Type: Renewal PW

Title: Leadership-class Computing Resources in Support of Very Large and Advanced Reservation Experiments for Ensemble-based Data Assimilation and Prediction Research

Principal Investigator: Xuguang Wang (University of Oklahoma)
Co-Investigators: Aaron Johnson (University of Oklahoma); Yongming Wang (University of Oklahoma); Nick Gasperoni (University of Oklahoma)

Field of Science: Meteorology; Atmospheric Sciences

Abstract:
This Pathways research allocation proposal seeks critical Frontera resources to support very large and advanced reservation experiments by University of Oklahoma Multiscale data Assimilation and Predictability (MAP) Lab. These experiments aim to advance the ensemble based data assimilation (DA) and ensemble prediction research to improve convective scale numerical weather prediction over the Continental US. The topics included are (a) evaluating the effectiveness of the valid time shifting (VTS) method in improving ensemble-based DA through Hazardous Weather Testbed (HWT) real-time forecast experiments, and (b) using past forecast cases to generate skillful post-processed probabilistic forecasts of severe weather hazards Both of these research topics are funded through competitive proposals. 220.2k SUs from Frontera are requested to support large scale and advanced reservation ensemble-based data assimilation and ensemble forecast experiments to address the scientific goals of these projects by the MAP research lab. The experiments will be running with numerical models with grid spacing of 3km over the large Continental US domain, A 40-member parallel ensemble forecasts during the data assimilation cycling and 10-member parallel ensemble forecasts with longer lead times initialized at the end of the data assimilation cycling. Scaling tests have shown that forecast system can make efficient use of Frontera resources as the dominating model ensemble component of the forecast system scales well to more than 200,000-400,000 cores on Frontera. Frontera is the only suitable resource the proposing team can identify to perform the large scale and time sensitive experiments. The proposal team has no access to other resources to perform the proposed experiments.

Type: Renewal PW

Title: Magnetic Reconnection Localized in the Dawn-Dusk Direction of Earth's Magnetotail

Principal Investigator: Yi-Hsin Liu (Dartmouth College)
Co-Investigators: Xiaocan Li (Dartmouth College)

Field of Science: Magnetospheric Physics

Abstract:
The earthward ejecta of the near-earth magnetotail reconnection is dipolarizing flux bundles (DFBs), flux tubes with an intense magnetic field. Observations show that the DFBs are embedded in fast earthward flows called bursty bulk flows (BBFs), and they are localized in the azimuthal (i.e., dawn-dusk) direction with an extent of ~< 3 RE. These fast earthward flows have been associated with Pi2 pulsations and the geomagnetic substorm current wedge. A localized DFB that propagates earthward could originate from an azimuthally localized reconnection x-line, where the frozen-in condition is violated. In this proposal, we plan to conduct a thorough study on the kinetic process of this scenario, which by itself will make a transformative advance in understanding the fundamental nature of three-dimensional (3D) reconnection x-lines with a limited spatial extent. i.e., Note that this is dramatically different from a 2D model where the x-line extent is “infinitely long” because of the translational invariance in the out-of-plane direction. Based on the observation input, we will induce localized x-lines in the tail geometry in 3D particle-in-cell (PIC) simulations, and then we study the spread, morphology, and interaction of these localized x-lines.

Type: New PW

Title: Towards improving hurricane storm surge modeling through the use of satellite-informed wind fields

Principal Investigator: Ethan Kubatko (Ohio State University (OSU))
Co-Investigators:

Field of Science: Natural and Man-Made Hazard Mitigation; Environmental and Ocean Systems

Abstract:
This proposal aims to employ the requested computational resources to support the use of measurements made available by NASA's first-of-its-kind Earth Venture, CYGNSS (CYclone Global Navigation Satellite System) mission for the improved prediction of hurricane storm surge, which can aid to increase readiness, to minimize damage incurred to human life,
and to mitigate severe economic ramifications. This requires a multi-pronged simulation, modelling, analysis and retrieval framework — which includes the use of the ADvanced CIRCulation (ADCIRC) storm surge model and the extended NASA CYGNSS End-to-End simulator and predictor.

Type: New PW

Title: DFT- and ML-Based Mechanistic Analysis of the Roles of Novel Base Metal Complexes in Stereoselective Catalytic Transformations

Principal Investigator: Oleg Larionov (University of Texas at San Antonio)
Co-Investigators:

Field of Science: Organic and Macromolecular Chemistry

Abstract:
Transition metal-catalyzed cross-coupling reactions have revolutionized construction of carbon–carbon and carbon–heteroatom bonds, yet the mechanistic underpinnings of the catalytic processes have remained poorly understood, especially in the case of stereoselective transformations. We aim to develop comprehensive understanding of base metal (e.g., copper and nickel) catalyzed stereoselective processes for the construction of carbon-carbon and carbon–heteroatom (e.g., sulfur) bonds, using in depth density functional theory-based computational and machine learning studies. The proposed work is expected to streamline the analysis and prediction of stereochemical outcomes of stereoselective catalytic transformations and guide the development of general models of catalytic transition metal-catalyzed reactions.

Type: New PW

Title: Application of MD Simulations to Rationally Design PROTACs

Principal Investigator: Jin Wang (Baylor College of Medicine (BCM))
Co-Investigators:

Field of Science: Chemistry

Abstract:
A PROTAC is a heterobifunctional molecule that can bind both a targeted protein and an E3 ubiquitin ligase to facilitate the formation of a ternary complex, leading to ubiquitination and ultimate degradation of the target protein. Compared with oligonucleotide and CRISPR therapeutics that face in vivo delivery challenges, PROTACs are small molecule therapeutics that provide opportunities to achieve broadly applicable body-wide protein knockdown. However, the current design and development of PROTACs is highly empirical due to the complicated nature of the E3 ligase complex formed. We will apply MD simulations to understand the structure-activity relationship of PROTACs and validate the computational modeling with experimental data. Our ultimate goal for this project is to develop a rational computational approach for PROTAC development.

Type: New PW

Title: SwitchIT: Pushing the Limits of computational Rovibrational Molecular Spectroscopy Simultaneously with Respect to System Size, Convergence Accuracy, and Number of Computed States

Principal Investigator: Janos Sarka (Texas Tech University (TTU))
Co-Investigators: Bill Poirier (Texas Tech University (TTU))

Field of Science: Physical Chemistry

Abstract:
Methods for solving the Schrödinger equation without approximation are in high demand but are notoriously computationally expensive. In practical terms, there are just three primary factors that currently limit what can be achieved: 1) system size/dimensionality; 2) energy level excitation; and 3) numerical convergence accuracy. Broadly speaking, current methods can deliver on any two of these three goals, but achieving all three at once remains an enormous challenge. In a recent paper [JTCC, 17, 7732-7744 (2021)], we demonstrated how to "hit the trifecta" in the context of molecular vibrational spectroscopy calculations. In particular, we implemented a new methodology in the SwitchIT code, and computed the lowest 1000 vibrational states for the six-atom acetonitrile molecule (CH3CN), to a numerical convergence of accuracy 10^{-2} cm^{-1} or better. These calculations encompass all vibrational states throughout most of the dynamically relevant range (i.e., up to ~4250 cm^{-1} above the ground state), computed in full quantum dimensionality (12 dimensions), to near spectroscopic accuracy. To our knowledge, no such vibrational spectroscopy calculation has ever previously been performed. Here, we propose to extend our recent investigation of CH3CN to compute the first 10,000 vibrational states—thereby covering the entire dynamically relevant range. Also, we would like to apply SwitchIT to another spectroscopically relevant and challenging system—i.e., the vibrational tunneling dynamics of malonaldehyde. This project is currently supported by two grants, one from NSF (CHE-1665370) and another from the Robert A. Welch Foundation (D-1523).

Type: Renewal PW

Title: Prediction of functional defect properties in materials for clean energy applications

Principal Investigator: Bilge Yildiz (Massachusetts Institute of Technology (MIT))
Co-Investigators:

Field of Science: Materials Research

Abstract:
We request a renewal of our research allocation on Frontera supercomputer for the prediction of functional defect properties in materials for clean energy applications. We mainly focus on three research topics: (1) bipolaronic superconductivity in hydrogen doped transition metal oxides, (2) improving durability and performance of solid oxide electrolyzers by controlling surface composition on oxygen electrodes, and (3) investigation of the Al2O3|Al interface structure for designing superior hydrogen permeation barriers. These projects require massive density functional theory (DFT) calculations, namely (1,2) density functional theory with Hubbard correction (DFT+U) to calculate defect chemistry and electronic structure, and (3) DFT-based Monte Carlo (MC) simulations to assess atomic-scale structure of Al2O3|Al interface. We expect that information obtained using ab initio modeling will help to identify the most promising material combinations and guide our experimental studies on tuning superconductivity by hydrogen doping, solid oxide electrolyzers, and hydrogen permeation barriers. In our calculations, we will primarily exploit VASP and LAMMPS computational packages designed to run on high-performance parallel supercomputers.

Type: New PW

Title: Materials genomic search for new quantum host compounds and high-throughput quantum materials characterization

Principal Investigator: Ju Li (Massachusetts Institute of Technology (MIT))
Co-Investigators:

Field of Science: Materials Research

Abstract:
New quantum materials and qubit control mechanisms would considerably accelerate the development of quantum technologies. In this proposal, we propose to conduct a materials genomic search for new host compounds and color center qubits for quantum technologies as well as employ machine learning paradigms to elastic strain engineering of nuclear spin-based quantum devices. It is of immense scientific and technological interest to extend our previous work to the emerging field of quantum devices.

Type: New PW

Title: First-Principles Studies of Excited-State Phenomena in Quasi-Two-Dimensional Materials

Principal Investigator: Felipe Jornada (Stanford University)
Co-Investigators:

Field of Science: Materials Research

Abstract:
This is a proposal for a Pathways allocation at Frontera. These resources will be used to explore new domains of research and scale our current computational methodologies in thefield of computational materials science. Our proposal utilizes parameter-free methods and massively parallel computer calculations to understand the excited-state properties of novel 2D materials. We are particularly interested in understanding the interplay between structural properties and electronic and optical excitations in such 2D systems. Specifically, our proposal addresses the general trends arising when two monolayer materials are stacked on top of each other, forming moiré potentials that localize electrons and excitons. We also seek to understand the role of lattice vibrations (phonons) in the scattering of excitons in such systems. Finally, we also seek to understand the nature of magnetic defects in 2D materials, and their experimental signature. Alltogether, our proposal addresses challenging scientific problems which have not yet been accessible with the level of prediction possible with state-of-the-art first-principles computational approaches. It also addresses emerging questions in the field of atomically thin materials, and has the possibility of impacting future photovoltaic materials and quantum science.

Type: Renewal PW

Title: Continent-scale InSAR velocity fields for volcanology and tectonics

Principal Investigator: falk amelung (University of Miami)
Co-Investigators:

Field of Science: Earth Sciences

Abstract:
We request a Frontera allocation for continent-wide InSAR processing for tectonics and volcanology. Continent-scale InSAR requires the processing of several 100TB of data. The science questions to be addressed are (1) how deformation from the India-Eurasia continental collision is distributed in Tibet, and (2) how rainwater infiltrated into the ground from anomalous precipitation affects volcanic unrest.

Type: New PW

Title: Direct numerical simulation of compressible shear layers with streamwise curvature and density variation

Principal Investigator: Robert Childs (National Aeronautics and Space Administration (NASA))
Co-Investigators:

Field of Science: Engineering Systems

Abstract:
Compressible, variable density turbulent mixing occurs in a wide variety of modern engineering applications, and has been a research topic of interest for several decades. Many aerospace applications also involve external, high-speed jet plumes that are affected by multiple complex turbulence mechanisms. While turbulence model corrections for the compressibility, variable density, and rotation and curvature effects observed in these flows exist, these models have not been developed systematically. Often, modeling options are proposed and demonstrated in flows which include only the one mechanism of interest. As such, application of these corrections in combination exacerbates model form uncertainty. A deeper, fundamental understanding of the turbulent mixing at the intersection of these parameters is required to improve the predictive capability of computational fluid dynamics (CFD). The proposed work addresses the challenge of characterizing turbulent mixing under such complex conditions by providing valuable data to inform the current understanding of turbulence physics. High-resolution large eddy simulations (LES) and direct numerical simulations (DNS) of the canonical spatially developing shear layer with the addition of streamwise curvature will pursued to fully investigate turbulent flow physics at the largest and smallest scales.

Type: Renewal PW

Title: Frontera Pathways: Calculation of electron collisions with molecular targets using the convergent close-coupling method

Principal Investigator: Barry Schneider (National Institute of Standards and Technology (NIST))
Co-Investigators: Igor Bray (Curtin University); Dmitri Fursa (Curtin University); Liam Scarlett (Curtin University)

Field of Science: Atomic, Molecular, and Optical Physics

Abstract:
The highly accurate Molecular Convergent Close Coupling method will be used to compute electron scattering cross sections for a number of small diatomic molecules where accurate data is needed for applications to plasma modeling in fusion, astrophysics and lighting.

Type: New PW

Title: Large scale simulations of collisionless plasma turbulence

Principal Investigator: Anna Tenerani (University of Texas at Austin (UT) (UT Austin))
Co-Investigators:

Field of Science: Physics

Abstract:
This project has the goal to investigate the interplay between kinetic physics and large scale nonlinear dynamics in turbulent systems such as the solar wind. This goal has long been a theoretical and numerical challenge of plasma physics due to the intrinsic multi-scale nature of plasmas. Our plan is to push the envelope of state-of-the-art hybrid and full Particle In Cell (PIC) codes to study kinetic effects in large scale turbulent systems, including performing the first fully PIC simulations of low frequency Alfvenic fluctuations. Results from this work will advance the understanding of the processes that govern the turbulent cascade and particle energization, and of how such processes affect the macroscopic dynamics of collisionless magnetized plasmas.

Type: New PW

Title: Sparse SYK model and gravity duals

Principal Investigator: Elena Caceres (University of Texas at Austin (UT) (UT Austin))
Co-Investigators: Anderson Misobuchi (University of Texas at Austin (UT) (UT Austin))

Field of Science: Theoretical Physics

Abstract:
We propose to study a class of quantum systems known as sparse SYK models. These systems exhibit quantum chaos and other properties that identify them as potential holographic duals of black holes. The holographic duality has revolutionized our understanding of quantum gravity. It is relevant to explain fundamental questions in physics regarding the very early stages of the universe and the interior of black holes. One of the challenges we face in understanding foundational questions in this duality is the lack of explicit quantum models with a holographic dual. The sparse SYK models are a new class of quantum systems conjectured to have gravity duals. We will carry out several projects to achieve a solid understanding of the sparse SYK models and their connection to quantum gravity. This will be achieved by computing physical observables and performing a state-of-the-art numerical simulation of sparse SYK.

Type: New LSCP

Title: Galaxy: A global platform for biological analysis and outbreak surveillance

Principal Investigator: Anton Nekrutenko (Penn State University (PSU))
Co-Investigators: Enis Afgan (Johns Hopkins University)

Field of Science: Advanced Scientific Computing

Abstract:
For over a decade, the Galaxy Project (https://galaxyproject.org/) has worked to solve key issues plaguing modern data intensive biology—the inability of researchers to access cutting-edge analysis methods, to share analysis results transparently, and to precisely reproduce complex computational analyses. Galaxy has become one of the largest and most widely used open source platforms for biological data science. Promoting openness and collaboration in all facets of the project, from technical decisions to training and leadership, has enabled us to build a vibrant community of users, developers, system engineers, and educators who continuously contribute new software features, add the latest tools, adopt to the most modern infrastructure, author training materials, and lead research and training workshops. Genomics research is continuously evolving, and current challenges include the rapid growth in size and complexity of new datasets and the continuing expansion in the breadth of research areas capable of generating high throughput data.

Most importantly, Galaxy is not a project led by a single PI, lab, or an institution. It is a community of users, developers, and infrastructure administrators that work together to provide a unique, freely available, high performance data analysis environment serving the full range of biological questions as well as other disciplines (see https://galaxyproject.org/use/). The allocation request aims at significantly improving the capability of our service to allow for the full range of data analysis scenarios currently present in modern biology.

Type: Renewal LSCP

Title: LSCP Support for the SolFER DRIVE Center

Principal Investigator: William Daughton (Los Alamos National Laboratory (LANL))
Co-Investigators:

Field of Science: Solar Terrestrial Research

Abstract:
SolFER (Solar Flare Energy Release) is a multi-institution collaboration funded by NASA's DRIVE program to study the explosive release of magnetic energy in solar flares and the associated production of energetic particles. It brings together 12 institutions and > 50 researchers with expertise in observation, theory, numerical modeling, and computer science. This LSCP proposal seeks computational resources for the theory and modeling aspects of SolFER as well as access to an archival system to facilitate comparisons of simulations with observations. Our team employs a rich set of numerical tools (particle-in-cell, hybrid, magnetohydrodynamics, and more) and has substantial experience in performing simulations on leadership supercomputing facilities. In the three-year project, we will explore several key aspects of solar flare energy release, including onset, the heating and acceleration of both ions and electrons, and energetic particle transport in the flaring region.

Type: Renewal LSCP

Title: IceCube Computing on Frontera

Principal Investigator: Francis Halzen (University of Wisconsin Madison (UW Madison))
Co-Investigators: Benedikt Riedel (University of Wisconsin Madison (UW Madison))

Field of Science: Astronomical Sciences

Abstract:
The IceCube Neutrino Observatory (ICNO) located at the U.S. Amundsen-Scott South Pole Station. The ICNO transformed one cubic kilometer of natural ice (at the depth from 1.4 to 2.4 km) into a giant Cherenkov emission detector, thus creating the world's largest neutrino detector above energies of approximately 10 GeV. Since its completion in 2010, the ICNO has detected neutrinos with energies spanning more than six orders of magnitude, from 10 GeV to beyond 5 PeV for the first time. (GeV = one billion electron volts; TeV = one trillion electron volts; and PeV = one quadrillion electron volts.) In 2017, the ICNO detected a neutrino with an energy of 290 TeV and its origin was pinpointed (again for the first time) to a blazar at a distance of about 3.5 million light years. This detection triggered an extensive campaign involving some twenty space- and ground-based telescopes that launched a new era in multi-messenger detection.

Multi-messenger detections depend heavily being able to model the detector behavior to signal and background. This requires significant computing resources, including GPU resources. This allocation will help IceCube produce more background simulation to get closer to the goal of parity between data collected and data simulated.

Type: Renewal LSCP

Title: Frontera Computing for the Compact Muon Solenoid at the Large Hadron Collider

Principal Investigator: Tulika Bose (University of Wisconsin Madison (UW Madison))
Co-Investigators: Mia Liu (Purdue University); Tulika Bose (University of Wisconsin Madison (UW Madison))

Field of Science: Elementary Particle Physics

Abstract:
The Compact Muon Solenoid (CMS) is one of the two general-purpose particle physics detectors at the Large Hadron Collider (LHC). The CMS Collaboration co-discovered the Higgs boson in 2012, has provided constraints on many models of new physics, and has made many precise measurements of the properties of known particles. 1070 scientific papers have been submitted to date. We request a renewal of our allocation on Frontera to continue our large- scale simulations of proton collisions, with an allocation sufficiently large to generate nearly 2B events, which would be about 5% of the total simulated data set planned by CMS for the year beginning March 1, 2022. This effort will also allow us to demonstrate the use of Frontera resources at very large scales in preparation for meeting the needs of CMS at the planned High Luminosity LHC.