Type: New
Title: "3D Imaging of Strong Interaction Nambu-Goldstone Bosons"

Principal Investigator: Yong Zhao, Argonne National Laboratory
Co-Investigators: Dennis Bollweg, Brookhaven National Laboratory
Peter Boyle, Brookhaven National Laboratory
Ian Cloët, Argonne National Laboratory
Xiang Gao, Argonne National Laboratory
Swagato Mukherjee, Brookhaven National Laboratory
Qi Shi, Brookhaven National Laboratory
Rui Zhang, Argonne National Laboratory

Scientific Discipline: Physics

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): HPE Cray EX - Intel Exascale Compute Blade Nodes (150,000 Aurora node-hours)

Research Summary: The visible universe is primarily composed of protons and neutrons which bind together to form nuclei and account for over 99% of the mass of all visible matter. However, nuclei as we know them would not exist without an intriguing strongly interacting particle called the pion, which plays a key role as the carrier of the strong nuclear force over distance scales greater than the size of the proton. Experimental research, coupled with significant advances in theory, have revealed that strongly interacting particles such as protons, neutrons, and pions are composed of elementary particles called quarks and gluons whose interactions are described by quantum chromodynamics (QCD). QCD is therefore responsible for the formation of atomic nuclei and as such, almost all visible matter in the universe.

With this INCITE project, researchers will carry out lattice QCD calculations of the 3D structures of the pion and kaon, which are the Nambu-Goldstone bosons in strong interactions. Using a lattice QCD Lagrangian that preserves chiral symmetry, the team will determine their electromagnetic form factors at high momentum transfer, transverse-momentum-dependent (TMD) wave functions, and parton distribution functions. These calculations are aimed at providing comparisons and predictions for experimental programs such as the Jefferson Lab (JLab) 12 GeV upgrade and the future Electron-Ion Collider (EIC). The results will deepen the understanding of the strong interaction and confinement, and provide comprehensive 3D imaging of the pion and kaon. The team will also use their findings to extract the Collins-Soper kernel for TMD evolution, which is a crucial input for the global analysis of proton TMDs from the JLab and EIC experiments.

Type: Renewal
Title: "Ab Initio Investigation of Disorder and Defects in Structural 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
Swarnava Ghosh, Oak Ridge National Laboratory
Ka-Ming Tam, Louisiana State University
Hanna Terletska, Middle Tennessee State University
Yang Wang, Carnegie Mellon University

Scientific Discipline: Materials

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (450,000 Frontier node-hours)

Research Summary: The goal of this project is to gain a quantitative understanding of the role of disorder and defects in alloys and functional materials beyond the ideal zero temperature ground state. To achieve this, the project combines density functional theory calculations with statistical mechanical methods and data driven models. These calculations feature a high-level data dependent part and a compute intensive part that allows the scaling of exascale-class systems.

In 2024 the project will continue research focused in the areas of high entropy alloys and oxides. Where appropriate, the calculations will include a new capability to perform electron transport calculations.

The results from this project are expected to continue to advance the robustness of quantum technologies and processes, as well as an understanding of stability in the structure of quantum materials.

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

Scientific Discipline: Physics

INCITE Allocation:

Site:	Argonne National Laboratory
Machine (Allocation):	HPE Cray EX - Intel Exascale Compute Blade Nodes (500,000 Aurora node-hours)
Site:	Oak Ridge National Laboratory
Machine (Allocation):	HPE-Cray EX (1,000,000 Frontier node-hours)

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

Type: New
Title: "A Climate-Informed, Large-scale, and High-resolution Inundation Modeling Framework"

Principal Investigator: Sudershan Gangrade, Oak Ridge National Laboratory
Co-Investigators: Shih-Chieh Kao, Oak Ridge National Laboratory
Mario Morales-Hernandez, I3A-University of Zaragoza
Ganesh Ghimire, Oak Ridge National Laboratory
Michael Kelleher, Oak Ridge National Laboratory
Matthew Norman, Oak Ridge National Laboratory

Scientific Discipline: Earth Science

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

Research Summary: Climate change is strengthening the intensity, frequency, and magnitude of extreme rainfall events. This poses a unique challenge for flood risk management, especially since there are limited tools and data to address this threat. Simulation of flood inundation relies on the integration of atmospheric, hydrologic, and hydrodynamic models in a format that is not usually available to decision-makers.

Modeling capabilities at the scale of large floods are desired to understanding the risk they pose, but such scale and spatial resolution has been challenging because of cost and power. This project proposes a high-resolution inundation model using TRITON, an open-source multi-GPU model for 2D inundation. The model's framework will assess climate-informed flood hazards and the risk to population and infrastructure. By taking advantage of the computing power Frontier holds, the project will advance the current limits of flood inundation modeling to necessary scales.

The framework will approach the inundation analysis using both historic and future climate conditions, generating high-resolution, climate-informed probabilistic flood maps. This will identify vulnerable locations, infrastructure improvements, and emergency preparedness.

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

Principal Investigator: Ivaylo Ivanov, Georgia State University

Scientific Discipline: Biological Sciences

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (450,000 Frontier node-hours)

Research Summary: Transcription complexes (complementary to DNA) are dynamic machines whose function and regulation underlie all of gene expression. Gene expression governs many fundamental aspects of cell biology and the loss of transcription control within it is a hallmark of cancers and other diseases. Gene expression is also intertwined with other vital DNA repair pathways that maintain the genome. Understanding the inner workings of this molecular complex is a great challenge in the biomedical sciences.

To overcome this barrier, this project will leverage cutting-edge computational modeling methods to simulate these complexes over wide time and length scales. This will be done by combining data from genetics and biochemistry with computational analysis methods. The project will also employ new methods to define the dynamic communities and mechanisms in these assemblies.

This project will impact understanding of human disease etiology and treatments. The work will subdivided to fulfil two milestones: build a structured model of communication pathways and switches that underpin the activators of RNA Polymerase, which copes DNA to RNA, and uncover the structure for coordination in the TC-NER pathway, which repairs damaged sites in transcription strands.

Overall, the project will provide unified knowledge of the assembly, dynamics, and function of key gene regulatory complexes.

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

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

Scientific Discipline: Materials Science

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

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

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

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

Scientific Discipline: Physics

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): HPE Cray EX - Intel Exascale Compute Blade Nodes (1,200,000 Aurora node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (1,000,000 Frontier node-hours)

Research Summary: This project, aiming to address fundamental questions in elementary particle physics, consists of three related themes: (1) the hadronic vacuum polarization contribution to the anomalous magnetic moment of the muon ("muon g – 2"); (2) semileptonic decays of B and D mesons ("heavy quark"); and (3) violation of charge conjugation parity symmetry in the kaon system ("CP violation").

The calculations performed in this work directly support extensive ongoing experimental efforts. The project uses numerical simulations constructed from the lattice gauge theory formulation of quantum chromodynamics. In some cases, the calculations 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 for particle physics.

Type: New
Title: "Advancing Fusion and Fission Energy through 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
John Tramm, Argonne National Laboratory
Patrick Shriwise, Argonne National Laboratory
Paul Romano, Argonne National Laboratory

Scientific Discipline: Engineering

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

Research Summary: Advanced nuclear energy holds promise as a reliable, carbon-free energy source capable of meeting our nation's commitments to addressing climate change. A wave of investment in fission and fusion power within the United States and around the world indicates an important maturation of academic research projects intothe commercial space. 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 large-scale multi-physics phenomena. First of a kind, full-corehybrid Reynolds Averaged Navier Stokes (RANS) and Large Eddy Simulation (LES) of fission reactors will be conducted on Frontier. Simulation of unprecedented scale will be conducted for fusion energy systems will be conducted approaching full-device multiphysics modeling of breeder blankets and for a novel retic-ulated foam tritium extraction system.

This research is situated at the opportune moment for leadership computing facilities to impact the trajectory of advanced nuclear. These first-of-a-kind large scale simulations will usher in a new era where such simulations are possible and firmly establish the nuclear field as a leader in exascale computing.

Type: New
Title: "AFQMC Beyond main group chemistry: Toward simulations of PSII and Nitrogenase"

Principal Investigator: Richard Friesner, Columbia University
Co-Investigators: David Reichman, Columbia University
James Shee, Rice University

Scientific Discipline: Chemistry

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (700,000 Frontier node-hours)

Research Summary: Predictive calculations of systems governed by the laws of quantum mechanics represent a grand challenge in science. The project aims to deploy highly accurate quantum Monte Carlo calculations (outcome-predictions based on action) to study transition metal-containing molecular systems from first principles. This will produce thermochemical reference values to investigate the process of water splitting and nitrogen reduction.

This proposal describes a set of calculations unprecedented in size and complexity, that would establish a quantum Monte Carlo formalism as a needed benchmark method for transition metal chemistry. A second goal hopes to simulate the conversion of water to oxygen with high efficiency using sunlight, a model for how solar energy can be harvested.

The project's results will bring to fruition many technological breakthroughs to help many mechanical processes more sustainable and affect the daily lives of citizens.

Large, parallel GPU supercomputers of the exascale-class are necessary for these achievements to be possible.

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

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

Scientific Discipline: Materials Science

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): HPE Cray EX - Intel Exascale Compute Blade Nodes (825,000 Aurora node-hours)

Research Summary: This project advances scalable manufacturing of quantum materials and ultrafast control of their emergent properties on demand using AI-guided exascale quantum dynamics simulations in tandem with state-of-the-art x-ray, electron-beam, and neutron experiments at DOE facilities:

(1) Self-assembly of layered material (LM) metastructures (i.e., atomically thin origami) for scalable and robust manufacturing of quantum emitters for future quantum information science and technology.
(2) Picosecond optical, electrical and mechanical control of symmetry breaking in topological ferroelectric skyrmion, skyrmionium and meron for emerging ultralow-power polar "topotronics".

As part of their work, the researchers perform reactive molecular dynamics simulations to computationally manufacture these materials, followed by nonadiabatic quantum molecular dynamics and neural-network quantum molecular dynamics (NNQMD) simulations to study their ultrafast control guided by AI.

The team's computational breakthrough, the Allegro-Legato NNQMD model, built on the Allegro model by Boris Kozinsky's group at Harvard—with state-of-the-art accuracy, speed and robustness based on group-theoretical equivariance, locality of descriptors, and sharpness-aware minimization of loss landscape—enables unprecedentedly large spatiotemporal-scale NNQMD simulations with spectroscopically stable trajectories to explain the highest-resolution inelastic neutron scattering experiment.

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

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

Scientific Discipline: Materials Science

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): HPE Cray EX - Intel Exascale Compute Blade Nodes (300,000 Aurora node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (1,000,000 Frontier node-hours)

Research Summary: The main objective of this project is to perform transformative quantum-accurate, billion atom molecular dynamics (MD) simulations on exascale DOE computers Frontier and Aurora to uncover the fundamental physics of carbon at extreme pressures and temperatures. The discovery science enabled by exascale computing is uniquely coupled to several experimental projects, led by the PI and his experimental collaborators, aimed at observing the phenomena, predicted by the team's simulations. The team's scientific goals are to design compressive pathways towards synthesis of elusive and long-sought post-diamond BC8 phase of carbon; uncover kinetics effects in phase transformations to BC8 phase from diamond and amorphous carbon in explicit, billion atom, double-shock simulations at micrometer and nanosecond time scales. They also seek to uncover fundamental mechanisms of inelastic deformations in shock compressed diamond and determine the origin of anomalous persistence of crystalline anisotropy at extreme compressions of diamond up to its melting line in multi-billion-atom simulations of split-shock wave propagation. Finally, they are working to investigate fundamental physics of shock melting and refreezing and determine the effect of refreeze microstructure on modulating initially planar second shock in multi-billion atom single and double shock simulations.

Type: New
Title: "Clinical Foundation LLMs for Scaling Public Health Surveillance"

Principal Investigator: Silvia Crivelli, Lawrence Berkeley National Laboratory
Co-Investigators: Rafael Zamora-Resendiz, Lawrence Berkeley National Laboratory

Scientific Discipline: Biological Sciences

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

Research Summary: Current advances in AI have the potential to revolutionize biomedical science and address emerging challenges in healthcare. Clinical language models can accelerate research in this field and improve healthcare for millions of patients.

A wealth of clinical predictive models that apply machine learning methods on structured data from EHR have been proposed to help physicians integrate large amounts of information. Most of these models do not use the unstructured notes in the EHR that are rich in detail. Recent studies have shown the need to include these notes to advance precision medicine.

This project aims to use the computational resources of Frontier to leverage the power of large language models in healthcare. By developing a foundation model for clinical language using the Veteran Affair's Corporate Data Warehouse, or CDW, the team aims to increase the size of clinical large language models by tens of billions in parameter and the training clinical corpus to billions of documents. This information-rich corpus of over 20 years' worth of clinical text for 23 million patients will enable the analysis of current language models.

The project will investigate and research how well large language models capture measures of healthcare like demographics and medical interventions. The investigation will provide insight toward building a better "map of disease progression" for the U.S. veteran population and tracing impacts of medical interventions on patient health.

Type: New
Title: "COMbining Deep-Learning with Physics-Based affinIty estimatiOn 3 (COMPBIO3)"

Principal Investigator: Peter Coveney, University College London
Co-Investigators: Shantenu Jha, Brookhaven National Laboratory
Philip Fowler, University of Oxford
Ola Engkvist, AstraZeneca
Eric Stahlberg, Frederick National Laboratory
Dilip Asthagiri, Oak Ridge National Laboratory
Balint Joo, Oak Ridge National Laboratory
Tom Beck, Oak Ridge National Laboratory
Rick Stevens, Argonne National Laboratory

Scientific Discipline: Biological Sciences

INCITE Allocation:

Site:	Argonne National Laboratory
Machine (Allocation):	HPE Apollo 6500 (80,000 Polaris node-hours)
Site:	Argonne National Laboratory
Machine (Allocation):	HPE Cray EX - Intel Exascale Compute Blade Nodes (250,000 Aurora node-hours)
Site:	Oak Ridge National Laboratory
Machine (Allocation):	HPE-Cray EX (1,000,000 Frontier node-hours)

Research Summary: This team will use exascale supercomputers for developing a personalized digital twin of the human body. They will simulate the entire cardiovascular system of the human body, and thus will afford clinicians the ability to make personalized predictions about treatment outcomes. Further they will combine machine learning and physics-based methods to accelerate the process of drug discovery.

The advent of exascale computing has opened up immense possibilities to realize a fully personalized digital twin (DT) of the human body. DT technology will not only enable clinicians to make reliable and actionable predictions to support clinical decision making, but it will also facilitate the adoption of informed lifestyle choices that support healthy ageing and wellbeing. To address any challenges, this team's goal is to advance the modeling and simulation of the human body in health and disease such that they are at the forefront of the development of human DTs for applications in personalized medicine and healthcare. This requires access to large-scale computing resources. This team developed a method called IMPECCABLE that couples ML and PB methods to accelerate the drug discovery process, each compensating for the limitations of the other. The main goal of this project is to implement IMPECCABLE at scale on exascale machines and identify potential drug candidates for various target proteins. In addition to the drug design aspect, the team also aims to develop a related method enabling them to assess drug resistance in target proteins.

Type: New
Title: "Commerical Aircraft High Lift Scale-Resolving CFD Simulations"

Principal Investigator: Adam Clark, Boeing Commerical Airplanes
Co-Investigators: Konrad Goc, The Boeing Company
Jeffrey Slotnick, The Boeing Company
Andrew Cary, The Boeing Company
Joerg Gablonsky, The Boeing Company
Sanjeeb Bose, Cadence Design Systems

Scientific Discipline: Engineering

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

Research Summary: There is a concerted effort in the aerospace industry to address the societal need to reduce airplane emissions, noise, and tackle related issues to the climate change imperative. Commercial aviation is a critical component of the global economic infrastructure and greenhouse gas emissions.

The take-off and landing phases of aircraft operations are critical considerations for low-speed aerodynamic design because they directly impact the overall levels of noise, fuel efficiency, and the corresponding emissions. Improving the ability to accurately simulate the class of challenging flow physics associated with low-speed flows can significantly increase aerodynamic efficiency and reduce certification time and costs. This, in turn, will enable more fuel efficient and environmentally friendly aircraft to be deployed quickly.

This project's effort focuses on using Cascade Technology's flow solver to perform large-scale simulations on 3D airplane configurations that will determine appropriate grid requirements for various flight conditions. A second focus will help predict the aerodynamic impact of small-scale ice accumulation on the wing during flight, which has not been previously attainable.

Exascale data produced by these impressive simulations will inform modeling guidance for government and industry applications. This effort is a necessary first step toward realizing the simulation requirements within the grand challenge problem.

Type: New
Title: "Democratizing AI by Training Deployable Open-source Language Models"

Principal Investigator: Abhinav Bhatele, University of Maryland
Co-Investigators: Tom Goldstein, University of Maryland
Harshitha Menon, Lawrence Livermore National Laboratory

Scientific Discipline: Computer Science

INCITE Allocation:

Site:	Argonne National Laboratory
Machine (Allocation):	HPE Apollo 6500 (100,000 Polaris node-hours)
Site:	Argonne National Laboratory
Machine (Allocation):	HPE Cray EX - Intel Exascale Compute Blade Nodes (50,000 Aurora node-hours)
Site:	Oak Ridge National Laboratory
Machine (Allocation):	HPE-Cray EX (600,000 Frontier node-hours)

Research Summary: Artificial intelligence (AI), and deep learning (DL) in particular, is rapidly becoming pervasive in almost all areas of computer science, and is even being used to assist computational science modeling and simulations. At the forefront of this development are large language models (LLMs). The challenges the team seeks to address in this project originate from the fact that large models do not fit on a single CPU/GPU and/or take a long time to train. Scaling the training of large neural networks to extreme levels of parallelism requires parallelizing and optimizing different computational and communication motifs such as dense and sparse tensor computations, irregular communication patterns, load imbalance issues, and fast filesystem access.

The team will use a sizeable INCITE allocation across the three platforms (Polaris, Aurora, and Frontier) to advance research in three directions. First, the scaling of parallel training of deep learning models to a large number of GPUs is non-trivial. They plan to use their framework, AxoNN, to analyze and optimize the performance and portability of training, fine-tuning, and inference. Second, they plan to explore efficient alternatives for transformer models for language modeling. They intend to train variants of modern language model architectures that are directly aimed at usability constraints in smaller academic laboratories. The team is focused on variants with smaller memory footprints and adaptive compute capabilities at deployment to enable more research and development in the fields of machine learning and NLP. Third, they propose to fine-tune trained models for several downstream tasks. The team plans to utilize the trained models for several HPC-related tasks such as improving portability and studying performance explainability.

Type: New
Title: "DNS and Surrogate DNS for NO_x and Flame Stabilization in NH_3/H_2 Gas Turbines"

Principal Investigator: Martin Rieth, Sandia National Laboratories
Co-Investigators: Jacqueline Chen, Sandia National Laboratories
Ki Sung Jung, Sandia National Laboratories
Bruce Perry, National Renewable Energy Laboratory
Bruno Soriano, Sandia National Laboratories
Marc Day, National Renewable Energy Laboratory

Scientific Discipline: Chemistry

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (900,000 Frontier node-hours)

Research Summary: As part of the U.S. National Clean Hydrogen Strategy and Roadmap and DOE Hydrogen Program Plan, gas turbines fired with hydrogen and ammonia will provide a promising, carbon-free alternative to firing of natural gas in dispatchable power generation. While carbon dioxide emissions are eliminated from the combustion process with these fuels, nitrogen oxide emissions (NO_x) pose a significant challenge. The research team proposes a series of direct numerical simulations (DNS) to shed light on the combustion process and emission formation of advanced combustion concepts that show promise in mitigating NO_x emissions with ammonia and hydrogen fuels. One of the most promising strategies is the so-called rich-quench-lean (RQL) staged combustion system, where the combustion process is divided into two stages. Such a system also allows for fuel-flexibility, which is a necessity for viably ramping up hydrogen and ammonia adoption to replace natural gas. With ammonia-based fuels, typically the first stage of the combustor features a fuel-rich flame and a central recirculation region to aid with flame stabilization. The proposed DNS aim to provide such understanding by featuring two distinct but relevant computational configurations of the staged combustion system: 1) a simplification of the second stage derived from a real gas turbine combustor (downscaled while retaining relevant timescales), 2) a bluff-body laboratory experiment representing the first stage. Results obtained will augment the experimental measurements with fully-resolved data valuable to the modeling community. After validation of the numerical setup, this configuration will be extended to higher pressures, relevant to gas turbine operation for which experimental data does not exists. This unique data will allow unprecedented insight into the details of the flame stabilization process and the impact of the recirculation regions on the formation of emissions at realistic pressures. All data generated in this project will be shared with the broader reacting flow modeling community to aid the development of predictive models for the design, development and optimization of efficient low-NO_x engines for carbon-free power generation.

Type: New
Title: "DNS of Transonic Shock-Induced Flow Separation"

Principal Investigator: Sanjeeb Bose, Cascade Technologies, Inc.
Co-Investigators: Parviz Moin, Stanford University

Scientific Discipline: Engineering

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (700,000 Frontier node-hours)

Research Summary: The use of computational fluid dynamics (CFD) in the aerospace industry has been a key tool for engineering design, impacting turbomachinery and aerodynamic applications by reducing the need for rig and wind tunnel tests. Flow predictions from state-of-the-art CFD solvers, however, are still unable to comply with the accuracy and computational efficiency requirements demanded by the industry.

Despite its salience and significance, the prediction of separated flow regimes remains a pacing challenge for simulation. The modeling challenge is complicated by the interaction of adverse pressure gradients and the presence of shockwaves. An experiment at Sandia National Laboratories recently provided a validation data set for numerical simulations that specifically target the physics of shock-induced boundary layer separation. There are outstanding issues from the simulation associated with strong non-equilibrium effects that are not well captured and necessitate a brute-force approach to achieve accurate results.

This project proposes to conduct a series of direct numerical simulations of the Sandia experiments across several set points about this separation boundary. The simulations will help anchor the ability of first principles-based calculations to characterize the boundary, while informing necessary resolution requirements.

The data will be made available to help support ongoing non-equilibrium wall and subgrid-scale modeling efforts, regarding flow regimes, to facilitate more cost-effective simulation approaches.

Type: New
Title: "Earthquake System Science Research on Seismic Hazard Analysis and Risk Reduction"

Principal Investigator: Yehuda Ben-Zion, University of Southern California
Co-Investigators: Kim Olsen, San Diego State University
Yifeng Cui, San Diego Supercomputer Center
Philip Maechling, Southern California Earthquake Center

Scientific Discipline: Earth Science

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (700,000 Frontier node-hours)

Research Summary: The widespread devastation caused by the recent earthquakes in Turkey provides a reminder of the urgent need to understand risks posed by corresponding large earthquakes in California and other seismically active areas. This project will perform physics-based earthquake simulations that help scientists and the earthquake engineering community anticipate the effects of earthquakes.

While large earthquakes near major urban areas in California are inevitable, the risk of hazards becoming societal catastrophes can be reduced by dramatically improving hazard estimates and their effects on the built environment. This will enable improved design and construction practices, transforming California into an earthquake-resilient society.

The use of Frontier for this project will advance the modeling of the interaction of seismic energy propagation with the built environment, moving toward better risk reduction. The project will include broadband physics-based earthquake simulations that will help the earthquake engineering community anticipate the effects of large earthquakes.

The results can be used to mitigate risk to urban populations and infrastructure by revealing vital vulnerabilities and illuminating pathways to more effective earthquake-resilient designs.

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

Principal Investigator: Peter Caldwell, Lawrence Livermore National Laboratory
Co-Investigators: Mark Taylor, Sandia National Laboratories
Chris Terai, Lawrence Livermore National Laboratory
Oksana Guba, Sandia National Laboratories
Ben Hillman, Sandia National Laboratories
Sarat Sreepathi, Oak Ridge National Laboratory
Xingqiu Yuan, Argonne National Laboratory
Dave Bader, Lawrence Livermore National Laboratory
Ruby Leung, Pacific Northwest National Laboratory

Scientific Discipline: Earth Science

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): HPE Cray EX - Intel Exascale Compute Blade Nodes (500,000 Aurora node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (1,000,000 Frontier node-hours)

Research Summary: This project is 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. E3SM is a collaborative effort across eight national laboratories and twelve academic institutions working towards the development of a cutting-edge Earth system model for the most demanding climate research applications.

The main goal of this year's INCITE proposal is to perform an unprecedented pair of decadal-scale climate simulations with atmospheric grid spacing of 3.25 km. This is two orders of magnitude finer than most climate models and will greatly improve our model predictions. One reason for this is that the team will explicitly resolve mountains, coastlines, and storms, which will allow the team to capture climate impacts that aren't captured by conventional climate models. Fine resolution will also allow the team to explicitly resolve deep convection, which plays a central role in determining how much warming the team will experience for a given CO_2 increase. The thing that makes these runs groundbreaking is their duration – many groups have done simulations at this resolution of a month to a year in length, but these runs are too short to separate climate change signal from weather noise. Long simulations are also needed to sample extreme events, which are by definition rare. The decadal-scale simulations planned for this proposal will enable statistically-robust analysis of climate impacts using a global storm-resolving simulation for the first time.

Type: New
Title: "Establishing Digital Twins for High-Throughput Cellular Analysis in Whole Blood"

Principal Investigator: Amanda Randles, Duke University
Co-Investigators: Lydia Sohn, University of California, Berkeley

Scientific Discipline: Biological Sciences

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): HPE Cray EX - Intel Exascale Compute Blade Nodes (60,000 Aurora node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (240,000 Frontier node-hours)

Research Summary: It has been well established that mechanical properties of cells change with differentiation, chronological age, and disease state. Specifically, a positive correlation between increased cell deformability and heightened metastatic potential has been observed for breast cancer cells. More broadly, the changes caused by many cancers within the cell are manifest in measurable biophysical properties, such as optical deformability and size. Being able to screen and accurately characterize many cells would allow cancer researchers to quickly identify potentially deleterious mechano-phenotypes.

To better understand this concept, this team developed a series of in vitro based techniques. Atomic-force microscopy (AFM) and micropipette aspiration are the gold standard for performing mechanical measurements on cells. However, they are limited in terms of throughput. Given these drawbacks, these researchers have turned to microfluidic platforms to extract mechanical properties from specific cell types with high throughput. Mechano-phenotyping platforms can now quantify four fundamental biophysical properties: diameter, resistance to compressive deformation, transverse deformation, and recovery from deformation in a label-free manner.

The team's work addresses three key challenges facing cellular simulations. First, being able to establish a precise and validated method for a digital twin of the microfluidic device. Second, the team will extend this capability by creating a framework for robustly capturing cellular behavior across the ensemble of potential red blood cell configurations. Finally, the team will set a computationally optimized method by integrating this framework with their adaptive physics refinement method that enables cellular resolution to be captured over large domains. Together, these advances will allow a robust digital twin for a wide range of microvascular and microfluidic applications for systems targeting whole blood analysis.

Type: New
Title: "ExaCortex: Exascale Reconstruction of Human Cerebral Cortex"

Principal Investigator: Nicola Ferrier, Argonne National Laboratory
Co-Investigators: Jeff Lichtman, Harvard University

Scientific Discipline: Biological Sciences

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): HPE Cray EX - Intel Exascale Compute Blade Nodes (250,000 Aurora node-hours)

Research Summary: While the functions carried out by most of the vital organs in humans are unremarkable, the human brain clearly separates us from the rest of life on the planet. It's a vastly complicated tissue and little is known about its cellular microstructure; particularly its synaptic circuits are almost completely unexplored. These circuits underlie the unparalleled capabilities of the human mind, and when disrupted, likely underlie some of the incurable disorders of brain function.

Three advances make it possible to pursue a precise understanding of the structure of the brain today: next-generation electron microscopes are capable of imaging with multiple beams simultaneously to speed the enormous task of imaging tissue at high resolution; accelerator-based computing is pushing supercomputers to exascale and beyond; and large deep learning models are quickly outperforming humans at laborious tasks such as identifying neurons in imaged data. This INCITE proposal aims to leverage all of these to produce datasets of human brain connectivity at unprecedented scale, for analysis within a separately funded neuroscience-driven project, and to publish the data via ALCF's Globus-based data sharing facilities.

While we acknowledge that reconstruction of a whole human brain with eighty billion neurons is a task for microscopes and supercomputers one or two generations beyond those available today, our work today necessarily pushes the boundaries toward achieving those future goals. This extreme-scale, AI-driven project extends this team's earlier Aurora Early Science project to adapt their neural network-based segmentation code for Polaris and Aurora. Already team has found that trained models have the ability to generalize across datasets, though fine-tuning is of course required; amid the ocean of data processed in this INCITE project, the team hopes this work enables steps towards a foundation model for segmentation, capable of superior performance across future EM datasets with minimal fine-tuning.

Type: New
Title: "Exascale Ab Initio Simulations of Out-of-Equilibrium Quantum Materials"

Principal Investigator: Panchapakesan Ganesh, Oak Ridge National Laboratory
Co-Investigators: David Lingerfelt, Oak Ridge National Laboratory
Jacek Jakowski, Oak Ridge National Laboratory
Jerzy Bernholc, North Carolina State University
Wenchang Lu, North Carolina State University
Emil Briggs, North Carolina State University

Scientific Discipline: Materials Science

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (175,000 Frontier node-hours)

Research Summary: Facilitating a greater understanding of the far-from-equilibrium response of chemical and material systems to external perturbations (motion brought by external force) is critical to the continuing advancement of energy-related technologies. These include solar cell technologies and quantum information processing.

Simulation methods have been developed that are technically capable of fully capturing the evolutions of these system responses but are cost-prohibitive in practice.

The goal of this project is to develop and apply these quantum and mixed-quantum dynamics at a scale to realistic systems and relevant materials. This will be achieved by considering the role of structure in the materials and the influence exerted on the material by its environment. This method will model the dynamics of charge in realistic materials and environments to describe material responses and transformations.

This requires the computational power that exascale-class systems present for speed and scaling.

The approach will answer key fundamental questions pertaining to dynamics of charge in quantum materials, enabling novel quantum information processing.

Type: New
Title: "Exascale Catalytic Chemistry"

Principal Investigator: David Bross, Argonne National Laboratory
Co-Investigators: Eric Bylaska, Pacific Northwest National Laboratory
C. Franklin Goldsmith, Brown University
Branko Ruscic, Argonne National Laboratory
Khachik Sargsyan, Sandia National Laboratories
Duo Song, Pacific Northwest National Laboratories
Richard West, Northeastern University
Judit Zádor, Sandia National Laboratories

Scientific Discipline: Chemistry

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): HPE Cray EX - Intel Exascale Compute Blade Nodes (425,000 Aurora node-hours)

Research Summary: The primary goal of this INCITE project is to enable routine construction of predictive microkinetic models for heterogenous catalysis systems by developing an open access database using tools developed within the ECC project.

This work will facilitate and significantly speed up the quantitative description of crucial gas-phase and coupled heterogeneous catalyst/gas-phase chemical systems. Such tools promise to enable revolutionary advances in predictive catalysis, crucial to addressing DOE grand challenges including both energy storage and chemical transformations. The researchers will construct a consistent database of values that enable reaction network tools to construct predictive values for heterogenous catalysis through interrelated thrusts of reaction network generation and analysis, potential energy surface exploration, advanced thermochemical properties, and beyond density functional theory (DFT) methods.

The team has three primary scientific objectives that will enable the construction of the underlying database that outside researchers can then use to generate predictive microkinetic models: (1) to calculate a large ensemble of reactions at a baseline density functional theory level of accuracy that is sufficiently detailed to enable the team's reaction network tools to make predictions, (2) to vastly reduce the uncertainty in temperature dependence of entropic considerations of adsorbate thermochemistry in this database by calculating a comprehensive consistent set of species with fully anharmonic partition functions, and (3) to investigate and reduce the uncertainty from DFT simulations by employing beyond DFT methods and validating the subsequent improvement in microkinetic modeling against experiment.

Type: New
Title: "Exascale Cosmology: Lighting Up the Dark Universe"

Principal Investigator: Katrin Heitmann, Argonne National Laboratory
Co-Investigators: Salman Habib, Argonne National Laboratory
Zarija Lukic, Lawrence Berkeley National Laboratory
Nicholas Frontiere, Argonne National Laboratory

Scientific Discipline: Physics

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): HPE Cray EX - Intel Exascale Compute Blade Nodes (375,000 Aurora node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX 800,000 Frontier node-hours)

Research Summary: The Universe is dominated by its "dark" sector, with two mysterious components accounting for 95 percent of the cosmic matter-energy content. The dark energy component is the cause of a yet to be understood late-time cosmic acceleration. The dark matter component dominates over normal matter, and while its gravitational presence is confirmed via multiple observations, it eludes direct detection because it does not appear to emit or absorb light. Major sky surveys are ongoing and being constructed by a large international community to unravel the physics of the dark Universe and to investigate other fundamental cosmological questions. Large-scale simulations that connect the physics of the dark sector to observations in the visible domain are essential to this global endeavor. Such simulations are the basis of synthetic sky catalogs that are crucial to developing and testing analysis capabilities for the surveys, delivering predictions for the nonlinear regime of structure formation inaccessible by any other means, and helping determine the systematics error budget, a critical task to ensure that the anticipated level of cosmological constraints can be attained.

This INCITE project will usher in a new era of cosmological simulations by fully exploiting the power of DOE's Frontier and Aurora supercomputers. The team will employ two exascale-ready cosmology codes: the Hardware/Hybrid Accelerated Cosmology Code (HACC) and Nyx. The team's simulations will be transformed into synthetic sky catalogs across wavebands and provide predictions for a range of cosmological observables using both direct analysis performed on simulations as well as transfer learning combining the strengths of all the simulations. The scientific results will be an important input for all major ongoing and upcoming U.S.-led cosmological surveys, including DOE's Dark Energy Spectroscopic Instrument (DESI); NSF and DOE's Rubin's Legacy Survey of Space and Time (LSST), South Pole Telescope (SPT), and CMB-S4; and NASA's Spectro-Photometer for the History of the Universe, Epoch of Reionization, and Ices Explorer (SPHEREx) and the Nancy Grace Roman Space Telescope.

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

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

Scientific Discipline: Physics

INCITE Allocation:

Site:	Argonne National Laboratory
Machine (Allocation):	HPE Apollo 6500 (100,000 Polaris node-hours)
Site:	Argonne National Laboratory
Machine (Allocation):	HPE Cray EX - Intel Exascale Compute Blade Nodes (450,000 Aurora node-hours)
Site:	Oak Ridge National Laboratory
Machine (Allocation):	HPE-Cray EX (1,000,000 Frontier node-hours)

Research Summary: The goal of this INCITE project is to employ the electromagnetic edge gyrokinetic PIC code XGC to perform two-pronged, but inter-related, fundamental edge physics studies of critical importance to the successful operation of ITER and to the design of Fusion Power Plants (FPPs). The first prong is the mitigation of high stationary heat-flux densities that will damage material walls while maintaining the high edge plasma pedestal within a safe operational window. The second prong is avoiding explosive transient power-flow to material walls caused by edge localized mode (ELM) crash. To achieve these goals, leadership-class compute-power is required to address the current game changing INCITE studies that include important but computationally expensive ingredients: i) the addition of tungsten impurity particles that are sputtered from ITER's material wall as a third species along with deuterium and tritium fuel particles; and ii) the capability for plasma detachment from the divertor plates.

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

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

Scientific Discipline: Physics

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): HPE Apollo 6500 (75,000 Polaris node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (400,000 Frontier node-hours)

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

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

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

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

Scientific Discipline: Physics

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

Research Summary: This project strives to develop the challenging capability for predication and real-time control of energetic particle confinement in burning plasmas. The study will combine state-of-the-art exascale power and the prominent, experimentally-validated AI/Deep Learning software.

The accurate identification and effective control of plasma instabilities that cause energy particle loss is important for the ignition of burning when developing clean fusion energy. This proposal seeks a deep-learning based surrogate model as an instability and transport simulator for real-time applications related to fusion energy. This will help navigate the problem of building a simulation that matches the required speed for real-time applications.

The proposed simulation will address the key physics identified by current simulations to improve the physics-based understanding of energy particle interactions with burning thermal plasmas. This includes advancing an understanding of energy particle transport and coupling with plasmas.

The project will open a new direction of bringing accurate physics-based instability information from the exascale simulations into modern fusion devices, geared toward clean and abundant fusion energy.

Type: New
Title: "Exascale Simulation of Correlated Election-Phonon Coupling in Quantum Materials"

Principal Investigator: Zhenglu Li, University of Southern California
Co-Investigators: Mauro Del Ben, Lawrence Berkeley National Laboratory

Scientific Discipline: Materials Science

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (450,000 Frontier node-hours)

Research Summary: Coupling between phonons (waves of atomic vibrational energy) and correlated electrons drives a spectrum of important phenomena in quantum materials. These include superconductivity and charge-density waves. Their understanding, however, remains elusive due to the lack of methodology behind electron-electron and electron-phonon interactions.

This project will take the GW-Bethe-Salpeter-equation, or GW-BSE, a general quantum theoretical tool, and apply it to the study of electron-phonon coupling to capture how this correlation effects quantum materials. This will optimize the performance of GW calculations to advance computational quantum materials research.

This proposal expects to advance the fundamental understanding of electron-phonon coupling in correlated materials using the computational approach of exascale-class systems, including Frontier. The expected achievements will redefine current boundaries of electron-phonon coupling research and the materials science computation at scale.

The project enables the largest-scale materials science computation, potentially leading to discoveries of new materials and designs of next-generation electronics.

Type: New
Title: "Exascale Simulations of Binary Neutron-Star Mergers "

Principal Investigator: Philipp Mösta, University of Amsterdam
Co-Investigators: Swapnil Shankar, University of Amsterdam
Sanjana Curtis, University of Chicago
Erik Schnetter, Perimeter Institute of Theoretical Physics
Roland Haas, National Center for Supercomputing Applications

Scientific Discipline: Physics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (500,000 Frontier node-hours)

Research Summary: The era of multimessenger astronomy has been inaugurated with the detection of gravitational waves from two merging neutron stars by aLIGO/VIRGO in combination with optical, infrared and γ-ray observationsof the same event. Together these observations have begun to revolutionize the understanding of short γ-ray bursts, of the physics of neutron stars, and of the origin of the heavy elements, like silver, gold, andplatinum. However, they also pose many pressing questions: What was the fate of the binary aftercoalescence? Which mechanisms generated the observed electromagnetic signals?

For this INCITE project, the team will make use of the Frontier supercomputer to address these questions. They will employ 579938 node-hours and perform state-of-the-art general-relativistic magnetohydrodynamic neutron-star merger simulations to predict the electromagnetic and nucleosynthetic signatures of these events. This process will help maximize the science return from observations of GW170817 and similar future events. The simulations will be the first of their kind and include general relativity, magnetic field and plasma effects, a microphysical equation of state and M1 neutrino transport. The codebase has been deployed and is currently being optimized for Frontier. It has been extensively used on Summit and the largest CPU machines in Europe and the US (BlueWaters, Frontera, SuperMUC) to produce high-impact science. With this INCITE allocation the team plans to build on this success.

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

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

Scientific Discipline: Materials Science

INCITE Allocation:

Site:	Argonne National Laboratory
Machine (Allocation):	HPE Apollo 6500 (190,000 Polaris node-hours)
Site:	Argonne National Laboratory
Machine (Allocation):	HPE Cray EX - Intel Exascale Compute Blade Nodes (400,000 Aurora node-hours)
Site:	Oak Ridge National Laboratory
Machine (Allocation):	HPE-Cray EX (600,000 Frontier node-hours)

Research Summary: This project is focused on being able to reliably predict, understand, and realize desired phenomena in specific, real materials. Advances are critical to help meet the challenges of reducing energy, realizing new technologies, and identifying the optimum materials for specific applications.

The team's focus is on materials and properties where commonly used electronic structure methods are thought to be inaccurate due to their inherent approximations and where insight from benchmark accuracy calculations is needed, such as two-dimensional nanomaterials and "quantum materials". Calculations are performed using the open-source QMCPACK code that implements Quantum Monte Carlo (QMC) algorithms. These methods are highly accurate and avoid the majority of problems of standard electronic structure methods, but at the trade-off of considerable additional computational cost.

Type: New
Title: "Extreme Resolution Brain Image Segmentation"

Principal Investigator: Evan Calabrese, Duke University
Co-Investigators: Isaac Lyngaas, Oak Ridge National Laboratory
Xiao Wang, Oak Ridge National Laboratory
Muralikrishnan Gopalakrishnan Meena, Oak Ridge National Laboratory
Yuankai Huo, Vanderbilt University
G. Allan Johnson, Duke University
Robert Williams, University of Tennessee Health Science Center
Thomas Beck, Oak Ridge National Laboratory

Scientific Discipline: Biological Sciences

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

Research Summary: A critical challenge in the field of neuroscience is understanding the structural brain changes that occur as a result of neurodevelopmental diseases like Alzheimer's disease (AD). These changes can serve as quantitative biomarkers for determining disease risk and assessing the efficiency of treatments.

Deep-learning image segmentation techniques have not been thoroughly developed for ultra-high resolution and multi-contrast brain imaging data. Existing techniques focused on typical human brain imaging data are not appropriate for the substantially higher resolution and larger number of image contrasts available for mouse brain imaging.

This project aims to develop AI image segmentation techniques for the unexplored space of high-resolution multi-model mouse brain imaging datasets. Due to large amounts of data and image contrasts, combined with the difficult image segmentation task, training of these models requires exascale-class systems. This project will allow high-throughput brain structural analysis in mouse models of Alzheimer's disease, providing new insights into the neuroanatomic underpinnings of neurodegeneration, the main feature of many neurological diseases.

Type: Renewal
Title: "Feedback and Energetics from Magnetized AGN Jets in Galaxy Groups and Clusters"

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

Scientific Discipline: Physics

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

Research Summary: The goal of this project is to understand how galaxies evolve and regulate themselves. The team will do this by simulating the feedback from supernovae and supermassive black holes on the diffuse plasma that surrounds galaxies, and in particular focus on the most massive galaxies in the universe. The team will, for the first time, fully utilize the capabilities of Frontier to explore the self-regulation of massive galaxies in groups and clusters using magnetized jet feedback from supermassive black holes. The successful completion and analysis of these calculations will revolutionize the team's understanding of AGN feedback and the self-regulation of galaxies within groups and clusters. This will be important in astrophysics for the interpretation of observations of galaxies and their environments, for the development of subgrid models in simulations of cosmological structure formation, and more generally in the team's theoretical understanding of the growth and evolution of galaxy populations over cosmic time.

Type: New
Title: "First-principle simulation of MHD modes with energetic particles in fusion experiments"

Principal Investigator: Chang Liu, Princeton Plasma Physics Laboratory
Co-Investigators: Stephen Jardin, Princeton Plasma Physics Laboratory
Nathaniel Ferraro, Princeton Plasma Physics Laboratory
Jin Chen, Princeton Plasma Physics Laboratory
Seegyoung Seol, Rensselaer Polytechnic Institute

Scientific Discipline: Physics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (240,000 Frontier node-hours)

Research Summary: The interaction between high-energy particles, such as runaway electrons, and instabilities in plasma, is of paramount importance to the operation of magnetic fusion reactors. These instabilities, including acoustic modes (modes that travel far distances), can become unstable due to the presence of energetic ions and electrons. This can lead to energy deconfinement and heat load on plasma-facing components.

The presence of high-energy particles themselves influence other instabilities.

Simulating the nonlinear behavior of these instabilities requires high-performance computers due to the range of timescales involved in the system's dynamics. This project aims to use Frontier to do just that, with the objective of understanding the comprehensive physics behind these interactions and explaining phenomena in fusion experiments.

The project addresses critical issues in the field of magnetic confined plasma physics, which in turn are vital for advancing fusion energy. The results are expected to have significant impact and will serve for future experimental investigations in fusion.

Fusion power is widely regarded as a promising clean energy source. This project will likely answer key questions toward more sustainable energy.

Type: New
Title: "Flight-Scale Simulations of a Transport Aircraft in High-Lift Conditions"

Principal Investigator: Eric Nielsen, NASA Langley Research Center
Co-Investigators: Li Wang, NASA Langley Research Center

Scientific Discipline: Engineering

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): HPE Cray EX - Intel Exascale Compute Blade Nodes (350,000 Aurora node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (1,000,000 Frontier node-hours)

Research Summary: According to the Federal Aviation Administration, the commercial aviation industry plays a key role in the overall health of the U.S. economy, which motivates a strong need to maintain leadership in this critical industry. One of the key cost drivers in the design and certification of a new transport aircraft is the ability to reliably and accurately predict the maximum lift the vehicle can achieve, particularly during the takeoff and landing phases of flight. For this reason, the global aerospace industry has identified the accurate prediction of high-lift flows using computational fluid dynamics as a top priority.

Historically, certification requirements for a new aircraft have been met through wind tunnel experiments and flight test campaigns. A substantial portion of a typical flight test campaign required for certification focuses on the low-speed performance characteristics associated with the takeoff and landing phases of flight. A current goal for the aircraft industry is to unambiguously demonstrate consistently accurate predictive computations of high-lift flows. If this objective can be realized, computations may facilitate a simulation-based approach to certification, thereby significantly reducing the cost of bringing a new aircraft to market while continuing to meet strict safety guidelines.

The exascale-class Frontier and Aurora systems offer unique and timely computational power to evaluate the viability of high-fidelity, eddy-resolving methods as an enabling technology for the use of computations in aircraft certification. In this effort, NASA Langley Research Center proposes a series of high-lift simulations supporting a grid refinement study at flight-relevant conditions. The simulations align with planned wind tunnel testing at the National Transonic Facility. NASA computational resources will be used to perform simulations on coarser mesh levels with relatively large time steps, while Frontier and Aurora will be used to evaluate solutions on substantially finer meshes with appropriately smaller time steps. Successful execution offers the potential to dramatically reduce costs associated with extensive physical testing campaigns, accelerating the time to market for new designs and ultimately ensuring that the U.S. remains positioned at the forefront of the global aviation community.

Type: New
Title: "Flow Fields Controlled Structuring of Ionizable Polymers"

Principal Investigator: Gary S. Grest, Sandia National Laboratories
Co-Investigators: Dvora Perahia, Clemson University
Stan Moore, Sandia National Laboratories

Scientific Discipline: Materials Science

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): HPE Apollo 6500 (190,000 Polaris node-hours)
Site: Argonne National Laboratory
Machine (Allocation): HPE Cray EX - Intel Exascale Compute Blade Nodes (300,000 Aurora node-hours)

Research Summary: Polymers are ubiquitous in modern life and are the cornerstone of numerous technologies. Nevertheless, the same properties that drive their uses pose a challenge to their assembly into viable materials. Full realization of their potential requires control over the collective motion of macromolecules in highly inhomogeneous large systems, that are often processed into viable materials under flow. Though pathways for processing of macromolecules have been developed, achieving sub-molecular control over their structure and response remains highly desired, and presents a key challenge to the design and manufacturing of smart responsive polymeric materials.

This work will use exascale computing to determine the fundamental response of structured ionizable polymers for energy applications, to flow. The research will elucidate new physics concepts that quantify the interrelation of responses across length scales, from atomistic to macroscopic, impacting processing and upcycling of a technologically important class of materials. Using fully atomistic classical molecular dynamics simulations, the project will generate compute-polymeric systems of structured ionizable block co-polymers, comparable in molecular weights to polymers measured in neutron scattering experiments. The structure and dynamics of these materials in their quiescent state will first be resolved, followed by nonequilibrium studies of these systems under flow. The understanding of the quiescent polymers will provide fundamental insight into their structure and dynamics that will be correlated with their response to flow.

The projected results will correlate the structure and dynamics of distinctive segments of structured polymers including their ionic blocks and non-ionic blocks in their quiescent state and under flow with the resulting macroscopic properties. These results will answer a fundamental polymer physics challenge of understanding the collective response of inhomogeneous systems controlled by distinctive energy length scales, while contributing directly to enhancing processing conditions of polymers for energy applications.

Type: New
Title: "Foundation Models for Molecular Design for Energy Storage and Conversion"

Principal Investigator: Venkatasubramanian Viswanathan, University of Michigan
Co-Investigators: Arvind Ramanathan, Argonne National Laboratory
Bharath Ramsundar, Deep Forest Sciences
Natalia Vassilieva, Cerebras Systems

Scientific Discipline: Energy Technologies

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

Research Summary: Energy storage and conversion devices require electrolyte materials that enable functionality for various applications. Designing electrolytes for electric vehicles, grid storage, and electric aircraft presents a myriad of unique challenges for each target application. It is critical to design domain-specific energy storage materials to electrify transportation and industrial processes to create a sustainable and electrified future.

Current energy storage materials development is hindered by expensive experiments that limit exploration to a small set of known synthesizable and readily available materials. To address the unique demands of developing batteries for electric mobility and grid storage applications, such as high energy density, low cost, safety, scalability, and power density, it is essential to explore a much larger chemical space than the few hundred currently considered. Foundation models offer a solution to both the exploration and evaluation issues: these models use self-supervised pre-training strategies to leverage unlabeled datasets and learn representations of data that can be applied to downstream tasks. Large unlabeled datasets of billions of synthesizable molecules are readily available. This INCITE project will scale up the training of foundation models to the largest available chemical libraries to achieve accuracy similar to quantum mechanical computational methods and apply these to the electrolyte design problem.

The foundation models will be embedded into the team's automated materials design workflow, AutoMat, to develop new energy storage materials for electric mobility and grid storage applications. Designing a good electrolyte involves optimizing for multiple properties (e.g., conductivity, voltage stability) over a large, high-dimensional design space. The team will investigate how emergent behavior observed in large-scale training of foundation models can be leveraged to posit better electrolyte compositions. The team's work holds tremendous potential for revolutionizing electrolyte design and advancing the fields of energy storage and transportation.

Type: New
Title: "Foundation Models for Predictive Molecular Epidemiology"

Principal Investigator: Arvind Ramanathan Nakano, Argonne National Laboratory
Co-Investigators: Rick Stevens, Argonne National Laboratory
Ian Foster, Argonne National Laboratory
James Davis, Argonne National Laboratory
Christopher Henry, Argonne National Laboratory
Thomas Brettin, Argonne National Laboratory
Anima Anandkumar, California Institute of Technology and NVIDIA Inc.
Thomas Gibbs, NVIDIA Inc.
Nicholas Chia, Mayo Clinic
Azton Wells, Argonne National Laboratory
Maulik Shukla, Argonne National Laboratory
Logan Ward, Argonne National Laboratory
Venkatram Vishwanath, Argonne National Laboratory

Scientific Discipline: Biological Sciences

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): HPE Apollo 6500 (50,000 Polaris node-hours)
Site: Argonne National Laboratory
Machine (Allocation): HPE Cray EX - Intel Exascale Compute Blade Nodes (270,000 Aurora node-hours)

Research Summary: The potential for extant and emerging pathogens to become global health crises necessitates the development of novel methods for proactively engaging these threats before they become pandemic. Recent advances in machine learning and artificial intelligence—specifically, large language models (LLMs)—provide powerful tools for predictive modeling and monitoring of pathogens of concern. The team's prior work developing Genome-scale Language Models (GenSLMs) demonstrated the potential for LLMs to predict future SARS-CoV-2 variants of concern prior to their emergence by modeling the evolutionary process. In this project the team builds on that work by scaling GenSLMs beyond the (relatively) simple SARS-CoV-2 to multi-segmented viruses and comparatively enormous bacterial genomes, and even further to more complex eukaryotic organisms including yeast and humans.

This project will thus increase biopreparedness by providing a continuous watchlist of pandemic-potential variants across several different pathogens; and will additionally benefit the community by making GenSLM models, data, and code available to a broad user base, who can fine-tune our foundation models for their own downstream predictive tasks.

Type: New
Title: "Frontier Universe: Astrophysics and Cosmology from Reionization to Cosmic Noon"

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/FermiLab
Reuben Budiardja, Oak Ridge National Laboratory
Damon McDougall, Advanced Micro Devices
Bruno Villasenor, Advanced Micro Devices

Scientific Discipline: Physics

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

Research Summary: The advent of exascale computing with Frontier coincides with the arrival of an unparalleled cosmological experiment in the Dark Energy Survey Instrument and the most powerful observatory ever flown in James Webb Space Telescope. For the first time, the scientific synergy of these facilities will enable researchers to answer the question: How does the combination of cosmology and astrophysics connect the formation of galaxies, the reionization of cosmic hydrogen, and the growth of large-scale structure over the first three billion years of cosmic history? The proposed set of simulations dubbed the "Frontier Universe" will answer this question by using the GPU-native, MPI-parallelized code Cholla to simulate a statistical volume of the universe almost 2 billion light-years across with spatially constant resolution sufficient to capture all the relevant physics to follow inhomogeneous cosmic reionization and model the observational signatures of large-scale structure via absorption line signatures of intergalactic hydrogen gas (the "Lyman-αForest"). The combination of volume, resolution, and physics will allow us to compare directly with both DESI observations of the Lyman-αForest and JWST observations of reionization, anchoring the team's theoretical calculations with experiments spanning billions of years of cosmic time. The Frontier Universe simulations will therefore be the first ever to simultaneously capture how the topology of reionization in the first billion years of cosmic history relates to the structure of the intergalactic medium (IGM) several billion years later. With the combined power of Frontier and Cholla, the Frontier Universe will include dozens of such simulations and will become the largest ever cosmological simulation suite by orders of magnitude. Only Frontier could possibly conduct this scientific program. This award will continue the team's efforts to leverage leadership class computational facilities at the interface of cosmology and astrophysics, which have been demonstrated to be successful and have led to a variety of refereed publications acknowledging INCITE. The team has multiple complementary grants from NASA to conduct this important work, with funding continuing over the duration of their proposed INCITE program.

Type: New
Title: "Global Adjoint Tomography"

Principal Investigator: Jeroen Tromp, Princeton University
Co-Investigators: Daniel Peter, KAUST

Scientific Discipline: Earth Science

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (450,000 Frontier node-hours)

Research Summary: The primary objective of seismic Full Waveform Inversion (FWI) is to achieve a precise match between simulated and observed seismograms. This is accomplished through an iterative process that involves constructing a model of the Earth's interior based on the principles of seismic wave propagation. By leveraging modern numerical methods and high-performance computers, FWI has made significant advancements over the past decade. FWI enables the computation of Fréchet derivatives of a predefined misfit function with respect to a selected set of model parameters. This is achieved by convolving a "forward" wavefield, generated by aseismic source, with a fictitious "adjoint" wavefield that incorporates time-reversed measurements of differences between observed and simulated seismograms at all receivers. By leveraging these derivatives, FWI aims to utilize every detail in a seismogram to gain insights into Earth's dynamics, including the nature of hotspots, the forces driving plate motions, and the occurrence of earthquakes. Detailed maps of Earth's interior are also crucial for accurate hydrocarbon localization, seismic hazard assessment in earthquake-prone regions, and nuclear explosion detection.

Thanks to previous allocations from the INCITE program, we have achieved significant milestones. Furthermore, the team's recent INCITE allocation has significantly reduced the computational cost of seismic tomography by implementing cross-talk-free source encoding. Traditionally, earthquake tomography scales linearly with the number of seismic sources. However, with source encoding, a single "super source" is employed, which is subsequently disentangled after simulation to update the model. Consequently, a significantly higher number of model iterations can be performed, leading to convergence toward a final model.

This INCITE projects seeks to pioneer the next-generation global source inversions by utilizing a comprehensive 3D global Green function database. Secondly, the team aims to conduct high-iteration global tomography using source encoding, thereby maximizing the convergence potential of the inversion process. Lastly, the team aims to integrate both source and structural inversions to achieve a more comprehensive understanding of Earth's subsurface.

Type: New
Title: "Heterogeneous Catalysis as a Collective Phenomenon within a Dynamic Ensemble of Sites"

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

Scientific Discipline: Chemistry

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): HPE Apollo 6500 (250,000 Polaris node-hours)

Research Summary: Chemical production is the single largest consumer of energy in U.S. manufacturing. The development of more efficient catalysts has the potential to reduce the energy use of many chemical production processes. While theory in catalysis remains more descriptive than predictive, scientists have recently shown that theory becomes more predictive if we change the paradigm of how heterogeneous catalysis is described. 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, that can be largely driven by highly active metastable states rather than the ground state.

With this INCITE project, the team will address the nature of the catalytic interface in reaction conditions, attainable swarms of mechanistic pathways, and routes of deactivation. They will make predictions toward improved activities, selectivity, and stabilities and test them experimentally. To carry out their computational work, the team 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 use primarily density functional theory (DFT) within VASP. In electrocatalysis, the electrolyte and electrochemical potential will be included. The team will develop and employ machine learning tools to replace costly DFT calculations wherever possible, using the large amount of data generated by this research.

Ultimately, the team will develop fundamental theory of heterogeneous thermal and electrocatalysis, and a realistic statistical and dynamical description of the catalytic interface in reaction conditions. This will enable the understanding of catalytic mechanisms, and the design of new efficient catalysts.

Type: New
Title: "Hadron physics from first principles"

Principal Investigator: Kostas Orginos, William & Mary
Co-Investigators: Robert Edwards, Jefferson Lab
David Richards, Jefferson Lab
Christopher Monahan, William & Mary
Balint Joo, Oak Ridge National Laboratory
Anatoly Radyushkin, Old Dominion University
Jianwei Qiu, Jefferson Lab
Frank Winter, Jefferson Lab
Savvas Zafeiropoulos, Centre National de la Recherche Scientifique
Eloy Romero, Jefferson Lab
Herve Dutrieux , William & Mary
Joseph Karpie, Jefferson Lab

Scientific Discipline: Physics

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

Research Summary: The research team will use Frontier to compute the structure of strongly-coupled hadronic states directly from quantum chromodynamics (QCD). These calculations will provide essential theoretical support to the experimental program of the Thomas Jefferson National Accelerator Facility (Jefferson Lab) and to the future Electron Ion Collider (EIC) at Brookhaven National Laboratory. The team will generate resources of direct benefit to others working in the computational nuclear physics community that will broaden the impact of this proposal, from complementary aspects of proton structure to form factors relevant to upcoming long-baseline neutrino science at Fermilab and the Deep Underground Neutrino Experiment.

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

Type: New
Title: "Heterogeneous Reaction Dynamics for Energy Storage and Hydrogen Production"

Principal Investigator: Boris Kozinsky, Harvard University

Scientific Discipline: Materials Science

INCITE Allocation:

Site:	Argonne National Laboratory
Machine (Allocation):	HPE Apollo 6500 (100,000 Polaris node-hours)
Site:	Argonne National Laboratory
Machine (Allocation):	HPE Cray EX - Intel Exascale Compute Blade Nodes (50,000 Aurora node-hours)
Site:	Oak Ridge National Laboratory
Machine (Allocation):	HPE-Cray EX (300,000 Frontier node-hours)

Research Summary: Heterogeneous catalysis is central to the production of hydrogen and more generally, catalytic production of chemicals consumes 30% of global energy used in manufacturing. Li-ion battery systems are becoming primary systems for storing energy in stationary and transportation applications. Optimizing the performance and durability, while reducing overall cost, is therefore key to advancing these technologies for sustainable energy infrastructure. Microscopic chemical and mechanical processes that critically determine performance and degradation of batteries and catalysts occur at interfaces and are poorly understood due to the inability of experimental characterization to probe surface and interface phenomena at atomistic resolution. Molecular dynamics (MD) simulations can enable faster and more detailed mechanistic insights, but have been until recently limited by the accuracy-cost tradeoff — ab initio methods are accurate but expensive, while empirical classical force-fields are fast but inaccurate. To break through this tradeoff, the team will deploy the team's new state-of-the-art machine learning (ML) methods to construct reliable and accurate force fields, trained on accurate quantum electronic structure (DFT) calculations and perform record-scale and -speed MD simulations of battery and catalytic interfaces. The team proposes to generate previously inaccessible atomistic understanding of interfacial reactions on two fronts: (1) solid-state electrolytes reacting with electrodes, and (2) reactive atmospheres over heterogeneous catalysts, both at experimentally relevant time- and length-scales. These efforts will yield critical information regarding processes like battery degradation and transport at interfaces, and active-site selectively and stability for hydrogen production.

Type: New
Title: "Heteropolymer Design Harnessing New and Emerging Computing Technologies"

Principal Investigator: Vikram Mulligan, Flatiron Institute
Co-Investigators: Douglas Renfrew, Flatiron Institute
Hans Melo, Menten AI
Yuri Alexeev, Argonne National Laboratory

Scientific Discipline: Chemistry

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): HPE Cray EX - Intel Exascale Compute Blade Nodes (375,000 Aurora node-hours)

Research Summary: Advances in computational protein design have enabled researchers to design exotic heteropolymers that can be built from thousands of synthetic building blocks beyond the 20 canonical amino acids from which natural proteins are built. This has opened up new possibilities for designing lifesaving drugs tailored to perfectly recognize their targets, exotic nanomaterials with structure crafted at the level of the atom, and enzymes able to catalyze industrially useful chemical reactions for greener manufacturing. However, certain challenges remain, the biggest being computational tractability: heteropolymer design involves NP-hard optimization problems that are solved during the computational design phase and again during the computational validation phase.

With this INCITE project, researchers aim to improve classical computational methods for heteropolymer design and validation to better harness modern computing hardware. This will make more challenging, higher-complexity design problems tractable, and will permit exploration of new, higher-cost approaches that could improve accuracy and generality. The team will leverage DOE supercomputers to test and apply their new software at scale, and to explore new algorithms that become conceivable when certain tractability limits are surpassed. Mindful that classical computers will always have their limits with NP-hard problems, the team will adapt these methods to take advantage of quantum computing hardware for the most poorly scaling optimization steps in their pipeline. Since the quantum computers that can help solve these problems have not yet been built, DOE supercomputers will allow the team to simulate quantum algorithms on classical hardware to determine feasibility of the approach, scaling as problems grow large, and the impact of noise of the sort that one encounters on real quantum hardware. Finally, the researchers will apply these methods to difficult problems in drug and enzyme scaffold design, using supercomputers to design and validate exotic molecules, which will subsequently be synthesized and characterized in the wet lab. Ultimately, their research will provide industry and academic users with powerful new tools for producing useful, functional new molecules that are currently beyond the reach of present-day design approaches.

Type: New
Title: "High Impact Nucleon Matrix Elements Affected by Nπ Excited States"

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

Scientific Discipline: Physics

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

Research Summary: The standard model of elementary particles, including the most recent understanding of neutrino masses and mixing, is extremely successful in describing all phenomena up to the TeV scale at the Large Hadron Collider, or LHC, in Geneva.

Nevertheless, new and unknown physics is required to explain three profound mysteries: observed matter-antimatter asymmetry of the universe, dark matter, and dark energy.

The goal of this project is to obtain high precision results for inputs needed in three different searches for physics beyond the standard model. These inputs touch on direct-detection experiments searching for dark matter and mechanisms that explain matter-antimatter asymmetry in the observed universe.

The proposed calculations for this project much optimize Frontier computing power to effectively hit the improved parameters and boundaries previous experiments have developed using INCITE. Previous calculations have been too small to explain the complete absence of antimatter in the universe.

The desired results will increase the reach of experiments searching for novel changes in the neutrino sector and continue solving the mysteries of dark matter and dark energy.

Type: New
Title: "High Reynolds Number Hypersonic Transition Control via Porous Walls"

Principal Investigator: Carlo Scalo, Purdue University
Co-Investigator: Matteo Ruggeri, Purdue University

Scientific Discipline: Engineering

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

Research Summary: This INCITE project seeks to create a direct numerical simulation (DNS) dataset capturing all the relevant processes involved in hypersonic boundary layer transition (including free-stream noise, receptivity, modal growth, and turbulent breakdown) in support of a recent experimental test campaign carried out at the Air Force Research Labs demonstrating passive transition control with the use of porous walls.

Simulations will be carried out using a high-scalable block-spectral code at Reynolds numbers of up to 22.9×10^6, which is prohibitively expensive for typical high-performance computing systems.

The resulting dataset will lead to a deeper understanding of the onset of second-mode waves on a flat plate (as opposed to conical geometries, which are more commonly studied) and their acoustic suppression via wall porosity under realistic flow conditions. This has strong implications for hypersonic vehicle design and thermal management specifically. Lower-order models, including wall-resolved large eddy simulations (LES), are not reliable at these extreme flow conditions, warranting the use of large-scale DNS approaches. The work relies on years of experience in developing techniques for acoustic-based passive control of external and internal flows for hypersonic applications.

The dataset created by this project will support the development of data-driven turbulence models, such as graph-neural-network-based machine learning algorithms to extract sub-filter-scale (LES) or total (Reynolds-averaged Navier-Stokes) turbulent stresses.

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

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

Scientific Discipline: Physics

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

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

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

Type: New
Title: "Hole, Electron and Exciton Transport in Organic Conductors by Non-orthogonal Configuration Interaction"

Principal Investigator: Coen de Graaf, Universitat Rovira i Virgili
Co-Investigators: Tjerk P. Straatsma, Oak Ridge National Laboratory
Carmen Sousa, University of Barcelona
Xavi Lopez, Universitat Rovira I Virgili
Ria Broer, University of Groningen
Jordi Ribas, University of Barcelona
Merce Deumal, University of Barcelona

Scientific Discipline: Chemistry

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

Research Summary: The replacement of traditional fossil fuels with alternative renewable energy sources is of fundamental importance to reduce the emission of carbon into the atmosphere. Carbon capture and its storage or conversation into other products is equally important.

Increasing the efficiency of sunlight conversion into electrical current or its storage into high-energy compounds are two ways to reduce societal dependency on fossil hydrocarbons. Silicon-based solar cells and perovskite solar cells have both been used efficiently in energy production at low cost, but both still suffer from shortcomings, mostly stability-wise.

This project studies the hole and electron mobility in transport layers of organic and perovskite cells. The code for this project is ready to explore these layers from a different perspective than conventional theory, using the computational power of Frontier.

The results will likely help advance design rules for materials with improved energy transfers, a step toward significant reduction of carbon emissions.

Type: New
Title: "Horizon-scale Variability Modeling for the EHT"

Principal Investigator: Benjamin Prather, Los Alamos National Laboratory
Co-Investigators: Charles Gammie, University of Illinois
Vedant Dhruv, University of Illinois

Scientific Discipline: Physics

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

Research Summary: The Event Horizon Telescope (EHT) collaboration recently published the first resolved images of the black holes M87* and Sgr A*, and observations are ongoing to produce further images, and potentially videos, of these sources. One of the most fruitful methods of understanding the EHT's results is by simulating the accreting plasma using general relativistic magnetohydrodynamics (GRMHD). Existing simulations accurately reproduce the observed image morphology and polarization, lending insight into the black hole's spin, as well as the magnetization (and soon tilt) of the accretion disk. However, current-generation simulations do not accurately capture the observed brightness variability of SgrA*, predicting it to be much more variable than is observed – as a result, no model matches all the available observations of this object. This project aims to understand and potentially resolve the discrepancy, using state-of-the-art models of SgrA*, run at high resolution and including the non-ideal fluid effects likely present in a collisionless plasma. It will produce the highest-resolution libraries to date of ideal and non-ideal GRMHD simulations, which will be useful not only to understand variability, but to better understand EHT observations for years to come.

Type: New
Title: "Improving radiation therapy treatment planning using deep learning"

Principal Investigator: Thibault Marin, Massachusetts General Hospital
Co-Investigators: Georges El Fakhri, Massachusetts General Hospital

Scientific Discipline: Biological Sciences

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

Research Summary: While radiation therapy (RT) is one of the main local treatment modalities for most solid tumors asneoadjuvant, adjuvant or definitive therapy, achieving consistently good treatment outcomes for patients with highly infiltrative tumors or for inoperable patients remains challenging. This challenge is in part due to inadequacy of current imaging to guide a physiologic definition of RT target volumes.

This team aims to study the role of functional, multi-modality cancer imaging in improving personalized RT target definition andtherefore efficacy of RT, using sarcoma as a model disease for proof of concept. Conventionally, the RT target volumes are defined by the visible extent of gross tumor volume (GTV)and expansion by standardmargins to define the clinical target volume (CTV) based on potential subclinical microscopic spread, localinvasive capacity of the tumor and imaging-pathology correlation. Standard imaging does not adequately visualize microscopic extension. Therefore, CTV is presently defined byguidelines and clinical judgment, yielding significant inter-physician variability in many tumor sites, especially sarcomas

With this project, the team proposes to develop deep learning methods to assist radiologists and radiation oncologists in the contouring of tumor volume for treatment planning.This project can significantly improve radiation therapy practice, by reducing variability in treatment planning and enabling faster contouring for physicians, thanks to assisted delineation.

Type: New
Title: "Interface-Resolved Simulations of Scalar Transport in Turbulent Bubbly Flows"

Principal Investigator: Parisa Mirbod, University of Illinois at Chicago
Co-Investigators: Luca Brandt, KTH Royal Institute of Technology
Nicolò Scapin, Princeton University

Scientific Discipline: Engineering

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): HPE Apollo 6500 (50,000 Polaris node-hours)

Research Summary: Despite the wide range of applications involving bubbly flows, there is a lack of quantitative understanding regarding fluxes and mixing in turbulent flows. This understanding is crucial for accurate predictions and advancements in engineering systems/devices. This INCITE project aims to address this gap by conducting direct numerical simulations (DNS) to study and quantify turbulence kinetic energy and diffusive scalar fields in gravity-driven turbulent bubbly suspensions.

In various natural and practical applications, bubbly flows are integral to processes involving heat and mass transfer, as well as chemical reactions. However, a detailed quantitative comprehension of fluxes and mixing in these turbulent flows is essential for accurate predictions and technological progress in engineering. Thus, a key objective of this INCITE project is to employ fully-resolved direct numerical simulations (DNS) to investigate and measure the transport mechanisms of turbulence kinetic energy and a diffusive scalar field in gravity-driven turbulent bubbly suspensions.

This entails resolving all pertinent scales, including the bubble diameter, as well as the Kolmogorov and Bachelor scales, which correspond to the smallest vortices and scalar filaments in the flow, respectively. The team aims to facilitate high-performance computing (HPC) interface-resolved DNS of bubbly turbulent flows with passive scalars, focusing on scenarios with realistically low values of diffusivities.

This INCITE project outlines a systematic approach to uncover new theories and computational models for the dynamics of passive scalars in turbulence induced by bubbles. These complex interactions will be scrutinized through fully-resolved simulations. Unlike laboratory experiments, numerical studies allow for the isolation of specific physical processes. To minimize variations in bubble deformation resulting from changes in the Galilei number, the team will conduct simulations with varying surface tension. Consequently, if the bubble size increases (Galilei number), the surface tension will also increase, thereby maintaining a roughly consistent bubble deformation.

Type: New
Title: "Large-scale Multiphysics Simulations for Optimized Design of Fusion Devices"

Principal Investigator: Arpan Sircar, Oak Ridge National Laboratory
Co-Investigators: Vittorio Badalassi, Oak Ridge National Laboratory
Katarzyna Borowiec, Oak Ridge National Laboratory
Jin Whan Bae, Oak Ridge National Laboratory

Scientific Discipline: Engineering

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (500,000 Frontier node-hours)

Research Summary: The development of fusion power devices has been recently accelerating due to key breakthroughs in several technologies, such as high temperatures superconducting magnets, successes of advanced fusion machines such as Jet and W7X, and a refined understanding of plasma physics. However, key challenges remain on the path to a fusion pilot plant (FPP), even for the well-studied tokamak concept. The operating conditions of FPP are extremely challenging, and a robust first wall and blanket system is essential to withstand high heat and particle fluxes under irradiation conditions and to guarantee enough tritium breeding. Balance must be kept between irradiation resistance, temperature limits, and influence on the tritium breeding ratio. This balance is further influenced by magnetohydrodynamics (MHD) effects on the fluid flowing in the blanket experiencing powerful magnetic fields (up to 20 Tesla) in the latest compact designs, such as the ARC-class devices from Commonwealth Fusion Systems. There is clearly a need to optimize intrinsically multiphysics problems to achieve an optimal design. Further, the new technology advancements in fusion with 20 Tesla magnets present unexplored MHD regimes, which must be studied with fully resolved numerical simulations. The team proposes implementing and enhancing the software FERMI (Fusion Energy Reactor Models Integrator) developed by the authors and collaborators to develop new MHD models for high-field compact tokamaks and perform the first accurate, high-fidelity simulations of fusion reactor blankets and their optimization in Frontier. The open-source computational fluid dynamics (CFD) tool, OpenFOAM (included in the FERMI suite), will be used here to investigate the effects of MHD using large eddy simulations (LES). The GPU capability and scalability of OpenFOAM have been demonstrated on Summit, and a clear pathway is defined to port that capability onto the Frontier architecture. The team will use scale-resolved computations, which could not be carried out before on other computing architectures due to the lack of resources, to understand the fundamental effects of MHD on engineering parameters such as pressure drop and heat transfer. Then they will proceed to multiphysics simulations using conjugate heat transfer (CHT) and conjugate electromagnetics (CEM) analysis using the unique capabilities of FERMI in coupling CHT + CEM analysis with interfacing to fusion neutronics capability. An improved fundamental MHD understanding coupled with tight multiphysics simulations will then be used to optimize the designs of tokamak fusion devices.

Type: New
Title: "Learning Common Sense Reasoning through Large Scale Video Generation"

Principal Investigator: Pieter Abbeel, University of California, Berkeley

Scientific Discipline: Computer Science

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

Research Summary: Over the past year, the field of generative AI has witnessed remarkable advancements through the scaling of large models in various domains, including visual understanding. Although these models have demonstrated impressive capabilities in reasoning and understanding, they still lack common sense. This aspect of intelligence is necessary to build a fundamental grounding in the world.

Videos, on the other hand, provide a wealth of information surrounding human behavior, 3D structures, and entity interactions. This project seeks to harness the richness of videos, hypothesizing that large-scale neural networks capable of generating high-quality videos can develop a central understanding of common sense. Video data is available in abundance on the internet, on which to effectively process and train these models.

The project aims to train and study large-scale video generation models to aid AI systems in developing this common sense. The desired result will be a video model that can extend its accumulated knowledge of the world to ground language models in more accurate reasoning and content creation. The project will also investigate the video generation capabilities of these models at varying sizes and how those relate to robotics.

Training large-scale video models requires a large, state-of-the-art computational cluster, making the Frontier allocation an imperative part of this research. Previous experiments have demonstrated that these video generation models can scale to the parameters needed to achieve these goals.

Type: Renewal
Title: "Lipid Shuttling Molecular Machines Enabling Functions of Human Cell Membranes"

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

Scientific Discipline: Biological Sciences

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

Research Summary: Through this project, the team will continue addressing the grand challenge in biomedicine and biophysics that focuses on the fundamental biological cell processes of establishing and maintaining the relevant properties and compositions of its membranes in the changing environment produced by its physiological function. The team has been leveraging the recognition that for the molecular machines involved in these vital tasks the membrane lipids are both the medium in which their activity is enabled, and the substrate that is being acted on to establish, restore and maintain the composition. They will use computation to learn how specific proteins in the membranes of the team's cells work to maintain the properties needed for life and health. Understanding how they function will enable repair in disease, and the engineering of proteins with new functional applications.

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

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

Type: New
Title: "LSDalton Discovers New Organic Photovoltaic Devices"

Principal Investigator: Kurt V. Mikkelsen, University of Copenhagen

Scientific Discipline: Chemistry

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

Research Summary: Organic photovoltaics (OPV) have significant advantages over inorganic photovoltaics by being lightweight, low-cost, flexible and free from heavy metals. This advantage places OPV as a very attractive PV technology in the years to come. The purpose of this project is to develop stable and efficient OPV devices. The researchers will focus their attention on boron subphthalocyanines that can act as light harvesters, electron donors or acceptors needed to obtain accurate molecular properties for selecting the optimal systems. The project combines theoretical modeling and substantial computational efforts for obtaining tools and database to design new and efficient OPV.

Electronic structure calculations of a wide range of molecular properties are today an integrated part of many branches of molecular sciences. The coupled–cluster (CC) model is the state–of–the–art wave function method, and, for small molecular systems, various molecular properties have been computed to an accuracy challenging experimental results. However, the application range of CC methods has so far been limited to small molecular systems due to their computational scaling with system size. For this reason, density functional theory (DFT) has developed into a work horse for large–scale applications. The major drawback of DFT calculations is that they generally do not possess the accuracy and the predictive power of the CC methods. The objective of the proposed project is to extend the application range of accurate modeling techniques in chemistry and molecular sciences by making the CC methods applicable to large molecular systems and ready-to-use on the supercomputers of tomorrow.

Type: New
Title: "Mechanisms of β-arrestin Activation"

Principal Investigator: Lei Shi, National Institutes of Health
Co-Investigators: Van Ngo, Oak Ridge National Laboratory
Jonathan Javitch, Columbia University
Robert Lefkowitz, Duke University Medical Center

Scientific Discipline: Biological Sciences

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

Research Summary: β-arrestins (βarr) regulate the signaling and trafficking of G protein-coupled receptors (GPCRs). They also play key roles as multifunctional scaffold proteins and signal transducers and are implicated in numerous diseases and disorders. Although much progress has been made in understanding the functional roles of βarr, structural and kinetic insights into the mechanism by which ligand-mediated GPCR activation enables βarr coupling and activation are just emerging. βarr's C-terminal tail (βarr tail), which binds clathrin and adaptin to mediate receptor endocytosis, and is also directly involved in scaffolding signaling kinases, is released by the C-tail of a GPCR, phosphorylated on multiple sites (Rp tail). Understanding the timing and mechanism of this release process and its relationship to receptor engagement and other structural rearrangements within βarr will facilitate deeper insight into βarr-mediated signaling pathways and potential therapeutic targets.

The team will use temperature replica-exchange molecular dynamics (TREMD) simulations to study the mechanism of βarr1. TREMD overcomes the multiple-minima problem by exchanging non-interacting replicas of the system at various temperatures, allowing efficient sampling of the probability distributions of a canonical ensemble for a wide temperature range. Models of βarr1 with its unwound C-tail (predicted from Rosetta) with/without the Rp tail are solvated with explicit waters, resulting in large systems with ~ 278,000 atoms each. The team will use NAMD for TREMD since NAMD has been shown to scale reasonably well over a large number of GPU nodes and has been tested on Frontier. To properly sample such large systems, a substantial number of replicas must be used to enable proper exchange rates among replicas so that sampling convergence can be achieved within reasonable runtimes. The team's preliminary TREMD runs indicated 200 replicas are necessary to achieve adequate acceptance ratio of about 40% per sampling time so that a significant sampling speed-up can be obtained. This scale of simulations is far beyond the capability of local high-performance computing clusters, such as those at NIH, Columbia University, or Duke University, and requires the leadership computation capability provided by INCITE (Frontier) to obtain reasonable convergence of sampling data.

Type: New
Title: "Nonequilibrium Chemical Order in High-Entropy Alloys"

Principal Investigator: Rodrigo Freitas, Massachusetts Institute of Technology

Scientific Discipline: Materials Science

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (350,000 Frontier node-hours)

Research Summary: Excessive trial-and-error currently dominates the manufacturing and processing of a new class of promising metallic alloys. This occurs because simulations have historically been performed under assumptions that limit their relevance in the practicalities of the industry.

A distinctive feature of high-entropy alloys, a metallic chemical mixture with at least five elements, is their chemical disorder. This exists because high-entropy alloys form solid solutions in which chemical elements are spread out randomly. Solid solutions are further affected by chemical short-range order, or SRO, which changes the alloy's energy and composition.

This project builds on recent developments toward a predictive approach to investigate SRO at appropriate length and time scales. One of the outcomes was the development of a learning machine that can quantitatively reduce the SRO in electronic structure calculations. The objective is to uncover the underpinning science of nonequilibrium chemical SRO in solid solutions. Opening the door to this connection requires rigorous performance brought by exascale systems.

This project will eliminate many assumptions that exist in the production of metallic alloys and create a more cost-effective and sustainable manufacturing process.

Type: New
Title: "Novel Calculation of Nucleon Generalized Form Factors in Lattice QCD at the Physical Point"

Principal Investigator: Martha Constantinou, Temple University
Co-Investigators: Constantia Alexandrou, University of Cyprus and The Cyprus Institute

Scientific Discipline: Physics

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): HPE Apollo 6500 (315,000 Polaris node-hours)

Research Summary: This project aims to evaluate key quantities so as to probe nucleon structure with unprecedented accuracy using lattice quantum chromodynamics. The work will enable a continuum extrapolation directly from the physical pion mass, thereby advancing the state-of-the-art. In particular, the continuum limit will be obtainable without the need to combine data with heavier-than-physical point simulations—thus avoiding a chiral extrapolation that introduces a systematic error difficult to quantify for for the baryon sector.

The researchers will employ their well-developed methodology to construct quark correlation functions yielding a broad set of quantities, primarily focusing on the generalized form factors up to three covariant derivatives and extracting up to the fourth Mellin moments. In addition to generalized form factors, nucleon form factors will be obtained without extra computational cost.

The project is fully aligned with a central milestone of nuclear physics—that is, to address important questions of how properties of the nucleon emerge directly from the dynamics of its constituents, recently reaffirmed by The National Academies of Sciences, Engineering, and Medicine.

Type: New
Title: "Nuclear and Hypernuclear Interactions from Lattice QCD"

Principal Investigator: Michael Wagman, FermiLab
Co-Investigators: Zohreh Davoudi, University of Maryland
William Detmold, Massachusetts Institute of Technology
Marc Illa, University of Washington
William Jay, Massachusetts Institute of Technology
Assumpta Parreno, University of Barcelona
Robert Perry, University of Barcelona
Phiala Shanahan, Massachusetts Institute of Technology

Scientific Discipline: Physics

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

Research Summary: Quantum Chromodynamics (QCD) is the underlying theory of the strong interaction, responsible for the binding of neutrons and protons to form atomic nuclei and, at a more fundamental level, for the binding of up and down light quarks to form nucleons. Extending our knowledge of nucleons and nuclei to systems containing strange quarks is difficult due to their short lifetimes, but is of vital importance for understanding a variety of nuclear and astrophysical processes. Only a few strange nuclei have been experimentally produced, while there is still no conclusive evidence for the existence of several long-predicted exotic states containing strange quarks, such as the *H*-dibaryon. Given the impossibility of obtaining analytical solutions for QCD in the low-energy regime, relevant for the study of such exotic states, we propose to calculate the interactions between baryons such as the proton and neutron and their more exotic strangeness-containing cousins (hyperons) using the numerical technique of lattice QCD (LQCD).

The Nuclear Physics from Lattice QCD (NPLQCD) collaboration, which supports this project, has led the development of lattice QCD for nuclear physics. The project director is less than 10 years post-PhD. Five other members of the project team are early career scientists, and two team members are current DOE Early Career award holders. This proposed work builds on the team's demonstrated progress towards lattice-QCD calculations of nuclei and on the long-term investment in lattice-QCD software and algorithms through the USQCD SciDAC and ECP software projects that have ensured readiness for Frontier.

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

Principal Investigator: Kenneth Jansen, University of Colorado Boulder
Co-Investigators: Jed Brown, University of Colorado Boulder
John Evans, University of Colorado Boulder
Alireza Doostan, University of Colorado Boulder
Stephen Becker, University of Colorado Boulder

Scientific Discipline: Engineering

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): HPE Cray EX - Intel Exascale Compute Blade Nodes (375,000 Aurora node-hours)

Research Summary: This project is motivated by the fact that the vertical tail of a commercial airplane is a significant contributor to the overall drag and fuel cost during cruise, and the sizing of this component is dictated by engine-out operations which require large surfaces to produce the necessary restoring force. A more effective system that uses flow control can utilize smaller surfaces, resulting in reduced drag and fuel cost during standard operations ($0.3B per year for large commercial airlines).

Building upon current and previous work leveraging DOE supercomputers, the team will use this INCITE project to advance the current state of the art for online data analytics and machine learning applied to large-scale computational fluid dynamics (CFD) simulations. They plan 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 new flow solver designed for GPUs with distributed and online data analytics and training algorithms, the team's research 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.

The team's work aims to extend neural net sub-grid stress (SGS) models for large eddy simulation (LES) beyond canonical turbulent flows. By continuing their prior flat plate direct numerical simulation (DNS) within a new GPU-based solver coupled with online learning of wall-bounded flows with increasing complexity and scale, the researchers can provide training data for SGS closures that is currently unavailable to the community. Using the DNS of a boundary layer over flat plate, they will develop an SGS neural net model capable of accurately predicting flows of increasing complexity. Finally, to evaluate the trained SGS model on a previously unseen flow, they will perform LES of the turbulent boundary layer over an airfoil with flow separation and a second LES of a vertical tail/rudder assembly. This is a particularly relevant flow case for the aerospace and renewable energy industries, therefore making a predictive closure extremely valuable.

Type: New
Title: "OpenFold-Powered Machine Learning of Protein-Protein Interactions and Complexes"

Principal Investigator: Mohammed AlQuraishi, Columbia University
Co-Investigator: Zhao Zhang, Texas Advanced Computing Center

Scientific Discipline: Biological Sciences

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

Research Summary: Protein-protein interactions (PPIs) underpin most biological processes. Despite the major role they play in disease, most PPIs in humans are not well understood. Biophysically, PPIs can be classified as idiosyncratic (driven by binding surfaces unique to individual proteins) or as canonical (driven by surfaces reused by members of homologous protein families to bind peptides on partner proteins). Idiosyncratic PPIs are often high-affinity and form stable complexes while canonical PPIs are often transient, low-affinity, and vary minutely across domains to drive signaling logic. While both PPIs are studied by high-throughput experimental methods, the cost, complexity, and insensitivity of these methods, and the enormity of PPI space, have resulted in <20% coverage of the human interactome and sparse coverage of most other species.

To advance our understanding of PPIs, this INCITE project will use artificial intelligence (AI) to develop tools that predict interactions between any two proteins and make these tools widely available to the biology community. The research team will use DOE supercomputers to build computational methods for identifying novel idiosyncratic and canonical PPIs by combining multiple tiers of direct and indirect binding data with supervised and unsupervised machine learning models that account for varying degrees of experimental evidence. To conduct this research, the team developed OpenFold, a trainable implementation of AlphaFold2 (an AI tool used for predicting protein structures).

The researchers will tackle PPI prediction by building three types of models: (1) a supervised model for predicting idiosyncratic PPIs; (2) a supervised model for predicting canonical peptide-mediated PPIs; and (3) an unsupervised model for predicting canonical peptide-mediated PPIs. The team has produced preliminary results for all three models that support their validity. Their idiosyncratic PPI model aims to help identify novel protein complexes and human/human pathogen PPIs for drug targeting. Similarly, their canonical PPI models are designed to help unravel signaling networks and their dysregulation in disease by modeling the effects of mutations on PPIs. The proposed models thus have the potential to be as transformative to protein interactomes as AlphaFold2 has been to protein structure.

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

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

Co-Investigators:
Jochen Autschbach, University at Buffalo, SUNY
Anastasia Borschevsky, University of Groningen
Miroslav Ilias, Matej Bel University
Hans Jorgen Aagaard Jensen, University of Southern Denmark
Kirk Peterson, Washington State University
Michal Repisky, University of Tromsø/The Arctic University of Norway
Trond Saue, Université Toulouse III-Paul Sabatier
Stefan Knecht, ETH Zürich
Ayaki Sunaga, Kyoto University
Valerie Vallet, Centre National de la Recherche Scientifique
Johann Pototschnig, Université Toulouse III-Paul Sabatier

Scientific Discipline: Chemistry

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

Research Summary: The goal of PRECISE is to study frontier aspects of the physics and chemistry of molecules containing heavy elements, started out in the 2020 INCITE project PRECISE. Accurate treatment of molecular energies and properties of these elements requires inclusion of both relativistic and electron correlation effects, and has only recently become feasible due to our realization of a relativistic coupled cluster implementation that has been designed specifically for massively parallel GPU-accelerated supercomputers. In this project the team focuses on applications relevant to catalysis by studying the behavior of clusters of noble metals, consider biological applications with models for the tungstoenzymes occurring in hyper-thermophilic archaea, and on cases where experiments are extremely difficult to perform, such as the superheavy elements which are now synthesized by mankind, often atom by atom. The unparalleled hardware capabilities of Summit and of Frontier are indispensable for achieving converged results that are of fundamental importance for obtaining quantitatively accurate data. The applications will set a new standard for accurate modeling of heavy elements and fill a large gap in the set of computational benchmark data for molecular systems. Filling this gap is essential in the development of density functionals that can specifically target heavy elements.

Type: New
Title: "The Progenitor-explosion Connection in Core-collapse Supernovae"

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

Scientific Discipline: Physics

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

Research Summary: Core-collapse supernovae, the explosive final moments of massive stars, are complex events yielding a bright and energetic explosion from the birth of a neutron star or black hole. The explosion creates and ejects many chemical elements, including the primary constituents of the Earth, thus dominating the production of elements from oxygen to iron throughout the universe.

This project aims to utilize the exascale era of computing, when the 3D simulations with sufficient physical detail necessary to understand these explosions and their byproducts are now possible. The simulations have two goals: understanding how these explosions depend on the interior structure of the star, and understanding how proto-neutron star wind develops after the onset of explosion. This phase makes critical contributions to how the explosion produces heavy elements.

Only by using Frontier to extend the simulations until the explosion matures will the study uncover detailed isotopic and elemental compositions of the material ejected by the supernova.

Type: New
Title: "QCD under Extreme Conditions"

Principal Investigator: Zoltan Fodor, Pennsylvania State University
Co-Investigators: Rene Bellwied, University of Houston
Claudia Ratti, University of Houston
Szabolcs Borsanyi, Wuppertal University
Ingo Tews, Los Alamos National Laboratory
Sandor Katz, Eotvos University
Volodymyr Vovchenko, University of Houston
Paolo Parotto, University of Turin

Scientific Discipline: Physics

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): HPE Cray EX - Intel Exascale Compute Blade Nodes (400,000 Aurora node-hours)

Research Summary: This work aims to advance knowledge of the phase diagram and equation of state of strong interactions, by means of first-principle simulations. The researchers' main goals are to locate the critical endpoint and explore the strongly interacting high-density regime relevant to neutron stars and their mergers—some of the main unsolved problems in the theory of strong interactions.

Ordinary hadronic matter undergoes a transition to a deconfined phase, quark-gluon plasma, at extremely high temperature or densities. In the universe, the reverse transition took place a few microseconds after the Big Bang: the basic building blocks of nature, the hadrons, were formed at this time. The Large Hadron Collider Heavy Ion program recreates this transition in the laboratory. Its DOE-funded detector upgrade will enable us to improve the precision in the data and thus search for new phenomena, such as experimental evidence for near criticality in the QCD transition. This project will compute experimental signatures to the onset of chiral critical behavior such as fluctuations of conserved charges.

A hydrodynamic description of the strongly interacting plasma requires the local equation of state at nonzero light and strange density. This project will compute it in the continuum limit with physical quark masses.

Brookhaven's Relativistic Heavy Ion Collider explores the same transition in a broad range of densities, searching for a critical point in the QCD phase diagram—a difficult task, since there are no first principles to predict its location; direct simulations at finite density have remained elusive because of a sign problem. Thanks to a recent algorithmic development, these simulations, run with physical quark masses, can overcome this barrier and scan the phase diagram for features such as the cross-over line and the critical end point.

Type: New
Title: "Radiation General Relativistic MHD Simulations of Accretion Disk Outbursts"

Principal Investigator: Matthew Liska, Harvard-Smithsonian Center for Astrophysics
Co-Investigators: Gibwa Musoke, University of Amsterdam
Oliver Porth, University of Amsterdam
Bart Ripperda, Princeton University

Scientific Discipline: Physics

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

Research Summary: A key feature of black holes, objects that have captured the interest of scientists and the public for decades, is their accretion disks. These disks are made of gas and dust and orbit black holes at extreme speeds. As these materials grow closer to the hole itself, they heat up and emit high-energy radiation, including gamma rays.

Understanding the radiative processes of black hole accretion disks provides valuable information about the physical processes occurring in the vicinity of the holes. This information can also be used to study a wide range of astrophysical phenomena, such as the evolution of galaxies.

This project will examine the impact of radiative processes that occur as the X-rays emitted by accretion disks change in shape and intensity. The exact physics of those changes, known as spectral state transitions, are not fully understood but are thought to involve complex interactions between the radiation, magnetic fields, and plasma in the accretion disk. The project will conduct the first radiative magnetohydrodynamics simulations of an accretion disk outburst.

To understand these extreme systems, it is necessary to perform high-resolution radiative simulations that account for effects from both general relativity and magnetic fields on the accretion flow. Only exascale systems, namely Frontier, have the computational power and memory to model the radiation-matter interaction of these disks. By running these simulations on Frontier, the team will gain insight into the fundamental physics driving the changes to black holes.

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

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

Scientific Discipline: Materials Science

INCITE Allocation:

Site:	Argonne National Laboratory
Machine (Allocation):	HPE Apollo 6500 (50,000 Polaris node-hours)
Site:	Argonne National Laboratory
Machine (Allocation):	HPE Cray EX - Intel Exascale Compute Blade Nodes (375,000 Aurora node-hours)
Site:	Oak Ridge National Laboratory
Machine (Allocation):	HPE-Cray EX (800,000 Frontier node-hours)

Research Summary: Accretion of plasma by black holes powers all of the most luminous objects in the universe, including x-ray binaries and active galactic nuclei. However, the inner regions of luminous accretion flows are dominated by radiation, and therefore modeling these sources requires solving the equations of general relativistic radiation magnetohydrodynamics (GR radiation MHD).

This project uses a new performance-portable version of the Athena++ astrophysical MHD code to perform the first calculations of radiation-dominated accretion on black holes using full transport methods and realistic opacities.

Unique aspects of the research include a new GR radiation MHD algorithm based on direct solution of the time-dependent radiation transfer equation, rather than approximate closure methods as have been used in the past. This method employs a novel geodesic mesh to resolve the radiation field over hundreds of angles in each computational grid cell. Moreover, as part of a NASA-funded Theory and Computational Network (TCAN), the researchers' methods are being extended to include frequency-dependent transport, as well as accurate models for frequency-dependent emissivities and opacities accounting for atomic transitions in photoionized astrophysical plasmas.

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

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

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

Scientific Discipline: Earth Science

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

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

Type: New
Title: "Resolving Cosmic Ray Transport by Pushing the Frontier of MHD Turbulence"

Principal Investigator: Drummond Fielding, Cornell University
Co-Investigators: Philipp Kempski, Princeton University
Eliot Quataert, Princeton University
Philipp Grete, Hamburg Observatory
Alexander Philippov, University of Maryland, College Park
Matthew Kunz, Princeton University
James Stone, Institute for Advanced Study

Scientific Discipline: Physics

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): HPE Cray EX - Intel Exascale Compute Blade Nodes (200,000 Aurora node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (700,000 Frontier node-hours)

Research Summary: Cosmic rays (CRs) are high-energy charged particles that pervade the universe and play a crucial role in shaping galaxies and their surroundings. Although incredibly low in number, their combined energy density rivals the kinetic, thermal, and magnetic energy in galaxies, underscoring their significance. CRs are accelerated and injected into the interstellar medium, where they become confined by magnetic fields. This confinement regulates CR transport, determining CR escape from and feedback on astrophysical sources.

CR transport remains an open problem. The leading theories of how CRs scatter and propagate have significant theoretical uncertainties and inconsistencies with observations. This work aims to resolve the long-standing "CR transport problem" using pioneering exascale simulations that model, for the first time, the propagation of CRs over a broad range of energies through fully resolved patches of the turbulent magnetized interstellar medium.

These simulations will reveal the key physics of how CRs interact with and scatter magnetic fields, enabling us to develop a new predictive model for CR transport. The same calculations will provide fundamental new insights into the nature of magnetohydrodynamic (MHD) turbulence in astrophysical plasmas.

This research will transform our understanding of CR transport and feedback, MHD turbulence theory, and the regulation of star formation and black hole growth within galaxies, paving the way for a new generation of galaxy-formation simulations that incorporate self-consistent CR feedback and more realistic plasma physics.

Type: New
Title: "Resolving Stratified Turbulence at Large Prandt Numbers"

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

Scientific Discipline: Engineering

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

Research Summary: Stably stratified turbulence, or SST, is a model used to understand turbulent flows influenced by density stratification, resulting in highly intermittent behavior across multiple scales. Studying SST has important implications for multiple fields, including pollution mitigation and deep-sea mining. The range of dynamically relevant length scales is large, requiring leadership-class computing resources.

The project proposes to study turbulent flow in a stably-stratified fluid using massive-scale numerical simulations. The study will involve the 3D, time-dependent solution of the Navier-Stokes equation (fluid movement) with the non-hydrostatic Boussinesq approximation (horizontal distance between two points) at high resolution. At this time, the resolution needed is only available using Frontier.

The research objective is to develop an improved fundamental understanding of how the behavior of SST is affected by low density. One key area where this study's results may have significant impact is accurately representing the mixing of heat in the ocean, an outstanding area of uncertainty in global climate models.

Type: New
Title: "Scalable Deep Learning for Phonon Contribution in Non-Zero Temperature Alloys"

Principal Investigator: Massimiliano (Max) Lupo Pasini, Oak Ridge National Laboratory
Co-Investigators: Jong Youl Choi, Oak Ridge National Laboratory
Kshitij Mehta, Oak Ridge National Laboratory
Junqi Yin, Oak Ridge National Laboratory
Markus Eisenbach, Oak Ridge National Laboratory
Yongqiang Cheng, Oak Ridge National Laboratory

Scientific Discipline: Materials Science

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

Research Summary: Phonons are essential in atomic modeling as they provide a fundamental framework for understanding the vibrational properties, energy transport, structural stability, spectroscopy, and material behavior of solids in realistic physical conditions that go beyond the ideal, ordered, zero temperature ground state. Their study contributes to advancing our knowledge of materials and helps in the design and optimization of novel materials for various technological applications. To accurately capture the effect of the atomic disorder on temperature-dependent properties of the alloys, the number of atoms in the crystal must be sufficiently large (i.e., thousands of atoms). State-of-the-art density functional theory (DFT) methods are computationally expensive on large crystals with thousands of atoms, and their expensive computational cost precludes their utilization for a thorough understanding of phonons even on exascale US-DOE supercomputers. In this context, artificial intelligence (AI) is essential to reduce the computational complexity of the exploration of the high dimensional parameter spaces associated with first principle calculations.

To overcome this daunting computational barrier of exploring large chemical spaces for design of alloys with improved functional behaviors at non-zero temperatures, the team will develop scalable, accurate, and generalizable deep learning (DL) surrogate models to predict phonons' behavior as a function of the atomic arrangement and temperature. The trained surrogate model will enable an AI-accelerated design of refractory high-entropy alloys with desired properties and functionalities.

Type: New
Title: "State-of-the-Art High-Resolution 3D Simulations of Core-Collapse Supernovae"

Principal Investigator: Adam Burrows, Princeton
Co-Investigators: David Vartanyan, Carnegie Institution
Christopher White, Center for Computational Astrophysics
Matthew Coleman, Stevens Institute of Technology

Scientific Discipline: Physics

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): HPE Apollo 6500 (250,000 Polaris node-hours)
Site: Argonne National Laboratory
Machine (Allocation): HPE Cray EX - Intel Exascale Compute Blade Nodes (750,000 Aurora node-hours)

Research Summary: Core-collapse supernova explosions dramatically announce the death of massive stars; give birth to neutron stars and black holes; are the source of many of the elements of Nature; inject mass, energy, and momentum into the interstellar medium generate cosmic rays; and are one source of interstellar grains. They are central agents of change in the Universe and a core topic of theoretical astrophysics.

The overarching goal of this INCITE project is to create, analyze, publish, and curate a large suite of state-of-the-art long-term 3D core-collapse supernova explosion simulations that will constitute the standard 3D model of core-collapse supernova explosions for years to come. Most previous simulations were for short duration that did not allow one to witness the completion of the explosion. The codes were too slow and the computational resources too meager. But now, after more than sixty years of progress, we find ourselves at a pivotal time in the theory of core-collapse supernova when sophisticated 3D radiation/hydrodynamic codes, such as the team's code Fornax, and high-performance resources such as Aurora and Polaris are converging to enable many, long-duration, and high-resolution simulations of the explosion of the cores of a wide spectrum of massive stars.

This will be the culmination of a decades-long quest to understand the mechanism of explosion and the mapping between massive-star progenitors, their observational signatures, and their larger astronomical products and impact. All the simulations will be unprecedented, as will be their scientific impact, and they will be analyzed to derive the explosion energies, residual neutron star properties (e.g., mass, kicks, and spins), ejecta debris fields, nucleosynthesis, neutrino and gravitational-wave signatures, and physical and progenitor correlations and mappings.

Type: New
Title: "Study of Turbulence Intermittency Using Exascale Simulation and Machine Learning"

Principal Investigator: Pui Kuen Yeung, Georgia Institute of Technology
Co-Investigators: Katepalli Sreenivasan, New York University
Charles Meneveau, The Johns Hopkins University
Daniel Livescu, Los Alamos National Laboratory

Scientific Discipline: Engineering

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

Research Summary: Exascale computing resources on Frontier at OLCF will be deployed to advance fundamental under-standing in three-dimensional fluid flow, using a combination of state-of-the-art direct numerical simulation algorithms in combination with new and promising advances in physics-informed machine learning. The simulations will reach a word-leading resolution of 32768^3(3.5×10^{13}) using the suite of GESTS (GPU-enabled Extreme Scale Turbulence Simulations) codes developed by the PI's team through the CAAR pro-gram for Frontier. The code is in Fortran and is highly optimized specifically for the Frontier architecture, especially in its OpenMP offloading, memory management and communication protocols.

Turbulence is a complex system characterized by nonlinear interactions among a large number of degrees of freedom. The complexity increases even further in applications where the most important physics occurs in a reference frame moving with the disorderly fluid motion, or when knowledge of the mixing of material or properties transported by the flow is of critical interest. While computational resource requirements are daunting, a combination of advanced GPU computing and the viability of shorter simulation segments for the study of small-scale physics have created a new range of exciting opportunities.

The scale of the problem and close coordination among the project partners will also help push the next frontier for machine learning in the subject of turbulence. The science impact of this work will be further enhanced through public data sharing as part of a funded NSF project with very successful record in providing data access for the wider research community, including experimentalists.

Type: New
Title: "System level view at the disease with atomic resolution"

Principal Investigator: Dmytro (Dima) Kozakov, Stony Brook University
Co-Investigators: Julie Mitchell, Oak Ridge National Laboratory
Andrew Emili, Oregon Health and Science University
Pawel Polak, Stony Brook University
Matthew Torres, Georgia Institute of Technology

Scientific Discipline: Biological Sciences

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (700,000 Frontier node-hours)

Research Summary: The coming years promise major improvements in understanding the molecular mechanisms of disease and the development of therapeutics. This progress will be based on exponential increase in the amount of information on molecules in the cell using throutput techniques and the unprecedented availability of computing power. This presents an urgent need to enable the machine learning and physics-based molecular tools to take advantage of this large body of knowledge in computational biology.

This project aims to harness the computational power of Frontier to understand system-level implication of diseases using molecular modeling software tools. This goal will be reached by combining mass multi-omics data with high throughput deep learning pipelines to model macromolecular interactions in healthy and disease states, focused on proteins.

The project will employ a physics-aware machine learning pipeline to analyze data from disease datasets, including for Sars-COV2, Alzheimer disease, and cancers. The elements of this pipeline will be finetuned for multiple protein-based interactions. Training and running these protein complex models require the computational power of Frontier.

The research will give insight to the organization of various diseases. Resources for modeling these molecular interactions will be made available to the community.

Type: New
Title: "Toward In-Service Realism: DNS of Roughness Effects on Vital Turbine Film-Cooling"

Principal Investigator: Richard Sandberg, University of Melbourne
Co-Investigators: Melissa Kozul, University of Melbourne
Tom Jelly, University of Melbourne
Pawel Przytarski, University of Melbourne
Massimiliano Nardini, University of Melbourne
Aamir Shabbir, General Electric Aerospace
Sriram Shankaran, General Electric Aerospace
William Solomon, General Electric Aerospace
Paul Vitt, General Electric Aerospace
Greg Sluyter, General Electric Aerospace

Scientific Discipline: Engineering

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (700,000 Frontier node-hours)

Research Summary: The efficiency of a gas turbine (GT) can be raised by increasing the turbine inlet temperature (TiT). An increase of 100°F (56°C) in TiT can provide an increase of 2-4% in simple-cycle efficiency. A key enabler for higher TiT is turbine cooling. Modern turbine blades, in addition to internal cooling technologies, employ so called film cooling, where purposely shaped holes eject cooler fluid extracted from the compressor to generate a thin layer of coolant that protects the blade surface from the main path hot gas. Surface roughness, occurring either through additive manufacturing or in operation due to fouling/erosion can significantly alter film development and thus efficiency and component durability. Understanding and accurately predicting roughness effects on film cooling in GT flows is particularly challenging though, for two reasons. How realistic surface roughness interacts with and affects film in conjunction with those phenomena is far from understood and no sufficiently accurate models exist. For that reason, more coolant is typically extracted from the compressor than needed, reducing overall efficiency. Given that in 2019 in the USA alone GTs produced 38.4% of all power generated (1.58×109 MWh) and burned 18×109 barrels of jet fuel, this lack of knowledge has a tremendous impact on cost and emissions. Therefore, any engine performance improvements realized through better understanding and prediction of roughness effects on film cooling can have a fuel-spend advantage of order billion-$, together with a significant emission benefit, and would also increase the viability of costlier, more sustainably sourced fuels. Better predictions could also substantially increase operability and durability of GTs, as just a 2% error in metal temperature prediction can half the blade life.

Type: New
Title: "Tuning Assembly of Renewable Biocomposites for Additive Manufacturing"

Principal Investigator: Jeremy Smith, University of Tennessee
Co-Investigators: Micholas Smith, University of Tennessee
Monojoy Goswami, Oak Ridge National Laboratory
Arnold Tharrington, Oak Ridge National Laboratory
Shalini Jayaraman Rukmani, University of Tennessee/Oak Ridge National Laboratory

Scientific Discipline: Energy Technologies

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

Research Summary: Large-scale additive manufacturing (AM) is a promising and energy-efficient manufacturing technique for the future technologies in Energy Earthshot (EE) applications. Especially for custom and complex parts, composites are primary materials for the varieties of EE applications. These composites require tailored properties for optimal processing capabilities, superior materials characteristics and low cost. Current materials for large-scale AM are relatively expensive with ahigh carbon footprint and low recyclability. This motivates the investigation of alternative, renewable, sustainable low-energy materials large-scale AM. Among forest-based biomaterials, cellulose nanofiber (CNF)polymer composites have shown tremendous promise for high-performance AM material design. However, due to a lack of fundamental understanding of these biocomposites, questions remain concerning the directed nanoscale material modifications needed to optimize these materials for EE applications. A significant challenge facing the assembly of CNF biocomposites is that, to avoid irreversible agglomeration generated CNFs must currently be stored in highly dilute solutions and then dried for incorporation into composites.

The overarching goal of this project is to develop in-silico design principles of solvents for CNF dispersion by determining the structure, energetics and thermodynamics of CNF interactions in solution. Molecular dynamics (MD) simulations are capable of revealing determining the forces driving CNF assembly and dispersion at atomic detail. However, computational limitations have hitherto restricted atomistic MD to classical (unbiased) simulations of single CNFs. Here, using the scaling capability of Frontier at OLCF, the team will apply MD to obtain the first atomistic simulation models of CNFs interacting in solution. The result should be a clear understanding of the interplay between molecular interactions and the thermodynamic forces and kinetic pathways that drive CNF dispersion and aggregation in solution and how these interactions change with solvent modification. The simulations will help guide the rational design of solvents that can tune CNF assembly in biocomposite design.

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

Principal Investigator: Sharon Glotzer, University of Michigan

Scientific Discipline: Materials Science

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (900,000 Frontier node-hours)

Research Summary: From chocolate to steel, the properties and behavior of any crystalline material depend directly on the quality of the crystal, which itself depends on the crystal's formation. The material can be composed of particles ranging from the atomic to the colloidal side. Thus, the ability to predict and control crystallization across scales is of paramount importance.

Nucleation and growth are the primary mechanisms proposed for crystallization without a seed or surface from which the crystal can develop. Yet, detailed studies of these processes are limited, and our understanding of crystallization remains incomplete.

Thus, simulation can play a critical role in guiding material synthesis for crystals. This project aims to discover the rules by which particles at different scales assemble into crystals, as well as the role of particle shapes and interactions during assembly.

Crystallization requires extremely large and long simulations, and several runs must be sampled. With resources on Frontier, the project will carry out a computational study of crystallization pathways of the most diverse crystal structures that has ever been done. Crystals are prevalent in nature and industrial applications of huge variety.

The findings will be of immediate interest to materials and cellular biophysics communities, and transferable to engineering and chemistry communities specializing in general crystallization.