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

Principal Investigator: Mark Taylor, Sandia National Laboratories
Co-Investigators: David Bader, Lawrence Livermore National Laboratory
Robert Jacob, Argonne National Laboratory
Phil Jones, Los Alamos National Laboratory
Lai-Yung Leung, Pacific Northwest National Laboratory
Julie McClean, University of California, San Diego
Matthew Norman, Oak Ridge National Laboratory
Phil Rasch, Pacific Northwest National Laboratory
Todd Ringler, Los Alamos National Laboratory
Pat Worley, Oak Ridge National Laboratory

Scientific Discipline: Earth Science: Climate Research

INCITE Allocation: **278,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (150,000,000 processor hours)
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (128,000,000 processor hours)

Research Summary:
This INCITE project focuses on two science questions that can be answered with the ACME v1 model and DOE capability computing resources:

1. Water Cycle: How will more realistic portrayals of features important to the water cycle (resolution, clouds, aerosols, snowpack, river routing, land use) affect river flow and associated freshwater supplies at the watershed scale?

2. Cryosphere Systems: Could a dynamical instability in the Antarctic Ice Sheet be triggered within the next 40 years?

For the water cycle question, the team hypothesizes that changes in river flow over the last 40 years have been dominated primarily by land management, water management and climate change associated with aerosol forcing, but that during the next 40 years, increasing atmospheric greenhouse gas concentrations will produce changes to river flow with signatures that dominate those other forcing agents. The goal is to simulate the changes in the hydrological cycle with a specific focus on precipitation and surface water in orographically complex regions such as the western United States and the headwaters of the Amazon. For the cyrosphere, the objective is to examine the near-term risk 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. The experiment would be the first fully coupled global simulation to include dynamic ice shelf-ocean interactions for addressing the potential instability associated with grounding line dynamics in marine ice sheets around Antarctica.

Type: New
Title: "Adaptive DES of a Vertical Tail/Rudder Assembly with Active Flow Control"

Principal Investigator: Kenneth E. Jansen, University of Colorado Boulder
Co-Investigators: Jed Brown, University of Colorado Boulder
John Evans, University of Colorado Boulder
Michel Rasquin, Cenaero
Onkar Sahni, Rensselaer Polytechnic Institute
Mark Shephard, Rensselaer Polytechnic Institute

Scientific Discipline: Engineering: Aerodynamics

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 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 $300 million per year. With this INCITE award, researchers propose to perform adaptive detached eddy simulations of synthetic jet active flow control on a vertical tail/rudder assembly. The simulations will provide insight into open scientific questions on 3D active flow control through a significant range of Reynolds numbers.

This effort builds on 2 ESP and 4 INCITE campaigns where computational models of a vertical tail/rudder assembly with 12 synthetic jets were validated against experiments, but at a Reynolds number 53 times smaller than flight conditions. The team will attempt a similar simulation, on Mira, at a five times higher Reynolds number, which will give insight required to eventually carry out the first-ever, flight Reynolds number DES validated against experiments.

Synthetic jet flow control may also prove effective in increasing or decreasing the lift on time scales rapid enough to offset the unsteady wind environment that wind turbines operate in. This would reduce the unsteady loads that are detrimental not only to wind turbine blades but also to the gearboxes used to convert wind energy to electric power. Understanding the fundamental flow physics of these synthetic jets is essential to these and other applications.

The computational approach used for these simulations is a 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: New
Title: "Advanced quantum Monte Carlo simulations of iron-based superconductors"

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

Scientific Discipline: Materials Science: Condensed Matter and Materials

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

Research Summary:
Reliable and controlled simulations of correlated electron materials remain one of the most challenging frontiers of contemporary condensed matter physics. If the behavior and functionalities of correlated systems could be predicted accurately, the "materials by design" concept could be extended to this most fascinating and technologically important class of materials. This would accelerate the search for superconductors with higher transition temperatures, critical rare earth magnet replacements, thermoelectrics with increased efficiency and multiferroics with optimized functionality, and thus have large-scale economic impacts.

This multi-year project will extend the understanding of superconductivity in iron-based materials, a key class of correlated systems important for the development of new energy-related technologies. Large-scale dynamic cluster quantum Monte Carlo simulations of multi-orbital Hubbard models will be used to investigate the nature of the pairing mechanism that gives rise to superconductivity in iron-based materials, explore spin, orbital, and nematic fluctuations in these systems, and study the unusually high transition temperature of monolayer iron-selenide superconductors.

Using its state-of-the-art DCA++ code along with several new algorithmic advances, the team will be able to take full advantage of petascale computation to address this frontier problem. Moreover, this project will demonstrate a significant advance in the general ability to simulate the physics of correlated electron systems and thus open new avenues in extending the materials-by-design concept to this most fascinating and technologically important class of materials.

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

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

Scientific Discipline: Earth Science

INCITE Allocation: **115,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (115,000,000 processor hours)

Research Summary:

Several questions of crucial importance to society involve the behavior of two or more fluids within a solid porous medium. Relevant applications include the geologic storage of carbon dioxide to counteract greenhouse gas emissions, land-atmosphere interactions with linkages to global climate processes, geothermal energy processes, hydraulic fracturing, and enhanced oil recovery. Mechanistic models are relied upon to answer such questions, to make predictions of future states, and to engineer solutions. In the context of these applications, the potential impact of improved mathematical models is broad.

The goal of this project is to use digital rock physics techniques to advance multiscale models for two-fluid flow that are consistent across disparate length scales and resolve the operative physics with higher fidelity than existing models. Recent theoretical, experimental, and computational developments offer the opportunity to improve macroscale models by synthesizing information from different scales to better describe the physics.

The main objective is to execute a set of simulations designed to resolve critical outstanding issues associated with the description of multiphase porous medium flows. The team's codes efficiently use Titan's GPUs, and have demonstrated scalability to thousands of nodes on Titan. The project team has the expertise and experience to ensure that simulations will achieve a high level of performance on Summit when it becomes available. The simulation campaign will generate data that cannot be obtained from other sources, and is needed to overcome important modeling challenge.

Type: New
Title: "All-atom Simulations of Photosynthetic and Respiratory Energy Conversion"

Principal Investigator: Klaus Schulten, University of Illinois at Urbana-Champaign
Co-Investigator: Abhishek Singharoy, 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 and biomedical technologies: the harvesting of solar energy in a photosynthetic organelle and energy conversion in mitochondrial respiration.

Much of the energy used in fundamental cellular functions for most life on Earth is provided either by the absorption of sunlight in light-harvesting membrane domains of plants and bacteria, known as chloroplasts in plants, or through the intake of nutrients in higher organisms. Biomolecular simulations of an entire photosynthetic apparatus, such as the chromatophore, or that of the respiratory complexes require petascale computing resources in order to reveal, on the one hand, how the function of hundreds of proteins are integrated across an entire network, and, on the other hand, how efficient energy conversion is achieved in nature.

Using atomic-level molecular dynamics, the research team will perform simulations of an entire photosynthetic organelle, the 100-million atom chromatophore. 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 will simulate Complex I, one of the most prominent bioenergetics systems in eukaryotic organisms, to explore the mechanism for efficient membrane-wide electron and proton transfer processes, a key step in the life-sustaining yield of ATP to biological cells.

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

Principal Investigator: Michael Zingale, Stony Brook University
Co-Investigators: Ann Almgren, Lawrence Berkeley National Laboratory
John Bell, Lawrence Berkeley National Laboratory
Alan Calder, Stony Brook University
Brian Friesen, Lawrence Berkley National Laboratory
William Hix, Oak Ridge National Laboratory
Adam Jacobs, Stony Brook University
Daniel Kasen, University of California, Berkeley
Max Katz, Stony Brook University
Eric Lentz, University of Tennessee
Christopher Malone, Los Alamos National Laboratory
Bronson Messer, Oak Ridge National Laboratory
Anthony Mezzacappa, Lawrence Berkely National Laboratory
Thomas Papatheodore, Oak Ridge National Laboratory
Stan Woosley, University of California, Santa Cruz
Weiqun Zhang, Lawrence Berkeley National Laboratory

Scientific Discipline: Physics: Astrophysics

INCITE Allocation: **45,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (45,000,000 processor hours)

Research Summary:
The research team will carry out a comprehensive study of stellar explosions and their precursors using a suite of state-of-the-art application codes. Progenitor models to be explored include Type Ia supernovae, the physics of X-ray bursts, the radiative ablation in black widow pulsars, and core-collapse supernovae. Simulating these systems can provide insight into stellar phenomena observed in the night sky and the formation of the universe over billions of years.

The team's simulation codes, Maestro and Castro, are well tuned to Titan, using a hybrid approach to parallelism, and considerable progress has been made in targeting effective use of GPUs.

Fundamental uncertainties to be investigated include the nature of Type Ia supernovae's progenitor—which has never been observed directly, matter's behavior under the extreme density of a neutron star, the nuclear burning leading up toa low-mass core-collapse supernovae, and the inferred mass of a pulsar in a binary system.

Type: New
Title: "Biophysical Principles of Functional Synaptic Plasticity in the Neocortex"

Principal Investigator: Eilif Muller, École Polytechnique Fédérale de Lausanne
Co-Investigators: Fabien Delalondre, École Polytechnique Fédérale de Lausanne
Michael Graupner, Paris Descartes University
Kathryn Hess, École Polytechnique Fédérale de Lausanne
Henry Markram, École Polytechnique Fédérale de Lausanne
Felix Schuermann, École Polytechnique Fédérale de Lausanne
Idan Segev, Hebrew University Jerusalem

Scientific Discipline: Biological Sciences: Neuroscience

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

Research Summary:
During our lifetimes, our brains undergo continuous changes as a consequence of our experiences. Synaptic plasticity—the biological process by which brain activity leads to changes in synaptic connections—is thought to be central to learning and memory. However, little is known about how this process shapes the specialization of biological neural networks.

For this INCITE project, researchers from École Polytechnique Fédérale de Lausanne will use Mira to advance the understanding of these fundamental mechanisms of the brain's neocortex. The team will carry out large-scale simulations of recently uncovered biophysical principles underlying synaptic plasticity in reconstructions of a neocortical microcircuit (Markram et al., 2015; 10.1016/j.cell.2015.09.029) consisting of around 200,000 neurons and 260 million synapses. The aim is to shed light on the synergistic functional principles that shape plasticity in realistic cortical circuits. To support these computationally intensive simulations, they will pursue several key technological developments, including job execution optimizations, and the implementation of an efficient and scalable checkpointing/restart strategy.

The team is targeting three scientific milestones: (1) characterizing the role of NMDA receptor spikes in plasticity induction; (2) characterizing the dynamics of neuronal assembly formation and maintenance; and (3) characterizing the computational impact of synaptic plasticity in common signal processing tasks. In addition to improving our understanding of the brain, this research could help inform the development of more optimized deep learning methods, as well as new learning paradigms for neuromorphic hardware.

Type: New
Title: "Collider Physics at the Precision Frontier"

Principal Investigator: Radja Boughezal, Argonne National Laboratory
Co-Investigator: Frank Petriello, Northwestern University

Scientific Discipline: Physics: Particle 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:
The detailed scrutiny of the Higgs boson and other searches for subtle deviations from the Standard Model of particle physics are reliant on increasingly intricate and precise measurements and theoretical calculations. Numerous examples show that perturbative Quantum Chromodynamics (QCD) computations with percent-level precision are essential to understanding the massive amount of data being produced by experiments at the Large Hadron Collider (LHC), but achieving predictions at this precision is an enormous theoretical and computational challenge.

For this INCITE project, researchers will use the N-jettiness framework, a novel approach to precision perturbative QCD calculations. The framework enables the efficient use of high-performance computing systems to perform computations needed to interpret increasingly precise data from the LHC and future colliders. The team's approach has already led to some of the first high-precision QCD predictions for several benchmark LHC processes, and the first comprehensive comparison of high-precision QCD predictions to jet data at the LHC. The combination of DOE supercomputers and the N-jettiness framework has made these prohibitively difficult calculations possible, and there is great potential for similar rapid progress in other areas.

The team's calculations will address several of the most pressing LHC needs for precision predictions, and will help answer some of the most significant questions facing particle physics. The researchers will also demonstrate that the N-jettiness framework can meet the precision goals set by future colliders by providing the first high-precision predictions for jet production in electron-ion collisions. Ultimately, results from this project will advance our knowledge of nature at the smallest scales and may reveal deviations between measurements and the Standard Model of particle physics.

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

Research Summary:
The goal of this project is to push the accuracy and scalability frontiers on the quantum mechanical calculation of realistic materials to advance lithium battery and solar fuel generation technologies. Using highly accurate quantum Monte Carlo (QMC) calculations together with a new approach for scalable multi-configurational wavefunction determination, the variational subspace valence bond (VSVB) method, the team aims to study surface reactions on transition metal oxides. Both QMC and VSVB are highly parallel and well suited to execution on the latest supercomputer resources.

The durable storage of substantial quantities of energy typically requires chemical bond formation and breaking. These reactions frequently occur on the surface of transition metal oxides, which often exhibit strong correlation and charge localization due to d electrons, which are in turn embedded in, and interact with, an extended electronic system. This combination of factors explains why the accurate first principles treatment of surface reactions has remained a challenge, with mean field approaches such as density functional theory (DFT) requiring various corrections.

Using QMC+VSVB, the team proposes to calculate adsorption energies at key steps in the oxygen reduction and evolution reactions on lithium-iron and lithium-manganese oxide surfaces, as well as in the carbon dioxide reduction on cuprous oxide surfaces. These highly accurate energies will allow the team to evaluate the accuracies of various existing corrections to DFT in order to inform future modeling efforts. Additionally, these highly accurate energies will also enable the team to determine rate limitations in these surface reactions, and surface-dependence of the activity.

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

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

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:

Heterogeneous 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 optimal materials for applications, such as water splitting, the production of clean fuels, and energy storage. However, the properties of interfaces are seldom explicitly included in *ab initio* models, due to the complexity and cost of the associated calculations.

With this multiyear INCITE project, researchers are developing accurate and efficient computational methods to study the interfaces present in realistic materials. The team has optimized the Qbox and WEST codes for Mira to enable calculations of opto-electronic (e.g., photoemission and absorption) and vibrational spectra (e.g., sum frequency generation) integrated with large-scale *ab initio* molecular dynamics simulations. This capability, combined with the petascale power of Mira, provides a practical time-to-solution for identifying vibrational signatures of specific reaction pathways that occur at interfaces and for sampling many configurations from Qbox for input to many-body GW calculations with WEST.

The team's open-source computational protocols will enable accurate calculations of the electronic properties of electrolyte solutions and interfaces important to energy-related applications. Theorists and experimentalists alike can use analysis tools derived from the calculations to interpret experiments and to optimize materials properties to improve clean fuel production and solar energy applications. In addition, the 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.

Type: Renewal
Title: "Cosmic Reionization On Computers"

Principal Investigator: Nickolay Gnedin, Fermilab

Scientific Discipline: Physics: Astrophysics

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

Research Summary:
The study of cosmic reionization—the process of ionization of the bulk of cosmic gas by high-energy radiation from early galaxies—is considered one of the most promising areas of astrophysical research in the current decade. The Cosmic Reionization On Computers (CROC) project aims to produce numerical simulations of reionization that fully model all relevant physics, from radiative transfer to gas dynamics and star formation.

Forthcoming observations from terrestrially based radio arrays and state-of-the-art space telescopes, such as the soon-to-be-launched James Webb Space Telescope (JWST), will make existing theoretical models of reionization obsolete. Hence, the theoretical community is challenged with upgrading simulation technology to a qualitatively higher level to keep theory adequate for comparing with future observations.

The primary scientific goal of this project, expected to be achieved by 2018, is to expand simulation sets and make accurate predictions for the properties of reionization sources expected to be observed by the JWST. The simulation technology developed under the CROC project will provide the theoretical framework to explore such models against data not only from JWST and the Atacama Large Millimeter Array (ALMA), but from the next generation optical telescopes and the Hydrogen Epoch of Reionization Array (HERA) radio telescope.

Another important objective of this research is to make predictions for future observations of the redshifted 21-cm line of neutral hydrogen. That line, emitted by every hydrogen atom in the universe, will enable researchers using the HERA to map the full 3D distribution of neutral gas in the universe.

The team recently published findings which suggest that the global average 21-cm line signal was likely substantially weaker, when the universe was roughly one-tenth its current size, than predicted by an earlier analytical model. This affects the sensitivity requirements of upcoming surveys designed to detect that signal and helps observers make more accurate plans for future observational missions.

Type: New
Title: "Determining the role of AcrA in the bacterial multidrug efflux pump"

Principal Investigator: James C. Gumbart, Georgia Tech
Co-Investigators: Jerome Baudry, University of Tennessee, Knoxville
Jerry Parks, Oak Ridge National Laboratory

Scientific Discipline: Biological Sciences: Biophysics

INCITE Allocation: **38,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (38,000,000 processor hours)

Research Summary:
The development and spread of antibiotic resistance in bacteria is a universal threat to both humans and animals. New therapies against multidrug resistant infections are urgently needed. The majority of currently available antibiotics have low efficacy against Gram-negative pathogens because of active efflux of drugs pumped out of the bacterial cells by multidrug efflux transporters. These transporters are promising targets in the development of small molecule efflux inhibitors (EPIs) that could be used in combinations with antibiotics to improve their efficacy against Gram-negative pathogens. The long-term goal of the research team is to understand the molecular mechanism of drug efflux in Gram-negative bacteria and to develop approaches to inhibit multidrug efflux transporters. For this INCITE proposal, the team will focus on the role of the so-called adaptor protein AcrA, which links the inner- and outer-membrane components of the bacterial efflux pump, AcrB and TolC, respectively. AcrA is critical to the assembly process, yet how it bridges the gap between other components is presently unknown. Detailed free-energy calculations will be used to reveal how the energetic landscape of AcrA is altered upon binding to its partners in the efflux pump.

The team will also describe how AcrA's available conformational space is altered upon binding of novel EPIs designed by us and experimentally validated recently. Simulations will take advantage of recently developed, accurate models of the E. coli bacterial cell envelope, which include both membranes and the intervening cell wall in atomistic detail. Finally, to incorporate the flexibility of partners AcrB and TolC, the team will implement a replica-exchange variant of the enhanced sampling technique accelerated molecular dynamics (aMD) into NAMD. This variant, referred to as REX-aMD, will effectively permit millisecond-equivalent simulations on petascale resources. The expected outcome of the proposed studies is detailed understanding of how multidrug efflux pumps are assembled, aiding the design of new, precisely targeted EPIs that will either prevent the assembly of the pump or block its post-assembly functioning. These EPIs are expected to restore activities of already existing antibiotics and expand therapeutic options against multidrug resistant infections.

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

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

Scientific Discipline: Engineering: Fluids and Turbulence

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

Research Summary:
During long-duration, supersonic or hypersonic flight in the atmosphere, a 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.

The aim of this multiyear INCITE 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.

Their 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. The team has completed simulations of a turbulent inflow case and has collected a large statistical dataset on large-scale separation unsteadiness. Additional calculations will enable researchers to replicate experimental data and explore the possibility of mitigating aircraft unsteadiness at supersonic and hypersonic speeds with flow control mechanisms.

Type: New
Title: "DNS of Turbulent Multi-Phase Combustion Underlying Efficient Flexible Engines"

Principal Investigator: Jacqueline Chen, Sandia National Laboratories
Co-Investigators: Giulio Borghesi, Sandia National Laboratories
Andrea Gruber, SINTEF Energy Research, Norway
Hemanth Kolla, Sandia National Laboratories
Aditya Konduri, Sandia National Laboratories
Alex Krisman, Sandia National Laboratories
Ramanan Sankaran, Oak Ridge National Laboratory

Scientific Discipline: Chemistry: Combustion

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

Research Summary:
The efficiency of combustion systems can prevent further climate change, minimize harmful emissions, and ensure U.S. energy security. Because liquid hydrocarbon fuels have an unrivaled energy density, combustion will continue to provide 80% of the energy for the world for the next fifty years. While the high fuel efficiency of diesel engines warrants their use in ground transport and marine engines, they generate considerable emissions of nitrogen oxides (NO_X) and soot.

The development of simulation benchmarks for model development in large eddy simulations and Reynolds–averaged Navier–Stokes equations is essential to meet urgent government mandates on the reduction of CO_2 by 80% by 2050 and increased efficiency imposed by the Corporate Average Fuel Economy standard of 54 mpg for vehicles by 2025. Meeting these standards will require the development of new low-temperature premixed compression ignition engine concepts such as RCCI internal combustion for diverse fuel streams. The time frame for these novel concepts requires a significant improvement in the fidelity of computational engine models. The direct numerical simulation targets proposed will have significant scientific and engineering impact including the understanding and control of key turbulence-chemistry interactions.

The research team also has targets relevant to the development of engines for flexible power generation. The target simulations will resolve outstanding questions regarding the impact of hydrogen-rich fuels. Understanding and controlling NO formation and intrinsic flashback safety (i.e. undesirable flame propagation upstream near walls in the boundary layer), particularly for syngases, will enable the design of high efficiency gas turbines operating under variable loads and fuels while also satisfying stringent NO mandates.

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

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

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation: **65,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (65,000,000 processor hours)

Research Summary:
The recent generation of laboratory high-energy-density physics facilities, including both laser facilities and pulsed power systems, has open significant physics opportunities for both fusion and for experimentally modeling astrophysical plasmas. The goal of this INCITE project is to understand and model the dynamics of magnetic fields in these high-energy-density 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.

This INCITE project proposes to continue a set of projects funded at OLCF through the ALCC program (July 2015–June 2016) and INCITE (2016). We will conduct both full-kinetic particle-in-cell simulations (with our PSC code) and reduced magnetohydrodynamics (MHD) and extended MHD, including a detailed comparison of the two. Our work with HMHD will advance studies of magnetic reconnection in the large-system size, plasmoid-dominated regime. Our 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. Our 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 for 3-D simulations to benchmark this important astrophysical instability.

Type: New
Title: "Electronic Stopping in Condensed Matter under Ion Irradiation"

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

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation: **130,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (130,000,000 processor hours)

Research Summary:
Electronic stopping describes the transfer of kinetic energy from a highly energetic ion to electrons in condensed matter. This process induces massive electronic excitations in the target material through interaction with the charged particle's electric field. Understanding this phenomenon in condensed matter systems contributes important knowledge with implications in various modern technologies.

The team has developed a predictive computational framework to accurately calculate the electronic stopping power for a range of condensed matter systems. This project will use an extended version of this framework to investigate intricate details of electronic excitation dynamics under ion irradiations.

For this work, the team will employ their highly scalable implementation of real-time time-dependent density functional theory, optimized for MIRA, and with new numerical integrators added. The team aims to study (1) Secondary electron emission from aluminum and graphite due to radiation; and (2) Electronic excitations in water and DNA under irradiation of alpha-particles and carbon ions.

One application of this work concerns ion beam cancer therapies, where energetic ions are used to induce irreparable DNA damage in targeted cancer cells. Further progress requires a molecular-level understanding of electronic stopping in liquid water and in DNA under ion irradiations. These INCITE simulations will reveal molecular-level differences in the electronic excitations between proton radiation and that of other ions, allowing more informed decisions for designing future ion beam therapy facilities.

Type: Renewal
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, Oak Ridge National Laboratory
G. Malcom 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 of 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 the compute-intensive deterministic kernels that require the majority of the execution time and can utilize the thread-level parallelism at the Monte-Carlo level. Finite temperature effects will be modeled by sampling the energy landscape with the Wang-Landau 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 thermodynamics description of magnetism. The combined WL sampling and LSMS will lead to a realistic treatment of allows and functional materials.

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

Principal Investigator: Jonathan Aurnou, University of California, Los Angeles
Co-Investigators: Benjamin Brown, University of Colorado, Boulder
Bruce Buffett, University of California, Berkeley
Nicholas Featherstone, University of Colorado, Boulder
Gary Glatzmaier, University 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: **260,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (260,000,000 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 developments are being used to demonstrate that transformative physical changes occur in planetary and stellar simulations of dynamo action in fluids with realistic material properties. In addition, a survey of Jupiter's interior dynamics has enabled a massive $2{,}048^3$ class calculation that greatly exceeds previous 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.

The team hopes to engage the broader community by providing access to these singularly extreme datasets and, more broadly, to demonstrate the community-wide need for massive computational efforts to investigate the turbulent liquid-metal dynamo action that occurs in planets and stars.

Type: Renewal
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

Scientific Discipline: Physics: Nuclear Physics

INCITE Allocation: **194,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (194,000,000 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. Their goal is to achieve a microscopic understanding of QGP properties near the transition to ordinary nuclear matter. Using a state-of-the-art lattice quantum chromodynamics (QCD) approach, they believe that the requirements and conditions for the creation of nuclear and exotic matter in the universe can be determined.

Investigators are looking at several aspects of QCD that are of relevance at different times during the brief life of the QGP in heavy-ion collision experiments at RHIC and the LHC. For example, they plan to calculate electric charge fluctuations as a function of temperature, crucial in determining the chemical freeze-out temperature, after which the multiplicities of all measurable particle species are fixed.

One of the most sought-after quantities in the description of the QGP is the shear viscosity, the transport coefficient that parametrizes the non-ideal hydrodynamics of the plasma. A key milestone in this project is to calculate shear viscosity in full QCD. 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.

Type: Renewal
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: 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:

Effective strategies for improving the efficiency of biofuel and bioproducts production from plant cell wall lignocellulosic biomass via cellulose hydrolysis require a detailed understanding of the structure and dynamics of the biomass, a complex material composed of cellulose, hemicellulose, pectin, and lignin polymers.

To reduce biomass recalcitrance to hydrolysis by improving pretreatment and designing improved feedstock plants, a detailed understanding of biomass structure, mechanics, and response to pretreatment regimes is needed.

This multiyear INCITE project is simulating full lignocellulosic biomass systems, consisting of cellulose, lignin and hemicelluloses at both physiological and pretreatment conditions. The simulations are helping to obtain a detailed knowledge of the fundamental molecular organization, interactions, mechanics, and associations of bulk lignocellulosic biomass. Furthermore, simulations of pretreatments effects on biomass structure and dynamics permit 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: Jeroen Tromp, Princeton University
Co-Investigators: Ebru Bozdag, University of Nice Sophia Antipolis
Dimitri Komatitsch, The French National Centre for Scientific Research
Matthieu Lefebvre, Princeton University
Daniel Peter, Swiss Federal Institute of Technology Zurich, Switzerland

Scientific Discipline: Earth Science: Geological Sciences

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

Research Summary:
This multiyear 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.

The team has produced the first global adjoint tomography model, the results of 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. Additional petascale resources will enable continued iterative updating and an increase in the resolution of seismic images of the 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. Since then, the team has expanded its dataset to include 1,200 earthquakes and is using this larger dataset to understand challenges in data assimilation.

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 ≤ Mw ≤ 7.0. To date, the team has gathered data for more than 4,200 earthquakes and is working on their source inversions. They started with 27 s waves, and since the 12th iteration were using 17 s waves. The current aim is to go down to ~ 9 s and include more earthquakes in the inversion. Additionally, 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: "Global Radiation MHD Simulations of Massive Star Envelopes"

Principal Investigator: Lars Bildsten, University of California, Santa Barbara
Co-Investigators: Omer Blaes, University of California, Santa Barbara
Matteo Cantiello, University of California, Santa Barbara
Yan-Fei Jiang, Harvard University
Eliot Quataert, University of California, Berkeley
James Stone, Princeton University

Scientific Discipline: Physics: Astrophysics

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

Research Summary:
Massive stars play an important role in many astrophysical environments. The radiative and mechanical energy output from massive stars are important feedback mechanisms regulating star formation and the structure of the interstellar medium in galaxies. One property that is particularly critical to the evolution and fate of massive stars is the degree of mass loss during stellar evolution. This includes both relatively steady winds and dramatic episodic mass loss eruptions. The mass loss rates during different stages of massive star evolution have large impacts on a star's luminosity, lifetime, final fate (e.g., neutron star or black hole) and the properties of its resulting supernovae and nucleosynthesis.

The goal of this project is to study the global structure of the gaseous outer layers, or envelopes, of massive stars, accounting for different masses and different evolutionary stages. The team will conduct 3D radiation magnetohydrodynamic (MHD) simulations using the unique radiation code Athena++, which directly solves the time-dependent radiation transfer equation. The simulations will capture the global properties of the stars and winds, while still resolving the structure of the stellar atmosphere.

These multi-dimensional simulations will dramatically improve the understanding of the surface layers of massive stars, including mass loss via radiation-pressure driven winds. The results will be incorporated into 1D stellar evolution models to create more realistic massive star models, which will significantly improve our understanding of the structure and evolution of massive stars and lead to more realistic pre-supernova progenitor models for use in simulations of core-collapse supernovae.

Type: New
Title: "High-Order Methods for LES of Turbomachinery Flows"

Principal Investigator: Gorazd Medic, United Technologies Research Center
Co-Investigators: Jaime Peraire, Massachusetts Institute of Technology
Mani Sadeghi, Pratt & Whitney

Scientific Discipline: Engineering: Aerodynamics

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

Research Summary:
A better understanding of turbulent unsteady flows in turbomachinery is necessary for breakthroughs in the design of jet engines that will enable lower fuel burn. Owing to relatively high Reynolds numbers and complex wall-bounded geometries, the flow physics in turbomachinery are hard to predict. While the most popular technique to model the flows in turbomachinery is based on a Reynolds–averaged Navier–Stokes (RANS) approach, these models are not accurate for complex turbulent flows. However, direct numerical simulation (DNS) of turbulent flows at high Reynolds numbers will remain intractable for a long time.

With the increase in computing power, large eddy simulation (LES) emerges as a promising technique to improve both knowledge of complex flow physics and reliability of flow predictions. The central premise of LES is that large scales dominate the turbulent transport and energy budget, while strategies for dealing with the small scales include explicit subgrid-scale (SGS) models or implicit numerical dissipation referred to as implicit LES (ILES).

The team proposes a high-order computational fluid dynamics (CFD) code based on the hybridized discontinuous Galerkin (HDG) method for wall-resolved LES of complex turbulent flows in turbomachinery. Their approach will focus on comparing high-order LES solvers against an industrial code, evaluating ILES and explicit SGS models, analyzing numerical errors due to the grid inadequacy, improving in the scalability and robustness of the flow solvers, and analyzing wall-resolved LES predictions of flows for advancing compressor and fan designs.

The team plans to advance the state-of-the-art of CFD simulations for complex turbomachinery configurations at realistic Reynolds numbers starting with tens of thousands and then extending the size of simulations. Success in their LES computations will provide a strong case to accelerate investments in transformative high-fidelity simulations through the partnership of industries, universities, and the US government.

Type: New
Title: "High-Resolution Climate Change Simulations with the CESM"

Principal Investigator: Gerald Meehl, NCAR
Co-Investigators: Susan Bates, NCAR
John Dennis, NCAR
Warren Washington, NCAR

Scientific Discipline: Earth Science: Climate Research

INCITE Allocation: **215,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (215,000,000 processor hours)

Research Summary:
In support of the U.S. Department of Energy's Biological and Environmental Research program, the National Center for Atmospheric Research's (NCAR) Climate Change Prediction (CCP) group seeks to understand complex biological, climatic, and environmental systems across multiple spatial and temporal scales. Their work includes producing and analyzing suites of climate simulations with the Community Earth System Model (CESM), and comparing the results to larger multi-model datasets.

For this INCITE project, the CCP research team will use Mira to perform simulations with the CESM at the highest atmospheric and oceanic resolutions currently feasible for century-long climate simulations. Building on previous INCITE research, the team will analyze the simulations to address science challenges involving long-term climate change projections, future hurricanes and tropical cyclones, regional precipitation and temperature extremes, global and regional sea level rise, and response of the future atmospheric hydrological cycle. Four 100-year future scenario simulations will be integrated using the CESM with atmosphere/land horizontal resolution of approximately 0.25° and an ocean/sea ice resolution of approximately 1.0°. These simulations have been shown to be extremely useful in constraining future climate projections and identifying future climate states.

The overarching purposes of the research are to investigate climate variability and change, and to evaluate potential consequences of energy use strategies of direct relevance within the energy-climate nexus. This project's findings will be critical to the future climate change studies, including the International Panel on Climate Change's Sixth Assessment Report and U.S. National Climate Assessment.

Type: New
Title: "Lattice QCD"

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

Scientific Discipline: Physics: Nuclear Physics

INCITE Allocation: **358,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (240,000,000 processor hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (108,000,000 processor hours)

Research Summary:
The research team proposes to use the Argonne Leadership Class Computing Facility's BlueGene/Q, Mira, and the Oak Ridge Leadership Class Computing Facility's Cray, Titan, to address key science questions in nuclear and particle physics research, and to support and complement the major experimental programs in these areas. Focusing on the research priorities at the Energy and Intensity Frontiers, and in cold and hot nuclear physics, the team's program in quantum chromodynamics is essential to meeting milestones set out by the Office of Science. Leadership class computers will be used to sample the quantum fluctuations of the gluon fields, including the contributions from up, down, strange, and, in some cases, charmed quarks at their physical masses, with the fine-graining of spacetime sufficient to enable a complete quantification of uncertainties in crucial observables. These gluon configurations are common and essential components that are required to determine a wide range of physical quantities of importance in high energy and nuclear physics.

In particle physics, they will enable pushing the search for beyond-the-standard-model effects in flavor physics to yet higher energies. They will also enable new lattice calculations that are required throughout the DOE's coming Intensity Frontier program. In nuclear physics, the team is proposing a suite of calculations that are essential for the success of present and planned experiments at RHIC, Jlab, FRIB, LANL, ORNL and other national facilities. Its calculations are critical in guiding the search for exotic states of matter at the GlueX experiment, and in interpreting the results that will be obtained there.

Type: New
Title: "LES to Characterize Shock Boundary Layer Interaction in a 3D Transonic Turbofan"

Principal Investigator: Umesh Paliath, GE Global Research

Co-Investigators: Rathakrishnan Bhaskaran, GE Global Research
Gregory Laskowski, GE Aviation
Vittorio Michelassi, GE Aviation
Anupam Sharma, Iowa state University
Trevor Wood, GE Global Research

Scientific Discipline: Engineering: Aerodynamics

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

Research Summary:
GE Global Research's work on large eddy simulations (LES) has leveraged petascale computing to break barriers in accurately characterizing the key flow physics of multi-scale turbulent mixing in boundary layer and shear flows. The GE LES strategy has been to accelerate its industrial impact by pushing application/validation to realistic conditions and scale, addressing fundamental physics and source characterization challenges and to extend capability to handle complex system interactions.

With this INCITE award, GE, and Iowa State University will use LES to better understand the complexities involved in a real transonic turbofan geometry operating at a high Mach and Reynolds number. Specifically, the team will perform a parametric study of the shock boundary layer interaction problem on a canonical geometry to predict and understand the loss-generation mechanism. The team will then perform full-span fan blade simulations to accurately predict and understand the impact of shock-boundary layer interaction, secondary flows, and wake dynamics on fan blade aerodynamic and aeroacoustic performance. Results from these simulations will also provide a valuable resource for identifying deficiencies in and improving existing turbulence models.

This project will enable future simulations, looking at coupled nacelle-fan simulations as well as advanced engine architectures, such as open rotor configurations. These simulations are critical in enabling design and optimization of the next generation engines, and affect a step-change reduction in energy demand for future air travel.

Type: Renewal
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: **54,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (54,000,000 processor hours)

Research Summary:
The effect of radiation on the structure and dynamics of accretion flows onto compact objects is important to systems ranging from X-ray binaries to active galactic nuclei. While it is known that magnetohydrodynamic (MHD) processes dominate the angular momentum transport in such flows, and while numerical MHD simulations have revealed many important insights, whether any of the expectations of theory in the regime of radiation dominated accretion are borne out remains to be explored. With this INCITE award, a research team will calculate the structure of such flows, and make predictions about how accreting sources evolve and affect their environment.

The team has developed new and accurate numerical algorithms for time-dependent radiation transport (RT) that can be integrated into existing MHD codes to study the physics of radiation dominated flows. These methods have been implemented in a new version of a compressible MHD code, athena++, whose features include mesh refinement and new physics such as algorithms for general relativistic (GR) MHD in stationary spacetimes. This code shows excellent single core performance, and excellent weak scaling on Mira.

This project will use athena++ for a 2-year campaign to run three-dimensional radiation MHD simulations of accretion flows onto compact objects. The first goal is to complete a survey of the structure and dynamics of radiation dominated accretion as the mass accretion rate is varied from highly super-Eddington (the radiation dominated, slim disk regime) to sub-Eddington (the standard, thin disk regime). The team will investigate whether thermal and/or viscous instabilities, predicted over 40 years ago, actually occur in global models of MHD turbulent disks.

Type: Renewal
Title: "Many-Body Theory of Materials"

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

Scientific Discipline: Materials Science: Condensed Matter and Materials

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

Research Summary:

This team is confronting 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 applications and further development of the first-principles many-body quantum Monte Carlo (QMC) methods which all 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 modeling. 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.

This project addresses questions of the electronic structure and properties for two key classes of materials of strategic interest to DOE: correlated transitions metals and metal oxides that are foundational to many applications in energy storage and conversion as well as layered nanomaterials, including magnetic materials with applications in electronics and spintronics.

Type: New
Title: "Materials and Interfaces for Organic and Hybrid Photovoltaics"

Principal Investigator: Noa Marom, Carnegie Mellon University
Co-Investigators: Volker Blum, Duke University
Oliver Hofmann, Technical University Graz
Thomas Körzdörfer, University of Potsdam
Harald Oberhofer, Technical University Munich
Patrick Rinke, Aalto University
Alvaro Vazquez-Mayagoitia, Argonne National Laboratory

Scientific Discipline: Materials Science: Condensed Matter and Materials

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

Research Summary:
This project aims to advance the efficiency of organic and hybrid solar cells through computer-aided discovery and design of new materials and interfaces. The team's broadly applicable quantum mechanical framework will advance the field of computational materials science and broaden the community of researchers capable of using leadership computing resources. Their first-principles approaches are based on density-functional theory (DFT) and many-body perturbation theory (MBPT), which describe these materials and interfaces on the most fundamental, quantum mechanical level at which light-to-energy conversion takes place and on which structure-function relationships are established.

This international team of experts will conduct a large-scale computational campaign to derive structure property relations and design rules for crystal forms with high carrier mobility and high singlet fission efficiency; carrier harvesting interfaces with effective charge transfer and transport behavior; and hybrid perovskites with reduced toxicity and increased stability.

To search the infinitely vast configuration space of materials structure and composition, they will integrate the proven DFT code FHI-aims with three structure search methods, implemented as open source codes. These are based on different approaches to global optimization, namely genetic algorithm, basin hopping, and Bayesian optimization.

This research will advance the current state-of-the-art in first-principles simulations and allow researchers to reveal design rules for organic and hybrid materials with desired properties. The theoretical understanding developed in this project will catalyze the emergence of new design paradigms for next-generation solar cell technologies.

Type: New
Title: "Multiscale Physics of the Ablative Rayleigh-Taylor Instability"

Principal Investigator: Hussein Aluie, University of Rochester

Scientific Discipline: Engineering: Fluids and Turbulence

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

Research Summary:

The Rayleigh-Taylor Instability (RTI) occurs in a multitude of natural and engineered systems in which buoyancy forces exist. It plays an important role in astrophysical systems, in solar physics, and in oceanic flows. RTI is also a major impediment to current efforts in realizing nuclear fusion as a viable and virtually limitless energy source via inertial confinement fusion. As a physical phenomenon in its classical form, RTI occurs at the interface of a dense fluid on top of a lighter fluid subject to a upward acceleration field. It is manifested by the formation of upward rising bubbles of the lighter fluid and downward sinking spikes of the heavy fluid. Ablative RTI (aRTI) includes the additional physics of mass evaporation of the lighter fluid due to a heat source, such as a star, a laser, or the hot center of an imploded target. It occurs in many systems such as in supernova explosions and in laser accelerated targets.

It has long been believed that ablation has a stabilizing effect on the RTI, especially at small scales. This has been used as a reason by numerical modelers to ignore short wavelength perturbations. However, recent research strongly suggests that while ablation is stabilizing in the early linear stage of the evolution of RTI, it can exacerbate the instability, especially at small scales in the late nonlinear stage. If true, it may imply that present approaches to modeling aRTI flows need to be fundamentally revised.

Researchers plan to conduct a systematic investigation of the multiscale physics of ablative RTI through massive 2D and 3D simulations of single-mode, multi-mode, and broadband classical and ablative RTI (aRTI), using the spectral code, DiNuSUR. Objectives include the study of bubble growth rate and the evolution of RTI at various stages, in order to understand the effects of dimensionality and multiscale coupling on the instability growth. The proposed massive simulations will be the first of their kind.

Both timely and pressing, the proposed research has important ramifications to modeling efforts in implosion physics, astrophysics, and combustion science.

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

Principal Investigator: Thomas Miller, California Institute of Technology

Scientific Discipline: Chemistry: Physical

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

Thomas Miller will provide both fundamental understanding and prediction of high-conductivity, non-flammable, solid polymer electrolytes for lithium-ion batteries. As part of an established collaboration, Thomas Miller's proposed 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, and their ion transport characteristics will be measured and tested in full cells.

In the first year of activity, Miller's team will first screen a set of 500 chemically diverse classes of polymers for high ion conductivity and solubility under dilute salt conditions and 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 recently been developed and validated in the Miller group. In the second year of activity, 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. Success of this research effort will advance battery technologies that are critical for transportation and other large-scale energy storage applications. The team's research approach, in which the theoretical and computational predictions form the proposed work are seamlessly integrated with experimental synthesis and characterization, offers a powerful paradigm for the development of advanced materials.

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

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

Scientific Discipline: Physics: Nuclear Physics

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

Research Summary:
Predictions for the structure and reactions of nuclei, with assessed uncertainties, are important for the future of the nation's energy and security needs. Developing a comprehensive description of all nuclei (stable and unstable) and their reactions requires investigations of rare and exotic isotopes with unusual proton-to-neutron ratios that are difficult or impossible to produce and study experimentally.

The team performs state-of-the-art simulations to provide needed quantified predictions where direct experiment is not possible or is subject to large uncertainties. Such calculations are relevant to many applications in nuclear energy, nuclear security, and nuclear astrophysics, since rare nuclei lie at the heart of nucleosynthesis and energy generation in the stars.

This project uses complementary methods applicable to different regions of the nuclear chart, including Green's function Monte Carlo, Hamiltonian diagonalization (the no-core shell model), coupled cluster, and resonating group methods, in order to perform ab intio calculations of light- and medium-mass nuclei using realistic nucleon-nucleon and three-nucleon interactions.

The team's predictions will complement DOE's major investments in forefront experimental facilities. In particular, the team will complement future experiments at the Facility for Rare Isotope Beams (FRIB), under construction at Michigan State University, electron scattering experiments at Jefferson Laboratory, and neutrino scattering experiments at Fermilab.

Type: Renewal
Title: "Nucleation and growth of colloidal crystals"

Principal Investigator: Sharon Glotzer, University of Michigan

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. In its second year, this project will continue to explore 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 is carrying out the most in-depth computational study of nucleation and grown that has ever been undertaken. The team is seeking 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: "On the Physics of Three-Dimensional Unsteady Flow over Low Pressure Turbines"

Principal Investigator: Peter Vincent, Imperial College
Co-Investigators: Ralf-Dietmar Baier, MTU Aero Engines
Antony Jameson, Stanford University

Scientific Discipline: Engineering: Aerodynamics

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

Research Summary:

To reduce weight and lower greenhouse gas emissions, modern jet engines are designed to use as few low-pressure turbine blades as possible. However, as the number of blades is reduced, individual blades are subjected to higher loading, which can introduce complex, unsteady airflow patterns that lead to an increase in fuel consumption.

Using high-order computational fluid dynamics, the research team will be simulating flow over the MTU-T161 low-pressure turbine linear cascade under various operating conditions and at unprecedented scale and resolution. The team's open-source Python-based code, PyFR, combines highly accurate numerical methods with a highly flexible, portable, and scalable code implementation that makes efficient use of GPU accelerators.

Moreover, MTU Aero Engines will make a comprehensive experimental dataset openly available for the first time for this test case. Results will be used to validate the performance of high-order implicit large eddy simulation as a predictive technology for cascades and turbine blade rows. Results will also be used to obtain unprecedented insight into the physics of three-dimensional unsteady flow over low-pressure turbines, including the effect of inlet turbulence on transition, the effect of inlet wake generators on transition, the shape and behavior of the separation bubble on the suction-side of the blade, and the effect of non-parallel end walls on transition and losses.

Finally, results will provide an extended database to enable development of improved models for lower fidelity—but significantly cheaper—Reynolds-Averaged Navier–Stokes simulations of low-pressure turbine configurations.

Type: New
Title: "Parton Distribution Functions from Lattice QCD"

Principal Investigator: Constantia Alexandrou, The Cyprus Institute and University of Cyprus
Co-Investigator: Giannis Koutsou The Cyprus Institute

Scientific Discipline: Physics: Nuclear Physics

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

Research Summary:
Parton distribution functions (PDFs) encode essential information about the distribution of momentum and spin of quarks and gluons inside hadrons. Deep inelastic scattering experiments provide information on the quark PDFs of the nucleon and factorization allows one to separate a short-distance, hard sub-process, from the complex, soft structure of the nucleon. Ab initio computation of this soft long-distance structure is complex and the most suitable approach is via a numerical solution using a discretized formulation of Quantum Chromodynamics (QCD) on a Euclidean space-time lattice known as lattice QCD using Monte Carlo methods. However, PDFs are matrix elements of non-local bi-linears in the light-cone frame. Such matrix elements cannot be evaluated using a Euclidean space-time lattice.

Therefore, the standard approach in lattice QCD has been to compute moments of PDFs being restricted to a few lower moments that avoid mixing. Recently, a new approach has been proposed X. Ji to compute quasi-distributions that can be matched to PDFs in the large momentum limit. A direct evaluation of PDFs within lattice QCD can have profound implications on our understanding of the structure of the nucleon providing essential input for phenomenology and ongoing experiments.

In this INCITE project, the research team will use this new approach to compute the quasi-distributions using lattice QCD and then match them to PDFs. The team will employ gauge-field configurations simulated by the European Twisted Mass Collaboration with light, strange and charm quarks tuned to their physical values. These configurations are currently among a handful of simulations that provide the most complete description of the QCD vacuum. The group has already carried out an exploratory study using similar gauge configurations but with a pion mass of 373 MeV and has worked out the mass corrections required for the matching. A new smearing technique has been tested and shown to allow us to go to large enough momentum to take the large momentum limit. The renormalization of the quasi-distributions is currently under study using lattice perturbation theory where we expect results to be finalized before the start of the time allocation.

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

Principal Investigator: Leonid Oliker, Lawrence Berkeley National Laboratory
Co-Investigators: Peter Beckman, Argonne National Laboratory
Laura Carrington, San Diego Supercomputer Center
Bronis de Supinski, Lawrence Livermore National Laboratory
James Demmel, University of California, Berkeley
Jack Dongarra, University of Tennessee–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

Scientific Discipline: Computer Science

INCITE Allocation: **60,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (35,000,000 processor hours)
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (25,000,000 processor hours)

Research Summary:
Understanding how to efficiently use DOE leadership class systems is important due to the challenges of effectively managing extreme levels of concurrency as well as architectural heterogeneity. The performance research community can provide critical tools, runtimes, and methodologies that scientists can use to exploit leadership class machines. The team will have a Performance Evaluation and Analysis Consortium (PEAC) End Station to complete this project.

To facilitate further understanding of leadership class systems, Oliker's team will develop new programming models and runtime systems. Consortium members will conduct research into the programming models, runtime systems, tools, system evaluations and application analysis that support computational science on leadership computing platforms. Ultimately, this will allow scientists to maximize the speed—and therefore the impact—of these large-scale platforms.

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, UC Santa Cruz
Evan O'Connor, University of Toronto
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:
The process by which core-collapse supernovae (CCSN) are produced drives the development of the heavier elements, which are distributed throughout the universe after a massive star explodes under its own weight. Project researchers will conduct a comprehensive study of the mechanisms that cause core-collapse supernovae utilizing 3D magnetohydrodynamics (MHD) simulations of the collapse of rotating, magnetic stellar cores. Their earlier work has demonstrated the importance of turbulence in the supernova mechanism and, thus, drives this INCITE project, which is to treat MHD with the highest fidelity possible.

The team is presently running 3D simulations with the high-fidelity M1 neutrino transport using a state-of-the-art 20-solar mass (20 times the mass of our own sun) 1D progenitor model generated by the open-source MESA code. Some simulations include non-spherical velocity perturbations in the silicon- and oxygen-burning shells inspired by realistic convective burning in massive stars. Due to significant optimization of the M1 code, they have achieved even higher resolution in the 3D simulations than originally planned.

These simulations will allow researchers to probe the behavior and importance of turbulence in aiding supernova shock revival in the most realistic way yet, particularly in conjunction with simulations that include non-spherical progenitor perturbations. In addition, they will be the most physically-detailed and accurate CCSN simulations to include magnetorotational effects ever accomplished, with the potential for uncovering a robust and realistic CCSN explosion mechanism.

Type: New
Title: "Petascale Simulations for Layered Materials Genome"

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

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

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

Research Summary:
Functional layered materials (LMs) will dominate nanomaterials science in this century. The attractiveness of LMs lies not only in their outstanding electronic, optical, magnetic and chemical properties, but also in the possibility of tuning these properties in desired ways by building van der Waal heterostructures composed of unlimited combinations of atomically thin layers. With this INCITE project, researchers will perform 10,000-atom nonadiabatic quantum molecular dynamics (NAQMD) and billion-atom reactive molecular dynamics (RMD) simulations for computational synthesis and characterization of revolutionary layered materials.

These simulations will (1) aid the synthesis of stacked LMs by chemical vapor deposition, exfoliation, and intercalation, and (2) discover function-property-structure relationships in LMs with a special focus on far-from-equilibrium electronic processes.

This project carries over the success of two previous INCITE projects on scalable and fast petascale simulations to the paradigm of LM. This team has already performed the largest-ever RMD and quantum molecular dynamics (QMD) simulations on Mira by fully exploiting the system's core architecture.

The project will provide predictive theory, directly validated by X-ray laser experiments at Stanford's Linac Coherent Light Source (LCLS), to form a cornerstone of DOE's layered materials genome efforts. Function-property-structure relationships in stacked LMs span a wide range of length and time scales. Together, the leadership INCITE simulations and LCLS X-ray laser experiments will, for the first time, describe nonequilibrium dynamics in LMs at exactly the same spatiotemporal scales.

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

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

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation: **147,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (147,000,000 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 excessive laser-plasma instabilities (LPIs), which can absorb, deflect, or reflect laser light, causing potential disruptions and excess heat loads.

Because laser beams in IFE devices develop multiple-speckle patterns (which result when a beam is scattered by a medium), researchers must understand how multiple speckles interact with each other. The goal of this project is to perform large-scale simulations of laser-plasma interactions in 2D and 3D, using the highly mature particle-in-cell code OSIRIS, to simulate increasingly realistic beam effects, such as spatial incoherence (i.e., laser speckles) and temporal incoherence (laser smoothing techniques).

At the outset of this allocation, the team performed the first ever study on the relationship between LPI activities and the orientation of external magnetic fields, showing that a perpendicular external magnetic field is more effective for reducing laser plasma instabilities in inertial fusion plasmas than parallel external magnetic fields. They also performed large 2D simulations to investigate the effects of temporal incoherence on laser-plasma interactions, and to study laser-plasma interactions under shock ignition-relevant conditions.

Now, researchers will investigate interactions between multiple speckles in 3D for varying instabilities, by first studying laser-plasma interactions of a single-laser speckle in 3D, providing both comparison to previous 2D simulations, as well as experience. The computationally-intensive, multiple-speckle 3D simulations will study smaller speckles to understand the essential physics involved in these systems, and larger speckles to study the problem under National Ignition Facility-relevant conditions. They will provide, for the first time, insights into the 3D nature of these processes and lead to the eventual understanding and control of LPI's in IFE plasmas.

Type: New
Title: "Petascale simulations of short pulse laser interaction with metals"

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

Scientific Discipline: Engineering: Material Response

INCITE Allocation: **20,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (20,000,000 processor hours)

Research Summary:

Short pulse laser irradiation is a processing technique used in many material applications, including tuning the surface-wetting properties (from superhydrophilic to superhydrophobic), fabrication of black or colored metals, as well as strong enhancement of photoelectron and thermal emission from surfaces nanostructured by femtosecond laser irradiation.

While it is generally recognized that the laser-induced modification of surface properties is related to the generation of complex hierarchical nano- and micro-scale surface structures, detailed understanding of the relations between the basic mechanisms of laser interaction with materials is still lacking.

Using petascale atomistic simulations of short pulse laser interactions with metals, the research team will provide new information on the materials behavior under extreme non-equilibrium conditions of ultrafast heating and cooling, reveal the processes responsible for the generation of nanoparticles and formation of complex surface structures, and facilitate the development of new laser techniques. The results of the simulations will contribute to the fundamental understanding of the mechanisms of phase transformations and microstructure development under the highly non-equilibrium conditions created by short pulse 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 non-equilibrium 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: "PICSSAR - Particle-In-Cell Spectral Scalable Accurate Relativistic"

Principal Investigator: Jean-Luc Vay, Lawrence Berkeley National Laboratory
Co-Investigator: Henri Vincenti, Lawrence Berkeley National Laboratory and Commissariat a l'Energie Atomique, Saclay, France

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:
The advent of high-power PW femtosecond lasers has opened a new branch of physics called ultra-high intensity (UHI) physics. Once such a laser is focused on a solid target, the laser intensity can reach values as large as 10^{23}W.cm^{-2}, for which matter is fully ionized and turns into a plasma mirror that reflects the incident light. The corresponding laser electric field at focus is so high, that plasma mirror particles get accelerated to relativistic velocities upon reflection of the laser on its surface. A whole range of compact "tabletop" sources of high-energy particles and radiations may thus be produced from the interaction between this plasma mirror and the ultra-intense laser field at focus.

Understanding and controlling these compact particle and light sources will rely on the strong coupling of experiments and large-scale simulations using particle-in-cell (PIC) codes. However, standard PIC codes fail to accurately describe most UHI laser-plasma interaction regimes because the finite-difference Maxwell solver produces strong instabilities and noise when the accelerated particles move at relativistic velocities or when the produced short-wavelength radiations span broad emission angles and frequencies. Mitigation of these instabilities often requires spatial and temporal resolutions so high, they are not practical for realistic 3D modeling on current petascale, or possibly even exascale systems.

This INCITE team proposes to use highly precise pseudo-spectral methods to solve Maxwell's equations to enable realistic simulations of UHI regimes, using a new grid decomposition technique for very-high-order/pseudo-spectral electromagnetic solvers. This technique has been implemented in the team's PIC code, WARP+PXR, and benchmarked against standard methods. Scaling tests on Mira show the technique enables a massively parallel implementation of pseudo-spectral solvers on up to at least 400,000 cores.

Type: New
Title: "Predictive Simulations of Functional Materials"

Principal Investigator: Paul Kent, Oak Ridge National Laboratory
Co-Investigators: Anouar Benali, Argonne National Laboratory
Olle Heinonen, Argonne National Laboratory
Jaron Krogel, Oak Ridge National Laboratory
Lubos Mitas, North Carolina State University
Miguel Morales, Lawrence Livermore National Laboratory
Eric Neuscamman, University of California, Berkeley
Luke Shulenburger, Sandia National Laboratories

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation: **138,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (98,000,000 processor hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (40,000,000 processor hours)

Research Summary:
Today, the design of functional materials is greatly hindered by the limited predictive power of established quantum mechanics-based approaches. The strong coupling between charge, spin, orbital, and lattice degrees of freedom that results in desired functionalities also challenges established modeling approaches. For example, functionals for density functional theory calculations are used empirically in practice, while existing quantum many-body approaches do not offer the capabilities, accuracy, and general applicability that is desired.

This project will support the proposed BES Computational Materials Sciences Center for Predictive Simulation of Functional Materials. Kent's team will take advantage of recent developments in parameter free Quantum Monte Carlo (QMC) methods and use the open source QMCPACK code. The team will initially demonstrate and validate new QMC methods and algorithms that significantly improve on the state of the art. They propose calculation on functional materials which possess a wide spectrum of properties. The transition metal oxide materials they will investigate are of great interest to new electronics, energy conversion and transmission technologies. They have selected established benchmark materials as well as new materials systems where the predictions will be validated by new experimental works and characterization. This will provide a stringent and timely validation of the newly developed methods as well as provide a rich area for identifying new functionalities for energy-related technologies.

Type: New
Title: "Pushing the Limits of Quantum Chemistry Using the Supercomputers of Tomorrow"

Principal Investigator: Poul Jorgensen, Aarhus University
Co-Investigators: Dmytro Bykov, Aarhus University
Thomas Kjaeaard, Aarhus University
Kasper Kristensen, Aarhus University
Filip Pawlowski, Aarhus University

Scientific Discipline: Chemistry

INCITE Allocation: **75,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (75,000,000 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 smaller molecular systems, various molecular properties have been computed to an accuracy challenging experimental results. However, the application range of CC has so far been limited to small molecular systems due to their computational scaling with system size. For this reason, density function 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 CC methods.

The objective of the proposed project is to extend the application range of accurate modeling techniques in chemistry and molecular sciences by making the CC methods applicable to large molecular systems and ready-to-use on the supercomputers of tomorrow. The proposed project is a continuation of previous INCITE work.

The team plans to remove bottlenecks for Hartree-Fock equation optimization and orbital localization, which is essential to implement the team's Divide-Expand-Consolidate (DEC) algorithm. The algorithm's framework is well established for coupled cluster models, but the overall precision is still limited by memory constraints. By removing these bottlenecks, the team hopes to address molecular systems containing up to 100,000 basis functions.

All the team's goals involve the implementation of massively parallel algorithms which can efficiently utilize the entire Titan supercomputer when applied to large molecules. All developments will be implemented in the non-commercial LS-Dalton program package and thus become freely available to scientists in other fields.

Type: New
Title: "Quantification of Uncertainty in Seismic Hazard Using Physics-Based Simulations"

Principal Investigator: Thomas H. Jordan, University of Southern California
Co-Investigators: Scott Callaghan, University of Southern California
Yifeng Cui, San Diego Supercomputer Center
Christine A. Goulet, University of Southern California
Philip J. Maechling, University of Southern California
Kim B. Olsen, San Diego State University
Ricardo Taborda, University of Memphis

Scientific Discipline: Earth Science: Geological Sciences

INCITE Allocation: **141,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (96,000,000 processor hours)
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (45,000,000 processor hours)

Research Summary:
Human and economic risks in seismically active regions continue to increase as the number and scale of urban areas, and their dependence on interconnected infrastructure networks, continue to grow. Characterization of seismic hazards across a wide spectrum of forecasting and response times is the foundation on which most seismic risk-reduction strategies are developed.

The Southern California Earthquake Center (SCEC) conducts and coordinates fundamental and applied research on earthquake processes using southern California as its main natural laboratory. SCEC will use computing resources to advance and improve the accuracy of earthquake simulations as a means to better understand seismic hazard and assess seismic risk.

SCEC will pursue a two-year earthquake system science research program that will improve 3D earth models used in ground motion simulations, improve physics-based earthquake rupture and wave propagation models, and reduce uncertainties in broad-impact ensemble-based physics-based probabilistic seismic hazard analysis (PSHA) calculations called CyberShake. Their research activities will lead to more accurate physics-based scenario ground motion simulations and improved physics-based PSHA by adding new physical elements and enhancing existing features. The proposed code development will reduce the time-to-completion of key PSHA applications, allowing in-depth analysis of the factors controlling seismic hazards. The proposed research is expected to improve broad impact seismic hazard information products including seismic hazard maps and civil engineering design codes.

Type: New
Title: "The Rate of Spontaneous Plasma Reconnection"

Principal Investigator: Andrey Beresnyak, Naval Research Laboratory

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation: **52,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (52,000,000 processor hours)

Research Summary:
Magnetic reconnection is a topological rearrangement of magnetic field lines, leading to the release of magnetic energy, often associated with solar X-ray flares. One of the key questions dogging this field of study revolves around the reconnection rate, the velocity at which magnetic field lines converge in a current layer, which has been inconsistent between observations of the sun, fluid simulations and plasma simulations.

To gain greater insight into plasma reconnection, project researchers plan to use high-resolution Hall magnetohydrodynamic (MHD) simulations, a simple framework for electron-proton plasmas. Resolving whether plasma reconnection is inherently different from resistive MHD reconnection is a key to many space and solar physics phenomena, from reconnection in the solar corona to acceleration in high energy sources, like blazars or gamma ray bursts.

It has been suggested that ambient turbulence also enhances reconnection rate, so that relatively high observed rates could be explained by two completely different mechanisms: either plasma effects or ambient turbulence. Previously, the team performed 3D MHD simulations above the Lundquist number of 10^4, for the first time, and made the first measurements of 3D spontaneous reconnection rate in MHD in resistive-independent regime. The rate was around 0.015 of Alfven speed, a rate independent on resistivity and therefore corresponds to the so-called fast reconnection.

The team is trying to resolve the puzzle of plasma reconnection rates by working with a minimal model that includes plasma effects by Hall-MHD approximation and by conducting 3D simulations in a simple and universal setup with only two governing parameters. By simplifying the parameter space, they hope to figure large-scale reconnection rates for electron-proton plasma. Additionally, they will perform a single particle-in-cell (PIC) simulation that will exactly mimic parameters in the lowest-resolution Hall-MHD simulation in order to rectify the importance of electron physics on the reconnection rate.

Type: New
Title: "Reactive Mesoscale Simulations of Tribological Interfaces"

Principal Investigator: Subramanian Sankaranarayanan, Argonne National Laboratory
Co-Investigators: Henry Chan, Argonne National Laboratory
Mathew Cherukara, Argonne National Laboratory
Ali Edermir, Argonne National Laboratory
Badri Narayanan, Argonne National Laboratory
Kiran Sasikumar, Argonne National Laboratory

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

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

Research Summary:
Friction remains the primary mode of mechanical energy dissipation across diverse areas from energy technologies to geology to biology. Energy and material losses due to friction and wear are estimated at several billions of dollars annually. For this INCITE project, researchers from Argonne National Laboratory will use Mira to study friction laws and mechanisms between sliding mechanical interfaces, and to design new nanoscale lubricant materials for moving part assemblies.

The INCITE team's expertise in carrying out large-scale simulations of tribological interfaces, combined with the highly scalable molecular dynamics codes, LAMMPS and NAMD, will allow them to address this complex research challenge. As part of this work, the researchers seek to combine the accuracy and flexibility of electronic structure calculations with the speed of classical potentials. They will leverage recently developed tools that merge and exploit the best insights from first-principles physics, atomistic simulations, and machine-learning techniques for nanoscale materials simulations.

The team's methodological developments will enable accurate prediction of interatomic forces and thereby allow high-fidelity dynamical and statistical simulations of tribological interfaces; properties and functionalities of new lubricant materials; and pathways and mechanisms of their *in operando* synthesis and assembly. Their work has the potential to achieve paradigm-changing breakthroughs in materials design for tribological applications. Ultimately, the team's findings could lead to next-generation lubricant materials and technologies that provide innovative solutions to the nation's pressing environmental and energy challenges.

Type: New
Title: "Reliable Predictions of Actinide Chemistry at Different Scales"

Principal Investigator: David Dixon, University of Alabama
Co-Investigators: Jochen Autschbach, the University of Buffalo
Aurora Clark, Washington State University
Kirk Peterson, Washington State University
Gustavo Scuseria, Rice University
Wibe de Jong, Lawrence Berkeley National Laboratory

Scientific Discipline: Chemistry

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

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

Understanding the chemistry of the actinides is one of the core issues that must be addressed in order to develop appropriate technologies. The accurate calculation of the electronic structure, energetics, and spectroscopic properties of heavy element compounds is difficult and computationally demanding.

The team has broad experience in computational actinide chemistry and high-performance computers and will use these tools to address the complex problem of predicting the properties of actinide complexes. The team will extend its prior highly accurate coupled cluster CCSD(T) complete basis set extrapolated results for actinide compounds including high levels of correlation and relativistic effects, both scalar and spin-orbit. These results will be used as benchmarks to test other methods as well as to explain recent experimental results on the spectroscopy and reactions of small molecules.

The team also plans to develop new computational capabilities on advanced high-performance computer architectures and use them to study actinide complexes in various oxidation states in solution, at interfaces, and at the nanoscale.

Type: New
Title: "Revealing the Physics of Galactic Winds with Petascale GPU Simulations"

Principal Investigator: Brant Robertson, University of California, Santa Cruz
Co-Investigator: Evan Schneider, University of Arizona

Scientific Discipline: Physics: Astrophysics

INCITE Allocation: **46,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (46,000,000 processor hours)

Research Summary:

Understanding the role galactic-scale winds play in the formation and evolution of galaxies is a fundamental goal of current astrophysical research. Galactic winds, driven by energetic feedback processes associated with supernovae, regulate the baryonic content, star formation rates, and stellar masses of galaxies. To understand the properties of galaxies throughout cosmic time, astrophysical theory must endeavor to model the hydrodynamic processes that govern how gas is ejected from galaxies. The corresponding need for sophisticated simulations of galactic outflows was identified as a prime theoretical challenge in astrophysics for the next decade by the National Research Council.

This project aims to meet this challenge by leveraging Titan's GPU power to simulate galactic outflows with numerical models that allow for supersonic wind velocities, quantify the importance of radiative cooling for the multiphase structure of observed galactic outflows, and determine the mass and energy coupling of ISM gas to supernova-driven outflows.

To perform these simulations, the team will use the Computational Hydrodynamics on parLLel Architectures (Cholla) code (Schneider & Robertson 2015) that performs all its hydrodynamics calculations on GPUs. Cholla has demonstrated excellent weak scaling on up to ~90% of the entire Titan system (16,384 GPUs). Using Titan, Cholla can begin resolving the multiphase structure of galactic outflows and revealing how mass and energy are entrained into a hot wind.

The proposed simulations will greatly extend our physical understanding of galactic outflows by meeting a wide range of scientific goals. They will improve theoretical models for the mass and momentum loading of interstellar gas into baryonic outflows, and better characterize the multiphase structure of supernova-driven galactic winds. In addition, they have the potential to prove the validity of recently developed key analytic theories regarding the large-scale cooling of these winds. Such theories are critical for explaining the observations of large reservoirs of gas in galaxy halos begun to be observed in detail only in the past decade.

Type: New
Title: "Safe fusion energy: predictively modeling ITER radiation shielding"

Principal Investigator: Seth Johnson, Oak Ridge National Laboratory
Co-Investigators: Thomas Evans, Oak Ridge National Laboratory
Stephen Wilson, Oak Ridge National Laboratory

Scientific Discipline: Other: Nuclear Engineering

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

Research Summary:

The ITER project is an aggressive, international attempt to bring fusion energy power to a reality by constructing a production-scale tokamak reactor for engineering validation and groundbreaking plasma science. Behind schedule and over budget as a result of its complexity, ITER needs transformational engineering solutions that are far beyond the scale of traditional tools. In particular, current models cannot resolve the detailed radiation field inside the entire ITER building: they work only at unacceptably coarse scales, and even at these resolutions, they require model-to-model coupling that introduces unquantified space-energy-angle errors in the neutron flux source terms. Without proper shielding, this radiation risks the exposure of personnel and destruction of sensitive and expensive electronic equipment. The lack of a predictive shielding model will cause additional delays and cost overruns to the project, potentially undermining its viability and delaying its promise to bring new fusion science to fruition.

The research team proposes a radical solution for accurately modeling ITER's shielding design to ensure the viability of the project: to run the novel, scalable radiation transport software Denovo on Leadership Computing Facility resources in order to model the ITER facility at an unprecedented, but necessary, level of detail and scale.

The engineering solution we propose is beyond the scale of any similar simulations performed to date: the calculation in itself will be groundbreaking. It will use implementations and methods that are novel to this class of problems. The analyses of both JET and ITER will produce a trove of high-resolution data suitable for benchmarking lower-resolution models, accelerating future work in other plasma neutronics calculations beyond the scope of this work. The team expects multiple publications from the methods and their performance, from the validation against existing experimental data, and from the final ITER shielding calculation.

Type: New
Title: "Simulations of Dense Hydrogen and Helium"

Principal Investigator: David Ceperley, University of Illinois, Urbana-Champaign

Scientific Discipline: Materials Science: Condensed Matter and Materials

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

Research Summary:
The research team proposes a sequence of quantum Monte Carlo simulations of dense hydrogen and helium to understand their respective phase diagrams and make predictions that can be verified in laboratory experiments. Dense hydrogen and helium make up most of the mass of giant planets, so knowledge of their properties are essential for understanding but the conditions of temperature and pressure are not easily accessible experimentally. Hydrogen exhibits a rich phase diagram, but even rough estimates of the sequence of phase and their conditions is only now becoming known.

We have developed an accurate quantum Monte Carlo approach to simulate electron-ion systems starting from the bare Colomb interaction and able to make such simulations at a wide range of thermodynamics conditions. There has been sufficient computational and algorithmic progress such that errors can be controlled and truly ab initio predictions made. However, recent studies of the deuterium Hugoniot and the liquid-liquid transition in hydrogen and deuterium show significant discrepancies with respect to shock experiments conducted at Sandia and Lawrence Livermore national laboratories. It is important that such differences be resolved. The team plans new calculations to study these phenomena in dense liquid helium.

We use the Coupled-Electron-Ion Monte Carlo method as implemented in the codes BOPIMC and QMCPACK. The method employs several different parallelization strategies and is able to scale to many nodes efficiently. The QMCPACK software uses the GPUs on Titan efficiently, out-performing the CPU code by a factor of 4.5.

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

Principal Investigator: David Baker, University of Washington

Scientific Discipline: Chemistry: Biochemistry

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

Research Summary:
Proteins are large, complex molecules that drive virtually all cellular functions in living organisms. With the emergence of protein structure modeling tools, researchers have the capability to design proteins with targeted applications, such as treating diseases and catalyzing medically and industrially useful reactions. While progress is continually being made with such tools, the ability to sufficiently sample the vast conformational space remains a limiting factor.

The Rosetta software suite, developed at the University of Washington's Baker Laboratory, is designed to tackle to two difficult computational problems: the prediction of protein structure from amino acid sequences, and the design of new amino acid sequences to yield a desired function. With this multiyear INCITE project, researchers are using Mira to enhance Rosetta's ability to adequately sample the conformational space and address other emerging challenges in protein structure calculation and design. Only large supercomputers like Mira have the capacity and rapid interprocess communication ability to consider large numbers of conformational states simultaneously, in parallel, and to permit a sufficiently fast search for an optimal sequence.

The team's work includes improving the Rosetta energy function and further developing homology model refinement methods. In addition, the researchers are using Mira to design therapeutic peptides with unique, rigid folds that can bind to targets of interest, including influenza and other pathogens.

The overall goal of this project is to develop and apply new computational methods to better understand biomolecular structures and their function with atomic-level precision. Ultimately, this work will allow researchers to design new proteins to address challenges in medicine, energy, and technology.

Type: New
Title: "Turbulence mixing at high Schmidt number"

Principal Investigator: Pui Kuen Yeung, Georgia Tech
Co-Investigator: Toshiyuki Gotoh, Nogoya Institute of Technology

Scientific Discipline: Engineering: Fluids and Turbulunce

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

Research Summary:
The science focus in this project is on the study of the turbulent mixing of scalars with very low diffusivity, or very high Schmidt number, extended into regimes that have been difficult to reach. One specific target is to reach a Schmidt number of 512, which is comparable with that for salinity transport in the ocean, while retaining the flow properties that characterize high Reynolds number turbulence. A high Schmidt number is challenging for both experiment and computation because fluctuations arise at scales much smaller than those of the velocity field.

An innovative dual-grid, dual-communicator approach where scalar fields are computed using eighth-order compact finite difference methods in a computation-intensive code that is highly optimized using OpenACC on Titan is the key to a likely breakthrough. A second focus is the occurrence and topology of extreme events in scalar dissipation rate at high Reynolds number and moderately high Schmidt number. This work will likely provide definitive answers on questions such as Batchelor scaling, local isotropy and saturation of intermittency that have long remained obscure because of limited resolution and limited Schmidt number in previous works.

Type: New
Title: "Understanding How Multiscale Transport Determines Confinement in Burning Plasmas"

Principal Investigator: Christopher Holland, University of California, San Diego
Co-Investigators: Jeff Candy, General Atomics
Nathan Howard, Massachusetts Institute of Technology

Scientific Discipline: Physics: Plasma Physics

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

Research Summary:
The frontier of magnetized plasma microturbulence lies in understanding the dynamics of multiscale driftwave turbulence in fusion reactor-relevant regimes. In a reactor, the plasma will be unstable to nonlinearly coupled instabilities at both the ion and electron gyroradius scales.

The research team proposes leveraging validation-quality datasets from reactor-relevant DIII-D H-mode (high confinement) tokamak discharges, for which standard ion-scale simulations were unable to reproduce experimental electron heat fluxes, to begin a more rigorous validation of the multiscale gyrokinetic model and pushing into unexplored regimes. These studies will use multiscale gyrokinetic simulations with realistic ion-to-electron mass ratio, experimentally-derived inputs, and electromagnetic effects to compare predicted transport in multiple channels directly against experiment. The results of this work will begin to shed light on whether cross-scale coupling will play an important role in reactor-relevant regimes, helping to define the requirements for reliable prediction of ITER and beyond. To further investigate this issue, the team also proposes to attempt the first multiscale simulations of ITER plasmas. ITER is predicted (by state of-the-art reduced turbulence models) to have significant levels of electromagnetic, multiscale electron transport. They will assess the accuracy of these reduced-model predictions against first-principles electromagnetic multiscale gyrokinetic simulation.

To investigate the importance of multiscale turbulence in reactor-relevant conditions, the team plans to utilize the newly developed gyrokinetic code, CGYRO. This successor to the well-established code, GYRO, has been optimized for Titan and for performing multiscale simulations utilizing large numbers of ion species. The team seeks to take advantage of these optimizations to enable first-of-a-kind simulations of ITER and the first comparisons of multiscale predictions of thermal and particle transport to measurements from the DIII-D tokamak. Ultimately, the completion of this work will begin to shed light on the multiscale nature of turbulence in ITER and the multiscale nature of particle transport in tokamaks, both of which must be accurately predicted to realize the success of fusion as a viable commercial energy source.

Type: New
Title: "Understanding the Molecular Origin of Climate Change"

Principal Investigator: Subramanian Sankaranarayanan, Argonne National Laboratory
Co-Investigators: Henry Chan, Argonne National Laboratory
Mathew Cherukara, Argonne National Laboratory
Xiao-Min Lin, Argonne National Laboratory
Badri Narayanan, Argonne National Laboratory
Kiran Sasikumar, Argonne National Laboratory

Scientific Discipline: Chemistry: Environmental

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

Research Summary:
Understanding the phase behavior of water is central to climate change, as well as many other research areas, including geology, heterogeneous catalysis, corrosion, nanofluidics, and emerging energy technologies. Altering the state points (temperature, pressure, etc.) and introducing foreign surfaces/particles often results in phase transformation of water; the exact molecular origins of which is a topic of longstanding interest to researchers across the world.

To better understand and address the problems associated with climate change, researchers from Argonne National Laboratory will use Mira to carry out large-scale mesoscopic simulations of ice nucleation and growth under a variety of conditions. Their research aims to provide a molecular-level understanding of snowflake formation, and how it is impacted by the interaction between water and atmospheric pollutants.

Advances in machine learning and data science algorithms, combined with the DOE's powerful computing resources, have made it possible to tackle this challenging problem. The Argonne research team will develop well-trained and robust force fields to accurately and efficiently capture the molecular interactions in water. They will use the interaction models to simulate billions of water molecules and understand the molecular origins of trace pollutant influence on snowflake formation and growth. The outcome will have direct and profound implications for understanding the impact of atmospheric pollutants on global warming and climate change.

In addition, this project's findings will be of significance to a broad range of materials problems. For example, in battery research, an improved understanding of dendritic growth (analogous to snowflakes) at the electrode interfaces is critical to achieving optimal performance.

Type: New
Title: "Unraveling autoimmune diseases with adaptive protein simulation"

Principal Investigator: Cecilia Clementi, Rice University
Co-Investigators: Shantenu Jha, Rutgers University
Frank Noé, Freie Universitat Berlin
Jeremy Smith, Oak Ridge National Laboratory

Scientific Discipline: Biological Sciences: Biophysics

INCITE Allocation: **65,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (65,000,000 processor hours)

Research Summary:
The team will explore the molecular basis of autoimmune defects by employing adaptive molecular dynamics and Markov state modeling techniques on leadership supercomputing hardware. The adaptive immune system is responsible for recognizing antigens, which are parts of harmful substances (e.g., toxins, viruses, bacteria), and then neutralizing these substances. Understanding and being able to manipulate the function of the immune system is of utmost importance for society.

Despite its complexity, the immune system is governed by the interactions between only a few key proteins. Out of these, the MHCII is of prominent importance, as it is associated with more diseases than any other region of the human genome. In particular, specific MHCII mutants are responsible for autoimmune diseases, such as arthritis or diabetes. There is experimental evidence that the conformational dynamics of MHCII are key to the understanding of the molecular mechanism of antigen recognition. Furthermore, it appears that allosteric switches govern the binding of antigens, providing a template for the rational design of drugs for autoimmune diseases.

Understanding molecular mechanisms and conformational transitions is an ideal problem for molecular dynamics (MD) simulations. Previous simulations of this system have been on the 100 nanoseconds time scale. In a preliminary Director's Discretionary award on Titan, the team has generated simulation data of _300 _s. These results demonstrate the feasibility of the above aims and already reveals interesting yet preliminary biological insights. They now propose to explore conformational transitions of MHCII on timescales of tens of milliseconds. Their scientific results will comprise (1) the molecular mechanism of MHCII as it moves from its "ground state" conformation to antigen-presenting conformations, (2) the molecular mechanisms in dysfunctional and pathological MHCII mutants, and (3) suggestions to interfere with such dysfunction e.g. by the use of drugs that bind to allosteric sites. These results can significantly advance the field of immunology. In addition, we will achieve technological results such as establishing and further developing adaptive sampling and Markov state modeling methods.