**Type:** Renewal
**Title:** "Ab-initio Nuclear Structure and Nuclear Reactions"


**Principal Investigator:** Gaute Hagen, Oak Ridge National Laboratory
**Co-Investigators:** Joseph Carlson, Los Alamos National Laboratory
Serdar Elhatisari, Karamanoglu Mehmetbey University
Stefano Gandolfi, Los Alamos National Laboratory
Gustav Jansen, Oak Ridge National Laboratory
Dean Lee, Michigan State University
Alessandro Lovato, Argonne National Laboratory
Pieter Maris, Iowa State University
Hai Ah Nam, Los Alamos National Laboratory
Petr Navrátil, TRIUMF
Thomas Papenbrock, University of Tennessee, Knoxville
Saori Pastore, Los Alamos National Laboratory
Maria Piarulli, Washington University in St. Louis
James Vary, Iowa State University
Robert Wiringa, Argonne National Laboratory


**Scientific Discipline:** Physics: Nuclear Physics

**INCITE Allocation:**
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** IBM AC922 (590,000 Summit node-hours)
**Site:** Argonne National Laboratory
**Machine (Allocation):** Cray XC40 (1,500,000 Theta node-hours)


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

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

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

**Principal Investigator:** Ivaylo Ivanov, Georgia State University

**Scientific Discipline:** Biological Sciences: Biophysics

**INCITE Allocation:**
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** IBM AC922 (190,000 Summit node-hours)

**Research Summary:** Gene expression governs all important aspects of cell biology – it determines cell identity, growth, differentiation, and development. Understanding how gene expression is regulated constitutes a grand challenge in biomedical science. Ivanov's project aims to simulate the intricate molecular machinery in gene expression and uncover important gene regulatory mechanisms.

Ivanov and team will take advantage of new cryo-EM data and combine it with advanced computational modeling on the Summit supercomputer to elucidate the mechanisms of PICTFIID assembly, promoter recognition, DNA melting and the roles of general transcription factors therein. The team will examine the role of the factor TFIID, which serves as a platform to assemble the PIC machinery on promoter DNA. They will also delineate the role of the co-activator Mediator in stabilizing the PIC assembly and effecting transcription regulation. Both Mediator and TFIID have important regulatory roles in communicating signals from accessory proteins to the PIC. Ivanov's project aims to uncover the underlying mechanisms and unveil the corresponding allosteric networks. Achieving these goals will require simulations of unprecedented size (2–5 million atoms and hundreds of replicas) using advanced path optimization and sampling algorithms (e.g. the string method, ensemble MD simulations). The requisite simulation codes (NAMD and Amber) are available and have been extensively optimized and tested on the Summit platform. The team verified the codes' efficiency on V100 GPUs and readiness for leadership computing (scalability up to 1000 Summit nodes).

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


**Principal Investigator:** Andreas Kronfeld, Fermi National Accelerator Laboratory
**Co-Investigators:** Thomas Blum, University of Connecticut
Peter Boyle, Brookhaven National Laboratory
Norman Christ, Columbia University
Carleton DeTar, University of Utah
Aida El-Khadra, University of Illinois
Steven Gottlieb, Indiana University
William Jay, Fermi National Accelerator Laboratory
Chulwoo Jung, Brookhaven National Laboratory
Joseph Karpie, Columbia University
Christoph Lehner, Universität Regensburg
Andrew Lytle, University of Illinois
Ruth Van de Water, Fermi National Accelerator Laboratory


**Scientific Discipline:** Physics: Particle Physics

**INCITE Allocation:**
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** IBM AC922 (790,000 Summit node-hours)


**Research Summary:** Kronfield's project will assist the experimental effort to discover new, fundamental particles and interactions. Starting from the Standard Model, this project will perform high-precision numerical calculations. Results from their project will be compared with results of high-precision experiments. Discrepancies between theory and experiment will provide clues for new physical processes at work.

Kronfield's team will work to address fundamental questions in elementary particle physics. Their proposed calculations directly support extensive experimental efforts in this field. They will use numerical simulations of the lattice gauge theory formulation of quantum chromodynamics (lattice QCD). In some cases, the team also incorporate corrections from electromagnetism and the small difference in the up- and down-quark masses, because the precision of corresponding experiments requires these effects. The calculations are well aligned with the U.S. strategic plan, spelled out a few years ago in the report of the Particle Physics Project Prioritization Panel. Because of these important, ambitious goals the highest-capability supercomputers are necessary to make an impact. QCD is the component of the Standard Model of particle physics from which hadrons and atomic nuclei emerge.

**Type:** Renewal
**Title:** "Approaching Exascale Models of Astrophysical Explosions"


**Principal Investigator:** Michael Zingale, Stony Brook University
**Co-Investigators:** Ann Almgren, Lawrence Berkeley National Laboratory
Maria Barrios Sazo, Stony Brook University
John Bell, Lawrence Berkeley National Laboratory
Alan Calder, Stony Brook University
Kiran Eiden, University of California, Berkeley
Duoming Fan, Lawrence Berkeley National Laboratory
Alice Harpole, Stony Brook University
Maximilian Katz, NVIDIA
Andy Nonaka, Lawrence Berkeley National Laboratory
Jean Sexton, Lawrence Berkeley National Laboratory
Donald Willcox, Lawrence Berkeley National Laboratory


**Scientific Discipline:** Physics: Astrophysics

**INCITE Allocation:**
**Site:** Argonne National Laboratory
**Machine (Allocation):** HPE Apollo 6500 Gen10+ (100,000 Polaris node-hours)
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** IBM AC922 (590,000 Summit node-hours)


**Research Summary:** Building on more than a decade of work, this project, leveraging the Summit and Polaris supercomputers, aims to produce models of burning and flame propagation on neutron stars as models for x-ray bursts (XRBs), investigate white dwarf mergers and the role of magnetic fields, and explore the end state of massive star convection. These are all multiscale, multiphysics problems whose calculation requires the coupling of hydrodynamics, magnetic fields, reactions, gravity, and diffusion.

The team's XRB simulations will provide insight into the rapid proton capture process nucleosynthesis, connect with observations, and probe the structure of the underlying neutron star. A suite of white dwarf mergers, with and without magnetic fields, will be modeled, allowing the team to probe this system as a possible progenitor for Type Ia supernovae. Finally, the massive star research will provide important input (and an Open simulation framework) to the core collapse modeling community.

**Type:** New
**Title:** "Automatic Building Energy Modeling (AutoBEM)"

**Principal Investigator:** Joshua New, Oak Ridge National Laboratory
**Co-Investigators:** Andy Berres, Oak Ridge National Laboratory
Brett Bass, Oak Ridge National Laboratory

**Scientific Discipline:** Energy Technologies: Energy Efficiency

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

**Research Summary:** There are more than 125 million residential and commercial buildings in the U.S. consuming approximately $395 billion per year in energy bills, 73% of the nation's electricity (80% during peak generation), and 39% of the nation's greenhouse gas emissions. Building energy modeling can help identify energy conversation measures, but this approach suffers from the high transaction costs needed to create, refine, understand, and effectively utilize the models. For example, significant amounts of manual labor are required to construct one-off building models by hand, often repeatedly for different uses by different stakeholders.

With this INCITE project, researchers will advance the Automatic Building Energy Modeling (AutoBEM) project to extend existing capabilities for creating and simulating a model of every building in America (bit.ly/ModelAmerica) to estimate energy, emissions, and cost reductions of energy-efficient building technologies. AutoBEM (bit.ly/AutoBEM) is a suite of software tools that incorporates several data retrieval and scalable processing algorithms for defining properties about each building in a geographical area and synthesizing an OpenStudio and EnergyPlus building energy model.

Building on the research carried out with a 2020-2021 award from DOE's ASCR Leadership Computing Challenge, the AutoBEM team will continue to leverage DOE supercomputers to incorporate new data, methods, and stakeholder feedback to significantly improve crude, nation-scale building energy models toward investment-grade models. The researchers will also continue to work with stakeholders to make the resulting building energy models and analysis free and publicly available under a permissive license for use by any organization for any purpose. Ultimately, this project will deliver data products that aim to stimulate private sector activity towards more simulation-informed and grid-aware energy efficiency technologies necessary for a sustainable built environment.

**Type:** New
**Title:** "Climatype Clustering: A Longitudinal View of Environmental Change"


**Principal Investigator:** Daniel Jacobson, Oak Ridge National Laboratory
**Co-Investigators:** Peter Thornton, Oak Ridge National Laboratory
Wayne Joubert, Oak Ridge National Laboratory
Michael Garvin, Oak Ridge National Laboratory
David Kainer, Oak Ridge National Laboratory
John Lagergren, Oak Ridge National Laboratory
Mikaela Cashman, Oak Ridge National Laboratory
Verónica Melesse Vergara, Oak Ridge National Laboratory
Jean Merlet, Oak Ridge National Laboratory


**Scientific Discipline:** Biological Sciences: Systems Biology

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


**Research Summary:** Jacobson's team will capture and compare the monthly climate patterns across many environmental variables in one-year time windows over a 60-year time period for dry land geolocations across the Earth. In addition, the team will determine patterns of relative environmental stability and instability for all geolocations analyzed.

The challenges of world hunger and the expansion of biofuel products to address sustainable energy needs 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. Researchers now have the ability to design plant genotypes(cultivars) that are optimized for food or energy production, are stress resistant, and can be grown in targeted locations where they are likely to thrive. In order to improve understanding of climate zones and fine-scale geographic conditions, Jacobson's team will capture the daily climate patterns across many environmental variables for dry land geolocations across the planet. This will allow them to make accurate and unbiased assessments of environmentally correlated regions that can be used to address the problem of global food insecurity and to determine which environments are undergoing notable relativistic change and those that are stable. 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 substantial positive economic, political, and societal implications.

**Type:** New
**Title:** "COMPBIO2: COMbining deep-learning with Physics-Based affinIty estimatiOn 2"


**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:**
**Site:** Argonne National Laboratory
**Machine (Allocation):** Cray XC40 (1,000,000 Theta 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, the researchers have 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. The selected compounds are scored based on calculated binding free energies, and fed back into the deep learning algorithm to iteratively refine predictive capability.

This approach will have direct applicability in the pharmaceutical industry for quick identification of potent binders for a given target protein and binding pocket. Additionally, a machine learning-based method will enable assessment of the resistance of COVID-19 protein variants and their impact on existing vaccines and drugs.

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


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


**Scientific Discipline:** Materials Science: Condensed Matter and Materials

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


**Research Summary:** Correlated quantum materials exhibit novel properties that promise to revolutionize science and technology, but they require optimization to unleash their full potential. Maier's project will use high-end simulations to understand and predict the rich phenomenology in unconventional and topological superconductors and thus help accelerate the discovery of new and improved materials. With this goal in view, the team will carry out unprecedented numerical studies of multi-orbital Hubbard models, including variants with additional spin-orbit and electron-lattice interactions. They will study these models using implementations of advanced numerical algorithms, including the dynamic cluster, determinant quantum Monte Carlo, and density matrix renormalization group methods, which they have heavily optimized for ORNL's Summit supercomputer. The use of leadership computing will allow the team to go well beyond previous work and use cluster and lattice sizes large enough to provide reliable results.

This project will significantly impact the path to discovering new materials by using powerful and efficient numerical algorithms, with optimized implementations making full use of leadership computing, to push the limits of correlated quantum materials simulations. Using these methods, Maier's team will provide decisive answers to questions needed to understand the rich phenomenology observed in these systems and predict the circumstances under which these properties are optimized. The team's track record in delivering large-scale and high-impact computational science uniquely positions them to carry out this research and help the scientific community lay the foundation for revolutionary new advances in materials science.

**Type:** New
**Title:** "Decoding the IGM with Exascale Cholla Simulations"


**Principal Investigator:** Brant Robertson, University of California Santa Cruz
**Co-Investigators:** Evan Schneider, University of Pittsburgh
Piero Madau, University of California Santa Cruz
Nickolay Gnedin, University of Chicago and Fermi National Accelerator Laboratory
Reuben Budiardja, Oak Ridge National Laboratory
Damon McDougall, Advanced Micro Devices


**Scientific Discipline:** Physics: Astrophysics

**INCITE Allocation:**
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** IBM AC922 (390,000 Summit node-hours)


**Research Summary:** Using simulations of the formation of large-scale structures in the universe, Robertson and team will leverage the power of Summit to study the properties of the "cosmic web" in unprecedented detail. These simulations will be compared with observations from powerful facilities like the Dark Energy Spectroscopic Instrument (DESI) to learn about the nature of dark energy and dark matter.

The properties of the "cosmic web", the large-scale filamentary distribution of matter in the universe, are a critical probe for constraining cosmological physics including the nature of dark matter, the sum of the neutrino masses, and the process of cosmic reionization. Absorption line signatures of neutral hydrogen gas in the intergalactic medium (the "Lyman-$\alpha$ Forest") provide among the best constraints available from the cosmic web, but interpreting such observations requires detailed cosmological hydrodynamical simulations. Experiments like DESI commissioned this year will revolutionize this field, driving an urgent need for sophisticated, high-resolution simulations of the Lyman-$\alpha$ Forest. Robertson and team will perform an unprecedented series of cosmological simulations that use the GPU-native, MPI-parallelized code Cholla to model the cosmological formation of large-scale baryonic structures with unmatched detail. Given the sheer number of computational elements and the need for GPU acceleration, only Summit will have the power to perform this important work.

**Type:** New, Early Career
**Title:** "Deep Learning for Accurate and Cost-effective Imputation of Genotypes at Whole Genome Level"

**Principal Investigator:** Raquel Dias, The Scripps Research Institute
**Co-Investigators:** Ali Torkamani, The Scripps Research Institute

**Scientific Discipline:** Biological Sciences: Bioinformatics

**INCITE Allocation:**
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** IBM AC922 (690,000 Summit node-hours)

**Research Summary:** Genetic imputation is a standard tool in population genetics and genomic medicine, utilized in several contexts to go from sparse genetic data to near whole genome genetic data. Through this project, Dias's team will apply deep learning for scalable, accurate, and cost-effective imputation of genotypes at whole genome level.

Genetic imputation used in a variety of contexts to go from sparse genetic data to near whole genome genetic data. Traditional imputation tools use statistical techniques that rely on the availability of reference panels of dense genomes that often present access restrictions. Dias and team will use a deep learning-based approach for whole genome imputation. The approach consists of pre-trained autoencoders that are tiled across the human genome, simultaneously performing imputation, feature extraction and dimensionality reduction for downstream analyses with clinical and translational applications (e.g., genetic risk score calculation and genome wide association studies). Unlike statistical imputation tools, in which certain modelling rules must be predefined (e.g., phasing, recombination rates, mutation rates, and genotyping error rates), deep learning algorithms are built to automatically detect patterns in complex data. Additionally, the autoencoder-based imputation approach only requires a reference panel during training – only the neural network needs to be distributed for implementation. Thus, the neural network is portable and avoids privacy issues associated with standard statistical imputation. After expanding this approach across the whole genome, the team's work will provide a more cost-effective genotype imputation platform on whole genomic scale and thus beneficial for genome association studies and clinical applications in precision medicine. More robust results from autoencoder-based imputation will provide more insights on how deep learning can be integrated into imputation on whole genomic data, expanding clinical applications of genetic risk scores and improving preventive healthcare.

**Type:** Renewal
**Title:** "Design of Peptides and Proteins on Classical and Quantum Computing Hardware"


**Principal Investigator:** Vikram Mulligan, Flatiron Institute
**Co-Investigators:** Richard Bonneau, Flatiron Institute and New York University


**Scientific Discipline:** Biological Sciences

**INCITE Allocation:**
**Site:** Argonne National Laboratory
**Machine (Allocation):** Cray XC40 (1,000,000 Theta node-hours)
HPE Apollo 6500 Gen10+ (70,000 Polaris node-hours)


**Research Summary:** Artificial proteins and peptides represent a powerful and versatile class of molecules. The sequence of amino acid building blocks in such a molecule uniquely determines the fold of the molecule, and the fold uniquely determines the molecule's function. Unfortunately, the sequence-fold-function relationship is one that is computationally challenging to untangle, due the vastness of both the possible sequence space and the possible conformational space.

This project aims to reduce the computational and energetic costs of producing successful peptide macrocycle drugs or industrial enzymes using two approaches. First, the researchers will develop low-cost machine learning methods that can approximate the output of computationally expensive validation simulations, ultimately allowing users without access to large-scale resources to perform design and validation tasks on much more modest computing systems. Second, they will explore the use of quantum computing technologies as a means of solving the design problem at much lower energetic cost. This requires large-scale classical computing hardware both for carrying out quantum computing simulations during quantum algorithm development, and for performing computational validation of designs produced on current-generation quantum computing hardware.

Ultimately, this project aspires to decimate the computational and energetic cost of creating successful, computationally designed folding heteropolymers with useful functions in medicine and manufacturing, and to greatly enhance the accessibility of these computational design technologies to the scientific community.

**Type:** New
**Title:** "Dispersoid-based Strengthening of Plasma-facing Materials"

**Principal Investigator:** Aidan Thompson, Sandia National Laboratories

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

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

**Research Summary:** Tungsten containing microscopic carbide dispersions has proven to be a promising approach to designing fusion reactor materials, but many aspects of these materials are poorly understood. Leveraging the computational resources of the Summit machine, Thompson's team will advance the state-of-the-art in atomistic materials modeling of plasma material interactions, enabling accurate predictions of the material degradation mechanisms and providing much needed insight into experiments.

The divertor in the International Thermonuclear Experimental Reactor (ITER) is primarily composed of polycrystalline tungsten, but will contain impurities and complex microstructural features. A first category of impurities consists of intentionally added carbide dispersoids through the manufacturing process. Dispersion strengthened tungsten alloys are sought after as plasma facing materials (PFMs) due to their excellent mechanical properties, high thermal shock resistance, good high temperature stability. Experimental evidence shows excellent resistance to low energy highflux plasma irradiation. Degradation arising from plasma exposure, such as implanted hydrogen or helium, constitute a second category of impurities. The transport and trapping of hydrogen or helium within tungsten can be strongly enhanced or suppressed by the introduction of defects and other microstructural features, whether by design or due to plasma exposure. Experimental studies can elucidate some of these effects, but much remains to be learned. Extensive and largescale numerical studies from Thompson's team will help elucidate these effects, and probe how suitably engineered ZrC dispersions could strengthen the PFMs and improve their resistance to plasma species interaction and hydrogen retention.

**Type:** New
**Title:** "DNS of Performance-enhancing Riblets on Gas Turbine Compressor Blades"


**Principal Investigator:** Richard Sandberg, University of Melbourne
**Co-Investigators:** Ivan Marusic, University of Melbourne
Melissa Kozul, University of Melbourne
Tom Jelly, University of Melbourne
Pawel Przytarski, 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: Fluids and Turbulence

**INCITE Allocation:**
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** IBM AC922 (570,000 Summit node-hours)


**Research Summary:** Sandberg's team will leverage recent capability advances in performing first-principle based simulations to improve their understanding of how engineered surface textures improve the performance of gas turbine (GT) compressor blades. The new knowledge will inform modelling approaches for low fidelity industrial design tools, aiding global efforts to reduce fuel use and emissions. For example, the General Electric (GE) GT installed base burns $150B/yr in oil and gas. Every percentage point increase in combined cycle efficiency would reduce GE GT fuel costs by $1.5B/yr and reduce $CO_2$ emissions per MW by 1.5%. More efficient GTs would also increase the viability of costlier, more sustainably sourced fuels.

In GTs, the high-pressure compressor (HPC) experiences high levels of unsteadiness and turbulence, as well as high temperatures, pressures, and velocities. With this project, Sandberg and team will conduct first-principle based simulations of performance-enhancing textured surfaces as applied to HPC. For the first time, a systematic high-fidelity simulation campaign will be conducted of textured surfaces within complex HPC flow fields. The generated data will shed light on the detailed fundamental physical mechanisms associated with the effects of riblets in boundary layers exposed to curvature, pressure gradients and external perturbations in the form of freestream turbulence and wakes. The planned simulations are extremely computationally intensive and only possible with a highly efficient CFD solver, here HiPSTAR, developed by the PI and research group and extensively optimized for the GPU architecture of Summit, on a leadership computer facility.

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


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


**Scientific Discipline:** Physics: Astrophysics

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


**Research Summary:** Ultra-high-resolution imaging breakthroughs are revolutionizing our understanding of how black holes interact with their environments. The iconic image by the Event Horizon Telescope shows the "shadow" of the M87 black hole, silhouetted against the glowing plasma swirling around it. The basic dynamics of these accretion flows has been studied in general-relativistic magnetohydrodynamic (GRMHD) simulations that show the development of turbulence driven by the magnetorotational instability (MRI) and intermittent large magnetic structures.

However, in isolation such studies are inadequate because radiation is emitted by the electrons alone and we do not understand the electron kinetics. The only way to connect observations of accreting black holes to the physical nature of accretion flows, as revealed by the GRMHD simulations, is with detailed study of electron (and ion) kinetics. Using petascale 3D particle-in-cell simulations, this project investigates electron versus ion energization; nonthermal particle acceleration; and self-consistent synchrotron radiation, for three processes characteristic of black-hole accretion: MRI-driven turbulence, externally driven turbulence, and collisionless magnetic reconnection. These studies will be done in the relativistic or "semi-relativistic" (relativistic electrons but non-relativistic ions) regimes relevant to black-hole accretion flows.

This work takes a critical step toward understanding the behavior of black holes in the universe. Moreover, these simulations of 3D electron-ion MRI turbulence and reconnection have the potential to significantly advance computational plasma physics.

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


**Principal Investigator:** Mark Taylor, Sandia National Laboratories
**Co-Investigators:** Dave Bader, Lawrence Livermore National Laboratory
Luca Bertagna, Sandia National Laboratories
Peter Caldwell, Lawrence Livermore National Laboratory
Walter Hannah, Lawrence Livermore National Laboratory
Phil Jones, Los Alamos National Laboratory
L. Ruby Leung, Pacific Northwest National Laboratory
Matthew Norman, Oak Ridge National Laboratory
Sarat Sreepathi, Oak Ridge National Laboratory
Jayesh Krishna, Argonne National Laboratory


**Scientific Discipline:** Earth Science: Climate Research

**INCITE Allocation:**
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** IBM AC922 (620,000 Summit node-hours)


**Research Summary:** Taylor's team will work in support of the Energy Exascale Earth System Model (E3SM) project, a multi-laboratory project developing a leading-edge climate and Earth system model designed to address U.S. Department of Energy (DOE) mission needs and specifically targeting DOE Leadership Computing Facility resources now and in the future. The DOE is a leader in adoption of disruptive new computational architectures to support a range of Earth system science endeavors. Unique storm-resolving configurations of E3SM will leverage 2021 INCITE resources to make unprecedented estimates of our climate's sensitivity to elevated greenhouse gases to advance climate research. Uncertainty in the parameterization of large convective storms has been identified as a primary source of predictive uncertainty so this advancement should improve predictions. This simulation campaign is made possible due to E3SM's GPU performance, availability of pre-Exascale resources, specifically Summit, and clever experimental design.

**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: Plasma Physics

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

**Research Summary:** Lin's team will 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 and the prominent experimentally-validated AI/Deep Learning FRNN software. Because 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. However, these first-principles model simulations are generally not fast enough for real-time applications. In their project, Lin's team will develop a deep-learning based surrogate model as an instability and transport simulator for real-time applications and train it within the FRNN framework in a supervised manner using data from GTC global electromagnetic simulations of EP instability and transport.

**Type:** Renewal
**Title:** "Extreme Scale Multiphysics Models to Predict Metastatic Tumor Cell Fate"

**Principal Investigator:** Amanda Randles, Duke University

**Scientific Discipline:** Biological Sciences: Medical Science

**INCITE Allocation:**
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** IBM AC922 (330,000 Summit node-hours)

**Research Summary:** Cancer is the attributed cause of death in one in four cases in the United States and metastasis, a complex multistep process leading to the spread of tumors, is responsible for more than 90% of these deaths. Circulating tumor cell (CTC) survival in the bloodstream plays a key role in future arrest and seeding of metastatic sites and this survival is strongly influenced by exposure to varying hemodynamic forces, a mechanistic understanding of the shear forces experienced by a CTC or cluster of CTCs as it moves through the body and how that relates to cell survival remains an elusive goal. Current research efforts to uncover these mechanisms are fundamentally driven by in vitro and in silico experiments. One of the greatest challenges in this experiment-rich era of cancer research has been the ability to effectively analyze this information and isolate root causes of exhibited behaviors. Randles's team of computational researchers has complemented wet lab inquiry with high-resolution, fluid-structure-interaction simulations to address biomedical questions. The team's long-term goal is to establish an open source, easily extensible software tool to provide access to such methods in a way that allows even cancer researchers with limited coding experience to effectively complement their data with in silico enquiry to target individual properties in a way that wet lab approaches alone cannot achieve.

Predicting the trajectory of cancer cells through the body requires capturing system-level transport at cellular resolution which pushes the limits of today's supercomputers. To overcome this challenge, Randles's team has developed a new method that couples physics-based models across these different scales and leverages a hybrid CPU-GPU approach to maximize performance. Through algorithmic advances that efficiently use hardware on the Summit supercomputer and seamlessly integrate both multi-scale and multi-resolution models, the team established a finely resolved window with explicitly resolved cells to track a cancer cell through a large arterial network. They seek to leverage their novel, multiphysics algorithm that enables biomedical researchers to capture cell-specific phenomena over the long length-scales seen in the microvasculature or larger geometries to investigate properties influencing cell fate in complex vasculatures.

**Type:** New, Early Career
**Title:** "First-Principles Modeling of the Multi-wavelength Emission from Pulsars"

**Principal Investigator:** Yuran Chen, University of Colorado Boulder
**Co-Investigators:** Yajie Yuan, Flatiron Institute
Dmitri Uzdensky, University of Colorado Boulder

**Scientific Discipline:** Physics: Astrophysics

**INCITE Allocation:**
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** IBM AC922 (190,000 Summit node-hours)

**Research Summary:** Rapidly rotating neutron stars are some of the most extreme 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:** New, Early Career
**Title:** "First Principles Simulation of Hypersonic Flight"


**Principal Investigator:** Maninder Grover, Air Force Research Laboratory / University of Dayton Research Institute

**Co-Investigators:** Paolo Valentini, Air Force Research Laboratory / University of Dayton Research Institute
Ashley Verhoff, Air Force Research Laboratory
Nicholas Bisek, Air Force Research Laboratory


**Scientific Discipline:** Engineering: Aerodynamics

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


**Research Summary:** The aerothermodynamics of hypersonic flight is extremely complex. In recent years, there has been renewed interest in this field due to its implications on national security and military applications. 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.

With this INCITE project, these researchers will be able to conduct large-scale simulations of hypersonic flow fields based on the fundamental interactions of atoms and molecules in the gas. Through the use of massively parallel Direct Molecular Simulations (DMS), these researchers will enable the computation of flows around geometries at length scales at which experiments have been or will be done. Their first objective is to investigate a canonical hypersonic test case, namely the double-cone flow. Unlike similar calculations in the past, the sole input for this team's calculation will be the quantum mechanical potential energy surface (PES) that describes interactions between nitrogen molecules and atoms. The simulations will be conducted using a widely researched *ab initio* PES and its further recent refinement. The team's second objective of their research is to investigate a high-enthalpy nitrogen flow over a blunt wedge geometry in collaboration with experimentalists at Texas A & M University in order to characterize the refractive index of the gas under non-equilibrium conditions. Finally, the third objective of their research is to simulate air flows solely based on the various PESs that describe the interactions between the various air constituents. Arguably, the computations in the proposed research will produce the highest-fidelity computational fluid dynamics results obtained to date.

**Type:** New, Early Career
**Title:** "First-Principles Simulations of 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: Astrophysics

**INCITE Allocation:**
**Site:** Argonne National Laboratory
**Machine (Allocation):** Cray XC40 (1,000,000 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. A detailed understanding of the physical environment that produces this emission will deepen our knowledge of black holes themselves and of the matter in extreme conditions that surrounds them.

With this INCITE project, researchers will 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 will use the particle-in-cell code, TRISTAN-MP, to perform large-scale kinetic simulations focused on two aspects of the physics of plasmas near black holes.

For one study, the researchers will explore the development of turbulence and reconnection 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 image of the black hole "shadow" in the M87 galaxy.

For the second study, the team will investigate the self-consistent interplay of turbulence and radiation in the most magnetized regions around luminous black hole systems. They will assess the origin of the observed hard X-ray emission, and test whether black hole coronae are likely sources of ultra high energy cosmic rays, the most energetic particles in the Universe. On a more fundamental level, this study will advance our understanding of the plasma physics of turbulence and reconnection in the extreme relativistic conditions near black holes.

**Type:** Renewal
**Title:** "Global Adjoint Tomography"


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


**Scientific Discipline:** Earth Science: Geological Sciences

**INCITE Allocation:**
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** IBM AC922 (490,000 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:** "Heterogeneous Catalysis as a Collective Phenomenon Within Dynamic Ensembles of States"

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

**Scientific Discipline:** Chemistry: Catalytic

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

**Research Summary:** Chemical production is the single largest consumer of energy in U.S. manufacturing according to a 2015 DOE bandwidth study on energy use in the chemical industry. More efficient catalysts can reduce energy consumption for many processes, but the discovery and development of such catalysts continues to elude scientists.

The basis of this INCITE 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 this dynamism, the interface presents a fluxional ensemble of many states (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.

This project operates within this new paradigm. In collaboration with experiment, the researchers aim to elucidate the true dynamic nature of catalytic interfaces in reaction conditions, in which hundreds of dynamically interchanging metastable sites collectively govern the catalytic outcome. Several thermal and electro-catalytic processes and catalysts will be addressed, illuminating physically relevant design strategies for more effective catalysts. Predictions toward improved activities, selectivity, and stabilities will be made and experimentally tested.

To do so, the researchers will use and further develop methods of grand canonical global optimization for the discovery of dynamic ensembles in realistic reaction conditions. For electronic structure calculations, they will primarily use density functional theory (DFT) within the Vienna Ab initio Simulation Package (VASP), and, if necessary, higher-level ab initio theory with embedding. The team will develop machine learning tools to replace costly DFT calculations wherever possible, using the large amount of data the researchers have accumulated and will continue to generate with this project.

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


**Principal Investigator:** Choongseock Chang, Princeton Plasma Physics Laboratory
**Co-Investigators:** Mark Adams, Lawrence Berkeley National Laboratory
Luis Chacon, Los Alamos National Laboratory
R. Michael Churchill, Princeton Plasma Physics Laboratory
Stéphane Ethier, Princeton Plasma Physics Laboratory
Robert Hager, Princeton Plasma Physics Laboratory
Scott Klasky, Oak Ridge National Laboratory
Seung-Hoe Ku, Princeton Plasma Physics Laboratory
Scott Parker, University of Colorado
Aaron Scheinberg, Jubilee Development
Mark Shephard, Rensselaer Polytechnic Institute
Sarat Sreepathi, Oak Ridge National Laboratory
Benjamin Sturdevant, Princeton Plasma Physics Laboratory


**Scientific Discipline:** Physics: Plasma Physics

**INCITE Allocation:**
**Site:** Argonne National Laboratory
**Machine (Allocation):** Cray XC40 (1,300,000 Theta node-hours)
HPE Apollo 6500 Gen10+ (140,000 Polaris node-hours)
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** IBM AC922 (790,000 Summit node-hours)


**Research Summary:** This project uses use the gyrokinetic particle-in-cell code XGC to study two fundamental edge physics issues critical to the success of ITER and the magnetic fusion energy programs: (1) understanding and thus promoting innovative ways to achieve the transition from low- to high-confinement mode operation; and (2) a high-enough plasma edge pedestal in the high-mode with a wall heat-flux density below the material limit.

Achieving ITER's goal of a 10-fold energy gain depends critically on resolving these two issues. The nonlocal, multiscale, nonlinear plasma physics across the open and closed magnetic field geometries, which demand unstructured triangular mesh and neutral particle recycling, make the problem an extremely large one that requires trillions of marker particles for ITER.

Based on previous INCITE allocations, for physics the project will focus on the large-size effect (compared to the ion gyroradius) in the Fusion Power Operation phase (FPO) of ITER and in future magnetic-fusion reactors.

**Type:** Renewal
**Title:** "High-Speed Turbulence with Shocks Over Non-Adiabatic and Flexible Walls"

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

**Scientific Discipline:** Engineering

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

**Research Summary:** This INCITE project is focused on supersonic turbulent boundary layers and their interaction with shock waves. The project is aimed at uncovering flow physics, producing validation data for lower-fidelity simulation approaches, and supporting the development of improved predictive theory. The project is specifically focused on how high-speed turbulent boundary layers and shock/boundary-layer interactions (SBLI) are affected by additional factors including non-adiabatic and non-rigid walls as well as the presence of cross flow. The project makes use of two different codes that both solve the compressible Navier-Stokes equations. The hybrid code uses high-order numerics on structured Cartesian grids while the uPDE code is an unstructured finite-volume code with the ability to handle moving boundaries and fluid-structure interaction.

The data from the turbulent boundary layer simulations have been used to inspire and validate an improved method to make engineering predictions of the skin friction and heat transfer in supersonic turbulent boundary layers. The new method produces estimates to within 5-8% accuracy across all Mach numbers and wall thermal conditions, compared with about 10-15% accuracy of existing state-of-the-art methods at some conditions.

The data from the shock/boundary-layer interaction simulations have been used to build a deeper understanding into the effects of three-dimensionality on these flows. The addition of a cross flow increases the size of the separated flow region without increasing the low-frequency unsteadiness of the interaction.

**Type:** New
**Title:** "Implementing a Dispersive Interaction Database through Quantum Monte Carlo"


**Principal Investigator:** Matteo Barborini, University of Luxembourg
**Co-Investigators:** Alexandre Tkatchenko, University of Luxembourg
Jaron Krogel, Oak Ridge National Laboratory
Leonardo Medrano Sandonas, University of Luxembourg
David Rogers, Oak Ridge National Laboratory
Matej Ditte, University of Luxembourg


**Scientific Discipline:** Chemistry: Physical

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


**Research Summary:** In the design of advanced molecular materials and in the discovery of new drugs, it is crucial to explore in an accurate and extensive way the chemical compound space—the phase space containing all feasible molecular compositions and conformations. Moreover, the understanding of how the various chemical and physical properties behave in and out-of-equilibrium is fundamental to reconstruct possible interaction patterns and the formation paths of stable conformers.

In this regard, non-covalent van der Waals (vdW) interactions play a crucial role for the qualitatively correct and quantitatively accurate description of not only the binding processes, but also of the structural, kinetic and spectroscopic, properties of an extensive set of molecules and materials. While there have been many attempts to model these interactions and overcome prohibitively high computational costs, the vdW models rely on accurate benchmark calculations. Moreover, in order to improve vdW models, reference calculations must be extended to large supramolecular complexes with an increase of the computational cost.

This project aims to create a new database of non-covalent interactions, in and out of equilibrium with a combination of density functional theory (DFT) with many-body-dispersion method (DFT+MBD) and the diffusion Monte Carlo (DMC) method. The database will include an accurate evaluation of the interaction energies via diffusion Monte Carlo (DMC). Through DMC calculations the researchers will be able to obtain extremely accurate interaction energies with a relative error of approximately 5%, overcoming the computational limitations that arise in traditional high-level quantum chemistry methods. This work will provide reference data for more accurate vdW models, and will be able to establish for the first time an extendable procedure to generate highly accurate databases via a combined DFT+MBD and DMC workflow.

**Type:** New
**Title:** "The Importance of Prandtl Number in Stratified Turbulence"


**Principal Investigator:** Stephen de Bruyn Kops, University of Massachusetts
**Co-Investigators:** Colm-Cille Caulfield, University of Cambridge
Miles Couchman, University of Cambridge
Rich Kerswell, University of Cambridge
James Riley, University of Washington


**Scientific Discipline:** Engineering: Fluids and Turbulence

**INCITE Allocation:**
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** IBM AC922 (280,000 Summit node-hours)


**Research Summary:** Through this project de Bruyn Kops's team will investigate the effects of fluid properties on turbulence and mixing in flows strongly affected by density gradients, which include the stratosphere, the lower atmosphere at night, and the deep ocean. Stably stratied turbulence (SST) is a model for understanding fluid flows that, due to strong, ambient stable density stratication, are highly intermittent and anisotropic at large scales. Studying SST is fundamental research with important implications for climate modeling, pollution mitigation, deep sea mining, and military operations of cold land or ice. SST is also valuable for enhancing fundamental turbulence theory on turbulent/non-turbulent interfaces, internal intermittency, and anisotropic multi-scale energetics.

The team believes modeling fluid flows is synergistic with understanding them. The data sets generated with INCITE resources will be used in conjunction with the team's extensive existing databases to carry out the modeling component of this project.

This project will include a study of turbulent flow in a stably-stratied fluid mimicking thermally stratied water 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 unprecedented numerical resolution which, at the present time, can only be carried out using the computer resources available in the INCITE Program.

**Type:** New
**Title:** "Insights on Proton Structure from Lattice QCD: GPDs Beyond Leading Twist"


**Principal Investigator:** Martha Constantinou, Temple University
**Co-Investigators:** Krzysztof Cichy, Adam Mickiewicz University
Kyriakos Hadjiyiannakou, University of Cyprus
Andreas Metz, Temple University


**Scientific Discipline:** Physics: Nuclear Physics

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


**Research Summary:** More than 99% of the mass of the visible matter resides in atomic nuclei and therefore in nucleons. Nucleons are complicated bound states of quarks and gluons (partons), the fundamental degrees of freedom of quantum chromodynamics (QCD), the theory of the strong interaction. The structure of nucleons is among the most important and active research areas in hadronic physics for several decades. The first experimental evidence of a partonic substructure of the proton emerged from measurements of deep-inelastic electron-proton scattering (DIS) in the 1960s. The DIS cross section can be parameterized in terms of structure functions. QCD factorization theorems allow one to separate it into a perturbative and a non-perturbative part. The latter is given by parton distribution functions (PDFs), which are therefore fundamental quantities characterizing proton structure. For the description of the full 3-D proton structure one needs to also consider generalized distribution functions (GPDs) and transverse momentum distributions (TMDs) entering in various high-energy processes.

Constantinou's team will undertake a ground-breaking research program on the proton GPDs including higher-twist effects. The numerical simulations will be performed with quark masses as encountered in nature. a pioneering research program using the quasi-distributions approach to obtain the proton GPDs using state-of-the-art numerical simulation with quark masses fixed to their physical value. This program includes, twist-2 and twist-3 GPDs, and the flavor decomposition of their forward kinematic limit (PDFs). Some of these quantities will be obtained for the first time ever, and others for the first time at the physical point. The proposed calculations are computationally very challenging, as one must include calculations of disconnected diagrams. Therefore, acquiring the requested resources is critical to achieve the scientific goals of this groundbreaking line of research.

**Type:** New
**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: Physical

**INCITE Allocation:**
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** IBM AC922 (540,000 Summit 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 $CO_2$. But turnover numbers and stability are not as optimal as they should be for large-scale application of the photocatalysis for $CO_2$ reduction, implying a certain urge for improvement. 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:** New, Early Career
**Title:** "Internal Structure of Strong Interaction Nambu-Goldstone Bosons"


**Principal Investigator:** Yong Zhao, Argonne National Laboratory
**Co-Investigators:** Peter Boyle, Brookhaven National Laboratory
Ian Cloet, Argonne National Laboratory
Xiang Gao, Brookhaven National Laboratory
Andrew Hanlon, Brookhaven National Laboratory
Swagato Mukherjee, Brookhaven National Laboratory
Philipp Scior, Brookhaven National Laboratory
Sergey Syritsyn, Stony Brook University


**Scientific Discipline:** Physics: Nuclear Physics

**INCITE Allocation:**
**Site:** Argonne National Laboratory
**Machine (Allocation):** HPE Apollo 6500 Gen10+ (200,000 Polaris node-hours)


**Research Summary:** This project aims to carry out precision lattice QCD calculations of the inner structures of the pion and kaon—the Nambu-Goldstone bosons in strong interactions—in order to determine their electromagnetic form factors, Fock-space distribution amplitudes, parton distribution functions, and generalized parton distributions. These calculations are intended to provide experimental programs, such as the Jefferson Lab (JLab) 12 GeV upgrade and the future Electron-Ion Collider (EIC), with comparisons and predictions.

The results will help answer fundamental questions regarding spontaneous chiral symmetry breaking in strong interactions, flavor symmetry violation, color confinement, and the origin of the mass of hadrons. Additionally, the distribution amplitudes are important inputs for deeply virtual meson production processes that are used to map out 3D images of the proton.

**Type:** New, Early Career
**Title:** "Interplay Between Cell/Dendrite and Grain Length Scales as Spot Melts Solidify"


**Principal Investigator:** Stephen DeWitt, Oak Ridge National Laboratory
**Co-Investigators:** Christopher Newman, Los Alamos National Laboratory
Stephen Nichols, Oak Ridge National Laboratory
Jean-Luc Fattebert, Oak Ridge National Laboratory
Balasubramaniam Radhakrishnan, Oak Ridge National Laboratory
James Belak, Lawrence Livermore National Laboratory
John Turner, Oak Ridge National Laboratory


**Scientific Discipline:** Materials Science: Condensed Matter and Materials

**INCITE Allocation:**
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** IBM AC922 (370,000 Summit node-hours)


**Research Summary:** This project simulates the solidification process during additive manufacturing to better understand how small structural features inside a metal alloy interact. These structural features determine the properties of the material and improved control of these features can lead to reliable additively manufactured parts with optimized properties

Additive manufacturing techniques for metal alloys are revolutionizing engineering aspects of product design and manufacturing as well as fundamental materials science research. Current computational research into the scientific and technological aspects of solidification during additive manufacturing typically follows a multiscale approach, separately considering phenomena at the part scale, the melt pool/grain scale, and the dendrite/cell scale. This multiscale approach is largely driven by computational cost considerations, although the inherent scale separation assumptions are called into question by the overlap of the length scales of the relevant physics. As part of ExaAM, the additive manufacturing application development project in the US Department of Energy's Exascale Computing Project, DeWitt's team has an alternate strategy that avoids the inherent limitations of the multiscale framing. They propose an unprecedented approach to examine the interplay between microstructure evolution at the cell/dendrite scale and the melt pool/grain scale: to use the scalable phase-field simulation software Tusas on Leadership Computing Facility resources to directly simulate solidification in 3D at the melt pool scale while simultaneously resolving cell/dendrite features.

**Type:** New
**Title:** "Large Scale Simulation of Disorder in Alloys and Functional Materials"


**Principal Investigator:** Markus Eisenbach, Oak Ridge National Laboratory
**Co-Investigators:** Valentino Cooper, Oak Ridge National Laboratory
Mina Yoon, Oak Ridge National Laboratory
Ka Min, Louisiana State University
Hanna Terletska, Middle Tennessee State University
Yang Wang, Carnegie Mellon University


**Scientific Discipline:** Materials Science: Condensed Matter and Materials

**INCITE Allocation:**
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** IBM AC922 (480,000 Summit 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. Eisenbach's team will employ 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.

The goal of this project is to gain a first principles based, quantitative understanding of the role of disorder and defects in alloys and functional materials beyond the ideal, ordered, zero temperature ground state. To achieve this goal, Eisenbach's team will combine density functional theory-based ab initio calculations with statistical mechanics methods and first principles data driven models. The calculations for disordered materials, statistical sampling of configuration distributions and the generation of first principles data for model generation share as common features a high-level data dependent stochastic part and a compute intensive deterministic kernel, that will allow the exposure of multiple levels of parallelism, scaling towards the exascale. In this project the team will investigate partially overlapping classes of important material that are significant from both a basic science point as well as for their potential technological applications. Thus, the team will focus on the statistical physics and functional behavior of high entropy alloys and high entropy oxides, magnetic functional materials with spin-orbit interactions that lead to complex spin order (skyrmions) and quantum states (topological insulators and Weyl semimetals) and disorder driven phenomena in photovoltaic semiconductors.

**Type:** Renewal
**Title:** "Large-Scale Simulations of Light-Activated Matter"


**Principal Investigator:** Giulia Galli, University of Chicago and Argonne National Laboratory
**Co-Investigators:** Marco Govoni, Argonne National Laboratory
Francois Gygi, University of California Davis


**Scientific Discipline:** Materials: Micro

**INCITE Allocation:**
**Site:** Argonne National Laboratory
**Machine (Allocation):** Cray XC40 (600,000 Theta node-hours)
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** IBM AC922 (290,000 Summit node-hours)


**Research Summary:** This project carries out large-scale quantum simulations of light-activated processes in materials so as to tackle two classes of problems: the design of (1) sustainable materials that efficiently capture and convert solar energy, and (2) materials to build novel, optically addressable quantum platforms, including quantum sensors.

The project carries out simulations of electronic excited state properties of heterogeneous materials—including defects and interfaces—by coupling first-principles molecular dynamics and electronic structure methods beyond density functional theory, as implemented in the Qbox and WEST open-source codes.

Applications of interest include point defects in wide band gap semiconductors for the realization of qubit and quantum sensors, as well as assemblies of nanostructured building-blocks in materials used for solar energy absorption. Predictions of the structural and electronic properties of heterogeneous systems will be compared to experiment to obtain an integrated mechanistic understanding of the interaction of defective and nanostructured materials with light, in addition to validated data for systems of interest for sustainability and quantum technologies.

**Type:** Renewal
**Title:** "Long Term 3D Simulations of Core-collapse Supernovae"


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


**Scientific Discipline:** Physics: Astrophysics

**INCITE Allocation:**
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** IBM AC922 (390,000 Summit node-hours)


**Research Summary:** Core-collapse supernovae, the explosive final moments of massive stars, are complex, dynamic, multi-physics events yielding a bright and energetic explosion from the birth of a neutron star or black hole. The 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 we are 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. However, the number of extant 3D simulations with adequate physics is small and none have been run until the explosion matures more than a second after the proto-neutron star forms.

Hix's team will run state of the art simulations that extend through all of the element creation process that occur in these supernovae to better understand the elements made. The 3D supernova simulations proposed here have two goals. First, the team seeks to understand the impact of stellar rotation on the explosion mechanism of core-collapse supernovae and the associated observables. Second, they seek to understand the development of the proto-neutron star wind following the onset of explosion.

**Type:** New
**Title:** "Multi-ion Turbulence in Burning Plasma Experiments"


**Principal Investigator:** Emily Belli, General Atomics
**Co-Investigators:** Jeff Candy, General Atomics
George Fann, Oak Ridge National Laboratory
Gary Staebler, General Atomics


**Scientific Discipline:** Physics: Plasma Physics

**INCITE Allocation:**
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** IBM AC922 (540,000 Summit node-hours)


**Research Summary:** Realizing the potential of nuclear fusion to provide a clean, limitless source of energy requires good confinement of the heat in the plasma to achieve self-sustaining fusion power. Multiscale turbulence simulations of hydrogen fuel isotopes and helium fusion byproducts are used to predict energy losses for next-generation reactors like ITER. Present-day tokamak experiments typically use a single hydrogen isotope (deuterium), while future burning plasma experiments like ITER will use a fuel mixture consisting of 50% deuterium (D) and 50% tritium (T) to increase the thermonuclear cross section, yielding a higher fusion power output at a lower temperature. D-T tokamak experiments have only been done a few times over the past few decades. Thus, theory and modeling will be important in planning for the ramp-up stages in ITER from hydrogen to deuterium to reactor-level D-T.

Belli's team will use complex multi-ion simulations to model energy losses due to turbulent transport and maximize fusion performance. The simulations will model the cross-species interactions between the deuterium and tritium fuel ions, fusion helium ash impurity, wall impurities (beryllium and tungsten), and electrons. The mechanisms that drive the ion transport (including heavy tungsten ions) will be studied for high-confinement mode (H-mode) operating scenarios in both the central core, which is dominated by ion-scale turbulence, and in the outer core/edge, where multiscale turbulence (which spans ion to electron scales) exists. These simulations are particularly challenging because of the need to resolve the long space and time scales of high-Z impurities together with the short space and time scales of the much lighter electrons.

**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: Aerodynamics

**INCITE Allocation:**
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** IBM AC922 (690,000 Summit 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, new approaches to EDL are necessary in order to support delivery of substantially larger payloads to the surface. Nielsen's team leverages high fidelity simulation to understand the complex physics associated with controlled, decelerating descent through the Martian atmosphere during the critical supersonic-to-transonic-to-subsonic phase. Nielsen's team will conduct simulations building up to a full six degree-of-freedom, closed-loop controlled-flight, computational fluid dynamics simulation of a human-scale Mars lander as it uses retropropulsion to decelerate through the most critical portion of its descent trajectory. This effort will leverage the efficiency of GPU-based leadership-class resources to perform high-fidelity simulations at flight-relevant physical and time scales. The work directly supports NASA efforts to characterize environments and requisite computational modeling approaches to enable implementation of the technology into a flight vehicle.

**Type:** New, Early Career
**Title:** "New Window into Tropical Meteorology with Global 1 km Atmosphere-Ocean Simulations"


**Principal Investigator:** Inna Polichtchouk, European Centre for Medium-Range Weather Forecasts (ECMWF)

**Co-Investigators:** Ioan Hadade, ECMWF
Nils Wedi, ECMWF
Valentine Anantharaj, National Center for Computational Sciences
Frederic Vitart, ECMWF
Kristian Mogensen, ECMWF


**Scientific Discipline:** Earth Science: Climate

**INCITE Allocation:**
**Site:** Argonne National Laboratory
**Machine (Allocation):** HPE Apollo 6500 Gen10+ (50,000 Polaris node-hours)
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** IBM AC922 (520,000 Summit node-hours)


**Research Summary:** The project will investigate how better forecasts of extreme weather events, such as tropical cyclones (TCs), can be achieved via unprecedented simulations which represent the Earth's atmosphere and oceans with very fine detail. The outcome of this project will contribute to solving the top global threats in the next decade—extreme weather and climate action failure.

Performing the world's first-ever GPU-enabled global subseasonal nonhydrostatic simulations of the atmosphere at 1 km resolution coupled to an eddy-permitting ocean, this work seeks to answer fundamental questions: How does the meso-scale permitting ocean, when coupled to a convection permitting atmosphere, impact TC and Madden Julian Oscillation (MJO) representation? What is the impact of relaxing the hydrostatic approximation on the simulated convection, and thus on the TC and the MJO representation? What advantages, if any, does the 1 km resolution present over the more affordable 3-4 km resolution for representing the Earth's weather and climate?

Further, the project will address whether explicitly resolving deep convection while simultaneously coupling to the ocean significantly improves forecast skill of the MJO and TCs in comparison to current models, as well as remote influence of the MJO on extremes and teleconnections between the MJO and other atmospheric features.

**Type:** New
**Title:** "Next-Generation 3D Core-Collapse Supernova"


**Principal Investigator:** Adam Burrows, Princeton University
**Co-Investigators:** David Vartanyan, University of California Berkeley
Matt Coleman, Princeton University
Chris White, Princeton University
Aaron Skinner, Lawrence Livermore National Laboratory


**Scientific Discipline:** Physics: Astrophysics

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


**Research Summary:** The supernova explosions of massive stars, the so-called core-collapse supernovae (CCSNe), have been theoretically studied for more than half a century and observationally studied even longer. What has emerged in the modern era of CCSN theory is that the structure of the progenitor star, turbulence, and symmetry-breaking in the core after bounce, and the details of the neutrino-matter interaction are all key and determinative of the outcome of a collapse.

With the recent availability of leadership-class high-performance computing platforms with petaflop (soon to be exaflop) capability, and with sophisticated codes such as Fornax, researchers are now able to perform multiple simulations per year in the full 3D of nature to definitively explore the mechanism of this central phenomenon in theoretical astrophysics. With this new INCITE project, this team will conduct not only a full suite of 3D simulations for the spectrum of progenitor stars, but carry out these simulations for approximately five times the physical time possible with previous INCITE allocations all the way to the asymptotic state. 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:** "Next-Generation Modeling for the EHT"


**Principal Investigator:** Charles Gammie, Univ. of Illinois at Urbana-Champaign
**Co-Investigators:** Jason Dexter, University of Colorado Boulder
Ben S. Prather, Univ. of Illinois at Urbana-Champaign


**Scientific Discipline:** Physics: Astrophysics

**INCITE Allocation:**
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** IBM AC922 (410,000 Summit node-hours)


**Research Summary:** Gammie and team will generate state-of-the-art theoretical models of gas flow around black holes. The models will enable physical interpretation of resolved images and movies of black holes from the Event Horizon Telescope (EHT).

The EHT collaboration recently published the first resolved image of a black hole, and continues to take data, analyze results, and publish high-impact papers. Interpretation of EHT data is heavily reliant on simulations of plasma flow close to the black hole event horizon. Gammie's campaign would generate a library of 181 new, high-resolution, ideal General Relativistic Magnetohydrodynamic (GRMHD) simulations using the open-source KHARMA code. KHARMA is designed for efficient execution on CPUs and GPUs, using the Kokkos library for performance portability, via the Parthenon framework from Los Alamos National Laboratory. This simulation library would enlarge and more densely sample model parameter space and address persistent concerns about convergence. The campaign would also generate a library of nonideal GRMHD models using the open-source `grim` code, which was developed by members of the team. `grim` achieves performance portability using the ArrayFire library.

**Type:** New, Early Career
**Title:** "Nuclear Femtography: Parton Distribution Functions for the Electron-Ion Collider"


**Principal Investigator:** Phiala Shanahan, Massachusetts Institute of Technology
**Co-Investigators:** Zohreh Davoudi, University of Maryland
William Detmold, Massachusetts Institute of Technology
Assumpta Parreño, University of Barcelona
Michael Wagman, Fermi National Accelerator Facility
Frank Winter, Thomas Jefferson National Accelerator Facility


**Scientific Discipline:** Physics: Nuclear Physics

**INCITE Allocation:**
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** IBM AC922 (650,000 Summit node-hours)


**Research Summary:** Shananhan and team will work to reveal the structure of light nuclei in terms of the most fundamental quark and gluon constituents encoded in the theory of the strong interactions, quantum chromodynamics (QCD). The results of the proposed work will directly impact the DOE experimental program, and in particular the design, and future science program, of the planned Electron-Ion Collider.

In particular, Shanahan's team will undertake the first calculation of nuclear parton distribution functions (PDFs) with fully-quantified uncertainties from the underlying theory of the strong interactions between quarks and gluons, or QCD. The unpolarized and polarized PDFs that they target through variational lattice QCD calculations are among the most fundamental quantities that encapsulate knowledge of nuclear structure. The team's project will be used in global PDF fits and markedly increase the precision with which nuclear PDFs are known. This work will enable the uncertainties on the nuclear PDFs to be reduced by a factor of 3 or more in specific kinematic regions, as is necessary for experiments at the Electron-Ion Collider (EIC) which aim to achieve new understanding of novel QCD dynamics at high parton density. The work will also enable the development of QCD benchmarks that define theory predictions and precision goals for measurements of gluonic contributions to nuclear structure at the EIC. Finally, it will enable improvements in studies characterizing the quark-gluon plasma via hard probes at the Relativistic Heavy Ion Collider and at the Large Hadron Collider, and first insight into the QCD mechanisms that drive the modifications of proton and neutron structure in the nuclear medium, constraining models of nuclear effects in the PDFs.

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


**Principal Investigator:** Aurel Bulgac, University of Washington
**Co-Investigators:** Piotr Magierski, Warsaw University of Technology
Kenneth Roche, Pacific Northwest National Laboratory
Gauillaume Scamps, Université Libre de Bruxelles
Kazuyuki Sekizawa, Tokyo Institute of Technology
Ionel Stetcu, Los Alamos National Laboratory
Gabriel Wlazłowski, Warsaw University of Technology


**Scientific Discipline:** Chemistry: Physical

**INCITE Allocation:**
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** IBM AC922 (140,000 Summit node-hours)
**Site:** Argonne National Laboratory
**Machine (Allocation):** HPE Apollo 6500 Gen10+ (400,000 Polaris node-hours)


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

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

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

**Type:** New
**Title:** "Online Machine Learning for Large-Scale Turbulent Simulations"


**Principal Investigator:** Kenneth Jansen, University of Colorado Boulder
**Co-Investigators:** John Evans, University of Colorado Boulder
Jed Brown, University of Colorado Boulder
Stephen Becker, University of Colorado Boulder
Alireza Doostan, University of Colorado Boulder
Sam Partee, Hewlett Packard Enterprise


**Scientific Discipline:** Engineering: Fluids and Turbulence

**INCITE Allocation:**
**Site:** Argonne National Laboratory
**Machine (Allocation):** Cray XC40 (1,200,000 Theta node-hours)


**Research Summary:** Building on work being performed as part of Argonne's Aurora Early Science Program (ESP), the project seeks to advance the current state of the art for online data analytics and machine learning (ML) applied to large-scale computational fluid dynamics simulations, as well as to develop more predictive lower-fidelity (and thus less computationally expensive) turbulence models for flows of interest to the aerospace, automotive, and renewable energy industries.

Through the integration of a mature flow solver already scaled to more than 3 million processes with distributed and online data analytics and training algorithms, this work will greatly enhance the confidence in lower-fidelity models and enable engineers to obtain more accurate solutions to complex flows outside the reach of today's modeling capabilities.

Using tools developed under the ESP allocation to extend beyond canonical turbulent flows neural net sub-grid stress (SGS) models for large eddy simulation, (LES) the researchers will perform two direct numerical simulations coupled with online learning of wall-bounded flows with increasing complexity and scale so as to provide training data for SGS closures. Hence the team will develop a neural net SGS model capable of accurately predicting flows of increasing complexity and that surpasses current state-of-the-art closures. LES on the same flows computed by DNS will validate the accuracy of the newly trained SGS model. Finally, to evaluate the trained SGS model on a previously unseen flow, the team will perform LES of the turbulent boundary layer over an airfoil with flow separation—a particularly relevant flow case for the aerospace and renewable energy industries, therefore making a predictive closure extremely valuable.

**Type:** New
**Title:** "Pioneering High-Fidelity Full-Core Simulations at Exascale"


**Principal Investigator:** Elia Merzari, Pennsylvania State University
**Co-Investigators:** Paul Fischer, University of Illinois at Urbana Champaign
Misun Min, Argonne National Laboratory
April Novak, Argonne National Laboratory
Jun Fang, Argonne National Laboratory


**Scientific Discipline:** Engineering: Fluids and Turbulence

**INCITE Allocation:**
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** IBM AC922 (440,000 Summit node-hours)


**Research Summary:** To accelerate the deployment of small modular nuclear reactors and advanced reactors, Merzari and team will leverage the novel fluid dynamics code NekRS to deliver simulations of unprecedented scale. The simulations are aimed at providing critical understanding and model development for core-wide phenomena, impossible with current architectures or experiments alone.

Advanced nuclear energy holds promise as a reliable, carbon-free energy source capable of meeting the nation's commitments to addressing climate change. The design, certification, and licensing of novel reactor concepts pose formidable hurdles to the successful deployment of new technologies. The high cost of integral-effect nuclear experiments necessitates the use of high-fidelity numerical simulations to ensure the viability of nuclear energy in a clean energy portfolio.

The objective of this research is to provide the high-fidelity simulation capabilities essential to this mission by developing unprecedented insight into core-wide phenomena in rod bundle nuclear reactors. First of a kind, full-core Large Eddy Simulation (LES) of nuclear reactors will be conducted on Summit. A high-resolution LES database will be used to inform low-resolution industry analysis methods for two challenge problems critical to the development of advanced nuclear – inter-assembly mixing in Light Water Small Modular Reactors (SMRs) and inter-assembly heat transfer in Sodium Fast Reactors (SFRs). This work will target simulations 1000× larger than competing work in our field, and only with capability computing and petascale-level resources can these insights be gained.

**Type:** Renewal
**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, Los Alamos National Laboratory

**Scientific Discipline:** Physics: High Energy Physics

**INCITE Allocation:**
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** IBM AC922 (440,000 Summit node-hours)

**Research Summary:** The standard model (SM) of elementary particles, including the recent understanding of neutrino masses and mixing, has been extremely successful in describing all phenomena up to the TeV scale probed at the Large Hadron Collider (LHC) in Geneva. At the same time new, and as yet unknown, physics is required to explain three profound mysteries: the observed matter-antimatter asymmetry of the universe, dark matter and dark energy. A profound mystery is the almost total absence of antimatter in the observed universe, whose explanation requires much larger violation of charge-conjugation-parity (CP) symmetry than exists in established theory.

Gupta's team will calculate the form factors (the momentum dependent strength of the coupling of neutrinos to nucleons) for the neutrino experiments, and the matrix elements of CP violation operators that give the size of their contribution to the neutron electric dipole moment. These calculations will increase the reach of experiments searching for novel CP violation in the neutrino sector and in neutron electric dipole moment.

**Type:** Renewal
**Title:** "Predicting Ion Transport Kinetics at Complex Interfaces for Energy Storage"


**Principal Investigator:** Brandon Wood, Lawrence Livermore National Laboratory
**Co-Investigators:** Tae Wook Heo, Lawrence Livermore National Laboratory
Liwen (Sabrina) Wan, Lawrence Livermore National Laboratory
ShinYoung Kang, Lawrence Livermore National Laboratory
Boris Kozinsky, Harvard University
Nicole Adelstein, San Francisco State University


**Scientific Discipline:** Materials Science

**INCITE Allocation:**
**Site:** Argonne National Laboratory
**Machine (Allocation):** Cray XC40 (1,000,000 Theta node-hours)
HPE Apollo 6500 Gen10+ (120,000 Polaris node-hours)


**Research Summary:** Ion transport kinetics critically define the performance of a wide variety of emerging energy storage solutions. For solid-state devices in particular, ion transport can be heavily influenced by interfaces between different phases or grains, which appear unavoidably from processing or cycling and influence transport in often-problematic ways. With this INCITE project, the researchers aim to integrate a validated multiscale modeling framework to study ion transport kinetics at complex interfaces in solid-state battery and hydrogen storage systems.

To achieve their goal, this team addresses three main objectives: 1) use large-scale quantum simulations to assemble training data for the development of machine-learning force fields based on local ion environments within solids, 2) apply the machine-learning force fields and advanced sampling techniques to compute ion diffusion across a wider variety of configurations, and 3) evaluate the dependence of ion transport on microstructures using mesoscale models. The project also leverages a suite of novel graph-theoretic tools to characterize atomic configurations of disordered interfaces and correlate local arrangements to key properties.

The multiscale simulations are being used to probe the relationship between physicochemical interface properties and ion transport kinetics, guiding rational engineering strategies for improving performance of advanced materials for grid and vehicular energy storage. This project renewal builds upon the team's previous efforts in simulating thermodynamic and kinetic aspects of hydrogen transport in composite structures for hydrogen storage, as well as lithium transport in a variety of polycrystalline solid-state battery materials.

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


**Principal Investigator:** Shiwei Zhang, Flatiron Institute; College of William & Mary
**Co-Investigators:** Richard Friesner, Columbia University
David Reichman, Columbia University
Steven White, University of California, Irvine


**Scientific Discipline:** Chemistry: Physical

**INCITE Allocation:**
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** IBM AC922 (680,000 Summit node-hours)


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

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

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

**Type:** New
**Title:** "Rational Design of More Effective Drugs with Reduced Side Effects"

**Principal Investigator:** Ron Dror, Stanford University

**Scientific Discipline:** Biological Sciences: Biophysics

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

**Research Summary:** Dror's team will use massively parallel simulations on Summit to determine how chemical compounds can cause drug receptors to stimulate beneficial cellular signaling pathways without stimulating harmful ones. They will then demonstrate how to use this information to design more effective drugs with fewer dangerous side effects.

One-third of all current drugs act by binding to G protein–coupled receptors (GPCRs), and these receptors also represent the largest class of targets for the development of new therapeutics. Medicines that cause a GPCR to selectively stimulate or selectively avoid stimulation of specific intracellular signaling proteins promise better treatments for diseases ranging from psychiatric and cardiovascular disorders to cancer and HIV. Designing such medicines has been difficult, however, because the mechanisms by which drug molecules can achieve such effects have remained unclear. Dror's team will use their refined methods to expand greatly on their previous findings. Taking advantage of newly available experimental data, they will extend their work to some of the most medically relevant GPCRs. They will determine mechanisms by which drugs could select among many signaling pathways, rather than only two. Dror's team will also employ these results to identify novel GPCR-targeted ompounds with unique and desirable pharmacological properties, which will then be assayed experimentally. The team will use their computational results to guide both pharmacological and spectroscopic experiments, which will in turn serve to validate their simulations.

**Type:** New, Early Career
**Title:** "Scalable Transformer Language Models for Drug Discovery"


**Principal Investigator:** Andrew Blanchard, Oak Ridge National Laboratory
**Co-Investigators:** Belinda Akpa, Oak Ridge National Laboratory
Debsindhu Bhowmik, Oak Ridge National Laboratory
Mayanka Chandra Shekar, Oak Ridge National Laboratory
Shang Gao, Oak Ridge National Laboratory
Jens Glaser, Oak Ridge National Laboratory
John Gounley, Oak Ridge National Laboratory
Isaac Lyngaas, Oak Ridge National Laboratory


**Scientific Discipline:** Biological Sciences: Bioinformatics

**INCITE Allocation:**
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** IBM AC922 (390,000 Summit node-hours)


**Research Summary:** Drug discovery efforts have an urgent need for models to propose new molecules coupled with the prediction of chemical properties using limited experimental data. To meet this need, Blanchard's team proposes to develop a Transformer model to learn generalizable features from large unlabeled compound libraries and then fine-tune for specific applications. Due to the high computational cost of Transformer models, which require thousands of GPU hours for pre-training, leadership computing facility resources are necessary for development and testing.

Computer-aided drug discovery is a combinatorially complex, multiple-objective, optimization problem requiring the estimation of a range of chemical properties to find molecules that are deliverable, safe, and effective. Supervised ML approaches, however, are ill-equipped to estimate multiple properties; each property prediction task requires the costly development of a large dataset and the design of a specific model. Blanchard's project will have a transformative impact by leveraging unlabeled data to pre-train a Transformer model capable of learning generalizable features. The pre-trained model can then be fine-tuned on limited experimental data to generate state-of-the-art results across a wide range of chemical property prediction tasks. The team will demonstrate their approach on two key applications: (1) the estimation of binding affinities for thousands of protein targets and (2) the estimation of chemical properties to parameterize a physiologically-based pharmacokinetic model. They will then use the fine-tuned model for property prediction to score molecules in the search for optimized drug candidates.

**Type:** Renewal
**Title:** "Towards Predictive Calculations of Functional and Quantum Materials"


**Principal Investigator:** Paul Kent, Oak Ridge National Laboratory
**Co-Investigators:** Anouar Benali, Argonne National Laboratory
Panchapakesan Ganesh, Oak Ridge National Laboratory
Olle Heinonen, Argonne 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: Nano

**INCITE Allocation:**
**Site:** Argonne National Laboratory
**Machine (Allocation):** Cray XC40 (1,000,000 Theta node-hours)
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** IBM AC922 (430,000 Summit node-hours)


**Research Summary:** This project aims to predict and better understand the quantum-mechanical properties of materials that display novel properties, including novel quantum phases. These materials are of outstanding fundamental scientific interest and present the potential for the development of new sensors and devices.

In all of the materials studied, small changes in composition, pressure, strain, doping, and applied field yield greatly altered properties, which is a challenge to simulation and modeling. This project therefore applies approaches based on Quantum Monte Carlo (QMC), as implemented in the open-source QMCPACK code. By directly solving the Schrödinger equation and by treating the electrons at a consistent highly-accurate many-body level, these methods can be applied to general elements and materials, while employing very few approximations.

Supported by the DOE BES Computational Materials Sciences Center for the Predictive Simulation of Functional Materials and core BES programs, this project operates alongside experimental collaborators to enable joint theory-experimental work.

**Type:** Renewal
**Title:** "Ultrafast Control of Functional Materials"


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


**Scientific Discipline:** Materials: Microscopic

**INCITE Allocation:**
**Site:** Argonne National Laboratory
**Machine (Allocation):** Cray XC40 (1,500,000 Theta node-hours)
HPE Apollo 6500 Gen10+ (200,000 Summit node-hours)


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

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

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

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

**Principal Investigator:** Sharon Glotzer, University of Michigan

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

**INCITE Allocation:**
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** IBM AC922 (690,000 Summit node-hours)

**Research Summary:** Glotzer's team will investigate the ways in which soft materials made of nanoparticles of different shapes and sizes self assemble into ordered crystals of extraordinary complexity and diversity. Using the fastest computers available, they aim to discover design rules that will lead to materials with new and exciting properties.

Glozter's team aims to discover the rules by which systems at different scale assemble into colloidal crystals and the role of particle shape(s) and interparticle interactions in determining both the kinetic and thermodynamic assembly pathways. Because crystallization studies require extremely large and long simulations, and many runs must be sampled to draw strong conclusions of statistical significance, these simulations require the capabilities of leadership class machines. With substantial resources from Summit, the team will carry out a computational study of crystallization pathways of the most diverse crystal structures that has ever been undertaken. The team's previous work based on INCITE allocations focused on classifying pre-nucleation motifs and focused mainly on hard anisotropic particles. Their focus in 2022 will be on studying particles with vastly different. By studying these disparate, experimentally accessible systems within the same project – asking identical questions and using identical methods of statistical analysis – Glotzer's team will learn not only about each class of systems but also, and more importantly, which features of assembly pathways are universal across materials class.

**Type:** New
**Title:** "Wall-resolved Large Eddy Simulation of the NASA CRM High-lift Configuration"

**Principal Investigator:** Zhi Jian Wang, Univ. of Kansas Center for Research, Inc.
**Co-Investigators:** Joshua Romero, NVIDIA Corporation
Nick Wyman, Cadence Design Systems

**Scientific Discipline:** Engineering: Aerodynamics

**INCITE Allocation:**
**Site:** Oak Ridge National Laboratory
**Machine (Allocation):** IBM AC922 (590,000 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).