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, Karamanoglu Mehmetbey University
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 Navrátil, TRIUMF
Thomas Papenbrock, University of Tennessee
Saori Pastore, Washington University in St. Louis
Maria Piarulli, Washington University in St. Louis
James Vary, Iowa State University
Robert Wiringa, Argonne National Laboratory

Scientific Discipline: Physics: Nuclear Physics

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (1,000,000 node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (550,000 node-hours)

Research Summary: Atomic nuclei are strongly interacting, quantum many-body systems displaying fascinating properties. They exhibit emergent phenomena characteristic of large complex systems while at the same time being laboratories of most fundamental laws of nature. Predictions for the structure and reactions of nuclei, with assessed uncertainties, are important for the future of the nation's energy and security needs.

Building on previous INCITE research, this project will employ advanced *ab initio* quantum many-body techniques coupled with applied mathematics and computer science methods to study a wide range of nuclei and to accurately describe the atomic nucleus from first principles, including their electroweak transitions and reactions important in both terrestrial experiments and astrophysical environments. The team's predictions will complement DOE's major investments in forefront experimental facilities, including existing low-energy nuclear physics facilities, Jefferson Laboratory, neutrino experiments, and the forthcoming Facility for Rare Isotope Beams (FRIB) under construction at Michigan State University. Ultimately, results from this INCITE project will help support and guide new experiments, 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

Scientific Discipline: Biological Sciences: Biophysics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (260,000 Summit node-hours)

Research Summary: RNA Polymerases (Pol I, II and III) constitute the centerpiece of the intricate molecular machinery that transcribes the genetic code into RNA and controls such diverse processes as cell differentiation, development, and responses to environmental change. Specifically, Pol II transcribes protein-coding genes into messenger RNA (mRNA). In turn, mRNA serves as a template for the synthesis of proteins by the ribosome. Therefore, Pol II functions as the critical intermediary in transforming the genetic code into the myriad of proteins that are the building blocks of all living organisms.

Gene transcription is a complex and highly regulated process. While structural knowledge is beginning to emerge, little is understood about the molecular-level mechanisms that underlie gene expression. At the same time, detailed mechanistic knowledge is essential to advance biomedical applications.

The principal aim of Ivanov's project is to unravel the molecular architecture and functional dynamics of transcription pre-initiation (PIC) complexes, which are critical for gene regulation. The team will take advantage of new cryo–electron microscopy data and combine it with advanced computational modeling on the Summit machine at OLCF to elucidate the mechanisms of PIC assembly, promoter recognition, DNA melting, and the roles of general transcription factors therein.

Type: Renewal
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
Alice Harpole, Stony Brook University
Max Katz, NVIDIA
Andy Nonaka, Lawrence Berkeley National Laboratory
Donald Willcox, Lawrence Berkeley National Laboratory

Scientific Discipline: Physics: Astrophysics

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

Research Summary: Zingale's research team will model astrophysical thermonuclear explosions, including Type Ia supernovae and x-ray bursts, using its open-source MaestroeX and Castro codes. Simulating these can provide insight into stellar phenomena observed in the night sky and the formation of elements throughout the history of the Universe.

MaestroeX 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 the reactions that accompany these events.

In the team's previous allocation, significant progress was made in code development, with all of the physics for the Castro x-ray burst and white dwarf mergers (including self-gravity) on the GPUs and a substantial portion of MaestroeX's hydrodynamics also on GPUs.

For Type Ia supernovae, the team is modeling all of the progenitor systems that are popular today. The team's interest in x-ray bursts also involves understanding the interplay of hydrodynamics and reactions. The team finished a set of 2D calculations that resolve the flame and follow its propagation across the neutron star, and the group is now performing the first-ever 3D simulations resolving the flame structure in x-ray bursts, a problem that will continue to be a highlight in the 2020 INCITE allocation.

Type: New
Title: "A Baseline for Global Weather and Climate Simulations at 1km Resolution"

Principal Investigator: Nils Wedi, European Centre for Medium-Range Weather Forecasts

Co-Investigators: Peter Dueben, European Centre for Medium-Range Weather Forecasts
Peter Bauer, European Centre for Medium-Range Weather Forecasts
Valentine Anantharaj, Oak Ridge National Laboratory

Scientific Discipline: Earth Science: Climate Research

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (500,000 Summit node-hours)

Research Summary: It is one of the major sources of uncertainty for both weather and climate predictions that important features of the atmosphere, such as deep convection, cannot be resolved explicitly within existing weather and climate models due to the limited grid spacing of these models. Deep convection is seen as crucial in regulating the vertical redistribution of energy, momentum, and heat, and the community of weather and climate modeling is striving for the "quantum leap" of climate science to allow for long-range simulations of the global atmosphere at O(1 km) resolution that represent deep convection explicitly within the simulation.

Until today, the limited performance of supercomputers and the challenge of making efficient use of highly parallel high-performance computing systems did not allow for the use of O(1km) resolution with state-of-the-art global weather and climate models, and hence the explicit representation of convection could only be realised in limited areas, thus lacking the feedback of fundamental energy exchanges onto the larger scales.

This project will deliver this "quantum leap" forward in simulating and understanding the Earth's weather and climate. The world's first climate timescale simulation at O(1 km) resolution will explain how resolved deep convection feeds back on global dynamics of the atmosphere on an annual timescale, thus providing a baseline reference and guidance for the worldwide climate modeling community.

Type: New
Title: "Characterization of Strongly Interacting Matter through Fluctuations"

Principal Investigator: Claudia Ratti, University of Houston
Co-Investigators: Rene Bellwied, University of Houston
Sandor Katz, Eotvos University Budapest
Szabolcs Borsanyi, University of Wuppertal
Zoltan Fodor, University of Wuppertal

Scientific Discipline: Physics: Nuclear Physics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (510,000 Summit node-hours)

Research Summary: The main purpose of heavy-ion collisions is to test the theory of strong interactions in quantum chromodynamics (QCD) in the high-temperature/density phase. It is expected that a transition occurred immediately after the Big Bang in which matter converted from a state of quarks and gluons to a state of massive color-neutral particles, the hadrons, which populate the Universe today.

Ratti's team is providing theoretical support to the near-term experimental programs at the Relativistic Heavy Ion Collider and the Large Hadron Collider, which produce strongly interacting matter under extreme conditions, by simulating relevant observables from first principles.

This project will extend the validity of the equation of state to larger values of μ_B and provide the behavior of higher order fluctuations at finite density. It will also help the researchers determine whether chiral symmetry restoration occurs in heavy-ion collisions, what the effective degrees of freedom are in the vicinity of the phase transition, and which exotic states contribute to QCD thermodynamics.

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

Principal Investigator: Cass T. Miller, University of North Carolina at Chapel Hill
Co-Investigators: Jan F. Prins, University of North Carolina at Chapel Hill
William G. Gray, University of North Carolina at Chapel Hill

Scientific Discipline: Engineering: Fluids and Turbulence

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (340,000 Summit 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. However, traditional models for understanding these systems 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.

A prior INCITE allocation resulted in a rigorous derivation and computational confirmation of a hysteretic-free equation of state involving capillary pressure that applies to both equilibrium and dynamic conditions; the establishment of the precision in thermodynamically constrained averaging theory (TCAT) variables as a function of domain size; a new evolution equation for the geometric orientation tensor; a promising approximation for the velocity of the fluid–fluid interface; the formulation of evolution and constraint equations for mean and Gaussian curvature; and substantial progress on computational confirmation of the new theoretical developments.

In this project, the team will develop a macroscale simulator implementing the new TCAT model and paving the way for rigorous evaluation and validation of the entire model and not just the component parts individually. The researchers anticipate that this work will hasten the development of a new generation of TCAT-model-based simulators yielding higher fidelity simulation of multiphase porous medium systems than is possible using current approaches.

Type: New
Title: "Colloidal Crystallization Pathways"

Principal Investigator: Sharon C. Glotzer, University of Michigan

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

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (800,000 Summit node-hours)

Research Summary: 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. Simulation can play a critical role in guiding material design and providing understanding that cannot yet come from experiments.

With substantial resources from Summit, Glotzer's team will carry out the most in-depth computational study of colloidal crystallization pathways that has ever been undertaken. Expanding on work carried out with previous INCITE support, a particular focus of this project will be on the role of precrystallization motifs or structures in nanoparticles—pathways that involve liquid-liquid phase separation—and critical behavior in protein crystallization not seen in simple liquids.

A central goal of this study is to understand what conditions lead to multistep pathways and rich precrystallization behavior in hard particles and biological materials. The team's approaches and tools are transferable and will be of immediate and even broader interest to the materials, engineering, and chemistry communities interested in crystallization (e.g., of atoms, molecules, and proteins).

Type: New
Title: "Computational Physical Genomics: Exploring Potential Novel Cancer Therapies"

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

Scientific Discipline: Biological Sciences: Biophysics

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

Research Summary: With the ultimate aim of exploring novel therapies potentially applicable to a broad spectrum of human cancers, this project combines high-performance computing with laboratory experiments and preclinical studies to model and study physical genomics. "Physical genomics" refers to the functional structure of interphase DNA and how it is affected by ambient conditions within a cell's nucleus, inside which DNA is compacted into chromatin. Understanding chromatin folding and how it is affected by physico-chemical factors is important both for early-stage cancer detection and the rational design of new cancer treatments.

Partial wave spectroscopic (PWS) microscopy as an optical imaging technique has revealed mass-fractal-like heterogeneous chromatin packing with a global impact on gene expression. To explain such heterogeneous chromatin packing, the researchers have developed a mathematical model called a self-returning random walk (SRRW), which provides a new theoretical framework to understand chromatin folding. Related findings suggest the potential of macrogenomic engineering for cancer treatment—i.e., using physico-chemical strategies to regulate chomatin packing for whole-scale transcriptional engineering that constrains the adaptive potential of neoplastic cells. Achieving this goal requires a more detailed molecular description of chromatin folding beyond the SRRW model.

To this end, this work will build a high-fidelity computational model of chromatin to investigate the interplay between different folding mechanisms and to decipher the effects of genetic and epigenetic codes on the self-organization of the human genome. It will also extend the current static model into a dynamic one that leverages the dynamic PWS imaging technique developed in a previous INCITE allocation. This research could yield significantly improved understanding of chromatin folding and the cause of cancer, while also providing new insights and strategies to develop genetic therapeutics that target specific domains and networks of our genome.

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

Principal Investigator: Thomas Maier, Oak Ridge National Laboratory
Co-Investigators: Steven Johnston, University of Tennessee, Knoxville
Satoshi Okamoto, Oak Ridge National Laboratory
Gonzalo Alvarez, Oak Ridge National Laboratory
Thomas Schulthess, Swiss National Supercomputing Centre
Douglas Scalapino, University of California, Santa Barbara
Eduardo D'Azevedo, Oak Ridge National Laboratory

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (900,000 Summit 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 Summit, 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.

Following on from a prior INCITE allocation, the team will carry out numerical simulations of multi-orbital Hubbard models of unconventional superconductors and realistic spin models of quantum spin liquids. For the unconventional superconductors, the goal is to provide insight into the respective roles of magnetic, charge, orbital, and lattice degrees of freedom in shaping pairing correlations. For the quantum spin liquids, the aim is to understand materials proposed to realize the celebrated Kitaev quantum spin liquid and the role of competing interactions. Key scientific outcomes of this work will be the development of physical models that describe the mechanism(s) leading to high-temperature superconductivity and the factors that determine the critical temperature T_c and clear guidelines for identifying materials realizing a Kitaev spin liquid.

Type: New
Title: "Decoding the Physics of the Intergalactic Medium"

Principal Investigator: Zarija Lukic, Lawrence Berkeley National Laboratory
Co-Investigators: Ann Almgren, Lawrence Berkeley National Laboratory
Christopher Daley, Lawrence Berkeley National Laboratory
Frederick Davies, University of California, Santa Barbara
Dmitriy Morozov, Lawrence Berkeley National Laboratory
Andrew Myers, Lawrence Berkeley National Laboratory
Jose Onorbe, University of Madrid
Hannah Ross, Lawrence Berkeley National Laboratory
Jean Sexton, Lawrence Berkeley National Laboratory
Weiqun Zhang, Lawrence Berkeley National Laboratory
Joseph Hennawi, University of California, Santa Barbara

Scientific Discipline: Physics: Astrophysics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (500,000 Summit node-hours)

Research Summary: The intergalactic medium (IGM) is the rarefied gas that fills the vast volumes between the galaxies in the universe. Physical effects, ranging from the nature of dark matter to the radiation from star-forming galaxies and quasars, set the observable properties of the IGM, making the IGM a powerful probe of both fundamental physics and astrophysics. To extract scientific insights, confronting observations of the IGM with numerical simulations is a necessity.

Lukic's team will perform a comprehensive set of simulations that will simultaneously constrain the properties of dark matter and characterize the epoch of reionization. The three large simulations the team proposes will be state-of-the-art and a dramatic improvement over current simulation suites both in size and physical accuracy. The team expects these simulations to be analyzed for years and inform many cosmological and astrophysical applications, such as different statistics of the Lyman-alpha and Lyman-beta forest, 21-cm modeling, and constraints on the nature of dark matter.

Type: New
Title: "Direct Numerical Simulations of High-Pressure Turbine Stages with Endwalls"

Principal Investigator: Richard Sandberg, The University of Melbourne
Co-Investigators: Yuxin Zhang, General Electric Aviation
Aamir Shabbir, General Electric Aviation
Sriram Shankaran, General Electric Aviation
Yaomin Zhao, University of Melbourne

Scientific Discipline: Engineering: Fluids and Turbulence

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (525,000 Summit node-hours)

Research Summary: Gas turbines are—and will continue to be—the backbone of aircraft propulsion, power generation, and mechanical drive due to their power density (i.e., thrust per unit engine weight), efficiency, and ability to adjust to rapidly varying loads. In the US alone, the natural gas and oil burn summed up to 27×10^{12} cubic feet and 6.3×10^{9} barrels of oil equivalent respectively in 2015. Therefore, even at the current fuel price, a small engine performance improvement does have a fuel-spend advantage of the billion-dollar order, together with a significant CO_2 emission benefit.

The Melbourne/GE team is exploiting the capability of the very efficient computational fluid dynamics code, the High-Performance Solver for Turbulence and Aeroacoustic Research (HiPSTAR) developed by Sandberg's research group, to perform the first-of-a-kind direct numerical simulation of high-pressure turbine stages with realistic geometry and at engine-relevant conditions.

The generated data will shed light on the detailed fundamental flow physics—in particular the behavior of transitional and turbulent boundary layers affected by large-scale violent freestream turbulence—under strong pressure gradient and curvature. It will also help evaluate and develop lower-order models readily applicable to gas turbine designs. With the results, it will be possible to identify opportunities to increase turbine aerothermal efficiency by 2–4 percent and extend hot-gas-path durability. This would translate into combined cycle efficiency gains of 0.4–0.8 percent and thus have a significant economic and environmental impact.

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

Principal Investigator: Jacqueline Chen, Sandia National Laboratories
Co-Investigators: Tarek Echekki, North Carolina State University
Martin Rieth, Sandia National Laboratories
Alex Aiken, Stanford University
Elliott Slaughter, Stanford University
Ramanan Sankaran, Oak Ridge National Laboratory
Myoungku Lee, Sandia National Laboratories
Aditya Konduri, Indian Institute of Science

Scientific Discipline: Chemistry: Combustion

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (600,000 Summit node-hours)

Research Summary: Engines for future industrial power and heat generation, ground transport of freight, and propulsion 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, combustion is governed by strong "turbulence-chemistry" interactions spanning a wide range of aerothermochemical conditions and coupled with multiphase spray physics.

Chen's team plans to continue work that was started in previous INCITE allocations, performing direct numerical simulations (DNS) of turbulent premixed spray autoignition in jet flames, varying the ambient temperature. The team will also perform DNS of turbulent premixed high-Karlovitz-number piloted jet flames at more intense turbulence conditions than was feasible in the past.

The team will initially target a lean methane air premixed jet flame at a Reynolds number of 21,079 based on recent experiments as part of a parameter study, with the Reynolds number based on an earlier DNS study in the same configuration. A significant portion of the effort will be to explore the use and fidelity of DNS in principal component (PC) composition space. If successful, this new approach of transporting PCs rather than species and temperature in reacting flow DNS will lead to enormous computational savings by as much as two orders of magnitude. The team will use the DNS data generated from the premixed flame to construct the set of in situ–derived PCs and to tabulate their transport properties and reaction rates.

Type: New
Title: "Electronic Stopping Simulation of Complex Systems"

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

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (2,000,000 node-hours)

Research Summary: Electronic stopping describes the transfer of kinetic energy from highly energetic charged particles to electrons in matter. This process results in massive electronic excitations within the target material.

Although the researchers' first-principles simulation approach—based on non-equilibrium real-time time-dependent density functional theory (RT-TDDFT)— has brought great success to modeling electronic stopping of light ion projectiles like protons, situations with heavier high-Z ion projectiles (i.e., ion projectiles featuring a large number of protons) present challenges. With this project, the researchers intend to advance their approach so as to study electronic stopping processes of complex systems for which going beyond typical-linear response theory formalism is necessary.

In particular, this work aims (1) to advance our understanding of electronic stopping with heavy high-Z ion projectiles in solids, (2) to investigate how hot electrons stimulate defect diffusion in magnesium oxide under proton, electron, and photo irradiation, and (3) to investigate details of electronic excitation dynamics of solvated DNA under ion irradiation of protons, alpha-particles, and carbon ions in the context of emerging ion beam cancer therapy, especially in comparison to electronic excitations under typical photon irradiation.

Type: Renewal
Title: "Enabling the Design of Drugs that Achieve Good Effects without Bad Ones"

Principal Investigator: Ron Dror, Stanford University

Scientific Discipline: Biological Sciences: Biophysics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (690,000 Summit 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.

In a prior INCITE allocation, Dror's team made substantial progress in determining how GPCRs affect the conformational ensemble of β-arrestin signaling proteins and also identified—for the first time—distinct intracellular GPCR conformations that have clear preferences for coupling to different intracellular signaling proteins. The team used the results to rationally design ligands with desired signaling profiles.

In this project, the team will continue focusing on identifying GPCR conformations that stimulate arrestin signaling more than G-protein signaling or G-protein signaling more than arrestin signaling. Determining such conformations is critical to enabling the rational design of GPCR-targeted drugs that achieve the desired effects with fewer side effects.

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

Principal Investigator: Mark Taylor, Sandia National Laboratories
Co-Investigators: David Bader, Lawrence Livermore National Laboratory
Karthik Balaguru, Pacific Northwest National Laboratory
Peter Caldwell, Lawrence Livermore National Laboratory
Walter Hannah, Lawrence Livermore National Laboratory
Christopher Jones, Pacific Northwest National Laboratory
Lai-Yung Ruby Leung, Pacific Northwest National Laboratory
Jungmin Lee, Lawrence Livermore National Laboratory
Matthew Norman, Oak Ridge National Laboratory
Stephen Price, Los Alamos National Laboratory
Mike Pritchard, University of California Irvine
Sarat Sreepathi, Oak Ridge National Laboratory
Luke Van Roekel, Los Alamos National Laboratory

Scientific Discipline: Earth Science: Climate Research

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (1,800,000 node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (1,000,000 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) How will more realistic portrayals of the water cycle's important features (resolution, clouds, aerosols, snowpack, river routing, land use) affect river flow and associated freshwater supplies at the watershed scale? (2) In cryosphere systems, what are the impacts of ocean-ice interactions on Antarctic ice shelf melting and the implications for ice sheet dynamics and sea level rise?

For the water cycle question, 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 the cryosphere question, the simulations assess the potential for significant increases in sub-ice shelf melt rates in response to past, ongoing, and future changes in global climate (and associated regional changes in the Southern Ocean).

Type: New
Title: "Exascale Artificial Intelligence to Accelerate Scientific Discovery"

Principal Investigator: Robert Patton, Oak Ridge National Laboratory
Co-Investigators: Thomas Potok, Oak Ridge National Laboratory
Steven Young, Oak Ridge National Laboratory
Catherine Schuman, Oak Ridge National Laboratory
Travis Johnston, Oak Ridge National Laboratory
Seung-Hwan Lim, Oak Ridge National Laboratory
Maxim Ziatdinov, Oak Ridge National Laboratory
Sergei Kalinin, Oak Ridge National Laboratory
Joel Saltz, Stony Brook University

Scientific Discipline: Computer Science: Computer Science

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (250,000 Summit node-hours)

Research Summary: Many scientific research applications rely on the analysis of imagery produced using scientific instruments such as microscopes. This analysis benefits from neural networks because, unlike other computer vision approaches, this approach does not rely on hand-engineered features. Instead, neural networks learn the features needed for the image-processing task from the data.

In this project, Patton's team will use the Multinode Evolutionary Neural Networks for Deep Learning and the Evolutionary Optimization of Neuromorphic Systems, which are artificial intelligence systems, to accelerate understanding of two different application areas: (1) nanoscale material fabrication using scanning transmission electron microscopy (STEM) imagery and (2) cancer research and treatment using digital pathology imagery.

The results of this work could bring real-time, image-based feedback for STEM significantly closer to a reality and enable the linking of pathology images and cancer registry abstracts to create a unique, population-wide, molecular view of cancer.

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): Cray XC40 (1,000,000 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: Renewal
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
Yehuda Ben-Zion, University of Southern California

Scientific Discipline: Earth Science: Geological Sciences

INCITE Allocation:

Site:	Argonne National Laboratory
Machine (Allocation):	Cray XC40 (500,000 node-hours)
Site:	Oak Ridge National Laboratory
Machine (Allocation):	IBM AC922 (300,000 node-hours)

Research Summary: Accurate seismic hazard assessments help inform and prepare society for earthquakes, enabling the development of design and mitigation strategies that save lives and reduce economic losses in the event of a major earthquake. The advancement of earthquake modeling and simulation tools 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) are working to enhance their earthquake simulation and hazard mapping tools to provide the best possible information in terms of earthquake ground motion and seismic hazard. This involves extending the SCEC software ecosystem, including CyberShake, for example, 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. A significant part of the research involves the integration and testing of new and improved simulation elements in the codes to model topography, realistic material rheology and inelasticity, 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. 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-class 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 Principles Investigation of Solid State Phase Transitions"

Principal Investigator: Markus Eisenbach, Oak Ridge National Laboratory
Co-Investigators: Valentino R. Cooper, Oak Ridge National Laboratory
Ying Wai Li, Los Alamos National Laboratory
Od Khorgolkhuu Odbadrakh, University of Tennessee, Knoxville
G. Malcolm Stocks, Oak Ridge National Laboratory
Ka Ming Tam, Louisiana State University
Yang Wang, Pittsburgh Supercomputing Center

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (500,000 Summit 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.

In a previous INCITE allocation, Eisenbach's team defined atomic-level stresses and showed, for the first time, that the dominant origin of solid solution strengthening that had been observed in these alloys is not principally due to the number of elements but results from the charge transfer between neighboring lattice sites in these alloys.

During 2020, the team will continue the research focused in these areas: ferroelectric materials, transition metal alloys, and disorder-driven functional materials. The team will expand the materials studied as well as concentrate on additional properties that will require additional statistics that will be enabled by access to Summit. In addition, the team will use the capabilities of full-potential locally self-consistent multiple scattering to accurately calculate the total energies and forces in large simulation cells that will allow the team to include the efects of local relaxations in multicomponent, solid-solution, concentrated high-entropy alloys.

Type: Renewal
Title: "Global Adjoint Tomography"

Principal Investigator: Jeroen Tromp, Princeton University
Co-Investigators: Ebru Bozdag, Colorado School of Mines
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 (450,000 Summit node-hours)

Research Summary: Information about Earth's interior comes from seismograms recorded at its surface. Seismic imaging based on spectral-element and adjoint-state 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.

Tromp's project addresses the long-standing challenge of imaging Earth's interior at the global scale based on full-waveform inversion. The team combines 3D simulations of global seismic wave propagation with the assimilation of seismographic data from an exhaustive earthquake catalog. These simulations will result in a much improved Earth model with drastically sharper contrasts around regions of interest. An anticipated impact on community paradigms includes sophisticated GPU-enabled open-source software freely distributed to the seismological community via the Computational Infrastructure for Geodynamics.

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

Principal Investigator: Choongseok Chang, Princeton Plasma Physics Laboratory
Co-Investigators: Mark Adams, Lawrence Berkeley National Laboratory
Luis Chacon, Los Alamos National Laboratory
Ed D'Azevedo, Oak Ridge National Laboratory
Stephane Ethier, Princeton Plasma Physics Laboratory
Robert Hager, Princeton Plasma Physics Laboratory
Scott Klasky, Oak Ridge National Laboratory
Seung-Hoe Ku, Princeton Plasma Physics Laboratory
Scott Parker, University of Colorado
Aaron Scheinberg, Princeton Plasma Physics Laboratory
Mark Shephard, Rensselaer Polytechnic Institute,
Sarat Sreepathi, Oak Ridge National Laboratory
Patrick Worley, PHWorley Consulting

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): IBM AC922 (970,000 node-hours)

Research Summary: This multi-year INCITE project seeks to advance the understanding of the edge plasma physics critical to 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 and future fusion reactors. In particular, they are performing studies on three high-priority challenges: (1) quantifying the narrowness of the heat-flux width on the ITER divertor material plates in the high-confinement mode (H-mode) operation during tenfold energy gain operation; (2) understanding the basic physics behind the low-to-high mode L-H transition and pedestal formation at the edge, which is necessary to achieve a tenfold energy gain in ITER; and (3) studying the control of edge localized instabilities that could damage the material wall in ITER and future magnetic fusion reactors. 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 Fidelity Study of Impact of Complex Flows on High Pressure Turbines"

Principal Investigator: Michal Osusky, GE Research
Co-Investigators: Rathakrishnan Bhaskaran, GE Research
Gustavo Ledezma, GE Research
Carlos Velez, GE Research
Sriram Shankaran, GE Aviation
Greg Sluyter, GE Aviation

Scientific Discipline: Engineering: Fluids and Turbulence

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (590,000 Summit node-hours)

Research Summary: Advances in computational fluid dynamics technology have enabled the aerothermal design of gas turbines used in aircraft engines and power generation equipment to achieve previously unattainable performance. Insatiable customer demands for lower cost of fuel consumption (higher thermal efficiency) and parts (maintenance and repair) result in increased operating temperatures in the high-pressure turbine (HPT) within very tight design margins.

Further design improvements demand understanding the complex flow physics that impact gas turbine performance—specifically the phenomena of flow mixing, boundary layer transition, separated flows, multiscale flow structures, and coupling between HPT components (e.g., stator/rotor interaction).

The GE team will leverage large eddy simulation capabilities to study the physics in a coupled stator/rotor HPT architecture in high fidelity and resolve the wake interactions and boundary layer transition. The competitive impact of design insight through this study includes improving efficiency (reducing fuel consumption) in jet engines and heavy-duty gas turbines as well as guiding opportunities to exploit additive and other advanced manufacturing capabilities.

Type: New
Title: "High-Performance Computation for Fusion Energy Wall Erosion Diagnostics"

Principal Investigator: Stuart Loch, Auburn University
Co-Investigators: David Ennis, Auburn University
Connor Balance, Queen's University of Belfast

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (400,000 Summit node-hours)

Research Summary: Current and next-generation fusion energy experiments use tungsten plasma-facing components (PFCs) to withstand the high heat loads on the plasma-wall interfaces. Determining the erosion and redeposition of this wall material is a critical issue for the success of fusion as an energy source. The potential for eroded tungsten atoms to transport into in the core plasma could quench the fusion reaction.

The diagnosis of erosion and redeposition of tungsten PFCs needs accurate ionization and excitation atomic data, which can only be calculated with large-scale computational facilities.

Loch's team will use Summit to produce accurate tungsten erosion and redeposition diagnostics for fusion tokamak experiments such as the DIII-D tokamak in California. The project is also of relevance for world-wide efforts on fusion energy, such as the ITER experiment under construction in France.

Type: New
Title: "High-Speed Turbulence with Shocks over Non-Adiabatic and Flexible Walls"

Principal Investigator: Johan Larsson, University of Maryland
Co-Investigators: Ivan Bermejo-Moreno, University of Southern California

Scientific Discipline: Engineering: Aerodynamics

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (2,000,000 node-hours)

Research Summary: This project investigates how supersonic wall-bounded turbulent flows are affected by the thermal wall boundary condition and how they interact with flexible walls. High-fidelity simulations at different Mach numbers, Reynolds numbers, and imposed wall temperatures will be used to create a database that advances the theoretical description of how the mean velocity profile scales with these factors. As current theories fail at high Mach numbers for either strongly cooled walls or nearly adiabatic walls, the results of this work will be used to develop a predictive model that remains accurate across all flow conditions. This, in turn, will lead to improved modeling techniques for near-wall turbulence and improved semi-empirical friction.

This project will also consider the interaction between supersonic turbulent boundary layers and shockwaves in the presence of rigid and flexible walls, and will create highly resolved reference data for two such cases (axisymmetric and planar interactions). These data will be used to assess and validate modeling techniques for near-wall turbulence in the context of large eddy simulations.

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

Principal Investigator: Zhihong Lin, University of California, Irvine

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (600,000 Summit node-hours)

Research Summary: Lin's project addresses the key physics identified by the current Scientific Discovery through Advanced Computing Center for Integrated Simulation of Energetic Particles in Burning Plasmas to improve physics understanding of energetic particle (EP) confinement and EP interactions with burning thermal plasmas. Since ignition relies on self-heating by energetic fusion products (α-particles), EP confinement is a critical issue for the international burning plasma ITER experiment—the crucial next step in the quest for clean and abundant fusion energy.

EP pressure gradients can readily excite mesoscale EP instabilities that can degrade overall plasma confinement and threaten the machine's integrity. EP could also strongly influence thermal plasma dynamics, including the microturbulence responsible for turbulent transport of thermal plasmas and macroscopic magnetohydrodynamic (MHD) modes, potentially leading to disastrous disruptions. In return, microturbulence and MHD modes can affect EP confinement. Providing an EP predictive capability requires an improvement in the understanding of EP physics by breaking the complex EP dynamics into these critical and cohesive components:

1. EP transport by mesoscale turbulence driven by EP pressure gradients and
2. EP coupling with microturbulence and macroscopic MHD modes driven by thermal plasmas.

The team will perform exascale simulations using the flagship gyrokinetic toroidal code, or GTC, to improve physics understanding of EP confinement and EP interactions with burning thermal plasmas. The project will develop a multiscale and multiphysics simulation for a predictive capability of EP physics in fusion plasmas and deliver an EP module incorporating both first-principles simulations and high fidelity reduced transport models to the future fusion whole-device modelling project.

Type: New
Title: "Large-Scale First Principles Calculations of Dislocation Core Energetics in Al and Mg"

Principal Investigator: Vikram Gavini, University of Michigan
Co-Investigators: Phani Motamarri, University of Michigan

Scientific Discipline: Engineering: Material Response

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (360,000 Summit node-hours)

Research Summary: Since the bronze age, mankind has been creating metals with desirable properties using basic metallurgical processes of alloying and "heating and beating," thereby altering their plasticity and failure properties. It is only in the last hundred years that scientists have obtained insights into the fundamental origins of crystalline plasticity.

New lightweight structural materials are critically required to reduce energy consumption and the carbon footprint in the automotive and aerospace sectors. However, a predictive dislocation-based theory of crystalline plasticity, vital for the computational design of next-generation lightweight structural alloys, is still elusive due to the extraordinary challenges posed by the multiscale physics ranging over a vast span of interacting length scales.

Gavini's team seeks to conduct fundamental investigations into the core energetics of dislocations in aluminum and magnesium using large-scale, real-space, finite-element-based Kohn-Sham density functional theory calculations (DFT-FE). The excellent parallel scalability and throughput performance of the numerical algorithms implemented in DFT-FE, combined with advantages of FE discretization in handling arbitrary boundary conditions, complex geometries, and systematic convergent behavior of the FE basis sets, allows the team to conduct the proposed simulations on dislocation energetics for the first time on Summit GPU nodes, which has not been possible heretofore.

Type: New
Title: "Lattice QCD"

Principal Investigator: Andreas Kronfeld, 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 Urbana–Champaign
Anna Hasenfratz, University of Colorado
Christoph Lehner, Universität Regensburg & Brookhaven National Laboratory
Swagato Mukherjee, Brookhaven National Laboratory
Konstantinos Orginos, College of William and Mary

Scientific Discipline: Physics: Particle Physics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (750,000 Summit node-hours)

Research Summary: The calculations geared to high-energy physics are well aligned with the US strategic plan, spelled out in the report of the Particle Physics Project Prioritization Panel. Likewise, those geared to nuclear physics are also well aligned with the US strategic plan, spelled out the long-range plan of the Nuclear Science Advisory Committee.

Kronfeld's team will perform work of interest to both fields. For example, nucleon form factors pertain to neutrino-oscillation experiments at Fermilab and to electron-proton scattering experiments at Jefferson Laboratory. A forward-looking program of calculations of parton distribution functions are relevant to the Large Hadron Collider at CERN and to the planned Electron-Ion Collider.

In the area of flavor physics, the team aims for subpercent precision on many quantities, and in the area of hot-dense quantum chromodynamics, it aims to elucidate experimental results from the Beam Energy Scan at the Lawrence Berkeley National Laboratory Relativistic Heavy-Ion Collider.

Type: New
Title: "Long Term 3D Simulations of Core-Collapse Supernovae"

Principal Investigator: William Raphael Hix, Oak Ridge National Laboratory
Co-Investigators: Stephen Bruenn, Florida Atlantic University
Eric Lentz, University of Tennessee
James Austin Harris, Oak Ridge National Laboratory
Anthony Mezzacappa, University of Tennessee

Scientific Discipline: Physics: Astrophysics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (660,000 Summit node-hours)

Research Summary: Core-collapse supernovae—the explosive final moments of massive stars—are complex, dynamic multiphysics events yielding a bright and energetic explosion and a newborn neutron star or black hole. The central engine of a core-collapse supernova generates rare transient signals in gravitational waves and neutrinos. The explosion creates and ejects many chemical elements, including the primary constituents of the Earth, dominating the production of elements from oxygen to iron throughout the Universe.

The core-collapse supernova problem has been a computational challenge for several decades, and today the world is entering an era in which the well-resolved, symmetry-free, 3D simulations with sufficient physical detail and coupling required to understand these complex stellar explosions and their byproducts are now possible. However, the number of extant 3D simulations with adequate physics is small, and none have been run until the explosion matures more than a second after the proto-neutron star forms.

Hix's project aims to explore and bring understanding of the impact of stellar rotation on the explosion mechanism of core-collapse supernovae and the associated observables, as well as the development of the proto-neutron star wind following the onset of explosion. These studies will directly support and guide the experimental efforts at the Facility for Rare Isotope Beams, expected to open in 2021, and similar facilities by helping to establish the sites of the r-process and p-process.

Type: Renewal
Title: "Molecular Dynamics of Motor–Protein Networks in Cellular Energy Metabolism"

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

Scientific Discipline: Biological Sciences: Biophysics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (230,000 Summit node-hours)

Research Summary: This INCITE project investigates two biomolecular systems, each of which promises a significant impact on US energy and health issues: (1) conformational transitions involved in mitochondrial protein complexes and (2) membrane-wide energy conversion in the chromatophore of purple bacteria. These exemplify, respectively, processes fundamental to respiration in animals and photosynthesis in plants.

Following a successful transition path sampling simulation of conformational transitions in a V-type ATPase under a previous allocation, Singharoy's team now embarks on simulating a complete F-type ATPase (also called Complex V), using an analogous Replica Exchange Molecular Dynamics methodology. The group is also simulating entire biological membranes from the simplest of photosynthetic organisms (e.g., purple photosynthetic bacteria) in atomic detail.

The results of simulating Complex V will bring an understanding of the molecular details of coupling between the ATP-reaction and proton transport events between the soluble and transmembrane arms. In addition, by simulating entire biological membranes, the team will gain and understanding of the long-range diffusion characteristics of 12 charge carriers in cytochrome c_2 and quinone that are involved simultaneously in the photosynthesis process.

Type: New
Title: "Novel Methods for Complex Excited-State Phenomena in Functional Materials"

Principal Investigator: Jack R. Deslippe, Lawrence Berkeley National Laboratory
Co-Investigators: Steven G. Louie, University of California, Berkeley; Lawrence Berkeley National Laboratory
Jeffrey B. Neaton, University of California, Berkeley; Lawrence Berkeley National Laboratory
James R. Chelikowsky, University of Texas, Austin)
Diana Y. Qiu, Lawrence Berkeley National Laboratory; Yale University
Felipe H. da Jornada, Lawrence Berkeley National Laboratory
Sivan Refaely-Abramson, Weizmann Institute of Science

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (400,000 Summit node-hours)

Research Summary: Many of the present technologies on which global industries are based, such as silicon technology for computers or optoelectronics and photovoltaics, will become increasingly more advanced with the advent of new technologies that are based on devices built from complex and functional materials. These new devices represent a broad class of systems which exhibit unique and controllable electronic and optical properties triggered by atomic arrangements specifically engineered at the nanoscale level.

Deslippe's team will apply and advance state-of-the-art ab initio approaches to understand and predict complex excited-state phenomena in novel and functional materials. The team will explore various types of systems of structural complexity and emerging scientific interest to understand the underlying interactions dominating their optoelectronic properties and the structural dependencies of those interactions, thus identifying principles to rationally design new materials with optimal properties.

Type: New
Title: "Nuclear Matter Dynamics in Real Time and the Heaviest Elements in Nature"

Principal Investigator: Aurel Bulgac, University of Washington
Co-Investigators: 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
Gabriel Wlazłowski, Warsaw University of Technology

Scientific Discipline: Chemistry: Physical

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

Research Summary: Nuclear physics is poised to answer fundamental questions about nature, but these questions are complex and the answers require the latest developments in theory, high-performance computing, and new emerging compute elements and architectures.

Bulgac's team will use the full quantum mechanical predictive tools needed to quantitatively describe nuclear fission, collisions of heavy ions, and fusion—including the total kinetic energy released, the properties and excitation energies of the fission fragments, their masses, charges, excitation energies, angular momenta, the spectra of emitted neutrons, the multinucleon, and the energy transfer in low and medium energy heavy-ion collisions.

The microscopic description of low-energy heavy-ion reactions, in particular the calculation of fusion cross-sections and of nucleon transfer cross-sections, has fundamental and practical importance. These reactions are relevant for the physics at the Facility for Rare Isotopes Beams and many other laboratories in US and across the world for further pursuing the quest for superheavy elements, for extending the periodic table of elements, and for explaining the origin and the abundance of chemical elements in the Universe.

Type: Renewal
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
Han Wen, University of Rochester

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (1,000,000 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.

The INCITE project is harnessing the power of DOE leadership computing resources to study the kinetic evolution of LPI on meaningful spatial and temporal scales directly relevant to various IFE scenarios. Using the popular PIC code OSIRIS, the team is performing fully kinetic simulations that will help advance research at the National Ignition Facility and other IFE experiments (e.g., direct drive and shock ignition studies at the OMEGA facility at the University of Rochester).

Type: Renewal
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): Cray XC40 (600,000 node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (110,000 node-hours)

Research Summary: Relativistic plasma mirrors (PM), produced when a high-power laser hits a solid target, can provide very promising compact sources of relativistic electron, ions, and very intense extreme ultraviolet Doppler harmonic light sources.

This project aims to show, in silico and using massively parallel pseudo-spectral particle-in-cell (PIC) simulations, that such PMs can provide a simple and common elegant solution to three long-standing challenges of ultrahigh-intensity (UHI) physics.

These three challenges are: (1) Can we produce high-charge compact electron accelerators with high beam quality that will be essential to push forward the horizons of high energy science? (2) Can we produce efficient and very compact high-energy ion accelerators to democratize cancer hadron-therapy? (3) Can we reach extreme light intensities approaching the Schwinger limit of approximately 10^{29}W·cm^{-2}, beyond which light self-focuses in vacuum and electron-positrons pairs are produced?

Type: New
Title: "PRECISE: Predictive Electronic Structure Modeling of Heavy Elements"

Principal Investigator: Lucas Visscher, Vrije Universiteit Amsterdam
Co-Investigators: Anastasia Borschevsky, University of Groningen
Wibe Albert de Jong, Lawrence Berkeley National Laboratory
André Severo Pereira Gomes, CNRS and University of Lille
Miroslav Iliaš, Matej Bel University
Hans Jørgen Aagaard Jensen, University of Southern Denmark
Dmitry Liakh, Oak Ridge National Laboratory
Valeria Pershina, GSI Helmholtzzentrum für Schwerionenforschung
Michal Repisky, University of Tromsø
Trond Saue, Université Paul Sabatier Toulouse III
Valérie Vallet, CNRS and University of Lille

Scientific Discipline: Chemistry: Physical

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (400,000 Summit node-hours)

Research Summary: In this project, an international team will study frontier aspects of the physics and chemistry of molecules containing one or more heavy elements. The accurate treatment of molecular energies and properties of these elements requires inclusion of both relativistic and electron correlation effects. This has only recently become feasible due to the team's realization of a relativistic coupled cluster implementation that has been designed specifically for massively parallel GPU-accelerated supercomputers as part of the OLCF's Center for Accelerated Application Readiness program for Summit.

These applications will aid in the search for new physics beyond the Standard Model, unravel the complicated chemistry and spectroscopy of f-elements, and provide predictions for the chemical properties of superheavy elements. The project aims to set a new standard for accurate modelling of heavy elements and fill a large gap in the set of computational benchmark data for molecular systems. Filling this gap is for instance essential in the development of density functionals that can specifically target heavy elements. The project will thereby have an impact on computational chemistry that goes far beyond the results of the individual studies.

Type: New
Title: "Predictive Chemistry of Realistic Systems for Advanced Nuclear Energy"

Principal Investigator: David Dixon, The University of Alabama
Co-Investigators: Aurora Clark, Washington State University
Kirk Peterson, Washington State University
Xiaosong Li, University of Washington

Scientific Discipline: Chemistry: Inorganic

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (500,000 Summit node-hours)

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

Understanding the chemistry of the actinides is one of the core issues that must be addressed in order to develop appropriate technologies, but the difficulty and expense in doing experiments on very rare and highly radioactive materials makes simulation a critical component of any program in actinide science to improve safety and reduce costs.

In this project, Dixon's team will extend its highly accurate coupled cluster CCSD(T) extrapolated complete basis set results for actinide compounds and develop new computational capabilities to study actinide complexes in various oxidation states in solution, at interfaces, and at the nanoscale. Specific areas include hydrolysis, aggregation reactions, separation systems, and the properties of interfaces. These studies will afford the team unique insights into the solvation of actinides and how to treat collective weak interactions, which are important in the formation of nanoparticles, colloids, and other phase transformation phenomena that can impact the design of separations systems.

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

Principal Investigator: Shiwei Zhang, Flatiron Institute; College of William & 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 (550,000 Summit 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 the advent of petascale and exascale computing presents a unique opportunity to make fundamental progress on this problem. The project of Zhang's team 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 that 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 computational and 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.

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

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

Scientific Discipline: Physics: Astrophysics

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (1,800,000 node-hours)

Research Summary: This work aims to advance our understanding of the physical mechanisms that drive the large mass loss rate for Wolf-Rayet (WR) stars—stars that are hotter and typically have a higher Eddington ratio than the massive stars studied in previous INCITE allocations.

Previous studies carried out 3D global radiation hydrodynamic simulations with initial envelope structures covering a wide range of parameter space for massive stars, and quantified the effects of enhanced opacity resulting from the turbulent broadening of the lines on the mass loss rate and envelope structures. Researchers also examined the envelope structures of a 20 solar mass star when the luminosity reaches 40% of the Eddington value for electron scattering opacity.

This allocation will be used to study the envelopes of a 40 solar mass star, setting the stage for research into how the star's mass loss rate and envelope structure depend on rotation.

Type: New
Title: "Reionization and Its Impact on the Local Universe: Witnessing Our Own Cosmic Dawn"

Principal Investigator: Pierre Ocvirk, Observatoire Astronomique de Strasbourg
Co-Investigators: Paul R. Shapiro, University of Texas
Dominique Aubert, Observatoire Astronomique de Strasbourg
Stefan Gottloeber, Leibniz-Institut für Astrophysik
Ilian T. Iliev, University of Sussex
Jenny Sorce, Centre de Recherche Astrophysique de Lyon
Gustavo Yepes, Universidad Autonoma de Madrid
Romain Teyssier, University of Zurich
Kyungjin Ahn, Chosun University

Scientific Discipline: Physics: Astrophysics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (600,000 Summit node-hours)

Research Summary: When the first stars and galaxies formed more than 100 million years after the Big Bang, they released ultraviolet radiation that ripped apart hydrogen atoms in the intergalactic medium and heated gas there to 10,000 K, while polluting the pristine, primordial gas with the first heavy elements ("metals") produced by the same massive stars. This created a patchwork of ionized zones that grew over the first billion years until they overlapped and the universe was fully reionized. This epoch of reionization is one of the last windows of cosmic time subject to direct detection and a critical missing link in galaxy formation theory.

Ocvirk's team will perform frontier simulations of the reionization of the Local Universe to probe the cosmological evolution of the Universe at large by comparing theory with observations to link the properties of the nearest galaxies today with their origin in the history of global reionization at high redshift. The team will simulate the fully-coupled radiation-hydrodynamical-gravitational N-body evolution of the local Universe in a volume 300 million light-years across, centered on the Milky Way, with the world-leading resolution of $8{,}192^3$ particles and $8{,}192^3$ cells, as required to resolve the formation of feedback-suppressed dwarf galaxies in a volume large enough to model global reionization.

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

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

Scientific Discipline: Physics: Astrophysics

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

Research Summary: In August 2017, gravitational waves (GWs) from a merger of binary neutron stars were detected for the first time, accompanied by optical/UV electromagnetic "kilonova" emission (due to the radioactive decay of r-process elements synthesized in the ejecta) and by a radio, x-ray, and gamma-ray flare (due to a jetted outflow). To meaningfully interpret this exciting discovery and make predictions for future GW detections and their electromagnetic counterparts, Tchekhovskoy's team will simulate the long-term evolution of a magnetized turbulent merger remnant accretion disk and its outflows.

Summit will also allow the team to carry out the long-awaited, truly thin tilted disks simulations with $h/r = 0.02$ to determine whether inner regions of such disks align with the black hole by the purely general relativistic Bardeen-Petterson effect.

Both goals push the limits of physics and computation in preparation for future exascale systems and will lead to a better understanding of magnetized black hole accretion systems, especially in regards to recent paradigm-shifting results obtained by the team that suggest that at large tilt values, the disk breaks or tears apart, potentially leading to a substantially higher disk radiative efficiency accompanied by flaring events.

Type: New
Title: "Solvent-Lignocellulose Interactions for 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): IBM AC922 (400,000 Summit node-hours)

Research Summary: Due to the robust 3D structures of secondary plant cell walls, biomass is recalcitrant to conversion to biofuels and other high-value bioproducts. This recalcitrance can be, in principle, overcome by solvent pretreatment. Three classes of solvent-based pretreatments are of particular interest: organic cosolvents, ionic liquids, and deep eutectic solvents. Each of these has been shown experimentally to increase the efficiency of biomass conversion to bioproducts relative to previous methods.

Smith's team will apply state-of-the-art adaptive sampling molecular dynamics simulations on Summit to determine structural changes to cellulose and lignin together with the free energy of binding between biomass polymers in seven different pretreatment solvents (and water) derived from organic cosolvents, ionic liquids, and deep eutectic solvents.

The simulations will provide atomic-scale details of biomass-solvent interactions, which will lead to a quantitative determination of the physical properties required of effective biomass solvents. Furthermore, the simulations will serve as a means to rationalize a wide range of ongoing experimental studies.

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

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

Scientific Discipline: Biological Sciences: Biophysics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (550,000 Summit node-hours)

Research Summary: Fundamental mechanisms in cell function and communication (e.g., in the brain) are understood only phenotypically based on inferences from experiments that do not reach down to molecular scale. This is clearly not an ideal position from which to address disease, attempt to mitigate the effects of toxic environments, or employ the richness of biological templates to guide nanotechnology or the design of complex molecular machines.

The discovery and quantifications of the underlying fundamental molecular processes that are needed to accomplish these important tasks is a grand challenge in current biomedicine and biophysics.

In this project, Weinstein's team will use computational simulation and analysis to take advantage of the precious structural and functional data provided by crystallography, nuclear magnetic resonance spectroscopy, ultra-resolution microscopy, and cryo–electron microscopy at the required atomic or near-atomic resolution in order to uncover and quantify the dynamic molecular mechanisms of complex molecular machines.

By using advanced mechanistic analyses of trajectories from molecular dynamics dynamics simulations at unprecedented scales, the team will discover the molecular mechanisms of the functions and properties that are found in eukaryotic but not prokaryotic neurotransmitter transporters in the same (neurotransmitter:sodium symporters) class (e.g., the switch of activity from reuptake to efflux) in order to achieve a novel level of understanding of biological functions and to enable designs of synthetic analogs of such molecular machines with specifically engineered properties and functions.

Type: New
Title: "The Structure and Interactions of Nucleons from the Standard Model"

Principal Investigator: André Walker-Loud, Lawrence Berkeley National Laboratory
Co-Investigators:
Colin Morningstar, Carnegie Mellon University
Amy Nicholson, University of North Carolina at Chapel Hill
John Bulava, Souther Denmark University
Kate Clark, NVIDIA
Evan Berkowitz, Forschungszentrum Julich
Chris Bouchard, University of Glasgow
Chia Cheng Chang, RIKEN and University of California, Berkeley
Arjun Gambhir, Lawrence Livermore National Laboratory
Ben Hoerz, Lawrence Berkeley National Laboratory
Dean Howarth, Boston University
Chris Koerber, University of California, Berkeley
Ken McElvain, University of California, Berkeley
Henry Monge-Camacho, University of North Carolina at Chapel Hill
Enrico Rinaldi, RIKEN
Andrew Hanlon, Mainz University

Scientific Discipline: Physics: Nuclear Physics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (500,000 Summit node-hours)

Research Summary: Walker-Loud's team will perform lattice quantum chromodynamics calculations relevant to the broader nuclear physics community and the search for new physics. Building on the progress the team made in calculations of nucleon structure and two-nucleon interactions on Summit, combined with state-of-the-art techniques in two-particle spectroscopy, the team will conclude its study of the nucleon axial form factor and calculate two-nucleon scattering phase shifts at $m_\pi \sim 200$ MeV.

It is widely believed that computing finite volume spectra using correlation matrix methods with variationally-optimized operators, which has been highly successful for calculations of mesonic scattering, will be necessary to resolve discrepancies and reliably control systematics in the two-nucleon system. These calculations will be unprecedented and crucial for the interpretation of several high-profile experiments utilizing nuclei in the search for new physics, as well as the broader goal of understanding nuclear physics from first principles.

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

Principal Investigator: Adam Burrows, Princeton University
Co-Investigators:

Scientific Discipline: Physics: Astrophysics

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (2,000,000 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.

Since the 1960s, there has been an agonizingly slow march towards demonstrating a robust mechanism of supernovae explosion. 2D simulations of supernovae have supported the theory that capturing a small fraction of the neutrinos emitted during collapse powers the explosions, but detailed 3D calculations proving this paradigm are lacking. With the power of leadership-class supercomputers and continued advances in software, researchers now have the capabilities to tackle this longstanding challenge in nuclear astrophysics.

This multi-year INCITE project is addressing whether and how 3D supernova explosion models differ from their 2D counterparts. The researchers are using the 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 50-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 Predictive Simulations of Functional and Quantum 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
Ye Luo, Argonne National Laboratory
Lubos Mitas, North Carolina State University
Eric Neuscamman, University of California, Berkeley
Fernando Reboredo, Oak Ridge National Laboratory
Luke Shulenburger, Sandia National Laboratories
Miguel Morales, Lawrence Livermore National Laboratory

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (1,500,000 node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (400,000 node-hours)

Research Summary: Our ability to understand, predict, and design functional and quantum materials is severely hindered by the limited predictive power of computational quantum-mechanical approaches. For functional materials, the strong couplings between electron charge, spin, and the atomic positions that yield novel functionality make predictive simulations a grand challenge. For quantum materials—solids with exotic physical properties arising from the quantum-mechanical nature of their constituent electrons—the challenge is even greater.

This project aims to demonstrate significant progress towards the establishment a truly predictive, empirical, and external-parameter-free materials-specific theory, applying newly developed techniques based on quantum Monte Carlo (QMC). By directly solving the Schrödinger equation, these techniques can be used with general materials and employ very few approximations.

Centered around the open-source QMCPACK code and supported by the DOE BES Computational Materials Sciences Center for the Predictive Simulation of Functional Materials, the project focuses on the development, application, validation, and dissemination of empirical parameter-free methods and open-source codes to predict and explain the properties of functional materials for energy applications. To demonstrate a truly predictive and validated framework, it performs calculations on complex materials that possess a wide spectrum of properties, benefiting both fundamental science and new electronics, energy storage, conversion, and quantum technologies.

Type: New
Title: "Towards Understanding Instability Mechanisms of Axial Compressors"

Principal Investigator: Charles Hirsch, Numeca International

Scientific Discipline: Engineering: Fluids and Turbulence

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (305,000 Summit node-hours)

Research Summary: Energy transformation systems rely on rotating machines, such as gas turbines, transforming chemical energy from combustion into mechanical energy, to efficiently drive electrical generators or aircraft engines. Their impact on the environment is significant and reduction of emissions and fuel consumption are critical to the continued growth and sustainability of the global energy conversion process. Key factors in the reduction in emissions and fuel consumption are tied to the performance of the gas turbine components, namely compressor, combustor and turbine components and their operating range.

The present project is focused on compressor performance limits, which condition the stability and operating range of the whole of the gas turbine system. Of particular interest is the mechanisms leading to the onset of stall and the subsequent appearance and propagation of rotating stall configurations in axial compressors.

This knowledge will help industrial turbomachinery designers understand and potentially delay or avoid the onset of stall, resulting in components with robust stall margins and operating ranges with higher efficiency. In addition, by collecting and feeding these new data towards design methodologies based on engineering methods, either empirical or Reynolds-averaged Navier-Stokes equations, optimizations with enhanced knowledge and significant potential energy savings will be made possible.

The industrial partners Dresser-Rand and Concepts NREC are contributing to the data analysis and to the potential integration of the gained knowledge into their design process and design tools.

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

Principal Investigator: Joseph Oefelein, Georgia Institute of Technology
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 (400,000 Summit 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. The goal is to establish an improved understanding of turbulent multiphase injection, mixing, and combustion processes at 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).

In a prior INCITE project, Oefelein's team performed a series of staging studies to verify the performance and accuracy of the coupled system of submodels required for LOX/CH_4 mixing layer calculations. This project uses the marked improvement in speed and capacity provided by the OLCF Summit platform to establish new databases with increased detail in both physics and dimensionality at the same high-pressure, high-Reynolds-number conditions present in actual engines.

In the 2020 INCITE project, Oefelein's team will perform direct numerical simulations (DNS) of LOX/CH_4 mixing layer dynamics at supercritical pressures and investigate trends from these. In addition, the team will perform hybrid DNS and large eddy simulations (LES) of LOX/H_2 and LOX/CH_4 shear-coaxial and swirl-coaxial injection processes with acoustic excitation and LES of transverse instabilities in a multielement laboratory-scale combustion chamber.

Type: New
Title: "Ultrafast Control of Functional Materials"

Principal Investigator: Priya Vashishta, University of Southern California
Co-Investigators: Rajiv K. Kalia, University of Southern California
Aiichiro Nakano, University of Southern California

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

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (2,000,000 node-hours)

Research Summary: Recent advancements in ultrafast materials science have raised the possibility of using femtosecond light pulses to switch emergent properties of quantum materials on demand. Such ultrafast and high-quantum-efficiency switching of material properties (e.g., polarization and conductivity) has the potential to revolutionize future information and energy technologies using non-equilibrium processes in quantum materials. With this INCITE project, researchers from the University of Southern California will leverage leadership-scale quantum dynamics simulations, machine learning, and x-ray free-electron laser (XFEL) experimental data to extend the frontier of ultrafast materials science.

State-of-the-art XFEL and ultrafast electron diffraction (UED) experiments now provide unprecedented capability to observe light-induced material dynamics with sub-nanometer spatial and femtosecond time resolutions. By observing the motions of electrons and atoms at their natural time scales, these experiments will help accelerate ultrafast control of quantum-material properties. Understanding the complex far-from-equilibrium quantum dynamics from first principles, however, poses an enormous computational challenge that necessitates the use of leadership computing resources.

Building on the success of previous INCITE awards, the University of Southern California team will use the Theta supercomputer to predict ultrafast function-property-structure relationships that dictate light control of emergent material properties in complex nanostructures composed of three classes of advanced functional materials: (1) layered-material heterostructures and magic-angle heterostacks; (2) novel chalcogenide perovskites; and (3) topological skyrmions superlattices. The researchers will perform 10^4-atom nonadiabatic quantum molecular dynamics (NAQMD) and billion-atom reactive molecular dynamics (RMD) simulations that will not only mirror far-from-equilibrium electronic and lattice dynamics in next-generation XFEL experiments at the forthcoming Linac Coherent Light Source (LCLS-II) at exactly the same space and time scales, but also provide fundamental understanding of their structural transition pathways and electronic origins, which is critical for the advancement of emerging ultrafast materials science.