Type: New
Title: "Ab-initio Nuclear Structure and Nuclear Reactions"

Principal Investigator: Gaute Hagen, Oak Ridge National Laboratory
Co-Investigators: Joseph Carlson, Los Alamos National Laboratory
Serdar Elhatisari, Helmholtz Institute for Radiation and Nuclear Physics
Stefano Gandolfi, Los Alamos National Laboratory
Gustav Jansen, Oak Ridge National Laboratory
Dean Lee, Michigan State University
Alessandro Lovato, Argonne National Laboratory
Pieter Maris, Iowa State University
Hai Ah Nam, Los Alamos National Laboratory
Petr Navratil, TRIUMF
Thomas Papenbrock, University of Tennessee
Saori Pastore, Los Alamos National Laboratory
Maria Piarulli, Washington University in St. Louis
Steven Pieper, Argonne National Laboratory
James Vary, Iowa State University
Robert Wiringa, Argonne National Laboratory

Scientific Discipline: Physics: Nuclear Physics

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (3,500,000 node-hours)
Cray XC40 (650,000 node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (3,500,000 node-hours)
IBM AC922 (364,000 node-hours)

Research Summary: Atomic nuclei are strongly interacting, quantum many-body systems that display fascinating properties. Building on previous INCITE research, this project focuses solely on *ab initio* approaches to nuclear structure and reactions that apply interactions from effective field theories and quantum chromodynamics. The researchers will use advanced quantum many-body methods to accurately describe and predict properties of the atomic nucleus from first principles, including their electroweak transitions and reactions important to both terrestrial experiments and astrophysical environments. The performed calculations will make predictions for and guide new experiments at major DOE facilities, explain observed phenomena, and potentially propel the discovery of new laws of nature.

Type: New
Title: "Advanced Computational Modeling of Molecular Machines in Gene Regulation"

Principal Investigator: Ivaylo Ivanov, Georgia State University
Co-Investigators:

Scientific Discipline: Biological Sciences: Biophysics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (220,000 node-hours)

Research Summary: Gene transcription, the first step of gene expression, is a complex and highly regulated process. While structural knowledge is beginning to emerge, little is understood about the molecular-level mechanisms of the process. At the same time, detailed mechanistic knowledge is essential to advance biomedical applications. Importantly, the biochemical pathways that orchestrate the expression and repair of genes are intricately intertwined.

This project will provide new insights into transcription initiation and the essential regulatory mechanisms controlling gene expression. Ivanov's team will take advantage of new cryo-electron microscopy data and combine it with advanced computational modeling on the Summit machine to elucidate the mechanisms of transcription pre-initiation complex assembly, promoter recognition, DNA melting, and the roles of general transcription factors therein.

Achieving these goals will require simulations of unprecedented size—more than 2 million atoms and hundreds of replicas—using advanced path optimization and sampling algorithms (e.g. the string method, ensemble MD simulations, metadynamics).

Improved understanding of gene transcription holds the promise of transformational advances not only in fundamental science but also in understanding human diseases and developing new therapeutic strategies.

Type: Renewal
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, Flatiron Institute

Scientific Discipline: Chemistry: Biochemistry

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (5,000,000 node-hours)
Cray XC40 (715,000 node-hours)

Research Summary: Researchers from the University of Washington's Baker lab have pioneered the prediction of protein structure and the design of new amino acid sequences that enable new proteins folds and functions. Past INCITE allocations have improved the accuracy and versatility of Rosetta, the software suite for modeling biomolecular structures that forms the core of the team's workflow, opening new frontiers in the rational design of macromolecular materials, catalysts, and therapeutics.

The researchers currently have three specific aims: (1) to improve the Rosetta software's energetic model, with a particular focus on enhancing the accuracy of their design algorithms; (2) to improve the design algorithms themselves, with applications to materials, catalysts, and therapeutics; and (3) to generalize their energy model and algorithms to permit the design of protein-like synthetic heteropolymers bearing capabilities far beyond those of natural proteins.

This INCITE project will allow for rapid cycles that validate improvements made to the team's method, as well as for applications to real-world problems in materials science and medicine. The impact will be the creation of larger molecules more specific to their targets than their smaller counterparts, ultimately yielding more potent drugs with fewer side effects.

Type: New
Title: "Advancing Electronic Stopping Simulation: From Solids to DNA"

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:
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (4,180,000 node-hours)
Cray XC40 (1,000,000 node-hours)

Research Summary: Electronic stopping describes the transfer of kinetic energy from highly energetic ions to electrons in matter. This process results in massive electronic excitations within the target material through interactions with the charged projectile's electric field. The researchers will use first-principles simulations to address a few outstanding challenges in modeling and theories of electronic stopping as well as to answer outstanding scientific questions in how DNA responds to ionizing radiations. Although significant progress has been made for modeling electronic stopping in solids, we as a community still lack understanding for how the electrons of projectile ions are involved in electronic stopping especially for heavy projectile ions. Building on our prior INCITE work, the new simulation method can be also used to model electronic stopping of large complex systems like DNA. In particular, a molecular-level understanding of electronic stopping process as it occurs in liquid water and solvated DNA under ion irradiation is developed in the context of ion beam cancer therapy.

The researchers will use this award (1) to further advance modeling of electronic stopping and to study hot-electron initiated ion dynamics for swift heavy ion projectiles in solids, and (2) to use their predictive framework to investigate the intricate details of electronic excitation dynamics of solvated DNA under ion radiation (as compared to electronic excitations under typical photon irradiation used for radiation oncology). Their highly scalable implementation of real-time time-dependent density functional theory code has been further optimized, putting the team in a good position to execute highly complex, massively parallel simulations.

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
Doreen Fan, Lawrence Berkeley National Laboratory
Brian Friesen, Lawrence Berkeley National Laboratory
Alice Harpole, University of Southampton
Adam Jacobs, Michigan State University
Max Katz, NVIDIA
Andy Nonaka, Lawrence Berkeley National Laboratory
Don Wilcox, Stony Brook University

Scientific Discipline: Physics: Astrophysics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (1,500,000 node-hours)
IBM AC922 (105,000 node-hours)

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

Maestro and Castro are 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 the Type Ia supernovae's progenitor—which has never been observed directly. The team will explore a wide variety of models to assess their feasibility, including the highest resolution white dwarf merger to date. The team's X-ray burst work will focus on the interplay between hydrodynamics and reactions, helping to uncover the nature of flame propagation within the neutron star's dense nuclear matter.

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

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

Scientific Discipline: Physics: Astrophysics

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (6,750,000 node-hours)

Research Summary: Magnetic reconnection and turbulence play significant roles in a wide variety of plasma environments, from tokamaks to Earth's magnetosphere to the solar corona and to distant astrophysical sources where they can power intense γ-ray flares. They are both fundamental plasma processes with important consequences, including the conversion of electromagnetic energy to particle kinetic energy. Besides heating the plasma, these processes can drive nonthermal particle acceleration (NTPA), resulting in a power-law particle energy distribution extending to very high energies.

Understanding these mechanisms in relativistic collisionless plasmas is especially important for high-energy astrophysical sources, where the existence of nonthermal particle populations is inferred from observations of nonthermal power-law radiation spectra. The acceleration mechanism, however, is a subject of continuing debate.

With this INCITE project, researchers are studying relativistic particle energization and resulting radiative signatures in reconnecting and turbulent plasmas, with the ultimate goal of determining the conditions and mechanisms operating in astrophysical sources. To conduct the research, the team is using its open-source, particle-in-cell (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. The massively parallel, 3D PIC simulations of reconnection and turbulence are allowing the team to examine the viability of these two promising mechanisms as potential efficient astrophysical accelerators of large numbers of particles to ultrarelativistic energies sufficient to explain observed radiation.

The combination of recent astronomical observations of high-energy radiation and the ability to demonstrate NTPA on DOE's leadership-class supercomputers, along with the broad relevance of reconnection and turbulence to fundamental plasma physics, make this investigation timely and scientifically urgent.

Type: New
Title: "Bringing NE Regulatory Workflow on a Path to Exascale: LES Validation for PANDA"

Principal Investigator: Aleksandr Obabko, Argonne National Laboratory
Co-Investigators: Christopher Boyd, US Nuclear Regulatory Commission
Paul Fischer, University of Illinois at Urbana-Champaign
Elia Merzari, Argonne National Laboratory
Ketan Mittal, University of Illinois at Urbana-Champaign
Ananias Tomboulides, Aristotle University of Thessaloniki
Yiqi Yu, Argonne National Laboratory

Scientific Discipline: Other: Nuclear Energy

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (17,700,000 node-hours)

Research Summary: Safer nuclear energy power promises to become a reliable, carbon-free resource capable of meeting our nation's and the world's energy needs. Numerical simulation has been an intrinsic part of nuclear engineering research, design, and licensing of existing and proposed conventional nuclear power plants. The nuclear modeling and simulation tools available today, however, are mostly low-dimensional and only valid for conditions close to the original experiments. In fact, many represent incremental improvements to decades-old legacy codes.

This project seeks to address these issues through the development, deployment, verification, and validation of higher-fidelity computational capabilities for analyzing, modeling, simulating, and predicting complex thermo-fluid phenomena. Doing so will help advance nuclear power capabilities by resolving technical, cost, safety, and licensing issues. Higher-fidelity, advanced thermal hydraulics codes will help simulate nuclear systems with well-defined and validated prediction capabilities. In particular, prediction of mixed convection flows and their associated uncertainties involves the accurate computation of thermal and species mixing governed by energy and mass mixed convection in a coolant flow over a complex geometry of next-generation nuclear reactors.

The researchers will work closely with the Nuclear Regulatory Commission on high-performance computing applications of Nek5000 large-eddy simulations for PANDA benchmark and experiment modifications so as to advance state-of-the-art modeling and improve the safety of scalable carbon-free energy options.

Type: New
Title: "Closing, Evaluating, and Validating Multiphase Flow Models in Porous Medium Systems"

Principal Investigator: Cass Miller, University of North Carolina
Co-Investigators: William Gray, University of North Carolina
Jan Prins, University of North Carolina

Scientific Discipline: Engineering: Fluids and Turbulence

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (620,000 node-hours)
IBM AC922 (61,000 node-hours)

Research Summary: Multiphase porous medium systems arise routinely in natural and engineered systems and span applications in the geosciences, process engineering, and the biomedical field. These systems share many common scientific traits, including the existence of interfaces between phases and common curves that form where three phases meet.

Traditional models for understanding these systems, however, suffer from a lack of connection to the microscale, where the physics are better understood, than at the macroscale, where the models are formulated and solved.

Miller's team seeks to bridge these two scales by using leadership-class computing to develop a new generation of multiphase flow models for porous medium systems. The team's theory, known as the thermodynamically constrained averaging theory (TCAT), is consistent across length scales, constrained by the second law of thermodynamics, and hysteretic free. To complete the theory and render the work suitable for application, closure relations must be developed in a specific form, evaluated, and validated. This work will pair computing with experimental approaches, to complete and validate a two-fluid flow TCAT model.

Simulations will be performed using a highly efficient and scalable lattice-Boltzmann simulator. The lattice-Boltzmann simulator has recently been extended to three-fluid phases, another focus of the project. Three-fluid systems arise, for example, in contaminant remediation, petroleum and gas recovery, and carbon sequestration.

Type: New
Title: "Computational Studies of Correlated Quantum Materials"

Principal Investigator: Thomas Maier, Oak Ridge National Laboratory
Co-Investigators: Gonzalo Alvarez, Oak Ridge National Laboratory
Ed D'Azevedo, Oak Ridge National Laboratory
Steven Johnston, University of Tennessee, Knoxville
Satoshi Okamoto, Oak Ridge National Laboratory
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:
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (1,200,000 node-hours)
IBM AC922 (900,000 node-hours)

Research Summary: Correlated quantum materials are key components to developing new technologies but require optimization to reach their full potential. Leveraging state-of-the-art numerical algorithms on leadership-class supercomputers, Maier's team will provide important new insights into the mechanisms leading to the complex phases and physical behavior observed in unconventional superconductors and quantum spin liquids.

The importance of applying a complementary set of advanced algorithms and the use of high-end computing is related to the remarkable myriad of nearly degenerate quantum states in correlated systems and the limitations of the individual approaches. Only the combined application of different and complementary techniques, in conjunction with large-scale, high-performance computing, will permit a complete, conclusive, and reliable picture of the physics of these systems.

On a broader level, this capability is necessary to allow DOE and the scientific community to lay the foundation for revolutionary new advances in energy-related technologies by solving long-standing problems in quantum condensed matter physics.

Type: Renewal
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 Universität Darmstadt
Luis Zepeda-Ruiz, Lawrence Livermore National Laboratory

Scientific Discipline: Engineering: Material Response

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (17,000,000 node-hours)

Research Summary: With this INCITE project, researchers are using 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.

At present, *in situ* microscopy observations are possible only in thin electron-transparent films — where neither strain hardening nor dislocation patterns are observed. MD simulations are currently 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 had 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 team's approach combines very large MD simulations and detailed on-the-fly and post-processing analyses and characterizations of underlying events in the life of atoms and dislocations that, taken together, define crystal plasticity response. Their cross-scale simulations are simultaneously large enough to be representative of a macroscopic crystal plasticity and yet fully detailed tracing every "jiggle" of atomic motion. Ultimately, the team's computations will provide definitive data on the origin of staged strain hardening and on the nature of dislocation patterns, while also increasing the understanding of material strength and other technologically relevant mechanical properties.

Type: New
Title: "Decoding an 80-year-old Inverse Problem with Distributed Deep Learning"

Principal Investigator: Nouamane Laanait, Oak Ridge National Laboratory
Co-Investigators: Albina Borisevich, Oak Ridge National Laboratory
Alexander Sergeev, Uber Technologies
Sean Treichler, NVIDIA
Junqi Yin, Oak Ridge National Laboratory

Scientific Discipline: Other: Data science

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (350,000 node-hours)

Research Summary: Future technological advances in computing and energy depend critically on our ability to determine the local atomic structure of materials. Currently, scientists quantitatively access a material's local structure at length scales of 10^{-3} meters with X-ray and neutron diffraction, instead of the 10^{-10} meters of spatial resolution needed for continuing advances in materials science.

Standing in the way of routine access to materials' local properties with atomic resolution is the oldest and arguably the most challenging inverse problem in physics. Namely, reconstructing the 3D atomic configurations of a material by inverting electron diffraction patterns from picometer-size samples acquired with modern scanning transmission electron microscopes.

Laanait's team will train a deep learning algorithm to decode the material information present in electron pico-diffraction patterns and use it to create a universal approach to decoding local structural properties of materials. The project will draw from one of the largest scientific databases ever employed for deep learning at scale.

Type: New
Title: "DNS of Turbulent Combustion Towards Efficient Engines with In Situ Analytics"

Principal Investigator: Jacqueline Chen, Sandia National Laboratories
Co-Investigators: Alex Aiken, Stanford University
Giulio Borghesi, Sandia National Laboratories
Tarek Echekki, North Carolina State University
Aditya Konduri, Sandia National Laboratories
Martin Rieth, Sandia National Laboratories
Ramanan Sankaran, Oak Ridge National Laboratory
Elliott Slaughter, SLAC National Accelerator Laboratory

Scientific Discipline: Chemistry: Combustion

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (641,000 node-hours)

Research Summary: Engines for future industrial power and heat generation, ground transport of freight, and civilian and military aero-transport are pushing the boundaries of technology to obtain greater efficiency, reduced emissions, reduced signatures, and increased reliability. Specifically, at limiting ignition, flame propagation, and flame stabilization conditions, the stability of combustion is governed by strong 'turbulence-chemistry' interactions spanning a wide range of aero-thermo-chemical conditions and coupled with multi-phase spray physics.

Direct numerical simulation (DNS) at relevant conditions coupled with novel in situ data science methods can be used to better understand the underlying turbulence-chemistry interactions that govern spray diesel combustion and fuel chemistry effects on highly turbulent premixed flame propagation. The new physical insights gleaned from DNS will be used to develop predictive models for the design of efficient, clean and flexible engines for power generation, ground transportation, and for airplanes and air-breathing hypersonic propulsion.

Type: New
Title: "DNS Reference Data for Turbulence Model Development on the Bachalo-Johnson ATB"

Principal Investigator: Koen Hillewaert, Cenaero
Co-Investigators: Matthias Ihme, Stanford University

Scientific Discipline: Engineering: Aerodynamics

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (7,875,000 node-hours)

Research Summary: Today, the design and optimization of most internal and external flows rely on low-fidelity, statistically averaged turbulence models, commonly known as RANS. RANS are the most accurate approach currently affordable to industry. The limited availability of high-quality reference data on complex flows hinders improvement of RANS, or further turbulence model development.

To generate an exhaustive database that can be used for not only the validation of turbulence models, but also for their development and calibration, this project undertakes direct numerical simulations of the Bachalo-Johnson axisymmetric transonic bump at a Reynolds number of 1 million. This test case has been extensively used to validate turbulence models in the presence of shock-boundary layer interaction and shock-induced separation. The modeling of these phenomena is critical for aeronautical and aircraft engine companies.

An extensive DNS dataset, capable of reconstructing all RANS turbulence modeling terms, will be cross-validated using two codes of very different nature, and an extensive span-dependence study will be performed up to the full circumference.

Type: New
Title: "Dynamic Nanocluster Catalysis"

Principal Investigator: Anastassia Alexandrova, UCLA
Co-Investigators: Philippe Sautet, UCLA

Scientific Discipline: Chemistry: Catalytic

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

Research Summary: Today, heterogeneous catalysis is used in more than 90 percent of all chemical manufacturing processes. Catalytic materials enable selective formation of desired products at rates that are commercially viable. Catalysis is not only important for the production of chemicals, materials, and food, but also essential for pollution control, medical applications, and the development of sustainable energy solutions. Therefore, research on catalysis is a continuing developing area, which involves different sciences, such as chemistry, surface science, and materials science.

Small clusters of noble metals secured on supporting surfaces can be remarkable catalysts, with properties tunable through their size, nature of the support, and reaction conditions. The opportunities to improve the design of such catalysts are therefore vast. This INCITE project will use computation to understand and design the most powerful, selective, stable, and yet economical catalysts based on surface-mounted small clusters of transition metals. The exploration of such catalytic interfaces, which are incredibly complex and best represented as ensembles of many geometric states, requires the power and scale of DOE leadership-class supercomputers.

The research team will pursue the development and consolidation of protocols and efficient methods to enable the computational description of surface-mounted cluster catalysts in a statistical ensemble representation in realistic conditions. All the properties of cluster catalysts (e.g., reaction rates, stabilities, spectral signatures) will then be ensemble-averages, which can be used to explain existing experiments, or predict outcomes of new experiments.

Once the protocols and models are developed, the researchers will computationally manipulate the catalyst systems by varying temperature, partial pressures of gases, and cluster size to achieve the exposure of the most active binding sites and desired catalytic efficiency. The work will be done using ab initio methods and density functional theory (DFT) with and without periodic boundary conditions, as well as the team's in-house methods for modeling materials in conditions relevant to their practical use, in conjunction with chemical bonding analysis tools. The team's results will be used to inform experimental efforts to improve the performance of catalysts.

Type: New
Title: "Enabling Human Exploration of the Red Planet"

Principal Investigator: Eric Nielsen, NASA
Co-Investigators: Ashley Korzun, NASA

Scientific Discipline: Engineering: Aerodynamics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (181,000 node-hours)

Research Summary: Recent work at NASA has focused on development of technologies that enable delivery of significantly larger payloads to the surface of Mars. The goal of this project is to assist in advancing the understanding of the underlying flow physics associated with novel approaches to aerodynamic and propulsive deceleration for atmospheric entry on Mars.

Nielsen's team will apply advanced computing to create high-fidelity simulation of retropropulsion aerodynamics, which is necessary for human space exploration, at flight-relevant scale. Currently, investigations of retropropulsion aerodynamics in ground testing require substantial compromises on physical scale, instrumentation and data products, configuration, and environments. The problem is further complicated by the very low pressure, density, and carbon dioxide-dominate composition of the Martian atmosphere. The inability to fully simulate relevant physics through ground testing requires a strong reliance on high-fidelity computational analyses to identify and evolve the knowledge basis for retropropulsion aerodynamics. Simulating the interactions between the atmosphere and the retropropulsion exhaust plumes at sufficient spatial resolution requires leadership-class computational capabilities.

The proposed research will yield data that is unachievable with other resources, identifying the limits of dependence on spatial resolution and applicability of detached eddy simulation methods for the problem of retropropulsion in atmospheric environments and increasing understanding of how interactions between the Martian atmosphere and retrorocket exhaust plumes affect the ability to control and guide the vehicle to a safe landing.

Type: New
Title: "Enabling the Design of Drugs That Achieve Good Effects Without Bad Ones"

Principal Investigator: Ron Dror, Stanford University
Co-Investigators:

Scientific Discipline: Biological Sciences: Biophysics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (4,540,000 node-hours)
IBM AC922 (400,000 node-hours)

Research Summary: One-third of all existing drugs target G protein–coupled receptors (GPCRs), but designing effective, safe drugs for these receptors remains challenging. A major current effort in drug discovery involves a search for "functionally selective" ligands that promote signaling of a given GPCR through desired pathways while avoiding signaling through undesirable pathways responsible for dangerous side effects.

Using massively parallel simulations on Titan and Summit, Dror's team will explore how drug receptors select which signaling proteins to activate. Additionally, the work will shed light on how a GPCR affects the structure and motion of various signaling proteins, including arrestins, and how drug-induced changes in GPCR conformation and phosphorylation state can alter these effects.

The simulations will run on GPUs, using the AMBER code, which has been optimized to achieve very high single-node efficiency. Our simulations will utilize recently developed multidimensional replica exchange methods, which achieve excellent scaling across large numbers of nodes and high sampling efficiency.

The results will enable the development of finely tuned medicines that elicit more desired effects with fewer side effects, providing a foundation for the design of safer and more effective treatments for a wide variety of diseases.

Type: New
Title: "Energy Exascale Earth System Model"

Principal Investigator: Mark Taylor, Sandia National Laboratories
Co-Investigators: David Bader, Lawrence Livermore National Laboratory
Peter Caldwell, Lawrence Berkeley National Laboratory
Jean-Christophe Golaz, Lawrence Livermore National Laboratory
Walter Hannah, Lawrence Livermore National Laboratory
Christopher Jones, Pacific Northwest National Laboratory
Noel Keen, Lawrence Berkeley National Laboratory
Ruby Leung, Pacific Northwest National Laboratory
Wuyin Lin, Brookhaven National Laboratory
Matthew Norman, Oak Ridge National Laboratory
Mark Petersen, Los Alamos National Laboratory
Stephen Price, Los Alamos National Laboratory

Scientific Discipline: Earth Science: Climate Research

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (2,354,000 node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (700,000 node-hours)

Research Summary: This INCITE project supports the Energy Exascale Earth System Model (E3SM) model, a multi-laboratory project developing a leading-edge climate and Earth system and driven by three grand challenge questions, two of which are the focus of this project as they can be answered using the E3SM 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? (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), the team aims to examine 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 global simulation to include dynamic ice shelf-ocean interactions.

Type: Renewal
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:
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (9,375,000 node-hours)
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (281,000 node-hours)

Research Summary: Core-collapse supernovae (CCSNe) are the most extreme laboratories for nuclear physics in the universe. Stellar core collapse and the violent explosions that follow give birth to neutron stars and black holes, and in the process synthesize most of the elements heavier than helium throughout the universe. Despite the key role CCSNe play in astrophysics, the physical mechanism that causes these explosions is still not fully understood.

This multi-year INCITE project is using DOE leadership computing resources to perform extreme-scale simulations aimed at transforming our understanding of supernovae. The team's comprehensive, end-to-end investigation involves carrying out 3D magnetohydrodynamics 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. This research will also enable an intensive comparison to observations through the calculation of gravitational wave emission, detailed nucleosynthesis, and electromagnetic radiative transfer.

In addition, the team is developing and employing 3D massive stellar progenitor models at the point of core-collapse to address whether rotation and magnetic fields aid successful explosions for "normal" CCSNe, and to explore the impact of realistic initial conditions on nucleosynthesis in CCSNe. The team's findings will inform our understanding of the characteristics of newborn pulsars and magnetars — information that can be directly compared to observational data.

Ultimately, this project will help researchers address whether plausible rotation rates and magnetic field strengths influence the CCSNe mechanism and determine the impact that realistic 3D progenitor structures have on the CCSNe mechanism and observables.

Type: New
Title: "Extreme-Scale Simulations for Advanced Seismic Ground Motion and Hazard Modeling"

Principal Investigator: Christine Goulet, University of Southern California
Co-Investigators: Yifeng Cui, San Diego Supercomputer Center
Philip Maechling, University of Southern California
Kim Olsen, San Diego State University
Doriam Restrepo, Universidad EAFIT
John Vidale, University of Southern California

Scientific Discipline: Earth Science: Geological Sciences

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (1,620,000 node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (134,000 node-hours)

Research Summary: Accurate seismic hazard assessment helps inform and prepare society for earthquakes, enabling the development of design and mitigation strategies that save lives in the event of a major earthquake. The advancement of earthquake modeling and simulations is critical to reducing uncertainties and improving the accuracy of seismic hazard assessments.

With this INCITE project, researchers from the Southern California Earthquake Center (SCEC) will enhance their earthquake simulation and hazard mapping tools to provide the best possible information in terms of earthquake ground motion and seismic hazard assessment. Specifically, they plan to extend their software ecosystem, including CyberShake, to the next level of fidelity by advancing its capabilities to resolve shaking estimates and related uncertainties across a broadband range of frequencies of engineering interest (i.e., 0–20 Hz).

To enable the computation of broadband seismic hazard maps, the team will improve their computational codes' ability to accurately simulate high-frequency shaking. This effort requires the integration of new and improved simulation elements to model topography, realistic material inelasticities, and the stochastic representation of the heterogeneous portions of the Earth's crustal structure. It will also require the development of new processing workflows to address the added complexity. Furthermore, the team will gradually expand the geographical extent of their model to cover a larger portion of the U.S. West Coast. The larger simulation domains, higher resolution grids, and new physics models implemented in their codes will pose new challenges that can only be addressed with DOE's leadership-scale computing resources.

The modeling enhancements in the SCEC software ecosystem will increase the accuracy of simulations, reduce scientific uncertainties, and broaden the usefulness of these software tools in engineering applications.

Type: Renewal
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:
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (1,000,000 node-hours)
IBM AC922 (30,000 node-hours)

Research Summary: As the transistor size in microelectronics keeps shrinking in accordance with Moore's law, heat generation from the on-die interconnect has become a major issue that threatens to impede further downscaling of electronic devices.

Currently, continuum diffusion models with heavy parameterization are used to study this problem. However, as the nanocontact becomes a few nanometers wide, it is clear the continuum model is no longer adequate. In this INCITE project, the team will build on its past work applying 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.

To date, Wang's team has fully established the procedure to calculate the quantum transport for a system with thousands of atoms. This involves four distinct steps: the construction of the atomic structure for the interconnect; the LS3DF calculation of the system charge density and potential; the linear equation solution of the system states at a given energy; and the linear combination of the system states to construct the scattering states which satisfy the boundary condition at the electrodes.

Through new large-scale, high-fidelity simulations, the team is poised to address the following fundamental questions: (1) At what size limit will the classical approach based on Matthiessen's rule no longer be valid? (2) How large is the wave function interference effect? How sensitive does the resistivity depend on the shape of interconnect? (3) What are the effects of defect, amorphous, and surface scattering? (4) To build a better small-size interconnect, what is more important: the bulk resistivity or density of state at the Fermi energy? (5) Where is the heat generated within the interconnect at the atomic level?

Type: Renewal
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:
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (3,000,000 node-hours)
IBM AC922 (200,000 node-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: Renewal
Title: "FDTD Simulations to Facilitate Early-Stage Human Cancer Detection"

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

Scientific Discipline: Biological Sciences: Medical Science

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (5,000,000 node-hours)

Research Summary: The ultimate goal of this research is to develop a low-cost, high-throughput optical microscopic technique that can sense macromolecular alterations and thereby predict human cancer risk at a very early stage. The team has developed a novel optical microscopy technique, Partial Wave Spectroscopic (PWS) microscopy, which has been shown to be capable of detecting static intracellular nanoarchitectural alterations associated with early-stage cancers that are not accessible by conventional microscopy. Thus far, they have employed PWS to successfully quantify cancer risks across seven different organs (lung, colon, pancreas, esophagus, prostate, ovary, and thyroid) in approximately 800 human patients.

Importantly, in addition to static nanoarchitectural changes, abnormal movement of macromolecular complexes within cells is another signature of pathological changes, including early-stage cancer development. However, the team's current PWS technique can only provide information about a cell's nanostructures in its static form.

With this INCITE project, the team is using computational modeling to build upon static PWS to develop a new technique, dynamic PWS, which can sense and quantify macromolecular motions in live cells. By combining static and dynamic PWS, the researchers aim to improve the sensitivity and specificity of PWS detection of early-stage cancers. Furthermore, this will provide insights into the macromolecular behavior within live cells, thereby potentially assisting in the development of novel cancer therapeutics that regulate chromatin structure and dynamics.

The team's primary computational tool, Angora, is literally "a microscope in a computer." Its physics kernel implements the three-dimensional finite-difference time-domain (FDTD) solution of Maxwell's equations on nanometer voxels within the simulated biological cell. This is followed by rigorous integral transformations to synthesize full-color pixels at the image plane of the simulated microscope located centimeters away. Optimized for parallel processing on Argonne's Mira supercomputer, Angora is capable of solving for more than one trillion vector electromagnetic field components. High-fidelity modeling of dynamic PWS requires the scale and power of DOE leadership computing resources.

Type: Renewal
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:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (700,000 node-hours)

Research Summary: This multiyear project addresses the long-standing challenge of imaging Earth's interior based on full waveform inversion on a global scale, which has so far remained a challenge mainly due to computational limitations. To date, the team has gathered data for more than 4,200 earthquakes and is working on their source inversions.

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.

For the requested allocation Summit, Tromp's team plans to use all available data for earthquakes with magnitudes ≥5:5; use entire 180 min three-component seismograms, capturing one surface-wave orbit; use data with a shortest period of ~ 9 s, with the long-term goal of eventually reaching ~ 1 s; use a more complete physical parameterization, addressing transverse isotropy with a random symmetry axis, anelasticity, topography on internal boundaries such as the core-mantle boundary, and finite-source effects; facilitate uncertainty quantification; take advantage of machine learning, artificial intelligence, and deep learning algorithms to extract maximal information from seismic data; interpret results using data mining, feature extraction and visualization; and use workflow stabilization and management to automate the workflow.

Type: Renewal
Title: "High-Fidelity Gyrokinetic Simulation of Tokamak and ITER Edge Physics"

Principal Investigator: Choong-Seock Chang, Princeton Plasma Physics Laboratory
Co-Investigators: Stephen Abbot, NVIDIA
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 Ku, Princeton Plasma Physics Laboratory
Scott Parker, University of Colorado
Mark Shephard, Rensselaer Polytechnic Institute

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation:

Site:	Argonne National Laboratory
Machine (Allocation):	Cray XC40 (1,500,000 node-hours)
Site:	Oak Ridge National Laboratory
Machine (Allocation):	Cray XK7 (3,500,000 node-hours)
Site:	Oak Ridge National Laboratory
Machine (Allocation):	IBM AC922 (1,050,000 node-hours)

Research Summary: This multi-year INCITE project seeks to advance the understanding of the edge plasma physics in fusion reactors, with a focus on ITER, an international collaboration to design, construct, and assemble a burning plasma experiment that can demonstrate the scientific and technological feasibility of fusion.

The team is applying its 5D gyrokinetic particle code, XGC1, on DOE leadership computing resources to address some of the most difficult plasma physics questions facing ITER. In particular, they are performing studies on two high-priority challenges: (1) the peak heat-flux density on the ITER divertor target plates in the high-confinement mode (H-mode) operation with a tenfold energy gain, and (2) the achievability of the H-mode plasma condition (i.e., achieving the low-to-high mode L-H transition at edge) that can initiate the tenfold energy gain process. These large-scale studies are time-urgent for the successful planning of ITER operation and require an intensive, concentrated computing effort using extreme-scale supercomputers.

Type: New
Title: "High-Resolution Climate Sensitivity and Prediction Simulations with the CESM"

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

Scientific Discipline: Earth Science: Climate Research

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (13,250,000 node-hours)

Research Summary: The focus of current research conducted by the Climate Change Prediction group at the National Center for Atmospheric Research (NCAR) is encapsulated in the Cooperative Agreement To Analyze variabiLity, change, and predictabilitY in the earth SysTem (CATALYST) effort. CATALYST represents a sustained commitment to perform foundational research that advances a robust understanding of modes of variability and change using models, observations, and process studies.

For 2019, the team has designed a set of three simulation subprojects to assess parametric and structural uncertainty in earth system models, and to provide efficient guidance for future projects focused on longer timescale predictability.

The first employs the Cloud-Associated Parametrizations Testbed (CAPT), a framework that provides a computationally efficient method to identify parametrization errors in earth system simulations, so as to investigate error growth in the coupled system. The second investigates the robustness of the Labrador Sea coupled climate in CESM1.3 with respect to important factors like resolution, initialization, and parameter settings. It is motivated by the very tight interactions suspected to exist between multiple components (including atmosphere, ocean, sea-ice, and the Greenland ice sheet) of the earth system in the North Atlantic climate. The third studies in detail the sensitivity of the Atlantic Meridional Overturning Circulation to climate model resolution by examining the result of freshwater forcing into the subpolar North Atlantic.

These simulations will advance our understanding of externally forced changes in the earth system over multiple temporal and spatial scales, and of predictability and variability themselves.

Type: New
Title: "High Resolution Study of Intermittency in Turbulence and Turbulent Mixing"

Principal Investigator: Pui Kuen Yeung, Georgia Tech
Co-Investigators: Toshiyuiki Gotoh, Nagoya Institute of Technology
Katepalli Sreenivasan, New York University

Scientific Discipline: Engineering: Fluids and Turbulence

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (1,000,000 node-hours)

Research Summary: Capability resources on Summit will be applied to large-scale simulations of turbulence and turbulent mixing in two closely-related areas where higher resolution is needed. Both problems will be addressed using numerical simulations of unprecedented size and a new simulation code equipped with fine-grained asynchronism that takes maximum advantage of Summit's architecture.

The first science focus of this project is the study of intermittency and extreme events, with small-scale resolution in both space and time meeting or slightly exceeding the stringent standards suggested by recent work which used up to $8,192^3$ grid points. The proposed simulations at the scale of $18,432^3$ (5.8 trillion) and the Reynolds number will be high enough to provide further testing for some recently proposed scaling relations. In particular, the proposed simulations will address the scaling of extreme events in dissipation and enstrophy, the scaling exponents of local averages with a central role in intermittency theory, as well as the distinctive effects of intense straining and rotation on the local structure of many flow properties in small-scale turbulence relevant to a variety of flow geometries.

The second science focus is to extend the study of intermittency and extreme events to the turbulent mixing of passive scalar quantities in the moderately diffusive regime, which is applicable to fluctuations of species concentration and temperature in many reacting flow systems. A strong emphasis is again placed on high resolution, using $9,216^3$ grid points at a spatial resolution 4.5 times higher than previous work under similar conditions. The proposed simulation will provide detailed information on fluctuations of scalar dissipation rate, which could not be resolved adequately in previous work. The new data will provide a new and much-needed test concerning whether prior observations of departures of the scalar field from the classical theory of local isotropy may have been contaminated by the effects of resolution.

Type: New
Title: "Hot-dense Lattice QCD for RHIC and LHC"

Principal Investigator: Swagato Mukherjee, Brookhaven National Laboratory
Co-Investigators: Alexei Bazavov, Michigan State University
Olaf Kaczmarek, Bielefeld University, Germany
Frithjof Karsch, Brookhaven National Laboratory
Rasmus Larsen, Brookhaven National Laboratory
Peter Petreczky, Brookhaven National Laboratory
Patrick Steinbrecher, Brookhaven National Laboratory
Christian Schmidt, Bielefeld University, Germany

Scientific Discipline: Physics: Nuclear Physics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (900,000 node-hours)

Research Summary: The upcoming Beam Energy Scan program (BES-II) of the Relativistic Heavy-Ion Collider (RHIC) experiment at Brookhaven National Laboratory will search for the quantum chromodynamics (QCD) critical point, a landmark where ordinary hadronic-matter and quark-gluon plasma become indistinguishable. Starting from the fundamental theory of quarks and gluons, Mukherjee's team will provide more stringent constraints on the location of the QCD critical point in the phase-diagram of the strong-interaction matter; thereby, guiding the experimental search.

The non-Gaussian cumulants of conserved charge fluctuations are computed starting from the fundamental theory of strong interaction— QCD— using large-scale numerical calculations of the lattice-regularized version of the theory. Using state-of-the-art lattice QCD calculations, the team will provide the QCD-based results for the non-Gaussian cumulants of conserved charge fluctuations, which can directly be confronted with experimental findings in ultra-relativistic heavy-ion experiments at RHIC and the Large Hadron Collider in Switzerland. Furthermore, QCD-based calculations of these cumulants will enable determination of phase-structure and bulk thermodynamic properties of hot-dense QCD matter and provide the QCD-inputs needed to decipher data from BES-II.

These computations will be carried out on the Summit supercomputer at the Oak Ridge National Laboratory, using the team's highly-optimized heterogeneous software.

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

Principal Investigator: Rommie Amaro, University of California, San Diego
Co-Investigators:

Scientific Discipline: Biological Sciences: Biophysics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (800,000 node-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: Renewal
Title: "INtegrated and Scalable PredictIon of REsistance (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:
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (3,100,000 node-hours)

Research Summary: Cancer is the second leading cause of death in the United States, accounting for nearly 25 percent of all deaths. Targeted kinase inhibitors play an increasingly prominent role in the treatment of cancer and account for a significant fraction of the $37 billion U.S. market for oncology drugs in the last decade.

Unfortunately, the development of resistance limits the benefits patients can derive from their treatment. Resistance to therapeutics is responsible for more than 90 percent of deaths in patients with metastatic cancer. Mutations in the therapeutic target drive drug resistance in many patients; in some commonly targeted kinases such as Abl, missense mutations are the mechanism of resistance in as many as 90 percent of cases.

This project aims to lay the foundations for the use of molecular simulation and machine learning to guide precision cancer therapy, in which therapy is tailored to provide maximum benefit to individual patients based on the genetic information about their particular cancer. It is vital that such an approach is based on predictive methods as the vast majority of clinically observed mutations are rare, essentially ensuring that catalog-building alone will be insufficient for making therapeutic decisions.

While the team's central objective is to quantify the potential for a compound to elicit resistance and to predict potential resistance conferring mutations which have not yet arisen, the knowledge gained can also be used to design better small-molecule inhibitors as second- and third-line targeted therapies

Type: New
Title: "Integrated Simulation of Energetic Particles in Burning Plasmas"

Principal Investigator: Zhihong Lin, University of California, Irvine
Co-Investigators:

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (740,000 node-hours)

Research Summary: Energetic Particle (EP) confinement is a critical issue for the international ITER nuclear fusion reactor experiment – the crucial next step in the quest for clean and abundant energy—since ignition relies on self-heating by energetic fusion products. Due to the strong coupling of EP with burning thermal plasmas, plasma confinement property in the ignition regime is one of the most uncertain factors when extrapolating from existing fusion devices to the ITER tokamak.

To develop a predictive capability for the EP confinement, a SciDAC ISEP (Integrated Simulation of Energetic Particles) Center led by Lin aims to improve understanding of EP transport and EP coupling with thermal plasmas through integrated simulation using the multi-physics code GTC. The team will focus on two areas:

1. *EP transport due to mesoscale turbulence driven by EP pressure gradients*: Performing long-time simulation to determine EP profiles consistent with the EP turbulence, and to characterize the intermittency and transient EP heat load on the wall and divertor.

2. *EP coupling with microturbulence and macroscopic magnetohydrodynamic (MHD) modes driven by thermal plasmas*: Performing multi-physics simulations to study the effects of microturbulence and MHD modes on EP confinement, and in turn, the effects of EP on microturbulence and MHD modes.

The verification and validation of results will address all levels in the hierarchy of EP physics from fundamental to reduced constituents in the EP module. GTC simulations will be compared with gyrokinetic continuum code GYRO and MHD hybrid code FAR3D for verification. Full physics simulations will be compared to experimental measurements including eigenmode properties, instability threshold, spectral intensity, density and temperature fluctuations, and energetic particle transport in real and velocity space.

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

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

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (750,000 node-hours)

Research Summary: TAE Technologies' ultimate goal is to develop the world's first commercializable fusion-powered generator for carbon-free baseline electricity production. To this end, TAE has a large and active experimental, theoretical, and computational fusion plasma research program centered around the field-reversed configuration (FRC) magnetic topology. The main goals of the company's FRC research program are to study the confinement of energy at high electron temperatures in its C-2W experiment, and to master the plasma control methods that will be needed to increase the plasma temperature to commercializable fusion conditions in a future device.

The current INCITE allocation enables two strategic computing initiatives that directly support TAE's research program: (1) the development of the ANC kinetic micro-turbulence code to understand energy confinement in FRC plasmas, and (2) the development of the FPIC kinetic macro-stability code to model the global stability of FRC plasmas and to study plasma control methods that could be deployed on C-2W and future devices. These two initiatives are the most computationally demanding components of TAE's overarching strategic computing goal to develop a Whole Device Model (WDM) of FRC plasmas. The WDM is a hierarchy of models covering multiple time and space scales that will eventually allow TAE researchers to perform high-fidelity predictive simulations of FRC fusion experiments.

After making a number of physics model advances and numerical algorithm improvements in the first year of the INCITE allocation, the research team will continue their efforts to advance the scientific progress of the C-2W experimental program via simulation of both macroscopic plasma stability and micro-turbulent particle and energy transport. This includes using the FPIC and ANC codes to explore new experimental parameter regimes, to accelerate the optimization of experimental operating scenarios, and to predict stable and efficient operating points for future FRC reactor design concepts.

Type: New
Title: "Laminar-Turbulent Transition in Swept-Wing Boundary Layers"

Principal Investigator: Lian Duan, Missouri University of Science and Technology
Co-Investigators: Meelan Choudhari, NASA Langley
Fei Li, NASA Langley

Scientific Discipline: Engineering: Aerodynamics

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (6,000,000 node-hours)

Research Summary: Skin-friction drag accounts for approximately one half of the total drag for long-haul transport aircraft. Due to the substantial increase in drag in the course of laminar-turbulent transition, delay of crossflow-influenced transition in swept-wing boundary layers via laminar flow technology is a leading contender for reducing the aircraft fuel burn.

This project harnesses the computational power of Mira to enable petascale direct numerical simulations of the entire crossflow transition process—from the laminar regime through transition to the fully turbulent regime—over a transonic natural-laminar-flow wing at high chord Reynolds numbers relevant to the transport aircraft. In particular, the work will focus on generating a detailed knowledge base that will address the existing gaps in crossflow transition prediction, including (1) the excitation and control of crossflow instabilities via discrete roughness elements (DREs), and (2) the laminar breakdown of crossflow vortices preceding the onset of turbulent flow and the properties of developed turbulence in the post-transitional region.

This project will significantly advance our ability to predict and control laminar-turbulent transition in three-dimensional boundary layers. It will also help delineate the limitations of the current prediction tools, providing a basis to develop alternate models for cases in which those tools are either inapplicable or lead to unacceptable predictive errors. Beyond aerospace engineering, this work will more broadly impact the design of devices involving three-dimensional transitional and turbulent boundary layers, such as turbomachinery and wind turbines.

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

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

Scientific Discipline: Engineering: Aerodynamics

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (24,000,000 node-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-scale 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) and the high-lift JAXA Standard Model (JSM), which are community research models for commercial transport aircraft. The high-fidelity simulation of the NASA CRM is considered a grand challenge problem for computational fluid dynamics.

Successful calculation of these engineering flows would facilitate the use of high-fidelity simulation techniques to help design future aircraft, particularly in take-off and landing configurations that have been difficult to predict using lower fidelity techniques.

Type: Renewal
Title: "Lattice QCD"

Principal Investigator: Paul Mackenzie, Fermilab
Co-Investigators: Richard Brower, Boston University
Norman Christ, Columbia University
Carleton DeTar, University of Utah
William Detmold, Massachusetts Institute of Technology
Robert Edwards, Jefferson Laboratory
Aida El-Khadra, University of Illinois at Urbana-Champaign
Anna Hasenfratz, University of Colorado Boulder
Andreas Kronfeld, Fermilab
Christoph Lehner, Brookhaven National Laboratory
Swagato Mukhergee, Brookhaven National Laboratory
Kostas Orginos, William & Mary

Scientific Discipline: Physics: High Energy Physics

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (24,000,000 node-hours)
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (1,600,000 node-hours)

Research Summary: Using DOE leadership computing resources, this INCITE project is addressing key science questions in high-energy and nuclear physics research to support and complement major experimental programs in these areas. The team's research in lattice quantum chromodynamics (QCD) addresses fundamental questions in high energy and nuclear physics that are essential to meeting a number of DOE Office of Science milestones.

A central objective of the 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. The configurations will enable researchers to push the search for new effects in flavor physics to yet higher energies. They also enable lattice calculations required throughout the DOE's Intensity Frontier program, such as Fermilab's Muon g-2 and neutrino scattering experiments.

A second target for this project is to calculate the fluctuations in conserved quantities, such as electric charge, baryon number, and strangeness in the quark gluon plasma produced at Brookhaven National Laboratory's Relativistic Heavy Ion Collider (RHIC) and CERN's Large Hadron Collider. These fluctuations provide valuable information about this new state of matter, and are an important signal for the QCD phase transition sought in the Beam Energy Scan being carried out at RHIC.

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

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

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (16,000,000 node-hours)
Cray XC40 (1,000,000 node-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 structure-function relationships are established. By combining massively parallel quantum-mechanical calculations with modern machine learning techniques and optimization algorithms, the researchers 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 innovations will produce a general, broadly applicable framework for structure search and computational design of functional materials that will benefit and broaden the community of researchers capable of using leadership computing resources to advance materials science for energy applications. Significant progress has already been made in elucidating structure-property relationships and associated methodological development, leading to numerous publications and awards.

Type: New
Title: "Molecular Dynamics of Motor-protein Networks in Cellular Energy Metabolism"

Principal Investigator: Abhishek Singharoy, Arizona State University
Co-Investigators: James Phillips, University of Illinois, Urbana-Champaign

Scientific Discipline: Biological Sciences: Biophysics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (300,000 node-hours)

Research Summary: Inspired by the capability of motor proteins to address the energy needs of living cells, this project aims to investigate two related biomolecular systems, which have a significant impact on addressing US energy and biomedical interests: (1) the evolutionary design principle of chemical energy-to-mechanical work conversion in biological motors, namely in the ATP synthase family of proteins, and (2) capturing these motors in action within large-scale bioenergetic networks, such as within sub-micron-sized cellular organelles. Together, these computations will deliver in all-atom detail the machinery for energy metabolism in living cells, and their associated disorders resulting in cellular ageing and death.

To capture the design principles of a living cell's biological motors, molecular dynamics simulations will be performed on Summit, employing the so-called string with swarms-of-trajectories method, to describe the mechanism of fuel (ATP) consumption and reaction-product (ADP+Pi) release by ATP synthase

Additionally, ATP synthase contributes to a much larger network of membrane-embedded bioenergtic proteins that line the photosynthetic and respiratory pathways. Using photosynthesis in purple bacteria as a prototype for such bioenergetic networks, simulations will be employed to determine how hundreds of proteins within the chromatophore organelle are entrained to work in synergy with ATP synthase and ultimately to convert the energy from sunlight into ATP.

These computations push the envelope of all-atom simulations to the cellular scale and simultaneously derive innovations in artificial energy technologies.

Type: New
Title: "Nanotribology: Molecular Dynamics Screening of Monolayer Chemistry"

Principal Investigator: Peter Cummings, Vanderbilt University
Co-Investigators: Christopher Iacovella, Vanderbilt University
Clare McCabe, Vanderbilt University

Scientific Discipline: Materials Science: Nanoscience

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (1,500,000 node-hours)

Research Summary: Understanding how to effectively lubricate mechanical systems at the nanoscale is essential for the development of next-generation devices. Cummings' team will use the Titan supercomputer to screen multicomponent monolayer films to identify chemistries that provide optimal nanoscale lubrication and to better understand the relationship between structures and properties.

Multicomponent monolayers present a vast parameter landscape that is infeasible to characterize through a purely experimental approach. As such, molecular dynamics simulations provide a tool for not only efficiently screening tens of thousands of potential monolayer chemistries, but also providing a molecular-level vision of the underlying mechanisms for these behaviors.

Using its toolkit, MoSDeF (molecular simulation and design framework), the team will execute a workflow that involves running thousands of simulations, in an ensemble-style screening, with large numbers of jobs grouped into a single execution script. For this study, simulation results will be used to examine the role of terminal group functionalization, chain length, composition, and functionality of the chain backbones on monolayer tribological properties, focusing on binary chain mixtures. Analysis of these characteristics will point toward promising monolayer chemistries for long-term nanoscale lubrication for advanced systems.

Type: New
Title: "New Frontiers for Material Modeling via Machine Learning Techniques with Quantum Monte Carlo"

Principal Investigator: Dario Alfe, University College London
Co-Investigators: Gerit Brandenburg, University of Goettingen
Gabor Csanyi, University of Cambridge
Angelos Michaelides, University College London
Andrea Zen, University College London

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (1,210,000 node-hours)
IBM AC922 (40,000 node-hours)

Research Summary: The design of new materials is entering a new era. For this project, the team will use quantum Monte Carlo (QMC) techniques to provide high accuracy data for the adsorption of water on graphene, with possible applications to water purification, desalination and drug delivery.

Water is ubiquitous in nature, and the accurate evaluation of its interaction with graphitic carbon is of fundamental importance for nanotechnology. Other theoretical approaches are not accurate enough to correctly describe the interaction of water with extended graphitic surfaces. Taking advantage of the recent QMC developments, the team will generate urgently needed high-level water–graphitic carbon interaction energies.

Subsequently, a machine learning potential will be built on these data, enabling the first demonstrably accurate simulations for the wetting of graphene or flow of water through carbon nanotubes.

Type: New
Title: "N-jettiness Subtraction for Precision Collider Phenomenology"

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

Scientific Discipline: Physics: High Energy Physics

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (1,250,000 node-hours)
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (400,000 node-hours)

Research Summary: With this INCITE project, researchers will enable the high-precision perturbative quantum chromodynamics (QCD) calculations needed to interpret increasingly precise data from the Large Hadron Collider (LHC) and future colliders, such as a proposed Electron-Ion Collider (EIC). The team's computations will address longstanding questions in understanding the spin structure of the proton, and could potentially help reveal deviations between measurements and the Standard Model of particle physics.

To carry out the work, the researchers will use their N-jettiness framework, a novel approach to precision perturbative QCD calculations that is especially adapted to run on high-performance computing systems. With a previous INCITE allocation, the research team's use of the framework led to the first high-precision QCD predictions for several benchmark LHC processes and advanced the understanding of hadron collider data spanning several fields.

The team will now apply the N-jettiness framework on DOE leadership systems to predict time-reversal violating asymmetries in vector-boson plus jet production, which have never before been measured and are an experimental focus of the current LHC run. The researchers also aim to provide precision predictions for polarization asymmetries in jet and hadron production at current experiments and at the future EIC, which will help address the longstanding puzzle of how the spin of the proton is composed from its partonic constituents. Furthermore, they plan to carry out a detailed study of the power corrections to the factorization formula that underlies the N-jettiness approach, and that are currently the subject of intense community interest.

Type: Renewal
Title: "Nucleation and Growth of Colloidal Crystals"

Principal Investigator: Sharon Glotzer, University of Michigan

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

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (1,160,000 node-hours)
IBM AC922 (395,000 node-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: "Petascale Simulations for Layered Materials Genome"

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

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

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (12,500,000 node-hours)

Research Summary: Functional layered materials (LMs) will dominate nanomaterials science in this century. The attractiveness of LMs lies not only in their outstanding electronic, optical, magnetic and chemical properties, but also in the possibility of tuning these properties in desired ways by building van der Waal heterostructures composed of unlimited combinations of atomically thin layers. With this INCITE project, researchers 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, advancing the DOE's LMs genome efforts: (1) aid the synthesis of stacked LMs by chemical vapor deposition (CVD), exfoliation, and intercalation; and (2) discover function-property-structure relationships in LMs with a special focus on far-from-equilibrium electronic processes.

Following highly successful NAQMD and RMD simulations studying shape fluctuation and structural phase transitions in photo-excited transition metal dichalcogenide LMs, and liquid phase exfoliation and intercalation of LMs, the researchers will use NAQMD simulations to study chemical reactions on LMs and RMD simulations to study CVD growth.

Type: New
Title: "Petascale Simulations of Kinetic Effects in IFE Plasmas"

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

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (1,500,000 node-hours)

Research Summary: Inertial fusion energy (IFE) devices hold incredible promise as a source of clean and sustainable energy, but there are significant obstacles to obtaining and harnessing IFE in a controllable manner.

A comprehensive model of laser-plasma instabilities (LPI) is crucial to the success of any IFE scheme, but one so far remains elusive. The physics involved in these processes (including both wave-wave and wave-particle interactions) is complex and highly nonlinear, necessitating the use of nonlinear kinetic computer models, such as fully explicit particle-in-cell (PIC) simulations. The ultimate goal—a long-standing challenge—is a constructed hierarchy of kinetic, fluid, and other reduced description approaches capable of modeling full spatial and temporal scales. Kinetic modeling has not yet yielded sufficiently complete understanding across the array of scales necessary to make strong connections with more approximate models and experiments.

This INCITE project uses the popular PIC code OSIRIS to study the kinetic evolution of LPI on meaningful spatial and temporal scales directly relevant to various IFE scenarios. The work, rich in basic science, promises to make a significant impact in the IFE community.

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:
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (830,000 node-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: New
Title: "PLASM-IN-SILICO: HPC Modeling of High-Intensity Laser-Solid Interaction"

Principal Investigator: Jean-Luc Vay, Lawrence Berkeley National Laboratory
Co-Investigators: Henri Vincenti, Commissariat à l'Energie Atomique

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (8,000,000 node-hours)
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (600,000 node-hours)

Research Summary: The advent of petawatt (PW) lasers has made it possible to achieve light intensities at which matter is completely ionized into a plasma made of a collection of electrons and ions. This technology has laid the groundwork for a new, promising but still largely unexplored branch of physics called ultra-high-intensity (UHI) physics, which investigates light-matter interactions at extreme intensities to understand the complex laws governing plasma dynamics in ultra-relativistic regimes. So far, progress in the UHI physics has largely relied on the strong interplay between experiments performed using high-power lasers and first-principles, particle-in-cell (PIC) simulations of the laser-plasma interactions.

With this INCITE project, researchers aim to develop novel solutions employing PW lasers to solve three major challenges in UHI physics: (1) to attain extreme light intensities to unravel new quantum electrodynamics regimes where vacuum breaks down; (2) to achieve efficient compact electron accelerators to advance high energy science; and (3) to achieve compact ion accelerators for cheaper cancer hadron therapy. In particular, the research team seeks to show that so-called relativistic plasma mirrors, which are produced when a high-power laser hits a solid target, can provide simple and elegant paths to solving these challenges.

The researchers will carry out massively parallel simulations using their PIC code, WARP(X)/PICSAR, on DOE's leadership-class supercomputers to devise and validate novel and readily applicable solutions based on plasma mirrors. The team will make use of their recent transformative developments in first-principles simulation of UHI laser-plasma interactions that enabled the 3D modeling of plasma mirror sources with high-fidelity on current petascale and future exascale supercomputers. They will establish close collaborations with experimental teams at PW laser facilities in the U.S. and Europe to enable experimental validation of these solutions.

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
Fernando Reboredo, Oak Ridge National Laboratory
Luke Shulenburger, Sandia National Laboratories

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation:

Site:	Argonne National Laboratory
Machine (Allocation):	Cray XC40 (1,750,000 node-hours)
Site:	Oak Ridge National Laboratory
Machine (Allocation):	Cray XK7 (1,000,000 node-hours)
	IBM AC922 (100,000 node-hours)

Research Summary: Our ability to understand, design, or optimize functional materials is hindered by the limited predictive power of established quantum mechanics-based approaches for important classes of functional materials. In these materials, the strong coupling between charge, spin, orbital, and lattice degrees of freedom that results in desired functionalities requires highly accurate calculations.

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 advance the state of the art. The team is performing calculations on challenging new materials systems in coordination with new experimental synthesis and characterization. This project will continue to advance efforts to identify new functionalities for energy-related technologies.

Type: New
Title: "The Proton's Structure and the Search for New Physics"

Principal Investigator: Andre Walker-Loud, Lawrence Berkeley National Laboratory

Co-Investigators:
Evan Berkowitz, Jülich Research Centre
Chris Bouchard, University of Glasgow
David Brantley, Lawrence Berkeley National Laboratory
Chia Cheng Chang, Lawrence Berkeley National Laboratory
Kate Clark, NVIDIA
Arjun Gambhir, Lawrence Livermore National Laboratory
Nicolas Garron, University of Liverpool
Thorsten Kurth, Lawrence Berkeley National Laboratory
Ken McElvain, University of California, Berkeley
Chris Monahan, University of Washington
Henry Monge-Camacho, Lawrence Berkeley National Laboratory
Amy Nicholson, University of North Carolina
Enrico Rinaldi, Brookhaven National Laboratory

Scientific Discipline: Physics: Nuclear Physics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (700,000 node-hours)

Research Summary: Walker-Loud's team will perform a series of lattice quantum chromodynamics (QCD) calculations relevant to the broader nuclear physics community and the search for new physics. For the first time, the team will determine the nucleon axial form factor with the precision required by experiments exploring the origin of matter. Additionally, the team will determine the resources necessary to predict the neutron lifetime and the proton size with the precision needed to identify new physics.

Utilizing a new technique for calculating matrix elements inspired by the Feynman-Hellman (FH) theorem, which has been successfully applied to a computation of the nucleon axial charge, the team will calculate a variety of nucleon structure quantities, including the axial and electromagnetic form factors, and extract the corresponding radii, for which there are current experimental discrepancies and hints of new physics beyond the Standard Model.

Type: New
Title: "Quantum Simulations of Photosystem II and Cuprate Superconductivity"

Principal Investigator: Shiwei, Zhang, College of William and Mary
Co-Investigators: Richard Friesner, Columbia University
David Reichman, Columbia University
Steven White, University of California, Irvine

Scientific Discipline: Chemistry: Physical

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (262,000 node-hours)

Research Summary: Predictive calculations in many-body systems governed by the laws of quantum mechanics represent a grand challenge in science. The combination of methodological developments and leadership-class computing presents a unique opportunity to make fundamental progress on this problem. The focus of this project concerns two transition-metal oxide systems crucial to energy science: the catalytic site of Photosystem II (PSII) and cuprate high-temperature superconductors (HTSC).

PSII is a protein complex in plants which converts water to oxygen with high efficiency using light and has the potential to serve as a functional model for how solar energy can be harvested in order to perform useful work. The proposed theoretical investigations aim to supplement experimental findings to provide a complete understanding of the structure, function, and mechanism of PSII. This will facilitate the design of artificial analogs with similarly high catalytic efficacy.

HTSC materials have the potential to revolutionize many energy-related technologies. However, the underlying physics is not well understood. Going beyond simple models, Zhang's team plans to produce more accurate physical predictions via direct calculations of the chemically realistic copper oxide system. The effort aims to bring about key insights towards the solution of a long-standing problem, provide a benchmark for simpler models, and explore a path to the rational design of new materials.

The team's code was recently ported to utilize graphical processing units, achieving speed-ups of roughly two orders of magnitude and parallel efficiency greater than 98 percent across multiple nodes.

Type: New
Title: "Radiation Hydrodynamic Simulations of Massive Stars with Rotation"

Principal Investigator: Lars Bildsten, University of California, Santa Barbara
Co-Investigators: Matteo Cantiello, Flatiron Institute
Yan-Fei Jiang, University of California, Santa Barbara
Eliot Quataert, University of California, Berkeley
Stephen Ro, University of California, Berkeley

Scientific Discipline: Physics: Astrophysics

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (1,300,000 node-hours)

Research Summary: Massive stars play an important role in many astrophysical environments. Along with supernovae, they produce the majority of the heavy elements in nature, seeding the universe with the ashes of nuclear burning from which planets form and life is made.

While previous INCITE research—including recent global radiation hydrodynamic simulations that indicated the importance of helium opacity peak to outbursts of Luminous Blue Variables—has improved our understanding of massive stars' behavior, many of their puzzles remain unsolved.

This project executes three-dimensional global radiation hydrodynamic simulations of Wolf-Rayet star envelopes by directly solving the time-dependent radiation transfer equation along discrete rays. These simulations will resolve the convection developed around the iron opacity bump region due to the super-Eddington radiation flux and probe the mechanism to drive the large mass loss rate for these stars.

By coupling the rotation, convection, and three-dimensional radiative transfer self-consistently, the researchers will also carry out the first sets of simulations to study the effects of rotation on the envelope structures and mass loss. The results will be incorporated into one-dimensional stellar evolution models to create more realistic massive star models and supernovae progenitors, which will significantly improve our understanding of the structures and evolutions of massive stars.

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

Principal Investigator: Subramanian Sankaranarayanan, Argonne National Laboratory

Co-Investigators: Henry Chan, Argonne National Laboratory
Mathew Cherukara, Argonne National Laboratory
Ali Erdemir, Argonne National Laboratory
Ganesh Kamath, Argonne National Laboratory
Troy Loeffler, Argonne National Laboratory
Badri Narayanan, Argonne National Laboratory
Kiran Sasikumar, Argonne National Laboratory

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

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (650,000 node-hours)

Research Summary: Friction and wear remain the primary causes of mechanical energy dissipation across diverse application areas ranging from energy technologies to geology to biology. The energy and material losses due to friction and wear are estimated to cost several billions of dollars annually. With a better understanding of friction at the nanoscale and mesoscale, researchers can develop advanced lubricant materials that can significantly reduce such losses.

With this INCITE project, researchers will use the highly parallelizable molecular dynamics code, LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator), to advance the fundamental understanding of friction laws and mechanisms between sliding mechanical interfaces. They will leverage DOE leadership computing resources along with insights from first-principles physics, atomistic simulations and machine learning techniques to develop new, well-trained and robust force fields for accurately and efficiently capturing the molecular interactions in tribological interfaces.

The team's research will focus on two types of lubricants: (1) a new class of hybrid nanoscale lubricants (2-D materials and nanoparticles) and (2) adaptive self-organizing coatings. The researchers will use new first-principles-based interatomic potentials to enable precise predictions of interatomic forces and thereby allow high-fidelity, large-scale dynamical and statistical simulations of tribological interfaces, properties, and functionalities of new lubricants, as well as pathways and mechanisms of their in operando synthesis and assembly. Their findings are expected to have direct and profound implications for understanding mesoscale dynamics in tribological systems, which will lead to significant energy savings for a wide variety of applications.

Type: New
Title: "Real-Time Non-Equilibrium Dynamics of Strongly Interacting Nuclear Matter"

Principal Investigator: Aurel Bulgac, University of Washington
Co-Investigators: Satoshi Chiba, Tokyo Institute of Technology
Chikako Ishizuka, Tokyo Institute of Technology
Piotr Magierski, Warsaw University of Technology
Kenneth Roche, Pacific Northwest National Laboratory
Nicolas Schunck, Lawrence Livermore National Laboratory
Kazuyuki Sekizawa, Niigata University
Ionel Stetcu, Los Alamos National Laboratory

Scientific Discipline: Physics: Nuclear Physics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (275,000 node-hours)

Research Summary: This INCITE project will use full quantum mechanical predictive tools needed to quantitatively and comprehensively describe nuclear fission, collisions of heavy ions, and fusion, research that could help explain the origin and abundance of chemical elements used for medical, safety, and national security applications, energy production, nuclear non-proliferation and attribution, and nuclear forensics.

The overarching goal of the proposed work is to advance the nuclear physics community's ability to describe and predict complex non-stationary processes of strongly interacting quantum many-body systems using state-of-the-art microscopic approaches. Bulgac's team will use the most advanced numerical and software implementations to extend Density Functional Theory to superfluid systems and time-dependent phenomena for a range of non-equilibrium nuclear processes. The team will also perform the implementation of fluctuations and dissipation within the time-dependent density functional framework in a fully quantum mechanical approach for the first time. Fluctuations are indispensable in order to predict the distributions of the final products and their properties within a genuine microscopic quantum approach.

These results are relevant to experiments such as those performed at the Facility for Rare Isotopes Beams for extending the periodic table of elements, for pursuing the search for superheavy elements, and for explaining the origin and abundance of chemical elements in the Universe.

Type: New
Title: "Search for New Physics Using Precision Tests of the Standard Model"

Principal Investigator: Norman Christ, Columbia University
Co-Investigators: Peter Boyle, University of Edinburgh
Carleton Detar, University of Utah
Aida El-Khadra, University of Illinois, Urbana-Champaign
Xu Feng, Peking University
Elvira Gamiz, University of Granada
Steve Gottlieb, Indiana University
Andreas Juettner, University of Southampton
Chulwoo Jung, Brookhaven National Laboratory
Andreas Kronfield, Fermi National Laboratory
Christoph Lehner, Brookhaven National Laboratory
Robert Mawhinney, Columbia University
Ethan Neil, University of Colorado
Ruth VandeWater, Fermi National Laboratory

Scientific Discipline: Physics: High Energy Physics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (850,000 node-hours)

Research Summary: Scientific knowledge of the most fundamental elementary particles and forces in nature is incomplete. This team is carrying out high-precision calculations that are essential in the ongoing experimental search for new, more fundamental laws of nature.

The team proposes two sets of high-priority calculations on Summit that will improve precision Standard Model calculations and contribute to the search for a more complete theory:

(1) Calculate rare decays of the bottom quark using a new, large ensemble of gluon-field configurations based on highly-improved staggered sea quarks, intended for high-precision heavy-flavor calculations.

(2) Generate a new ensemble of gluon-field configurations based on chiral quarks with a smaller lattice spacing and with a five times larger lattice volume than previously achieved with chiral sea quarks. This ensemble will then be used for calculations of the anomalous magnetic moment of the muon and rare phenomena involving strange quarks, quantities central to particle physics phenomenology.

Type: New
Title: "Shock-Induced Multi-Material Mixing"

Principal Investigator: Sanjiva Lele, Stanford University
Co-Investigators:

Scientific Discipline: Engineering: Fluids and Turbulence

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (4,500,000 node-hours)

Research Summary: Shock-induced turbulent mixing is important in high-speed propulsion and inertial confinement fusion, but turbulence under such conditions remains poorly understood. This INCITE project performs high-resolution simulations of shock-induced turbulent mixing that results from Richtmyer-Meshkov (RM) instability.

The simulations focus on the interaction of a planar shockwave with a nominally planar fluid interface that is at an inclination with respect to the shockwave. They build on recent results that suggest anomalous energy scaling in compressible variable-density flows arising from the RM instability. This research is the first to establish a new regime of mode-coupling in shock-induced mixing and quantify the effects of compressibility and the fundamental compressible energy transfer mechanisms.

A critical milestone for the turbulence community, this work will create a benchmark-quality database for shock-induced missing that is validated against experiments, and for which the effect of the numerical method is carefully quantified and shown to be small. The results will advance the state of the art in simulations of RM instability-driven mixing and help improve engineering models of variable density-turbulence, which will enable innovations in new combustion devices and propulsion systems.

Type: New
Title: "Simulating Neutron Star Binary Merger Remnant Disks and Tilted Thin Disks"

Principal Investigator: Alexander Tchekhovskoy, Northwestern University
Co-Investigators: Francois Foucart, University of New Hampshire
Dimitrios Giannios, Purdue University
Daniel Kasen, Lawrence Berkeley National Laboratory
Matthew Liska, University of Amsterdam

Scientific Discipline: Physics: Astrophysics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (850,000 node-hours)

Research Summary: Unleashing the GPU power of the Summit supercomputer, Tchekhovskoy's team will address two longstanding mysteries: (1) how do neutron star collisions produce heavy elements, such as gold and platinum? (2) How do black holes break up luminous disks of gas that feed them, and does this make the disks much brighter than previously thought?

(1) In August 2017, gravitational waves from a merger of binary neutron stars were detected for the first time. To meaningfully interpret this exciting discovery and make predictions for future gravitational waves detections, Tchekhovskoy's team will simulate the long-term evolution of a merger remnant accretion disk and its outflows, which are launched by large-scale magnetic fields and magnetized turbulence.

(2) Luminous accretion disks around rapidly rotating black holes convert up to 30 percent of rest-mass energy into radiation, vastly exceeding the efficiency of nuclear fusion. The disks are typically tilted relative to the black hole midplane to some degree, yet the effects of the tilt on the black hole growth and energy release are poorly understood. The primary difficulty of studying such disks numerically is the need to dynamically resolve their extremely small thickness even as they move through the computational grid. Summit is the first machine capable of sustaining long-awaited, extremely thin tilted disks simulations by enabling a factor of 10 leap in resolution. The team will simulate the thinnest tilted disks to date using their 3D GR magnetohydrodynamic (GRMHD) code H-AMR.

Type: New
Title: "Solvent Disruption of Biomass for the Production of Biofuels and Bioproducts"

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

Scientific Discipline: Biological Sciences: Biophysics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (1,000,000 node-hours)
IBM AC922 (100,000 node-hours)

Research Summary: Plant cell wall biomass consists mostly of lignin, cellulose and hemicellulose — lignocellulosic biopolymers that are potential sources of clean, renewable biofuels and other high-value chemicals. However, the complex 3D structure of plant biomass makes it recalcitrant to deconstruction.

This recalcitrance can be overcome by thermochemically pretreating biomass. Recently, the utilization of novel organic cosolvent pretreatments has shown great promise in the conversion of plant biomass to fuels and other bioproducts. However, a physicochemical understanding of how (co)solvent conditions reduce recalcitrance is lacking.

In previous supercomputer-driven work Smith's team has demonstrated how key processes that impede the deconstruction of biomass are driven by solvation thermodynamics, including lignin-cellulose association, lignin aggregation, and cellulose fibril coalescence. This project proposes to apply state-of-the-art molecular dynamics simulation on the Titan and Summit supercomputers to determine the free energy of binding between biomass polymers in selected industrially-relevant pretreatment solvents.

The simulations will furnish a molecular-level description of biomass-solvent interactions, leading to a quantitative determination of the physical properties that make a biomass solvent effective. Furthermore, simulations will advance a rationalization of a wide range of experimental data.

Type: New
Title: "Structural Elements in the Evolution of Mechanisms in Substance Transporters"

Principal Investigator: Harel Weinstein, Weill Cornell Medical College
Co-Investigators: George Khelashvili, Weill Cornell Medical College

Scientific Discipline: Biological Sciences: Biophysics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (1,320,000 node-hours)

Research Summary: A powerful combination of advanced experimental and computational approaches has made it possible to explore important phenomena for the development of medicine and molecular-level technology. This proposal leverages these novel insights to discover new ways to modulate the activities of essential signaling machines in the nervous system and brain and proven modes of molecular engineering of complex chemical energy-driven molecular machines.

The team reasons that both mechanism elucidation and molecular engineering efforts will benefit from understanding how nature has solved the specific problems in the evolution of complex functional systems. For the transporter systems the team studies, this seems to have occurred through the addition of small structural elements to simpler templates, such as the bacterial homologs of the neurotransmitter transporters, and by introducing structural organization, such as the oligomerization of the eukaryotic transporters to enable additional functions.

The requested allocation will be used for atomistic large-scale ensemble molecular dynamics simulations using the ACEMD software, which has been optimized to run on GPUs.

Successful project completion will enable the presentation of a prototype for practical utilization of structural changes in the evolution from the bacterial LeuT-like transporters to the human Neurotransmitter: Sodium-Symporters as a novel approach to regulation and modulation of functional phenotypes in membrane-embedded, molecular machines.

Type: New
Title: "Three-dimensional Simulations of Rotating and Non-rotating Core-collapse Supernovae"

Principal Investigator: W. Raph Hix, Oak Ridge National Laboratory
Co-Investigators: Stephen Bruenn, Florida Atlantic University
James Harris, Oak Ridge National Laboratory
Eric Lentz, University of Tennessee, Knoxville
Anthony Mezzacappa, Oak Ridge National Laboratory

Scientific Discipline: Physics: Astrophysics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (1,920,000 node-hours)

Research Summary: Core-collapse supernovae, the explosive final moments of massive stars, are complex, dynamic, multi-physics events yielding a bright and energetic explosion from the birth of a neutron star or black hole.

The team's 3D simulations will explore the late phase of the explosions that mark the end of the lives of stars much more massive than the sun and how the supernovae of rotating stars differ from nonrotating stars. Simulation results will answer questions related to the impact of stellar rotation on the explosion mechanism of core-collapse supernovae and the associated observables. Additionally, the work will increase understanding of the development of the proto-neutron star wind following the onset of explosion.

These simulations will be performed using the team's Chimera multi-physics supernova code. Chimera contains all of the relevant physics required for core-collapse supernova simulations, including transport of energy by neutrinos and the required neutrino–matter interactions, general relativity and self-gravity, nuclear burning and nuclear equations of state, and 3D fluid dynamics.

Type: New
Title: "Towards a Definitive Model of Core-Collapse Supernova Explosions"

Principal Investigator: Adam Burrows, Princeton University
Co-Investigators: Joshua Dolence, Los Alamos National Laboratory
David Radice, Princeton University
Michael Aaron Skinner, Lawrence Livermore National Laboratory

Scientific Discipline: Physics: Astrophysics

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (1,750,000 node-hours)

Research Summary: Core-collapse supernovae dramatically announce the death of massive stars and the birth of neutron stars. During this violent process, a combination of high-density nuclear physics, multi-dimensional hydrodynamics, radiation transport, and neutrino physics determines whether and how the star explodes. However, though it is thought that capturing a small fraction of the neutrinos emitted during collapse powers such explosions, and though detailed 2D simulations provide strong supporting evidence, detailed 3D calculations that prove this to be the case are lacking. Lack of access to sufficient computational resources has hindered progress toward the demonstration of a robust explosion mechanism since the 1960s.

This INCITE project addresses whether and how 3D supernova explosion models differ from their 2D counterparts. The researchers will use the new state-of-the-art, highly scalable, 3D radiation-hydrodynamics simulation code Fornax to determine if the neutrino mechanism is a robust explanation for supernova explosions and the stellar progenitor dependence of their observables, resolving a fifty-year-old problem in nuclear astrophysics.

A solution will benefit ongoing efforts of observers and instrument designers in the U.S. and around the world engaged in projects to determine the origin of the elements, measure gravitational waves, and interpret laboratory nuclear reaction rate measurements in light of stellar nucleosynthesis.

Type: New
Title: "Towards Ultimate Rayleigh-Benard Convection"

Principal Investigator: Janet Scheel, Occidental College
Co-Investigators: Kartik Iyer, New York University
Joerg Schumacher, Technische Universitaet Ilmenau
Katepalli Sreenivasan, New York University

Scientific Discipline: Engineering: Fluids and Turbulence

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): IBM Blue Gene/Q (12,500,000 node-hours)

Research Summary: Turbulent convection is an important area of research in fluid dynamics with applications to diverse phenomena in nature and technology, ranging from chip cooling devices and heat exchangers in power plants to convection in the Earth's atmosphere, core, and oceans all the way to convection in the Sun and other stars. The turbulent Rayleigh-Bénard convection (RBC) model is at the core of all these turbulent flows. It can be studied in a controlled manner, but still has enough complexity to contain the key features of convective turbulence.

This INCITE project aims to shed light on the ultimate regime of convective turbulence in which the boundary layers become fully turbulent, resulting in significantly enhanced turbulent heat transfer. There are theoretical predictions and some recent experimental evidence of a possible transition into this regime, but three-dimensional simulations have not been able to capture the ultimate regime yet.

The research team will advance direct numerical simulations (DNS) to this new level of turbulence at Rayleigh numbers that have never been accessed before numerically. Their efforts are based on the Nek5000 spectral element software package, which was developed for solving flow equations on massively parallel supercomputers. In order to obtain the necessary high Rayleigh numbers of $Ra \geq 10^{16}$ for the ultimate regime at a Prandtl number $Pr = 0.7$, the researchers will take an unconventional step and study RBC in very slender cylindrical cells with an aspect ratio (diameter/height) of 1/10.

The team's DNS will provide new insights into the global structure of the convection flow and into the details of the increasingly intermittent boundary layer dynamics. The data obtained in this project will also help to resolve the contradictory experimental results for the onset of the transition to the ultimate regime. Ultimately, the team's study will provide a better understanding of the heat and momentum transport as a function of Rayleigh number. As such, their findings will be transformational in the domain of fluid dynamics with a variety of important applications.

Type: New
Title: "Turbulent Scalar-Mixing and Combustion in Supercritical Fluids"

Principal Investigator: Joseph Oefelein, Georgia Tech
Co-Investigators: Ramanan Sankaran, Oak Ridge National Laboratory

Scientific Discipline: Engineering: Fluids and Turbulence

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (1,050,000 node-hours)

Research Summary: This project focuses on developing a detailed understanding of supercritical fluid phenomena relevant to injection, mixing, and combustion of propellants under the high-pressure, highly-turbulent conditions of advanced propulsion and power systems.

Using a combination of the Large Eddy Simulation (LES) and Direct Numerical Simulation (DNS) techniques, Oefelein's team will simulate the high-pressure, high-Reynolds-number conditions encountered in advanced propulsion and power systems (e.g., liquid rocket, gas turbine, and reciprocating internal-combustion engines). This requires the formulation of refined theories, which must then be combined with the development and validation of advanced models. Thus, the objective of this project is to establish a progressive hierarchy of detailed simulations that enable both scientific discovery and the development of predictive models.

Calculations will be performed using the RAPTOR code, which is designed for both LES and DNS of the complex flow physics. The theoretical framework solves the fully-coupled conservation equations of mass, momentum, total-energy, and species for a chemically reacting flow.

The proposed calculations will provide a unique set of data to study supercritical fluid phenomena at conditions identical to those in actual engines. This will provide the foundation required to effectively develop the coupled set of sub-models required for the design of advanced systems. Results will provide new scientific insights on how liquid fuels and/or oxidizers behave at supercritical pressures in advanced propulsion and power systems.

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:
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (3,500,000 node-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: New
Title: "Unprecedented scales with ECMWF's medium-range weather prediction model"

Principal Investigator: Nils Wedi, European Center for Medium-Range Weather Forecasts
Co-Investigators: Peter Bauer, European Center for Medium-Range Weather Forecasts

Scientific Discipline: Earth Science: Climate Research

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (102,000 node-hours)

Research Summary: Advances in high-performance computing have brought climate research to the point where it is now possible to replace crude statistical models of crucial climate processes with more fundamental principles. Wedi's team will pave the way towards answering two fundamental questions related to the future design of global circulation models—the Integrated Forecasting System (IFS) in particular.

The first goal is a push towards global 1-kilometer simulations of weather and climate, which would substantially improve the diurnal cycle of convection, the representation of the interaction with orography and valley flows, and the appropriate use of high-resolution, land-use characteristics available from the latest satellite missions. All these efforts should result in better local predictions of high-impact weather. In a second stage, this work will compare the performance of the IFS spectral transform based dynamical core relying on large scale FFT and matrix-matrix multiplications with the newly developed IFS finite-volume module operating on an identical grid. This comparison will establish the first quantitative assessment of time- vs energy-to-solution of two highly representative state-of-the-art algorithmic formulations in numerical weather prediction.

Secondly, the team will establish and compare the scaling performance of key components and algorithms that account for the bulk of computation and data communication by successively replacing them with GPU-adapted versions. This fundamentally establishes the use of hybrid technology for numerical weather prediction and climate research using frontier simulations that fully exploit memory, interconnect, and cluster size resources that are not available anywhere else in the world.

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:
Site: Oak Ridge National Laboratory
Machine (Allocation): Cray XK7 (2,800,000 node-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.