Type: New
Title: "Accelerated Climate Modeling for Energy (ACME)"

Principal Investigator: Mark Taylor, Sandia National Laboratories
Co-Investigators: David Bader, Lawrence Livermore National Laboratory
Robert Jacob, Argonne National Laboratory
Ruby Leung, Pacific Northwest National Laboratory
Matthew Norman, Oak Ridge National Laboratory
Philip Rasch, Pacific Northwest National Laboratory
William Riley, Lawrence Berkeley National Laboratory
Todd Ringler, Los Alamos National Laboratory
Peter Thornton, Oak Ridge National Laboratory
Luke Van Roekel, Los Alamos National Laboratory
Charlie Zender, University of California, Irvine

Scientific Discipline: Earth Science: Climate Research

INCITE Allocation: **179,230,769 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (89,230,769 processor hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (90,000,000 processor hours)

Research Summary:
This INCITE project supports the Accelerated Climate Modeling for Energy (ACME) model, a multi-laboratory project developing a leading-edge climate and Earth system and driven by three grand challenges, two of which are the focus of this project using the ACME v1 model: (1) in the water cycle, how will more realistic portrayals of its important features (e.g., resolution, clouds, aerosols) affect river flow and associated freshwater supplies at the watershed scale?, and (2) in cryosphere systems, could a dynamic instability in the Antarctic Ice Sheet be triggered within the next 40 years?

For (1), the team's objective is to simulate 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 Amazon headwaters. For (2), ACME examines the near-term risk of initiating the dynamic instability and onset of the Antarctic Ice Sheet's collapse due to rapid melting by adjacent warming waters —the first fully coupled simulation to include dynamic ice shelf-ocean interactions.

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

Principal Investigator: Kenneth Jansen, University of Colorado, Boulder
Co-Investigators: Michael Amitay, Rensselaer Polytechnic Institute
Jed Brown, University of Colorado, Boulder
Christopher Carothers, Rensselaer Polytechnic Institute
John Evans, University of Colorado, Boulder
John Farnsworth, University of Colorado, Boulder
Michel Rasquin, University of Colorado, Boulder
Onkar Sahni, Rensselaer Polytechnic Institute
Mark Shephard, Rensselaer Polytechnic Institute
Cameron Smith, Rensselaer Polytechnic Institute
Philippe Spalart, Boeing
Edward Whalen, Boeing

Scientific Discipline: Engineering: Aerodynamics

INCITE Allocation: **207,692,308 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (200,000,000 processor hours)
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (7,692,308 processor hours)

Research Summary:
This effort builds upon multiple INCITE and Early Science Program campaigns where computational models of a vertical tail and rudder assembly with 12 synthetic jets were validated against experiments at a Reynolds number of 3.5e5, 53 times smaller than flight conditions. Using Mira and Theta, researchers will perform a suite of similar simulations at two- and four-times higher Reynolds number comparing synthetic jets and sweeping jets at two different spacings. This will provide the insight required to use exascale computing to carry out the first-ever flight Reynolds number delayed detached eddy simulation validated against experiments. Flow simulations of unprecedented scale and complexity are made possible by combining a highly scalable computational fluid dynamics (CFD) solver with anisotropically adapted unstructured grids on Mira and Theta.

Type: New
Title: "Advancing Design & Structure Prediction of Proteins & Peptides"

Principal Investigator: David Baker, University of Washington
Co-Investigators: Frank DiMaio, University of Washington
Andrew Leaver-Fay, University of North Carolina
Vikram Mulligan, University of Washington

Scientific Discipline: Chemistry: Biochemistry

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

Research Summary:
Researchers from the University of Washington's Baker Lab are pioneering the development of computational methods to predict protein and peptide structures, and to design those with new structures and functions. The core of the team's workflow is Rosetta, a software suite used for modeling biomolecular structures. Using previous INCITE awards, the team made significant progress developing and applying Rosetta to predict structures from amino acid sequences, and to design amino acid sequences that are able to fold into novel structures with new, desired functions. With this project, they will address emerging challenges by further improving the software, including the continued development of its energy function (the heart of all the Rosetta tools).

The team aims to tackle two new challenges within the energy function: improving its ability for de novo protein design and enabling it to precisely handle more general types of biomolecules. They will also continue work to improve the intelligence of Rosetta's design methods, which will help enable more robust protein design by eliminating many of the common design artifacts that must currently be filtered out of the design pool. Finally, the team will use this INCITE allocation to develop design methods for various non-canonical building blocks. This will enable researchers to computationally design binders to targets of therapeutic interest that could significantly reduce experimental costs. The broader impacts of this research will address challenges in biological and materials sciences, including the design of new therapeutics to combat disease.

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

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

Scientific Discipline: Earth Science: Geological Sciences

INCITE Allocation: **100,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (100,000,000 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: Renewal
Title: "All-atom Simulations of Photosynthetic and Respiratory Energy Conversion"

Principal Investigator: Abhishek Singharoy, Arizona State University
Co-Investigators: Klaus Schulten (deceased), University of Illinois at Urbana-Champaign

Scientific Discipline: Biology: Biophysics

INCITE Allocation: **80,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (80,000,000 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 has performed 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
Maria Barrios-Sazo, Stony Brook University
John Bell, Lawrence Berkeley National Laboratory
Alan Calder, Stony Brook University
Brian Friesen, Lawrence Berkley National Laboratory
Adam Jacobs, Michigan State University
Max Katz, Stony Brook University
Christopher Malone, Los Alamos National Laboratory
Andy Nonaka, Lawrence Berkley National Laboratory
Donald Wilcox, Stony Brook University
Weiqun Zhang, Lawrence Berkley National Laboratory

Scientific Discipline: Physics: Astrophysics

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

Research Summary: The research team will model astrophysical thermonuclear explosions, including Type Ia supernovae and X-ray bursts. Their open source application codes, Maestro and Castro, have been developed to take advantage of the hybrid architecture of the OLCF machines. Simulating these systems can provide insight into stellar phenomena observed in the night sky and the formation elements throughout the history of the Universe.

Maestro and Castro designed to model both the early subsonic, convection-dominated phase that precedes stellar explosions as well as the explosive dynamics and complex interplay of hydrodynamics, gravity, and reactions that accompanies these events.

Fundamental uncertainties to be investigated include the nature of Type Ia supernovae's progenitor—which has never been observed directly. They will explore all the current models to assess their feasibility. The team's X-ray burst work will help uncover the nature of the underlying neutron star, informing them about dense nuclear matter.

Type: New
Title: "Astrophysical Particle Accelerators: Magnetic Reconnection and Turbulence"

Principal Investigator: Dmitri Uzdensky, University of Colorado
Co-Investigators: Mitch Begelman, University of Colorado
Gregory Werner, University of Colorado
Vladimir Zhdankin, University of Colorado

Scientific Discipline: Physics: Astrophysics

INCITE Allocation: **98,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (98,000,000 processor hours)

Research Summary:
This project investigates nonthermal particle acceleration (NTPA) by magnetic reconnection and turbulence in three-dimensional (3D) relativistic plasmas relevant to astrophysical sources of intense bursts of high-energy X-rays and gamma-rays. Using petascale particle-in-cell (PIC) computer simulations, the research team is characterizing the particle energy distributions resulting from NTPA (or the lack thereof) as a function of plasma conditions. Based on completed simulations, the team is well-positioned to address several important questions regarding the fundamental viability of reconnection- and turbulence-driven NTPA as an explanation of observed high-energy emission, and thus to significantly advance the field of high-energy astrophysics. In addition, the empirical characterization of relativistic NTPA from reconnection and turbulence across a wide range of plasma conditions will help in modeling these astrophysical systems on larger scales and will guide our theoretical understanding of the key physical processes involved in particle acceleration.

This research seeks to advance understanding of fundamental energy exchange processes in plasmas. Energy exchange (e.g., between particles and fields) is one of the most important consequences of magnetic reconnection and turbulence, playing crucial roles in astrophysical systems, solar flares, the Earth's magnetosphere, and in magnetic fusion devices. The project employs the team's open-source PIC code Zeltron, which is capable of self-consistently incorporating the radiation reaction force to model cases where radiative losses significantly alter system dynamics and NTPA.

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

Principal Investigator: Eilif Muller, Blue Brain Project, EPFL
Co-Investigators: Fabien Delalondre, Blue Brain Project, EPFL
Michael Graupner, Paris Descartes
Kathryn Hess, Blue Brain Project, EPFL
Henry Markram, Blue Brain Project, EPFL
Felix Schuermann, Blue Brain Project, EPFL
Idan Segev, Hebrew University Jerusalem

Scientific Discipline: Biological Sciences: Neuroscience

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

For this INCITE project, researchers from École Polytechnique Fédérale de Lausanne are focused on advancing our understanding of these fundamental mechanisms of the brain's neocortex. The team is carrying 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.

The team is also using DOE supercomputers to characterize: (1) the role of NMDA receptor spikes in plasticity induction; (2) the dynamics of neuronal assembly formation and maintenance; and (3) 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 enhanced deep learning methods, as well as new learning paradigms for neuromorphic hardware.

Type: New
Title: "Co-evolutionary Networks: From Genome to 3D Proteome"

Principal Investigator: Daniel Jacobson, Oak Ridge National Laboratory
Co-Investigators: Xiaolin Cheng, Oak Ridge National Laboratory
Stephen DiFazio, West Virginia University
Wayne Joubert, Oak Ridge National Laboratory
Julie Mitchell, Oak Ridge National Laboratory
Jeremy Smith, Oak Ridge National Laboratory
Tim Tschaplinski, Oak Ridge National Laboratory
Gerald Tuskan, Oak Ridge National Laboratory

Scientific Discipline: Biological Sciences: Systems Biology

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

Research Summary: Fuels converted from cellulosic biomass offer one alternative to conventional energy sources, and supplementing fossil fuels with ethanol or other biofuels derived from bioenergy crops would benefit economic growth and energy security of the U.S. Short rotation woody crops, such as *Populus* species and hybrids, are expected to be an important renewable feedstock for biofuels production in the future due to their relatively low delivered cost.

Genetic effects of variants of these organisms can be viewed as the result of historic selective pressure and current environmental as well as epigenetic interactions, and, as such, their co-occurrence can be seen as genome-wide associations in a number of different manners. Jacobson's team will use these genome-wide associations, in combination with homology modeling, molecular dynamics, protein-protein docking and small molecule-protein docking to predict the structural interactions between proteins and small molecules in the cell for an unprecedented view of the 3D interactions among the components of the cellular machinery.

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

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

Scientific Discipline: Physics: Particle Physics

INCITE Allocation: **98,076,923 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (95,000,000 processor hours)
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (3,076,923 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 experimental data from the Large Hadron Collider (LHC), but achieving such precise predictions is an enormous theoretical and computational challenge.

For this INCITE project, researchers are using the N-jettiness framework, a novel approach to precision perturbative QCD calculations. The framework enables the efficient use of HPC 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 LHC's most pressing needs for precision predictions, and will help answer some of the most significant questions in 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: New
Title: "Computational Studies of Spin-Fluctuation Fingerprints in Cuprates"

Principal Investigator: Thomas Maier, Oak Ridge National Laboratory
Co-Investigators: Douglas Scalapino, University of California, Santa Barbara
Thomas Schulthess, Swiss Federal Institute of Technology Zurich, Switzerland

Scientific Discipline: Materials Science: Condensed Matter and Materials

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

Research Summary: This project carries out simulations of cuprate high-temperature superconductors with the goal of understanding the mechanism that leads to their behavior. These materials hold promise for revolutionizing many energy related technologies, but optimization is necessary for broader deployment and this requires a detailed understanding of their properties.

The team is specifically interested in understanding of the pairing mechanism, which is responsible for superconductivity in the cuprate high-temperature superconductors, and thus provide insight in the search for new superconducting materials. They will use a state-of-the art dynamic cluster quantum Monte Carlo algorithm implemented on leadership class computing hardware to carry out numerical simulations of these systems.

While there is common agreement that superconductivity in these systems is mediated by repulsive interactions, there is still debate as to whether or not this mechanism can be framed in terms of the exchange of spin-fluctuations. Driven by the physics of strong Coulomb interactions, these systems pose one of the most challenging problems for condensed matter theory. With the growing efficiency of numerical algorithms and the rapidly increasing computational power, modeling and simulation has played an important role in addressing this challenge. Previous simulations of simple models have found that the pairing interaction that gives rise to superconductivity is mediated by the exchange of spin-fluctuations. The aim of this project is to determine the fingerprints of a spin-fluctuation interaction in the dynamic behavior of experimentally accessible observables, a crucial step in establishing the theory of high-temperature superconductivity.

Type: New
Title: "Convective Turbulence in Liquid Sodium"

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

Scientific Discipline: Engineering: Fluids and Turbulence

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

Research Summary:
Turbulent Rayleigh-Bénard convection (RBC) is a type of heat transfer in which a constant temperature difference is maintained for a horizontal layer of fluid, heated from below. Because the fluid is confined, thin thermal and velocity boundary layers form near the top and bottom plates. One of the central unsolved problems in turbulent RBC is finding the transition to turbulence in these thin boundary layers. Simulations of turbulent RBC at high Rayleigh and low Prandtl numbers will help determine heat transport properties and predict transition parameters.

This INCITE project, will continue earlier research to advance numerical investigations of RBC to a parameter regime (Rayleigh number and Prandtl number) that has not been accessed before. The study's two main scientific objectives are to determine what happens to the flow for liquid sodium at high Rayleigh numbers, and how the Nusselt number and Reynolds number scale with the Rayleigh number.

The previous year's INCITE data provides preliminary supporting results that a new flow state exists for liquid sodium for a range of Rayleigh numbers $Ra > 10^7$. The team will run longer simulations at the same Rayleigh number to validate these results and run higher Rayleigh numbers to better understand this trend. Numerical simulations of turbulent RBC are based on the Nek5000 spectral element software package developed for solving the fluid flow equations on massively parallel supercomputers.

Simulations of turbulent heated convection at high Rayleigh and low Prandtl numbers will help researchers determine heat transport properties, in general, and the transition parameters for a turbulent boundary layer. Low-Prandtl-number convection has direct application to convection in liquid metals, such as gallium or sodium, and can shed light on convection in earth's liquid metal core and in the sun.

Type: New
Title: "Crystal Plasticity from First Principles"

Principal Investigator: Vasily Bulatov, Lawrence Livermore National Laboratory
Co-Investigators: Tomas Oppelstrup, Lawrence Livermore National Laboratory
Alexander Stukowski, Technische University Darmstadt
Luis Zepeda-Ruiz, Lawrence Livermore National Laboratory

Scientific Discipline: Engineering: Material Response

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

Research Summary:
The research team will use large-scale molecular dynamics (MD) simulations to settle two long-standing controversies in classical physical metallurgy: (1) the microscopic origin of strain hardening, and (2) the nature and geometric character of dislocation patterns. Widely divergent theories have been advanced about these two phenomena, some "classical" theories even being mutually contradictory. The disarray persists because scientists are unable to test crystal plasticity properties while simultaneously (*in situ*) observing the underlying dynamics of atoms and dislocations, which are line defects in the crystal lattice known to be responsible for crystal plasticity.

In situ microscopy observations are possible only in thin electron-transparent films — where neither strain hardening nor dislocation patterns are observed. At present, MD simulations offer the only means to permit, in principle, simultaneous mechanical testing of bulk crystal plasticity *in silico* and fully detailed *in situ* observation of the underlying atomic dynamics. Because of their immense computational cost, direct MD simulations of crystal plasticity have been regarded as impossible. However, the team, in applying a newly established simulation capability, has demonstrated that direct cross-scale MD simulations of plasticity and strength of tantalum metal are feasible. The project objective now is to address three stages of strain hardening and the nature of dislocation patterns using cross-scale rather than multi-scale simulations. This effort will also increase understanding of the strength of structural materials.

Type: New
Title: "Differential Diffusion and Double Diffusive Phenomena in Turbulence"

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

Scientific Discipline: Engineering: Fluids and Turbulence

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

Research Summary:
This INCITE project seeks to pursue fundamental advances in understanding of turbulent flow phenomena, in two closely-related problem areas that are important but not well or little investigated in the past. Both problems will be addressed using numerical simulations at resolution up to 8192^3, i.e., half-a-trillion grid points, which is feasible only on multi-Peta flop capability machines.

The code to be deployed is a recently extended version of one which uses OpenMP 4.5 on GPUs and has been proven to scale very well on Titan, achieving a GPU to CPU speedup of up to 5X at the scale of 8192 Titan nodes. A major focus of code development has been the use of asynchronous execution between CPU and GPU for three-dimensional compact finite difference calculations. These optimizations are greatly facilitated by the Cray compiler implementation of OpenMP 4.5 on Titan.

One science focus in this project is differential diffusion i.e. the turbulent mixing of two passive scalars with different molecular diffusivities, in the regime of low diffusivity (high Schmidt number). This is a parameter regime which occurs for mixing in many liquids, and, more importantly, temperature and salinity in the ocean whose diffusivities differ by a factor of 100. A second science focus is to generalize to active scalars which can modify the flow field substantially, as for temperature and salinity in the ocean which can lead to either stabilizing or de-stabilizing density stratification. Studies of stratification are known in the literature but only in parameter ranges characteristic of the atmosphere but not the ocean, with high Schmidt number again being a major challenge.

Type: New
Title: "DNS of Multi-Stage Multi-Mode Combustion Towards 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: **80,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (80,000,000 processor hours)

Research Summary:

More efficient 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.

In this INCITE project, Chen's team proposes petascale direct numerical simulation (DNS) of multi-stage mixed-mode turbulent combustion to elucidate key physics that govern autoignition and flame stabilization in engines and to provide benchmark data for combustion model development under the conditions of next generation engines, which operate near combustion limits to maximize efficiency and to minimize harmful emissions.

Targets will provide fundamental insights into key turbulence-chemistry interactions required for predictive model development of fuel efficient flexible engines for transportation and power generation. The development of direct numerical simulation benchmarks for model development in LES and RANS is essential to vastly improve the fidelity of computational engine models that enable simulation based optimization and design, shortening the time-to-market and increasing American competitiveness.

Type: Renewal
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: **50,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (50,000,000 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: "Extreme-scale Simulation of Supernovae and Magnetars from Realistic Progenitors"

Principal Investigator: Sean Couch, Michigan State University
Co-Investigators: Andrew Christlieb, Michigan State University
Evan O'Connor, Stockholm University
Kuo-Chuan Pan, Michigan State University
Luke Roberts, Michigan State University
MacKenzie Warren, Michigan State University

Scientific Discipline: Physics: Astrophysics

INCITE Allocation: **159,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (150,000,000 processor hours)
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (9,000,000 processor hours)

Research Summary:
Core-collapse supernovae (CCSNe) are the explosive deaths of massive stars that drive cosmic chemical evolution and the formation of compact objects. But the mechanism driving these explosions is still uncertain. This project will transform our understanding of supernovae through extreme-scale simulations.

This comprehensive, end-to-end investigation will utilize 3D MHD CCSNe simulations with sophisticated multidimensional neutrino transport and the most realistic initial conditions ever adopted for CCSNe to study the effects of rotation, magnetic fields, and progenitor asphericity on CCSNe. In addition, a multi-year progressive investigation will develop and employ 3D massive stellar progenitor models at the point of core-collapse and address whether rotation and magnetic fields aid successful explosions for "normal" CCSNe. The impact of realistic initial conditions on nucleosynthesis in CCSNe will also be explored.

Results will directly inform our understanding of the characteristics of newborn pulsars and magnetars, information that can be directly compared to observational data. The project will also address whether plausible rotation rates and magnetic field strengths influence the CCSNe mechanism and what impact realistic 3D progenitor structures have on the CCSNe mechanism and observables.

Type: New
Title: "Finite Difference Time Domain Simulations to Facilitate Early-Stage Human Cancer"

Principal Investigator: Allen Taflove, Northwestern University
Co-Investigators: Vadim Backman, Northwestern University
Wei Jiang, Argonne National Laboratory
Di Zhang, Northwestern University

Scientific Discipline: Biological Science: Computational Electromagnetics/ Biomedical Sciences

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

Research Summary:
Early-stage cancer detection has been widely recognized as one of the most critical factors to successfully treat cancer and reduce mortality. Current gold standards for diagnosing cancer target existing tumorous tissue and cells. These techniques are not efficient in detecting cancer before formation of the tumor, since very early cancerous alterations occur at macromolecule scales. The ultimate goal of this research is to develop a low-cost, high-throughput optical microscopic technique that can sense macromolecular alterations and predict cancer risk at a very early stage.

Facilitated by finite-difference time-domain (FDTD) computational solutions of Maxwell's equations, this research group has developed the novel technique, Partial Wave Spectroscopic (PWS) microscopy, that can detect static, intracellular, nano-architectural alterations not accessible by conventional microscopy. Researchers propose to extend FDTD's capabilities to develop a dynamic component to PWS that will, in combination with static PWS, provide insights into macromolecular behavior in live cells. Because a dynamic PWS requires numerical methods to simulate optical imaging systems, the group's FDTD software package, Angora—literally "a microscope in a computer"—will be applied to its development.

The proposed research could significantly improve early-stage detection of several different cancers (e.g., lung, colon, pancreas, esophagus, prostate, and ovaries) and benefit the public by reducing mortality rates. Additionally, it could provide tools to reveal fundamental macromolecular behaviors during pathological processes that are critical for the development of therapeutics targeting these behaviors.

Type: New
Title: "First Principle Simulations of On-Die Interconnects and Their Heat Generations"

Principal Investigator: Lin-Wang Wang, Lawrence Berkeley National Laboratory
Co-Investigators: Laurent Bellaiche, University of Arkansas

Scientific Discipline: Materials Science: Nanoelectronics

INCITE Allocation: **27,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (27,000,000 processor hours)

Research Summary: As the transistor size keeps shrinking in microelectronics following the Moore's law, the heat generation from the on-die interconnect has become a major issue, and can threaten further downscaling of electronic devices. The interconnect has bypassed the computing units and is the number one heat generating source on a chip. If this problem is not solved, it has a potential to halt the future developments of electronic industry, thus has a major impact in the society.

Currently, continuum diffusion models with heavy parameterization are used to study this problem. However, as the nanocontact becomes a few nm wide, it is clear the continuum model is no longer adequate. In this INCITE project, the team proposes to use first principle simulations to study the heat generation mechanism in an on-die nanocontact.

This proposal is based on previous experience in large-scale electronic structure calculations for nanosystems. The ready-to-use codes were developed in previous INCITE projects and have been optimized for the Titan machine. Through the proposed large scale high fidelity simulations, we hope to address the following fundamental questions: (1) what is the atomic structure in a nanocontact? What kind of crystal imperfections will be formed there: void, point defect, grain boundary, or amorphousness? (2) What is its I-V curve? What is the main heat generation source, one of the above defects, or the Cu/liner interface? (3) What is the optimal nanocontact shape to reduce the resistance? (4) How strong is the electromigration effect, and how that could damage a nano-contact?

Type: New
Title: "First Principles Investigation of Solid State Phase Transitions"

Principal Investigator: Markus Eisenbach, Oak Ridge National Laboratory
Co-Investigators: Valentino Cooper, Oak Ridge National Laboratory
Mark Jarrell, Louisiana State University
Ying Wai Li, Oak Ridge National Laboratory
Od 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: **95,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (95,000,000 processor hours)

Research Summary: Disorder is present in all real materials, but while in many cases idealized systems give a good description of a material's properties, in some classes of materials high degrees of disorder can lead to qualitatively new physics. This project explores these exciting new properties such as phase transitions in the magnetic and electronic states and mechanical properties that are controlled by disorder and temperature. The team seeks to provide first principles calculations of disorder driven phenomena in solid state systems.

The team will achieve this goal by applying density functional based ab initio methods in conjunction with statistical physics methods. The calculations performed using first principles Wang-Landau and typical medium embedding share as a common feature a high level averaging part and a compute intensive deterministic kernel, that will allow the exposure of multiple levels of parallelism, scaling towards the exascale.

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: New
Title: "Global Adjoint Tomography"

Principal Investigator: Jeroen Tromp, Princeton University
Co-Investigators: Ebru Bozdag, Colorado School of Mines
Dimitri Komatitsch, University of Aix-Marseille
Matthieu Lefebvre, Princeton University
Daniel Peter, King Abdullah University of Science and Technology

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: Information about Earth's interior comes from seismograms recorded at its surface. Seismic imaging based on spectral-element and adjoint methods has enabled assimilation of this information for the construction of 3D (an)elastic Earth models. These methods account for the physics of wave excitation and propagation by numerically solving the equations of motion, and require the execution of complex computational procedures that challenge the most advanced high-performance computing systems. Current research is petascale; future research will require exascale capabilities.

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.

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: Renewal
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, University of California, Santa Barbara
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, but poor understanding of mass loss is one of the biggest uncertainties in massive star evolution. Winds from these stars depends on surface layer structure, including the effects of hydrodynamic and/or magnetohydrodynamic (MHD) instabilities that can only be understood via 3D global radiation MHD simulations.

Using the unique radiation code Athena++, the team will conduct these simulations to study the global structure of the gaseous outer layers, or envelopes, of massive stars. Higher resolution near the iron opacity peak— increases in opacity due to atomic transitions of iron—resolves 3D turbulent structures due to convection; and relatively lower resolution at large radii captures the extended envelope and radiation driven outflow. These researchers hope to capture the photosphere within the simulation to predict observational properties directly.

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

Type: New
Title: "Hadron Structure from Lattice QCD"

Principal Investigator: Konstantinos Orginos, College of William & Mary
Co-Investigators: Michael Engelhardt, NMSU
Hue-Wen Lin, MSU
Keh-Fei Liu, University of Kentucky
David Richards, Jefferson National Laboratory

Scientific Discipline: Physics: Nuclear Physics

INCITE Allocation: **155,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (55,000,000 processor hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (100,000,000 processor hours)

Research Summary: This project will study the structure of hadrons using first principles with a newly developed theoretical approach that allows us for the first time to achieve a complete 3D image of the hadron using the fundamental theory known as Quantum Chromodynamics. These studies employ Monte Carlo computations and are only possible with leadership class computing facilities.

This work will provide essential theoretical support to the current (JLab 12 GeV) and future (Electron Ion Collider) experimental program in hadronic physics. Orginos's project is essential in achieving the physics goals set forward in the recent Nuclear Physics Long Range plan.

Leadership class computers are required in order to capitalize on configurations, generated by USQCD, that sample the QCD vacuum fluctuations, allowing researchers to determine the properties of hadrons from first principles. In this project, the team is employing state of the art methods, developed recently, that allow researchers to have a complete picture of the hadron for the first time. First, they will compute the distribution of momentum of the constituents of a hadron along the direction of its motion by determining the longitudinal momentum distribution functions. By studying the transverse momentum parton distribution functions, they will image the hadron in the transverse plane to its direction of motion. Therefore, they will achieve a full 3D imaging of the hadron. Finally, the same methodology will allow the team to study the distribution of angular momentum of the hadron among its constituents.

Type: New
Title: "High-Accuracy LES of a Multistage Compressor Using Discontinuous Galerkin"

Principal Investigator: Koen Hillewaert, Cenaero
Co-Investigators: Sophie Mouriaux, Safran
Michel Rasquin, Cenaero
Ariane Frère, Cenaero

Scientific Discipline: Engineering: Aerodynamics

INCITE Allocation: **78,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (78,000,000 processor hours)

Research Summary:
Jet engine design relies on statistically averaged turbulence models. Known as RANS, these models constitute the most accurate, computationally affordable approach available, but have important limitations, particularly in the area of very complex geometries and off-design conditions. Industry would therefore like to complement their simulation tools with more accurate approaches such as large-eddy simulations (LES), which compute the largest turbulent flow features directly and models the smallest ones. Low-order finite-volume methods, typically tailored for RANS, continue to be used to solve for geometrical complexity. But in academia, LES is typically performed using much more accurate, yet geometrically inflexible, discretization methods.

Recently, unstructured, discontinuous, high-order methods have emerged that bridge the gap between academic accuracy and industrial geometrical complexity, thereby providing a much better suited discretization for industrial LES. This project represents the first use of such a high-order unstructured method for the LES of an actual machine, a transonic high-pressure multistage axial compressor. The computational approach used for these simulations is the discontinuous Galerkin flow solver Argo.

The first objective is to vastly improve the resolution and accuracy with respect to previous RANS and LES studies, providing an unprecedented and reliable insight into flow, particularly features such as leakage flows and stall, which are notoriously hard to capture. This new approach will allow industry to reliably predict jet engine performance, before constructing costly prototypes. Furthermore, this project will provide important information for future uptake of LES in industry and constitute a milestone and reference in their development.

Type: Renewal
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: **264,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (264,000,000 processor hours)

Research Summary:

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. CCP's work includes producing and analyzing suites of climate simulations with the Community Earth System Model (CESM) and then comparing the results to larger multi-model datasets.

For 2018, the team intends to further clarify the effects of small-scale regional features and interactions across spatial scales, especially how they influence high-impact events in climate, by proceeding with CESM1.3 simulations using a 0.25° atmosphere/land coupled to a 0.1° ocean/ice resolution. This is pioneering work with the CESM, representing the forefront of Earth system modeling capabilities, and has the potential for being transformative within the climate projection discipline. The completion of these century-long experiments with CESM at its highest possible atmosphere and ocean resolution will create a rich climate modeling database available not only to members of the CCP team, but also to climate scientists at DOE labs and universities to mine for analysis of related climate variability and climate change problems.

The overarching purposes of the research are to investigate climate variability and change related to high-impact events. This project's findings will be critical to future climate change studies, both of national and international interest.

Type: New
Title: "High-Accuracy Quantum Approaches for Predictions of Catalysis on Solids"

Principal Investigator: Maria Chan, Argonne National Laboratory
Co-Investigators: Anouar Benali, Argonne National Laboratory
Ken Jordan, University of Pittsburgh
Ye Luo, Argonne National Laboratory

Scientific Discipline: Chemistry: Catalytic

INCITE Allocation: **46,615,384 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (42,000,000 processor hours)
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (4,615,384 processor hours)

Research Summary:
The catalytic and photocatalytic splitting of water to H_2 and O_2 as well as CO_2's reduction to organic fuels are of increasing significance for solar energy capture, fuel production and storage, and carbon sequestration — heightening the importance of a predictive modeling approach for understanding fundamental reaction mechanisms and the catalytic properties of target and potential catalysts for these reactions. However, in quantum mechanics (QM)-based modeling of catalytic processes, different approximations often yield widely disparate results, necessitating the development of a computational approach that both aids in error and uncertainty quantification (UQ) and predicts reaction and barrier energies to high accuracy.

Project objectives are to (1) perform high-accuracy quantum Monte Carlo (QMC) calculations of water splitting and CO_2 reduction catalysis on earth-abundant transition metals and transition metal oxides, (2) enable periodic multi-determinant trial wavefunctions for QMC calculations, and (3) quantify the uncertainties and systematic errors of various QM-based surface catalysis approaches using multifidelity analysis and comparison with QMC calculations. The result will be unprecedented accuracy and robust UQ for predictive modeling and design of solid catalysts. By accurately determining catalytic surface reaction mechanisms and energetics, we seek to enable prediction of reaction rates and selectivities; point to key characteristics that determine these reactivity properties; and promote rigorous computational catalyst design for water splitting and CO_2 reduction. Our codes will also enable full utilization of peta- to exascale HPC systems for catalysis applications.

Type: New
Title: "High-fidelity Gyrokinetic Simulation of Tokamak and ITER Edge Physics"

Principal Investigator: C.S. Chang, Princeton Plasma Physics Laboratory
Co-Investigators: Stephen Abbot, Oak Ridge National Laboratory
Mark Adams, Lawrence Berkeley National Laboratory
Luis Chacon, Los Alamos National Laboratory
Stephanie Ethier, Princeton Plasma Physics Laboratory
Robert Hager, Princeton Plasma Physics Laboratory
Scott Klasky, Oak Ridge National Laboratory
Tuomas Koskela, Lawrence Berkeley National Laboratory
Seung-Hoe, Princeton Plasma Physics Laboratory
Scott Parker, University of Colorado
Mark Shephard, Rensselaer Polytechnic Institute

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation: **161,538,462 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (61,538,462 processor hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (100,000,000 processor hours)

Research Summary: The success of the ITER program is of the highest relevance to the DOE mission. An important theoretical aspect of the US contribution to ITER is expected to be from first-principles-based extreme scale simulations. Two of the most critical challenges for ITER boundary plasma, which need to be studied from first-principles-based extreme scale simulation, are (i) external heating power requirement for the H-mode operation, and (ii) its ability to withstand the steady-state exhaust-heat deposited by the plasma in a narrow strip on the divertor target plates. These questions will be directly addressed using high-fidelity first-principles based models through the application of the edge gyrokinetic code XGC1 executing at extreme scale on Titan-Summit at OLCF and Theta-Aurora at ALCF. These large-scale studies are time-urgent for successful planning of ITER operation and require intensive, concentrated computing effort with many continuous check-point restarts.

Type: New
Title: "Influenza Druggability and Transmissibility through the Computational Microscope"

Principal Investigator: Rommie Amaro, University of California, San Diego

Scientific Discipline: Biological Sciences: Biophysics

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

Research Summary: Both seasonal and pandemic influenza have been responsible for millions of deaths worldwide. The emergence of new highly transmissible pandemic strains is highly probable given the recent 2009 H1N1 "swine flu" pandemic and the imminent threat of the highly pathogenic avian influenza H5N1.

Molecular dynamics (MD) simulations of this massive H1N1 pandemic strain influenza virus system of about 180 million atoms conducted on NCSA Blue Waters provided unprecedented insights into the mechanisms of influenza virulence and drug resistance. Based on the team's preliminary data, they hypothesized an explanation of flu transmissibility based on dynamics at the atomic scale. The whole virus simulation revealed the cooperativity among the disparate sites. As a follow-up to this exciting work, the team now proposes to run two additional whole virion simulations: H1N1 with short stalk NA (swapped in from avian H5N1, mimicking viral reassortment) and H1N1 with short stalk NA (again swapped from avian H5N1) and sialic acid bound to the NA 2nd binding site. Both systems consist of ~180 million atoms. An INCITE leadership-class allocation is critical because typical (XSEDE) supercomputer allocations do not permit the simulation of atomistic models of this size and scale. A comprehensive analysis will be performed to comparatively examine the dynamic changes, multisite cooperativity, and ensemble-averaged electrostatic potentials of each virion and to determine how those dynamic and electrostatic potentials influence the association kinetics with host-cell glycan receptors.

Together, large-scale biological simulations and emerging analysis approaches set the stage for exciting data-driven biophysical and biomedical research wherein key biological processes at the organism level can be directly inferred from the small changes at the atomic scale.

Type: New
Title: "INtegrated and Scalable PredictIon of REsistanace (INSPIRE)"

Principal Investigator:	Peter Coveney, University College London
Co-Investigators:	John Chodera, Memorial Sloan Kettering Cancer Center Shantenu Jha, Rutgers University Rick Stevens, Argonne National Laboratory Herman Van Vlijmen, Janssen, Pharmaceutical Companies of Johnson & Johnson
Scientific Discipline:	Biological Sciences: Biophysics
INCITE Allocation:	**80,000,000 processor hours**
Site:	Oak Ridge National Laboratory
Machine (Allocation):	Cray XK7 (80,000,000 processor hours)

Research Summary: Both seasonal and pandemic influenza have been responsible for millions of deaths worldwide. The emergence of new highly transmissible pandemic strains is highly probable given the recent 2009 H1N1 "swine flu" pandemic and the imminent threat of the highly pathogenic avian influenza H5N1.

Molecular dynamics (MD) simulations of this massive H1N1 pandemic strain influenza virus system of about 180 million atoms conducted on NCSA Blue Waters provided unprecedented insights into the mechanisms of influenza virulence and drug resistance. Based on the team's preliminary data, they hypothesized an explanation of flu transmissibility based on dynamics at the atomic scale. The whole virus simulation revealed the cooperativity among the disparate sites. As a follow-up to this exciting work, the team now proposes to run two additional whole virion simulations: H1N1 with short stalk NA (swapped in from avian H5N1, mimicking viral reassortment) and H1N1 with short stalk NA (again swapped from avian H5N1) and sialic acid bound to the NA 2nd binding site. Both systems consist of ~180 million atoms. An INCITE leadership-class allocation is critical because typical (XSEDE) supercomputer allocations do not permit the simulation of atomistic models of this size and scale.

Together, large-scale biological simulations and emerging analysis approaches set the stage for exciting data-driven biophysical and biomedical research wherein key biological processes at the organism level can be directly inferred from the small changes at the atomic scale.

Type: New
Title: "Kinetic Simulation of FRC Stability and Transport"

Principal Investigator: Sean Dettrick, TAE Technologies, Inc
Co-Investigators: David Leinweber, TAE Technologies, Inc
Toshiki Tajima, TAE Technologies, Inc/University of California, Irvine

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation: **30,769,230 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (30,769,230 processor hours)

Research Summary:
Magnetic confinement fusion offers the prospect of a carbon-neutral, environmentally responsible, and inexhaustible energy source. As part of an innovative class of magnetically confined fusion plasma experiments, researchers at Tri Alpha Energy (TAE) recently have shown that the confinement of energy improves with increasing plasma temperature. Following the development of an advanced Field Reversed Configuration (FRC) magnetic confinement device to contain the hot plasma needed to fuel fusion, TAE is now building a new device, named C-2W, to study the confinement of energy at still higher temperatures and inform the design of a prototype reactor.

Two strategic computing initiatives are underway at TAE to support the C-2W experimental program. The first is the development of a first-principles code to study the micro-stability of the plasma, namely kinetic microturbulence—the chief cause of heat losses from the plasma. The second is the development of a kinetic code to study macro-stability properties of the plasma. Together, the codes span orders of magnitude of spatiotemporal scales, to find stable operating points in advanced parameter regimes and to make quantitative predictions of the turbulent losses.

With this INCITE award, the TAE team will use DOE computing resources to (1) validate the codes against the experiment, (2) mitigate experimental risk inherent in the exploration of new parameter regimes, (3) accelerate the optimization of C-2W operating scenarios, and (4) use validated models to predict stable and efficient operating points for future FRC reactor design concepts.

Type: New
Title: "Large-Eddy Simulation for the Prediction and Control of Impinging Jet Noise"

Principal Investigator: Joseph Nichols, University of Minnesota

Scientific Discipline: Engineering: Fluids and Turbulence

INCITE Allocation: **81,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (81,000,000 processor hours)

Research Summary:
This project is motivated by the need for innovative strategies to reduce the noise produced by the high-speed exhaust jets of aircraft engines, among the loudest human-created sources of noise. Recent high-fidelity simulations performed at ALCF have demonstrated the predictive power of unstructured large-eddy simulations (LES) for aeroacoustics involving complex geometry. This project hopes to push beyond this previous work to develop groundbreaking prescriptive platforms for aeroacoustic design.

To control jet noise, the team will investigate the flow and noise associated with a supersonic jet impinging perpendicularly on a flat wall, modified by a ring of 16 microjet actuators that surround the nozzle lip. This problem is relevant to a number of aerospace and industrial applications, and contains complex interactions between turbulence, shocks, the wall, and acoustic feedback. The flow configuration, including microjets, is precisely represented by unstructured meshes.

The geometry exactly matches that of an experiment underway at state-of-the-art aeroacoustic test facilities at the Florida Center for Advanced Aero-Propulsion (FCAAP) at Florida State University, by a group with whom the team is collaborating. The physics of the compressible turbulent flow are captured accurately using high-fidelity LES with an explicit subgrid scale model. Data extracted from these simulations will be used to construct reduced-order models, which will then be used to control new simulations through dynamic forcing of the microjets.

In addition to applications such as helping to make jet engines quieter, the information derived from this project provides unique and deep insights about the inner mechanisms and hidden dynamics of turbulent flows, in general.

Type: New
Title: "Large Scale and Efficient Ultraviolet Light Emitting Diode Design with NEMO5"

Principal Investigator: Gerhard Klimeck, Purdue University
Co-Investigators: Tillmann Kubis, Purdue University

Scientific Discipline: Materials Science: Nanoelectronics

INCITE Allocation: **26,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (26,000,000 processor hours)

Research Summary:

Although ultraviolet light (UV-C) is critical for failsafe disinfection, all relevant UV-C light sources are inefficient, short lived and use poisonous mercury. The task of this project is to identify a UV-C LED design that can scale to large areas, has high efficiency and output power, and avoids bio-unsafe materials.

Klimeck's team's project supports research and design of UV-C light emitting diodes (LEDs) that give LED- typical high efficiencies, emit disinfecting UV-C light on large surfaces, and consist of bio-safe materials. The material of choice of this task is hexagonal boron nitride (hBN). This material has been used industrially for decades. Thanks to its bio-safety, it is even applied in cosmetic products. This 2D wide band gap semiconductor has been subject to various use studies in 2D UV-LEDs. Important experimental milestones such as the verification of UV-light emission, n- and p-type doping in hBN, the fabrication of high quality hBN layers, etc., have been reported in high-ranking journals over the last 5 years. Therefore, this work will assess possible metal-hBN contacts and determine promising hBN LED device designs with highest output efficiency and disinfection-sufficient output power.

Over the past 20 years the Klimeck research team has built up a suite of Nanoelectronic Modeling Tools (NEMO) at Texas Instruments, NASA JPL, and now at Purdue. They will use Titan to conduct parameterization of the LED materials and their combinations.

Type: New
Title: "Large-Eddy Simulation of a Commercial Transport Aircraft Model"

Principal Investigator: Parviz Moin, Stanford University
Co-Investigators: George Park, University of Pennsylvania

Scientific Discipline: Engineering: Aerodynamics

INCITE Allocation: **240,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (240,000,000 processor hours)

Research Summary:
This project seeks to perform large-eddy simulation (LES) of flow over a realistic aircraft geometry. The team's aim is to demonstrate, for the first time, the predictive capability of low-dissipation LES methodologies for practical external aerodynamics configurations. The major obstacle in accomplishing this goal is the presence of energetic near-wall eddies with diminishing length scales as one approaches the wall. Resolving such small but dynamically important near-wall eddies is infeasible even with the supercomputers to be introduced in the next decade. The team is addressing this issue by modeling the effect of the small-scale near-wall turbulence on the large-scales resolvable fluid motion in the outer portion of the boundary layer. This concept of wall modeling is now deemed indispensable for enabling predictive but affordable LES of practical aeronautical flows. However, application of wall-modeled LES (WMLES) to date has been confined largely to studies of canonical flows involving relatively low Reynolds numbers and mostly two-dimensional geometries. To this end, the team plans to conduct WMLES of the National Aeronautics and Space Administration (NASA) Common Research Model (CRM), which is a widely used community research model for a commercial transport aircraft. High-fidelity simulation of the NASA CRM is considered a grand challenge problem for computational fluid dynamics.

This project aims at producing the first demonstration of low-dissipation LES codes with the ability to perform scale-resolving calculations of a practical 3D external aerodynamics configuration. This milestone would point a new path to future aircraft design and engineering analysis, where low-dissipation LES has long been excluded for cost and stability considerations despite its superior predictive capability.

Type: Renewal
Title: "Lattice QCD"

Principal Investigator: Paul Mackenzie, Fermilab
Co-Investigators: Richard Brower, Boston University
Norman Christ, Columbia University
William Detmold, MIT
Robert Edwards, 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: **444,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (344,000,000 processor hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (100,000,000 processor hours)

Research Summary:
Using Mira and Titan, the team is addressing key science questions in high-energy and nuclear physics research 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 research in lattice quantum chromodynamics (QCD) addresses fundamental questions in high-energy and nuclear physics and relates directly to major experimental programs in these fields essential to meeting a number of Office of Science milestones.

A central objective of this project is to generate gauge configurations, which are representative samples of the QCD ground state used by the more than 100 U.S. QCD theoretical physicists to determine a wide range of physical quantities of importance in high-energy and nuclear physics. In high-energy physics, the configurations will enable researchers to push the search for new effects in flavor physics to yet higher energies. In nuclear physics, the team's suite of calculations can enable success of present and planned experiments at RHIC, Jlab, FRIB, LANL, ORNL, and other national facilities, including to guide the search for exotic states of matter at GlueX.

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 Korzdorfer, 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: **260,769,231 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (230,000,000 processor hours)
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (30,769,231 processor hours)

Research Summary:
With this project, researchers are conducting a large-scale computational campaign to discover and design new materials and interfaces that will advance the efficiency of organic and hybrid solar cells. To do so, the team is developing first-principles approaches, based on density functional theory and many-body perturbation theory, to describe materials and interfaces on the most fundamental level at which solar energy conversion takes place and at which structure-function relationships are established. By combining massively parallel quantum-mechanical calculations with modern machine learning techniques and optimization algorithms, they aim to predict and design new advanced functional photovoltaic materials and hetero-structures.

Ultimately, this research will enable transformative advances in the understanding of organic and hybrid photovoltaic materials, and the technology needed to harness their power for affordable, large-scale solar cells. The project's methodological advances will produce a general, broadly applicable first principles framework for structure search and computational design of functional materials that will broaden the community of researchers capable of using leadership computing resources to advance materials science for energy applications.

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

Principal Investigator: Yosuke Kanai, University of North Carolina at Chapel Hill
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: **155,384,615 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (140,000,000 processor hours)
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (15,384,615 processor hours)

Research Summary:
Electronic stopping describes the transfer of kinetic energy from very fast ions, like protons, to electrons in condensed matter. This process induces massive electronic excitations within the target material through interactions with the charged projectile's electric field. Understanding this phenomenon in condensed matter is critical to advancing various technological and medical applications.

Building upon previous INCITE work, researchers will use this award to (1) advance the first-principles electronic stopping modeling capabilities for high-Z heavy ions in semiconductors and (2) to use their predictive framework to investigate intricate details of electronic excitation dynamics of DNA under light-ion irradiation. The team will use their highly scalable implementation of real-time, time-dependent density functional theory to achieve ambitious computational goals, such as simulating a structurally complex system of hydrated DNA with more than 10,000 electrons and more than 2 million basis functions.

Ultimately, the team's work will provide predictive and quantitative computational insights into the interactions of fast ions with various materials. This knowledge has the potential to improve a variety of applications, including focused-ion beam microscopes, proton-beam cancer therapies, and the manufacturing of quantum bits and other advanced electronics.

Type: New
Title: "Multiscale Modeling of Magnetic Reconnection in Space and Laboratory Plasmas"

Principal Investigator: William Daughton, Los Alamos National Laboratory
Co-Investigators: Robert Bird, Los Alamos National Laboratory
Fan Guo, Los Alamos National Laboratory
Ari Le, Los Alamos National Laboratory
Adam Stanier, Los Alamos National Laboratory

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation: **24,061,538 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (24,061,538 processor hours)

Research Summary:
Magnetic reconnection, the mechanism by which magnetic field lines change their connectivity, leads to the explosive release of magnetic energy into plasma kinetic energy. In the laboratory, reconnection has implications for magnetic fusion devices; in space, it can lead to plasma transport from solar winds into the Earth's magnetosphere, which is a key driver of space weather and can lead to satellite damage. This project will shed new light on both the physics and consequences of magnetic reconnection.

Reconnection is a truly multiscale and, therefore, formidable phenomenon, due to the cross-scale coupling between global plasma dynamics and small-scale electron and ion kinetic physics. This research will address several fundamental open questions about reconnection using multiscale, first-principles, kinetic modeling through fully kinetic particle-in-cell simulations on the ALCF's supercomputer, Theta. These simulations will use more realistic configurations suitable for comparison with new laboratory experiments and spacecraft observations, providing critical new insights into the physics of magnetic reconnection.

In addition to providing a better understanding of reconnection events in magnetic fusion energy devices and space plasmas, information derived from these simulations will advance the capabilities of facilities conducting next-generation magnetic reconnection experiments, such as FLARE, at the Princeton Plasma Physics Laboratory, and T-REX, at the University of Wisconsin. Further numerical simulations will support two DOE Office of Science Opportunities in Basic Plasma Science grants to model reconnection in laboratory experiments.

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

Principal Investigator: Hussein Aluie, University of Rochester

Scientific Discipline: Engineering: Fluids and Turbulence

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

Research Summary:

The Rayleigh-Taylor Instability (RTI) is a ubiquitous flow phenomenon occurring in numerous natural and engineered systems in which buoyancy forces exist. RTI is a major obstacle to current efforts to realize nuclear fusion as a viable and virtually limitless energy source via inertial confinement fusion (ICF); thus, DOE's ICF program is making a significant effort to account for RTI's effects in large-scale simulations of ICF implosions in both two and three dimensions. Another factor is ablation (or mass evaporation) caused by a heat source such as a laser or the hot spot in laser-driven plasmas that occurs in many RTI flows (e.g., supernova explosions, molecular clouds).

Small-scale perturbations in the ablative RTI (aRTI) are often neglected because they are linearly stable when their wavelength is shorter than a linear cutoff. Using our previous allocation, we have shown that linearly stable modes of any wavelength can be destabilized. This instability regime requires finite amplitude initial perturbations, and linearly stable aRTI modes are more easily destabilized in 3D than in 2D. One surprising result: for conditions found in laser fusion targets, short-wavelength aRTI modes are more efficient at driving the mixing of ablated material throughout the target because the nonlinear bubble density increases with the wave number, and small-scale bubbles carry a larger mass flux of mixed material. These findings have important ramifications for modeling efforts in implosion physics, astrophysics, and combustion science.

Research objectives for 2018 include simulating: (1) a suite of two- and three-mode perturbations to address how ablation changes RTI evolution, and (2) a suite of broad-band turbulent mixing.

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

Principal Investigator: Gaute Hagen, Oak Ridge National Laboratory
Co-Investigators: Joseph Carlson, Los Alamos National Laboratory
Serdar Elhatisari, University of Bonn
Charles Horowitz, Indiana University
Gustav Jansen, Oak Ridge National Laboratory
Dean Lee, North Carolina State University
Alessandro Lovato, Argonne National Laboratory
Pieter Maris, Iowa State University
Hai Ah Nam, Los Alamos National Laboratory
Petr Navratil, TRIUMF
Steven Pieper, Argonne National Laboratory
Nicolas Schunck, Lawrence Livermore National Laboratory
James Vary, Iowa State University
Robert Wiringa, Argonne National Laboratory

Scientific Discipline: Physics: Nuclear Physics

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

Research Summary:
Atomic nuclei are strongly interacting, quantum many-body systems displaying fascinating properties: they exhibit emergent phenomena characteristic of large complex systems while at the same time being laboratories of most fundamental laws of nature. Using advanced applied mathematics, computer science, and physics, the project objective is to accurately describe the atomic nucleus in its entirety. To this end, the research team treats a wide range of nuclei, studying their electroweak transitions and reactions as these are important in both terrestrial experiments and astrophysical environments and will enable predictions for basic science and for applications in nuclear energy, nuclear security, and nuclear astrophysics.

Type: New
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: Renewal
Title: "On the Physics of Three-Dimensional Unsteady Flow over Low Pressure Turbines"

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

Scientific Discipline: Engineering: Aerodynamics

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

Research Summary: This INCITE project is using the high-order accurate open-source CFD solver PyFR to undertake compressible scale-resolving simulations of flow over a Low Pressure Turbine (LPT) cascade. Specifically, they are undertaking simulations of flow over the MTU-T161 LPT linear cascade with expanding end walls. Simulations from this project are of an unprecedented scale and resolution compared to previous studies. Moreover, MTU Aero Engines have made openly available, for the first time, a comprehensive set of experimental data for this test case, such that detailed comparisons can be made between computational and experimental results.

The team has demonstrated that PyFR can perform the required simulations in an acceptable resource envelope. Results from preliminary simulations indicate that analogous final production simulations, along with the work planned for year two, will have significant impact in three ways. Firstly, it will demonstrate the utility of high-order scale-resolving simulations as a predictive technology for LPT cascades, enabling industry to develop perspective on the impact of scale-resolving simulations for LPT design. Secondly, it will allow unprecedented insight into the 3D unsteady flow physics associated with LPT cascades, including the effect of end-walls. Thirdly, it will provide a unique dataset that can be used to develop improved turbulence models for relatively inexpensive Reynolds Averaged Navier-Stokes (RANS) simulations of LPT cascades. Taken together, the work will seed a step-change in LPT design capability; lowering overall cost and time-to-design by reducing reliance on expensive wind-tunnel testing, and improving overall performance by leveraging increased physical insight and more accurate RANS models. Such a step change is required, now, to help realize the ambitious green aviation objectives set out by the EU Clean Sky and NASA Environmentally Responsible Aviation projects.

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

Principal Investigator: Constantia Alexandrou, The Cyprus Institute and University of Cyprus
Co-Investigators: 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:
Protons are the most abundant particles of the visible matter in the Universe. This project studies through large scale simulations of the theory of strong interactions, Quantum Chromodynamics (QCD), fundamental properties of the proton such as its size and the momentum and spin distribution of its constituents, the quarks.

Parton distribution functions (PDFs) encode essential information about the distribution of momentum and spin of quarks and gluons inside hadrons. 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 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. They 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.

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: **89,230,769 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (45,000,000 processor hours)
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (9,230,769 processor hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (35,000,000 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 team will have a 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 Simulations for Layered Materials Genome"

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

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

INCITE Allocation: **200,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (200,000,000 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 Waals heterostructures composed of unlimited combinations of atomically thin layers. For 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 LMs.

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 team has already performed the largest-ever RMD and quantum molecular dynamics (QMD) simulations on Mira by fully exploiting the system's core architecture. For this project, they have designed simulation engines that will continue to scale on future computing platforms based on a common algorithmic framework called divide-conquer-recombine, significantly reducing computational cost in QMD and increasing accuracy in RMD simulations.

Results will provide predictive theory, directly validated by ultrafast 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 simulations and LCLS X-ray laser experiments will, for the first time, describe non-equilibrium dynamics in LMs at exactly the same spatiotemporal scales.

Type: Renewal
Title: "Petascale Simulations of Short Pulse Laser Interaction with Metals"

Principal Investigator: Leonid Zhigilei, University of Virginia
Co-Investigators: 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, like tuning the surface-wetting properties, fabrication of black or colored metals, and 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: Renewal
Title: " PICSSAR"

Principal Investigator: Jean-Luc Vay, Lawrence Berkeley National Laboratory
Co-Investigators: Henri Vincenti, Lawrence Berkeley National Laboratory

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation: **88,615,384 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (80,000,000 processor hours)
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (8,615,384 processor hours)

Research Summary:
The success of PetaWatt laser facilities that aim to control promising ultra-short particle (electrons, ions) and X-UV light sources from Ultra-High Intensity (UHI) laser-plasma mirror interactions, will rely on the strong coupling between experiments and large-scale simulations with particle-in-cell (PIC) codes. But standard PIC codes partly fail to accurately describe most UHI laser-plasma interaction regimes because the finite-difference time domain (FDTD) Maxwell solver is too inaccurate.

To address this challenge, researchers are using highly precise very high-order pseudo-spectral methods to solve Maxwell's equations. Despite their high accuracy, legacy pseudo-spectral methods employing global Fast Fourier Transforms (FFT) have hardly been used in large-scale 2D/3D simulations due to their inefficiency at scaling beyond tens of thousands of cores. To break this barrier, a pioneering grid decomposition technique was recently proposed for pseudo-spectral FFT-based electromagnetic solvers, which was first validated by extensive analytical work and then implemented in the PIC code Warp+PXR.

In accordance with the initial overarching project goal to design, optimize, and control the next generation of particle and light sources produced by UHI laser interactions on plasma mirrors, researchers will now use the potential of the new code to develop innovative schemes harnessing the full potential of plasma mirror sources in promising application experiments.

Type: Renewal
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: **140,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (100,000,000 processor hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (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.

This project supports DOE's Center for Predictive Simulation of Functional Materials, which focuses on the development, application, validation, and dissemination of parameter-free methods and open source codes to predict and explain the properties of functional materials for energy applications. Using the open source QMCPACK code, the researchers are demonstrating and validating new quantum Monte Carlo (QMC) methods and algorithms that will significantly improve on the state of the art. The team is performing calculations on 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, and advance efforts to identify new functionalities for energy-related technologies.

Type: Renewal
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: **126,000,000 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (30,000,000 processor hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (96,000,000 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's two-year earthquake system science research program seeks to 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 calculations called CyberShake.

Type: Renewal
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: Physical

INCITE Allocation: **75,000,000 processor hours**
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (75,000,000 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 and for chemical reactions in solution.

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

Principal Investigator: Brant Robertson, University of California, Santa Cruz
Co-Investigators: 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: "Galactic winds" are large-scale outflows of mass and momentum from galaxies, and are thought to originate from thermal pressure- or momentum-driven expansion of gas as a result of supernova explosions from the deaths of massive stars or other star formation-related feedback mechanisms. Almost all modern theories of galaxy formation invoke galactic winds to regulate the gas content of low-mass galaxies, keeping them faint and helping to reconcile the meager abundance of dwarf galaxies relative to the number of low-mass dark matter halos expected from cosmological simulations.

Understanding galactic winds through simulations is extraordinarily dicult as the hydrodynamics, radiative cooling, and other physics of the winds must be well-resolved (on ~ few parsec scales) everywhere in the flow that extends kiloparsecs above the galaxy before it merges with the circumgalactic medium. The linear dynamic range is therefore several up to ~ ten thousand, which nominally requires tens of billions of cells over the volume surrounding the galactic disk to simulate. Since the winds consist of a multiphase medium that includes hot and cold components outflowing at high velocities, capturing all relevant hydrodynamical processes in the wind is best addressed through enormous fixed-grid Eulerian simulation methods.

This INCITE project is specifically designed to test the physical mechanisms that launch galactic-scale outflows and shape their observed properties by leveraging the unique power of Titan and the cutting-edge technology of the team's GPU-native Cholla code to simulate winds in global simulations of isolated galaxies.

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

Johnson's 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 they 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.

Type: New
Title: "The Free Energy Landscapes Governing Membrane Protein Function"

Principal Investigator: Benoit Roux, University of Chicago
Co-Investigator: Chris Chipot, University of Illinois at Urbana-Champaign
Giacomo Fiorin, Temple University

Scientific Discipline: Biological Sciences: Biophysics

INCITE Allocation: **92,307,692 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (92,307,692 processor hours)

Research Summary:
Large membrane proteins involved in transport and cellular signaling are critical for life. The objective of this research is to elucidate the mechanism that underlies their function at the molecular level. This proposal is focused on three prototypical important membrane proteins: the ATP-driven sarcoplasmic endoplasmic reticulum calcium pump SERCA, the voltage-activated potassium channel, and the voltage-activated phosphatase CiVSP. A complete understanding of how these proteins carry out their function will rely heavily on characterizing conformational transitions. However, such conformational transition pathways, and their associated free energies, are challenging to determine directly from experiments due to their transient, short-lived states.

To determine functionally important conformational transition pathways and characterize the energetics associated with these structural changes, researchers will utilize the unifying concept of free energy landscape. Considerable progress has already been made in discovering the transition pathways of these systems using the string method simulations. However, a more complete understanding of their mechanism requires a quantitative characterization of the pathways and free energy landscapes that govern motions along them. This vision can be achieved by leveraging the information from classical molecular dynamics simulations of atomic-resolution models.

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

Type: New
Title: "Towards Predictive Exascale Wind Farm Simulations"

Principal Investigator: Michael Sprague, NREL
Co-Investigators: Shreyas Ananthan, NREL
Matt Barone, Sandia National Laboratories
Stefan Domino, Sandia National Laboratories
Simon Hammond, Sandia National Laboratories
Stephen Thomas, NREL

Scientific Discipline: Energy Technologies: Wind Energy

INCITE Allocation: **114,615,385 processor hours**
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (110,000,000 processor hours)
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (4,615,385 processor hours)

Research Summary:
Greater use of wind resources for electric power generation — reaching 30% of U.S. electrical supply — will have profound impacts: strengthening U.S. energy security through greater diversity in supply, providing cost-competitive electricity to key regions, reducing greenhouse-gas emissions, and reducing water used in thermo-electric power generation. However, a key challenge to wide-scale deployment of wind energy in the utility grid *without subsidies* is predicting and minimizing plant-level energy losses, which are currently estimated to be 20% in relatively flat areas and much higher in regions of complex terrain. Current simulation tools and methods for modeling wind plant performance fall far short because of insufficient model fidelity and inadequate treatment of key phenomena, combined with a lack of needed computational power necessary.

Objectives of this research are to advance both the development of a next-generation wind farm simulation capability and also the understanding of how this capability can be applied to important science questions challenging the wind energy community. The team has three large-scale simulation activities it deems as necessary steps on the path to exascale-class wind farm simulations: demonstrate time-to-solution improvements for atmospheric boundary layer simulations on a next-generation platform; demonstrate and evaluate improvements to linear-solver performance for large-aspect-ratio meshes; and perform "hero"-type simulations of a fully resolved wind turbine — expected to be the highest-fidelity turbine simulations to date.

Type: Renewal
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.

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. 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.

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. 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: Renewal
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: This project investigates the molecular mechanism of MHCII, an important peptide exchanger in the adaptive immune system responsible for the correct recognition of antigens, such as viruses or bacteria. 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 Discretion award on TITAN the team generated simulation data of ~300 μs. These results demonstrate the feasibility of the above aims and already reveal interesting yet preliminary biological insights. The team now proposes to explore conformational transitions of MHCII on timescales of tens of milliseconds.

As an integral component of a larger collaboration between world leading experts in computation, theory, and experiment, this project does not only have the potential to have a high impact on the field of immunology, but also to serve as a case study demonstrating the capabilities of unbiased enhanced molecular dynamics simulations.