

Type: New PW

Title: Subseasonal to Interannual Prediction Experiments with the Unified Forecast System (UFS)

Principal Investigator: Benjamin Cash (George Mason University)

Co-Investigators: Chulsu Shin (George Mason University); Erik Swenson (George Mason University)

Field of Science: Climate Dynamics

Abstract:

The importance of the interactions among the components of the Earth system - atmosphere, ocean, waves, sea ice, land surface, and others - in influencing weather and climate is increasingly recognized. Therefore, operational numerical weather prediction systems are now moving towards coupled Earth system models to provide forecast guidance on all time scales from hours to seasons, and project the evolution of the climate over even longer time scales from years to decades.

The numerical experiments presented here will support our newly-funded NOAA Weather Program Office (WPO) project entitled "The Road to the Seasonal Forecast System: Improving Prediction of Precipitation Extremes" (end date 8/31/2025). The next generation seasonal forecast application, the UFS Seasonal Forecast System version 1 (SFSv1), is currently slated for operations in Q2FY25. The SFSv1 will replace the decades-old operational seasonal forecast application, the Coupled Forecast System, version 2 (CFSv2), and will hopefully represent a significant step forward in NOAA's seasonal forecast capabilities. Our work represents a critical step in the development of the SFSv1

Type: New PW

Title: Simulating Multi-Scale Tropical Convection and its Effects at Storm Resolving Scales

Principal Investigator: Xingying Huang (University Corp. for Atmospheric Research (UCAR) (National Center for Atmospheric Research) (NCAR))

Co-Investigators: William Skamarock (UCAR); Andrew Gettelman (UCAR); David Randall (Colorado State University)

Field of Science: Global Atmospheric Research

Abstract:

Next-generation Global Storm Resolving Models (GSRMs) with horizontal resolutions provide a cutting-edge way to understand weather and climate events across scales for better-informed climate impacts. In this work, we apply the recently developed and validated CAM (Community Atmosphere Model) - MPAS (the Model for Prediction Across Scales) modeling framework, based on the open-source Community Earth System Model (CESM2), to examine the tropical convection features at storm resolving scale over the refined western Pacific region at 3 km grid spacing.

This region features a series of regimes that need to be simulated well for both weather and climate prediction, and complex multi-scale organization of cloud and storm systems from individual convective towers, to 10-100km scale convective complexes, to tropical cyclones, all embedded in large scale atmospheric waves driven by the General Circulation. The storms interact with land and ocean, particularly elevated terrain of the Maritime Continent (Indonesia). This region also affects global circulation patterns by driving the tropical overturning circulation, with remote effects, for example, on the west coast of North America. Getting the multi-scale interactions in this region correct at high resolution is a critical and unsolved problem.

Type: Renewal PW

Title: Structure elucidation of novel molecular substances via machine learning and nuclear magnetic resonance spectroscopy

Principal Investigator: Eric Jonas (University of Chicago)

Co-Investigators:

Field of Science: Chemistry

Abstract:

Small molecules are of vital importance in chemistry, biology, and society, but determining the structure of new molecules continues to be a challenge. Currently, spectroscopic techniques are used that require considerable human effort to interpret. Here we propose building on our recent success in automating this analysis for carbon nuclear magnetic resonance (NMR) spectroscopy to the more challenging proton NMR, which offers a significantly higher signal-to-noise ratio. We do this using ML and AI techniques developed in our research group, requesting both CPU time (for data generation) and GPU time (for scaling and development of novel models).

Type: New PW

Title: Plasma assisted ignition of hydrocarbon mixtures in turbulent flows

Principal Investigator: Fabrizio Bisetti (University of Texas at Austin (UT) (UT Austin))

Co-Investigators:

Field of Science: Fluid, Particulate, and Hydraulic Systems

Abstract:

Low temperature plasma (LTP) ignition is one of the most promising technologies to increase ignition efficiency and reliability in combustion systems. We seek a fundamental understanding of the ignition mechanism of hydrocarbon mixtures under homogeneous isotropic turbulence using low temperature plasma discharges. Under the support of NSF and DOE awards, we consider hydrocarbon mixtures using a newly developed plasma kinetics mechanism in a pin-to-pin configuration. The simulations will be executed leveraging a plasma and reactive flow solver that uses mesh refinement library AMReX. AMReX provides a framework to deal with the challenges arising from the multiscale nature of LTP in turbulent flows. The code displays good scaling behavior on Frontera under the configurations of interest. The adaptive mesh refinement is essential to reduce the problem size and computational resources by orders of magnitude. To support this work, about 250,000 SU in Frontera and 20.2 TB on Ranch are requested.

\end{abstract}

Type: Renewal

PW

Title: Reproducible preprocessing of open neuroimaging data

Principal Investigator: Russell Poldrack (Stanford University)

Co-Investigators: Christopher Markiewicz (Stanford University)

Field of Science: Behavioral and Neural Sciences

Abstract:

Brain imaging techniques, particularly magnetic resonance imaging (MRI), have provided growing insight into the ways that the structure and function of the brain give rise to the human mind, and the ways in which brain functions go awry in mental health disorders. These data are increasingly shared in an open manner, which greatly benefits the scientific community. However, the variability in processing of these data across different groups has the potential to reduce reproducibility of research results. We propose to use a set of well-established tools for quality control and preprocessing of functional magnetic resonance imaging datasets to consistently preprocess all of the more than 330 relevant datasets in the OpenNeuro data archive. This will provide a broad group of researchers with analysis-ready data, enabling the pursuit of a wide range of neuroscientific questions.

Type: Renewal

PW

Title: First-principles Study on Strongly Correlated and Energy Storage Materials

Principal Investigator: Xin Li (Harvard University)

Co-Investigators:

Field of Science: Materials Research

Abstract:

Energy storage plays a crucial role in the clean energy revolution of the twenty-first century. Advanced electrochemical energy storage technologies are essential to any future implementation of broad-base clean energy. With the discovery of more new unconventional superconductors, the possibility of new superconductor materials with high T_c attracts people's interest. High-throughput computational simulations are not only less expensive and time-consuming as compared to experiments, but also efficient to test new ideas in the materials design schema. Such computational approaches are an ideal guide for the experimental discovery of new functional materials. At the Li laboratory at Harvard University, computation and experiment are merged under this principle. The main research goal of this proposal is to develop the material understanding and design needed to supply Li lab experimentalists with the strategic guidance to recognize practical next-generation superconductive and energy storage materials.

Type: New PW

Title: Optimization of Plasma Chemistry Modeling for Etching Processes of Semiconductor Devices via Deep Learning

Principal Investigator: Roberto Longo Pazos (Tokyo Electron Limited USA)

Co-Investigators: Gregory Hartmann (University of Texas at Austin (UT) (UT Austin))

Field of Science: Materials Research

Abstract:

This project is part of much broader research currently being performed here at Tokyo Electron America, Inc., in the fields of atomic layer etching (ALE) and atomic layer deposition (ALD) for semiconductor device manufacturing. Current standards of the industry use 5 or 3 nm as the length of the channel materials, with the critical length of 1 nm already breaking on the horizon. Atomic scale precision in device fabrication is now an absolute necessity to the reduction in device dimensions. ALE and ALD are the complementary techniques that are being considered as most promising for achieving such 1 nm critical length. The key is to enable the control of the process at the atomic scale. ALE removes single layers of material using sequential self-limiting chemical surface reactions, either thermally activated or using plasma ions in the removal step.

The overall goal of this research is to create a computational platform for accelerating the development of ALE and ALD techniques in device manufacturing. To achieve this, the first step must necessarily be the study of the surface reactions undergone by large numbers of molecular precursors in a variety of surfaces under specific conditions, in order to develop an extensive knowledge of the characteristics and the surface modifications induced by each precursor, such as thickness, reaction energy thresholds, impact on the material, sticking coefficients, cross sections, etc. Such properties will ultimately dictate the feasibility of the ALE process with atomic scale control. The present Pathways allocation application is intended mainly to acquire the extensive datasets required for developing Deep Learning-based interatomic potentials, by using our first-principles quantum chemistry codes. We intend to apply modern Deep Learning techniques to optimize the modeling of plasma etching processes by downscaling the required simulation time needed by accurate but computationally expensive first-principles methods. The details of our proposed research are detailed in the main document of this application.

Type: New PW

Title: Computational Design of Hydrogen-Resistant Metal Alloys

Principal Investigator: Konstantin Klyukin (Auburn University)

Co-Investigators:

Field of Science: Materials Research

Abstract:

The exploration of a vast space of compositions that are potentially good structural hydrogen-resistant alloys is an insurmountable challenge to experimental analysis or traditional first-principles calculations. Our approach will use first-principles calculations of atomic and electronic structure, and machine learning methods to assess the most robust descriptors to hydrogen solubility in metal alloys. The use of interpretable descriptors will help to formulate design guidelines and facilitate the discovery of novel promising compositions by using machine learning predictive models and high-throughput screening.

Type: New PW

Title: Predictive Characterization for the Additive Manufacture of Complex Metallic Alloys

Principal Investigator: Ganesh Balasubramanian (Lehigh University)

Co-Investigators:

Field of Science: Materials Research

Abstract:

Multi-principal element alloys (MPEAs) represent a radical new class of materials that, unlike conventional alloys, are concentrated solid-solutions generally consisting of multiple (≥ 5) principal elements in significant proportions. Certain MPEAs, e.g., $\text{Co}_{33}\text{W}_{07}\text{Al}_{33}\text{Nb}_{24}\text{Cr}_{03}$, have exhibited superior hardness and mechanical strength that are unattainable from traditional alloys. These promising properties have encouraged their use as a laser cladded coating material to engineer surfaces of components exposed to severe environments. However, uneven mixing and microstructure evolution of the MPEA melt under rapid cooling have contributed to poor quality and formation of cracks in the coating. Since the dynamics of the molten alloy is fundamentally driven by the diffusion of the elemental species in the MPEA, correlating atomistic properties (e.g. diffusion coefficient) to system-scale processing parameters (e.g. laser power) has posed as a major impediment, that remains unaddressed. In response to this challenge, the PI proposes to establish a predictive framework correlating processing to structure and properties by coupling findings from first principles and molecular dynamics simulations of the alloy with uncertainty quantification and experimental validation, geared towards proposing optimal manufacturing parameters to enhance the quality of the laser deposited MPEA clads.

Type: New PW

Title: Layered materials for quantum technology

Principal Investigator: Efthimios Kaxiras (Harvard University)

Co-Investigators:

Field of Science: Materials Research

Abstract:

Complex assemblies of van der Waals (vdW) bonded two-dimensional materials, nano-structures, nanowires, and color-center defects offer unique opportunities to realize properties unattainable in any single quantum material, as well as flexible and transparent quantum devices. Recent works have demonstrated wafer-scale flexible circuitry with stable electrical performance under an ultra-small bending radius of using mixed-dimensional van der Waals (vdW) materials, and further realized exponential-sensitivity temperature sensors and binary-logic inverters using all-vdW materials. Flexible device modalities have as yet not been extended to quantum technology, and have obvious applications in bio-integrated quantum sensing. For applications such as quantum bio-sensing, low-dimensional material heterostructures are able to overcome the mismatch between soft tissue and stiff electronics, permitting bio-integrated quantum sensors capable of continuous physiological signal monitoring. Two-dimensional materials can be insulators, semiconductors, and metals, permitting complete device fabrication from Van der Waals bonded heterostructures of two-dimensional components. Such heterostructures permit application of nearly arbitrary static strain states, yielding a degree of system design freedom comparable to lithographic patterning.

Type: Renewal

PW

Title: High Fidelity Hurricane Storm Surge and Ocean Modeling

Principal Investigator: Eirik Valseth (University of Texas at Austin (UT) (UT Austin))

Co-Investigators: Clinton N. Dawson (University of Texas at Austin (UT) (UT Austin))

Field of Science: Computational Mathematics

Abstract:

In this project, we seek to continue our exploration of the use of large-scale, multi-core computing for the modeling of hurricane storm surge on the Louisiana and Texas (LATEX) coastal regions using high fidelity finite element meshes. Furthermore, we plan to also focus our efforts on larger global ocean models and their use in modeling of global tidal flows.

Type: New PW

Title: Model-constrained deep learning methods for large-scale complex science and engineering problems

Principal Investigator: Tan Bui (University of Texas at Austin (UT) (UT Austin))

Co-Investigators:

Field of Science: Computational Mathematics

Abstract:

While Deep Learning, a subset of machine learning, has proved to be state-of-the-art approach in many fields of computer sciences such as computer vision, speech recognition, natural language processing, etc, it is still in its infancy in computational science and engineering communities. Unlike computational applied math methods in which solution accuracy and reliability are guaranteed under regularity conditions, deep learning in its present state is often far from providing accurate predictions for inverse problems in engineering and science applications.

The following, we argue, are among the main reasons. First, scalable approaches for designing the network architecture are not available, thus hours or days may be required to tune hyperparameters. Second, standard deep learning methods are not capable of respecting the underlying mathematical models with limited data.

Third, for machine learning methods that serve as a basis for design, control, discovery, and decision-making, their solutions must be equipped with the degree of confidence. However, quantifying the uncertainty in machine learning solution remains challenging and an open problem facing the computational science and engineering community.

Thus, there is a critical need to develop reliable, robust, and model-aware deep learning methods to tackle complex, natural, engineered, and science systems in order to continue the pace of scientific discoveries and to promote the progress of science.

The objective of this project is to:

1) equip deep learning with the underlying mathematical models to improve generalization error, especially for low data regime, 2) achieve comparable accuracy with traditional forward/inverse computational methods while taking a fraction of the cost; and 3) quantify the uncertainty in deep learning for forward/inverse solutions.

Forward/inverse seismic wave propagation and magnetohydrodynamics---problems in NSF portfolio--- are chosen as the demanding testbed for our developments.

Type: New PW

Title: Simulating slab-plume interaction with realistic mantle convection models

Principal Investigator: Dave Stegman (University of California San Diego (UCSD) (UC San Diego))

Co-Investigators:

Field of Science: Geophysics

Abstract:

We propose to use high resolution numerical models to reproduce the subduction of slabs, the rising of plumes, the tilting of plume conduits and its potentiality of producing hotspot tracks. With the presence of Samoan plume and considering the slow seismic anomalies, the rheology could be complex. We plan to apply non-Newtonian rheology and melt-dependent viscosity in the models. The mantle convection models will also be used to simulate seismic anisotropy. By comparing with observation, the model results will provide key constraints on the distribution of slab and plume as well as their interaction. The revealed mantle flow history will be critical for studying the travel of Samoan plume.

Type: Renewal

PW

Title: Exploration of the Energy Landscape of Nisin-Membrane Interaction

Principal Investigator: Ulrich Hansmann (University of Oklahoma (OU))

Co-Investigators:

Field of Science: Biochemistry and Molecular Structure and Function

Abstract:

The 34-residue long nisin protein is widely utilized in the food industry, as it is highly effective, safe, and naturally produced food preservative. Because of its strong antibacterial activity toward many gram-positive bacteria, it has the potential to be used as an antibiotic drug. However, its adaption in drug design is limited by a lack of understanding on the mechanism by which it is efficacious. Continuing our previous investigations into the energy landscapes of protein folding and aggregation, we will use molecular dynamics to study the pore formation mechanism of nisin in bacterial and cancerous cell membranes, to identify the factors that affect the stability of the pore, and to probe the interaction between nisin and the membrane.

Type: Renewal

PW

Title: Mechanism of Ca²⁺-evoked synaptic vesicle fusion

Principal Investigator: Jose Rizo-Rey (University of Texas Southwestern Medical Center (UTSW) (UT Southwestern))

Co-Investigators:

Field of Science: Neuroscience Biology

Abstract:

The mechanism of neurotransmitter release by Ca²⁺-evoked synaptic vesicle fusion has been extensively studied for three decades, yielding critical insights into the functions of the core components of the release machinery. The SNAREs syntaxin-1, synaptobrevin and SNAP-25 play a critical role in membrane fusion by forming a tight SNARE complex that brings the membranes together, and synaptotagmin-1 acts as the Ca²⁺-sensor that trigger release. However, the mechanism of membrane fusion remains highly unclear. This application proposes to perform all-atom molecular dynamics simulations in the microsecond time scale to investigate how the SNAREs trigger fast, Ca²⁺-dependent membrane fusion in a tight interplay with synaptotagmin-1.

Type: Renewal

PW

Title: Investigation of Mechanical and Thermal Properties of TMDs using Parametrized MD Force Fields

Principal Investigator: Horacio Espinosa (Northwestern University)

Co-Investigators:

Field of Science: Mechanics and Materials

Abstract:

Transition metal dichalcogenides (TMDs), a family of two-dimensional materials, have shown unique optical, electrical, and thermal properties that enable emergent applications in batteries, solar cells, electronics, and sensors. In all these applications, failure by fracture as well as thermal effects are major concerns. Under this project, the aim is to advance the fundamental knowledge of thermo-mechanical properties of transition metal dichalcogenides, and to establish robust experimental and computational protocols that are applicable to similar studies on other nanomaterials. Specifically, the work done on MoSe₂ under project MSS21004 is extended to a library of TMDs. In the same line, effect of strain and grain boundaries on thermal transport would be explored.

Type: Renewal

PW

Title: Renewal for PHY20032: First-principles study of many-body interactions and excited-state properties in two-dimensional

Principal Investigator: Diana Qiu (Yale University)

Co-Investigators:

Field of Science: Condensed Matter Physics

Abstract:

Two-dimensional (2D) materials are the subject of significant ongoing research for technological applications in electronics, optoelectronics, valleytronics, and energy. Under optical excitation, 2D materials in general exhibit strong electron-hole interactions due to the strong spatial variations in the screening of the Coulomb interaction, as well as reduced total screening and electronic confinement resulting from the dimensionality reduction. It is thus very important to accurately calculate and thoroughly understand the many-electron properties of 2D materials for developing devices based on such materials. Our group is actively focused on studying the effect of many-body interactions on the excited state properties of materials in reduced dimensions and complex functional materials. Particular emphasis is placed on engineering optical excitations of 2D materials by inducing and controlling structural/chemical defects, aiming to provide an understanding of fundamental processes such as charge/energy transfer between heterointerfaces and guidelines for designing 2D systems for technological applications. Our group is also engaged in developing high-performance first-principles quantum physics methods based on the GW-Bethe-Salpeter-Equation (BSE) approach to calculate many-electron interaction effects for a broad range of material systems with a current focus on novel efficient algorithms for solving BSE including non-uniform spatial sampling schemes, finite momentum excitons, time-dependent approaches, and electron-hole interactions in core-level spectra. Three specific research topics will be investigated on the renewed Frontera Pathway allocation. In the first project, we will propose a scheme for calculating the exciton-phonon interactions in 2D materials. In the second project, we will use the GW-BSE method to study the chirality induced spin selectivity at the interface of chiral and achiral materials. Lastly, we will explore the effects of molecular adsorption and structural defects on the excitonic features and valley polarization of 2D materials using the ab initio GW-BSE approach.

Type: New LSCP

Title: Discovery and Measurement at the Energy Frontier with the ATLAS Detector at the CERN Large Hadron Collider

Principal Investigator: Rui Wang (Argonne National Laboratory (ANL))

Co-Investigators: Rob Gardner (University of Chicago)

Field of Science: Elementary Particle Physics

Abstract:

The goal of high energy physics researchers is to understand the fundamental nature of matter and the basic forces through which it interacts. The ATLAS experiment at the Large Hadron Collider (the world's highest energy proton collider) offers a rich data set for exploring particle physics at the highest available energies.

The discovery of interesting phenomena requires studying very rare processes which occur at rates of one out of every billion or more collisions. ATLAS collects dataset at O(petabytes) per year to look for a tiny fraction of important collisions. This poses significant computational challenges, including generating and simulating all physics processes of interest in great detail and with very high statistics (2 to 3 times the size of the real data).

Frontera offers a unique opportunity to accelerate the physics reach of the current data set while modeling the future conditions relevant for the High Luminosity LHC upgrade, scheduled to begin operations in 2029. We would like to exploit the CPU and GPU capacity of Frontera to contribute to ATLAS Run 3 simulation production, accelerate discovery for the collaboration, and solve the challenges for HL-LHC operation on event generation, software trigger and workflow.