



Type: New
Title: "Ab Initio Foundation Models for Riboswitch Inhibitors in RNA-Targeted Therapeutics"

Principal Investigator: Jean-Philip Piquemal, Sorbonne University
Co-Investigators: Kevin Gasperich, Qubit Pharmaceuticals Inc.
Louis Lagardere, Sorbonne University
Krystel El Hage, Qubit Pharmaceuticals Inc.

Scientific Discipline: Chemistry

INCITE Allocation:

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

Research Summary: This project brings the power of next-generation supercomputers directly to the front lines of drug discovery, targeting two of medicine's toughest challenges: RNA-based regulation and metal-containing therapies. Riboswitches are tiny RNA "switches" inside bacteria and human cells that turn genes on or off when they bind specific molecules or metal ions. Because of their precision and specificity, riboswitches offer a path to new antibiotics and anticancer drugs, but their behavior depends on subtle, hard-to-predict quantum effects.

The team will use the nation's fastest machines to generate the world's most detailed quantum dataset of RNA-ion interactions (magnesium, calcium, zinc) and metal-drug-DNA complexes (such as the chemotherapy agent cisplatin). The researchers will build and validate an unprecedented library of ion-binding data using cutting-edge Quantum Monte Carlo simulations. Those results will train FeNNix-Bio, the team's specialized foundation model, to predict how charge transfer, polarization, and metal coordination shape molecular function. By capturing the full quantum nature of these interactions, their approach will drastically reduce the time and cost needed to identify promising drug candidates. Researchers everywhere will gain a publicly accessible computational platform that delivers — for the first time — reliable, high-accuracy predictions for riboswitch inhibitors and metal-based therapeutics. In doing so, this work will accelerate the development of safer antibiotics, more effective cancer treatments, and ultimately pave the way for personalized medicines that harness the fundamental rules of quantum chemistry.



Type: New
Title: "Ab Initio Theory Derived High-Fidelity Kinetics Databases"

Principal Investigator: Sarah Elliott, Argonne National Laboratory
Co-Investigators: Clayton Mulvihill, Baylor University
Luna Pratali Maffei, Politecnico di Milano
Andreas Copan, University of Georgia
Carlo Cavallotti, Politecnico di Milano
Yuri Georgievski, Argonne National Laboratory

Scientific Discipline: Chemistry

INCITE Allocation:

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

Research Summary: Gas-phase chemical kinetic modeling is paramount in numerous applications, including atmospheric chemistry, particle synthesis, combustion, pyrolysis, plasmas, chemical vapor deposition, and astrochemistry. These kinetic models are used to better understand the global chemical conversions occurring in these environments and thereby help optimize the devices and processes of interest. Underlying such modeling efforts are chemical kinetic mechanisms, which can comprise thousands of species participating in many thousands of reactions. Existing chemical mechanisms are often largely empirical in nature, being derived from fairly crude rate rules. This empiricism severely limits their predictive capabilities outside their explicit range of validation. Ultimately, researchers would like to use AI to develop improved mechanisms, but effective AI requires much more substantive and accurate databases of rate constants than currently exist.

To remedy this situation, this project proposes to generate large-scale state-of-the-art first-principles theory-based kinetics databases using the Argonne Leadership Computing Facility's Aurora exascale supercomputer. The team's open source code, AutoMech, will first be utilized to assimilate the data from several publicly available databases of structures and energies, which will then be improved through higher-accuracy quantum chemical calculations. The improved energetic data will then be transformed into a database of rate constants and thermochemical properties (the building blocks of kinetic mechanisms) through master equation simulations with the team's MESS code. Moreover, this kinetic database will be greatly expanded to better represent radicals, whose reactions play a central role in chemical conversion processes. Through the unique capabilities of the ALCF, an unprecedented number of reactions will be studied at the highest feasible levels of accuracy. The open-source database generated in this project will enable enhanced simulations in a wide range of applications. Furthermore, it is expected to reveal exciting new possibilities for the development of effective AI models for gas-phase kinetics.



Type: New
Title: "Ab-initio Nuclear Structure and Nuclear Reactions"

Principal Investigator: Gaute Hagen, Oak Ridge National Laboratory
Co-Investigators:

Scientific Discipline: Physics: Nuclear 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 (1,200,000 Aurora node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE Cray EX (1,000,000 Frontier node-hours)

Research Summary: This proposal targets experiments and science at ATLAS (Argonne National Laboratory), the Facility for Rare Isotope Beams (FRIB), CEBAF (Jefferson Laboratory), the Deep Underground Neutrino Experiment (DUNE), and the ton-scale detector (LEGEND-1000) for neutrinoless double beta-decay. We are targeting the science outlined in 2023 the Long-Range Plan for Nuclear Science, and will enable science not available previously and accelerate scientific discovery through high-performance computing. The proposed computations will lead to significant improvements in the simulation capabilities of atomic nuclei and nuclear matter, and their reactions with neutrinos and electrons. We will advance our understanding of nuclear phenomena by targeting predictive capabilities regarding structure and reactions of light nuclei and few-nucleon systems, precision calculations of nuclear matrix elements for fundamental symmetries, neutrino and electron interactions in nuclei, and properties of nuclei and nuclear matter. We will employ advanced ab initio quantum many-body techniques coupled with applied mathematics and computer science methods targeted for efficient use of large-scale high performance computing environments. We will also perform state-of-the-art simulations to provide quantified predictions where direct experiment is not possible or is subject to large uncertainties. Such calculations are relevant to many applications in nuclear energy, nuclear security, and nuclear astrophysics, since rare nuclei lie at the heart of nucleosynthesis and energy generation in stars.



Type: New
Title: "AbacusAurora: N-Body Simulations for a New Generation of Cosmic Surveys"

Principal Investigator: Daniel Eisenstein, Harvard University
Co-Investigators: Sownak Bose, Durham University
Joseph DeRose, Lawrence Berkeley National Laboratory
Benedikt Diemer, University of Maryland
Lehman Garrison, Flatiron Institute
Boryana Hadzhiyska, Lawrence Berkeley National Laboratory
Alexander Johnson, Harvard University
Alexie Leauthaud, University of California Santa Cruz

Scientific Discipline: Physics: Astrophysics

INCITE Allocation:

Site: Argonne National Laboratory
Machine (Allocation): HPE Cray EX - Intel Exascale Compute Blade Nodes (510,000 Aurora node-hours)

Research Summary: We will produce the world's largest cosmological N-body simulation, a flagship run of 35 trillion particles designed to model the cosmological large-scale structure of the coming generation of observational surveys. Such simulations are a key component of cosmological analyses, used to connect the underlying theory to the complexity of late-time clustering, to estimate both statistical and systematic errors, and to design novel statistics. Building on our past AbacusSummit suite, the AbacusAurora project will leverage the speed and accuracy of the Abacus code as well as our past experience in generating feature-rich and highly used data products. An important opportunity of these new simulations is the deployment of a novel framework for the assignment of mock galaxies to such simulations, which we use to address key shortcomings in past modeling. We expect that the merger trees resulting from this framework will be of great utility in modeling the clustering bias and assembly bias of a wide range of galaxy populations. This flagship simulation will cover the huge volume of modern surveys while preserving sufficient mass resolution to track the array of smaller galaxies that allow these surveys to obtain a sharper view of large-scale structure. We will provide outputs both in time slices and along light cones so as to provide easy connections to observational modeling. A companion suite of 200 smaller simulations will allow us to explore the dependence of results on cosmological parameters. Through AbacusAurora, we will provide the simulation foundation sought by a wide range of analyses of dark energy, dark matter, and general cosmology.



Type: New
Title: "Advanced Computational Modeling of Molecular Machines in Nucleotide Excision 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: Understanding genome maintenance at the molecular level, is a grand challenge for structural biology and biomedicine. Our INCITE project leverages recent experimental breakthroughs from cryo-electron microscopy, advances in GPU-accelerated computing and new integrative modeling methods to address the above long-standing grand challenge specifically for the nucleotide excision repair (NER) genome maintenance pathway. By harnessing the computational power of Frontier, we aim to generate predictive, atomic-resolution models of nucleotide excision repair complexes and uncover the principles that govern genome maintenance and disease susceptibility. Mechanistic understanding of NER will not only advance basic science but also inform strategies for cancer therapy, genotoxic stress response, and precision medicine.



Type: New
Title: "Advanced Simulations of Multi-Orbital Superconductors"

Principal Investigator: Thomas Maier, Oak Ridge National Laboratory
Co-Investigators: Steven Johnston, University of Tennessee
Philip Dee, 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 (840,000 Frontier node-hours)

Research Summary: This project will perform advanced simulations of correlated quantum materials to deliver unprecedented understanding of their exotic emergent properties, focusing on multi-orbital superconductivity induced by strong electronic interactions. By using state-of-the-art quantum manybody approaches and leveraging leadership-class exascale computing, the simulations will properly account for the competing interactions in these systems and deliver unprecedented understanding of how their intricate balance gives rise to the emergence of exotic phases such as superconductivity.

The delicate balance between strong and competing interactions in correlated quantum materials and their ensuing nearly degenerate energy landscape give rise to complex many-body dynamics and entanglement, leading to novel emergent phases like superconductivity, quantum spin liquids, and topological states. These exotic properties can have revolutionary impact on many technologies, ranging from next-generation microelectronic devices to energy-efficient power transmission solutions to novel quantum information systems. The key challenge is to understand and reliably predict the behavior of quantum materials to accelerate discoveries of new materials with optimized properties. This goal can only be achieved by using leadership computing and efficient implementations of manybody methods that can treat the complex interactions accurately and resolve the nearly degenerate energy landscape driving the behavior of these materials.

By using a state-of-the-art dynamic cluster quantum Monte Carlo implementation, this project will leverage leadership computing on the Department of Energy's Frontier supercomputer to push the limits of quantum materials simulations and provide new insight into multi-orbital superconductivity in nickelate and copper-oxide materials by delivering physical models that describe the mechanism for superconductivity in these systems. At a broader level, the project will help uncover how the intricate interplay between strong correlations and orbital degrees of freedom leads to emergent phenomena in quantum materials. This type of information is critical for accelerating the path to discovery of new materials with optimized properties and their deployment in advanced energy-related technologies.



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

Principal Investigator: Andreas Kronfeld, Fermi National Accelerator Laboratory
Co-Investigators: Thomas Blum, University of Connecticut
Peter Boyle, Brookhaven National Laboratory
En-Hung Chao, Columbia University
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
Shaun Lahert, University of Utah
Christoph Lehner, University of Regensburg
Andrew Lytle, University of Illinois Urbana-Champaign
Robert Mawhinney, Columbia University
Ethan Neil, University of Colorado

Scientific Discipline: Physics

INCITE Allocation:

Site: Argonne National Laboratory
Machine (Allocation): HPE Cray EX - Intel Exascale Compute Blade Nodes
(2,000,000 Aurora node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE Cray EX (1,000,000 Frontier node-hours)

Research Summary: Starting from the Standard Model of elementary particles, this project performs high-precision numerical calculations, so that the results can be compared with results of high-precision experiments. Any discrepancies between theory and experiment will provide clues for as-yet undiscovered physical processes at work. We use the lattice gauge theory formulation of quantum chromodynamics (QCD), which is the modern theory of the strong nuclear force. The lattice formulation allows a mathematically rigorous, computationally feasible and improvable approach to obtaining reliable estimates of properties of hadrons, such as proton, neutrons, and more exotic particles (such as those studied in our work). The results of this project are needed to interpret many experiments carried out at particle accelerators. These include measurements of the anomalous magnetic moment of the muon, which is sensitive to quantum imprints from all known and unknown particles. Other facets of our project—namely decays of B and K mesons and of the tau lepton—are also sensitive to as-yet unknown force. The calculations have been carefully selected for their impact on 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: Renewal
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
Daniel Moore, Lawrence Livermore National Laboratory
Omar Hussien, Lawrence Livermore National Laboratory
Ian Winter, Lawrence Livermore National Laboratory

Scientific Discipline: Materials Science

INCITE Allocation:

Site: Argonne National Laboratory
Machine (Allocation): HPE Apollo 6500 (100,000 Polaris node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE Cray EX (500,000 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: Renewal
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 many-body systems governed by the laws of quantum mechanics, especially systems containing transition metals, represent a grand challenge in computational science. The combination of methodological developments and the advent of petaflop and exascale computing presents a unique opportunity to make fundamental progress on this problem. This renewal aims to continue our work in simulating strongly correlated systems containing transition metals in biology, such as the oxygen-evolving complex (OEC) of Photosystem II (PSII) and FeMoCo core of Nitrogenases. A second, complementary goal is to provide $O(1000)$ theoretical reference values for a broad range of observables for both main group and transition metals species, which will be crucial in developing faster approximate methods (particularly Density Functional Theory (DFT)-based) approaches to produce reliable predictions on systems on the order of thousands atoms.



Type: New
Title: "AI-Controlled Adaptive Modeling of Subsurface Geothermal Systems"

Principal Investigator: David Trebotich, Lawrence Berkeley National Laboratory
Co-Investigators: Marcus Noack, Lawrence Berkeley National Laboratory
Sergi Molins, Lawrence Berkeley National Laboratory

Scientific Discipline: Engineering

INCITE Allocation:

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

Research Summary: Enhanced geothermal systems (EGS) represent a promising approach that can provide new methods to access Earth's internal heat. Extracting heat from deep rock formations has traditionally required a rock mass that is both naturally hot and permeable so that hot fluids could be produced at commercially interesting rates. Lacking sufficient permeability in hot rock, the approach in EGS is to enhance permeability through the use of stimulation methods so as to create a fracture network through which fluid can flow and from which heat can be extracted. The promise of Enhanced Geothermal Systems (EGS) is effective, economic, and at-scale recovery of the heat that is ubiquitously available at depth. The challenge of EGS is to create an engineered circulation system, inexpensively, at-will, anywhere, that is robust, long-lived, and has minimal environmental impact. This typically requires elevating distributed fracture permeability from the sub-microDarcy to milliDarcy levels, maintaining permeability, and using methods guaranteed to be successful and independent of the subsurface environment.

The overall goal of this project is to simulate the multiphysics processes involved in flow and heat transfer in subsurface fractures relevant to geothermal energy extraction. Conventional subsurface modeling occurs at the reservoir, or field scale, comprising a continuum model with averaged bulk properties that takes an effective medium approach to subsurface heterogeneity. However, the success of geothermal energy extraction relies on stimulated fracture networks that create and maintain explicit fluid contact with heterogeneous hot rock. Sustained permeability in these fracture networks would be ideal but the actual subsurface conditions are far from a consistent bulk property due to heterogeneous nature of fractured systems. Therefore, we propose a capability that would allow for explicit pore scale resolution of these fracture networks, yielding more accurate prediction of the thermal energy that can be extracted from surrounding hot rock. Our capability is based on an efficient hybrid pore-continuum model that is optimized to align pore scale resolution only with long narrow fractures of finite aperture while leaving the interstitial hot rock between fractures at a more computationally-efficient coarse, continuum model (Darcy). In addition, we include outer loop AI-control of inner loop forward simulation that adapts the continuum model to local pore scale subsurface conditions.



Type: New
Title: "AI-facilitated Global Profile Prediction in Tokamak Plasma"

Principal Investigator: Robert Hager, Princeton Plasma Physics Laboratory
Co-Investigators: Seung-Hoe Ku, Princeton Plasma Physics Laboratory

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation:

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

Research Summary: This INCITE project aims to enable first-principles prediction of temperature and density profiles across fusion devices, from the plasma core to plasma-facing components. It addresses the limitations of current scaling laws and reduced fluid models by combining exascale computing on Frontier and Aurora with advanced core and edge plasma algorithms. The approach couples a machine-learned surrogate—trained on PORTALS/CGYRO core simulations—with iterative edge calculations using the full-f XGC code. The surrogate provides fast inner boundary conditions, while XGC resolves scrape-off-layer physics, impurity radiation, and exhaust-heat handling.

Using techniques such as time-telescoping, adaptive turbulence seeding, and ML-accelerated convergence, the project seeks to find steady-state profiles efficiently. Deliverables include a verified workflow for Aurora, a library of core–edge simulations for future tokamak and spherical-tokamak concepts, and an open, compressed dataset for AI tools. The results will help guide pilot-plant design by providing quantitative predictions of heat-flux limits, impurity tolerances, actuator requirements, and achievable fusion gain, while establishing a scalable, mixed-fidelity framework applicable to future fusion devices.



Type: Renewal
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 Cray EX - Intel Exascale Compute Blade Nodes (3,000,000 Aurora node-hours)

Site: Argonne National Laboratory

Machine (Allocation): HPE Apollo 6500 (75,000 Polaris 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: New
Title: "Building SOTA Foundation Models for Precision and Preventive Medicine"

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

Scientific Discipline: Biological Sciences: Medical 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 (700,000 Frontier node-hours)

Research Summary: Clinical large language models (LLMs) have the potential to advance medical science by enabling more accurate characterization of patient populations and supporting early detection of disease progression. However, current clinical LLMs are limited by short context windows and insufficient exposure to long-term, comprehensive health histories, restricting their ability to model the complex temporal patterns present in real-world clinical data.

Through a partnership between the Department of Energy (DOE) and the Department of Veterans Affairs (VA), this project leverages more than 20 years of electronic health record (EHR) data from millions of Veterans. Using an INCITE allocation, we developed two VA-specific LLMs—a 1.62B-parameter and a 13.6B-parameter model—pre-trained entirely on VA data and now being fine-tuned on four major clinical applications. Despite this progress, their 4,096-token context window allows them to process only a small portion of average patient histories, which commonly exceed 126,000 tokens.

To overcome these limitations, this project will scale clinical LLMs using exascale computing resources. We will develop the X-FORGE platform for efficient training, build a 100-billion-parameter energy-efficient foundation model capable of handling long EHR contexts, and apply the resulting model to two high-impact tasks: identifying patients at elevated risk of suicide and modeling frailty progression. The project will also develop explainability techniques to support clinical interpretation and ensure transparent model behavior for VA clinicians.



Type: New

Title: "Characterizing the Effect of Drugs Targeting the Elevator Transport Mechanism"

Principal Investigator: Emad Tajkhorshid, University of Illinois Urbana-Champaign

Scientific Discipline: Biological Sciences

INCITE Allocation:

Site: Oak Ridge National Laboratory

Machine (Allocation): HPE Cray EX (1,200,000 Frontier node-hours)

Research Summary: Transporters are proteins that act as cellular gatekeepers, allowing small molecules to cross the mostly impermeable membranes that surround cells and organelles. Because of their central role in cellular function, transporters are common targets for pharmaceutical drugs, and transporter malfunction is often associated with disease. The translocation of small molecules across membranes by transporters is achieved through coordinated, large-scale conformational changes, which are grouped into a handful of canonical transport mechanisms. A representative "elevator"-type transporter is NaCT, a human citrate transporter that has been implicated as a potential drug target for treatment of obesity and type 2 diabetes. Using an advanced molecular dynamics (MD)-based approach previously developed in our lab and resources provided by a SummitPLUS award, we recently structurally and thermodynamically characterized the elevator mechanism of NaCT. Cryoelectron microscopy structures solved in the lab of our collaborator Da-Neng Wang (New York University) have recently captured NaCT with two drug-like compounds bound to two distinct locations: (1) in the central binding pocket of NaCT and (2) at an allosteric site, wedged between two mobile domains of NaCT. We here propose using our MD-based approach to characterize in detail how these two compounds perturb the elevator transport mechanism of NaCT. The inhibitor binding sites of NaCT represent two unique drug targeting strategies that are relevant to all elevator transporters, and our results will offer key insights into the relative effectiveness of these two strategies.



Type: New
Title: "COMbining Deep-Learning with Physics-Based AffinIty EstimatiOn 4 (COMPBIO4)"

Principal Investigator: Peter Coveney, University College London
Co-Investigators: Shantenu Jha, Pacific Northwest National Laboratory
Philip Fowler, University of Oxford
Ola Engkvist, Astra Zeneca
Eric Stahlberg, MD Anderson Cancer Center
Mariano Vazquez, ELEM Biotech
Dilip Asthagiri, Oak Ridge National Laboratory
Antigoni Georgiadou, Oak Ridge National Laboratory
Francis Joseph Alexander, Argonne National Laboratory
Tom Beck, Oak Ridge National Laboratory
Rick L Stevens, Argonne National Laboratory

Scientific Discipline: Biological Sciences: Medical Science

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

Research Summary: The advent of exascale computing and advances in artificial intelligence (AI) have opened up immense possibilities to realize a fully personalized digital twin (DT) of the human body. DT technology will not only enable clinicians to make reliable and actionable predictions to support clinical decision-making, but it will also facilitate the adoption of informed lifestyle choices that support healthy ageing and well-being. However, achieving this aim is challenging.

To address this challenge, our research goal is to advance the modeling and simulation of the human body in health and disease such that we 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. We aim to combine multiple scales of human biology through simulation combined with AI to deliver actionable outcomes in the medical context. In this project, we focus our attention on two specific use cases of human DTs at two different scales: (a) drug discovery and personalized medicine (molecular scale) and (b) hemodynamics (organ scale).



Type: New
Title: "Computational Prediction of Phase Diagrams for Metallic Alloys"

Principal Investigator: Rodrigo Freitas, Massachusetts Institute of Technology

Scientific Discipline: Materials Science

INCITE Allocation:

Site: Oak Ridge National Laboratory
Machine (Allocation): HPE Cray EX (544,768 Frontier node-hours)

Research Summary: Phase diagrams are essential tools in materials science. They map out the conditions under which different phases of a material are stable—information that is critical for designing new materials, understanding their behavior during processing, and optimizing their performance in applications ranging from jet engines to microelectronics. Despite their importance, experimentally measured phase diagrams are only available for a small fraction of known materials, and virtually none exist for the complex alloys that dominate modern materials research, such as high-entropy alloys and other multicomponent systems.

This project aims to address that gap using a fully predictive, computational approach. By combining machine learning with physics-based modeling and large-scale molecular simulations, we will calculate accurate phase diagrams directly from quantum mechanics—without relying on any experimental fitting or empirical parameters. Our approach uses machine-learned interatomic potentials trained on density functional theory data, along with advanced methods for calculating thermodynamic free energies across temperature and composition. This enables the prediction of phase stability for materials that have never been synthesized, and for which experimental phase data is not available.

Using the Frontier supercomputer at Oak Ridge National Laboratory, we will generate more than 2,500 new phase diagrams for binary, ternary, and quaternary alloys. These include key structural materials such as refractory metals, lightweight alloys, and high-temperature alloys relevant to aerospace and energy systems. The results will form the largest collection of first-principles-based phase diagrams ever produced. All data will be made publicly available, providing a new foundation for materials discovery and design. This project has the potential to transform how we explore material systems—replacing time-consuming trial-and-error with predictive modeling at unprecedented scale and fidelity.

Type: New

Title: "Digital Twins of Heterogeneous Reaction Dynamics in Catalysts and Batteries"

Principal Investigator: Boris Kozinsky, Harvard University

Co-Investigators: Joonho Lee, Harvard University, Chuck Witt, Harvard University

Scientific Discipline: Materials Science: Nanoscience

INCITE Allocation:

Site: Argonne National Laboratory

Machine (Allocation): HPE Cray EX - Intel Exascale Compute Blade Nodes (430,000 Aurora node-hours)

Site: Argonne National Laboratory

Machine HPE Apollo 6500 (150,000 Polaris node-hours)

(Allocation):Site: Oak Ridge National Laboratory

Machine (Allocation): HPE Cray EX (400,000 Frontier node-hours)

Research Summary: Heterogeneous reactions are central to the materials and devices that underpin modern energy technologies. Thermal catalysis is vital for hydrogen production, and catalytic chemical manufacturing consumes a major share of global industrial energy. Li-ion batteries have become key systems for stationary and transportation energy storage, and heterogeneous or surface reactions also govern ceramic synthesis, metallurgical microstructure evolution, and nanomaterial deposition. Yet the atomistic interfacial processes that drive performance and degradation in batteries and catalysts remain poorly understood because experimental techniques cannot probe them with sufficient resolution.

Molecular dynamics simulations can reveal these mechanisms, and machine-learning interatomic potentials (MLIPs) are increasingly used to support such simulations. However, MLIP accuracy is limited by errors in density functional theory (DFT) training data, especially for catalyst surface reactions and electrochemical processes. To address these limitations, the project will use the phaseless auxiliary field quantum Monte Carlo (ph-AFQMC) method, a highly accurate many-body approach suited to large-scale computation. The resulting data will enable predictive, foundation-level MLIP models.

Using these improved MLIPs, the project will provide atomistic insight into interfacial reactions in two key areas: (1) ionic transport, chemical evolution, and micromechanical processes at Li-ion solid electrolyte–electrode interfaces involving Li anodes and layered oxide cathodes with sulfide electrolytes; and (2) the geometry, stability, and evolution of active sites in Pt/CeO₂ nanoparticle catalysts under realistic water–gas shift reaction conditions.

These simulations will deliver quantum-accurate, atomic-scale understanding at realistic electrode dimensions, offering critical insight for mitigating battery degradation and improving catalytic performance in energy storage and chemical conversion.



Type: New
Title: "DNS of Flameholding in Cavity Stabilized Hypersonic Combustion"

Principal Investigator: Jackie Chen, Sandia National Laboratories
Co-Investigators: Pino Martin, Dridam LLC
Cristian Lacey, Sandia National Laboratories
David Muir, Dridam Consulting, LLC

Scientific Discipline: Chemistry

INCITE Allocation:

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

Research Summary: Supersonic combustion ramjet (scramjet) engines are one of the few types of propulsion devices that can reach hypersonic speeds. However, these engines face several challenges that make them difficult to operate effectively. One major issue is that the time available for mixing fuel and air is very short, which can lead to uneven burning and unstable flames. Additionally, the flow of air and fuel can become chaotic, causing fluctuations that create areas with too much or too little fuel, affecting how well the engine burns the fuel. To address these challenges, we will perform a detailed study using advanced computer simulations to better understand how turbulence and chemical reactions interact in scramjet engines. We plan to test different conditions by changing the mixture of fuel and air and the velocity of the air entering the combustor relative to that of the injected fuel. This will capture the physical mechanisms that influence flame stability and the overall performance of the engine. The datasets generated from these simulations will be valuable for improving existing predictive models of scramjet engines with machine learning-based closure models. Moreover, this information will be shared with the scientific community to help augment foundation models for science.



Type: New
Title: "DNS of Shock-Induced Instabilities Over Hypersonic Control Surfaces"

Principal Investigator: Carlo Scalo, Purdue University
Co-Investigators: Lian Duan, The Ohio State University

Scientific Discipline: Domain: Engineering

INCITE Allocation:

Site: Argonne National Laboratory
Machine (Allocation): HPE Cray EX - Intel Exascale Compute Blade Nodes
(315,000 Aurora node-hours)
HPE Apollo 6500 (150,000 Polaris node-hours)

Research Summary:

The INCITE proposal aims to generate a Direct Numerical Simulation (DNS) dataset to study shock wave boundary layer interactions (SWBLI), starting with a ramp configuration and later the High-Speed Army Reference Vehicle (HARV). These simulations involve billions of grid points and millions of iterations, requiring top-tier supercomputers due to their computational demands. A highly scalable block-spectral code, upgraded for multi-platform use and tested on ALCF's Polaris and Aurora systems, will perform the computations, demonstrating nearly perfect weak scaling up to 512 Aurora nodes—sufficient for the HARV's fine mesh.

The resulting dataset will improve understanding of turbulence onset from shock waves on both simple and complex geometries, with implications for hypersonic vehicle design and thermal management. Analysis of subfilter-scale quantities will support the development of new LES and wall-modeled LES (WMLES) models, as wall-resolved LES remains unreliable under extreme flow conditions. The work builds on Dr. Scalo's extensive experience in turbulence modeling and shock-capturing methods for hypersonic flows.

The dataset will be shared through publications, conferences, and a public SFTP server hosted by Dr. Scalo's lab. It may also aid in developing or replacing CFD solvers with machine learning-based turbulence modeling methods.



Type: Renewal
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 (400,000 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: Renewal
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.

Over the past year, our INCITE project has yielded substantial progress in uncovering how drugs that bind to a G protein-coupled receptor (GPCR) can selectively stimulate certain intracellular signaling pathways without stimulating other pathways controlled by the same GPCR. These results will facilitate the rational design of safer and more effective therapeutics for chronic pain and other diseases. By harnessing Frontier's exceptional computational capabilities, we have conducted large-scale molecular dynamics simulations that revealed previously uncharacterized mechanisms by which a GPCR can selectively stimulate different G protein subtypes, depending on which drug is bound to the GPCR. For example, we identified a distinct active conformation (structure) of an opioid receptor that couples more favorably to the G protein Gz than to other G proteins. This previously unobserved Gz-favoring conformation provides atomic-level insight into how to design a drug to selectively stimulate Gz, or to selectively avoid stimulating Gz. We have made efficient use of our current allocation, optimized the performance of our simulation code, and established a streamlined analysis workflow. Specifically, we have significantly reduced the memory footprint of our multidimensional replica exchange molecular dynamics (M-REMD) simulations, enabling very efficient parallel execution on over 20,000 GCDs. Building on these accomplishments, we are well-positioned to continue this research at leadership-class scale in the upcoming allocation year. To maximize the impact of our computational studies, we maintain close collaborations with world-class experimental groups at multiple institutions, allowing us to use our computational results to design drug candidates and guide pharmacological experiments.



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

Principal Investigator: Aaron Donahue, Lawrence Livermore National Laboratory
Co-Investigators: Chris Terai, Lawrence Livermore National Laboratory
Mark Taylor, Sandia National Laboratories
Thomas Clevenger, Sandia National Laboratories
Naser Mahfouz, Pacific Northwest National Laboratory
Walter Hannah, Lawrence Livermore National Laboratory
Peter Bogenschutz, Lawrence Livermore National Laboratory
Peter Caldwell, Lawrence Livermore National Laboratory
Ruby Leung, Pacific Northwest National Laboratory
Azamat Mаметjanov, Argonne National Laboratory
Sarat Sreepathi, Oak Ridge National Laboratory
Susannah Burrows, Pacific Northwest 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 (600,000 Frontier node-hours)

Research Summary: SCREAM is a global atmospheric model designed to operate at kilometer-scale resolutions. By utilizing a resolution 30 times finer than most other models, SCREAM delivers more precise predictions and offers detailed, location-specific insights essential for understanding both local and global atmospheric phenomena. However, this high level of detail requires significant computational power, limiting its use to leadership-class computational systems. The objective of this project is to evaluate SCREAM using real-world simulations over the continental United States at an unprecedented 200-meter resolution.



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

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

Scientific Discipline: Earth Science

INCITE Allocation:

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

Research Summary: Major earthquakes continue to pose a significant risk to urban infrastructure and critical facilities, presenting ongoing challenges across the Department of Energy mission space. Traditional seismic hazard assessments rely on empirical models derived from limited historical ground motion records, often from distant locations. While these models offer broad statistical estimates, they are unable to capture the complex spatial variability of ground motions driven by rupture dynamics, wave propagation through heterogeneous geologic media, and local site conditions. Recent advances in high-performance computing have made physics-based simulations a viable and increasingly important alternative. The Earthquake SIMulation (EQSIM) framework, developed through the DOE Exascale Computing Project, enables high-resolution, physics-based regional-scale simulations of large earthquakes in realistic three-dimensional geologic settings at frequencies up to 10 Hz. EQSIM integrates rupture modeling, seismic wave propagation, and infrastructure response within a scalable workflow optimized for GPU-accelerated exascale platforms such as Frontier. Building on previous large-scale simulations, including magnitude 7.0 events on the Hayward fault and a limited number of magnitude 7.5 San Andreas fault rupture scenarios, this project will focus on expanding simulations of large earthquakes on the San Andreas fault, and initiate new simulations for the New Madrid and Newport Inglewood faults. The proposed simulations will provide extensive data that are key to understanding and predicting regional ground motion variability, and region-specific infrastructure risk. The results of our simulations are expected to significantly increase the applicability of the physics-based deterministic approach to seismic hazard assessment and to resilience improvements of the DOE critical infrastructure. All results will be included in the open-access LBNL-PEER ground motion database. This work will extend the database to new high-risk regions and support the broader application of deterministic simulations in seismic hazard assessment and infrastructure resilience planning.



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

Principal Investigator: Amanda Randles, Duke University
Co-Investigators:

Scientific Discipline: Biological Sciences: Medical Science

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: New
Title: "Evaluating the Performance of the Quantum Approximate Optimization Algorithm"

Principal Investigator: Abid Khan, JPMorgan Chase
Co-Investigators: Minzhao Liu, JPMorgan Chase
Sami Boulebnane, JPMorgan Chase
Ruslan Shaydulin, JPMorgan Chase
Jeffrey Larson, Argonne National Laboratory

Scientific Discipline: Computer Science

INCITE Allocation:

Site: Argonne National Laboratory
Machine (Allocation): HPE Apollo 6500 (40,000 Polaris node-hours)
Site: Argonne National Laboratory
Machine (Allocation): HPE Cray EX - Intel Exascale Compute Blade Nodes (200,000 Aurora node-hours)

Research Summary: Strong theoretical evidence exists for the power of quantum computers to tackle a wide range of problems out of the reach of classical techniques. Among the many applications of quantum computing, a particularly promising domain is optimization due to the ubiquity and high impact of optimization problems. The Quantum Approximate Optimization Algorithm (QAOA) has emerged as a promising approach for solving combinatorial optimization problems with some evidence suggesting it may offer a quantum advantage on early fault-tolerant quantum computers. However, QAOA is challenging to study analytically, motivating the use of numerical methods that require supercomputers, as it involves exponentially expensive simulations of quantum systems.

In this project, researchers will develop numerical techniques to predict QAOA performance for arbitrarily large problems. The team's techniques can compute finite-size corrections to the infinite-size-limit QAOA performance, where the infinite-size performance was computed in prior work. The outcome of this research will be two-fold. First, the computed quantities would enable accurate QAOA performance estimation at large problem sizes beyond classical simulability, which would, in turn, allow resource estimation, concrete comparisons with classical solvers, and clarification of the requirements for quantum advantage in optimization. Second, the resulting values would allow the calculation of optimal QAOA hyperparameters without actually performing QAOA optimization via classical simulation or quantum execution. Together, these findings would provide evidence for the potential for QAOA to serve as a credible candidate for achieving quantum advantage.



Type: Renewal
Title: "Exascale Quantum-AI Molecular Dynamics for Covalent Drug Discovery"

Principal Investigator: Giuseppe Barca, Australian National University

Scientific Discipline: Chemistry

INCITE Allocation:

Site: Oak Ridge National Laboratory
Machine (Allocation): HPE Cray EX (395,700 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: Xishuo Wei, 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 (1,000,000 Aurora node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE Cray EX (1,000,000 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. During the last one and half years, significant progress has been made on GTC simulations of EP turbulence, SGTC training, and FRNN development as highlighted in several publications including a paper in the prestigious Physical Review Letters and in two oral talks (out of a worldwide total of 5) on the EP physics at the biennial IAEA Fusion Energy Conferences. The large scale GTC simulations for AEs in DIII-D tokamak has finished. Equilibrium data for thousands of DIII-D experiments for coupled microturbulence-AE-kink/fishbone simulations have been progressed, and our team are ready to carry out the production runs. GTC has been fully optimized and are scalable on Frontier and Aurora, thanks to fruitful collaboration with INCITE liaisons, the experts from ALCF, OLCF, AMD, and Intel.



Type: New
Title: "Exascale Simulations of Compact Binary Mergers"

Principal Investigator: David Radice, The Pennsylvania State University
Co-Investigators:

Scientific Discipline: Physics: Nuclear Physics

INCITE Allocation:

Site: Argonne National Laboratory
Machine (Allocation): HPE Cray EX - Intel Exascale Compute Blade Nodes
(1,000,000 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 few years, LIGO will undergo a series of upgrades that will double its sensitivity. In 2027, following the upgrades, LIGO will start its 5th 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 Webb Space Telescope. The combined gravitational-wave and electromagnetic data from these observations will encode the answers to some of the most pressing questions in high-energy and nuclear astrophysics.

The aim of this project is to perform large compact binary merger simulations to unlock them. The team will perform general-relativistic, hydrodynamics, very-high-resolution simulations of tidally interacting neutron stars over more than 20 orbits, 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. This team will also perform general-relativistic, global, magnetohydrodynamics simulations of merging neutron stars at unprecedented resolution to study the turbulence and dynamo action resulting from the magnetorotational instability in the remnant. These simulations will be used to quantify the impact of turbulent-viscous torques on the post-merger gravitational-wave signal, as well as the viability of remnant massive neutron stars as engines for gamma-ray bursts and kilonovae.



Type: New

Title: "Exascale Simulations of Excited-State Phenomena in Quantum Materials"

Principal Investigator: Zhenglu Li, University of Southern California
Co-Investigators: Mauro Del Ben, Lawrence Berkeley National Laboratory
Felipe H. da Jornada, Stanford University
Steven G. Louie, University of California, Berkeley
Jeffrey B. Neaton, Lawrence Berkeley National Laboratory
Diana Y. Qiu, Yale University

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation:

Site: Argonne National Laboratory
Machine (Allocation): HPE Cray EX – Intel Exascale Compute Blade Nodes
(400,000 Aurora node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE Cray EX (450,000 Frontier node-hours)

Research Summary: The overarching goal of this project is to apply and advance the state-of-the-art ab initio many-body Green's function approaches for understanding and predicting excited-state phenomena in quantum materials. Multiparticle interactions such as electron-electron, electron-hole, electron-phonon couplings drive many exotic quantum phases and orders and are essential in excited-state scattering and quantum decoherence processes.

Accurate first-principles descriptions of these many-body interactions and excited-state phenomena pose grand challenges in theoretical formulation and software implementation, and have high demands for massive computational resources. This project develops and applies advanced computational methodologies including the GW method, GW-Bethe-Salpeter equation method, GW perturbation theory, and time-dependent GW approach to study quasiparticle excitations, optical properties, time-dependent and nonequilibrium phenomena, multiparticle excitations, and coupling between phonons and correlated electrons and excitons. The computation in this project can efficiently utilize exascale supercomputing resources, aiming to gain deep understanding, at the many-electron interacting level, of how phonons interact with excited states, how strongly correlated excitonic states develop in two-dimensional materials, and how we can engineer excited states in quantum materials.



Type: New
Title: "Exascale Simulations of Injection Mixing and Combustion in Supersonic Flows "

Principal Investigator: Joseph Oefelein, Georgia Institute of Technology
Co-Investigators: Dhruv Purushotham, Georgia Institute of Technology

Scientific Discipline: Engineering

INCITE Allocation:

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

Research Summary: Advanced propulsion systems for aviation are rapidly moving toward internal high-speed flow environments that involve complex shock-wave/boundary-layer interactions intermingled with integrated fuel injection and flame holding strategies, e.g., gas turbines for supersonic transport, rotating detonation engines, and scramjets. Simultaneously, there is emphasis on the development of Sustainable Aviation Fuels (SAFs) derived from sources such as renewable biomass or waste streams to reduce the carbon footprint of air travel. Current trends combined with advanced computational capabilities respectively warrant and enable more detailed investigations of fuel-air injection, mixing, and combustion processes in these environments that include detailed consideration of complex hydrocarbon fuel blends combined with transient near-wall boundary-layer and heat transfer processes. The calculations proposed under this grant are designed to provide a detailed quantitative understanding of these processes and the complex interactions between them that lead to unreliable operation and performance losses. In addition to new fundamental insights, these investigations will provide new findings toward the development and reliable use of affordable and predictive engineering models for these systems and documented databases for model validation.



Type: New
Title: "Exascale Simulations of Laser Plasma Interactions Driven by Structured Light"

Principal Investigator: Frank Tsung, University of California, Los Angeles
Co-Investigators: John Palastro, University of Rochester, Paulo Alves, University of California, Los Angeles, Kyle Miller University of Rochester

Scientific Discipline: Fusion

INCITE Allocation:

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

Recent years have brought major advances in controlling the spatial and temporal structure of laser pulses, enabling new research areas. These include beams with realistic fusion beam smoothing, "flying focus" pulses where the peak intensity moves at superluminal or subluminal speeds, beams with orbital angular momentum, and lasers with spatially varying polarization. Intense particle beams can also be produced using flying foci and chromatic lenses.

While the vacuum behavior of such lasers and beams is well understood, their interactions with plasmas are only beginning to be explored. The INCITE project has upgraded the OSIRIS particle-in-cell code to launch lasers with arbitrary spatial-temporal profiles (ASTRL pulses). Using this capability, the team proposes computational studies to build understanding of these interactions and develop near-term applications.

The research aims to advance compact and efficient plasma-based accelerators and light sources, ultrahigh-power lasers via Raman and Brillouin amplification, and control of laser-plasma instabilities in inertial fusion targets using bandwidth.

The team is utilizing computing resources on Polaris at Argonne National Laboratory, where they have already demonstrated positive scaling and high productivity.



Type: New
Title: "Exascale-enabled Simulation of Cavitation for Medicine and Beyond"

Principal Investigator: Spencer Bryngelson, Georgia Institute of Technology
Co-Investigators: Tim Colonius, California Institute of Technology
Mauro Rodriguez, Brown University
Reuben Budiardja, Oak Ridge National Laboratory
Fang Liu, Georgia Institute of Technology

Scientific Discipline: Engineering

INCITE Allocation:

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

Research Summary: Disperse multiphase flows—flows laden with droplets, particles, and/or bubbles—are ubiquitous in nature and engineering devices. Modeling these flows is crucial in solving problems ranging from understanding ocean and atmosphere transport to controlling disease spread to designing pebblebed nuclear reactors. Multiphase flows are linchpins for creating new medical treatments and developing new hydro-marine propulsors and energy sources.

Across these applications, first-principles predictive simulations of these flows are largely prohibitive due to the broad range of spatial and temporal scales involved. Even when molecularly thin interfaces are smeared to continuum scales, which is acceptable in many applications, one is still confronted with enormous scale separation from, for example, micron-sized bubbles to meter-scaled eddies and devices. Sub-grid-scale models for multiphase dispersions exist and can reduce the associated computational expense by several orders of magnitude. For example, the PIs have developed state-of-the-art models for cavitating bubbly flows. However, these models are only validated in the dilute limit for non-interacting spherical particles with simple internal physics. This is because the models rely upon analytic closures for the flow physics that have not yet been interrogated with full-resolution simulations or experiments.

Our effort will break this bottleneck by conducting the first simulations of large, realistic bubble dispersions and their cavitation dynamics. The simulation data will illuminate the physical interactions that give rise to larger collective behaviors. The data and its analysis can be used to develop and train next-generation sub-grid models using state-of-the-art statistical-inference and machine-learning inference techniques.



Type: New
Title: "Exploring the Frontiers of Black Hole Accretion and Feedback"

Principal Investigator: Eliot Quataert, Princeton University
Co-Investigators: James Stone, Institute for Advanced Study
Minghao Guo, Princeton University
Rajeskhar Mohapatra, Princeton University
Volker Springel, Max Planck Institute for Astrophysics

Scientific Discipline: Astrophysics

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

Research Summary: One of the most challenging computational problems in astrophysics and cosmology is understanding the impact of energy produced by black hole accretion on its environment. Remarkably, the smallest and densest objects in the Universe (black holes) dramatically reshape the environment in which they reside over length-scales billions of times larger than the black hole itself. Such 'feedback' influences the population of galaxies we observe. It also modifies the distribution of gas and dark matter throughout the Universe, observations of which are used to constrain cosmological parameters such as the properties of dark matter and dark energy. This proposal lays out an ambitious plan to leverage the unparalleled computational power of Frontier, our GPU-optimized general relativistic magnetohydrodynamic code AthenaK, and a new numerical method we have developed ('cyclic zoom'). We propose to carry out the first ab initio calculations of the impact of black hole feedback on structure formation that simultaneously resolve event horizon and galaxy scales over cosmologically interesting timescales (100 Myr). These calculations will use initial conditions drawn from both observations and cosmological simulations of structure formation, and they will provide fundamental new insights into how feedback from black holes via outflows and jets impacts galaxy formation. The same simulations will provide a new generation of event-horizon scale simulations of black hole accretion in the galaxy M87 free from the idealized initial conditions in previous models. These will be critical for interpreting existing and future observations of the massive black hole in M87 by the Event Horizon Telescope and other facilities.



Type: New
Title: "Extreme Plasmas at the Spacetime Frontier: Kinetic effects in Black hole Accretion"

Principal Investigator: Alexander Philippov, University of Maryland, College Park
Co-Investigators: Evgeny Gorbunov, University of Maryland, College Park
Hayk Hakobyan, Columbia University
Jens Mahlmann, Dartmouth University
Muni Zhou, Dartmouth University
Vladimir Zhdankin, University of Wisconsin, Madison
Alisa Galishnikova, Flatiron Institute
Vassilios Mewes, Oak Ridge National Laboratory

Scientific Discipline: Physics

INCITE Allocation:

Site: Oak Ridge National Laboratory
Machine (Allocation): HPE Cray EX (970,000 Frontier node-hours)

Research Summary: The most striking black hole observations (BH) observations to date are the radio global interferometric images by the Event Horizon Telescope (EHT), directly probing the relativistic plasma orbiting within a few event-horizon radii of the BH in the M87 galaxy, and the one at the center of our Galaxy -- the SgrA*. EHT observations revolutionize our understanding of extreme gravity and supermassive BHs in galactic centers. The difficulty in interpreting the observed emission, however, lies not in our knowledge of BHs themselves but in the physics of plasmas that produce the radiation. Since the accreting plasma around the sources observed by the EHT is effectively collisionless, rigorous models of the accretion onto these BHs require kinetic plasma physics. Moreover, using currently state-of-the-art single-fluid simulations to construct radio images requires ad hoc prescriptions for the distribution function of radiating electrons. This proposal aims to advance our understanding of the role of kinetic processes in shaping the observations of accretion flows near SMBHs by utilizing the supercomputing power of Frontier. We plan to conduct kinetic plasma turbulence simulations at an unprecedented level of realism and groundbreaking resolution. Through these simulations, we aim to connect the large-scale properties of turbulence in various regions of the accretion flows with the properties of electron energization and, ultimately, with observables, as well as develop a new foundational theory of collisionless accretion.



Type: New
Title: "FRAME-IDP: Framework for Reasoning Analytics & Modeling of Emergent biologics targeting Intrinsically Disordered Proteins"

Principal Investigator: Arvind Ramanathan, Argonne National Laboratory
Co-Investigators: Rick Stevens, Argonne National Laboratory
Thomas Brettin, Argonne National Laboratory
Bryan Dickinson, University of Chicago
Kunle Odunsi, University of Chicago
Abhishek Pandey, Abbvie
Archit Vasan, Argonne National Laboratory
Heng Ma, Argonne National Laboratory
Matt Sinclair, Argonne National Laboratory
Moeen Meigooni, Argonne National Laboratory
Xinran Lia, Argonne National Laboratory
Venkatram Vishwanath, Argonne National Laboratory

Scientific Discipline: Biological Sciences

INCITE Allocation:

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

Research Summary: Intrinsically disordered proteins (IDPs) and regions (IDRs) play critical roles in cancer signaling but have historically evaded therapeutic targeting due to their structural plasticity. The FRAME-IDP project is pioneering a transformative strategy for designing biologics that leverage—rather than circumvent—this disorder. Focusing on five cancer-relevant IDP targets (NMNAT2, WHSC1, CSF1R, NLRP3, NBS1), the team is integrating generative AI, exascale molecular simulations, and experimental validation into a unified discovery framework. Project goals include using a retrieval-augmented generation pipeline to identify pathway-specific interfaces for targeted binder design; coupling coarse-grained and all-atom molecular dynamics with Markov state modeling to characterize conformational ensembles; implementing generative diffusion models and inverse folding techniques to create biologics for evaluation through AI-guided simulations and experimental feedback; and driving optimization through reinforcement learning and preference-based methods. This INCITE project directly aligns with the ARPA-H IDEAL initiative and DOE’s mission in AI-enabled biosciences. The team’s work will establish a scalable, generalizable platform for IDP-targeted drug discovery, with downstream applications in neurodegeneration, virology, and immunology. By turning the “undruggable” nature of IDPs into a feature, FRAME-IDP aims to redefine therapeutic design and accelerate discovery pipelines for next-generation biologics.



Type: New
Title: "Frontier Forest: Probing New Physics with the Intergalactic Medium"

Principal Investigator: Brant Robertson, University of California, Santa Cruz
Co-Investigators: Evan Schneider, University of Pittsburgh
Piero Madau, University of California, Santa Cruz
Yuan-Sen Ting, The Ohio State University
Nickolay Gnedin, Fermilab
Reuben Budiardja, Oak Ridge National Laboratory
Bruno Villaseñor, AMD
Tirthankar Ghosal, Oak Ridge National Laboratory

Scientific Discipline: Physics

INCITE Allocation:

Site: Oak Ridge National Laboratory
Machine (Allocation): HPE Cray EX (470,000 Frontier node-hours)

Research Summary: With the development of dramatic new observational capabilities that can survey millions of galaxies over a large fraction of the sky, our theoretical models used to interpret data have to become more advanced and cover a dramatically larger space of physical parameters. When new experiments discover new physics outside the range of expected results, we rely on detailed physical models to both explain the results and illuminate how exciting potential discoveries can be confirmed through predictions for other phenomenology. By inferring the expansion history of the universe through their Baryon Acoustic Oscillation measurements combined with other cosmological probes, the Dark Energy Survey Instrument team has claimed evidence for dynamical dark energy at the $\approx 3\sigma$ -level. Confirmation of this time-variable dark energy would force us to rewrite our standard models of particle physics and cosmology, and the onus to push for any potential confirmation requires us to understand how dynamical dark energy could affect other observables. The DESI results have posed the questions How would dynamical dark energy affect cosmological probes beyond the expansion history? and Can we hope to confirm dynamical dark energy observationally through further precision cosmological measurements?

The proposed set of simulations dubbed the "Frontier Forest" will answer these questions by using the GPU-native, MPI-parallelized code Cholla to simulate a statistical volume of the universe with spatially constant resolution sufficient to capture all the relevant scales for structure formation in dynamical dark energy cosmologies and model the observational signatures of large-scale structure via absorption line signatures of intergalactic hydrogen gas (the "Lyman- α Forest"). The combination of volume, resolution, and physics will allow us to compare directly with both DESI observations of the Lyman- α Forest, anchoring our theoretical calculations with experiments spanning billions of years of cosmic time. We will leverage advances in machine learning to augment the physics of our simulations and optimize our numerical studies in executing the most efficient scientific exploration possible.



Type: New
Title: "General Relativistic Radiation Magnetohydrodynamics of Tidal Disruptions"

Principal Investigator: Shane Davis, University of Virginia
Co-Investigators: James Stone, Institute for Advanced Study
Yan-Fei Jiang, Flatiron Institute
Xiaoshan Huang, California Institute of Technology
Lizhong Zhang, Institute for Advanced Study
Philip Chang, University of Wisconsin, Milwaukee
Enrico Ramirez-Ruiz, Lick Observatory
Yuhan Yao, University of California, Berkeley
Andrew Mummery, Institute for Advanced Study

Scientific Discipline: Physics: Astrophysics

INCITE Allocation:

Site: Argonne National Laboratory
Machine (Allocation): HPE Cray EX - Intel Exascale Compute Blade Nodes
(950,000 Aurora node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE Cray EX (250,000 Frontier node-hours)

Research Summary: A tidal disruption event occurs when a star's orbit is nudged by gravitational interactions with other stars so that it passes close enough to a supermassive black hole to be ripped apart by the black hole's gravitational force. A large fraction of the star can fall back onto the black hole over the subsequent year, forming accretion flows that are observed as luminous transients. Because the initial conditions are well understood, these systems are excellent laboratories for studying accretion, a ubiquitous process in astronomical sources. Careful modeling of these sources can also help us to discern the properties of the black hole causing the disruption. These systems, however, are challenging to model because they can be so luminous that the radiation forces from the light emitted can overcome even the gravity of the black hole, sculpting the flow and driving winds. Modeling these flows therefore requires state-of-the-art treatments of radiation physics, which are computationally expensive and require exascale computing to perform. Such calculations are critical at the current time because the NSF/DOE Rubin observatory starts observation in 2025 and will deliver a huge wealth of new data on these sources.



Type: New
Title: "Hadron Physics from First Principles"

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

Scientific Discipline: Physics: Nuclear Physics

INCITE Allocation:

	Site:
Machine (Allocation):	Argonne National Laboratory
Site:	HPE Cray EX – Intel Exascale Compute Blade Nodes (430,000 Aurora node-hours)
Machine (Allocation):	Oak Ridge National Laboratory
	HPE Cray EX (1,000,000 Frontier node-hours)

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

The main goal of the project is to compute the x-dependent, flavor-separated quark, and gluon generalized parton distributions (GPDs) of the nucleon and of the pion, 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: Renewal

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

Principal Investigator: Peter Petreczky, Brookhaven National Laboratory
Co-Investigators: Dennis Bollweg, Brookhaven National Laboratory
Jorge DaSilva, Brookhaven National Laboratory
Olaf Kaczmarek, Bielefeld University
Rasmus Larsen, Bielefeld University
Swagato Mukherjee, Brookhaven National Laboratory
Johannes Heinrich Weber, Technical Univ. of Darmstadt

Scientific Discipline: Physics

INCITE Allocation:

Site: Oak Ridge National Laboratory

Machine (Allocation): HPE Cray EX (1,000,000 Frontier node-hours)

Research Summary: The goal of this multi-year project is to provide first principle lattice QCD input for heavy flavor probes of strongly coupled quark gluons plasma formed in heavy ion collisions and studied by sPHENIX and STAR experiments at Relativistic Heavy Ion Collider, as well as by the experiments at Larger Hadron Collider. These inputs include the heavy quark diffusion coefficient, the in-medium quarkonia masses and widths, and the heavy quark potential. The calculations of these quantities involves: a) generation of the gauge configurations; b) calculations of the pertinent correlation functions on the generated gauge configurations; c) the analysis of the correlation functions and the extractions of the relevant quantities from them, such as quarkonium properties, heavy quark diffusion coefficient and the complex potential. The generation of the gauge configuration often requires leadership class resources. Because the generation of gauge configurations takes long time and computationally is very demanding a staged approach is taken: first we have generated gauge configurations on smaller volumes using various resources, including NERSC and ALLC allocation and then generate gauge configurations on large volume using INCITE allocation. The small volume calculations provide us with the first results on the quantities needed for the phenomenology and at the same time inform us about computational requirements for the large volume calculations and thus help to plan the future calculations. Through the calculations on the small volumes we obtained important results on the quarkonium masses and widths and the heavy quark diffusion coefficient.



Type: New
Title: "Heterogeneous Catalysis as a Collective Phenomenon On and Off Equilibrium"

Principal Investigator: Anastassia Alexandrova, University of California, Los Angeles

Co-Investigators: Philippe Sautet, University of California, Los Angeles

Scientific Discipline: Chemistry

INCITE Allocation:

Site: Argonne National Laboratory

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

Research Summary: Chemical production is the single largest consumer of energy in US manufacturing, according to the 2015 DOE Bandwidth Report, and the development of efficient catalysts for many processes remains a major challenge. Over recent years, researchers have shown that theory in catalysis, while being merely descriptive for a long time, becomes predictive if the paradigm of how we describe heterogeneous catalysis is changed. The basis of this project is the realization that a catalytic interface is in constant motion enabled by the reaction conditions (temperature and pressure of gases in thermal catalysis, or electrochemical potential, solvent and pH in electrocatalysis). Due to this dynamism, the interface presents a fluxional ensemble of many structural and stoichiometric states (rather than just one), each characterized by its catalytic activity, selectivity, and deactivation propensity. Catalysis, therefore, is a collective and highly dynamic phenomenon.

This INCITE project will develop frontier approaches and methods to describe catalysts as such. To achieve this, the team will use and further develop grand canonical sampling techniques for the discovery of dynamic ensembles in realistic reaction conditions and extend them to capture non-equilibrium effects. Electronic structure calculations will rely primarily on DFT within VASP. In electrocatalysis studies, the electrolyte and electrochemical potential will be included. Machine learning potentials will also be developed to replace costly DFT calculations wherever possible, using the large amount of data generated by the project.

Predicting new catalysts with this dynamic complexity is a frontier of catalysis science and is a central focus of this research. Catalytic reactions of interest are relevant to fuel production, chemical manufacturing, and efficient fuel cells.



Type: New
Title: "High-Energy Electrons Driven by High-Power Lasers for Strong-Field Physics"

Principal Investigator: Victor Malka, Weizmann Institute of Science

Scientific Discipline: Physics: Plasma Physics

INCITE Allocation:

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

Research Summary: The INCITE project proposes a coordinated numerical campaign to advance three areas in laser-wakefield acceleration (LWFA) and its applications. It focuses on optimizing dephasingless acceleration using spatio-temporally shaped axiparabola-reflected pulses, modeling beam coupling between staged wakefield accelerators, and interpreting strong-field Compton scattering experiments. The work uses large-scale particle-in-cell simulations with INCITE resources and is closely integrated with experimental programs at the Weizmann Institute, ELI-NP, and Lund University.

The project will apply Bayesian optimization and quasi-2D simulations to identify parameters for maintaining stable wake phase velocity, followed by full 3D simulations with realistic geometries. It will also study how an electron beam from a laser-driven stage can be injected into a beam-driven stage, examining focusing, nonlinear wakefield generation, and injection instabilities. Additionally, it will model interactions between LWFA electrons and backreflected laser pulses to predict photon yield and assess access to the strong-field QED regime. The results will support ongoing experiments, validate new acceleration concepts, and guide the design of future laser-based accelerators and radiation sources.



Type: New
Title: "High-Fidelity Gyrokinetic Turbulence AI Surrogates for Fusion Energy Stellarator Design"

Principal Investigator: Randy Churchill, Princeton Plasma Physics Laboratory
Co-Investigators: Prasanna Balaprakash, Oak Ridge National Laboratory
Anima Anandkumar, Caltech
Matthew Landreman, University of Maryland
Jong Choi, Oak Ridge National Laboratory
Valentin Duruisseaux, Caltech

Scientific Discipline: Physics

INCITE Allocation:

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

Research Summary: This project aims to revolutionize the design and analysis of fusion energy devices by developing a new generation of artificial intelligence (AI) surrogate models for plasma turbulence. Building upon recent successes in creating AI surrogates from gyrokinetic simulations, we propose to significantly advance predictive capability by utilizing high-fidelity simulations that include kinetic electron dynamics. Current state-of-the-art surrogates often rely on adiabatic electron models, which limit their accuracy for comprehensive transport studies involving both ions and electrons.

We will leverage the GPU-native gyrokinetic code GX to generate an unprecedentedly large dataset of over 1 million simulations across diverse stellarator geometries, this time incorporating kinetic electrons. These simulations are approximately 60 times more computationally intensive than their adiabatic counterparts, necessitating the leadership-class computational power of Frontier. Each simulation is projected to generate upwards of 800GB of data, primarily from saving the distribution function, with judicious choices to create a total dataset size on the order of (300)+ PB.

A key innovation of this project is the application of neural operator models directly to the complex, high-dimensional distribution function data. This approach promises to capture more of the underlying physics than previous methods. To manage the vast dataset and evolving models, we will explore and implement continual learning strategies, allowing for efficient ingestion of new simulation data and iterative improvement of the AI surrogates. The resulting high-fidelity AI surrogate will enable significantly faster and more accurate predictions of turbulent transport in fusion plasmas, directly impacting the optimization of stellarator designs and accelerating the path towards sustainable fusion energy. This research will also pioneer methods for large-scale scientific AI, tackling challenges in massive data handling and advanced model development on exascale platforms.



Type: Renewal
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, retired
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: Aerodynamics

INCITE Allocation:

Site: Argonne National Laboratory
Machine (Allocation): HPE Cray EX - Intel Exascale Compute Blade Nodes (400,000 Aurora node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE Cray EX (1,000,000 Frontier node-hours)

Research Summary: The aviation industry plays a critical role in the global economy and is committed to improve efficiency and reduce fuel burn. A key strategy for achieving significant reductions in fuel burn and emissions is a fundamental shift in propulsion system architecture to improve propulsive efficiency for commercial aircraft. As performance gains from increasing bypass ratios in ducted turbofans approach their limits, open fan propulsion offers a path toward a step change in improved efficiency.

Realizing the full benefits of open fan technology requires careful integration of the engine with the aircraft, particularly in wing-mounted configurations where the fully-coupled open fan+wing system needs to be optimized. In this project, NASA, Boeing, and GE Aerospace are collaborating to investigate the aerodynamic and installation challenges associated with aircraft-integrated open fan propulsion systems.

The effort focuses on developing a detailed understanding of the flow physics governing installed open fan propulsors through high-fidelity, turbulence-resolving simulations. The resulting data will be used to benchmark and improve computational design models using machine learning and physics-based approaches. These models will enable efficient design optimization across integrated propulsion-aircraft configurations. Resolving the complex turbulence and flow interactions requires simulations with billions of computational cells, making exascale computing resources provided by the INCITE program essential to project success.



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: Ria Broer, University of Groningen
Carmen Sousa, University of Barcelona
Jordi Ribas, University of Barcelona
Mercè Deumal, University of Barcelona
Xavier Lopez, Universitat Rovira I Virgili
Tjerk P. Straatsma, Oak Ridge National Laboratory

Scientific Discipline: Chemistry

INCITE Allocation:

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

Research Summary: The project aims to obtain theoretical insight into energy transfer as well as electron and hole transport processes in materials relevant to organic solar cells. For this purpose we study singlet fission, the generation of two excitonic states by the absorption of one photon; exciton transfer, the delocalization of an electronic excited state through the material; triplet separation, the first step towards two uncoupled pairs of charge carriers after singlet fission; hole and electron transport, the movement of the charge carriers towards the electrodes; and non-radiative recombination, two opposite charges meet and recombine.

In the first part of the project, we have been able to give a unique ab initio account of the full singlet fission process; all the way from the absorption of a photon, passing through the formation of a singlet coupled double triplet, to finally give two independent triplet states. A second important advancement has been the development of a many-electron tight binding model parametrized by the NOCI-F calculations performed on Frontier. This has given rise to the construction of model Hamiltonians of NOCI-F quality for systems with more than 300 atoms and 80 active electrons in 80 orbitals.

Intramolecular singlet fission and electron transfer is the third important pillar of the project and concentrates on acenes of increasing size bridged by the bicyclo(2,2,1)heptane group. The use of covalently linked chromophores has several advantages, among which the much wider variation of relative orientations of the fragments compared to molecular crystals is one of the most appealing.



Type: Renewal
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. This research focuses 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: "Impurity transport and core-edge integration in a stellarator fusion pilot plant"

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

Scientific Discipline: Physics

INCITE Allocation:

Site: Oak Ridge National Laboratory
Machine (Allocation): HPE Cray EX (1,100,000 Frontier 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 the fusion performance of Type One Energy's recently-developed Infinity Two fusion pilot plant concept. In particular, we will focus on the transport of non-fuel impurity ions, as well as radiative core-edge integration strategies for exhaust power handling.



Type: New
Title: "In situ dynamics of HIV-1 envelope glycoprotein"

Principal Investigator: Rommie Amaro, University of California, San Diego

Scientific Discipline: Biological Sciences

INCITE Allocation:

Site: Oak Ridge National Laboratory
Machine (Allocation): HPE Cray EX (1,228,800 Frontier node-hours)

Research Summary: We aim to use advanced molecular simulations to explore the structure and behavior of HIV-1, the virus that causes AIDS. Although HIV has been studied for decades, there are still many unanswered questions about how certain parts of the virus help it infect cells, avoid the immune system, and respond to treatments. One key part is the envelope glycoprotein (Env), which sits on the virus's surface and is the main target for neutralizing antibodies.

Recently, our team built the first complete, atom-level model of the HIV-1 Env that includes its sugar coating (called glycans), and we used this to build a detailed model of the entire HIV-1 virus — a massive system of about 250 million atoms. With the help of some of the world's most powerful supercomputers, we're now ready to run simulations that will let us "see" how the virus behaves in ways that experiments alone are unable to capture.

We will simulate three versions of the virus: the original model, a version with a different glycan pattern based on lab data, and a version that includes another important protein called matrix (MA), which lies beneath the membrane. These simulations will help us understand how the virus's outer layer protects it, how its components move and interact, and where potential weak spots might exist for vaccines or treatments.

By combining these massive simulations with advanced data analysis techniques, we hope to uncover insights that could directly inform future vaccine designs and antiviral therapies, while also pushing the boundaries of what's possible in molecular modeling.



Type: New

Title: "Large volume, phase-resolved simulations of galactic winds"

Principal Investigator: Benjamin Wibking, Michigan State University
Co-Investigators: Mark Krumholz, Australian National University
Chong-Chong He, Australian National University
Aditi Vijayan, Australian National University
Andrew Myers, Lawrence Berkeley National Laboratory

Scientific Discipline: Physics

INCITE Allocation:

Site: Oak Ridge National Laboratory

Machine (Allocation): HPE Cray EX (1,000,000 Frontier node-hours)

Research Summary: Supernova-driven galactic winds play a fundamental role in galaxy formation and evolution by transporting mass, energy, and metals from galactic disks into the circumgalactic medium (CGM). Despite their importance in shaping key galactic properties like the stellar mass function and mass-metallicity relation, our understanding of these winds remains limited due to unresolved questions about which galaxy types drive winds, their ejection rates, and the long-term fate of ejected material. Current simulations face significant challenges in simultaneously resolving both the large-scale wind structure (~ 10 - 100 kpc) and the complex internal phase structure of cool neutral and warm ionized clouds embedded within the supernova-heated working fluid (~ 10 pc scales). This proposal addresses these limitations through high-resolution simulations using the GPU-accelerated adaptive mesh radiation-magnetohydrodynamics code QUOKKA. We will simulate three representative galaxy types: a Milky Way-like disk galaxy, a steadily star-forming dwarf, and a gas-rich starburst dwarf. These systems span the galactic star formation main sequence and provide observational benchmarks. Each simulation will encompass volumes large enough to capture the full CGM while maintaining high resolution around galactic disks to resolve multi-phase gas dynamics. Our approach involves three generations of simulations with increasing physical complexity, beginning with magnetohydrodynamics, gravity, star formation, and supernova feedback, then incorporating stellar photoionization and photochemistry. This systematic approach will produce the first simulations capable of capturing wind phase structure at high resolution and fidelity across large dynamic ranges. The resulting comprehensive theory of galactic winds will quantitatively predict mass, energy, and metal ejection rates across different galaxy types and gas phases. These findings will enable development of robust sub-grid models for cosmological simulations and improved observational fitting models, advancing our fundamental understanding of galaxy evolution processes.



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

Principal Investigator: Marcos Sotomayor, University of Chicago

Scientific Discipline: Biological Sciences

INCITE Allocation:

Site: Argonne National Laboratory
Machine (Allocation): HPE Apollo 6500 (180,000 Polaris node-hours)
Site: Argonne National Laboratory
Machine (Allocation): HPE Cray EX - Intel Exascale Compute Blade Nodes (267,000 Aurora 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 involves tip-link filaments that pull on ion channels and associated proteins to trigger sensory responses. 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.

With this INCITE project, the team will perform multi-microsecond all-atom molecular dynamics simulations of experimentally obtained structural models, complemented with AlphaFold 2 and 3 structural predictions of two systems: the entire inner-ear tip-link filament and the transmembrane transduction apparatus. Their goals are to predict tip-link mechanics and to understand the gating mechanisms of the inner-ear hair-cell mechanotransduction apparatus. The team's simulations are particularly well suited for INCITE resources because massively parallel supercomputers are required to study and visualize the dynamics of large systems, including proteins, lipids, and ions, at physiologically relevant timescales for auditory transduction and mechanosensitive channel gating (10 microseconds). These simulations will help elucidate how hearing occurs at the molecular level, with implications for understanding and potentially treating inherited deafness.



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

Principal Investigator: James Austin Harris, Oak Ridge National Laboratory
Co-Investigators: W. Raphael Hix, Oak Ridge National Laboratory
Eirik Endeve, Oak Ridge National Laboratory
Vassilios Mewes, Oak Ridge National Laboratory
Steve Fromm, Oak Ridge National Laboratory
Margot Fitz Axen, Oak Ridge National Laboratory
Luca Boccioli, University of California, Berkeley
Eric Lentz, University of Tennessee
Michael Sandoval, Oak Ridge National Laboratory
Anthony Mezzacappa, University of Tennessee

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: "Mechanisms of Non-Equilibrium Ion Dynamics in Radiation Tolerant Alloys"

Principal Investigator: Mitchell Wood, Sandia National Laboratory
Co-Investigators: Gabrielle Koknat, Sandia National Laboratory
Megan McCarthy, Sandia National Laboratory
Raymond Clay III, Sandia National Laboratory

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation:

Site: Argonne National Laboratory
Machine (Allocation): HPE Apollo 6500 (300,000 Polaris node-hours)
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 (1,000,000 Frontier node-hours)

Research Summary: This project advances the frontiers of knowledge that underpin the nations' fusion energy capabilities by resolving one of the key limiting factors of a viable pilot plant; the survivability of plasma facing materials. One of the main challenges in understanding the cumulative effects of radiation damage in structural and functional materials lies in the ultrafast dynamics after an energetic collision with the lattice. The limited scientific understanding of degradation and component lifetime predictions when exposed to these environments stands as a roadblock to commercially available inertial and magnetic confinement fusion energy power plants. While the inherent length and timescale bottlenecks of our simulation methods are being addressed through ever-increasing computing resources, uncertainty about the underlying theories and model approximations remains, and hinders the ability to derive mechanistic insight into problems beyond the reach of experimental validation. Studies of materials in extreme environments are well situated for the atomistic molecular dynamics (MD) used here due to the short timescales of the associated governing mechanisms.



Type: New
Title: "Mechanistic Large Language Model for Biological Network Reasoning"

Principal Investigator: Daniel Jacobson, Oak Ridge National Laboratory
Co-Investigators: Feiyi Wang, Oak Ridge National Laboratory
Verónica Melesse Vergara, Oak Ridge National Laboratory

Scientific Discipline: Biological Sciences

INCITE Allocation:

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

Research Summary: Biological systems are governed not by individual genes acting alone, but by coordinated interactions among genes, proteins, metabolites, and regulatory elements. Understanding these mechanisms, how they operate, adapt, and fail, is essential for progress in medicine, agriculture, and biotechnology. This project uses the world's most powerful supercomputer, Frontier, to train a 400-billion parameter large language model (LLaMA 4 Maverick) that can learn and reason about these systems. Unlike traditional AI models trained on unstructured text, this model will be fine-tuned on structured biological networks that capture the relationships among molecules in cells and tissues. These networks include protein-protein interactions, transcriptional regulation, metabolic pathways, and gene expression data derived from human and model organisms. The model will learn from this multiplex network to predict how genes function together, how biological mechanisms are conserved or rewired across species, and how disease-associated genes connect to actionable pathways. The trained model will be further optimized using reinforcement learning to perform complex reasoning tasks, such as identifying causal regulators, reconstructing disrupted pathways in disease, and simulating evolutionary changes in biological systems. These capabilities will support interpretation of large-scale genomics and multi-omics data in human health and plant biology. This research will advance the state of the art in scientific AI and deepen our understanding of biology at a systems level. By training a biologically grounded language model at scale, this project lays the groundwork for AI systems that generate interpretable, testable hypotheses and accelerate discovery. The resulting models and tools will be open for scientific use, enabling new insights in biomedical research, evolutionary genomics, and trait engineering.



Type: New

Title: "Multi-million particle simulations of bio-inspired material micromachines"

Principal Investigator: Sharon Glotzer, University of Michigan

Scientific Discipline: Materials Science

INCITE Allocation:

Site: Oak Ridge National Laboratory

Machine (Allocation): HPE Cray EX (1,400,000 Frontier node-hours)

Research Summary: Biological tissues possess remarkable capabilities! They self-organize, adapt to local stimuli, and regenerate after damage. These behaviors emerge from complex interactions among active, deformable, and hierarchically organized components. Replicating such dynamics in synthetic systems remains a major challenge at the interface of soft matter physics, materials science, and cellular biophysics. In this project, we leverage massively parallel molecular dynamics simulations to study "flexicles," a computational model of active, deformable vesicles enclosing self-propelled particles, as a platform for designing responsive and hierarchical active materials.

Building on prior work demonstrating emergent behaviors of homogeneous flexicles, we now move toward biologically more relevant tissue-like conditions to investigate how heterogeneity, flexibility, activity, and confinement give rise to collective, adaptive phenomena. We introduce heterogeneity in mechanical properties across flexicle populations to probe how rigidity gradients influence collective migration, jamming, and cell-sorting-like behavior. We study quasi-2D flexicle assemblies under confinement, focusing on high-density states and their ability to spontaneously close wounds, with implications for modeling motility-driven self-repair. Lastly, we introduce a new level of hierarchy by encapsulating flexicle swarms in spherical (rigid and soft) confinements, exploring the role of topology, crowding, and confinement deformability in shaping collective states.

Our work will establish a systematic framework to understand and control emergent behaviors in active, deformable systems. It addresses key questions relevant to synthetic biology, tissue engineering, and active matter design, while pushing the limits of simulation capabilities. Results from this study will inform the design of biomimetic materials capable of autonomous response, contribute to fundamental theories of active phase behavior, and offer new directions for soft robotic and metamaterial systems.



Type: New
Title: "Multimodal Foundation Models for Materials"

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

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

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

Research Summary: The development of new materials is fundamental to technological progress, from electronics and medicine to clean energy and aerospace. However, traditional materials discovery is painfully slow—often taking decades to move from laboratory to real-world application. This project will develop breakthrough artificial intelligence models that can rapidly identify and design new materials across diverse applications. The team's "multimodal" foundation models will simultaneously process multiple types of information about materials creating a comprehensive understanding of how materials behave. The multimodal foundation model for materials will act as a powerful accelerator for materials discovery, enabling researchers to screen millions of potential materials. The models will be trained using Aurora and will support diverse materials discovery challenges in domains such as energy storage and electronics.



Type: New
Title: "Multiscale Light-Matter Dynamics in Quantum Materials"

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
(1,000,000 Aurora node-hours)

Research Summary: To reveal the fundamental mechanisms of light-matter dynamics in quantum materials, this project is using a multiscale approach that integrates first-principles nonadiabatic quantum molecular dynamics (NAQMD) and AI-accelerated neural-network quantum molecular dynamics (NNQMD) simulations, in tandem with X-ray, electron-beam, and neutron experiments at DOE facilities. The team will use this approach to study: (1) light-induced switching of topological ferroelectric moiré superlattices for future ultrafast, ultra-low-power ferroelectric "topotronics"; and (2) photochemical pathways in polymeric ceramic precursors for energy-efficient additive manufacturing of high-temperature ceramics.

Simulating multiple field and particle equations for light, electrons, and atoms over vast spatiotemporal scales is computationally demanding. To address this, the team employs exascale-demonstrated multiscale light-matter dynamics (MLMD) simulations that leverage hardware heterogeneity and low-precision arithmetic. Divide-conquer-recombine (DCR) algorithms split problems into spatial and physical subproblems with small dynamic ranges and minimal mutual information, which are mapped to hardware units with optimal characteristics. Metamodel-space algebra (MSA) keeps key data structures on their respective hardware units, minimizing communication and precision demands.

Within the DCR/MSA paradigm, MLMD software combines first-principles DC-MESH (divide-and-conquer Maxwell-Ehrenfest surface hopping) and AI-accelerated excited-state (XS)-NNQMD modules. DC-MESH integrates Maxwell-Ehrenfest dynamics for short-time light-electron coupling on GPUs and surface-hopping NAQMD for longer-time electron-atom coupling on CPUs, with minimal GPU-CPU communication via electronic occupation numbers, while XS-NNQMD extends accessible spatiotemporal scales by orders of magnitude. In previous work using 60,000 GPUs on Aurora, the DC-MESH and XS-NNQMD modules achieved nearly perfect scalability, with 1.87 exaflop/s performance for DC-MESH.



Type: New
Title: "Natural Language Prompt Guided Design of Functional de Novo Proteins"

Principal Investigator: Rama Ranganathan, University of Chicago
Co-Investigators: Ravi Madduri, Argonne National Laboratory

Scientific Discipline: Biological Sciences: Biophysics

INCITE Allocation:

Site: Argonne National Laboratory
Machine (Allocation): HPE Apollo 6500 (90,000 Polaris node-hours)
Site: Argonne National Laboratory
Machine (Allocation): HPE Cray EX - Intel Exascale Compute Blade Nodes (550,000 Aurora node-hours)

Research Summary: Proteins are nanoscale machines that carry out essentially all the chemical reactions necessary for life, and their fundamental properties—folding, binding, catalysis, signal transmission, and allosteric regulation—all emerge from a complex pattern of cooperative forces acting between constituent atoms. With the explosion of available sequence data and computational resources, deep generative models (DGMs) have emerged as a powerful tool to extract these patterns and learn the underlying design principles of biological macromolecules. The models can be both interpretive—capable of revealing the internal machinery of proteins—and generative—capable of designing novel proteins with controlled functional properties.

In this proposal, we describe the development and scaling of BioM3, the first multimodal DGM capable of natural language-prompted protein design. BioM3 aligns protein sequences with the scientific literature in a joint embedding space through contrastive learning, followed by refinement of the text embeddings to produce an interpretable representation. Once trained, BioM3 can then guide a conditional diffusion process to generate novel protein sequences from text prompts. Experimental tests show that the designed proteins work as specified by prompts both in vitro and in vivo and explore a vast space of alternate solutions for biological functions. These results inspire the work proposed here—to advance and scale BioM3 to become a general-use foundation model for engineering biological macromolecules. This work has the potential to provide new fundamental insights about protein mechanisms and to facilitate the production of novel molecules with applications in medicine, biotechnology, chemical engineering, and public health.



Type: Renewal
Title: "Nuclear Interactions from QCD"

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

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. The goals of this project are to compute two-nucleon scattering amplitudes, directly from the underlying theory of strong interactions, QCD, using lattice QCD. In addition to the two-nucleon interactions, which are key ingredients to the nuclear force and atomic nuclei, we will compute a number of related two-hadron interactions. These calculations represent the first reliable determinations of multi-hadron nuclear interactions at the physical pion mass and are a critical step toward building a robust connection between nuclear physics and the Standard Model of particle physics.



Type: New
Title: "Optimization of inlet diffusers to mitigate dynamic total-pressure distortion"

Principal Investigator: Parviz Moin, Stanford University
Co-Investigators: Sanjeeb Bose, Cadence Design Systems
Rahul Agrawal, Cadence Design Systems

Scientific Discipline: Engineering

INCITE Allocation:

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

Research Summary: Blended wing body configurations are emerging as a promising design for future military aircraft, offering improved aerodynamic efficiency and a compact airframe that enhances the overall thrust-to-weight ratio. By integrating the engines within the fuselage, these designs also reduce radar cross section and fuel consumption. However, such compact layouts require complex inlet systems, like serpentine ducts, which are capable of ingesting the large boundary layer that develops over the aircraft body. A major challenge with serpentine ducts is flow separation, induced by the high curvature walls at duct bends. This can lead to severe consequences, including flow distortion, increased stress on turbine blades, reduced stall margin, and in extreme cases, engine failure.

Flow through serpentine ducts leads to azimuthal distortion and increased pressure losses, which can negatively affect engine performance, as demonstrated by numerous studies. To mitigate these effects, researchers have explored shape optimization strategies. Shape Optimization methods using genetic algorithms and adjoint-based techniques have shown significant reductions in distortion. Only a few studies on shape optimization have been performed, via Reynolds-averaged Navier-Stokes simulations, which have shown limitations in the predictions of inlet distortions.

The objective of this numerical study is to maximize total pressure recovery and minimize azimuthal flow distortion at the SD-2 inlet using a combination of wall-modeled large eddy simulations (WMLES) and direct numerical simulations (DNS) integrated with surrogate optimization techniques for shape optimization. In addition, we aim to elucidate the impact of the inflow angle to the serpentine duct on the flow recovery, and the corresponding reduction of the flow distortion at the exit plane.



Type: New
Title: "Phenotype Anything Model"

Principal Investigator: Aristeidis Tsaris, Oak Ridge National Laboratory
Co-Investigators: Larry York, Oak Ridge National Laboratory
John Lagergren, Oak Ridge National Laboratory
Xiao Wang, Oak Ridge National Laboratory
Noah Fahlgren, Donald Danforth Plant Science Center
Brandon Sloan, Oak Ridge National Laboratory
Sharmin Majumder, Oak Ridge National Laboratory
Anika Tabassum, Oak Ridge National Laboratory
Malia Gehan, Donald Danforth Plant Science Center

Scientific Discipline: Biological Sciences

INCITE Allocation:

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

Research Summary: Biological systems are characterized by complex multi-scale interactions that span from molecules to entire ecosystems and present significant challenges for understanding and engineering. Leveraging the power of artificial intelligence (AI) at exascale, specifically through the development of foundation models for plant phenomics and genomics, offers an unprecedented opportunity to objectively map and interpret the intricate grammar of biological systems. The Advanced Plant Phenotyping Laboratory (APPL) at ORNL generates RGB, thermal, hyperspectral, 3D point cloud, and fluorescence imagery of both plant shoots and roots that are known to relate to aspects of plant morphology and physiology important for acquisition of critical materials and minerals, surviving drought, and the microbiome. However, image analysis of such multimodal data is challenging while deeper biological interpretations that use all information available in imagery do not exist. AI methods and models are needed to ingest and understand the vast amounts of time-series multimodal imagery available in the plant sciences across lab, greenhouse, agricultural, and landscape scales. In this work we develop the Phenotype Anything Model (PAM), a multimodal biological foundation model. PAM will learn generalizable spectral and morphological representations across spatial, spectral, and temporal dimensions across a range of plant species, especially bioenergy crops. We seek to create a single foundation model capable of understanding plant imagery from facilities such as APPL; multispectral UAV and satellite imagery; and root images. We have partnered to acquire diverse imagery from other phenotyping facilities and DOE Bioenergy Research Centers, and will investigate efficient methods to balance and prioritize data used for pre-training to boost model performance and generalizability.



Type: New
Title: "Predicting Evolutionary Pathways with Foundational Genome-Scale Language Models"

Principal Investigator: Azton Wells, Argonne National Laboratory
Co-Investigators:

Scientific Discipline: Biological Sciences: Bioinformatics

INCITE Allocation:

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

Research Summary: The emergence of genome-scale language models represents a transformative moment in computational biology, with AI-driven genomic discovery projected to generate \$13.65 billion in market value by 2029 and to have profound implications for advancing DOE's strategic missions in bioenergy, environmental remediation, and national security.

State-of-the-art DNA-based language models still suffer from fundamental limitations: narrow taxonomic representation, restricted context windows, and computational bottlenecks that prevent effective modeling of environmental microbes essential for DOE applications and limit understanding of long-range regulatory interactions crucial for engineering biological systems or chromosome-level modeling of evolutionary processes. This creates an unprecedented opportunity for DOE to leverage its unique advantages: diverse genomic datasets, exascale computing infrastructure, and a mission-driven focus on energy, environmental, and biosecurity applications.

This project will deliver the first comprehensive genome foundation model capable of whole-chromosome analysis across all domains of life, establishing DOE as the global leader in genome-scale AI and establishing the computational infrastructure necessary for next-generation biological discovery, while advancing DOE's AI for Science initiative and validating the transformative potential of exascale computing for scientific applications.



Type: New
Title: "Predicting Excited-States of Organic Semiconductor Crystals with GW+BSE and ML"

Principal Investigator: Noa Marom, Carnegie Mellon University
Co-Investigators: Mauro Del Ben, Lawrence Berkeley National Laboratory

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation:

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

Research Summary: Crystalline organic semiconductors are used for applications in optoelectronic devices such as solar cells, transistors, and displays. Key parameters for device performance derive from the excited-state properties of these materials, which determine how well they conduct electric current, how they interact with light, and how they convert photons to electrons and vice versa. Device applications require materials with unique combinations of properties that are hard to find. The team aims to discover promising candidate materials using computer simulations. This is challenging because calculating the excited-state properties of molecular crystals with hundreds of atoms in the unit cell is too time consuming and resource intensive to be able to screen a million materials. Machine learning (ML) can help bypass some of these costly calculations by constructing statistical models to predict the properties of interest. However, this typically requires very large amounts of training data. Innovative approaches are needed to train predictive ML models with a small amount of data.

To address this challenge, the team has developed an iterative approach whereby ML models help select materials for excited-state simulations. The data acquired is then used to construct improved ML models, which are subsequently used to select materials for the next round of simulations, and so on. This can maximize the chances of materials discovery and the accuracy of the ML models while minimizing the amount of costly simulations. This research is expected to advance device technology based on crystalline organic semiconductors.



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

Principal Investigator: Paul Kent, Oak Ridge National Laboratory
Co-Investigators: Raymond 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
Cody Melton, Sandia National Laboratories
Lubos Mitas, North Carolina State University
Fernando Reboredo, Oak Ridge National Laboratory
Brenda Rubenstein, Brown University
Kayahan Saritas, Oak Ridge National Laboratory
Hyeondeok Shin, Argonne Laboratory

Scientific Discipline: Materials Science

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 (500,000 Frontier node-hours)

Research Summary: One of the most significant challenges in theoretical and computational condensed matter physics is to be able to predict, understand, realize, and optimize desired properties in specific real materials. Computational and theoretical advances are needed to realize new phenomena for new quantum technologies and aid the identification of optimal materials with specific properties. Quantum materials -- materials that exhibit novel physical properties arising from the quantum mechanics of their electrons and the constituent atoms and structure of their host materials -- are both challenging to model accurately and of critical interest due to their novel physical properties and the possibility of enabling new quantum sensors, quantum computing devices, and new forms of electronics. This project will apply advanced quantum Monte Carlo (QMC) methods to meet the above challenges by providing benchmark accuracy predictions and analysis for highly topical quantum materials, while simultaneously advancing the state of the art. These materials and their properties are of both strong fundamental and technological interest and share the need for the highly accurate treatment of electron correlation of QMC and have properties that strongly and sensitively depend on the material's composition. Building on recent theoretical developments and efficient implementations, we will use the open source QMCPACK code for these calculations. Project members have developed this code for high GPU performance, performance portability between Frontier and Aurora.



Type: Renewal

Title: "Pushing the Frontier of Cosmic Ray Transport in Interstellar Turbulence"

Principal Investigator: Drummond B. Fielding, New York University
Co-Investigators: Philipp Kempfski, Princeton University
Eliot Quataert, Princeton University
Philipp Grete, University of Hamburg
Alexander A. Philippov, Univ. of Maryland, College Park
Matthew Kunz, Princeton University
James M. Stone, Institute for Advanced Study

Scientific Discipline: Physics

INCITE Allocation:

Site: Oak Ridge National Laboratory

Machine (Allocation): HPE Cray EX (875,000 Frontier node-hours)

Research Summary: This project aims to resolve the 50-year-old cosmic ray (CR) transport problem by testing a new paradigm where intermittent magnetic field structures—rather than traditional volume-filling small-amplitude waves—control CR propagation. Using unprecedented computational resources, we are developing predictive models of CR transport essential for understanding galaxy evolution and interpreting multi-wavelength observations from current and future missions. We successfully completed a groundbreaking 10,2403 magnetohydrodynamic (MHD) turbulence simulation on Frontier—the largest simulation of compressible weakguide field MHD turbulence ever performed. This flagship simulation enabled us to track billions of CR particles through turbulent magnetic fields, capturing for the first time the physics of CR scattering across four orders of magnitude in spatial scales from energy injection to magnetic reconnection.



Type: Renewal
Title: "QCD under Extreme Conditions"

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

Scientific Discipline: Physics: Nuclear Physics

INCITE Allocation:

Site: Argonne National Laboratory
Machine (Allocation): HPE Cray EX – Intel Exascale Compute Blade Nodes
(856,000 Aurora node-hours)

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

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

A hydrodynamic description of the strongly interacting plasma requires the local equation of state at nonzero light and strange density. This project will compute it in the continuum limit with physical quark masses. Brookhaven's Relativistic Heavy Ion Collider explores the same transition in a broad range of densities, searching for a critical point in the QCD phase diagram—a difficult task, since there are no first principles to predict its location; direct simulations at finite density have remained elusive because of a sign problem. Thanks to a recent algorithmic development, these simulations, run with physical quark masses, can overcome this barrier and scan the phase diagram for features such as the cross-over line and the critical end point.



Type: New
Title: "QMC-HAMM: High Accuracy Multiscale Models using Quantum Monte Carlo"

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

Scientific Discipline: Materials Science: Condensed Matter and Materials

INCITE Allocation:

Site: Argonne National Laboratory
Machine (Allocation): HPE Cray EX – Intel Exascale Compute Blade Nodes
(950,000 Aurora node-hours)

Research Summary: There has been a sea change in materials modeling as machine learning models have come to dominate the description of materials. These models have benefited from the easy availability of data from first principles density functional theory (DFT) calculations, which approximately describe the quantum mechanical properties of fundamental electrons and nuclei. Advances in machine learning have resulted in models that are near DFT in accuracy, resulting in a situation where the underlying data itself is the limiting factor in predictivity. This project focuses on developing models which use high accuracy data from quantum Monte Carlo to further enhance the ability to predict the properties of materials. This project is devoted to creating a set of community-serving software tools that enable one to link highly accurate many-electron microscopic quantum simulations with multiscale modeling that can achieve large length and time scales. A key distinction of this work is that electron correlation plays a critical role in the materials physics but is a crucial weakness for widely-used computational tools such as DFT. By starting with higher accuracy microscopic calculations and using modern methods of computing coarse-grained models, this platform will enable higher accuracy large-scale models than the standard techniques based on DFT.

With the objective of diversity in mind, three application areas are considered, based on impact and for fundamental interest. First is hydrogen at high pressure, which is relevant for fusion science and planetary interiors, and has an intricate phase diagram which is reminiscent of other materials. Second is the development of machine learning interatomic potentials for several materials, including lithium phosphates and 2D materials. Finally, the team will address a fundamental question in the physics of materials, examining the fundamental mechanisms of charge density waves, a phenomenon in which a material breaks symmetry spontaneously, often suddenly changing its properties significantly. On a broader scale, this proposal will enable cutting edge methodology that moves beyond the state of the art in materials modeling. High accuracy models will be produced, and improved practices will be developed. Each computation campaign will produce high accuracy data on the selected materials, which will be a valuable resource for other materials modelers; such data is scarce at best.



Type: New
Title: "Revolutionary Insights into Turbomachinery Analysis Using Exascale Computing"

Principal Investigator: Michael Borghi, NASA
Co-Investigators: Eric Nielsen, NASA
Li Wang, NASA

Scientific Discipline: Engineering

INCITE Allocation:

Site: Argonne National Laboratory
Machine (Allocation): HPE Cray EX - Intel Exascale Compute Blade Nodes
(780,000 Aurora node-hours)
Site: Oak Ridge National Laboratory
Machine (Allocation): HPE Cray EX (654,937 Frontier node-hours)

Research Summary: The U.S. commercial aviation industry is a strategic asset for the U.S. economy. Narrow-body aircraft, such as the Boeing 737 MAX and the Airbus A320neo, account for the largest share of the commercial aircraft market, primarily due to their reduced fuel consumption. The next-generation turbofan engine for narrow-body aircraft is targeted for service entry in the 2030s, with a projected 5-10% reduction in fuel burn compared to 2020 best-in-class narrow-body aircraft. Today, North America dominates the aircraft engine market. Achieving next-generation engine performance targets is critical to enabling U.S. industry to continue its leading role in the narrow-body aircraft market. To achieve the design goals of the next-generation aircraft engine, two fundamental questions must be answered: "What level of simulation accuracy is required? And what is the cost of those simulations?" Understanding the limitations of different modeling approaches is critical to reducing the cost of numerical simulation while still maintaining the necessary level of accuracy. This project will perform computational studies to address these questions and help inform the U.S. aerospace community. By comparing Unsteady Reynolds-Averaged Navier-Stokes (URANS) simulations with Hybrid-RANS Large-Eddy Simulations (LES) and Wall-Resolved LES, the strengths and weaknesses of each simulation approach can be quantified for a modern high-pressure compressor. This effort will also provide fundamental insights into the complex fluid-dynamics phenomena at play in the next generation of aircraft engines.



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 Torino

Scientific Discipline: Engineering: Fluids and Turbulence

INCITE Allocation:

Site: Argonne National Laboratory
Machine (Allocation): HPE Apollo 6500 (64,000 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 for accurate prediction and progress 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 using fully resolved direct numerical simulations (DNS). This requires resolving all relevant scales, including the bubble diameter and the Kolmogorov and Batchelor scales, which correspond to the smallest vortices and scalar filaments in the flow.

This research aims to enable high-performance computing (HPC) interface-resolved DNS of bubbly turbulent flows with passive scalars and realistically low diffusivities. Despite the wide range of applications of bubbly flows, we still lack a quantitative understanding of fluxes and mixing in turbulent regimes—knowledge that is essential for accurate prediction and technological advancement. Using DNS, this project studies and quantifies turbulence kinetic energy, diffusive scalar fields, and gravity-driven turbulent bubbly suspensions.



Type: New

Title: "Small-Scale Dynamo in the Interstellar Medium: Testing the Asymptotic Limits"

Principal Investigator: Mordecai-Mark Mac Low, American Museum of Natural History

Co-Investigators: Maarit Korpi-Lagg, Aalto University

Hsien Shang, Academia Sinica

Miikka Väisälä

Touko Puro, Aalto University

Frederick Gent, Aalto University and NORDITA

Scientific Discipline: Physics:

INCITE Allocation:

Site: Oak Ridge National Laboratory

Machine (Allocation): HPE Cray EX (400,000 Frontier node-hours)

Research Summary: Understanding magnetic fields in galaxies provides the necessary basis for fields of research ranging from the origin of the Sun and Earth through the star and planet formation process, to the evolution of galaxies over cosmic time, to the detection of signals of cosmic inflation through the foreground radiation of the Galaxy. Magnetic fields contribute as much energy to the interstellar medium (ISM) as thermal pressure, turbulent motions, and cosmic rays. Two dynamo processes determine the structure and origin of galactic magnetic fields. Turbulent velocity fluctuations in the interstellar medium produced largely by interacting supernova blastwaves drive a small-scale dynamo (SSD) that grows on the short eddy turnover time, while the differential rotation of the galactic disk drives a mean-field or large-scale dynamo (LSD) that grows on the long orbital timescale in the disk. Galaxies are observed to host magnetic fields with a typical total strength of around 15 microgauss. To model the full dynamo self-consistently requires a physically consistent model of the SSD. The ISM of galaxies is a high magnetic Prandtl number P_m fluid, meaning that the ratio of viscosity to resistivity is large. Numerical models of the LSD by our group and others show a ratio of mean field to fluctuating field far higher than observed. Idealized models of the SSD in isothermal, uniformly stirred fluids saturate at levels that appear to depend on P_m . Our models including the physics of supernova stirring and radiative heating and cooling in the ISM at modest P_m saturate at levels of only a few percent of equipartition. We hypothesize that the SSD saturation level in the SN-driven ISM depends directly on the magnetic Prandtl number P_m in the asymptotic limit of $P_m \gg 1$. This regime has never been explored because of the enormous resolution requirements, but testing this hypothesis is fundamental to our understanding of the ISM and galaxy evolution. We have developed a parallel GPU code to solve the equations of magnetohydrodynamics efficiently called Astaroth. We propose to use it for unprecedentedly high resolution models of the supernova-driven, magnetized ISM at extremely high P_m . Exploring this regime will reveal whether there is an asymptotic limit that can explain observed galactic magnetic fields. We have developed a parallel GPU code to solve the equations of magnetohydrodynamics efficiently.



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 Science
Christopher White, Flatiron Institute
Matthew Coleman, Princeton University

Scientific Discipline: Physics: Astrophysics

INCITE Allocation:

Site: Argonne National Laboratory
Machine (Allocation): HPE Apollo 6500 (400,000 Polaris node-hours)
Site: Argonne National Laboratory
Machine (Allocation): HPE Cray EX - Intel Exascale Compute Blade Nodes (2,450,000 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: Renewal

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
Matthew Torres, Georgia Institute of Technology
Pawel Polak, Stony Brook University

Scientific Discipline: Biological Sciences

INCITE Allocation:

Site: Oak Ridge National Laboratory

Machine (Allocation): HPE Cray EX (700,000 Frontier node-hours)

Research Summary: The coming years promise major improvements in understanding the molecular mechanisms of disease and the development of therapeutics. This progress will be based on exponential increase in the amount of information on molecules in the cell using throughput 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: "THESAN-ALT: Constraining Alternative Cosmologies During Reionization"

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

Scientific Discipline: Physics

INCITE Allocation:

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

Research Summary: While the standard model of cosmology (Λ CDM) has been successful in describing many aspects of the Universe, several high significance tensions have emerged in recent years. These include discrepancies in the measured value of the Hubble constant (Hubble tension), too steep density profiles in dark matter halo substructures, and an unexpectedly large number of massive, UVbright galaxies and supermassive black holes observed by the James Webb Space Telescope at high redshift. These findings challenge key assumptions of the standard model and motivate the investigation of alternative cosmological scenarios.

THESAN-ALT will explore the impact of three well-motivated extensions to Λ CDM on early structure formation, the timing and topology of reionization, the abundance and morphology of highredshift galaxies, and the thermal state of the intergalactic medium. Specifically, we will focus on early dark energy (EDE), self-interacting dark matter (SIDM), and cosmic strings. We will conduct large-scale galaxy formation simulations with GPU-accelerated radiation hydrodynamics (RHD) to model the coupled processes of galaxy formation and reionization in an extremely large volume of the Universe for each modification.

These simulations will match the resolution and numerical setup of the ongoing THESAN-XL project, which is based on a Λ CDM cosmology. This direct comparison will allow us to isolate the physical effects of each modification and generate testable predictions for upcoming observations by JWST, the Nancy Grace Roman Space Telescope, HERA, and future 21cm and line intensity mapping experiments. THESAN-ALT will provide a robust simulation-based framework for testing extensions to Λ CDM and interpreting future high redshift data.



Type: New
Title: "Three-Dimensional Imaging of the Nucleon Transverse Spin Structure"

Principal Investigator: Yong Zhao, Argonne National Laboratory
Co-Investigators: Dennis Bollweg, Brookhaven National Laboratory
Peter Boyle, Brookhaven National Laboratory
Xiang Gao, Brookhaven National Laboratory
Jinchen He, University of Maryland, College Park
Swagato Mukherjee, Brookhaven National Laboratory
Qi Shi, Brookhaven National Laboratory
Fei Yao, Brookhaven National Laboratory
Rui Zhang, Argonne National Laboratory

Scientific Discipline: Physics: Nuclear Physics

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

Research Summary: Quarks and gluons are the building blocks of protons and neutrons, collectively called nucleons. They are bound inside nucleons by the strong nuclear force, or quantum chromodynamics (QCD), which is also responsible for the formation of atomic nuclei and, as such, over 99% of visible matter in our universe. Central questions in QCD include uncovering the origin of the proton's mass and spin and understanding how QCD governs the confined motion and spatial distribution of quarks and gluons within the nucleon. These fundamental questions can all be profoundly informed by precise multi-dimensional imaging—tomography—of the proton. This endeavor lies at the heart of the scientific missions of the United States' flagship hadron physics facilities: Jefferson Lab and the forthcoming Electron-Ion Collider, which is to be constructed at Brookhaven National Laboratory.

This project will carry out the first lattice QCD calculation of the transverse-momentum-dependent partonic structure of a nucleon transversely polarized relative to its direction of motion. Specifically, this project will compute the quark transversity, worm-gear, and pretzelosity transverse-momentum parton distributions in 3D momentum space—key observables for imaging the transverse spin structure of the nucleon. To date, phenomenological knowledge of these distributions remains limited; thus, the calculations will provide critical theoretical input and predictive guidance for experiments at the Jefferson Lab 12 GeV upgrade and the future Electron-Ion Collider. These results will significantly advance our understanding of the origin of transverse proton spin and contribute to a comprehensive 3D tomography of the nucleon.



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: Tom Jelly, University of Melbourne
Melissa Kozul, University of Melbourne
Massimiliano Nardini, University of Melbourne
Pawel Przytarski, University of Melbourne
Marco Rosenzweig, University of Melbourne
Paul Vitt, General Electric Aerospace
Greg Sluyter, General Electric Aerospace
Sriram Shankaran, General Electric Aerospace
William Solomon, General Electric Aerospace
Arash Mousavi, General Electric Aerospace

Scientific Discipline: Engineering

INCITE Allocation:

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

Research Summary: This project tackles the challenge of modeling film cooling in the presence of realistic surface roughness under engine-relevant conditions, using high-fidelity, first-principles simulations. For the first time, a comprehensive computational campaign is being carried out on film-cooled high-pressure turbine blades featuring micron-scale roughness profiles derived from surface scan data of in-service high-pressure turbine vanes. So far, the resulting datasets have provided new insight into the complex interplay between film coolant evolution in the presence of surface irregularities, blade curvature, adverse pressure gradients, and external disturbances such as turbulence and wake interactions. Capturing these effects accurately requires extremely fine mesh resolution not only due to the wide range of hydrodynamic scales that must be resolved, but also the microscopic nature of the roughness features. As a result, these simulations require immense computational resources, made feasible only through our optimized HiPSTAR CFD solver running on state-of-the-art supercomputing infrastructure such as Frontier.



Type: New
Title: "Trustworthy multiscale adaptive probabilistic turbulence foundation models"

Principal Investigator: Pei Zhang, Oak Ridge National Laboratory
Co-Investigators: John Gounley, Oak Ridge National Laboratory
Junqi Yin, Oak Ridge National Laboratory
Paul Laiu, Oak Ridge National Laboratory
Murali Gopalakrishnan Meena, Oak Ridge National Laboratory
Stephen de Bruyn Kops, University of Massachusetts Amherst
Ramanan Sankaran, Oak Ridge National Laboratory

Scientific Discipline: Engineering

INCITE Allocation:

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

Research Summary: Turbulence remains a crucial yet unresolved challenge across a wide range of applications, including energy generation, materials science, earth sciences, and stellar evolution. Traditional physics-based approaches solve large sets of equations, demanding significant computing resources due to the need for extremely high spatiotemporal resolutions and carefully designed algorithms, to accommodate the stochastic, multiscale nature of turbulence. These high-resolution solutions also incur substantial archive storage and sharing costs. Deep learning models offer the potential for fast solutions and compact representations, but they often do not generalize well.

This project proposes to develop a trustworthy foundation model—a large-scale AI model trained on mass datasets—for turbulence, leveraging DOE's leadership-class supercomputers. During pretraining, the model captures the generic knowledge, enabling it to be fine-tuned to diverse downstream applications with minimal additional data and computing. This approach offers a promising path toward a generalizable, scalable, and unified solution with broad impacts across scientific domains.

We have demonstrated a proof-of-concept by developing a hierarchical Turbulence Transformer to represent the extreme multiscale features, and showcased the scalability of our codebase, MATEY, on Frontier with a novel sequence parallelism called RingX, achieving 1.1 EFLOPS performance with 32,768 GPUs. This INCITE allocation will enable full-scale training runs on larger datasets and model sizes. The resulting model will enhance our fundamental understanding of turbulence and accelerate the design of next-generation energy technologies.