Type: New

Title: "Ab Initio Investigation of Disorder and Defects in Structural and Functional Materials"

Principal Investigator: Markus Eisenbach, Oak Ridge National Laboratory

Co-Investigators: Valentino R. Cooper, Oak Ridge National Laboratory
Mina Yoon, Oak Ridge National Laboratory
Swarnava Ghosh, Oak Ridge National Laboratory
Ka-Ming Tam, Louisiana State University
Hanna Terletska, Middle Tennessee State University
Yang Wang, Carnegie Mellon University

Scientific Discipline: Materials

INCITE Allocation:

Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (290,000 Summit node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (250,000 Frontier node-hours)

Research Summary: Real materials show disorder at the atomic level and behave differently from perfect crystals that can be described readily with standard computational methods. The team employs high performance computing to explore the quantitative and qualitative changes in the behavior of electrons in materials due to disorder and finite temperature that can lead to new fundamental behavior. This INCITE allocation will provide computer resources to enable research in the Materials Theory, Modeling and Simulations Section at Oak Ridge National Laboratory, that is funded by the following DOE-BES awards: Advanced Theoretical and Computational Approaches for Quantum Materials (ERKCS92, PI: F. Reboredo), Simulation, Design, and Discovery of Complex Materials (ERKCS91, PI: V. R. Cooper), Understanding and Controlling Entanglement in Solid-State Systems via Atomic Scale Manipulation (ERKCK47, PI: S. Jesse), Growth Mechanisms and Controlled Synthesis of Nanomaterials (ERKCS81, PI: K. Xiao), and Quantum Science Center at ORNL.

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, Universität Bonn
Stefano Gandolfi, Los Alamos National Laboratory
Gustav R. Jansen, Oak Ridge National Laboratory
Dean J. Lee, Facility for Rare Isotope Beams and Michigan State University
Justin G. Lietz, Oak Ridge National Laboratory
Alessandro Lovato, Argonne National Laboratory
Pieter Maris, Iowa State University
Petr Navrátil, TRIUMF
Thomas Papenbrock, University of Tennessee and Oak Ridge National Laboratory
Saori Pastore, Washington University in St. Louis
Maria Piarulli, Washington University in St. Louis
James P. Vary, Iowa State University
Robert B. Wiringa, Argonne National Laboratory

Scientific Discipline: Physics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (690,000 Summit node-hours)
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (2,500,000 Theta node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (900,000 Frontier node-hours)

Research Summary: This INCITE project will lead to improvements in the simulation capabilities of atomic nuclei and nuclear matter, and their reactions with neutrinos and electrons. The team will advance their understanding of nuclear phenomena by targeting predictive capabilities regarding structure and reactions of nuclei, fundamental symmetries, and neutrino and electron interactions in nuclei. The project targets experiments and science at the Facility for Rare Isotope Beams (FRIB), Jefferson Laboratory (JLab), the Deep Underground Neutrino Experiment (DUNE), and ton-scale detectors for neutrinoless double β decay. The work will enable science not available previously and accelerate scientific discovery through high-performance computing. The team will perform state-of-the-art simulations to provide quantified predictions where direct experiment is not possible or is subject to large uncertainties. Such calculations are relevant to many applications in nuclear energy, nuclear security, and nuclear astrophysics, since rare nuclei lie at the heart of nucleosynthesis and energy generation in stars.

Type: New
Title: "Accurate Quantum Chemistry Study of Carbon Capture with Solid-Supported Amines"

Principal Investigator: Peng Xu, Ames Laboratory
Co-Investigators: Giuseppe Barca, Ames Laboratory
Mark Gordon, Iowa State University
Sarom Leang, EP Analytics
Buu Pham, Ames Laboratory
Tosaporn Sattasathuchana, Ames Laboratory

Scientific Discipline: Chemistry

INCITE Allocation:

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

Research Summary: With this project, researchers will perform high-level quantum chemistry calculations to elucidate the physisorption and chemisorption processes of CO_2 capture with amine-functionalized mesoporous silica nanoparticles. The team will provide insights and guidance for the rational design of solid sorbent with optimal balance of CO_2 capacity and oxidative stability.

The dramatic increase of atmospheric CO_2 concentration due to anthropogenic CO_2 emission resulting from over a century of fossil fuel combustion has been recognized by the Intergovernmental Panel on Climate Change (IPCC) as the primary source of modern climate changes and global warming. While technologies that can reduce the consumption of fossil fuels, increase energy efficiency, and use renewable energy sources (e.g., solar, wind) can bring down CO_2 emissions, carbon negative technologies, removing CO_2 at the source or from the atmosphere, need rapid development in order to address the scale of the current problem and achieve the challenging target set out in the Paris Agreement. Quantum mechanical (QM) simulations of target materials at their real length scale can uncover accurate atomistic insights that are difficult to obtain experimentally or overlooked by smaller or simplified models and provide guidelines to design desired materials. Research in this proposal will leverage the highly efficient and scalable, GPU-enabled, QM-based methods developed from the GAMESS Exascale Computing Project (ECP) to study and design amine-functionalized mesoporous silica nanoparticles (MSNs) for carbon capture applications.

Type: New
Title: "Advanced Computational Modeling of Molecular Machines in Nucleotide Excision Repair"

Principal Investigator: Ivaylo Ivanov, Georgia State University

Scientific Discipline: Biology

INCITE Allocation:

Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (290,000 Summit node-hours)

Research Summary: The project will leverage new computational and hybrid modeling approaches to provide unified knowledge of the assembly, dynamics and function of key complexes in nucleotide excision DNA repair – the most versatile pathway for removal of DNA damage from exposure to environmental carcinogens. The project will impact understanding of human disease etiology and treatments. The INCITE project will leverage new cryo-EM structures, data from genetics and biochemistry and combine these with novel computational modeling and analysis methods. The team's integrated strategy relies on extensive molecular dynamics (MD) simulations of key NER complexes in disparate functional states. The team also employ new graph-theoretical methods to define dynamic communities and allosteric mechanisms in vital NER assemblies.

The wide variety of lesions processed by NER has led to the evolution of a remarkably complex protein machinery. Defects in this machinery are associated with severe human genetic diseases – ultraviolet radiation sensitive syndrome, xeroderma pigmentosum, cerebro-oculo-facio-skeletal syndrome, trichothiodystrophy, and Cockayne syndrome. Yet, a basis for this striking heterogeneity in clinical outcomes has not emerged. Thus, unravelling NER mechanisms at the molecular level is a grand challenge in biomedical science. Equally important is understanding how NER is intertwined with other vital pathways that orchestrate the expression and repair of genes.

Type: New
Title: "Advanced Computing for Correlated Quantum Materials"

Principal Investigator: Thomas Maier, Oak Ridge National Laboratory
Co-Investigators: Steven Johnston, University of Tennessee, Knoxville
Gonzalo Alvarez, Oak Ridge National Laboratory
Peter Doak, Oak Ridge National Laboratory

Scientific Discipline: Materials

INCITE Allocation:

Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (720,000 Summit node-hours)

Research Summary: Correlated quantum materials show great promise for revolutionizing many energy-related technologies but require optimization to unleash their full potential.

This project will perform high-end simulations of correlated quantum materials, in order to understand, predict and optimize their complex behavior, and thus help accelerate development in this area. This project aims to understand and reliably predict the rich phenomenology in correlated quantum materials induced by multiple orbital degrees of freedom, geometric frustration, spin-orbit interactions, and electron-phonon coupling. With this goal in view, the team will conduct unprecedented numerical studies of multi-orbital Hubbard models, including variants on highly frustrated lattices and with additional spin-orbit and electron-phonon interactions. The team will study these models with advanced numerical algorithms, including the dynamic cluster, determinant quantum Monte Carlo, and density matrix renormalization group methods, using implementations that the team have heavily optimized for ORNL's Summit supercomputer. The use of leadership computing will allow the team to go well beyond previous work in terms of problem size and thus provide new insight into problems that have not been accessible before.

Type: New
Title: "Advances in Quark and Lepton Flavor Physics with Lattice QCD"

Principal Investigator: Andreas Kronfeld, Fermilab
Co-Investigators: Thomas Blum, University of Connecticut
Peter Boyle, Brookhaven National Laboratory
Norman Christ, Columbia University
Carleton DeTar, University of Utah
Aida Khadra, University of Illinois at Urbana-Champaign
Steven Gottlieb, Indiana University
William Jay, Massachusetts Institute of Technology
Luchang Jin, University of Connecticut
Chulwoo Jung, Brookhaven National Laboratory
Christoph Lehner, Universität Regensburg
Andrew Lytle, University of Illinois at Urbana-Champaign
Robert Mawhinney, Columbia University
Ruth Van de Water, Fermilab

Scientific Discipline: Physics

INCITE Allocation:

Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (1,000,000 Summit node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (1,250,000 Frontier node-hours)

Research Summary: Starting from the Standard Model of elementary particles, this project performs high-precision numerical calculations, so that the results can be compared with results of high-precision experiments. Any discrepancies between theory and experiment will provide clues for as-yet undiscovered physical processes at work. The calculations are well aligned with the U.S. strategic plan, spelled out several years ago in the report of the Particle Physics Project Prioritization Panel. Because of these important, ambitious goals the highest-capability supercomputers—Summit (OLCF), Frontier (OLCF), and Aurora (ALCF)—are necessary to make an impact.

Type: New
Title: "AI-Guided Exascale Simulations of Quantum Materials Manufacturing and Control"

Principal Investigator: Aiichiro Nakano, University of Southern California
Co-Investigators: Rajiv Kalia, University of Southern California
Ken-ichi Nomura, University of Southern California
Priya Vashishta, University of Southern California

Scientific Discipline: Materials Science

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): HPE Apollo 6500 (200,000 Polaris node-hours)

Research Summary: This project will boost scalable manufacturing of quantum materials and ultrafast control of their emergent properties on demand using AI-guided exascale quantum dynamics simulations. In particular, these efforts will focus on the self-assembly of layered material (LM) metastructures (i.e., atomically thin origami) for scalable and robust manufacturing of quantum emitters for future quantum information science and technology, as well as picosecond optical, electrical, and mechanical control of symmetry breaking in topological ferroelectric skyrmion, skyrmionium and meron for emerging ultralow-power polar "topotronics."

Hundred-thousand-atom nonadiabatic quantum molecular dynamics and billion-atom reactive molecular dynamics and excited-state neural-network quantum molecular dynamics simulations will significantly extend the scope of prototype Aurora Early Science Program simulations to a richer set of quantum material applications for LM quantum emitters and polar topotronics.

The simulations performed will not only mirror far-from-equilibrium electronic and lattice dynamics in x-ray free-electron laser (XFEL) and ultrafast electron diffraction (UED) experiments at the Stanford Linac Coherent Light Source at exactly the same space and time scales, but will also provide fundamental understanding of their structural transition pathways and electronic origins.

This work, directly validated by XFEL, UED and neutron experiments at DOE facilities, will enable future production of high-quality custom quantum material architectures for broad and critical applications to continued U.S. leadership in technology development, thereby addressing DOE Basic Research Needs for Transformative Manufacturing and Quantum Materials.

Type: New
Title: "Carbon at Extremes: Discovery Science with Exascale Computers"

Principal Investigator: Ivan Oleynik, University of South Florida
Co-Investigators: Aidan Thompson, Sandia National Laboratories
Mitchell Wood, Sandia National Laboratories
Stan Moore, Sandia National Laboratories
Anatoly Belonoshko, Royal Institute of Technology
Rahulkumar Gayatri, NERSC
Marius Millot, Lawrence Livermore National Laboratory
Sally Tracy, Carnegie Institution for Science

Scientific Discipline: Materials

INCITE Allocation:

Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (1,300,000 Frontier node-hours)

Research Summary: The main research objective of this project is to perform transformative quantum-accurate, billion atom MD simulations on exascale DOE computers Frontier and Aurora to uncover the fundamental physics of carbon at extreme pressures and temperatures. This research will be uniquely coupled to experiments aimed at observing the phenomena, predicted by the team's simulations.

Although the team has successfully synthesized post-diamond BC8 high-pressure phase of carbon in a couple of big, billion atom runs, most of the team's production simulations sampled transitions to final thermodynamic states using relatively small, several million-atom diamond and amorphous carbon samples. These simulations were performed in simplified isotropic hydrostatic compression approximation, which ignores the effects of crystalline anisotropy in uniaxial shock compressions. The limits of computational power did not allow the team to simulate the entire transformation pathways and uncover the kinetic effects of phase transitions. This game-changing step-up will further advance science frontiers by removing roadblocks of the team's previous simulations, thus allowing the team to effectively design experimental campaigns of very expensive, million-dollar experiments at NIF and Omega EP facilities.

Type: Renewal
Title: "COMbining deep-learning with Physics-Based affinIty estimatiOn 2 (COMPBIO2)"

Principal Investigator: Peter Coveney, University College London
Co-Investigators: Shantenu Jha, Rutgers University
Philip Fowler, University of Oxford
Rick Stevens, University of Chicago

Scientific Discipline: Learning

INCITE Allocation:
Machine (Allocation): HPE Apollo 6500 (75,000 Polaris node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (520,000 Frontier node-hours)

Research Summary: Coupling machine learning and physics-based methods, with this work researchers aim to accelerate the slow process of drug discovery, which typically lasts many years and costs billions of dollars—a major weakness in public health emergencies. Furthermore, virtual screening methods employed in drug discovery are currently hampered by their reliance on human intelligence in the application of chemical knowledge.

To overcome this, this team has developed a method called "IMPECCABLE" that involves sampling candidate compounds from both a billion-compound, synthetically accessible space, as well as from the output of a deep learning generative algorithm. It is an iterative method that loops its various modules consisting of a variety of physics-based scoring methods with increasing levels of accuracy as well as DL methods actively interacting with each other and becoming progressively more accurate in their predictions. The selected compounds are scored based on calculated binding free energies and fed back into the deep learning algorithm to iteratively refine predictive capability.

The approach this team takes will have direct applicability in the pharmaceutical industry for quick identification of potent binders for a given target protein and binding pocket. Using "IMPECCABLE," the team has been able to analyze several million compounds from a set of orderable compound libraries to discover an inhibitor for the main protease of SARS-CoV2.

Type: New
Title: "Convection-Permitting Climate-Scale Simulations for Extreme Event Modeling"

Principal Investigator: Rao Kotamarthi, Argonne National Laboratory
Co-Investigators: Jiali Wang, Argonne National Laboratory
Dimitrios Fytanidis, Argonne National Laboratory
Brandi Gamelin, Argonne National Laboratory
Chunyong Jung, Argonne National Laboratory
William Pringle, Argonne National Laboratory
Gokhan Sever, Argonne National Laboratory
Haochen Tan, Argonne National Laboratory

Scientific Discipline: Earth Science

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (1,500,000 Theta node-hours)
Site: Argonne National Laboratory
Machine (Allocation): HPE Apollo 6500 (100,000 Polaris node-hours)

Research Summary: The ability to assess the risk from extreme climate events is critical for developing adaptation and mitigation strategies that are often made at local and regional scales of the impacted region. Therefore, improved capabilities for predicting the frequency, duration, and extent of such events and their potential impacts for various locations across the continental United States is becoming increasingly necessary.

However, identifying and evaluating the risk in a warming climate requires long timescales for the simulation covering multiple decades and/or a large ensemble that covers a selected time slice. In addition, simulating extreme events and their impacts requires very high spatial resolution in the models, often covering several orders of magnitude, from hundreds of kilometers to tens of meters. Both these factors make these calculations computationally intensive.

With this INCITE project, researchers will use very high spatial-resolution regional-scale climate models to explore the physics underlying the formation and evolution of extremes in precipitation and temperature in the current and future climates under various greenhouse gas emission scenarios. The team's ultimate goal is to provide the research community with a large multi-petabyte dataset of climate simulations with well-characterized uncertainties and biases that can be used to realistically describe extreme events, understand the environmental drivers that contribute to these extremes, and estimate risk from these events at local scales. The results from this work will provide a unique database for performing further studies for developing AI-based emulators for extreme events and developing climate risk estimates at local scales from these events.

Type: New
Title: “Data-Driven Methods to Characterize Intermittency in Stratified Turbulence”

Principal Investigator: Stephen de Bruyn Kops, University of Massachusetts Amherst
Co-Investigators: James Riley, University of Washington
Andrew Bragg, Duke University
Colm-Cille Caulfield, University of Cambridge
Miles Couchman, Duke University

Scientific Discipline: Engineering

INCITE Allocation:

Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (600,000 Summit node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (190,000 Frontier node-hours)

Research Summary: Stably stratified turbulence is a model flow with important implications for pollution mitigation, deep sea mining, military operations over cold land or ice, and climate modeling. It is spatio-temporally intermittent and three dimensional with a large range of length scales, and so it requires multiple realizations of very large simulations to understand and model.

The team proposes a study of turbulent flow in a stably stratified fluid using massive-scale direct numerical simulations (MsDNS). The study will involve the three-dimensional, time-dependent solution of the Navier-Stokes equations with the non-hydrostatic Boussinesq approximation at numerical resolution which, at the present time, can only be carried out using the computer resources available in the INCITE Program. The reason that INCITE is required relates to two key aspects: first, the concept of dynamic range, that is, the ratio of the largest to smallest dynamically important length scales in a flow; and second, the fact that the Prandtl number Pr is significantly greater than one in parts of the team’s proposed DNS campaign, signifying that the density diffusivity is significantly smaller than the kinematic viscosity. Here the team considers $Pr = 1$ and 7, in order to compare the properties of turbulent intermittency in flows representative of air and water, respectively, which will thus inform turbulent research in both the atmosphere and ocean communities.

Type: New
Title: "The Discovery of Longitudinal and Temporal Climatype Patterns"

Principal Investigator: Daniel Jacobson, Oak Ridge National Laboratory
Co-Investigators: Wayne Joubert, Oak Ridge National Laboratory

Scientific Discipline: Energy

INCITE Allocation:

Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (210,000 Summit node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (800,000 Frontier node-hours)

Research Summary: A growing population will require a significant expansion of biofuel and food production (and a doubling in developing countries). These challenges necessitate detailed and accurate knowledge of environmental conditions on a global scale to rapidly establish crops in geographic regions that will maximize production and minimize costs. The application of high-performance computing and explainable-Artificial-Intelligence to these problems will make it possible to engineer crops that are more resource efficient, stress resistant, and better able to thrive in modified lands. This will have impacts on several areas of DOE BER sponsored research, including Bioenergy Research Centers, Plant-Microbe SFAs, Feedstock Genomics, and the Integrated Pennycress Resilience Project as well as having substantial positive economic, political, and societal implications.

The work proposed in this project builds on a series of new methods that the team has developed in previous ALCC and INCITE projects that are enabling them to determine the genomic architectures responsible for the adaptation of an organism to its environment and climate. The team is studying pathogen resistance in other projects and believe that it is possible to breed or genome edit for pathogen resistance. Thus, pathogens are outside the scope of this specific proposal. Populus, Panicum, and Thlaspi are the primary bioenergy genera targeted in this proposal. As bioenergy crops, Populus and Panicum are typically vegetatively propagated and Thlaspi is sewn as seeds (and is self or wind pollinated) so do not require the presence of specific pollinator species. Although Populus, Panicum, and Thlaspi are the team's initial targets, the team believes that the results and resources that will be developed in this project will be relevant to other bioenergy crops as well as many food crops and model plant species (including Arabidopsis).

Type: New
Title: "DNS of Wall-Bounded Magnetohydrodynamic Turbulence at High Reynolds Number"

Principal Investigator: Myoungkyu Lee, University of Alabama

Scientific Discipline: Engineering

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (700,000 Theta node-hours)

Research Summary: Understanding the fundamental physics of wall-bounded magnetohydrodynamic (MHD) turbulence is the key to developing multiple engineering applications, such as liquid metal blankets in nuclear fusion reactors. The study of such applications is challenging because operating conditions are often at a high Reynolds number. Therefore, either very high-fidelity experimental measurement systems or leadership-scale computing systems are required.

This project will perform direct numerical simulations (DNS) of wall-bounded MHD turbulence at high Reynolds numbers. Since DNS requires resolving the entire spectrum of length- and time-scales of turbulent flows, it is impractical to use for complicated scenarios. Instead, the researchers will study incompressible canonical channel flow at different flow speeds and magnetic field strengths & directions in both transient and statistically stationary states.

The high-fidelity data generated with this INCITE allocation will reveal the spectral behaviors of turbulent kinetic energy (TKE) as functions of fluid speed, the strength and direction of the magnetic field, and the wall-normal distances. Primarily, it will provide the life-cycle of TKE from its production and dissipation at different length scales while displaying the influence of large-scale motion on the near-wall flows in MHD turbulence. Additionally, the resulting high-fidelity data will be useable for developing and improving reduced-order models, such as RANS (Reynolds-averaged Navier-Stokes) models, subgrid stress models for large eddy simulation, and machine learning surrogates.

Type: Renewal
Title: "Electron Kinetic Plasma Physics of Black Hole Accretion Flows"

Principal Investigator: Dmitri Uzdensky, University of Colorado
Co-Investigators: Fabio Bacchini, KU Leuven
Mitchell Begelman, University of Colorado
Jason Dexter, University of Colorado
Nicolas Scepi, University of Southampton
Gregory Werner, University of Colorado
Vladimir Zhdankin, Flatiron Institute

Scientific Discipline: Physics

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (2,600,000 Theta node-hours)

Research Summary: Accretion flows around supermassive black holes at the centers of galaxies emit electromagnetic radiation that is critical to understanding these active galactic nuclei, which influence galactic evolution. Interpreting observed radiation, however, requires detailed modeling of the complex multi-scale plasma processes in accretion flows. Using petascale 3D particle-in-cell simulations, this project investigates electron versus ion energization, nonthermal particle acceleration, and self-consistent synchrotron radiation for plasma processes likely ubiquitous in black-hole accretion, including plasma turbulence driven by the magnetorotational instability (MRI) or other forces, and collisionless magnetic reconnection.

The team has identified three key links in the chain of plasma processes that lead from gravitational attraction of matter around a black hole to accretion and radiation. The development of the MRI leads to outward angular momentum transport that allows accretion; it also generates turbulence and current sheets leading to magnetic reconnection, both of which result in particle energization, hence also radiation.

The work takes a critical step toward understanding the behavior of black holes in the universe. The first-principles simulations of plasma processes and energy conversion mechanisms important in black hole accretion flows will be used to inform global magnetohydrodynamics computational and theoretical modeling, thus taking into account kinetic processes to predict radiation output for comparison to observations. Moreover, these kinetic simulations of 3D MRI turbulence and reconnection have the potential to significantly advance computational plasma physics.

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

Principal Investigator: Mark Taylor, Sandia National Laboratories
Co-Investigators: David Bader, Lawrence Livermore National Laboratory
Peter Caldwell, Lawrence Livermore National Laboratory
Oksana Guba, Sandia National Laboratories
Walter Hannah, Lawrence Livermore National Laboratory
Phil Jones, Los Alamos National Laboratory
L. Ruby Leung, Pacific Northwest National Laboratory
Mathew Norman, Oak Ridge National Laboratory
Sarat Sreepathi, Oak Ridge National Laboratory
Xingqiu Yuan, Argonne National Laboratory

Scientific Discipline: Earth Science

INCITE Allocation:

Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (450,000 Summit node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (1,250,000 Frontier node-hours)

Research Summary: The E3SM project is developing a next generation Earth System Model tailored specifically for DOE's Leadership Computing Facilities. Unique storm-resolving configurations of E3SM will leverage 2023 INCITE resources to make unprecedented estimates of the team's climate's sensitivity to elevated greenhouse gases to advance climate research. The advent of machines like Summit and Frontier- coupled with a rewrite of Earth system models to take advantage of new architectures - permits simulations that resolve individual storms yet also run long enough to separate climate signal from weather noise. In recognition of this impending opportunity, many modeling centers are focusing now on global storm-resolving global models (GSRMs). Most GSRMs cannot fully utilize Exascale architectures, however, so they are not ready to perform the multi-year simulations necessary to make robust climate predictions. E3SM is one of the first GSRMs designed to run efficiently on DOE's upcoming Exascale supercomputers. In 2023, the team proposes to extend the team's 2022 simulation campaign representing one of the first efforts to compute climate sensitivity to elevated greenhouse gases at global storm resolving resolution.

Type: New
Title: "EQSIM Regional-Scale Simulations for Earthquake Hazard and Risk Assessments"

Principal Investigator: David McCallen, Lawrence Berkeley National Laboratory
Co-Investigators: Arben Pitarka, Lawrence Livermore National Laboratory
Houjun Tang, Lawrence Berkeley National Laboratory
Rie Nakata, Lawrence Berkeley National Laboratory
Ramesh Pankajakshan, Lawrence Berkeley National Laboratory

Scientific Discipline: Earth Science

INCITE Allocation:

Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (1,000,000 Frontier node-hours)

Research Summary: Advanced high-performance computing is becoming a key tool for the prediction of earthquake hazard and risk on a regional scale. The large-scale research simulations proposed herein occur at the nexus of earth science and engineering and are focused on advancing the utilization of large-scale high-performance simulations in assessing site-specific regional earthquake hazard and risk. The proposed simulation activities consist of multidisciplinary, coupled geophysics and engineering simulations for regional-scale fault-to-structure modeling that starts from an earthquake fault rupture, propagates seismic waves through a heterogenous earth and finally represents the complex interaction between incident seismic waves and critical infrastructure systems at the surface/subsurface boundary. The proposed simulations have only recently become feasible as a result of major software and workflow advancements in the DOE Exascale Computing Project EQSIM application development, coupled with the advancements of the FRONTIER exaflop system. The EQSIM project has been focused on developing capabilities for the emerging exaflop systems with demonstrated performance on SUMMIT and early successful testing on CRUSHER. The simulation tasks proposed will yield new information on ground motion severity, its spatial variability, and building response in the near field of major earthquakes, the way incident seismic waves interact with critical infrastructure (as opposed to legacy simplified engineering idealizations) and the number fault rupture realizations that are required to fully characterize the risk to critical infrastructure. Finally, the unique suite of simulated ground motion datasets generated will be shared via open source for utilization by the broad earthquake research community of earth scientists and engineers to help promote additional research and practical utilization of synthetic ground motions.

Type: New
Title: "Establishing microfluidc digital twins for high throughput cellular analysis"

Principal Investigator: Amanda Randles, Duke University

Scientific Discipline: Biological

INCITE Allocation:

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

Research Summary: This work will establish a validated digital twin of microfluidic devices enabling high throughput calculation of a wide range of phenomarkers such as cell elasticity. By creating a virtual model of the device, tuning cell parameters so that the team mimics transport in the device and match their measured wCDI, the team can then extract quantities like Young's Modulus or wall shear stress directly from the simulation. This contribution is significant because it constitutes the first step along a continuum of research toward high throughput measuring of key quantities like cell stiffness.

The work proposed here will address three key challenges facing cellular simulations. First, the team will establish a clear and validated method for establishing a digital twin of the microfluidic device. By setting up a virtual replica of the device and tuning it to mimic the measured quantities, the team will be able to validate the model and use it to extract a wider range of metrics. Second, the team will extend this capability by establishing a framework for robustly capturing cellular behavior across the ensemble of potential red blood cell configurations. Finally, the team will establish a computationally optimized method by integrating this framework with the team's established adaptive physics refinement method that enables cellular resolution to be captured over large domains. Together, these advances will enable a robust digital twin to be created for a wide range of microvascular and microfluidic applications.

Type: New
Title: "Exascale Gyrokinetic Study of ITER Challenge on Power-Exhaust and ELM-Free Edge"

Principal Investigator: Choongseok Chang, Princeton Plasma Physics Laboratory
Co-Investigators: Scott Parker, University of Colorado at Boulder
Robert Hager, Princeton Plasma Physics Laboratory
Seung-Hoe Ku, Princeton Plasma Physics Laboratory
George Wilkie, Princeton Plasma Physics Laboratory
Scott Klasky, Oak Ridge National Laboratory
Aaron Scheinberg, Jubilee Development
Mark Shephard, RPI
Mark Adams, Lawrence Berkeley National Laboratory
Julien Dominski, Princeton Plasma Physics Laboratory
Kevin Huck, University of Oregon
Luis Chacon, Los Alamos National Laboratory
Sameer Shende, University of Oregon
Randy Michael Churchill, Princeton Plasma Physics Laboratory
Stephane Ethier, Princeton Plasma Physics Laboratory
Yang Chen, University of Colorado at Boulder

Scientific Discipline: Materials

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (1,000,000 Summit node-hours)
Site: Argonne National Laboratory
Machine (Allocation): HPE Apollo 6500 (300,000 Polaris node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (1,500,000 Frontier node-hours)

Research Summary: This INCITE project will employ the electromagnetic gyrokinetic particle-in-cell code XGC, with most of the important physics included, to perform two-pronged fundamental edge physics studies of critical importance to the successful operation of ITER and for the design of Fusion Power Plants (FPPs). The first is mitigating high stationary heat-flux densities that will damage material walls while maintaining the high edge plasma pedestal within a safe operational window. The second is avoiding explosive transient power-flow to material walls caused by edge localized mode (ELM) crash whose onset is influenced by the plasma condition near the wall. As has been demonstrated in previous INCITE-supported XGC-based studies in pure deuterium plasmas, an edge physics regime different from the present experimental tokamaks has been observed due to the greater size of ITER. Thus, projection of the physics observations from present tokamaks to ITER is unwarranted. These studies require more powerful computers due to the inclusion of several more critical physics elements that could not be handled by the previous INCITE resources.

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

Principal Investigator: Michael Zingale, Stony Brook University
Co-Investigators: Ann Almgren, Lawrence Berkeley National Laboratory
Alan Calder, Stony Brook University
Kiran Eiden, UC Berkeley
Eric Johnson, Stony Brook University
Max Katz, Stony Brook University
Andy Nonaka, Lawrence Berkeley National Laboratory
Alexander Smith Clark, Stony Brook University
Abigail Polin, Caltech
Jean Sexton, Lawrence Berkeley National Laboratory
Donald Willcox, Lawrence Berkeley National Laboratory

Scientific Discipline: Physics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (400,000 Summit node-hours)
Site: Argonne National Laboratory
Machine (Allocation): HPE Apollo 6500 (100,000 Polaris node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (300,000 Frontier node-hours)

Research Summary: This project will build upon the success of earlier INCITE awards that explored astrophysical thermonuclear explosions, in particular, Type Ia supernovae (SN Ia) and x-ray bursts (XRBs). The team will use their Castro code to carry out high-performance, robust, and accurate simulations to advance our understanding of XRBs and SN Ia, as well as related physics (thermonuclear combustion and detonations).

In the area of XRBs, the researchers will greatly expand their work to model thermonuclear flame propagation across the surface of a neutron star. They will explore larger reaction networks and the effect of magnetic fields, and push to model a larger fraction of the neutron star surface. For their SN Ia studies, the team will focus on the double-detonation model. Both XRBs and SN Ia are multiscale, multiphysics problems that rely on the interplay between reactions and hydrodynamics. The team's open-source Castro code has a new time-integration that is designed to strongly couple these processes, enabling the team to carry out accurate and efficient simulations of reacting flows.

Type: New
Title: "Exascale Simulation and Deep Learning Model for Energetic Particles in Burning Plasmas"

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

Scientific Discipline: Physics

INCITE Allocation:

Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (410,000 Summit node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (200,000 Frontier node-hours)

Research Summary: Through this INCITE project, the team proposes to develop the challenging capability for prediction and real-time control of energetic particle (EP) confinement in burning plasmas by combining exascale first-principles simulation and experimentally validated AI/Deep Learning software. The team proposes this INCITE project to develop the challenging capability for prediction and real-time control of energetic particle (EP) confinement in burning plasmas by combining the state-of-the-art exascale first-principles GTC simulation [Science, 1998] and the prominent experimentally validated AI/Deep Learning FRNN software [Nature, 2019]. 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. The accurate identification and effective control of plasma instabilities that cause EP loss is therefore important for successful fusion experiments. Due to the strong coupling of EP with burning thermal plasmas, accurate assessment of the plasma confinement properties in the ignition regime is one of the most uncertain factors when extrapolating from existing fusion devices to the ITER tokamak. Predictive EP capability will require exascale, integrated first-principles simulation of nonlinear interactions of multiple kinetic-magnetohydrodynamic (MHD) processes. These first-principles model simulations are, however, generally not fast enough for real-time applications. In the proposed project, a deep learning based surrogate model as an instability and transport simulator for real-time applications will be developed and trained within the FRNN framework in a supervised manner using data from GTC global electromagnetic simulations of EP instability and transport.

Type: New
Title: "Exascale Simulation of Photon-Matter Interactions"

Principal Investigator: Prineha Narang, University of California, Los Angeles
Co-Investigators: Felipe Jornada, Stanford University
Eran Rabani, University of California, Berkeley

Scientific Discipline: Materials

INCITE Allocation:

Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (200,000 Summit node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (50,000 Frontier node-hours)

Research Summary: The last decade has seen unprecedented progress in controlling matter at the atomic scale, enabled by the team's ability to predict the relationship between atomic structure and performance. The team will investigate the emergence of a similarly transformative concept: properties of materials and pathways of chemistry are modified by driving the system out of equilibrium with light. The team's work leverages the excellent GPU readiness of massively parallel codes in this INCITE program with demonstrated scalability on leadership-class supercomputing systems to tackle the next frontier of nonequilibrium materials and molecules.

The rapidly converging fields of quantum optics and electronic structure theory now opens the new field of polaritonically-controlled quantum matter and chemical dynamics and necessitates a unified approach to predict and computationally interrogate such strongly-correlated light-matter interactions. Combining concepts from both fields presents an opportunity to create a predictive theoretical and computational approach to elucidate mechanistic questions in cavity correlated matter. In the QED (also referred to as the polariton or ultrastrong coupling) regime, the original constituents of the system lose their individual identity and hybrid quasi-particles of novel character are formed. These new hybridized states, polaritons, of mixed light-matter character can dramatically change the ground and excited correlations and energy landscape, with important implications in physics and chemistry.

Type: New
Title: "Exascale Simulations of Quantum Materials"

Principal Investigator: Paul Kent, Oak Ridge National Laboratory
Co-Investigators: Anouar Benali, Argonne National Laboratory
Panchapakesan Ganesh, Oak Ridge National Laboratory
Jaron Krogel, Oak Ridge National Laboratory
Ye Luo, Argonne National Laboratory
Lubos Mitas, North Carolina State University
Fernando A. Reboredo, Oak Ridge National Laboratory
Brenda Rubenstein, Brown University
Luke Shulenburger, Sandia National Laboratories

Scientific Discipline: Materials

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): HPE Apollo 6500 (100,000 Polaris node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (1,000,000 Frontier node-hours)

Research Summary: To help meet the challenges of reducing energy, realizing new technologies, and identifying optimum materials for specific applications, advances in our ability to understand, predict, and realize desired phenomena in specific, real materials is critical. This demand is particularly strong for quantum materials – solids with exotic physical properties arising from the quantum mechanical properties of their constituent electrons – which promise to facilitate, e.g., new quantum sensors and devices, and new forms of low-power electronics. While databases of candidate materials have been created based on approximate calculations, it is now clear that more accurate and more computationally challenging methods need to be applied to refine this work, obtain detailed understanding, and to precisely identify high-impact experimental targets.

Accurate, quantum-mechanics based simulations of these materials are very challenging due to the role of spin-orbit interaction, magnetism, electronic charge, and their combined coupling to the material's structure. Through this INCITE project, the team proposes to apply quantum Monte Carlo (QMC) methods to address these challenges and provide reliable materials predictions for several classes of quantum materials of tremendous topical interest. For broader community impact beyond results on specific materials, they will also systematically compute properties of a small series of materials and publish the resultant database. This will help reveal underlying trends and serve as the reference requested by the theoretical quantum materials community.

Type: New
Title: "Extreme-Scale Data Assimilation for Predictive Flow Simulations"

Principal Investigator: Jonathan MacArt, University of Notre Dame
Co-Investigators: Justin Sirignano, University of Oxford

Scientific Discipline: Engineering

INCITE Allocation:

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

Research Summary: The project enables extreme-scale data assimilation for simulations of external aerodynamics, leveraging both high-fidelity numerical data and sparse experimental data. It advances the state-of-the-art for predictive accuracy, computational cost, and model-based design of real-world aerodynamic applications, which will enable faster and higher-risk design cycles.

The team has recently developed a theoretically optimal method for physics-constrained ML based on PDE-constrained optimization and adjoint PDEs. The proposed research will further develop these methods to enable extreme-scale, solver-in-the-loop data assimilation (DA). The team will test the learned models in turbulent flow problems relevant to aircraft drag reduction, high-efficiency wind turbine blades, and turbomachinery for energy conversion. Extending and proving the team's DA methods on leadership-class systems will enable simultaneous optimization over hundreds of configurations and flow parameters, which is necessary for highly generalizable models (that is, accurate and stable at conditions different from the training data) in high-dimensional parameter spaces such as turbulent flows. Additionally, leadership-class simulations will provide trusted data at high-enough Reynolds numbers to develop genuinely useful engineering models. Finally, the methodological and software improvements will enable extreme-scale DA in other fields such as atmospheric science, medicine, alternative fuels design, hypersonics, and materials science.

Type: New
Title: "Extreme-scale phenomena in turbulent dispersion and mixing"

Principal Investigator: Pui Kuen (P.K.) Yeung, Georgia Institute of Technology
Co-Investigators: Katepalli Sreenivasan, New York University
Charles Meneveau, The Johns Hopkins University

Scientific Discipline: Engineering

INCITE Allocation:

Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (1,400,000 Frontier node-hours)

Research Summary: Record-breaking simulations of fluid turbulence at the highest Reynolds number to-date, using the full power of Frontier, will be performed to investigate extreme events of dispersion and mixing at low molecular diffusivity. The work answers crucial fundamental questions, and large datasets will be shared publicly through an open turbulence database.

In this INCITE proposal, using the power of Frontier, the team plans to obtain precise solutions of the equations of motion for conditions of the largest scale separations possible. The team will leverage the extensive knowledge of the PI and co-PIs, and the PI's recent successes in algorithmic advancement on hardware identical to Frontier, to investigate the fundamental problems in turbulence. In both instances cited above, direct numerical simulations (DNS) of the exact equations of motion at record-breaking resolution will be designed to maximize advancements in physical understanding in part through detailed analyses of data that will also be made available per a large NSF-funded database project to interested members of the team's community. Their work on Lagrangian properties builds on the extensive DNS work of the past. The team will also investigate the subject with fresh perspectives on extreme conditions and fine-scale intermittency, considering both single particles and particle pairs. Secondly, the team will be able to simulate turbulent mixing of transported entities with very low molecular diffusivity, in a parameter range close to oceanic conditions that have never been approached before.

Type: New
Title: "Feedback and energetics from magnetized AGN jets in galaxy groups and clusters"

Principal Investigator: Brian O'Shea, Michigan State University
Co-Investigators: Philipp Grete, University of Hamburg
Forrest Glines, Los Alamos National Laboratory
Deovrat Prasad, Cardiff University

Scientific Discipline: Physics

INCITE Allocation:

Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (630,000 Frontier node-hours)

Research Summary: The goal of this project is to understand how galaxies evolve and regulate themselves. The team will do this by simulating the feedback from supernovae and supermassive black holes on the diffuse plasma that surrounds galaxies, and in particular focus on the most massive galaxies in the universe. The team will, for the first time, fully utilize the capabilities of Frontier to explore the self-regulation of massive galaxies in groups and clusters using magnetized jet feedback from supermassive black holes.

The successful completion and analysis of these calculations will revolutionize the team's understanding of AGN feedback and the self-regulation of galaxies within groups and clusters. This will be important in astrophysics for the interpretation of observations of galaxies and their environments, for the development of subgrid models in simulations of cosmological structure formation, and more generally in the team's theoretical understanding of the growth and evolution of galaxy populations over cosmic time.

Type: New
Title: "First-Principles Simulation of Hypersonic Flight"

Principal Investigator: Maninder Grover, University of Dayton Research Institute
Co-Investigators: Paolo Valentini, University of Dayton Research Institute
Nicholas Bisek, Air Force Research Laboratory

Scientific Discipline: Engineering

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (1,650,000 Theta node-hours)

Research Summary: It is clear that hypersonic flight has the potential to completely change the defense industry. However, much of the physics that characterizes hypersonic flight is still unknown or poorly characterized, particularly at regimes where strong thermo-chemical non-equilibrium is present. A key question is to understand how adequately reduced-order formulations, used in computational fluid dynamics design codes, can capture the strong coupling between the fluid mechanics of the gas flow, the local gas-phase thermochemical non-equilibrium, and the transport properties of the high-temperature gas. Traditionally, these physics have been intensely investigated separately by producing simplified models that tend to reproduce only certain aspects of the physics characterizing high-speed, reacting flows.

Large-scale computational tools have been developed that enable researchers to obtain entire hypersonic flow fields solely from the fundamental interactions of atoms and molecules in the gas. Such interactions are directly obtained from quantum mechanics. Hence, such solutions are from first-principles as they are free of any empiricism. This technique is called Direct Molecular Simulation (DMS). Through the use of massively-parallel DMS simulations, this project will enable the computation of flows around geometries at length scales at which experiments can be conducted. The goal of the project is to compare simulated atomic-level flow field details derived from quantum chemistry with experimentally captured data.

Type: New
Title: "First-Principles Electron Dynamics in Complex Systems"

Principal Investigator: Andre Schleife, University of Illinois at Urbana-Champaign
Co-Investigators: Yosuke Kanai, University of North Carolina at Chapel Hill

Scientific Discipline: Materials Science

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

Research Summary: In the conversion of solar photons to energy commodities like electricity and fuel, a predictive understanding of how excited electrons and electron-hole pairs (excitons) behave in complex matter—such as molecules on surfaces or defects in semiconductors—is central to designing and improving energy conversion processes at the atomistic level. For instance, the dynamics of excitons at the interface of semiconductors and catalytic molecules represents a critical knowledge void that impedes DOE mission-critical design of new materials for solar fuel generation. Excited electrons near defects in semiconductors increase defect mobility, laying the foundation of the recently emerging field of photo-ionics, with promise of high impact on DOE priorities such as batteries as well as materials design for quantum computing.

This project uses new advancements in real-time time-dependent density functional theory (RT-TDDFT) to reliably study high-impact scientific questions associated with the dynamics of electrons and ions in complex heterogeneous systems. In particular, the researchers seek to investigate how excitons dissociate at silicon-molecule interfaces, using a hybrid functional to approximate exchange and correlation within RT-TDDFT. The simulations generated will uncover the detailed mechanism of how the initial formation of a tightly bound exciton subsequently transitions to a charge-transfer exciton across the interface. If successful, this will enable greater understanding of the materials-dependence of the underlying femto- to picosecond timescale of exciton dynamics, allowing for direct comparison to experiment and facilitating acceleration of this process by materials design and selection.

Type: Renewal
Title: "First-Principles Modeling of the Multi-wavelength Emission from Pulsars"

Principal Investigator: Yuran Chen, Washington University in St. Louis
Co-Investigators: Yajie Yuan, Washington University in St. Louis
Dmitri Uzdensky, University of Colorado Boulder

Scientific Discipline: Physics

INCITE Allocation:

Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (279,000 Summit node-hours)

Research Summary: Rapidly objects in the universe and they can emit powerful radiation across the electromagnetic spectrum in extremely regular pulses. Chen's team will study comprehensively how neutron stars produce this radiation using large-scale first-principles simulations.

The team will take a two-pronged approach, examining both the large-scale global structure of the magnetosphere, as well as zooming in and exploring the detailed physics of local emission regions. The global approach will allow them to map the light curves of observed multi-wavelength radiation to the geometric configuration of the magnetosphere. The local approach will allow them to understand the interaction between radiation and plasma in unprecedented detail and compute the emergent electromagnetic spectrum.

This project is made possible by the team's state-of-the-art Particle-in-Cell (PIC) code Aperture, which harnesses the incredible computational power of GPUs. The INCITE allocation will allow them to perform petascale, first-principles simulations that have never been done before. These simulations will greatly advance their understanding of extreme relativistic plasma physics and can solve some of the most fundamental puzzles in the science of pulsars. They expect some of these results will also be applicable to other astrophysical systems such as accreting black holes and flaring magnetars.

Type: Renewal
Title: "Global Adjoint Tomography"

Principal Investigator: Jeroen Tromp, Princeton University
Co-Investigators: Shantenu Jha, Rutgers University
Daniel Peter, King Abdullah University
Matteo Turilli, Rutgers University

Scientific Discipline: Earth

INCITE Allocation:

Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (550,000 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: New
Title: "Hadron physics from first principles"

Principal Investigator: Kostas Orginos, William & Mary
Co-Investigators: Robert Edwards, Jefferson Laboratory
David Richards, Jefferson Laboratory
Christopher Monahan, William & Mary
Balint Joo, Jefferson Laboratory
Anatoly Radyushkin, Old Dominion University
Jianwei Qiu, Jefferson Laboratory
Frank Winter, Jefferson Laboratory
Savvas Zafeiropoulos, Centre National de la Recherche Scientifique (CNRS)
Raza Sufian, William & Mary
Eloy Romero, Jefferson Laboratory
Colin Egerer, Jefferson Laboratory

Scientific Discipline: Physics

INCITE Allocation:

Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (1,000,000 Frontier node-hours)

Research Summary: Through this INCITE project, the team will perform calculations of the properties of Hadrons (particles that interact strongly) from first principles using the fundamental theory of strong interactions know as Quantum ChromoDynamics (QCD). The team's project utilizes modern computational methods in order to obtain information about the internal structure, the interactions and the spectrum of Hadrons.

The team has two main goals. First, to compute the x-dependent, isovector light-quark generalized parton distributions (GPDs) of the nucleon, in the continuum and physical quark-mass limits of lattice QCD. Second, to provide a lattice determination of the flavor decomposition of the proton sea through isoscalar GPDs. Leadership class computing is critical for the team's goals, which will provide the ab initio answers to a question "essential for understanding the nature of visible matter" [1] and central to the Department of Energy's experimental nuclear physics program: how do quarks and gluons form the wide range of hadronic bound states the team observes in experiment?

Type: New
Title: "Heterogeneous Catalysis as a Collective Phenomenon within Dynamic Ensembles of States"

Principal Investigator: Philippe Sautet, University of California Los Angeles
Co-Investigators: Anastassia Alexandrova, University of California Los Angeles

Scientific Discipline: Chemistry

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (2,000,000 Theta node-hours)
Site: Argonne National Laboratory
Machine (Allocation): HPE Apollo 6500 (200,000 Polaris node-hours)

Research Summary: Chemical production is the single largest consumer of energy in US manufacturing, according to the 2015 DOE Bandwidth Report; but the development of efficient catalysts for many processes continues to elude catalyst scientists. The basis of this project is the realization that a catalytic interface in the steady state is in constant motion enabled by the reaction conditions (temperature and pressure of gases in thermal catalysis, or electrochemical potential, solvent and pH in electrocatalysis). Due to these dynamics, the interface presents a fluxional ensemble of many states and active sites (rather than just one), each characterized by its specific activity, selectivity, deactivation propensity, and operando spectral signatures. Catalysis, therefore, is a collective ensemble phenomenon, largely driven by highly active metastable states rather than the ground state.

Operating within this new paradigm, this project addresses the nature of the catalytic interface in reaction conditions, attainable swarms of mechanistic pathways, and routes of deactivation, for size-selected fluxional cluster catalysts deposited on supporting surfaces. Predictions toward improved activities, selectivity, and stabilities will be made and experimentally tested. Additionally, the researchers will probe several fundamental phenomena that are expected to shift the new paradigm even further: sintering of clusters on amorphous surfaces in the presence of adsorbates that is expected to be strongly driven by metastable states, interpretations of operando spectra in view of the apparently ensemble-averaged nature of the experimental signal, and broken scaling relations that point toward better cluster catalysts in counterintuitive ways.

The project will use and further develop methods of grand canonical global optimization for the discovery of dynamic ensembles in realistic reaction conditions and of global activity sampling, for the determination of the most active configurations of the catalyst. Machine learning tools will be developed to replace costly DFT calculations wherever possible.

Type: New
Title: "High-Resolution Ensemble 3D Structures of Genome across Tissues"

Principal Investigator: Jie Liang, University of Illinois at Chicago
Co-Investigators: Konstantinos Chronis, University of Illinois at Chicago

Scientific Discipline: Biology

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (1,500,000 Theta node-hours)
Site: Argonne National Laboratory
Machine (Allocation): HPE Apollo 6500 (125,000 Polaris node-hours)

Research Summary: Three-dimensional genome organization and modifications are the basis of cellular functions. Genomic DNAs that are approximately 2 meters in length in the form of chromosomes are packed into a cell nucleus 10-20 micrometers in diameter. They have to be properly folded such that the appropriate nuclear organization can be maintained and essential fundamental cellular processes such as regulation of gene expression and cellular specialization can proceed. 3D genome folding enables various genomic functions, allowing cells with identical genomic DNAs to differentiate into skin, bone, liver and other tissue types.

To understand the relationship between genome 3D structure and genome function, this project aims to carry out a large-scale computational campaign to construct detailed 3D genome-folding models. 3D models of different loci at unprecedented resolution and accuracy will enable examination of the structural basis of genome folding and genome functions, and will provide an atlas for discovering how genes at different loci form different spatial structures, how they define cellular states, and how they control gene expression. The researchers will extract structurally and functionally important relationships among genomic elements from experimental data based on physical principles of 3D chromatin folding, and will generate maps of driver interactomes of 3D chromatin folding for each locus along all chromosomes, providing a concise shortened list of putative causal interactions that can drive 3D chromatin folding. The work will also yield highly accurate and fine-resolution repertoire models of ensembles of single-cell 3D chromatin conformations for all genomic loci. Predicted 3D single-cell chromatin conformations will significantly extend coverage and resolution of what is accessible to single-cell experimental techniques, and the constructed ensemble of single-cell chromatin models will allow characterization of chromatin structural heterogeneity via identification of major structural clusters of chromatin conformations in subpopulations of cells.

Type: New
Title: "High-Z Impurity Transport in D-T Fusion Plasmas"

Principal Investigator: Emily Belli, General Atomics
Co-Investigators: Reuben Budiardja, Oak Ridge National Laboratory
Jeff Candy, General Atomics
Igor Sfiligoi, University of California, San Diego
Gary Staebler, General Atomics

Scientific Discipline: Physics

INCITE Allocation:

Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (400,000 Summit node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (370,000 Frontier node-hours)

Research Summary: Realizing the potential of nuclear fusion to provide a nearly limitless, zero-carbon power source requires good confinement of the energy in the plasma to achieve self-sustaining fusion power. Multiscale turbulence simulations of hydrogen fuel isotopes and multi-ion impurities will predict energy losses and optimize performance for next-generation reactors like ITER. Exceptional GPU scaling performance of CGYRO on Summit to capability-level has been demonstrated through previous ALCC and INCITE awards and is expected to carry-over to Frontier. These CGYRO simulations of JET DTE2 scenarios will provide a unique and timely opportunity for validation of models for multi-ion burning plasma turbulence and developing a predictive capability for ITER.

With global energy demands growing, nuclear fusion promises a potentially attractive solution as a nearly limitless, zero-carbon source of energy for the next generation. Magnetic confinement of plasmas in a tokamak is a leading approach for controlled nuclear fusion energy production in worldwide research programs. Good confinement of the thermal energy in the plasma is necessary for efficient, self-sustaining (burning) fusion power. Plasma confinement, however, is limited by slow particle and energy losses due to turbulence, driven by unstable waves triggered by plasma inhomogeneities, that can limit fusion performance. Understanding the underlying mechanisms that drive turbulence in burning plasmas is essential in designing next-generation tokamak fusion reactors like ITER with optimum confinement.

Type: New
Title: "High-Throughput Calculation of Materials Properties at Finite Temperature"

Principal Investigator: Chris Wolverton, Northwestern University

Scientific Discipline: Materials Science

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

Research Summary: Large-scale electronic structure calculations using density functional theory (DFT) have become an important workhorse in computational materials science. Increasing amounts of computed materials properties are being stored in large databases, which serve as a basis for many data-mining and machine learning efforts to design novel functional materials. Materials Project, AflowLib, and the Open Quantum Materials Database (OQMD) are only a few of the largest and most popular computational materials databases available to date. Data-driven materials design projects have recently not only led to the discovery of novel, improved materials, but also to a better understanding of the complex relationship between atomic structure and materials properties. However, the materials properties currently contained in these databases are limited to those obtained by rather simple ground state calculations—such as formation energies, electronic band-gaps, and structures—with no dynamical information. This poses a crucial limitation when it comes to the prediction of materials at ambient or higher temperatures. It is well known that effects arising from finite temperature are important for many materials properties such as electronic and heat transport, polymorphism, and dynamical stability, among others.

This project aims to address the above-mentioned limitations of currently available computational materials databases by vastly extending the range of materials properties such databases contain. To this end, this work will include dynamical data obtained from lattice dynamics calculations in a high-throughput fashion. Prohibitively expensive, conventional methods had so far prevented the calculation of force constants from DFT on a routine basis, but recent advances in modeling techniques finally bring this endeavor within reach.

For the very first time, the researchers will employ a highly efficient compressive sensing lattice dynamics technique on a large scale to extract both harmonic and anharmonic force constants up to the fourth order at a fraction of the computational cost compared to conventional methods. Single-point DFT calculations on several large super cells will be performed for each compound to generate the fitting data. The force constants will then be readily useable for computing a variety of materials properties, such as free energy, entropy, phonon dispersion, lattice thermal conductivity, and many more.

Type: New
Title: "Hybrid simulation of macroscopic instabilities with energetic particles in fusion plasma"

Principal Investigator: Chang Liu, Princeton Plasma Physics Laboratory
Co-Investigators: Stephen Jardin, Princeton Plasma Physics Laboratory
Amitava Bhattacharjee, Princeton Plasma Physics Laboratory

Scientific Discipline: Physics

INCITE Allocation:

Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (240,000 Summit node-hours)

Research Summary: Through this INCITE project, the team will use the M3D-C1-K code to conduct kinetic-MHD simulation for magnetohydrodynamics (MHD) instabilities excited by energetic ions or runaway electrons in tokamaks and stellarators. The goal is to understand the comprehensive nonlinear physics in current experiments and solve critical physics issues for ITER and future magnetic confinement fusion reactors.

M3D-C1-K is a hybrid code including a continuum solver for the MHD equations, and a particle simulation module using the PIC method. The MHD equations are discretized using a finite element method on a 3D unstructured mesh, which is generated and managed through the SCOREC library developed at Rensselaer Polytechnic Institute (RPI). The equations are solved as an initial value problem, and advanced in time through full implicit or semi-implicit methods. The time advance matrix is solved using the PETSC library by constructing a block-Jacobi preconditioner and calling GMRES iterative solver. The LU decomposition for each block is obtained using the MUMPS or the SuperLU libraries. The code is mainly developed using Fortran 90, with some new features including function and operator overloading. The interface to the SCOREC and PETSC libraries are developed using C++ with an object-oriented model. The teams have extensive experience in deploying the code on different architectures and diagnosing issues. The team has deployed the code on many HPCs before, including Edison, Hopper, Cori, Perlmutter, and AiMOS. The code can run on different machine architectures including Intel, AMD, IBM and Nvidia using compilers from GNU, Intel, PGI and Nvidia. The team has developed tools inside the code to analyze the computation time of each component and find the bottleneck of code running

Type: New
Title: "Hypersonic Turbulent Boundary Layers Over Parameterized Wall Conditions"

Principal Investigator: Lian Duan, The Ohio State University

Scientific Discipline: Engineering

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

Research Summary: This project aims to enable more accurate predictions for hypersonic boundary layer flows subject to the effects of pressure gradient and wall cooling. The research approach is to (i) develop a direct numerical simulation (DNS) database over parameterized wall conditions that include systematically and continuously varied surface curvature and wall temperature, and (ii) subsequently utilize this DNS database to both characterize the effects of pressure gradient and wall cooling on boundary-layer turbulence and perform a thorough evaluation of the existing turbulence models as well as the models that are currently under development.

The study will create a benchmark quality parameter-sweeping database that is essential to the training and testing of data-driven turbulence models. It will also derive flow statistics, including boundary layer profiles of mean flow, Reynolds stresses, velocity-temperature correlations, surface skin friction and heat flux, as well as various budget terms in the exact equations of turbulent kinetic energy (TKE) and Reynolds-stress transport. The evaluation of existing turbulence models will include a term-by-term comparison of TKE and Reynolds-stress budgets between DNS and the Reynolds-stress transport modelling, as well as an evaluation of the algebraic model for turbulent energy flux based on a priori and a posteriori assessments. The generated DNS datasets and turbulence statistics will be made available to other investigators to develop, improve, and validate turbulence models (both conventional and data-driven) for Reynolds-averaged Navier-Stokes equations.

Type: Renewal
Title: "Intermolecular energy and electron transfer by non-orthogonal configuration interaction"

Principal Investigator: Coen de Graaf, Universitat Rovira i Virgili
Co-Investigators: Carmen Sousa, Universitat de Barcelona
Tjerk Straatsma, Oak Ridge National Laboratory
Ria Broer, University of Groningen

Scientific Discipline: Chemistry

INCITE Allocation:

Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (650,000 Summit node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (170,000 Frontier node-hours)

Research Summary: Traditional silicon-based solar cells have become quite efficient both in production costs and conversion, but organic photovoltaics have several potential advantages such as lower production costs, portability, flexibility, and their light weight. Although efficiency is steadily increasing, the solar cells based on organic materials still need further development to become serious additions to the silicon-based cells. Where solar cells help to reduce the use of fossil fuels, photocatalytic complexes can reduce CO_2 to CO or any of the many hydrocarbons, eventually leading to negative emission rates of CO_2. De Graaf's team will study the electron and/or energy transfer in transition metal complexes with photocatalytic properties, in multiple exciton generation (as occurs in singlet fission), and in the dispersion of excitons in organic molecular crystals. The GronOR code is ready to attack these problems from a completely different point of view than those taken by the conventional theoretical approaches based on one-electron models or density functional theory. The team expects that the NOCI calculations can lead to crucial information to derive advanced design rules for materials with improved electron and energy transfer properties, which can be applied to improve the efficiency of organic solar cells, conducting polymers, organic light-emitting diodes, homogeneous catalysts for CO_2 reduction and other materials where these processes play an important role.

Type: Renewal
Title: "Kinetic Turbulence in Black Hole Accretion Flows and Coronae"

Principal Investigator: Luca Comisso, Columbia University
Co-Investigators: Daniel Groselj, Columbia University
Lorenzo Sironi, Columbia University

Scientific Discipline: Physics

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (700,000 Theta node-hours)

Research Summary: Supermassive black holes are believed to exist at the center of every galaxy, where they play a crucial role in the evolution of galaxies. While no particles or electromagnetic radiation can escape from black holes, electromagnetic radiation can be emitted from the accretion material surrounding and feeding the black hole, the so-called accretion flow.

The goal of this project is to study how magnetized plasma turbulence and magnetic reconnection—two of the most fundamental and ubiquitous plasma processes, which were historically studied separately, but have recently been shown to be inevitably interconnected—lead to heating and particle acceleration in the accretion flows feeding massive black holes. The team's proposed computational plan focuses on two aspects of the physics of plasmas near black holes.

The first aspect concerns the exploration of the turbulence and reconnection interplay in low-luminosity accretion flows to understand the efficiency and the mechanisms of electron heating and acceleration. This will be critical to producing physically motivated models that can be used to compare with observations such as the Event Horizon Telescope, which recently delivered the first-ever image of Sgr A*, the supermassive black hole located at the center of our galaxy.

The second aspect involves the investigation of the self-consistent interplay of turbulence and radiation in the most magnetized regions around luminous black hole systems. The team will assess the origin of the observed hard x-ray emission, and test whether black hole coronae are likely sources of ultrahigh-energy cosmic rays, the most energetic particles in the universe.

This team's project will advance our understanding of the plasma physics of turbulence and reconnection in the extreme relativistic conditions near black holes.

Type: New
Title: "Lipid shuttling molecular machines enabling functions of human cell membranes"

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

Scientific Discipline: Biology

INCITE Allocation:

Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (730,000 Summit node-hours)

Research Summary: The team will use computation to learn how specific proteins in the membranes of the team's cells work to maintain the properties needed for life and health. Understanding how they function will enable repair in disease, and the engineering of proteins with new functional applications.

The team's goals are to discover, quantify and develop blueprints for practical uses of, molecular and functional properties of key types of lipid-shuttling molecular machines: lipid scramblase and transporter proteins. Compelling reasons for achieving these goals include (1)-the great biological importance of what these molecular machines achieve as evidenced by their misfunction being involved in recognized genetic disorders of tissues and entire organs; (2)-their experimentally determined role in normal cell physiology based on membrane regulation; and (3)-their ability to serve as mechanistic templates for the biomimetic engineering of synthetic regulators of lipid membrane systems, lipid transport machines, and the creation of specific environments for biological function.

To attain the objectives and Milestones of this study, the major emphasis is on the collection and analysis of massive amounts of data from computational simulations and analysis/interpretation with machine-learning based approaches to trajectory analysis.

Type: New
Title: "Long term 3D simulations of core–collapse supernovae"

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

Scientific Discipline: Physics

INCITE Allocation:

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

Research Summary: Through this INCITE project, the team plans long running models of core-collapse supernovae to examine their neutrino and gravitational wave signals for potential detection by current and future observatories. The team will also examine the elemental production that occurs in supernova, especially the potential for elements heavier than iron to be made late in the explosion. Operator splitting (solving physics components separately, rather than simultaneously) and dimensional splitting (solving equations separately for the three spatial dimensions: r, ✓,) are the key themes to Chimera's computational approach to the multi-dimensional supernova problem.

Core-collapse supernovae, the explosive final moments of massive stars, are complex, dynamic, multi-physics events yielding a bright and energetic explosion from the birth of a neutron star or black hole. The 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 team is entering an era where the well-resolved, symmetry-free, three-dimensional (3D) simulations with sufficient physical detail and coupling necessary to understand these complex stellar explosions and their byproducts are now possible.

Type: New
Title: "A Multiphysics Approach for Guided Human-Scale Mars Lander Descent Simulations'

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

Scientific Discipline: Engineering

INCITE Allocation:

Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (20,000 Summit node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (1,000,000 Frontier node-hours)

Research Summary: The entry, descent, and landing (EDL) systems for the United States' nine successful landings on Mars have all relied heavily on extensions of technology developed for the Viking missions of the mid-1970s. To achieve human exploration on Mars, this effort aims to explore new EDL approaches to support delivery of substantially larger payloads to the surface. This investigation will be able to use wind tunnel data as a future validation source and support assessment of the state-of-the-art in current ground test and computational capabilities in simulating the retro propulsion problem. When combined with data generated on Summit in 2019, 2021, and 2022, the limitations in subscale static testing with inert simulant gases will be quantified.

Large physical scales and challenging operational environments greatly restrict the ability to develop databases with ground test facilities and terrestrial flight tests. Computational analysis will be the cornerstone of the development and substantiation of a powered descent system. Fully coupled, unsteady simulations will be performed for a full-scale retropropulsive vehicle traversing a controlled, decelerating trajectory while accounting for turbulence in the near-wall and off-body/plume regions and further complicated by extensive gas chemistry interactions between the Martian CO2/N2 atmosphere and the O2/CH4 engine exhaust. Closed-loop control will be accommodated using main engine throttling and a reaction control system. Along with data generated previously on Summit, the impacts of decelerating flight will be quantified for the first time. The proposed effort directly provides the capability for NASA to complete a feasibility assessment of the baseline human Mars EDL architecture and establish requirements for the methods and resources necessary to support a flight implementation.

Type: New
Title: "A new path to energy-scalable laser plasma accelerators"

Principal Investigator: Alexander Debus, Helmholtz-Zentrum Dresden-Rossendorf
Co-Investigators: Klaus Steiniger, Helmholtz-Zentrum Dresden-Rossendorf

Scientific Discipline: Physics

INCITE Allocation:

Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (1,000,000 Frontier node-hours)

Research Summary: PIConGPU simulations on Frontier will allow physicists to build realistic models of novel laser-plasma accelerators that can reach unprecedented particle energies. These open the path for compact, multi-TeV electron-positron colliders for answering fundamental questions of the universe.

The quest for advanced acceleration techniques for providing more compact accelerators is a grand challenge of particle accelerator physics. Addressing this challenge will allow to further scale up energies for high-energy physics, as well as enable accelerator technology to be more compact and commonly available, thus making it affordable for universities, hospitals, and industry to operate their own accelerator facilities. Particle accelerators have a broad impact on science, engineering, and medicine. State-of-the-art accelerators based on conventional radio-frequency (rf) -cavities are driving the most advanced x-ray FELs such as LCLS. In contrast, Laser-plasma accelerators (LPA) can make use of orders of magnitude larger acceleration fields in plasma structures than are achievable in conventional rf-cavities. Despite tremendous advances in LPAs with respect to beam energy, quality, charge and stability, sustaining scalability of compact LPAs for accelerating bright electron and positron beams to even higher electron energies is one of the yet to be solved key challenges of the field.

In pioneering studies at HZDR, the team found that these limitations can be overcome by a novel laser-plasma interaction geometry, Traveling-Wave Electron Acceleration (TWEAC). Relying on spatio-temporally shaped ultrashort, high-power laser pulses using existing laser technology, these laser pulses provide "flying" focal regions propagating at tunable velocities close to the speed of light without the need for laser guiding structures.

Type: Renewal
Title: "Next-Generation 3D Core-Collapse Supernova Simulations"

Principal Investigator: Adam Burrows, Princeton University
Co-Investigators: David Vartanyan, University of California Berkeley
Matt Coleman, Princeton University
Chris White, Princeton University

Scientific Discipline: Physics

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): Cray XC40 (2,500,000 Theta node-hours)
Site: Argonne National Laboratory
Machine (Allocation): HPE Apollo 6500 (300,000 Polaris node-hours)

Research Summary: Core-collapse supernova explosions accompany the deaths of massive stars. These explosions give birth to neutron stars and black holes and eject solar masses of heavy elements. However, determining the mechanism of explosion has been a half-century journey of great complexity.

Nevertheless, due in part to recent massive suite of 3D simulations performed using the team's code Fornax on HPC resources, the delayed neutrino-heating mechanism is emerging finally as a robust solution. However, models must not only be shown to explode, but the asymptotic state of the blast must be reached to determine many of the observables. Hence, the key goals of this INCITE project are to determine such observables as the explosion energies and neutron star residual masses. To accomplish this, the team is simulating a collection of massive-star progenitor models to late times after bounce. The team plans to double this long-term effort because of code speed-ups and improvements. Hence, the overall scientific goal of simulating 3D models to late times has not changed but has in fact been augmented.

As a byproduct of this investigation, the researchers will generate libraries of supernova simulation data; neutrino, nucleosynthetic, and gravitational-wave signatures; and the systematics of supernova explosion energy, neutron star mass, pulsar kicks and spins, and debris morphologies with progenitor. Hence, this INCITE project has been constructed to build on the team's recent palpable progress, capture this pivotal moment in theoretical astrophysics when codes and resources are aligning, and erect a standard model for core-collapse supernova explosions in the emerging era of the exascale.

Type: New
Title: "Photophysics of Excitons in Low Dimensional Organic-Inorganic Semiconductors"

Principal Investigator: Marina Filip, University of Oxford
Co-Investigators: Sivan Refaely-Abramson, Weizmann Institute of Science
Linn Leppert, University of Twente
Diana Qiu, Yale University
Mauro Del Ben, Lawrence Berkeley National Lab

Scientific Discipline: Materials

INCITE Allocation:

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

Research Summary: The team will use and develop upon first principles Green's functions-based methods to understand the photophysical properties of optically excited quasiparticles in complex low dimensional hybrid organic-inorganic semiconductors. The team's goal is to develop new methods and new intuition in order to design and discover new hybrid materials for optoelectronic and energy applications.

The team's project is structured in five main research objectives, all centered around developing a deep understanding of the photophysics of the organic-inorganic low-dimensional metal-halide perovskite and perovskite-related materials. The team has designed their research objectives to run continuously over two years. Of the five objectives, four focus on using many-body perturbation theory techniques to understand the optoelectronic properties of these complex systems, and specifically on elucidating the role of chemical and structural heterogeneity in the photophysics of this complex materials family. They therefore hone in on the structure-chemistry-property relationship in this family (O1), understanding how to accurately compute and probe the effect of disorder and chirality in these systems (O2), developing a framework to compute dynamical properties of excitations in these systems using first principles techniques (O3) and combining the knowledge and frameworks developed in O1-O3 to a sufficiently broad structural and chemical family of materials to delineate design rules and develop routes to design and discover new materials with bespoke properties (O4). The fifth objective (O5) is dedicated to the development of the necessary infrastructure to tackle these complex problems from first principles, specifically focused on continuing to optimize the BerkeleyGW code to allow the study of ever-larger and more complex systems and using the materials systems and scientific questions in O1-O4 to guide development directions.

Type: New
Title: "Precision calculations of matrix elements for Novel CP Violation Experiments"

Principal Investigator: Rajan Gupta, Los Alamos National Laboratory
Co-Investigators: Tanmoy Bhattacharya, Los Alamos National Laboratory
Vincenzo Cirigliano, University of Washington

Scientific Discipline: Physics

INCITE Allocation:

Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (100,000 Summit node-hours)

Research Summary: The observed universe has an almost total absence of antimatter, whose dynamical generation requires much larger violation of charge-conjugation-parity (CP) symmetry than exists in established theory. The proposed results increase the reach of experiments searching for novel CP violation in the neutrino sector and in neutron electric dipole moment. The team represents a balance in expertise between lattice QCD, phenomenology of CP violation, high performance computing, and code development and optimization (on Summit and Frontier).

The goal of this project is to calculate matrix elements (ME) within nucleon ground state that are needed to quantify CP violation in two sectors: neutrino mixing matrix and neutron electric dipole moment (nEDM). These ME will allow the team to probe beyond the standard model (BSM) physics in two different ways: In the first case, precision results for the axial form factors enter in the calculation of the neutrino-nucleus scattering cross-section and the neutrino flux that are needed for reaching the design precision of experiments such as SBN and DUNE at Fermilab. In the second, combined with the experimental bound [or result] for the nEDM, they put constraints on novel CP violating interactions at the TeV scale, and impact the analysis of whether baryogenesis is a credible mechanism for explaining the matter-antimatter asymmetry in the observed universe.

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

Principal Investigator: Andre Severo Pereira Gomes, Centre National de la Recherche Scientifique (CNRS)

Co-Investigators:
Jochen Autschbach, University at Buffalo, SUNY
Anastasia Borschevsky, University of Groningen
Miroslav Ilias, Matej Bel University
Hans Jorgen Aagaard Jensen, University of Southern Denmark
Kirk Peterson, Washington State University
Michal Repisky, University of Tromsø/The Arctic University of Norway
Trond Saue, Université Toulouse III-Paul Sabatier
Stefan Knecht, ETH Zürich
Ayaki Sunaga, Kyoto University
Valerie Vallet, Laboratoire de Physique des Lasers Atomes et Molecules (PhLAM)
Johann Pototschnig, Université Toulouse III-Paul Sabatier

Scientific Discipline: Chemistry

INCITE Allocation:

Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (490,000 Summit node-hours)

Research Summary: The PRECISE project will use highly accurate relativistic correlated electronic structure methods, implemented in a modern massively parallel gpu-accelerated code, to investigate different aspects of the chemistry and physics of transition metals and actinides, from their reactivity and spectroscopic signatures to their use as probes for physics beyond the Standard Model.

Accurate treatment of molecular energies and properties of these elements requires inclusion of both relativistic and electron correlation effects and 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 CAAR program for Summit and employed for the first time in the team's 2020 INCITE application.

Type: New
Title: "Radiation-Dominated Black Hole Accretion"

Principal Investigator: James Stone, Institute for Advanced Study
Co-Investigators: Shane Davis, University of Virginia
YanFei Jiang, Center for Computational Astrophysics, Flatiron Institute
Patrick Mullen, Institute for Advanced Study
Christopher White, Center for Computational Astrophysics, Flatiron Institute

Scientific Discipline: Physics

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): HPE Apollo 6500 (110,000 Polaris node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (1,000,000 Frontier node-hours)

Research Summary: Accretion of plasma by black holes powers all of the most luminous objects in the universe, including x-ray binaries and active galactic nuclei. In addition, the radiation and outflows produced by accreting black holes produces feedback on their environment, which in turn affects galaxy formation and limits the rate of growth of supermassive black holes in the early universe. It has long been known that the inner regions of luminous accretion flows are dominated by radiation, and therefore modeling these sources requires solving the equations of general relativistic radiation magneto-hydrodynamics (MHD). However, despite the importance of understanding luminous accretion flows for interpreting a variety of astronomical observations, very few calculations of this regime have been performed to date due to the complexity and cost of the methods.

With this INCITE project, the team will perform the first calculations of radiation-dominated accretion on black holes using full transport methods and realistic opacities. The researchers will survey the properties of accretion flows for both supermassive and stellar mass black holes for a variety of spins, tilt, and accretion rates. They will also study how relativistic jets and outflows produced by combination of magnetic fields and black hole spin are affected by strong radiation fields. To carry out this work, the team will use AthenaK, a new performance-portable version of the Athena++ astrophysical MHD code that uses Kokkos.

Their calculations, enabled by emerging exascale architectures, will push the frontier of state-of-the-art modeling of astrophysical accretion flows. The simulations will allow the first direct tests of theoretical models of luminous accretion disks, and moreover direct comparison to observations will test such important questions as whether spectral fitting methods to measure the mass and spin of black holes are reliable.

Type: New
Title: "Radiation transport general relativistic MHD simulations of transitional accretion disks"

Principal Investigator: Matthew Liska, Harvard University
Co-Investigators: Gibwa Musoke, University of Amsterdam
Oliver Porth, University of Amsterdam
Bar Ripperda, Flatiron Institute

Scientific Discipline: Physics

INCITE Allocation:

Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (750,000 Frontier node-hours)

Research Summary: This proposal aims to address how radiation pressure supported accretion disks get torn apart by a rapidly spinning black hole. The proposed numerical simulations will be the largest ever and will give the astrophysical community unique insights into fundamental plasma physics under extreme conditions and gravity. The team's work contributes to the training of the next-generation workforce (students and postdocs) highly qualified in carrying out radiative MHD modeling in the regimes from linear to nonlinear and into turbulent radiation-dominated regimes and with excellent physical insight into radiation-matter interactions of great interest to a wide range of DOE laboratories and basic science.

Using ORNL Frontier, the team proposes to carry out, analyze and ray-trace the next generation GRMHD simulations of the 'luminous-hard' and 'luminous-soft' BH accretion states, using the team's newly developed GRMHD radiation transport module. The unprecedented scale and complexity of these simulations requires exascale resources. This will lead to breakthroughs in understanding luminous black hole accretion disks and their radiation-driven outflows. The energetics of such outflows can be incorporated into cosmological simulations to better constrain black hole feedback and tighten the constraints on dark matter and energy. Ray-tracing of the simulation results will yield first-principles lightcurves and spectra, to be confronted against observational data to constrain strong-field gravity and extreme plasma physics. The proposed work pushes beyond the state of the art in the modeling of high-pressure plasma and radiation, coupled together by an advanced radiation-transport scheme.

Type: New
Title: "Rayleigh Taylor Mixing with Extreme Transport Property Contrasts"

Principal Investigator: Sanjiva Lele, Stanford University

Scientific Discipline: Engineering

INCITE Allocation:

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

Research Summary: Through this INCITE project, the team will develop a benchmark quality database of fully resolved compressible multi-species Rayleigh-Taylor (RT) instability with extreme transport property variations. The study will yield fundamental knowledge about RT turbulence behavior close to its quenching conditions, and guide future development of theory and turbulence models for variable density turbulence.

The goal of this INCITE proposal is to develop a benchmark quality database of fully resolved compressible multi-species Rayleigh-Taylor instability simulations with extreme transport property variations. The Rayleigh-Taylor Instability (RTI) occurs when fluids are accelerated opposite to their density gradient, causing small perturbations on the interface to grow and develop into "spikes" of heavy fluid and "bubbles" of light fluid. These spikes and bubbles interact with each other nonlinearly, break up and eventually the flow transitions into turbulence. However, in many situations, the Rayleigh Taylor (RT) instability may occur under conditions with large variations in density and fluid transport properties such as viscosity, thermal conductivity and mass diffusivity, either through temperature variations or differences in the fluid properties themselves. These conditions are commonly seen in Inertial Confinement Fusion (ICF), supernovae phenomena, Earth's mantle-core interactions and oceanic flows. Therefore, understanding how these instabilities develop under these conditions and how to mitigate their effects is of upmost importance. This proposal aims to advance the scientific understanding of RT turbulence under extreme property variations through accurate direct numerical simulations of this phenomena.

Type: New
Title: "Reactive Transport Controls on Fracture Evolution in Carbon Sequestration"

Principal Investigator: David Trebotich, Lawrence Berkeley National Laboratory
Co-Investigators: Sergi Molins, Lawrence Berkeley National Laboratory
Carl Steefel, Lawrence Berkeley National Laboratory
Randy Settgast, Lawrence Livermore National Laboratory

Scientific Discipline: Earth Science

INCITE Allocation:

Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (1,000,000 Frontier node-hours)

Research Summary: The geologic subsurface has constituted the nation's primary source of energy but now also provides a vast amount of storage critical to a low-carbon, secure energy future. Safe and efficient use of the subsurface requires sound understanding of and predictive capability for coupled thermal, hydrological, chemical and mechanical processes that control fracture evolution. The geologic subsurface has constituted the nation's primary source of energy but now also provides a vast amount of storage critical to a low-carbon and secure energy future. The safe and efficient use of the subsurface requires a sound understanding of and predictive capability for the coupled hydrological, chemical, thermal, and mechanical processes that control the success or failure of many energy-related endeavors including geologic CO_2 sequestration, petroleum extraction, geothermal energy, and nuclear waste isolation. The inherent multiscale nature of the subsurface, however, makes predictions of thermal, hydrological, chemical, and mechanical (THCM) processes difficult, particularly when relatively small-scale features like fractures or damage zones around wellbores can have a disproportionate effect on the larger scale system behavior. Wells are high-risk pathways for fluid leakage from geologic CO_2 storage reservoirs, because breaches in this engineered system have the potential to connect the reservoir groundwater resources and the atmosphere. The geologic carbon storage community has raised further concerns about wellbore stability because the acidic fluids associated with CO_2 storage is highly reactive with respect to the alkaline cement lining the borehole and meant to isolate the reservoir fluids from the overlying strata. This is particularly a concern in depleted oil and gas reservoirs that are used for CO_2 storage.

Type: New
Title: "Scalable Foundational Models for Transferable Generalist AI"

Principal Investigator: Irina Rish, University of Montreal, Mila - Quebec AI Institute
Co-Investigators: Stella Biderman, EleutherAI
Jenia Jitsev, Juelich Supercomputing Center / Research Center Juelich

Scientific Discipline: Computer Science

INCITE Allocation:

Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (990,000 Summit node-hours)

Research Summary: This project aims to train large-scale multi-modal deep neural network models, investigate their scaling laws and emergent behavior, and apply their generalization and knowledge transfer capabilities in a variety of practical applications.

The team's goal is to contribute to advancing AI from narrow to "broad" (general) while ensuring AI Safety and alignment with human values, and contribute towards advances in other fields (healthcare, biomedical sciences, and others) via developing generic, powerful large-scale models pretrained in a self-supervised manner on broad variety of datasets. Such models can serve as a foundation of transferable knowledge and can be used in a broad variety of applications ("downstream tasks") due to their drastically improved generalization abilities as compared to prior state-of-art in the field of AI. More specifically, building on recent successes in this area, the team plans to train large-scale neural network models called Transformers, which recently demonstrated impressive performance in language modeling and image processing; the team plans to evaluate their scaling with increasing model and pretraining dataset size, as well as the amount of compute available. Such models, also known as "foundation models", appear to improve their generalization and few-shot learning abilities with scale. The team plans to investigate this trend in more detail and identify the most promising approaches to scaling the architecture, and datasets. Next, they plan to extend these models to handle a much wider range of modalities beyond text and images, as well as various machine-learning tasks, and expand them towards adaptive, continually learning systems. Finally, the team plans to use the obtained foundation models for predictive modeling in several applications such as healthcare and brain imaging. As an outcome of this project, the team will obtain highly transferable multi-modal models that the team will make publicly available.

Type: New
Title: "Toward In-Service Realism: DNS of Gas Turbine Blades with Localized Roughness"

Principal Investigator: Richard Sandberg, University of Melbourne
Co-Investigators: Ivan Marusic, University of Melbourne
Melissa Kozul, University of Melbourne
Pawel Przytarski, University of Melbourne
Jake Leggett, University of Melbourne
Massimiliano Nardini, University of Melbourne
Aamir Shabbir, General Electric Aviation
Sriram Shankaran, General Electric Aviation
William Solomon, General Electric Aviation
Paul Vitt, General Electric Aviation

Scientific Discipline: Engineering

INCITE Allocation:

Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (410,000 Summit node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (320,000 Frontier node-hours)

Research Summary: This project will improve the team's understanding of how in-service roughness on turbine blades interacts with complex gas turbine flows by leveraging recent advances in first principle-based turbulence simulation capability. The new knowledge will help improve low fidelity industrial design tools and aid global efforts to reduce fuel use and emissions. Surface roughness affects fluid flow in many situations, from the atmospheric boundary layer always encountering rough surfaces, to many engineering applications where initially smooth surfaces may become rough due to fouling or erosion. An engineering application where roughness effects can significantly reduce efficiency (by up to 10% in several components) is the gas turbine (GT). Given that in 2019 in the USA alone GTs produced 38.4% of all power generated (1.58×109 MWh) and burned 18×109 barrels of jet fuel, roughness effects have a tremendous impact on cost and emissions. Therefore, any engine performance improvements realized through better understanding and prediction of roughness effects can have a fuel-spend advantage of order billion-$, together with a significant CO_2 emission benefit, and would also increase the viability of costlier, more sustainably sourced fuels.

Type: Renewal
Title: "Toward the rational design of more effective drugs with reduced side effects"

Principal Investigator: Ron Dror, Stanford University

Scientific Discipline: Biology

INCITE Allocation:

Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (630,000 Summit node-hours)

Research Summary: Chemical compounds that bind to G protein–coupled receptors (GPCRs), which represent the targets of nearly half of known drugs, activate several cellular signaling pathways mediated by both G proteins and arrestins.

In a phenomenon known as biased signaling, certain compounds can selectively activate specific G protein–mediated or arrestin–mediated signaling pathways, while avoiding other pathways controlled by the same GPCR. Leveraging this phenomenon is of tremendous medical importance, because, often, only one pathway leads to desired effects, while other pathways lead to harmful side effects. The molecular mechanism of biased signaling, however, has remained unknown, hindering the design of drugs with drastically reduced side effects. In this INCITE project, the team will use large-scale molecular dynamics (MD) simulations of GPCRs and their binding partners to address this question.

The team is using massively parallel simulations on Summit to identify molecular mechanisms by which different compounds that bind to the same drug target can stimulate different cellular signaling pathways. The team's goal is to enable the design of drugs that stimulate desired signaling pathways while avoiding undesired pathways, leading to safer and more effective treatments for a wide variety of diseases.

Type: New
Title: "Understanding Colloidal Crystallization Pathways and Processes"

Principal Investigator: Sharon Glotzer, University of Michigan

Scientific Discipline: Materials

INCITE Allocation:

Site: Oak Ridge National Laboratory
Machine (Allocation): IBM AC922 (410,000 Summit node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (730,000 Frontier node-hours)

Research Summary: Through this INCITE project, the team will investigate the ways in which nanoparticles of different shapes, sizes and composition self-assemble into materials of extraordinary structural complexity and diversity. Using the fastest computers available, the team aims to discover design rules that will lead to nanomaterials with new and exciting properties.

The team's aim in this proposal is to push the envelope of systems studied for crystallization to uncover potential novel assembly pathways and gain a more detailed understanding of crystallization that explains phenomena that elude description by current theories. The team proposes to study systems of increasing shape and interaction complexity including patchy polygons in two dimensions, proteins, flexible vesicles, and point particles interacting with oscillatory pair potentials. The team will compare and contrast the pathways these systems use to form complex crystals. Because of their differences, the team can find key insights not obtainable by studying any one system alone. The team's collective findings will be of immediate interest to the nanoparticle and colloidal assembly, condensed matter physics and protein crystallization communities. 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 the crystallization generally. The team's data sets and software will be made openly available for investigation by others.

Type: New

Title: "Unraveling How Lasers and Beams with Arbitrary Spatial and Temporal Structure Interact with Plasmas"

Principal Investigator: Paulo Alves, University of California Los Angeles

Co-Investigators: Warren Mori, University of California Los Angeles
Frank Tsung, University of California Los Angeles
John Palastro, University of Rochester
Xinlu Xu, Stanford Linear Accelerator Center

Scientific Discipline: Physics

INCITE Allocation:

Site: Argonne National Laboratory

Machine (Allocation): HPE Apollo 6500 (200,000 Polaris node-hours)

Research Summary: The past several years have seen tremendous progress in how to spatially and temporally structure laser pulses, which are rapidly opening up new research topics. These include laser pulses in which the peak intensity location moves at superluminal or subluminal speeds in vacuum (a flying focus), the phase fronts have corkscrew shapes (orbital angular momentum), and the polarization direction of the laser varies within the phase front of the laser. Furthermore, it is also possible to create intense particle beams with flying foci through the use of a chromatic lens. While the vacuum propagation properties of these lasers and particle beams are well-understood, the interactions of such lasers and beams with plasmas is just beginning to be understood.

The team leading this project has recently enhanced the particle-in-cell code OSIRIS to launch lasers with arbitrary spatial-temporal profiles. Using this capability, they are aiming to undertake a computational effort that lays the foundation for understanding such interactions while also developing near-term applications. The research will be discovery-driven, but with an eye towards making transformative progress in important applied areas: (i) making compact and efficient plasma-based accelerator and light sources, and (ii) generating ultra-high-power lasers through Raman and Brillouin amplification.

Type: Renewal
Title: "Wall-Resolved Large Eddy Simulation of the NASA CRM High-Lift Configuration"

Principal Investigator: Z.J. Wang, University of Kansas Center for Research, Inc.
Co-Investigators: Joshua Romero, NVIDIA Corporation
Nick Wyman, Cadence Design Systems

Scientific Discipline: Engineering

INCITE Allocation:

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

Research Summary: Wang's team will conduct a wall-resolved large eddy simulation of the NASA Common Research Model high-lift configuration using an implicit high-order unstructured-mesh compressible flow solver on Summit. This problem is considered a grand-challenge in aerospace engineering and the results will be very valuable in the development of turbulence models and wall models.

Very aggressive goals have been set by the U.S. and European Union to dramatically improve aircraft performance and reduce fuel burn and noise. However, many technology breakthroughs are needed to reach these goals. One such breakthrough in the next generation design tools is the use of large eddy simulation (LES) in understanding turbulent flow through jet engines and over high-lift configurations. To overcome the cost barrier of LES, University of Kansas researchers have been developing an unstructured-mesh based high-order LES solver, hpMusic, capable of handling complex geometries. Currently, this tool is used by KU's industrial partner GE to solve complex turbomachinery problems. Recent developments in implicit solution algorithms and wall-adaptive meshing have made it possible to conduct wall-resolved LES (WRLES) of high-lift configurations (HLC).