computational science research.

**Type:** New
**Title:** "First Lattice QCD Calculation of the I=2 Two-Nucleon Parity Violating Amplitude"


**Principal Investigator:** Andre Walker-Loud, Lawrence Berkeley National Laboratory
**Co-Investigators:** Evan Berkowitz, Lawrence Livermore National Laboratory
Wick Haxton, Univeristy of California, Berkeley, and LBNL
Thorsten Kurth, Lawrence Berkeley National Laboratory
Amy Nicholson, University of California, Berkeley
Joe Wasem, Lawrence Livermore National Laboratory


**Scientific Discipline:** Physics: Nuclear Physics

**INCITE Allocation:** **64,000,000 processor hours**
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** Cray XK7 (64,000,000 processor hours)


**Research Summary:**
The team will perform a high statistics calculation of the isospin-2 parity violating amplitude in the two-nucleon system. The lack of knowledge of this amplitude currently limits the physics the team can extract from the field's most precise measurements, on the p~ + p asymmetry. These calculations will provide important theoretical support for current and future experimental efforts such as the NPDGamma Experiment at ORNL.

An understanding of Hadronic Parity Violation (HPV) directly from the Standard Model of physics remains an outstanding theoretical challenge. The underlying weak interactions between the quarks are well understood. However, these interactions are masked by the non-perturbative nature of QCD, which describes the interactions between quarks and gluons that are bound into the observed hadrons. The least constrained of all the Standard Model currents is the hadronic neutral weak interaction, which is best studied in low-energy nuclear environments. The typical strength of this hadronic weak interaction is 7 orders of magnitude smaller than the typical QCD interactions, making it extremely challenging to measure experimentally. An improved theoretical understanding of these phenomena will be necessary to interpret the experimental results in terms of the underlying interactions. Lattice QCD is the only theoretical tool available to quantitatively determine these HPV quantities directly in terms of the Standard Model parameters.



This research is supported by the DOE Office of Science SciDAC 3 Initiative and the Early Career Award program.

**Type:** New
**Title:** "First Principles Based Statistical Physics of Alloys and Functional Materials"


**Principal Investigator:** Markus Eisenbach, Oak Ridge National Laboratory
**Co-Investigators:** Valentino Cooper, Oak Ridge National Laboratory
Ying Wai Li, Oak Ridge National Laboratory
Khorgolkhuu Odbadrakh, University of Tennessee, Knoxville
G. Malcolm Stocks, Oak Ridge National Laboratory
Yang Wang, Pittsburgh Supercomputing Center


**Scientific Discipline:** Materials Science: Condensed Matter and Materials

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


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

The team will investigate three important, overlapping classes of materials: magnetic materials, high entropy alloys and ferroelectric materials. These materials are of fundamental importance both to basic science as well as for potential technological applications.

First principles Wang-Landau allows the team to exploit the multiple levels of parallelism available in future architectures, as they depend on compute intensive deterministic kernels that require the majority of the execution time and can utilize the thread level parallelism of multi core CPUs and GPU accelerators and the coarse grained distributed memory parallelism at the Monte-Carlo level. Finite temperature effects will be modeled by sampling the energy landscape with the Wang-Landau (WL) statistical approach. The value of the energy at the sampled points will be determined by the Locally Self-consistent Multiple Scattering (LSMS) method. The efficiency of WL sampling, the speed of the LSMS, and the computing power of Titan combine to allow a truly first-principles thermodynamic description of magnetism. The combined WL sampling and LSMS will lead to a realistic treatment of alloys and functional materials.

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

**Principal Investigator:** Alexei Khokhlov, The University of Chicago
**Co-Investigators:** Marta Garcia, Argonne National Laboratory

**Scientific Discipline:** Chemistry: Combustion

**INCITE Allocation:** **140,000,000 processor hours**
**Site:** Argonne National Laboratory
**Machine (Allocation):** IBM Blue Gene/Q (140,000,000 processor hours)

**Research Summary:**
This research seeks to understand the fundamental physics of high-speed combustion, in particular flame acceleration and deflagration-to-detonation transition (DDT) in reactive gases. Because detonation occurs quickly and on a very small spatial scale compared to the size of the system, high-resolution, multidimensional simulations are the most feasible method by which to investigate the detailed physics of a DDT.

This study requires first-principles, compressible, reactive flow Navier-Stokes direct numerical simulations (DNS), which account for and explicitly resolve physical processes on a range of spatial scales, as well as attendant shocks and physical variables. Work on this project has been accomplished with a high-speed combustion and detonation code (HSCD) on Mira.

Using previous INCITE awards, researchers conducted the first 3D reactive flow Navier-Stokes DNS simulations of flame acceleration and DDT in a stoichiometric hydrogen-oxygen mixture in a 2.5 cm square pipe with smooth and rough walls. Wall roughness introduces additional turbulence which leads to a somewhat faster DDT and a drastic change in the location of the DDT from pre-heated gas ahead of the flame brush to hot spots inside it.

Validation of a physical model via simulations of reflected shock tube ignition delay experiments are in a very good agreement with physical experiments. An unexpected outcome of the studies has been the discovery of a universal acoustic mechanism responsible for the formation of hot spots and transition from strong to mild ignition behind reflected shocks in reactive gases.

This year's award continues validation and sensitivity studies, and incorporates the important effect of water condensation on the tube walls, which may be responsible for an observed slowdown of the flame and a delay in the DTT observed in the long tube experiments. This effect has never been considered in modeling of a DDT in hydrogen-oxygen mixtures.

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

**Type:** Renewal
**Title:** "Frontiers in Planetary and Stellar Magnetism Through High-Performance Computing"


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


**Scientific Discipline:** Earth Science: Geological Sciences

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


**Research Summary:**
This continuing INCITE project examines the interaction of convection, magnetism, and rotation within the context of three distinct solar-system bodies: the sun, Jupiter, and Earth. To address the limitations of present-day planetary and stellar dynamo models, a project research team of geo- and astrophysicists is developing state-of-the-art computational models to describe the interior dynamics of these systems, using *Rayleigh*, a pseudo-spectral code designed to study magnetohydrodynamic convection in spherical geometries.

Using the extrapolative power of Mira, the team has been able to construct high-resolution models and resolve a range of spatial scales previously inaccessible to numerical simulation. These will be used to demonstrate that transformative physical changes occur in planetary and stellar simulations of dynamo action in fluids with realistic material properties.

Currently, researchers are developing extreme models of rotating convection in the solar convection zone. The study has already shed light on factors that determine the typical velocity amplitudes and spectral distribution of solar convection, a major problem in solar physics.

A survey of Jovian interior dynamics simulations will lead to a massive $2{,}048^3$ class calculation that greatly exceeds previous Jovian modeling efforts. The models will be used to make detailed predictions of magnetic field morphology, thermal emission, and gravity field anomalies that can be tested via data from NASA's Juno mission to Jupiter.

Researchers hope to engage the broader community by providing access to these singularly extreme data sets and, more broadly, to demonstrate the community-wide need for massive computational efforts to investigate the realistic, turbulent liquid-metal dynamo action that occurs in planets and stars.

**Type:** New
**Title:** "Fundamental Properties of QCD Matter Produced at RHIC and the LHC"

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

**Scientific Discipline:** Physics: Nuclear Physics

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

**Research Summary:**

A few seconds after the Big Bang, the building blocks of matter emerged from a hot, energetic state known as the Quark-Gluon Plasma (QGP)—named for its composition of quark and gluon particles. These building blocks of matter are called hadron particles, and they form when gluons, which carry the strong nuclear force, bind quarks together.

Physicists are recreating the primordial conditions of the QGP experimentally through extreme temperatures and pressures generated in the Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratory in the United States, and the Large Hadron Collider (LHC) at CERN, in Europe. One unexpected discovery from experiments shows that the QGP is almost an ideal liquid, rather than a gaseous-like plasma, with the smallest shear viscosity over entropy density ratio ever observed. This suggests that the QGP is a strongly interacting system. The theory of strong interactions can be studied computationally through lattice Quantum Chromodynamics (QCD), a complex numerical approach to solving quark-gluon interactions.

In previous INCITE projects, this team made key contributions to the QGP research. By integrating and comparing results from the RHIC and LHC, their simulations determined the temperature at which hadrons form and uncovered other details of particle formation. Employing first-principles calculations, which rely on individual interactions at high computational demand, this team will use Mira to address some of the most fundamental unsolved questions in the field, such as a microscopic explanation of the QGP behavior and the propagation of conserved charges in the medium.

The resulting data should help scientists determine the strength of coupling between quarks and gluons in the QGP, how charges propagate through it, and whether the QGP is an ideal liquid. Resolving these and other questions related to the microscopic behavior of the QGP and its transition to hadrons will improve scientific understanding of particle interactions, and the formation of matter in the universe.

**Type:** New
**Title:** "A Generic Plant Cell Wall and its Deconstruction for Bioenergy"

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

**Research Summary:**

Rational strategies for improving the efficiency of the production of biofuels and bioproducts from plant cell wall lignocellulosic biomass via cellulose hydrolysis require a detailed understanding of the structure and dynamics of the biomass. Lignocellulosic biomass is a complex material composed of cellulose microfibrils laminated with hemicellulose, pectin, and lignin polymers.

To reduce biomass recalcitrance to hydrolysis by the improvement of pretreatment and the design of improved feedstock plants, a detailed understanding of biomass structure, mechanics, and response to pretreatment regimes is needed. During a previous INCITE award, the team led by Oak Ridge National Laboratory's (ORNL's) Jeremy Smith, applied molecular dynamics simulation to understand the structure and dynamics of lignin aggregates, of lignin precipitation on cellulose fibers, and of systems of lignin, cellulose and cellulases. During this time they also developed technology permitting the efficient simulation of multimillion atom biomolecular systems running on the Titan supercomputer at ORNL. This enabled them to propose to simulate full lignocellulosic biomass systems, consisting of cellulose, lignin and hemicelluloses at both physiological and pretreatment conditions.

The simulations performed will help obtain a detailed knowledge of the fundamental molecular organization, interactions, mechanics and associations of bulk lignocellulosic biomass. Furthermore, simulations will be performed of the effect of pretreatments on biomass structure and dynamics, permitting a rationalization of a wide range of experimental data. This work forms an integral part of a larger effort comprising the Bioenergy Science Center, the ORNL Biofuels Science Focus Area, and the Center for Lignocellulose Structure and Formation, aimed at integrating experimental and leadership-class computation to synergistically derive information on lignocellulosic assembly degradation at an unprecedented level of detail.

**Type:** Renewal
**Title:** "Global Adjoint Tomography"


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


**Scientific Discipline:** Earth Science: Geological Sciences

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


**Research Summary:**
This project addresses the long-standing challenge of imaging Earth's interior based on full waveform inversion on a global scale, which has so far remained a challenge mainly due to computational limitations. Using the Titan supercomputer at Oak Ridge National Laboratory, the team, led by Princeton University's Jereon Tromp, has performed 15 iterations for a global mantle and crustal model with transverse isotropy confined to the upper mantle, using seismic waves with a shortest period of ~ 17 s. Advances in seismology enabled by an allocation of the requested petascale resources include continuing iteratively updating and increasing the resolution of seismic images of our entire planet based on massive data assimilation accommodated by adjoint techniques.

The team started with a global dataset of 253 earthquakes with magnitudes in the range of 5.8 ≤ Mw ≤ 7.0. The current 15$^{th}$ iteration model will be the first generation "full waveform" global adjoint tomography model. During the 2016 allocation, they aim to include general anisotropy and anelasticity, which will provide better constraints on interactions between Earth's mantle and crust and related tectonic/geodynamical processes.

Their ultimate goal is to use all earthquakes recorded by permanent and temporary seismographic networks since 1995, using the global Centroid Moment-Tensor catalogue for earthquakes in the magnitude range of 5.5 ≤ $M_w$ ≤ 7.0. To date, the team has gathered data for about ~ 4,000 earthquakes and are working on their source inversions. They started with 27 s waves, and since the 12$^{th}$ iteration were using 17 s waves. The aim for the next year is to go down to ~ 9 s and include more earthquakes in the inversion. Meanwhile, they will continue optimizing the solver and improving the adjoint tomography workflow in conjunction with preparations for running higher-resolution simulations (~ 1 s) on the next-generation supercomputer Summit.

**Type:** New
**Title:** "GPU Accelerated LES of High-Pressure Turbine Stator-Rotor at Engine Conditions"

**Principal Investigator:** Vittorio Michelassi, GE
**Co-Investigators:** Gregory Laskowski, GE
Richard Sandberg, University of Southampton

**Scientific Discipline:** Energy Technologies: Energy Efficiency

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

**Research Summary:**
The goal of this project is to leverage recent advances in high-fidelity LES, validated by DNS, to compute the flow in a High-Pressure-Turbine (HPT) stage at large Reynolds numbers, turbulence intensities and length scales to move closer to engine conditions.

The program will investigate the accurate flow prediction in HPT. The team will first concentrate on the HPT first stage nozzle, challenging due to the interaction with large-scale turbulent flow structures from the combustion chamber that may provoke large losses and heat loads. The team will move to an HPT stage to capture the stator-rotor interaction and the concerted effect of random unsteadiness (turbulence), deterministic unsteadiness (wakes and shocks) and potential effects. The team will investigate how these phenomena affect boundary layer stability and ultimately losses and heat transfer. Finally, the team will move to a full radial span vane calculation to investigate end-wall flows and their span-wise penetration.

The high quality of the simulations will allow a better understanding of loss generation, of both momentum and enthalpy mixing and of the effect of secondary flows. The results will constitute a reference data-set able to indicate weaknesses in current HPT design and the associated lower-order CFD based design tools. The results will also help unlock performance increase opportunities and ways to improve the accuracy of lower-fidelity CFD tools, the workhorse in design loops for many years to come.

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


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


**Scientific Discipline:** Earth Science: Geological Sciences

**INCITE Allocation:** **190,000,000 processor hours**
**Site:** Argonne National Laboratory
**Machine (Allocation):** IBM Blue Gene/Q (90,000,000 processor hours)
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** Cray XK7 (100,000,000 processor hours)


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

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

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

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


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


**Scientific Discipline:** Materials Science: Condensed Matter and Materials

**INCITE Allocation:** **70,000,000 processor hours**
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** Cray XK7 (70,000,000 processor hours)


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

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

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

**Type:** New
**Title:** "Kinetic Simulations of Relativistic Radiative Magnetic Reconnection"


**Principal Investigator:** Dmitri Uzdensky, University of Colorado, Boulder
**Co-Investigators:** Mitchell Begelman, University of Colorado, Boulder
Benoit Cerutti, Princeton University
Krzysztof Nalewajko, Stanford University
Greg Werner, University of Colorado, Boulder


**Scientific Discipline:** Physics: Plasma Physics

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


**Research Summary:**
This project investigates radiative relativistic magnetic reconnection in collisionless electron-positron and electron-ion plasmas under conditions relevant to high-energy astrophysical environments, including the effects of strong radiative cooling. Reconnection is a fundamental plasma process of magnetic field rearrangement and relaxation, leading to rapid conversion of magnetic energy into thermal and nonthermal particle energy. It is important in natural and laboratory plasma environments, such as solar flares, Earth's magnetosphere, various astrophysical systems, and magnetic fusion devices. Understanding radiative magnetic reconnection will help advance the field of high-energy-density plasma physics—a key DOE science frontier.

Researchers will use petascale radiative particle-in-cell (PIC) plasma simulations to characterize nonthermal particle acceleration and the associated synchrotron and inverse-Compton radiation produced by energetic particles in the reconnecting system. The project team has developed the unique radiative PIC code, Zeltron, that self-consistently incorporates the radiation reaction force on relativistic particles. This will enable investigating reconnection in high-energy-density radiative regimes that have so far been inaccessible to direct kinetic simulations. A set of large 3D simulations of radiative relativistic magnetic reconnection in pair plasmas demonstrated excellent scalability of Zeltron in short test runs on Mira.

Results from this project will lead to advances in the understanding of fundamental plasma physics processes and have important implications for modern high-energy astrophysics. It will enable first-principles modeling of plasma energization and radiation in systems such as pulsar magnetospheres, gamma-ray bursts, and accretion flows and jets powered by black holes.

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


**Principal Investigator:** Anne Dord, GE Aviation
**Co-Investigators:** Greg Laskowski, GE Aviation
Lee Shunn, Cascade Technologies
Jin Yan, GE Global Research
Matthieu Masquelet, GE Global Research


**Scientific Discipline:** Engineering: Fluids and Turbulence

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


**Research Summary:**
This project looks at the complex physics of combustor liner flows to help aviation engineers develop cleaner, more efficient engines. Utilizing earlier results on the characteristics of multi-hole cooling flow on the transition piece, the part of the combustor liner that connects the main combustion zone and turbine, current simulations will use wall-modeled large-eddy simulations (LES) to analyze flow in single and multi-cup combustors.

An in-depth study of the detailed geometries of combustor systems requires computational fluid dynamics (CFD) resolutions achievable only on massively parallel computing platforms, such as Mira. This collaborative effort has investigated four geometries, thus far, using Cascade Technologies' CFD code, CharLES low-Mach "Helmholtz" solver, which performs reacting LES and reproduces the important interactions between chemistry, turbulence, and acoustics that occur in real-world gas turbine engines.

Understanding and predicting the aero-thermal flow field in combustors is a key step in designing and optimizing the architecture for better fuel efficiency, lower emissions and better performance. The first group of calculations used LES to model the behavior of an idealized configuration representative of combustor liners. This has enabled modelers to generate high-fidelity datasets that will be used to improve low-fidelity models available to designers. Next, simulations will use wall-modeled LES to analyze the flow in single- and multi-cup combustors.

Researchers will apply the same approach to a more complex configuration, involving a larger domain and more realistic flow characteristics. They will employ the results on an actual multi-cup General Electric rig, providing a vehicle with which to test the improved models developed in the first two steps of the program. This affords designers a better understanding of the complex unsteady processes governing the aerothermal field around combustor liners.

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

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

**Scientific Discipline:** Chemistry: Physical

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

**Research Summary:**

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

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

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

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

**Type:** Renewal
**Title:** "Lattice QCD"


**Principal Investigator:** Paul Mackenzie, Fermilab
**Co-Investigators:** Richard Brower, Boston University
Norman Christ, Columbia University
Frithjof Karsch, Brookhaven National Laboratory
Julius Kuti, University of California, San Diego
Kostas Orginos, College of William & Mary
David Richards, Jefferson Laboratory
Martin Savage, University of Washington
Robert Sugar, University of California, Santa Barbara


**Scientific Discipline:** Physics: Particle Physics

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


**Research Summary:**
For this INCITE project, researchers from the U.S. Quantum Chromodynamics (USQCD) Collaboration will advance exploration in lattice quantum chromodynamics (QCD), the theory of the strong interactions between quarks and gluons, which make up hadrons, such as protons, neutrons, and pions. In high-energy physics, precise lattice QCD calculations are required to investigate and validate the properties of the Standard Model of particle physics, and to search for new physics beyond the Standard Model.

The main objectives of the calculations are to generate gauge configurations of the gluon fields, which are representative samples of the QCD ground state, and use these configurations to calculate physical quantities. To date, this project has created 4,800 new gauge configurations which will be used to address fundamental questions in high-energy and nuclear physics. They are directly related to on-going major experimental programs, such as the GlueX experiment at the Thomas Jefferson National Accelerator Facility, the Relativistic Heavy Ion Collider at Brookhaven National Laboratory, and the Large Hadron Collider at CERN, in Switzerland.

The availability of petascale computers, such as Mira, has made it possible, for the first time, to perform calculations at the physical value of the pion mass on very fine lattices. These calculations, in turn, are having a major impact on Standard Model theory. Results from this project are essential for meeting milestones set by DOE's Office of Science.

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

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

**Scientific Discipline:** Physics: Plasma Physics

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

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

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

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

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

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

**Type:** New
**Title:** "Magnetohydrodynamic Models of Accretion Including Radiation Transport"


**Principal Investigator:** James Stone, Princeton University
**Co-Investigators:** Shane Davis, University of Virginia
Charles Gammie, University of Illinois at Urbana-Champaign
Yan-Fei Jiang, Harvard University
Eliot Quataert, University of California, Berkeley


**Scientific Discipline:** Physics: Astrophysics

**INCITE Allocation:** **47,000,000 processor hours**
**Site:** Argonne National Laboratory
**Machine (Allocation):** IBM Blue Gene/Q (47,000,000 processor hours)


**Research Summary:**
This project explores the largely ignored impact of radiation on accretion flow—the flow of objects, ranging from dust to planets, onto a compact object with a strong gravitational potential, like a supermassive black hole. For 20 years, such studies have focused on the magnetohydrodynamic (MHD) processes that drive angular momentum transport. However, scientists understand that angular momentum and radiation transport affect the structure and dynamics of accretion flow. Researchers will calculate the structure of such flows, and make predictions about how accreting sources evolve and affect their environment.

Leadership-class computers, like Mira, are the only resources that can explore these far-away phenomena at the scale and detailed needed. The team is using a new version of its compressible MHD code, Athena ++, which features new algorithms, such as those for general relativistic (GR) MHD in stationary spacetime. The code shows excellent single-core performance and weak scaling on Mira, making it possible to thoroughly explore 3D time-dependent radiation MHD simulations.

In the first of this two-year project, the team is completing a survey of the structure and dynamics of radiation-dominated accretion. They will investigate, for the first time, whether thermal and/or viscous instabilities, predicted over 40 years ago, actually occur in global models of MHD turbulent disks. Researchers will use these simulations to further investigate the effect of radiation on the production of jets and outflow from spinning black holes.

This will be the first time the physics of radiation-dominated accretion flows onto compact objects is computed using direct solutions of radiation transport equations rather than approximations. As such, the team's results are contributing to the understanding of the growth of supermassive black holes in the early universe, the effects of active galactic nuclei on galaxy formation, and the interpretation of observational data.

**Type:** New
**Title:** "Many-Body Theory of Materials"


**Principal Investigator:** Paul Kent, Oak Ridge National Laboratory
**Co-Investigators:** Valentino Cooper, Oak Ridge National Laboratory
Jaron Krogel, Oak Ridge National Laboratory
Fernando Reboredo, Oak Ridge National Laboratory


**Scientific Discipline:** Materials Science: Condensed Matter and Materials

**INCITE Allocation:** **70,000,000 processor hours**
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** Cray XK7 (70,000,000 processor hours)

## Research Summary:


The team plans to confront one of the grand challenges of materials science and condensed matter physics: the development of truly predictive and reliable quantum-mechanics-based methods in order to understand novel materials and to help design and optimize materials properties for technological deployment. The lack of sufficiently accurate or reliable methods significantly hinders progress in many areas of energy-related materials.

The team proposes application and further development of first-principles, many-body quantum Monte Carlo (QMC) methods which are already able to provide the required increase in predictive power over established methods for many materials. Furthermore, the methods are expected to be systematically convergable in the future, thus providing a key missing capability for materials modelling. Due to the emergence of petascale computing, QMC methods are increasingly able to study materials of significant electronic and structural complexity. They have seen a remarkable increase in use owing to their high scalability, and the utility of benchmark-quality data provided.

The team plans to address the challenging questions of electronic structure and properties for two key classes of materials of strategic importance to DOE: correlated transition metals and metal oxides that are foundational to many applications in energy storage and conversion and layered nanomaterials including magnetic materials with applications in electronics and spintronics.

The team was designed its investigations to be able to exploit the very high performance achievable on Titan's GPU architecture. The team's QMCPACK code is the only first-principles QMC code to efficiently exploit GPUs.

**Type:** New
**Title:** "Multi-Scale Plasma Turbulence"

**Principal Investigator:** Frank Jenko, University of California, Los Angeles

**Scientific Discipline:** Physics: Plasma Physics

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

**Research Summary:**

In contrast to our immediate environment on Earth, the majority of matter in the visible universe is in a plasma state—it consists of partially or fully ionized gas. Flows in these plasmas tend to be highly turbulent, exhibiting complex and fascinating nonlinear multi-scale effects.

Plasma physics is also at the heart of numerous technical applications, the most prominent of which is magnetic confinement fusion (MCF) research, the quest to recreate the Sun's power on Earth. MCF holds the promise of covering a large fraction of the world's future electricity demands in a safe and environmentally friendly way for generations to come.

Interestingly, a common link between space/astrophysics and MCF research is provided by the fact that one usually deals with weakly collisional plasmas. Such systems can only be adequately described in the context of kinetic theory, whose main quantity of interest is a distribution function in 6D position-velocity space (or phase space) for each particle species. However, many of these plasmas are strongly magnetized, and this often allows for the use of a reduced (5D) version of kinetics named gyrokinetics.

The main aim of the present project is to employ one of the world-leading gyrokinetic codes, GENE, to make major contributions regarding two Grand Challenge problems related to plasma turbulence—namely the understanding of turbulent dissipation in space/astrophysical plasmas as well as the development of a predictive theory of magnetic confinement in fusion plasmas.

Two major goals of the present project are to carry out the first systematic and fully resolved gyrokinetic study of turbulent heating in Alfvénic turbulence, with applications to solar wind turbulence as observed by spacecraft, as well as to prepare and perform the first "triple-scale" turbulence simulations for the near-edge pedestal region of tokamak plasmas, treating profile scales, ion scales, and electron scales self-consistently. The proposed simulations, involving an unprecedented level of multi-scale physics and thus realism, are truly ground-breaking and only feasible with the help of leadership computing facilities resources.

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

**Principal Investigator:** George Karniadakis, Brown University

**Scientific Discipline:** Biological Sciences: Biophysics

**INCITE Allocation:** **90,000,000 processor hours**
**Site:** Argonne National Laboratory
**Machine (Allocation):** IBM Blue Gene/Q (50,000,000 processor hours)
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** Cray XK7 (40,000,000 processor hours)

**Research Summary:**

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

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

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

**Type:** New
**Title:** "Next-Generation Nanostructured Polymer Electrolytes by Molecular Design"

**Principal Investigator:** Thomas Miller, California Institute of Technology

**Scientific Discipline:** Chemistry: Physical

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

**Research Summary:**
State-of-the-art rechargeable lithium-ion batteries contain a flammable mixture of alkyl carbonates that serves as the electrolyte solvent; about one in a million lithium-ion batteries exhibits catastrophic failure, usually initiated by combustion of the solvent, which strongly motivates the development of safer lithium batteries without flammable components. Solidification of electrolytes - though the use of polymer electrolyte materials - can reduce the flammability of the electrolyte material but generally results in lower ionic conductivity because the solvation shells become immobile.

To address these problems, the team will use INCITE computing resources, in collaboration with experimental synthesis and characterization efforts, to provide both fundamental understanding and prediction of high-conductivity, non-flammable, solid polymer electrolytes for lithium- ion batteries. The molecular simulation work will be performed in close connection with the efforts of synthetic chemists at Cornell (Geoff Coates), chemical engineers at UC Berkeley (Nitash Balsara), and polymer physicists at Caltech (Zhen-Gang Wang). The simulations will drive the screening and design of new polymer electrolytes, as well as the detailed understanding of ion diffusion mechanisms; promising polymer electrolyte candidates will then be synthesized in the laboratory (Coates), and their ion transport characteristics will be measured and tested in full cells (Balsara). Success of this research effort will advance battery technologies that are critical for transportation and other large-scale energy storage applications.

In the first year, the team will screen a set of 500 chemically diverse classes of polymers for high ion conductivity and solubility under dilute salt conditions, and will then screen over 5000 polymer sequences from the most-promising classes to identify specific polymer sequences that merit experimental synthesis and characterization. The screening of polymer materials will be employed using the Chemically Specific Dynamic Bond Percolation (CS-DBP) model, which has recently been developed and validated in the Miller group. In the second year, these candidate polymer sequences will be further investigated under conditions of moderate-to-high salt conditions, yielding fundamental insights into the mechanisms of ion-conductivity under practical conditions.

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


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


**Scientific Discipline:** Physics: Nuclear Physics

**INCITE Allocation:** **184,000,000 processor hours**
**Site:** Argonne National Laboratory
**Machine (Allocation):** IBM Blue Gene/Q (80,000,000 processor hours)
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** Cray XK7 (104,000,000 processor hours)


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

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

**Type:** New
**Title:** "Nulceation and Growth of Colloidal Crystals"

**Principal Investigator:** Sharon Glotzer, University of Michigan
**Co-Investigators:**

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

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

**Research Summary:**

The use of nanoparticles as building blocks for self-assembly enables new approaches to design materials with specific target applications. This project will discover the mechanisms by which simple, complex and aperiodic structures grown for a variety of particle shapes and potentials, yielding insights for the development of new nanomaterials.

The properties and behavior of crystalline materials depend directly on the quality of the crystals, which in turn depends on how the crystal formed. From Big Pharma to the chocolate industry, product quality depends on the ability to predict and control crystallization.

With substantial resources from Titan, this team plans to carry out the most in-depth computational study of nucleation and grown that has ever been undertaken. The team seeks to understand the nature of the processes by which fluids crystallize into complex colloidal crystals. Both the large system size and sampling complexity needed for these studies requires massively parallel computing systems.

The team's approaches will be of immediate and even broader interest to the materials, engineering and chemistry communities interested in crystallization.

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


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


**Scientific Discipline:** Computer Science

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


**Research Summary:**
This research team is dedicated to furthering understanding and development of leadership-class compute systems Blue Gene/Q and XK7. Their work is focused on five goals: (1) develop new programming models and runtime systems for emerging and future-generation leadership computing platforms that exploit thread-level parallelism and potential architectural heterogeneity; (2) update and extend performance evaluation of all systems using suites of standard and custom micro, kernel, and application benchmarks; (3) continue to port performance tools and performance middleware to the BG/Q and XK7, make them available to high-end computing users, and further develop the tools and middleware to support the scale and unique modes of parallelism of each system; (4) validate and modify performance prediction technologies to improve utility for production runs on each system; and (5) analyze and help optimize current or prospective application codes and potentially develop new parallel algorithms.

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


**Principal Investigator:** Sean Couch, Michigan State University
**Co-Investigators:** Almudena Arcones, TU Darmstadt
Emmanouil Chatzopoulos, University of Chicago
Carla Frohlich, North Carolina State University
Dongwook Lee, University of California, Santa Cruz
Evan O'Connor, North Carolina State University
Petros Tzeferacos, University of Chicago
J. Craig Wheeler, University of Texas at Austin


**Scientific Discipline:** Physics: Astrophysics

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


**Research Summary:**
Despite the importance of core-collapse supernovae (CCSNe) to our understanding of many aspects of the universe, the mechanism that reverses stellar core collapse and drives supernova explosions is not fully understood. The goal of this project is to carry out the most comprehensive study yet accomplished on the influence of magnetic fields and rotation in core-collapse supernovae (CCSNe). Using the multi-physics FLASH code on Mira, researchers will employ advanced 3D magnetohydrodynamics (MHD) simulations of rotating, magnetic stellar core collapse in an effort to uncover a robust explosion mechanism that matches observations.

Researchers are running two fine-grid full-star simulations, one non-rotating with zero initial magnetic field and one with moderate rotation and weak initial field strength. Given the recent realization of the important role plain hydrodynamic turbulence plays in the CCSNe mechanism, it was determined that a non-magnetic, non-rotating control simulation was crucial. The control proves valuable, both as a comparison to magnetorotational simulations and as a test of the resolution required to accurately model hydrodynamic turbulence in the CCSN context. Early indications suggest that the growth rate of the magnetic field strength in the magnetorotational simulation is faster than for the lower resolution case. Detailed analyses of both simulations are currently under way.

In preparation for 3D full-neutrino transport simulations, several 2D CCSNe simulations were conducted, which yielded significant scientific results. Specifically, it was found that, in purely Newtonian cases, no progenitor successfully explodes, while including an approximate treatment of relativistic gravity results in successful explosions for some progenitors.

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

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

**Scientific Discipline:** Physics: Plasma Physics

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

**Research Summary:**

Laser-initiated, or inertial fusion energy (IFE), holds incredible promise as a source of clean and sustainable energy. However, significant obstacles to delivering IFE remain, including the fact that IFE experiments have not achieved self-sustained ignition. This is attributed in large part to excessive laser-plasma instabilities (LPIs) encountered by the laser beams. LPIs, such as two-plasmon/high-frequency-hybrid instability (HFHI) and stimulated Raman scattering (SRS), can absorb, deflect, or reflect laser light, causing potential disruptions and excess heat loads. Therefore, developing an understanding of LPIs is crucial to the success of any IFE scheme.

LPI processes are complex, involving both wave-wave and wave-particle interactions. This project is focused on using fully nonlinear kinetic computer models to study high-energy density science relevant to IFE. The research team's OSIRIS code uses explicit particle-in-cell codes that are computationally intensive and capable of studying the kinetic evolution of LPIs on the desired spatial and time scales. Because laser beams in IFE devices are broken up into multiple speckles (a pattern that results when a beam is scattered by a medium), researchers must understand how multiple speckles interact with each other.

In 2015, the team completed 2D simulations of laser plasma interactions with multiple laser speckles. These simulations isolated and identified three processes for inter-speckle interaction that can trigger instability in the form of SRS. They also conducted the first-ever study to investigate the relationship between external magnetic fields and LPI reduction in current and future magnetic IFE experiments. Simulation results are, so far, consistent with experiment.

Now, researchers will study the interactions of multiple speckles in 3D for both HFHI and SRS instabilities. They will perform simulations using smaller speckles to understand the essential physics involved in these systems, and larger speckles to study the problem under National Ignition Facility-relevant conditions. These simulations reveal, for the first time, the 3D nature of these processes, and could lead to the understanding and control of LPIs in IFE plasmas.

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

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

**Scientific Discipline:** Materials Science: Condensed Matter and Materials

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

**Research Summary:**
Self-healing of cracks in brittle ceramics and glasses can dramatically increase the reliability and lifetime of structural components and reduce the maintenance costs in a broad range of energy technologies. The goal of this project is to achieve a detailed atomistic understanding of self-healing processes to determine the optimal size and spatial distribution of nanoparticles for self-healing of structural ceramics in energy applications at high service temperatures.

Researchers will perform petascale quantum molecular dynamics (QMD), reactive molecular dynamics (RMD), and mesoscale reactive dissipative particle dynamics (RDPD) simulations to study the self-healing capabilities of anticorrosion coatings for metals and ceramic nanocomposites. They also will perform RMD simulations to determine the mechanical properties of self-healing materials, like aluminum sponges.

Based on benchmarks and previous production runs on Mira, researchers have significantly improved the scalability, time-to-solution, and floating-point performance of QMD and RMD simulation codes. Time-to-solution was 60-times less than the previous state-of-the-art code.

Simulation results have revealed a novel nanostructural design for on-demand hydrogen production from water, advancing renewable energy technologies. And the team's largest QMD simulation has shown that orders-of-magnitude faster reactions with higher yields can be achieved by alloying aluminum (Al) particles with lithium (Li). During this investigation, researchers discovered a surprising autocatalytic behavior of the oxygens that bridge Li and Al, suggesting that Li-O-Al plays an active role in oxidation. This atomistic understanding of metal corrosion advances the proposed study of anticorrosion coatings for metals.

Novel self-healing materials will play vital roles in the design of components for high-temperature turbines, wind and solar energy, lighting applications, and medical implants.

**Type:** New
**Title:** "Petascale Simulations of Short Pulse Laser Nanostructuring of Metals"

**Principal Investigator:** Leonid Zhigilei, University of Virginia
**Co-Investigators:** Chengping Wu, University of Virginia

**Scientific Discipline:** Engineering: Material Response

**INCITE Allocation:** **10,000,000 processor hours**
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** Cray XK7 (10,000,000 processor hours)

**Research Summary:**

The goal of the petascale modeling of laser interactions with metal targets is to obtain detailed information on the mechanisms and kinetics of fast non-equilibrium structural and phase transformations triggered by the rapid laser energy deposition and responsible for the generation of complex hierarchical nano-/micro-scale surface morphology and unusual surface microstructure. The immediate impact of the proposed simulations will be in revealing the interrelation between the complex multi-scale processes in laser processing and facilitating the development of new laser techniques based on controlled surface modification at the nanoscale. At a more general level, the results of the simulations will contribute to the fundamental understanding of the mechanisms of phase transformations and microstructure development under highly non-equilibrium conditions created by the laser irradiation.

The simulations will be performed with a hybrid atomistic-continuum model that combines classical molecular dynamics method with a continuum description of laser excitation and subsequent relaxation of the excited electrons. The model provides a detailed atomic-level description of fast nonequilibrium phase and structural transformation in the irradiated targets and, at the same time, ensures an adequate description of the laser light absorption by the conduction band electrons, the energy transfer to the lattice due to the electron-phonon coupling, and the fast electron heat conduction in metals.

**Type:** New
**Title:** "Protein-Protein Binding Specificity"

**Principal Investigator:** Benoit Roux, University of Chicago
**Co-Investigators:** Chris Chipot, University of Illinois at Urbana-Champaign
Sunhwan Jo, Argonne National Laboratory

**Scientific Discipline:** Biological Sciences: Biophysics

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

**Research Summary:**

Protein-protein interactions are ubiquitous in many biological pathways and play an essential role in modulating cellular functions. However, computing the binding affinity of even two proteins to determine whether they will associate and form a stable complex is a technical challenge. This project aims to understand and predict protein-protein associations that govern biological processes at the atomic level using a molecular dynamics (MD) computational strategy, based on computationally intensive, all-atom models. Researchers are validating this computational method against a broad range of protein complexes to see if binding affinity can be predicted with quantitative accuracy.

Using NAMD scalable molecular dynamics software, the research team has developed a powerful and scalable computational method that breaks down binding calculations into several steps. It then expresses the binding free energy as a sum of free energies associated with each step that can be calculated from the replica-exchange MD (REMD) potential of mean force calculations, a type of energy change calculation. In REMD simulations conducted on Mira, an ensemble of replicas of the protein-protein interaction that cover a range of conditions is considered. This method increases the sampling efficacy of MD simulations.

The team is quantifying the binding affinity and binding entropy for several characteristic protein complexes, including cohesin-dockerin proteins that control the assembly of the cellulosome (enzyme complexes that facilitate the decomposition of plant cell walls) and are, therefore, important for energy production. By studying complexes of various size and flexibility, the team is advancing theory-modeling-simulation (TMS) technology. With an established TMS route to predicting protein-protein interactions, years of high-resolution structural data collected in large protein interactome databases could be leveraged to address fundamental biological questions and help solve the problem of rational protein design.

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


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


**Scientific Discipline:** Materials Science: Condensed Matter and Materials

**INCITE Allocation:** **170,000,000 processor hours**
**Site:** Argonne National Laboratory
**Machine (Allocation):** IBM Blue Gene/Q (90,000,000 processor hours)
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** Cray XK7 (80,000,000 processor hours)


**Research Summary:**
Due to its numerical expense, quantum Monte Carlo (QMC) methods were once limited to model systems of small atoms or molecules. Thanks to leadership-class resources such as Mira, QMC methods now allow for rigorous calculations of more complicated materials. This on-going INCITE award focuses on continuum-based QMC to model electronic structure and light nuclear-electronic systems related to heterogeneous catalysis of transition metal nanoparticles, phase transitions, properties of materials under pressure, and strongly correlated materials.

In their third year, researchers aim to study intermediate concentrations of iron-bearing perovskite (Pv) and post-perovskite (PPv) phases of magnesium silicate, of which the bulk of Earth's lower mantle is composed. Combining these intermediate iron concentration calculations with results from earlier studies, researchers may better understand the impact iron percentage has on the Pv-PPv phase transition, which explains many of the unusual properties observed in the core-mantle boundary layer. Results will also allow for the construction of an accurate QMC-based phase diagram of that transition, utilizing the QMCPACK code ported on Mira.

Work on platinum solids, nanoclusters and surfaces continues with final analysis of the surface energies of Pt(111) and Pt(100), surfaces important in surface and catalytic applications. The team will focus on developing benchmark estimates of extreme accuracy for the adsorption energies of key catalytic species on these surfaces. Successful validation will establish that QMC calculations, with carefully calibrated pseudopotentials, can effectively substitute for experiments in cases where experimental data are not available.

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


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


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

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


**Research Summary:**
The main goal of this research is to understand, at atomistic and molecular levels, the growth mechanisms and transport phenomena occurring at and across electrochemical interfaces, through the use of large-scale reactive molecular dynamics (MD) simulations. Breakthroughs in the fundamental understanding of these interfaces are urgently needed for the design and development of novel materials for energy applications.

The team's extensive expertise is in large atomistic-scale calculations of the interfacial properties of nanoscale materials, combined with the highly scalable LAMMPS and NAMD molecular dynamics software. This has placed them in the unprecedented position to address fundamental questions concerning electrochemical interfaces, in areas as diverse as materials synthesis and tribological interfaces.

The team has made significant advancements in understanding the dimensionality effects on the natural oxidation of iron nanoparticles, which are promising lithium-ion battery anodes. Earlier MD simulations in this area suggest that electric fields can form hollow oxide nanoparticles, which may lead to increased ionic mobility and more efficient energy transfer.

Working off of their molecular modeling of oxidation and corrosion, the team initiated a collaborative modeling effort between Argonne and the GE Global Research Center. Together, they will test the feasibility of using LAMMPS and a highly optimized version of the reactive force field approach, ReaxFF, to simulate hot corrosion, a sulfidation/oxidation process that affects aluminum and aluminum alloys, which is especially relevant to aircraft engines.

Continued development of these quantitative atomistic simulation models on the complexities of nanoscale corrosion problems will allow researchers to probe materials at finer levels of spatial resolution, while accurately capturing the dynamics of chemical reactions.

**Type:** New
**Title:** "Simulating Reionization of the Local Universe: Witnessing Our Own Cosmic Dawn"


**Principal Investigator:** Paul Shapiro, University of Texas at Austin
**Co-Investigators:** Kyungjin Ahn, Chosun University
Dominique Aubert, University of Strasbourg
Stefan Gottloeber, Leibniz-Institut fur Astrophysik Potsdam
Ilian Iliev, University of Sussex
Pierre Ocvirk, University of Strasbourg
Romain Teyssier, University of Zurich
Gustavo Yepes, Universidad Autonoma de Madrid


**Scientific Discipline:** Physics: Astrophysics

**INCITE Allocation:** **70,000,000 processor hours**
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** Cray XK7 (70,000,000 processor hours)


**Research Summary:**
Frontier simulations of the reionization of the local universe within 150 million light years of the Milky Way allow the team to probe the cosmological evolution of the universe at large by comparison of theory with observations of galaxies and their satellites in the Local Group.

The Local Group holds clues to the history of reionization. In fact, the theory of galaxy formation in the standard CDM model of cosmology overpredicts the abundance fo the known dwarf satellite galaxies in the Local Group, so reionization suppression is often used to explain this phenomenon. Deep surveys such as the Dark Energy Survey will test this by searching for under-luminous "missing" satellites of the Milky Way, while, for the Fermi Large Area Telescope, these same satellites are prime targets for the indirect detection of dark matter via gamma rays from annihilation.

To study reionization computationally, the team will use Titan to simulate the fully coupled radiation-hydrodynamical-gravitational N-body evolution of the Local Group and its surroundings, with world-leading resolution, as required to resolve the formation of feedback-supressed dwarf galaxies in a volume large enough to model global reionization. The team will use its new, massively parallel hybrid RAMSES-CUDATON code, solving radiative transfer and ionization rate equations on the GPUs to accelerate by orders of magnitude. This will advance significantly under the team's successful pathfinder simulation, CoDa (Cosmic Dawn), performed on Titan under a 2013 INCITE allocation. To boost resolution of dwarf galaxies further, the team will then use another new hybrid code, EMMA, to resimulate the same large volume, but zoom-in on the Local Group by using adaptive mesh refinement.

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

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

**Scientific Discipline:** Biology: Biophysics

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

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

Under this multiyear INCITE project, the research team is continuing to perform atomic-level molecular dynamics (MD) simulations of an entire photosynthetic organelle, called a chromatophore, 100 million atoms in size. The chromatophore simulations will provide insight into how requirements for structural stability, assembly, supramolecular organization, and efficient light-harvesting are balanced by photosynthetic systems and how competing functional constraints are met at the organelle scale. Additionally, the team is using the string method with a swarm of conventional MD simulations to find the minimum free energy pathway connecting the various adenosine diphosphate/ATP-bound ATP synthase conformations, studying how that pathway changes in well-studied ATP synthase mutants.

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

**Type:** Renewal
**Title:** "$SiO_2$ Fracture: Chemomechanics with a Machine Learning Hybrid QM/MM Scheme"

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

**Scientific Discipline:** Materials Science: Condensed Matter and Materials

**INCITE Allocation:** **126,000,000 processor hours**
**Site:** Argonne National Laboratory
**Machine (Allocation):** IBM Blue Gene/Q (126,000,000 processor hours)

**Research Summary:**
Understanding the chemo-mechanical phenomena that cause silicates to fracture would prove a great advantage to both enabling the process, as in large-scale mining, and eliminating it in products that rely on silicate materials. Researchers are utilizing advanced computing tools on Mira to better understand the behaviors that drive stress corrosion and chemically activated crack propagation at both the macro- and microscopic levels.

This multi-year INCITE project is pioneering simulation methodologies for predictive modelling of failure processes in oxides using a hybrid quantum mechanical/molecular mechanical (QM/MM) scheme to help describe the fracturing of silicon dioxide in a wet environment. On the method development side, the team is advancing a novel machine learning (ML) approach that significantly reduces the number of expensive QM calculations necessary per unit of simulated system time. This approach dramatically increases the efficiency of ongoing production calculations, reducing the computational cost anticipated for CY 2016 by approximately 40 percent for the same scientific milestones.

The simulations have shown, thus far, that cracks in silicon can initiate and propagate in the presence of oxygen, even if the energy supplied by the load is insufficient to create new fracture surfaces in pure systems. These results were confirmed by experiments that showed no evidence of cracking in oxygen-free conditions.

Continuing work on machine learning of QM forces is of key importance at this point in the project, as applications science and machine learning will converge to deliver much larger 3D modeling of silica/water systems. Simulation times will run much longer than is possible with current state-of-the-art, first-principles molecular dynamics approaches.

The results from this project have relevance for a broad range of applications in mining, photovoltaics, and biomedical implants. They are also expected to generate fundamental insights that could help rationalize and guide future materials design and novel algorithmic developments.

**Type:** New
**Title:** "Spin Dynamics of Strongly Correlated Materials"


**Principal Investigator:** Gabriel Kotliar, Rutgers University
**Co-Investigators:** Kristjan Haule, Rutgers University
Viktor Oudovenko, Rutgers University


**Scientific Discipline:** Chemistry: Physical

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


**Research Summary:**
A team from Rutgers University will perform first principles computational studies of the neutron scattering cross sections of strongly correlated materials of great importance for the US Department of Energy—essential research for improving nuclear fuels.

To tackle the complexity of this class of solids the team will use a highly parallel version of the Dynamical Mean Field Theory and Density Functional Theory (DMFT+DFT) program, which uses continuous time quantum Monte Carlo as the impurity solver. In a previous allocation, they were able to demonstrate the code's high degree of scalability and optimal performance on Oak Ridge National Laboratory's (ORNL's) Titan supercomputer.

With their improved code performance the researchers will investigate correlated actinides and iron pnictides, which exhibit high temperature superconductivity, with a particular focus on $PuCoGa_5$—plutonium-based superconductors—and related compounds in the actinide family, as well as FeSe superconductors in the iron pnictide family. The team's studies will identify the region of momentum and frequency where strong spin fluctuations exist, and their evolution with temperature. They will also perform structural relaxations and investigate the impact of lattice positions on the magnetic response, in addition to studying the impact of the spin fluctuations on superconductivity by incorporating them in an Eliashberg-like treatment.

The theoretical studies will be confronted with ongoing experimental efforts at neutron scattering facilities across the world including ORNL's Spallation Neutron Source, Los Alamos National Laboratory, and the Institute Laue-Langevin in France. Close contact with experimental groups will result in validation and improvement of the theoretical modeling, and simultaneously will allow a better design of the experiments.

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


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


**Scientific Discipline:** Materials Science: Condensed Matter and Materials

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


**Research Summary:**
Under this INCITE award, researchers are studying the behaviors of liquids and their solutes. Such studies are of paramount importance given that most chemical and biological processes occur in the liquid phase. High-fidelity quantum mechanics methods will be used to study water and ionic liquids, as well as the important processes that occur in them.

The team continues to examine solvated protons, halides, $NO_3^-$, $HSO_4^-$, $ClO_4^-$, and $SO_4^{-2}$, due to their importance in many aqueous chemical reactions. Further, ionic liquids are of interest for their potential to improve the mass and/or charge transport in dye-sensitized solar cells, and for their use as or with extractants, which separate complexes of the lanthanide elements.

Using the team's primary electronic structure code, GAMESS, on Mira, researchers are performing high-level correlated *ab initio* calculations to address the key issues of water structure and bonding, and the nature of solvation of electrolytes that contain ions. The methods used in these calculations are well-correlated electronic structure theory methods based on second order perturbation theory (MP2). In order to combine quantum mechanics (QM) methods with molecular dynamics (MD) simulations for complex systems, a fragment molecular orbital (FMO) method, which divides a molecular system into smaller units, runs alongside MP2 and exploits Mira's multi-level parallelism.

GAMESS is providing, for the first time, a systematic and highly accurate description and interpretation of these processes. During year one, researchers performed fully MP2 MD simulations for a proton solvated with 20 water molecules, developing a program to analyze intermolecular interactions during proton transfer. These will be compared to current replica exchange MD (REMD) simulations of the solvated proton, testing the ability of FMO2 (two-body FMO)/MP2 simulations with REMD to correctly describe the proton transfer and solvated proton decomposition processes.

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

**Principal Investigator:** David Baker, University of Washington

**Scientific Discipline:** Chemistry: Biochemistry

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

**Research Summary:**

While progress is being made in protein structure modeling, the ability to sufficiently sample conformation space, the relative positions of all atoms in 3D, is a limiting factor in protein structure prediction and design. This project aims to advance the simulation software suite ROSETTA, a pioneering tool for computational modeling of biomolecular structures and designs. Researchers plan to optimize the ROSETTA energy function, which provides an approximation of natural protein energetics. Calibration of the energy function can be improved by using molecular simulations predicting physical observables, such as the bulk properties of liquid. Computationally intensive simulations on Mira will further optimize calibration of the ROSETTA energy function for improved accuracy and precision on smaller computing platforms.

Previously, this project described a breakthrough in conformational sampling utilizing highly parallel computations on Mira, which determined the solution structures of proteins up to 40 kilodaltons, with limited experimental data. Only large supercomputers have the capacity and rapid inter-process communication ability to consider large numbers of conformational states simultaneously, in parallel, and to permit a sufficiently fast search for an optimal sequence.

The research will investigate how to refine models from structure prediction, given information about how the protein sequence varies across related organisms. More multistate design work will focus on generating catalytic and therapeutic peptides that bind to targets of interest—including influenza and other pathogens—and a massively parallel enzyme design protocol for the *de novo* design of novel enzymes and catalytic sites. Using both canonical and noncanonical building blocks, ROSETTA's parametric design tools to will help create self-assembling peptide helical bundles, small protein folds composed of several alpha helices that are usually nearly parallel or antiparallel to each other.

This research addresses contemporary issues in medicine, energy, and technology, including the development of protein therapeutics for a number of diseases, and the design of protein reagents to capture and destroy various pathogens and toxins.

**Type:** New
**Title:** "Unveiling the Behavior of $UO_2$ Under Extreme Physical Conditions"


**Principal Investigator:** Peter Littlewood, Argonne National Laboratory
**Co-Investigators:** Chris Benmore, Argonne National Laboratory
Thierry Deutsch, CEA Grenoble
Luigi Genovese, CEA Grenoble
Alejandro Lopez-Bezanilla, Argonne National Laboratory
Stephan Mohr, CEA Grenoble
Laura Ratcliff, Argonne National Laboratory
Lawrie Skinner, Stony Brook University
Johann Weber, Argonne National Laboratory


**Scientific Discipline:** Materials Science: Condensed Matter and Materials

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


**Research Summary:**
Operating safe nuclear power facilities is of the utmost importance. However, little is known about how nuclear fuel materials behave when reactor cores melt. The main objective of this INCITE award is to develop a fundamental understanding of the fluid dynamics, electronic structure, and mechanical properties of hot solid and molten nuclear systems.

Using a first-principles approach, researchers plan to pioneer the *ab initio* treatment of material systems under extreme conditions. Initially, the work will focus on uranium dioxide ($UO_2$). While the most widely used nuclear fuel, there remain large uncertainties associated with liquid $UO_2$ properties that are important for reactor-safety assessments.

Until recently, the nanometer length-scale interactions and picosecond timescales required to model the dynamics of large atomic clusters have rendered high-temperature molecular dynamics (MD) studies impractical. The team's BigDFT code is expected to significantly increase computational efficiency while decreasing the computational cost of the various structure analyses. Combining the code with Mira will allow, for the first time, accurate quantum MD calculations of large supercells at high temperatures.

Near-term results include the powerful capability to simulate the behavior of nuclear energy materials in relevant and extreme conditions. Such understanding, as the interplay between $UO_2$ and its zirconium cladding at the atomic scale, will allow researchers to design, test and deploy "accident-tolerant fuels" that do not react with their environments.