Type: Renewal
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 Muhkerjee, 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 (600,000 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 are carrying 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 aims to determine the 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 Science

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE Cray EX (560,000 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 2025 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: New
Title: "Ab initio modeling of polarized galactic CMB foreground emission"

Principal Investigator: Ka Ho Yuen, Los Alamos National Laboratory
Co-Investigators: Ka Wai, Los Alamos National Laboratory and University of Wisconsin-Madison
Alexei Kritsuk, University of California, San Diego
Raphael Flauger, University of California, San Diego
Alex Lazarian, University of Wisconsin-Madison
Andrey Beresnyak, Naval Research Laboratory

Scientific Discipline: Physics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE Cray EX (960,000 Frontier node-hours)

Research Summary: The search for the imprint of primordial gravitational waves on the cosmic microwave background (CMB) through precision measurements of the CMB polarization is an ambitious endeavour. It holds the potential to reveal information about the first fractions of a second of our Universe and provide insights into the mechanism responsible for the origin of structure in the Universe. However, the faint primordial signalis obscured by synchrotron radiation and polarized emission from dust in our galaxy. These foregrounds are brighter than the primordial signals at all frequencies, even in the cleanest patches of the sky. In addition, the primordial signal is subdominant to a signal generated by weak gravitational lensing of the CMB. Especially ground-based experiments will rely on their ability to remove this contribution, a process referred to as delensing. Delensing relies on non-Gaussian correlations in the data that may also be impacted by galactic foregrounds. Thus, reliable modeling of these ISM foregrounds, spanning scales from approximately 100 parsecs to 0.1 parsecs, is of crucial importance for the quest to detect gravitational waves from the early Universe.

The team will use the Frontier system to perform extensive simulations of multiphase interstellar turbulence, utilizing the AthenaK code. AthenaK is a performance-portable version of the Athena++ astrophysical MHD code, employing the Kokkos library to ensure compatibility with modern GPU-based HPC platforms. This project will significantly advance current methodologies by delivering high resolution simulations that can generate realistic maps of Galactic foreground emissions. These maps are invaluable for planning upcoming CMB experiments, such as CMB-S4 and LiteBIRD, as well as for the validation of analysis techniques for both existing and future experiments. In addition, the simulations will help improve our understanding of the physical processes within the interstellar medium, such as the gas and phase exchanges in interstellar media, and the cascade of multiphase, multi-physics magnetized turbulence.

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
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 (600,000 Aurora node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE Cray EX (1,000,000 Frontier node-hours)

Research Summary: This INCITE project is leveraging DOE supercomputers to improve the simulation capabilities of atomic nuclei and nuclear matter, and their reactions with neutrinos and electrons. The team aims to advance the 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 team is performing 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. The team's work will enable science not available previously and accelerate scientific discovery through high-performance computing.

Type: Renewal
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: Argonne National Laboratory
Machine (Allocation): HPE Cray EX - Intel Exascale Compute Blade Nodes (100,000 Aurora node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE Cray EX (1,300,000 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 needed to understand the risks they pose, but achieving this scale and spatial resolution has been challenging due to cost and power constraints. This project is developing 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 of DOE's exascale supercomputers, 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 help identify vulnerable locations, infrastructure improvements, and emergency preparedness measures.

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 (780,000 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: 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 (400,000 Frontier node-hours)

Research Summary: The project will leverage new computational and hybrid modeling approaches to provide unified knowledge of the assembly, dynamics and function of key gene regulatory complexes in the context of chromatin. Genomic DNA in cells forms chromatin whose fundamental repeating unit is the nucleosome. Nucleosome-incorporated DNA is generally inaccessible to DNA binding proteins. Predictably, nucleosome interactions have profound influence on all aspects of gene expression, including transcription and genome maintenance. Indeed, chromatin structure must be modulated for gene expression to occur in the first place, and gene regulation achieved by modification of the chromatin state is central to the field of epigenetics. Recent breakthroughs in cryo-EM, have visualized snapshots of transcription through chromatin. Nonetheless, cryo-EM, no matter how informative, still captures discrete intermediates from much larger conformational ensembles and, therefore, cannot unveil complete mechanisms. By coupling cryo-EM with state-of-the-art modeling, our INCITE project will overcome this barrier to progress in the field. Success of this project will shed light on how RNA polymerase II transcribes through a nucleosome without displacing it and losing its associated epigenetic modifications, and how elongation factors interact with the transcription machinery to maintain chromatin structure. The project will impact understanding of human disease etiology and treatments.

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

Principal Investigator: Andreas Kronfeld, Fermi National Accelerator Laboratory
Co-Investigators: Thomas Blum, University of Connecticut
Peter Boyle, Brookhaven National Laboratory
Norman Christ, Columbia University
Carleton DeTar, University of Utah
Aida El-Khadra, University of Illinois Urbana-Champaign
Steven Gottlieb, Indiana University
William Jay, Colorado State University
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, Fermi National Accelerator Laboratory

Scientific Discipline: Physics

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

Research Summary: This project, 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: Renewal
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: 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 (250,000 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 into the 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-their-kind, full-core hybrid Reynolds-averaged Navier-Stokes (RANS) calculations and large eddy simulation (LES) of fission reactors are being carried out on DOE supercomputers. Simulations of unprecedented scale are being conducted for fusion energy systems, approaching full-device multiphysics modeling of breeder blankets and for a novel reticulated 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: "Advancing Fusion Reactor Materials Through Exascale Simulations"

Principal Investigator: Tim Frolov, Lawrence Livermore National Laboratory
Co-Investigators: Flynn Walsh, Lawrence Livermore National Laboratory
Enze Chen, Stanford University
Ralf Drautz, Ruhr-Universität Bochum
Tomas Oppelstrup, Lawrence Livermore National Laboratory

Scientific Discipline: Materials Science

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): HPE Apollo 6500 (20,000 Polaris node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE Cray EX (980,000 Frontier node-hours)

Research Summary: The goal of this INCITE project is to make a breakthrough in our understanding of the brittle failure and plastic flow behavior of tungsten polycrystals, through exascale molecular dynamics simulations. The fundamental scientific discoveries revealed by the simulations are expected to be published in top-tier journals. The results of this research will also impact the broader Fusion Energy Science (FES) program through modeling of additively manufactured tungsten alloys. The team's cross-scale simulation approach will study tensile deformation of bulk crystals, high-angle tungsten GBs as a function of temperature, alloy segregation, and dislocation content in the bulk as well as in the GB plane. The researchers will coordinate these modeling efforts with the experimental additive manufacturing (AM) work at Lawrence Livermore National Laboratory and UCLA, funded through the GAMOW project, as well as with micromechanical tensile tests of AM W polycrystals performed at Lawrence Berkeley National Laboratory. These simulations are aimed at identifying the key parameters that can influence ductile or brittle failure of tungsten and suggest new strategies for mitigation of crack formation during additive manufacturing of tungsten alloys.

Type: New
Title: "Advancing Single Molecule Protein Sequencing: From Code to Clarity"

Principal Investigator: Aleksei Aksimentiev, Univ. of Illinois at Urbana-Champaign

Scientific Discipline: Biological Sciences

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

Research Summary: Single-molecule protein sequencing has the potential to revolutionize healthcare by providing the most detailed portrait of a biological cell. Nanopore sequencing, an established technique for single-molecule nucleic acid sequencing, holds the promise of providing a high-throughput, cost-effective protein sequencing method in which the amino acid sequence of individual proteins is read by measuring the blockage of the ionic current flowing through the nanopore as the protein chains translocate through the nanopore. However, nanopore sequencing of proteins presents unique challenges due to the heterogeneity in the physicochemical properties of the twenty standard amino acids and the diversity of post-translational modifications. The complexity of these chemical structures results in nanopore blockade currents that are difficult to interpret.

This project aims to lay the foundation for protein nanopore sequencing by developing a biophysical model that establishes a direct correlation between nanopore current signals and the amino acid sequences and post-translational modifications of the analyte proteins. Toward this goal, leadership DOE resources will be used to perform a massive set of all-atom molecular dynamics simulations of nanopore blockade currents. The simulations will provide the atomically precise data detailing the intricate dependence of the blockade current on the protein amino acid sequence, which will be used to develop a machine learning algorithm for accurate interpretation of single-molecule nanopore sequencing measurements. Establishing such an amino acid calling algorithm can enable transformative advances in various fields of research and engineering, including personalized medicine, drug discovery, biosecurity, and synthetic biology.

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 is advancing 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 are performing 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: New
Title: "AuroraGPT: A Large-Scale Foundation Model for Advancing Science"

Principal Investigator:	Rick Stevens, Argonne National Laboratory and The University of Chicago
Co-Investigators:	Ian Foster, Argonne National Laboratory
Scientific Discipline:	Computer Science
INCITE Allocation:	
Site:	Argonne National Laboratory
Machine (Allocation):	HPE Apollo 6500 (150,000 Polaris node-hours)
Site:	Argonne National Laboratory
Machine (Allocation):	HPE Cray EX - Intel Exascale Compute Blade Nodes (770,000 Aurora node-hours)

Research Summary: AuroraGPT is an ambitious pilot project to develop and improve methodologies that the science community can use to produce end-to-end pre-trained, and instruct-tuned and aligned models, as will be important for developing the type of general-purpose scientific foundation models advocated for in DOE's AI for Science planning process, and envisioned by the DOE FASST initiative. AuroraGPT aims to enhance the development and understanding of foundation models for science by exploring larger scientific corpora, more diverse types of data, and examining the role of modeling choices on the scientific reasoning tasks. The project's outcome has the potential to improve significantly how science is conducted by fostering a deeper integration of AI capabilities into research workflows. The AuroraGPT project will build a series of tools that assist researchers in making more informed and efficient scientific discoveries, greatly impacting the scientific landscape. The main tasks in the project include collecting and refining large-scale scientific datasets; building models at 8 billion to 400 billion or more parameter scales using general texts, code, and specific scientific data, and evaluating their performance on the Aurora and Polaris supercomputers; refining the models for deployment and introducing post-processing techniques such as instruct tuning and Reinforcement Learning for aligned chat-based interfaces; and evaluating the effectiveness of the models on scientific tasks. AuroraGPT offers a transformative opportunity to leverage AI for scientific discovery, potentially redefining problem-solving across various domains critical to the DOE's mission.

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

Principal Investigator: Ivan Oleynik, University of South Florida
Co-Investigators: Anatoly Belonoshko, KTH Royal Institute of Technology
Aidan Thompson, Sandia National Laboratories
Mitchell Wood, Sandia National Laboratories
Stan Moore, Sandia National Laboratories
Rahul Gayatri, NERSC
Marius Millot, Lawrence Livermore National Laboratory
Sally Tracy, Carnegie Institute 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 (800,000 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. The researchers 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: Renewal
Title: "COMbining deep-learning with Physics-Based affinIty esJmaJOn 3 (COMPBIO3)"

Principal Investigator: Peter V. 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 Cray EX - Intel Exascale Compute Blade Nodes (795,000 Aurora node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE Cray EX (1,000,000 Frontier node-hours)

Research Summary: This project is using exascale supercomputers to develop a personalized digital twin (DT) of the human body. The team 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 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, the INCITE 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. The 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: "Conjugate heat transfer effects in non-equilibrium rough wall boundary layers"

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

Scientific Discipline: Engineering

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE Cray EX (1,350,000 Frontier node-hours)

Research Summary: Hydrodynamically rough surfaces are common in many engineering and geophysical systems, including but not limited to icing on aircraft wings and wind turbine blades or molten deposition on turbomachinery components. In these examples, conjugate heat transfer effects between the rough wall boundary layers and the solid surfaces are important in controlling mass transfer rates (ice formation on wings or molten sand solidification on turbine blades) Accurately predicting these critical events is not possible without a detailed understanding of the heat transfer process in the presence of considerable surface roughness.

While many experimental and numerical tools exist to assess aerodynamic performance and flow characteristics over hydraulically smooth surfaces, few predictive computational tools exist to evaluate the impact of surface roughness and in particular, the impact of surface roughness on heat transfer. Empirical correlations for the impact of roughness on wall shear stress or heat transfer are often invoked, which do not necessarily generalize to other flow conditions and can incur significant errors. Recent work from the proposing group has demonstrated that if simulations are capable of resolving the length scales of the surface roughness, then it is possible to predict the aerodynamic characteristics such as the surface loading or the onset of boundary layer separation (Bornhoft et al 2024).

The proposed work aims to extend the predictive capabilities to include conjugate heat transfer effects in the presence of surface roughness. The proposed campaign will consist of two parts. First, the capability to predict conjugate heat transfer effects in rough-wall boundary layers will be validated against the experimental measurements of McCarrell et al (2018). This experiment measured surface temperatures over a roughness coupon placed on a flat plate subject to Joule heating, which simulations, including conjugate heat transfer effects, will aim to predict. Second, direct numerical simulations (DNS) including conjugate heat transfer effects over roughened NACA23012 airfoils will be performed at various angles of attack will be performed. This DNS database would fill a critical gap in the availability of present data for conjugate heat transfer effects in rough-wall boundary layers subjected to strong pressure gradients.

Type: New
Title: "Deep Learning Wall-Modeled LES for Aerodynamics and Wind Energy"

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

Scientific Discipline: Engineering

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

Research Summary: The project enables extreme-scale, solver-embedded deep learning for simulations of external aerodynamics, with particular applications to wind turbine blades, blade-rotor systems, and wind farms. It leverages both high-fidelity numerical data and sparse experimental data. It advances the state-of-the-art for predictive accuracy, computational cost, and model-based design of real-world aerodynamics applications, which will enable faster and higher-risk design cycles while reducing renewable energy costs in the wind energy sector.

Type: New
Title: "DNS and surrogate DNS mitigating N2O/NO in ammonia/hydrogen gas turbines"

Principal Investigator: Martin Rieth, Sandia National Laboratories
Co-Investigators: Jacqueline Chen, Sandia National Laboratories
Ki Sung Jung, Sandia National Laboratories
Seshu Yamajala, SLAC National Accelerator Lab
Elliott Slaughter, SLAC National Accelerator Lab
Alex Aiken, Stanford University

Scientific Discipline: Chemistry

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

Research Summary: Carbon-free fuels provide a promising route to reducing or even eliminating carbon dioxide emissions from power generation and transportation. Hydrogen and ammonia in particular are promising alternatives to natural gas in dispatchable power generation. However, significant challenges and open questions remain for the adoption of such fuels, in particular related to nitrogen oxide emissions. For ammonia, a so-called rich-quench-lean staged combustion system has shown to offer significant advantages with respect to flame stabilization, fuel flexibility and emissions. While significantly reducing nitrogen oxide emissions by burning ammonia fuel-rich in the first stage, ammonia slip that can occur in the first stage has significant negative impacts on emission formation. Such ammonia slip reacts with the second stage combustion process leading to fuel-bound nitrogen oxide formation counteracting the emission reductions gained from the two-stage operation. We propose a series of direct numerical simulations (DNS) and surrogate DNS to shed light on second stage combustion process, flame stabilization and emission formation under realistic RQL conditions with ammonia slip. The simulations will feature a jet-in-crossflow configuration as it is employed in the second stage of typical RQL combustion systems. Due to the high pressure at which gas turbine combustors typically operate, a detailed DNS of such a case is challenging, even on current supercomputing hardware. However, a novel time-dependent basis reduced order model on-the-fly surrogate DNS capability will allow for a parametric variation of the amount of ammonia slip. The simulations will provide a rich dataset that will allow unprecedented insight into the details of the flame stabilization and emission formation process in a realistic ammonia RQL scenario, as well as provide a wealth of data for further physics and data-driven model development to aid the development of predictive models for the design, development and optimization of efficient low-NOx engines for carbon-free power generation.

Type: New
Title: "Elastic properties of complex lipidomes"

Principal Investigator: Edward Lyman, University of Delaware
Co-Investigators: Van Ngo, Oak Ridge National Laboratory
Debsindhu Bhowmik, Oak Ridge National Laboratory

Scientific Discipline: Biological Sciences

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE Cray EX (766,000 Frontier node-hours)

Research Summary: Cellular membranes are built from a chemically diverse array of molecules called lipids. The lipids that compose a cell membrane are differentiated between the membranes of a single cell, between different cells within the human body and other multicellular organisms, and between different species across the tree of life. Although a comprehensive understanding of how and why "lipidomes" vary, they determine the material properties of cell membranes (stiffness, fluidity) and are intimately linked with disease states. This proposal builds on recent groundbreaking experimental work determining human lipidomes, and aims to link the details of lipid chemistry to these all important material properties. Massive supercomputing resources like those managed by the Department of Energy are necessary for this work, because the simulations must be large enough to observe the emergence of material properties from collective of lipids, and this demands simulations containing between two and five million atoms. The National labs of the DOE are among the only places in the world that house machines large enough for these simulations.

Type: New
Title: "Enabling the design of safer, more effective medicines"

Principal Investigator: Ron Dror, Stanford University

Scientific Discipline: Biological Sciences

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

Research Summary: We will use massively parallel simulations on Frontier to identify molecular mechanisms by which different drugs that bind to the same target can stimulate different cellular signaling pathways. We will also demonstrate how these results can be used to design drugs that stimulate desired signaling pathways while avoiding undesired pathways. This project will enable the rational design of more effective therapeutics with reduced side effects to treat a wide range of diseases.

One-third of all drugs act by binding to G protein–coupled receptors (GPCRs), and these receptors also represent the largest class of targets for the development of new therapeutics. Drugs that cause a GPCR to selectively stimulate or selectively avoid stimulation of specific intracellular signaling proteins promise better treatments for a wide range of medical conditions, including cardiovascular disease, cancer, mental health disorders, and chronic pain. Designing such medicines has proven difficult, however, because the molecular mechanisms by which drug molecules can achieve such effects have been unclear.

In recent INCITE projects, we identified some of these molecular mechanisms for the first time (Suomivuori et al., Science 2020; Latorraca et al., Cell 2020; Qu et al., Nature Chem. Biol. 2023; El Daibani et al., Nature Comm. 2023). We also developed methods to determine such mechanisms by effectively leveraging capability-class simulations on Frontier.

In this project, we will employ these methods to achieve several important goals. We will determine how drugs can cause the kappa opioid receptor to selectively stimulate signaling at one G protein subtype, facilitating the design of safe treatments for chronic pain. We will identify the mechanism by which drugs can selectively stimulate or block GPCR phosphorylation, which has a critical impact on downstream signaling. We will use our results to identify novel GPCR-targeted compounds with unique and desirable pharmacological properties. Our project will both address long-standing molecular biology questions and advance human health. Achieving our goals requires levels of parallelism that can only be achieved on leadership-class facilities. To maximize the impact of our computational studies, we have already established close collaborations with world-class experimental groups at multiple institutions.

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

Research Summary: SCREAM is a global atmosphere model with 3 km resolution. Using 30x finer resolution than most of its competitors yields more accurate predictions of the earth system and provides geographically specific information necessary for weather-impacts planning. Fine resolution is computationally expensive, however, so this model can only be run on leadership-class computing resources. The goal of this project is to provide, for the first time, decadal-scale real-world predictions using SCREAM.

Type: New
Title: "Enhancing Genomic Discoveries with GPU-Accelerated Computing"

Principal Investigator: Anurag Verma, Veterans Affairs
Co-Investigators: Ravi Madduri, Argonne National Laboratory
Alexis Rodriguez, Argonne National Laboratory
Scott Damrauer, Crescenz VA Medical Center
Benjamin Voight, Crescenz VA Medical Center
Jennifer Huffman, VA Palo Alto Health Care

Scientific Discipline: Biological Sciences

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

Research Summary: In our quest to better understand the basis of diseases, population-scale biobanks hold great promise. However, dealing with the amount of data involved poses several computational hurdles. This INCITE award aims to tackle these challenges by harnessing the capabilities of Graphics Processing Units (GPUs) to accelerate genomic discovery.

Conventional genomic data analysis is designed for computing resources that cannot keep up with the rapid expansion of genomic data. By creating and optimizing tools that utilize GPU technology, we can greatly accelerate processes like genome-wide association studies (GWAS), fine mapping, and multi-trait colocalization. These tools will empower researchers to efficiently and accurately identify causal variations associated with diseases and traits, offering insights into the genetic makeup of complex traits.

Moreover, our project emphasizes inclusivity by highlighting diversity. We will use the largest and most diverse biobank in the world, the VA Million Veteran Program, which includes over 650,000 individuals. Ensuring that genomic research benefits all communities, including those usually overlooked in studies, helps promote health equality and tackle healthcare disparities.

In essence, the advancement of discoveries through GPU-accelerated computing is poised to revolutionize genomic research and personalized medicine. By leveraging state-of-the-art GPU technology at leadership computing facilities, our goal is to speed up discoveries, enhance biomedical research findings, and make these findings available to the public at a rapid pace.

Type: Renewal
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 (200,000 Aurora node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE Cray EX (450,000 Frontier node-hours)

Research Summary: This project aims to leverage Advanced Physics Refinement (APR) to create a high-throughput mechano-phenotyping technology by establishing a digital twin of a microfluidic device and quantifying cellular behavior in complex 3D geometries with realistic red blood cell (RBC) backgrounds. The first goal is to develop a digital twin of the entire microfluidic device that can be coupled with in vitro devices to enable high-throughput mechano-phenotyping. The second goal is to create a protocol for quantifying likely cellular behavior across the full ensemble of potential RBC configurations in whole blood measures.

Type: Renewal
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 project leverages 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 the team acknowledges 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, their 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. The 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: Renewal
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: This INCITE project is enabling 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 is significantly speeding 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 are constructing 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's 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: Renewal
Title: "Exascale Gyrokinetic Study of ITER Challenge on Power-Exhaust and ELM-Free Edge"

Principal Investigator: CS Chang, 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
Julien Dominski, Princeton Plasma Physics Laboratory
Kevin Huck, University of Oregon
Luis Chacon, Los Alamos National Laboratory
Randy Michael Churchill, Princeton Plasma Physics Laboratory
Stephane Ethier, Princeton Plasma Physics Laboratory

Scientific Discipline: Physics

INCITE Allocation:

Site:	Argonne National Laboratory
Machine (Allocation):	HPE Apollo 6500 (200,000 Polaris node-hours)
Site:	Argonne National Laboratory
Machine (Allocation):	HPE Cray EX - Intel Exascale Compute Blade Nodes (1,000,000 Aurora node-hours)
Site:	Oak Ridge National Laboratory
Machine (Allocation):	HPE Cray EX (1,300,000 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 (50,000 Polaris node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE Cray EX (450,000 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 is using 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 are expanding their work to model thermonuclear flame propagation across the surface of a neutron star. They are exploring 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 is focusing 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 Quantum-AI Molecular Dynamics for Covalent Drug Discovery"

Principal Investigator: Giuseppe Barca, University of Melbourne
Co-Investigators: Jorge Gálvez Vallejo, Australian National University
Yasmin Shamsudin, QDX Technologies

Scientific Discipline: Chemistry

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE Cray EX (380,000 Frontier node-hours)

Research Summary: This INCITE initiative seeks to revolutionize molecular dynamics and drug discovery by creating the first exascale framework for ab initio reactive molecular dynamics (AIRMD) with quantum-level accuracy. By combining molecular fragmentation, machine-learned potentials, and advanced double-hybrid density functional theory (DHDFT) potentials, this framework will achieve unprecedented accuracy and scalability.

Our project leverages cutting-edge algorithms and software developed through the Exascale Computing Project and other high-performance computing grants. This hybrid Quantum-and-AI (QAI) framework will be instrumental in designing novel covalently binding therapeutics. Initially, we will validate our protocols using cysteine covalent binders for Bruton's Tyrosine Kinase (BTK), a crucial target in cancer treatment. Following successful validation, we will pioneer the development of covalent binders targeting the Human Epidermal Growth Factor Receptor 2 (HER2), a significant target in breast cancer therapy.

The framework's core innovation lies in using Bayesian Neural Networks (BNNs) trained on DHDFT data to estimate molecular forces, ensuring quantum-level accuracy. When the uncertainty of these estimates is high, the framework switches to direct DHDFT calculations, balancing efficiency and precision.

Our project aims to provide the research community with a powerful tool for quantum drug discovery. The resulting algorithms and codes will be integrated into the EXESS software, promoting widespread adoption and further innovation. By advancing the design of covalent drugs, this project has the potential to significantly impact cancer treatment, offering new hope for patients with resistant forms of the disease.

Type: Renewal
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 Plasma Physics Laboratory

Scientific Discipline: Physics

INCITE Allocation:

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

Research Summary: This project will develop the challenging capability for prediction and real-time control of energetic particle (EP) confinement in burning plasmas by combining the state-of-the-art exascale first-principles GTC simulation and the prominent experimentally validated AI/Deep Learning FRNN software.

Type: Renewal
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: Argonne National Laboratory
Machine (Allocation): HPE Cray EX - Intel Exascale Compute Blade Nodes (100,000 Aurora node-hours)
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 is applying the GW perturbation theory and GW-Bethe-Salpeter-equation, general quantum theoretical tools, 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.

The team's work aims to advance the fundamental understanding of electron-phonon coupling in correlated materials using the computational approach of exascale-class systems, including Frontier and Aurora. 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 Compact Binary Mergers"

Principal Investigator: David Radice, The Pennsylvania State University
Co-Investigators: Rossella Gamba, University of California, Berkeley
Maitraya Bhattacharyya, The Pennsylvania State University

Scientific Discipline: Physics

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

Research Summary: Compact binary mergers are related to some of the most pressing open problems in astrophysics, including the nature of gravity and matter under extreme conditions, the astrophysical site of production of the heavy elements, and the mechanism powering gamma-ray bursts. In the next years, the LIGO experiment will undergo a series of upgrades that will double its sensitivity. In 2027, following the upgrades, LIGO will start its fifth observing run (O5). LIGO will be joined by the Virgo detector in Italy and KAGRA in Japan to form an international network of detectors. A number of electromagnetic follow-up observations are planned, including with the Vera Rubin telescope, the Nancy Grace Roman Space Telescope, and the James Web Space Telescope. The combined gravitational-wave and electromagnetic data from these observations will encode the answer to some of the most pressing questions in high energy and nuclear astrophysics. The aim of this project is to perform compact binary merger simulations with unprecedented fidelity to unlock them. The team will perform simulations of precessing, eccentric binary black hole mergers and tidally interacting neutron stars at unprecedented resolutions, which will be used to develop new gravitational-wave data analysis pipelines. Such simulations are urgently needed, since systematic uncertainties in current models will dominate over statistical uncertainties for the high signal-to-noise ratio events expected in O5. General-relativistic neutrino-radiation magnetohydrodynamics simulations of a large number of configurations, some of which at very high resolutions, will be performed to characterize the electromagnetic counterpart to binary neutron star mergers. These will include the first full-Boltzmann neutrino-radiation magnetohydrodynamics simulations of these events and the first zoom-in simulations with up to 100 times higher resolution than any extant simulation and resolving, for the first time, the turbulence down to the neutrino viscous scale.

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

Principal Investigator: Paul Kent, Oak Ridge National Laboratory
Co-Investigators: Ray Clay, Sandia National Laboratories
Peter Doak, Oak Ridge 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
Kayahan Saritas, Oak Ridge National Laboratory

Scientific Discipline: Materials Science

INCITE Allocation:

Site:	Argonne National Laboratory
Machine (Allocation):	HPE Apollo 6500 (150,000 Polaris node-hours)
Site:	Argonne National Laboratory
Machine (Allocation):	HPE Cray EX - Intel Exascale Compute Blade Nodes (600,000 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, necessitating insights from benchmark accuracy calculations—particularly in areas 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: "Exascale Simulations of Rayleigh-Benard Convection"

Principal Investigator: Janet Scheel, Occidental College
Co-Investigators: Joerg Schumacher, Technical University of Ilmenau
Kartik Iyer, Michigan Technological University
Roshan Samuel, Technical University of Ilmenau
Katipalli Sreenivasan, New York University

Scientific Discipline: Engineering

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 (750,000 Aurora node-hours)

Research Summary: Many turbulent flows are driven by sustained temperature differences. Applications span a wide spectrum from heat exchangers in power plants and energy efficient indoor ventilation to convection in the Earth's atmosphere and oceans all the way to the Sun and other stars. Turbulent Rayleigh-Benard convection (RBC) is the paradigm for all these convection phenomena. In RBC, a fluid cell is kept at a constant temperature difference between top and bottom. The Rayleigh number measures the strength of convection. One of the key questions in RBC is that of the turbulent transport mechanisms of heat and momentum. Since the fluid is confined between rigid and/or impermeable walls, tiny boundary layers of the temperature and velocity fields will form in the vicinity of the walls. As the Rayleigh number increases, first the bulk becomes fully turbulent, while the boundary layers remain closer to laminar, although they become increasingly unsteady. There is a well-known theoretical scaling of Nusselt number, a measure of the heat transport, with a Rayleigh number that has been verified both experimentally and numerically. What is not well-understood is if the boundary layers become fully turbulent and the system then enters the ultimate regime of RBC for which the law of turbulent heat transport changes. This project advances the team's Direct Numerical Simulations (DNS) to Rayleigh numbers that have never been accessed before numerically. Their efforts are based on the nekRS spectral element software package which was developed for solving the flow equations on massively parallel GPU supercomputers. DNS will provide new insights into the global structure of the convection flow and the details of the boundary layer dynamics. The new data record will help to resolve the contradictory experimental results for the onset of the transition to the ultimate regime of convective turbulence in which the boundary layers become fully turbulent thus causing a significantly enhanced turbulent heat transfer. This study will provide new insights into the heat and momentum transport as a function of Rayleigh number and the transition to the ultimate regime. As such, research will be transformational in the domain of fluid dynamics with a variety of important applications in nature and technology.

Type: New
Title: "Expanding High-Fidelity CFD for Aircraft at the Corners of the Flight Envelope"

Principal Investigator: Adam Clark, The Boeing Company
Co-Investigators: Konrad Goc, The Boeing Company
Jeffrey Slotnick, The Boeing Company
Sanjeeb Bose, Cadence Design Systems

Scientific Discipline: Engineering

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

Research Summary: This project will explore the modelling requirements to meet required accuracy of external aerodynamics on commercial transport aircraft at flight Reynolds number using scale-resolving computational fluid dynamics. Validation work will be performed on problems encompassing transonic buffet and flight in icing. Understanding these requirements will enable this class of tools to be used early in the design process to enable better more fuel efficient designs.

Type: New
Title: "Experimental Realization of Certified Randomness from Quantum Supremacy"

Principal Investigator: Ruslan Shaydulin, JPMorgan Chase
Co-Investigators: Matthew DeCross, Quantinuum
Michael Foss-Feig, Quantinuum
Minzhao Liu, JPMorgan Chase
Pradeep Niroula, JPMorgan Chase
Marco Pistoia, JPMorgan Chase
Yuri Alexeev, Argonne National Laboratory
Travis Humble, Oak Ridge National Laboratory

Scientific Discipline: Computer Science

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

Research Summary: While quantum computers are expected to solve a wide range of practically important problems beyond the capabilities of classical computers, realizing this potential remains a challenge. This project considers the problem of generating true randomness, which is crucial for applications ranging from cryptography to public lotteries. At this task, quantum computers have an advantage over classical computers due to their intrinsic probabilistic nature. A fundamental problem shared by known methods of generating randomness is that a client in need of entropy often must trust a third-party or a black-box provider, a problem rendered severe in communications over public network with malicious adversaries. This has led to the formulation of "certified randomness," randomness that a skeptical client can independently verify with high confidence, without the need to check or trust the internal workings of the generator. While progress in quantum hardware has enabled experimental certified randomness, the known protocols have severe limitations in terms of practicality. The goal of this project is to implement a novel, more practical protocol for generating certified randomness, with generation performed on a quantum computer and certification on a classical supercomputer accessed through INCITE. This project will take a step towards improving practicality of a useful task performed by a gate-based quantum computer in conjunction with a classical supercomputer.

Type: Renewal
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 (100,000 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: "Fluid turbulence at the Exascale: Inertial range and low-diffusivity mixing"

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
Toshiyuki Gotoh, Nagoya Institute of Technology

Scientific Discipline: Engineering

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

Research Summary: Exascale computing resources on Frontier at OLCF will be deployed to advance fundamental understanding in three-dimensional turbulent fluid flow, using a combination of state-of-the-art direct numerical simulation algorithms, advanced turbulence theory, and physics-informed machine learning. The simulations will be at world-record resolution of 35 trillion grid points and will be conducted using a code highly optimized specifically for the Frontier architecture, especially in its OpenMP offloading, memory management and communication protocols, and demonstrated to very high levels of performance at or beyond half of the full size machine. Two major simulation campaigns are designed, to elucidate a number of long-standing puzzles where presence of massive scale separation as well as proper resolution of the small scales is crucial. The first is to extend the Reynolds number of isotropic turbulence simulations significantly at a resolution level sufficient for the analysis of intermittency in the inertial (intermediate) length scales, which is important for a proper assessment of corrections to classical theory needed to account for local fluctuations of high intensity. The second to to extend the Reynolds number, by a factor of 4, beyond recent studies of the mixing of passive contaminants with a low molecular diffusivity and examine the phenomenon of differential diffusion between contaminants with disparate diffusivities in a range with applications to oceanic and atmospheric phenomena.

Success in the project will be ground-breaking in Reynolds number in addition to grid resolution in the turbulence simulation community, worldwide. 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 type of data is well demonstrated in recent innovative studies of crucial aspects of scale similarity. Impact from the expected new data 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. About 0.9~PB of data will be transferred out of OLCF for this purpose, adding several large datasets to those of more moderate size already available at the Johns Hopkins Turbulence Database.

Type: New
Title: "Foundation Models for Crystals"

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

Scientific Discipline: Energy Technologies

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

Research Summary: Electrode materials are crucial for the performance of energy storage and conversion devices in various applications, such as electric vehicles, grid storage, and electric aircraft. However, each application has unique requirements, including conductivity, stability, and safety for electric vehicles; scalability and cost-effectiveness for grid storage; and light weight with high power density for electric aircraft. The high cost of experimentation and known stable crystals containing various amounts of the charge carrier (e.g. lithium, sodium) hinders the development of suitable energy storage materials to meet these demands. Advances in foundation models that leverage large unlabeled datasets offers a pathway to address this challenge. While existing foundation models have demonstrated state-of-the art performance for small molecules, the development of foundation models for crystals are still nascent. This project aims to develop a large-scale crystal dataset consisting of unrelaxed geometries leveraging symmetry-respecting encodings. Utilizing this dataset, the team will train a compute-optimal foundation model capable of accurately predicting thermodynamics, mechanical properties, thermal properties, enabling the efficient design of materials for energy storage and conversion.

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

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

Scientific Discipline: Biological Sciences

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): HPE Apollo 6500 (150,000 Polaris node-hours)
Site: Argonne National Laboratory
Machine (Allocation): HPE Cray EX - Intel Exascale Compute Blade Nodes (1,600,000 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: "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 (580,000 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: "Hadron physics from first principles"

Principal Investigator: Konstantinos Orginos, William & Mary University
Co-Investigators: Robert Edwards, Jefferson National Laboratory
David Richards, Jefferson National Laboratory
Christopher Monahan, William & Mary University
Anatoly Radyushkin, Old Dominion University
Jianwei Qiu, Jefferson National Laboratory
Frank Winter, Jefferson National Laboratory
Savvas Zafeiropoulos, CNRS
Eloy Romero, Jefferson National Laboratory
Herve Dutrieux, William & Mary University
Joseph Karpie, Jefferson National Laboratory

Scientific Discipline: Physics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE Cray EX (1,200,000 Frontier node-hours)

Research Summary: Using Lattice QCD we will perform calculations that 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. We 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 main goal of the project is to compute the x-dependent, flavor separated quark and gluon generalized parton distributions (GPDs) of the nucleon, in the continuum and physical quark-mass limits of lattice QCD. Leadership class computing is critical for our goals, which will provide the ab initio answers to the question of how quarks and gluons make up protons and neutrons which is central to the Department of Energy experimental nuclear physics program.

Type: New
Title: "Heavy quarks in QGP: lattice QCD inputs for RHIC and LHC"

Principal Investigator: Peter Petreczky, Brookhaven National Laboratory

Scientific Discipline: Physics

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE Cray EX (1,071,000 Frontier node-hours)

Research Summary: The project will study the properties of heavy quarks inside a new state of matter called Quark Gluon Plasma that existed few microseconds after the Big Bang and studied in the laboratories, including the Relativistic Heavy Ion Collider at Brookhaven National Laboratory. The project will aid our understanding of Quark Gluon Plasma created in laboratories.

Type: Renewal
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 Cray EX - Intel Exascale Compute Blade Nodes (50,000 Aurora node-hours)
Site:	Oak Ridge National Laboratory
Machine (Allocation):	HPE Cray EX (150,000 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 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, this INCITE project is deploying new state-of-the-art machine learning (ML) methods to construct reliable and accurate force fields, trained on accurate quantum electronic structure calculations and perform record-scale and -speed MD simulations of battery and catalytic interfaces. The team is using DOE supercomputers 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 such as battery degradation and transport at interfaces, and active site selectivity and stability for hydrogen production.

Type: Renewal
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, NVIDIA

Scientific Discipline: Chemistry

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): HPE Cray EX - Intel Exascale Compute Blade Nodes (1,500,000 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-Accuracy Quantum Simulations in Cancer Therapy Using Exascale Computing"

Principal Investigator: Anouar Benali, Qubit Pharmaceuticals
Co-Investigators: Jean-Philip Piquemal, Qubit Pharmaceuticals
Kevin Gasperich, Argonne National Laboratory

Scientific Discipline: Chemistry

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): HPE Cray EX - Intel Exascale Compute Blade Nodes (120,000 Aurora node-hours)

Research Summary: Cancer remains one of the most challenging diseases to treat, with treatments often taking decades to develop while costing millions of dollars in research. The complexity of cancer biology necessitates an understanding of the problem at a quantum level. Over the last decade, the design of cancer treatments has increasingly moved towards in silico methods, with bioinformatics playing a pivotal role. This shift has enabled the analysis of vast amounts of biological data and the simulation of complex biochemical interactions, accelerating the discovery and optimization of new treatments through AI/ML and QMMM-derived force fields. However, these methods often fail to capture strong correlations and weak interactions, which are crucial for understanding cancer cell mechanisms.

This project leverages high-accuracy Quantum Monte Carlo (QMC) simulations as implemented in the QMCPACK code, which has been specifically developed for exascale computing, to explore critical biochemical interactions in cancer therapy. By focusing on strong correlations and weak interactions—areas where traditional methods fall short—QMC aims to provide unprecedented insights into key cancer treatment mechanisms. Combining expertise in QMC methods, high-performance computing, drug design, and dataset development, the project's interdisciplinary team aims to advance the understanding of critical cancer-related processes and develop more effective treatments.

Type: New
Title: "High-Fidelity Simulations of Open Fan/Wing Integration for Sustainable Aviation"

Principal Investigator: Stephan Priebe, GE Aerospace Research
Co-Investigators: Adam Clark, Boeing
Gary Coleman, NASA
Ramakrishnan Kannan, Oak Ridge National Laboratory
Emanuel Setiawan, Boeing
Trevor Wood, GE Aerospace Research
Mujeeb Malik, NASA
Suryapratim Chakrabarti, GE Aerospace Research

Scientific Discipline: Engineering

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): HPE Cray EX - Intel Exascale Compute Blade Nodes (40,000 Aurora node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (800,000 Frontier node-hours)

Research Summary: The aviation industry has recognized the challenges of its contribution to greenhouse gas emissions while being a critical component of the global economic infrastructure. One of the key strategies to significantly reduce the environmental footprint of the aviation industry is to radically change the propulsion system architecture to minimize energy utilization required for future aircraft, and primarily for the dominant aircraft market segment. As the trend of increasing bypass ratio for ducted turbofans is asymptoting, an architecture change to open fan propulsion is needed to attain nearly optimal propulsive efficiency. To realize the fuel burn and emissions improvement potential of the open fan, the integration of the engine on the wing and aircraft must be optimized. In this project, NASA, Boeing, and GE Aerospace are engaging in a collaboration to investigate the challenge of integrating an open fan on an aircraft in a wing-mounted configuration, for which installation effects are a key risk to realizing the efficiency gains associated with this propulsion architecture. This project focuses on developing a deep understanding of flow physics of the aircraft-installed open fan propulsor through high-fidelity simulations. The simulation data generated will be used to benchmark and improve computational design models through machine learning and physics-based methods. The use of these models would allow for more efficient and practical design optimization for the open fan aircraft installation. Predictive capabilities of the improved models will be assessed on integrated propulsion and aircraft in various configurations and flow conditions. High-fidelity simulations of such configurations require tens of billions of cell volumes to fully resolve the turbulence and highly varying flow velocities in the propulsion system and the airplane components. Exascale computing capacity available under the INCITE program is critically required for the success of this project.

Type: New
Title: "High-Fidelity Turbulence-Based Predictions of Stellarator Reactor Performance"

Principal Investigator: Noah Mandell, Type One Energy
Co-Investigators: Walter Guttenfelder, Type One Energy
Antoine Cerfon, Type One Energy

Scientific Discipline: Physics

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

Research Summary: Fusion energy holds the promise of delivering substantial carbon-free baseload energy for the planet. In magnetic confinement fusion devices, turbulent transport of particles and heat degrades the efficiency of these machines, limiting their potential as net-energy sources. Stellarators are a type of magnetic fusion device with significant flexibility in the device geometry, which provides an opportunity to optimize the device to reduce transport and thereby improve efficiency. This would enable a transport-optimized stellarator to become the basis for commercial fusion energy generation.

The design and construction of such transport-optimized stellarators is a central goal of Type One Energy Group, Inc. Following decades of foundational Department of Energy research on the nature of turbulence in fusion plasmas, this INCITE project will use state-of-the-art multi-scale plasma turbulence simulations to predict and optimize fusion performance of new stellarator concepts being proposed for construction by Type One Energy. The results obtained with the proposed research will represent the most advanced transport physics basis required to design stellarator reactors that will be built by Type One Energy, accelerating the path to support the White House's Bold Decadal Vision for Commercial Fusion Energy.

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-Resolution GPU-Enabled SCREAM RRM Simulations for Extreme Weather and Climate Events"

Principal Investigator: Brandi Gamelin, Argonne National Laboratory
Co-Investigators: Dimitrios K. Fytanidis, Argonne National Laboratory
Gökhan Sever, Argonne National Laboratory
Vishwas Rao, Argonne National Laboratory
Jiali Wang, Argonne National Laboratory
Danqing Wu, Argonne National Laboratory

Scientific Discipline: Earth Science

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): HPE Apollo 6500 (150,000 Polaris node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE-Cray EX (300,000 Frontier node-hours)

Research Summary: The intensity and frequency of extreme events driven by Pacific Ocean variability has increased over time. Modeling the effects of Pacific Ocean surface temperature variability, coupled atmospheric dynamics, and long-term changes is crucial for understanding their influences on future extreme weather events in the United States, including the Pacific U.S. islands of Hawaii, Guam, Northern Mariana, and American Samoa. The insights gained will be critical for enhancing the resilience of energy systems, infrastructure, and communities against the impacts of extreme weather events.

This INCITE project will produce high-resolution datasets for regions extending from the U.S. and across the Pacific Ocean using DOE supercomputing resources to investigate the high impact of extreme weather and climate events extending into mid-century (2015-2055). The team will deploy the Simple Cloud Resolving E3SM Atmosphere Model (SCREAM) on DOE supercomputers over a global computational domain with regionally refined areas across the Pacific Ocean, the contiguous U.S. (CONUS), and particularly the U.S. islands, which are sorely underrepresented and lacking high-resolution data for future projections. This work will advance the availability of actionable data for the analysis of extreme weather events in the U.S. and ensure that the datasets generated by this work are publicly available. This unique set of simulations will also foster collaborative opportunities with other research organizations, and the generated dataset is expected to be valuable for numerous projects funded by DOE and other agencies—particularly for projects that are interested in risk, reliability, and resilience studies to inform infrastructure planning.

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

Principal Investigator: Chris Wolverton, Northwestern University
Co-Investigators: Yi Xia, Portland State University

Scientific Discipline: Materials Science

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): HPE Apollo 6500 (150,000 Polaris node-hours)

Research Summary: While evidently useful in materials design, current computational materials databases are mostly only available at zero temperature. Using a recently developed lattice dynamics method, this project aims to compute dynamical materials properties at finite temperature in a high-throughput fashion for thousands of compounds in the Open Quantum Materials Database.

Type: New
Title: "High-Throughput Lead Optimization with Amber"

Principal Investigator: Darrin York, Rutgers University

Scientific Discipline: Chemistry

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

Research Summary: The overall objective of this project is to address a major obstacle in computer-aided drug discovery and precision medicine: the absence of computational workflows capable of reliably identifying the most tight-binding ligands from a design pool of proposed compounds within 60 hours of wall-clock time (a typical time range required for a drug discovery team in industry). The researchers will develop and test a new adaptive framework for high-throughput lead optimization that integrates advanced methods and features in AMBER to achieve ligand-protein binding predictions. The framework will be optimized to run with unprecedented efficiency on advanced GPU supercomputing platforms such as Polaris.

Type: Renewal
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: Renewal
Title: "Hypersonic Transition Control via Porous and Wavy Walls at High Reynolds Numbers"

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

Scientific Discipline: Engineering

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): HPE Apollo 6500 (150,000 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 are carried out using a high-scalable block-spectral code at Reynolds numbers of up to 22.9 x 106 , 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 subfilter-scale (LES) or total (Reynolds-averaged Navier-Stokes) turbulent stresses.

Type: New
Title: "Improved confinement regimes for D-T fusion plasmas"

Principal Investigator: Emily Belli, General Atomics
Co-Investigators: Reuben Budiardja, Oak Ridge National Laboratory
Jeff Candy, General Atomics
Jeronimo Garcia, CEA (French Alternative Energies and Atomic Energy Commission)
Igor Sfiligoi, University of California San Diego

Scientific Discipline: Physics

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

Research Summary: Nuclear fusion holds tremendous promise for a nearly limitless, zero-carbon source of future energy. In a tokamak fusion reactor, good confinement of the thermal energy, or heat, in the plasma is needed to achieve self-sustaining (burning) fusion power. Confinement, however, is fundamentally limited by slow particle and energy losses due to turbulence that is driven by unstable plasma waves. Understanding the turbulence regimes expected in burning plasmas will help to develop scenarios that optimize fusion performance in next-generation reactors like ITER and other fusion pilot plants. Exascale computing resources on OLCF Frontier will be used to perform challenging multi-scale turbulence simulations of hydrogen plasma fuel ions and highly energetic fusion-born alpha (charged helium nuclei) particles with the CGYRO gyrokinetic code. The simulations will be used to predict energy and particle losses in improved, reactor-relevant, high-confinement regimes for burning plasmas from the recent fusion world-record-producing experiments on the JET tokamak. These simulations will span extreme space and time scales (over several orders of magnitude) to capture the highly complex and nonlinear interplay between the slow, large-scale dynamics of fuel ions and the fast, small-scale motion of the much lighter electrons in the fusion plasma. Research will focus on the role of hydrogenic fuel isotope, cross-interactions with energetic ions, and transport of impurities (from erosion of reactor wall materials) in improved confinement in future reactor scenarios. These simulations of JET experiments will provide a unique opportunity to assess the predictability of fusion plasmas close to ITER conditions.

Type: New
Title: "Large-Scale Simulations of Inner-Ear Mechanotransduction Complexes"

Principal Investigator: Marcos Sotomayor, University of Chicago

Scientific Discipline: Biological Sciences

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

Research Summary: Mechanotransduction is a process at the core of vertebrate hearing and balance. In this process, forces from sound and head movements are transduced into electrochemical signals that enable sensory perception. Inner-ear mechanotransduction takes place in hair cells and it involves tip-link filaments that pull on ion channels and associated proteins to trigger sensory perception. The inner-ear transduction apparatus is formed by tip-link components cadherin-23 and protocadherin-15, as well as membrane proteins TMIE, TMHS and TMC1 and the cytoplasmic proteins CIB2 and CIB3. Mutations to these proteins often result in inherited deafness and balance disorders. The elasticity of tip links, the pathway of force propagation from tip links to transduction channels, and the conformational changes of the transduction apparatus upon gating are unknown.

The researchers aim to perform multi-microsecond all-atom molecular dynamics simulations of experimentally obtained structural models complemented with AlphaFold 3 structural predictions of two systems: the entire inner-ear tip-link filament and the transmembrane transduction apparatus. In addition, we propose to use replica exchange molecular dynamics to sample TMC1 and related TMEM63/OSCA proteins states and identify their open-pore structures. The team aims to predict tip-link mechanics and to elucidate the gating mechanisms of the inner-ear hair-cell mechanotransduction apparatus. The simulations are particularly well-suited for INCITE resources as these require massively parallel supercomputers to enable users to study and visualize the dynamics of large systems including proteins, lipids, and ions in timescales that are physiologically relevant for auditory transduction and mechanosensitive channel gating (10 microseconds). This work will provide insight into how hearing happens at the molecular level with implications for the treatment of inherited deafness.

Type: New
Title: "Laser-Ion Acceleration Using Incoherent Combination of Pulses"

Principal Investigator: Davide Terzani, Lawrence Berkeley National Laboratory
Co-Investigators: Axel Huebl, Lawrence Berkeley National Laboratory
Lieselotte Obst-Huebl, Lawrence Berkeley National Laboratory
Jean-Luc Vay, Lawrence Berkeley National Laboratory
Stepan Bulanov, Lawrence Berkeley National Laboratory
Carl Schroeder, Lawrence Berkeley National Laboratory

Scientific Discipline: Physics

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

Research Summary: The interaction of a single ultra-short, ultra-intense laser pulse with solid targets produces immense electric fields capable of accelerating ion beams in ultra-compact setups. Such beams have several applications, including cancer therapy, where they can achieve the FLASH effect, and high energy density physics, a timely subject considering the rapid development of fusion plasmas. In this project, we explore the possibility of obtaining beams similar to those produced by a single high-energy pulse by using the incoherent combination of multiple low-energy laser pulses via a campaign of high-fidelity 3D simulations using WarpX, the particle-in-cell code that won the 2022 Gordon Bell Prize. The success of this project will open exciting avenues for producing high-repetition rate, high-energy, and ultrashort ion beams, bridging the gap between scientific experiments and their applications.

Type: New
Title: "MOFA: Generative AI-Driven MOF Discovery for Carbon Capture at Exascale"

Principal Investigator: Eliu Huerta, Argonne National Laboratory
Co-Investigators: Logan Ward, Argonne National Laboratory
Ian Foster, Argonne National Laboratory
Santanu Chaudhuri, University of Illinois Chicago

Scientific Discipline: Materials Science

INCITE Allocation:

Site:	Argonne National Laboratory
Machine (Allocation):	HPE Apollo 6500 (20,000 Polaris node-hours)
Site:	Argonne National Laboratory
Machine (Allocation):	HPE Cray EX - Intel Exascale Compute Blade Nodes (380,000 Aurora node-hours)
Site:	Oak Ridge National Laboratory
Machine (Allocation):	HPE Cray EX (370,000 Frontier node-hours)

Research Summary: This project will deliver MOFA, an exascale code for the discovery of new materials for carbon capture. MOFA will provide unique capabilities to enable accelerated in silico design of metal-organic frameworks (MOFs). Running at scale on Aurora and Frontier, the team will create and release a new MOF database through the Materials Data Facility, which includes MOF exemplars that are resilient to humid environments and exhibit enhanced affinity and selectivity for carbon dioxide.

MOFA will address the following grand challenges: 1) it will increase cross-platform GPU compatibility and performance by running at scale on Polaris (NVIDIA GPUs), Aurora (Intel GPUs),and Frontier (AMD GPUs); 2) it will combine generative AI, graph modeling, online learning, and Bayesian optimization to assemble MOFs with competitive properties for carbon capture, whose properties will be validated with state-of-the-art atomistic simulations; and 3) it will increase applicability for addressing materials development by rapidly converging to chemical design space regions where MOFs can be selected in terms of cost-effectiveness, synthesizability, and other manufacturing constraints. Ultimately, MOFA will enable scientists and industry partners to reduce time to solution and costs in the modeling of new materials for carbon capture by using cutting-edge generative AI and optimization methods, and robust HPC simulations in modern exascale computing environments.

Type: New
Title: "Multi-Resolution Genome Folding: Ensemble 3D Structures Across Diverse Tissues"

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

Scientific Discipline: Biological Sciences

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

Research Summary: 3D genome organization and modifications are fundamental to cellular functions. Genomic DNAs, typically 2 million base pairs long and organized into chromosomes, are compacted within a cell nucleus measuring 10-20 μm in diameter. Proper folding is crucial for maintaining nuclear organization and facilitating essential cellular processes such as gene expression regulation and cellular specialization.

To explore the relationship between genome 3D structure and function, the INCITE team will pursue a large-scale computational campaign aimed at constructing detailed 3D models of genome folding across four distinct cell types. These models will enable the team to investigate the structural basis of genome folding and its functional implications providing comprehensive maps of how genes at various loci adopt distinct spatial configurations, influence cellular states, and modulate gene expression. Additionally, they will generate highly accurate, fine-resolution ensemble models of single-cell 3D chromatin conformations for all genomic loci and diploid genomes. Their analysis will delineate tissue-specific master regulatory interactions and conserved interactions across cell types. It will also characterize chromatin structural heterogeneity by identifying major structural clusters in cell subpopulations. Moreover, the researchers will develop a high-quality database of enhancer-gene target pairs and train a machine learning predictor to identify such pairs genome-wide across various cell types. This approach is crucial for understanding genome topology, gene expression, and discovering potential causal genes for noncoding risk variants identified in genome-wide association studies.

Type: New
Title: "Nuclear Interactions from QCD"

Principal Investigator: Andre Walker-Loud, Lawrence Berkeley National Laboratory
Co-Investigators: John Bulava, DESY
Kate Clark, NVIDIA
Balint Joo, NVIDIA
Ken McElvain, University of California Berkeley
Aaron Meyer, University of California Berkeley
Henry Monge-Camacho, Oak Ridge National Laboratory
Colin Morningstar, Carnegie Mellon University
Amy Nicholson, University of North Carolina Chapel Hill
Pavlos Vranas, Lawrence Berkeley National Laboratory
Daniel Mohler, GSI
Steve Sharpe, University of Washington
Andrew Hanlon, Carnegie Mellon University
Fernando Romero-Lopez, MIT
Sungwoo Park, Lawrence Livermore National Laboratory
Renwick Hudspith, GSI

Scientific Discipline: Physics

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

Research Summary: Atomic nuclei, the building blocks of matter, provide an exciting experimental testbed for hints of new physics beyond the wildly successful Standard Model of Particle Physics (SM). Fully understanding the complex data emerging from these experimental and observational campaigns requires theoretical calculations of properties of nuclei and hadrons, the constituents of nuclei and other exotic matter, directly from the SM. Quantum Chromodynamics (QCD) is the theory of the strong force which governs the interactions underlying the formation of hadrons and nuclei. Lattice QCD, a formulation of QCD on a discretized spacetime, is currently our best tool for computing properties of matter directly from QCD, an intricate task that requires large-scale computer simulations at high-performance computing facilities. To advance our understanding of hadronic matter, this team proposes a series of unprecedented calculations using state-of-the art lattice QCD simulations to provide precise predictions about the interactions and properties of protons, neutrons, and hyperons. The results of these simulations are essential to understand the emergence of nuclear complexity from first principles. They are also critical for guiding and interpreting existing and future experimental efforts aimed at finding new physics beyond the SM, including neutrinoless double-beta decay and neutrino-nucleus scattering at DUNE. Furthermore, the insights gained from these simulations can shed light on exotic forms of matter that may be present in the extreme conditions provided by neutron stars.

Type: New
Title: "OLMo v.2.0"

Principal Investigator: Noah Smith, Allen Institute for Artificial Intelligence

Scientific Discipline: Computer Science

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

Research Summary: We seek computational resources to build an open language model, OLMo v.2.0. This effort will address the National AI Initiative's high-priority need for a widely accessible AI research cyberinfrastructure that would help to democratize the AI research and development landscape in the US, increasing diversity of talent and capacity for designing, building, and effectively using AI. Language models have the potential to transform scientific discovery, and open language models will enable broader understanding and improvement of future AI models. The rapidly advancing and transformative capabilities of these models—from synthesizing unstructured information to writing code to reasoning and solving problems—have been widely discussed, yet there is no concerted effort to steer them toward scientific use cases. Open models are the only viable way to transfer and specialize these technologies to other scientific disciplines (e.g., models trained on materials science literature and connected to relevant databases). Further, the best models currently available are proprietary and closed; direct experimentation to understand how they work is impossible for the scientific AI community, including current and next-generation researchers in the US.

Neural language models with billions of parameters and trained on trillions of words are now powering the fastest growing computing applications in history and generating discussion and debate across society. This project addresses a widely discussed need: AI scientists cannot study or improve those state-of-the-art models because the models' parameters, training data, code, and even documentation are not openly available. Building on our successful development of unique open language models (OLMo v.1.0 and v.1.7, strong models made available alongside their training data, code, and extensive documentation), the proposed model will also be made available to researchers. All components of the work will be shared along with software to support rigorous experimentation. The proposed model will be fully open to researchers along with open-source code for data management, training, inference, and interaction. Uniquely, our project emphasizes reproducibility, transparency, open data, and open evaluations, enabling the broader AI community to iterate and improve on our work to advance human-focused, trustworthy AI.

Type: Renewal
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 is using 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 are developing 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 is enhancing 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 extends 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 provide training data for SGS closures that is currently unavailable to the community. Using the DNS of a boundary layer over flat plate, they 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 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: "ORBIT: AI Foundation Model for Earth System Modeling"

Principal Investigator: Aris Tsaris, Oak Ridge National Laboratory
Co-Investigators: Dan Lu, Oak Ridge National Laboratory
Xiao Wang, Oak Ridge National Laboratory
Siyan Liu, Oak Ridge National Laboratory
Isaac Lyngaas, Oak Ridge National Laboratory
Moetasim Ashfaq, Oak Ridge National Laboratory
Jong Youl Choi, Oak Ridge National Laboratory
Dali Wang, Oak Ridge National Laboratory
Peter Thornton, Oak Ridge National Laboratory
Prasanna Balaprakash, Oak Ridge National Laboratory

Scientific Discipline: Earth Science

INCITE Allocation:
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE Cray EX (209,000 Frontier node-hours)

Research Summary: Accurately predicting the Earth system across various spatiotemporal scales is crucial for maintaining socio-ecological systems. Traditional physics-based models, while detailed, are computationally demanding and often fall short in prediction accuracy due to data integration challenges. Machine learning models trained on consistent datasets typically excel in singular modeling tasks yet lack the flexibility for diverse applications. To overcome these limitations, we developed the Oak Ridge Base Foundation Model for Earth System Predictability (ORBIT), an advanced vision-transformer model that scales up to 100 billion parameters and more than 90 climate variable channels, using a novel hybrid tensor-data orthogonal parallelism technique. As the largest model of its kind, ORBIT surpasses the current climate AI foundation model size by a thousandfold. Performance scaling tests conducted on the Frontier supercomputer have demonstrated that ORBIT's scaling efficiency is maintained at 81% to 96% across 24,576 AMD GPUs. We intend to train ORBIT to a larger scale, with a larger number of epochs, and use a larger dataset so that we can develop the largest, most efficient, and most accurate foundation model for Earth system prediction to date. These breakthroughs establish new advances in AI-driven climate modeling and demonstrate promise to significantly improve the Earth system predictability across various spatiotemporal scales.

Type: New
Title: "Probing the Primordial Universe with Exascale Simulations"

Principal Investigator: Nicholas Frontiere, Argonne National Laboratory
Co-Investigators: Michael Buehlmann, Argonne National Laboratory
JD Emberson, Argonne National Laboratory
Nesar Ramachandra, Argonne National Laboratory

Scientific Discipline: Physics

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 (1,000,000 Aurora node-hours)

Research Summary: Cosmological simulations are expanding our understanding of the early universe. Utilizing exascale computing systems, this project will conduct large-scale simulations with state-of-the-art accuracy and depth, essential for understanding primordial physics. The campaign involves running two comprehensive cosmological simulations to generate detailed synthetic galaxy catalogs. These simulations will mirror the universe's evolution and serve as critical tools for designing, optimizing, and validating analysis strategies for upcoming cosmic surveys, including the Dark Energy Spectroscopic Instrument (DESI), the Rubin Observatory's LSST, and NASA's SPHEREx mission. These surveys are set to explore fundamental questions about the universe's origins, including the nature of primordial non-Gaussianity (PNG), non-standard neutrino physics, and the dark sector. One simulation will act as a reference model, while the other, featuring PNG, will be blinded and provided to the scientific community as a challenge dataset. This approach ensures unbiased analysis and robust validation of theoretical models. Additionally, an ensemble of 32 paired simulations will create high-precision emulators for key cosmic observables, refining our understanding of the universe's initial conditions and the intricate web of cosmic structures. Performed using the Hardware/Hybrid Accelerated Cosmology Code (HACC), these simulations are optimized for supercomputing systems, ensuring efficient and scalable performance. The resulting data will offer high-fidelity predictions of galaxy properties and provide a comprehensive foundation for future research in cosmology. This project will not only advance knowledge of the universe's early stages but also exemplify the transformative potential of exascale computing in scientific discovery.

Type: New
Title: "Pushing the Frontier of Cosmic Ray Transport in Interstellar 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: Oak Ridge National Laboratory
Machine (Allocation): HPE Cray EX (600,000 Frontier node-hours)

Research Summary: We will determine the long debated source of cosmic ray scattering, which limits our understanding of galaxy formation and black hole growth, by running the largest simulations of magnetized turbulent astrophysical plasma. These simulations will adopt an anisotropic viscosity, appropriate for the low collisionality of the plasma in and around galaxies, that will allow us to study how this dissipation shapes both the magnetic and density structures. These structures are believed to play a central role in cosmic ray transport as well as the scattering of background radio sources, known as extreme scattering events. By studying both radio wave and cosmic ray transport in these groundbreaking realistic simulations we will be able to leverage the full power of the exascale computers to solve several of the most pressing unsolved questions in modern astrophysics.

Type: Renewal
Title: "QCD under Extreme Conditions"

Principal Investigator: Zoltan Fodor, Pennsylavania 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 is advancing knowledge of the phase diagram and equation of state of strong interactions, by means of first-principle simulations. The researchers' main goals are locating 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 enables them to improve the precision in the data and thus search for new phenomena, such as experimental evidence for near criticality in the QCD transition. The project continues 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 computes 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: "QMC-HAMM: High-Accuracy Multiscale Models Using Quantum Monte Carlo"

Principal Investigator: Lucas Wagner, University of Illinois
Co-Investigators: David Ceperley, University of Illinois at Urbana-Champaign
Elif Ertekin, University of Illinois at Urbana-Champaign

Scientific Discipline: Materials Science

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): HPE Cray EX - Intel Exascale Compute Blade Nodes (760,000 Aurora node-hours)

Research Summary: QMC-HAMM aims to simulate the detailed motion of electrons in materials. From these simulations, researchers then build up coarse-grained pictures of materials ranging from the interior of Jupiter, atomic-sized defects that emit and receive light, to ionic conductors to make the next highly efficient battery. INCITE resources will be used to obtain an unprecedentedly detailed picture of the motion of electrons, making our models more accurate, quantitative, and predictive. The data will be used by other researchers to improve their pictures of materials, and the models will be used to design and control the behavior of materials.

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

Principal Investigator: Mohammed AlQuraishi, Columbia University
Co-Investigators: Zhao Zhang, Rutgers University

Scientific Discipline: Biological Sciences

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): HPE Apollo 6500 (100,000 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 is leveraging 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 is using 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 are tackling 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. Their models thus have the potential to be as transformative to protein interactomes as AlphaFold2 has been to protein structure.

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: 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 (1,000,000 Aurora node-hours)
Site:	Oak Ridge National Laboratory
Machine (Allocation):	HPE Cray EX (1,00,000 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: New
Title: "Radiation General Relativistic MHD Simulations of Black Hole Coronae"

Principal Investigator: Matthew Liska, Harvard-Smithsonian Center for Astrophysicsi

Co-Investigators: Gibwa Musoke, Canadian Institute of Theoretical Astrophysics
Nick Kaaz, Northwestern University
Chris Bambic, Princeton University

Scientific Discipline: Physics

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

Research Summary: Black hole X-Ray binaries (BHXRBs) are fascinating cosmic systems where a stellar-mass black hole pulls in gas from a nearby star. This gas forms an accretion disk around the black hole, emitting mostly low-energy radiation. Alongside this disk, many BHXRBs have a corona, a super-hot, lowdensity plasma that emits high-energy radiation. The formation and behavior of this corona, especially during outbursts when BHXRBs switch between different spectral states, remain largely mysterious. In "hard" spectral states, the corona's high-energy radiation dominates, while in "soft" spectral states, the disk's low-energy radiation takes over. Understanding why the corona appears and disappears during these transitions is a significant challenge in astrophysics. Our new research proposal aims to study the evolution of the disk and corona in BHXRBs using advanced simulations running on 1000s of GPUs. These simulations will model the effects of gravity, gas dynamics, magnetic fields, and radiation in a single box. By doing so, we hope to uncover the role of magnetic fields and radiative processes in the corona and provide a clearer picture of its structure across different spectral states. This will help resolve current uncertainties and lead to a deeper understanding of black hole accretion disks and coronae. Our work will push the boundaries in scale and resolution using extremely detailed simulations featuring up to 20 billion cells. In particular, this extreme resolution will allow us to study the intricate dynamics of the movement of magnetic flux through the disk and corona. We expect that these simulations will pave the way for the next generation of simulations, providing even greater insights into BHXRBs and their fascinating observational signatures.

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 (1,300,000 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: "Scalar Transport in Turbulent Bubbly Flows: Insights from Interface-Resolved Simulations"

Principal Investigator: Parisa Mirbod, University of Illinois Chicago
Co-Investigators: Luca Brandt, Politecnico di Tornio

Scientific Discipline: Engineering

INCITE Allocation:
Site: Argonne National Laboratory
Machine (Allocation): HPE Apollo 6500 (60,000 Polaris node-hours)

Research Summary: In natural and practical applications, bubbly flows involving heat and mass transfer and chemical reactions play a critical role; yet we lack a quantitative understanding of fluxes and mixing in these turbulent flows, which is necessary to correctly predict them and produce advances in engineering technologies. A primary goal of this INCITE project is therefore to study and quantify the transport mechanisms of turbulence kinetic energy and of a diffusive scalar field in gravity-driven turbulent bubbly suspensions by using fully resolved direct numerical simulations (DNS). This implies resolving all relevant scales, including the bubble diameter, and the Kolmogorov and Bachelor scales, which correspond to the smallest vortices in the flow and the smallest scalar filaments in the flow. This research is intended to enable high performance computing (HPC) interface-resolved DNS of bubbly turbulent flows with passive scalars and realistically low values of diffusivities. Despite the multitude of applications bubbly flows have, we do not have a quantitative understanding of fluxes and mixing in turbulent flows, which is vital for correct predictions and engineering advances. Using DNS, this project studies and quantifies turbulence kinetic energy, diffusive scalar fields, and gravity-driven turbulent bubbly suspensions.

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

Principal Investigator: Adam Burrows, Princeton University
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 (3,000,000 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: "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 (450,000 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: "The progenitor-explosion connection in core collapse supernovae"

Principal Investigator: William Raphael Hix, Oak Ridge National Laboratory
Co-Investigators: Stephen Bruenn, Florida Atlantic University
James Austin Harris, Oak Ridge National Laboratory
Eric Lentz, University of Tennessee
Anthony 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: To better understand the deaths of massive stars as core-collapse supernovae, we plan a series of models to explore how the inner structure of a dying star, which is determined over the last days of the star's life, determines the power of the supernova explosion and the composition of the newly made nuclei that are ejected to form the next generation of stars and planets.

Type: New
Title: "THESAN-XL: Galaxy-Driven Large-Scale Reionization Simulations"

Principal Investigator: Oliver Zier, Massachusetts Institute of Technology
Co-Investigators: Rahul Kannan, York University
Aaron Smith, The University of Texas at Dallas
Mark Vogelsberger, Massachusetts Institute of Technology
Volker Springel, Max Planck Institute for Astrophysics
Ruediger Pakmor, Max Planck Institute for Astrophysics
Lars Hernquist, Harvard-Smithsonian Center for Astrophysics

Scientific Discipline: Physics

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

Research Summary: Understanding the formation and evolution of galaxies, the fundamental building blocks of cosmic structures, is crucial to discerning the history of the Universe. While the Hubble Space Telescope has provided extensive data on present-day galaxies, observing the initial stages of galaxy formation has been challenging. These early galaxies, formed within a billion years after the Big Bang, emitted abundant high-energy radiation that transformed the surrounding cold, neutral gas into a hot, ionized medium—a process known as cosmic reionization. Recent advancements in observational instruments such as the James Webb Space Telescope (JWST), Atacama Large Millimeter/submillimeter Array (ALMA), and Hydrogen Epoch of Reionization Array (HERA) are revolutionizing our understanding of primitive galaxies and the reionization process. This flood of data demands equally ambitious theoretical and numerical models for accurate interpretation.

The THESAN-XL project aims to meet this challenge by leveraging state-of-the-art galaxy formation models with novel radiation hydrodynamics (RHD) algorithms to simulate the coupled galaxy formation and reionization process in an extremely large volume of the Universe. This large volume will allow the study of the ionization of the intergalactic medium (IGM) on the largest scales and the investigation of rare objects that drive the patchiness of this process. Key objectives include studying the formation of massive galaxies, the impact of quasars on IGM properties, and providing longer sightlines for mock cosmological observations. These simulations will improve our understanding of Lyman-alpha forest transmission, line intensity mapping, and other signatures sensitive to large-scale ionized bubbles. Building on the original THESAN project, THESAN-XL will simulate volumes 64 and 512 times larger. This will set the stage for a new class of high-resolution, large-volume RHD simulations, providing invaluable models to accelerate our knowledge of the early Universe and help piece together a complete evolutionary picture of cosmic structure formation.

Type: Renewal
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): HPECray 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: "Trustworthy and Scalable Artificial Intelligence-Driven Modeling of Molten Salts"

Principal Investigator: Vyacheslav Bryantsev, Oak Ridge National Laboratory
Co-Investigators: Luke Gibson, Oak Ridge National Laboratory
Santanu Roy, Oak Ridge National Laboratory
Ada Sedova, Oak Ridge National Laboratory
Guannan Zhang, Oak Ridge National Laboratory
Lillian Chong, University of Pittsburgh

Scientific Discipline: Chemistry

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

Research Summary: The overarching goal of this proposal is the development of an open-source workflow that integrates cutting-edge, generative artificial intelligence (AI) methods with state-of-the-art, explicitly correlated, quantum mechanical (QM) calculations and molecular dynamics (MD) simulations to enable highly accurate modeling and efficient design of molten salts (MSs) systems. The proven success will simplify the costly, challenging, and time-consuming task of building experimental thermochemical and thermophysical databases for MSs by augmenting them with validated, high-quality, computational data. Aim 1 is to leverage ORNL-developed generative AI models, such as diffusion models, along with enhanced sampling workflows, to efficiently explore configurational space and enhance the development of machine learning interatomic potentials (MLIPs) by active learning through adaptive updates to the generative AI models. Aim 2 delves into improving the accuracy of MLIPs beyond the conventional density functional theory (DFT) calculations with highly accurate QM methods, such as Quantum Monte Carlo (QMC). The delta learning framework will be developed to use generative AI models to efficiently select from configurational space and minimize the number of expensive calculations required to correct for the differences between the energies and forces of the low-level and high-level QM methods. We will use Frontier at scale to develop, test, and deploy MLIPs trained on highly accurate QMC data, with the aim of creating a refinable foundational model able treat a wide range of MS compositions, temperatures, and mixtures. Aim 3 focuses on applying established and more advanced simulation techniques, such as thermodynamic integration (TI), for computing key thermodynamic and transport properties of molten salts compositions that are vital for different Molten Salt Reactor (MSR) concepts. The power of DOE leadership computing will be used to dramatically accelerate the development of new MS compositions and deployment of advanced nuclear energy technologies.

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

Principal Investigator: Jeremy Smith, University of Tennessee/Oak Ridge National Laboratory

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
Yan Yu, Oak Ridge National Laboratory

Scientific Discipline: Energy Technologies

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

Research Summary: Cellulose nanofibers (CNFs) are outstanding candidates for sustainable high-performance biocomposite applications using large-scale additive manufacturing (AM) with a low carbon footprint compared to traditional reinforcing materials. However, a major challenge in the assembly of CNF nanocomposites is their irreversible aggregation upon drying, resulting in degradation of their mechanical strength which requires them to be stored in highly dilute solutions, increasing transportation costs significantly. A lack of fundamental understanding of the physicochemical and thermodynamic forces that play a role in CNF aggregation hinders the rational design of co-solvents and surface modifications to reduce the inter-CNF interactions and increase dispersion in polymer matrices. Here, we will determine the structure, energetics, and thermodynamics of native and surface-modified CNFs during drying in candidate solvents with varying hydrogen bonding capabilities using enhanced sampling atomistic molecular dynamics (MD) simulations. The use of the FRONTIER supercomputer will permit multiple CNFs to be studied in solution. Further, coarse-grained simulations will be performed for micron-scale systems derived from the atomistic models to determine the microsecond time-scale CNF aggregation dynamics. Our findings will provide a molecular-level understanding of the thermodynamic forces and kinetic pathways that drive aggregation/dispersion of native and acetylated CNFs in various solvents during drying. The simulations will help guide the rational design of solvents and surface modifications that can tune CNF assembly in biocomposites for the circular bioeconomy.

Type: Renewal
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 (1,000,000 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.

Type: New
Title: "Using Exascale Computing for New Insights into High-Lift Ground Testing"

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 (500,000 Aurora node-hours)

Research Summary: Given the critical role of the U.S. commercial aviation industry in our national economy, it is imperative that the nation maintains its leadership in this area on the world stage. The ability to successfully and reliably predict high-lift flows experienced by modern transport aircraft is a top priority for the technical community. To certify a new aircraft for commercial service, manufacturers must demonstrate compliance with regulatory requirements, many of which focus on high-lift performance such as takeoff and landing. Historically, these requirements have been met through ground- and flight-test certification campaigns. The financial burden associated with such endeavors is estimated at nearly one billion U.S. dollars per aircraft design. However, regulatory agencies may accept computational results as a substitute for test data if the approach can be shown to be reliably accurate. In this INCITE effort, a NASA team is aiming to execute a computational campaign carefully coordinated with an ongoing series of wind-tunnel tests taking place at the National Transonic Facility located at NASA Langley Research Center. These activities support an important NASA milestone to be reported to Congress. The exascale-class Aurora system offers unique and timely computational power to tackle the challenging physics associated with high-lift flows. Successful execution of this effort offers the potential to dramatically reduce costs associated with extensive physical testing campaigns, accelerating the time to market for new aircraft designs and ultimately ensuring that the U.S. remains positioned at the forefront of the global aviation community.