Type: Renewal PW

Title: Pion Polarizability and Lattice QCD

Principal Investigator: Walter Wilcox (Baylor University (baylor.edu))
Co-Investigators: Frank Lee (George Washington University); Ronald Morgan (Baylor University)

Field of Science: Nuclear Physics

Abstract:
The amplitudes associated with many nuclear and elementary particle physics observables can be efficiently formed and measured using Monte Carlo lattice QCD (LQCD) four-point functions. These functions contain amplitudes associated with masses, electromagnetic charge radii, form factors and various types of particle polarizabilities. We propose a set of computer simulations to measure electric polarizabilities for charged kaons and neutral pions using LQCD four-point functions. We also propose extending these calculations to pion structure function function evaluations using the hadronic tensor approach.

Type: New PW

Title: Spring Land Surface and Subsurface Temperature Anomalies and Subsequent Downstream Late Spring-Summer Droughts/Floods in North America and East Asia

Principal Investigator: Yongkang Xue (University of California Los Angeles (ucla.edu))
Co-Investigators: HARA NAYAK (University of California Los Angeles (ucla.edu))

Field of Science: Atmospheric Sciences

Abstract:
The extreme climatic events, such as droughts and floods, can have serious socioeconomic impacts. The World Weather Research Programme and the World Climate Research Programme Sub-seasonal to Seasonal Prediction Project indicates that the subseasonal to seasonal (S2S) prediction, especially the drought and flood prediction, remained poor for years. Under the National Science Foundation (NSF) support, our NSF project aims to explore the idea for the first time to utilize the information of spring land surface temperature/subsurface temperature (LST/SUBT) anomalies over the high elevation areas in North America and East Asia for the prediction of late spring/summer droughts or floods. The results from this research are useful for disaster prediction, prevention, and mitigation. Under our NSF project support, we have employed an Earth system model to conduct a large number of numerical experiments to identify the role of the Tibetan Plateau and the Rocky Mountains LST/SUBT in affecting the drought/flood in many parts of the world, including the Southern Great Plains. So far, we have completed the first phase experiment, which focused on the effect of the Tibetan Plateau spring LST/SUBT. Currently we are focusing on the Rocky Mountains spring LST/SUBT effect which will require a large amount of computer resources to conduct several numerical experiments. Moreover, Experiments will also be conducted to test sea surface temperature effect, which is traditionally used in the weather/climate prediction, and will be compared with the LST/SUBT effect.

Type: Renewal 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 (utsa.edu))
Co-Investigators:

Field of Science: Organic and Macromolecular Chemistry

Abstract:
Transition metal- and photocatalyzed 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 catalyzed and photocatalyzed processes for the construction of carbon-carbon and carbon–heteroatom 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 outcomes of catalytic transformations and guide the development of general models of catalytic transition metal-catalyzed reactions.

Type: Renewal PW

Title: Correlated Effect in Twisted Materials

Principal Investigator: Allan MacDonald (University of Texas at Austin (utexas.edu))
Co-Investigators:

Field of Science: Condensed Matter Physics

Abstract:
Twisted multilayer van der Waals materials have been widely interested worldwide since the discovery of superconductivity in twisted bilayer graphene, which was predicted theoretically by our group. One of the most interesting phenomena is the strong electron-electron interactions due to the flatbands that appeared at a small twisted angle. Except for superconductivity, more exotic properties are discovered, including magnetism, topological phases, and correlated insulating states, etc. Exploring the physics of the twisted materials depends on various computational tools, for example, first principle density-functional-theory, Hartree-Fock method, and exact diagonalization of a huge matrices. We would like to motivate experimental work and engineered applications based on these effective and realistic simulations.

Type: New PW

Title: The Earth’s Global Magnetic Reconnection Configuration and Cusp Ion Signatures

Principal Investigator: Brandon Burkholder (University of Maryland Baltimore County (umbc.edu))
Co-Investigators:

Field of Science: Physics

Abstract:
Magnetic reconnection is the main driver of space weather at Earth. Understanding where and how reconnection occurs is a vital open question in space physics that is difficult to tackle because the reconnection process occurs on very small scales but its effects have global consequences for the magnetosphere. State-of-the-art global magnetosphere simulations are employed in this project to understand the interaction of different meso-scale processes in Earth's magnetosphere and how they lead to structure and dynamics of the global reconnection configuration. We also reconstruct observable signatures of the reconnection process to better understand spacecraft observations in key regions of the magnetosphere.

Type: New PW

Title: Ab initio excited state forces from GW/BSE and DFPT calculations: applications to perovskites and 2D materials

Principal Investigator: Rafael Del Grande (University of California Merced (ucmerced.edu))
Co-Investigators: David Strubbe (University of California Merced (ucmerced.edu))

Field of Science: Physics

Abstract:
While absorption of light has been long studied in electronic structure, the interactions of the resulting excited states with the lattice that cause light-induced structural changes remain hard to handle. This is an underlying phenomenon for photodegradation, Stokes shifts, exciton transport, and other photophysics, which can be studied via excited-state forces. Ismail-Beigi and Louie [Phys. Rev. Lett. 90, 076401 (2003)] developed an approximate theory combining quasiparticle and excitonic effects from GW and Bethe-Salpeter Equation (BSE) with electron-phonon interactions from Density Functional Perturbation Theory, but this approach has been little used. We revisit this theory, with improvements to the underlying approximations, and implement it in a practical workflow for BerkeleyGW. We make detailed tests of the validity of these approximations. Then we propose to explore two problems: (1) degradation mechanisms on perovskites: we found out that for the cubic phase of methylammonium lead iodide perovskite, low-frequency phonons couple to relevant excitons. We want to explore other phases of those materials as well light induced changes. (2) Exciton-phonon coupling in transition metal dichalcogenides: we want to explore how low energy excitons couple to phonons. In particular we have seen that for bilayer MoS2 the first exciton couples with the Layer Breathing Mode, which is important for the caracterization of the number of layers and their relative orientation in 2D materials.

Type: New LSCP

Title: The Atomic, Molecular and Optical Science Gateway

Principal Investigator: Barry Schneider (National Institute of Standards and Technology (nist.gov))
Co-Investigators: Sudhakar Pamidighantam (Indiana University Bloomington (indiana.edu)); Kathryn Hamilton (University of Colorado Denver)

Field of Science: Atomic, Molecular, and Optical Physics

Abstract:
The Atomic, Molecular and Optical Science (AMOS) Gateway project, is designed to provide the community with state-of-the-art resources to perform a variety of calculations of the energies and dynamical properties of atomic and molecular systems. The gateway also serves as an educational platform for AMOS and has been successfully used in a number of undergaduate and graduate programs in europe and australia. The AMOS Science gateway is accessible at https://AMOSGateway.org, and has been in production since May 2019. There are currently nine internationally recognized research groups participating in the gateway and the gateway has 385 registered users. It has the potential to reach a significantly larger user base as we deploy more mature and intuitive interfaces for the applications for research and training.

Type: New PW

Title: Simulations of Meteor Plasma Turbulence 2023-2024

Principal Investigator: Meers Oppenheim (Boston University (bu.edu))
Co-Investigators: William Longley (Boston University (bu.edu))

Field of Science: Solar Terrestrial Research

Abstract:
Every day billions of extremely small particles, typically weighing less than a grain of sand, impact the Earth's upper atmosphere. However, these particles seed the upper atmosphere with an array of metal ions and atoms which have important effects on the chemistry of the atmosphere and play a role in creating dust, which in turn seeds clouds Scientists use radar signals from meteors to measure upper-atmospheric winds, to estimate the impact of meteoric dust on the atmosphere, and to determine the origin and composition of meteoroids. Despite the frequency and importance of meteors, we have a limited understanding
of meteor physics and how to measure their characteristics and evolution. This prevents researchers from fully utilizing the abundant information that radars and cameras generate, and from understanding meteor effects on the atmosphere.
The proposed research will further develop the field of meteor physics through modeling meteor evolution from their point of entry into the atmosphere through their dissipation. It will use large-scale simulations to test our models and understanding of meteors. Space scientists and engineers
require a detailed understanding of the meteoroid
environment. Spacecraft designers need to know the distribution of particle orbits and masses in order to reduce potential hazards. Solar system scientists use meteoroid population characteristics to better understand the outer solar system and its evolution. Atmospheric scientists apply meteoroid data to estimate the amount of material
deposited in the upper atmosphere and its chemical evolution. A deeper understanding of meteor plasma physics will improve the broader scientific and engineering community's knowledge of meteor and upper atmosphere geoscience.

Type: Renewal PW

Title: Advanced Signal Processing and Machine Learning to Detect RNA Tails on DNA using 2D Nanopore Sensor

Principal Investigator: Jean-Pierre Leburton (University of Illinois Urbana-Champaign (illinois.edu))
Co-Investigators:

Field of Science: Biophysics

Abstract:
In this research, we will conduct an extensive investigation using molecular dynamics and device engineering to demonstrate the capabilities of 2D material membranes with nanopores to sequence DNA structures with RNA tails. The sensing technique will include the calculation of both ionic blocking currents and electronic currents along 2D membranes caused by the modified DNA structures during their translocation through the nanopore. Furthermore, advanced signal processing and machine learning will be employed to undermine the effect of noise and obtain a reliable signal
which can prove to be revolutionary in this field.

Type: New PW

Title: Numerical simulations of Rayleigh-Bénard sheared convection, and of turbulent convection in stars of spectral types from A to F

Principal Investigator: Michael Montgomery (University of Texas at Austin (utexas.edu))
Co-Investigators: Damian Fabbian (University of Vienna (univie.ac.at)); Andrea Caldiroli (University of Vienna (univie.ac.at)); Florian Zaussinger (Brandenburg University of Technology (tu-cottbus.de))

Field of Science: Stellar Astronomy and Astrophysics

Abstract:
This computing project will model the behavior of the atmospheres of stars that have an effective temperature from approximately 6600 K (spectral type F) to 9000 K (spectral type A), by using our radiation (magneto-)hydrodynamic code ANTARES [Muthsam et al., 2010]. We aim to obtain quantitative predictions regarding turbulent convection in these stars, and its detectable signatures. This extremely complex task can only be successfully achieved via the use of a powerful supercomputer such as “Frontera”, with its 8008 Intel ”Cascade Lake” compute nodes.

Type: Renewal PW

Title: Spectral function database for quantum materials using first principles calculations

Principal Investigator: David Vanderbilt (Rutgers University (rutgers.edu))
Co-Investigators: Subhasish Mandal (West Virginia University (wvu.edu)); David Vanderbilt (Rutgers University (rutgers.edu)); Kristjan Haule (Rutgers University (rutgers.edu))

Field of Science: Condensed Matter Physics

Abstract:
Discoveries of new quantum materials are crucial for technological advancement and economic development. The data-science tools recently became the newest scientific paradigm that can remarkably accelerate materials discovery. The physical properties of simpler materials can be well characterized in terms of a system of independent particles in the presence of an average potential, as done in Density Functional Theory (DFT). This has led to materials design, characterization, and database creation based on DFT, such that almost all existing materials databases developed in response to the Materials Genome initiative are built exclusively with DFT engines. For strongly correlated quantum materials, which cannot be treated in this averaged manner, DFT often fails. Various methods going beyond DFT, such as hybrid functionals, meta-GGAs, DFT+ dynamical mean-field theory (DMFT), and GW have been developed to describe the electronic structure of correlated materials, but it is not completely clear how accurate these methods can be expected to be when applied to a given strongly correlated solid. It is thus of pressing interest to compare their accuracy as they apply to different categories of materials. Here, we introduce a novel paradigm in which a chosen set of beyond-DFT methods is systematically and uniformly tested on a chosen class of materials. We have recently tested these methods on various classes of materials, head-to-head, and started to build a broad publicly available database with the results from these studies, hosted at NIST (beyond-DFT part of the JARVIS database). As we were populating the JARVIS beyond-DFT database it is becoming clear that eDMFT robustly outperforms other beyond-DFT methods used in the above studies, as it compares most favorably with experiments. Thus, the goal of this proposal allocation request is twofold. First is to continue testing the set of beyond-DFT ab initio methods (hybrid functionals, DFT+DMFT, and GW), and building up a database of spectral functions and optical properties, and their comparison to available experiments. The other goal is to scale up the DFT+eDMFT database. This allocation request is intended to continue the seed support to develop a culture of data-sharing in the spirit of the Materials Genome Initiative that will enable data-driven or data-intensive approaches to accelerate the discovery of 2D materials, their understanding, and related devices. Our Frontera project was initiated in 2019 in connection with a 2018 DMR-2D Data Framework supplement that funded a consortium of three collaborative NSF DMREF projects: 1629059 (Rutgers) + 1629079 (Tennessee); 1629346 (Rutgers) + 1629260 (Minnesota) + 1629477 (Penn State) + 1629457 (UCLA). The funding for this consortium is channeled via the Rutgers DMR-1954856 and DMR-1709229.

Type: New PW

Title: Nanocomposite Sensors Research

Principal Investigator: Eric Fahrenthold (Univresity of Texas at Austin)
Co-Investigators:

Field of Science: Physical Chemistry

Abstract:
Compact, low power sensors for explosive hazards detection are needed to provide improved protection for personnel and infrstructure. Basic research in this field can support fundamental improvements in the sensitivity and selectivity of explosive detection devices. Nanoscale sensors and quantum based sensing techniques offer important opportunities for scientific advances in compact low power sensors, and computational research can serve as a valuable complement to experiment in accelerating the development of new devices.

Type: Renewal PW

Title: Computational Infrastructure for Geodynamics - Community Code Scaling

Principal Investigator: Lorraine Hwang (University of California Davis (ucdavis.edu))
Co-Investigators: John Naliboff (New Mexico Institute of Mining and Technology (nmt.edu)); Timo Heister (Clemson University (clemson.edu)); Rene Gassmoeller (University of Florida (ufl.edu)); Hiroaki Matsui (University of California Davis (ucdavis.edu)); Arushi Saxena (University of Florida (ufl.edu))

Field of Science: Geophysics

Abstract:
The Computational Infrastructure for Geodynamics (CIG) is an NSF-funded organization dedicated to supporting the infrastructure for the development, maintenance and dissemination of a suite of high-quality, open-source software packages that are widely used in the geosciences to simulate the dynamics of the solid earth. An important mission of CIG is the development of computational capabilities in the scientific community we serve, particularly the use of modern numerical methods, software development methodologies, and high performance computing facilities. To achieve this goal, we aim to further the scalability of codes used in simulating the fluid flow in the Earth's mantle, the deformation of the lithosphere, and in the generation of the geodynamo with the goal of running large 3D simulations in studying the dynamics of the Earth's interior.

Type: New PW

Title: The role of flocculation in building land in river deltas – Theory of microscale processes and its impact on macroscale modeling at the Mississippi Delta

Principal Investigator: Michael Lamb (California Institute of Technology (caltech.edu))
Co-Investigators:

Field of Science: Geophysics

Abstract:
The purpose of this proposal is to apply for a Pathways allocation on Frontera's Cascade Lake (CLX) computational system, the world's top-ranked supercomputing resource. The main goal of this proposal is to use Frontera's high-performing computing resources to develop floc microscale theory and investigate its impact on macroscale earth surface evolution problems. This project includes the study of flocculated particle hydrodynamics, proposes a new theory to approximate cohesive materials transport using floc dynamics, and then applies the theory to the numerical model to simulate large-scale land accretion processes at the Mississippi River Delta system. The first study will advance our understanding on how the heterogeneity of the floc's internal structures impacts the flow around, hence changing the settling behavior of the flocculated particles. The second task will test and use the newly developed floc microscale theory to provide future predictions on macroscale river delta land evolutions. The observations and theories resulting from this work have the potential to be widely used in different geophysical and environmental flow applications and advance those theories in previous theoretical works. This work will also shed light on the development of future coastal engineering methods to preserve the precious land along the Louisiana coast, and other coastal areas with similar conditions over the world.

Type: Renewal PW

Title: Merging Magnetized Neutron Stars with Neutrino Transport

Principal Investigator: Steven Liebling (Long Island University (liu.edu))
Co-Investigators:

Field of Science: Gravitational Physics

Abstract:
This proposal renews that from last year using a distributed, adaptive mesh code, MHDuet, to solve the fully nonlinear, general relativistic, magnetohydrodynamics equations with an approximate neutrino scheme to model the merger of two magnetized neutron stars. This code incorporates large eddy simulation (LES) techniques that has been shown to converge the magnetic field amplification at merger from the Kelvin-Helmholtz instability. The proposed simulations extend those from last year by increasing the resolution and updating the neutrino treatment, in an effort to understand the multimessenger signals observed by gravitational wave (GW) observatories and conventional, electromagnetic (EM) telescopes. Such simulations are critical to extracting science from the wide spectrum of observations of GW170817, a neutron star binary merger that was observed in 2017 in both GW & EM bands, as well as future multimessenger observations.

Type: Renewal PW

Title: Sputtering of Graphitic Structures for Lifetime Estimates of Space Propulsion System

Principal Investigator: Huck Beng Chew (University of Illinois Urbana-Champaign (illinois.edu))
Co-Investigators:

Field of Science: Mechanics and Materials

Abstract:
The need for an efficient, high-thrust space propulsion system to augment or replace traditional chemical propulsion systems is of great national importance, and is paramount to advancing space supremacy of the United States. One of the candidate propulsion system for NASA's Artemis program and human space flight missions on Mars is the Hall Thruster, which is a high power electric propulsion (EP) system. Even though EP has been an integral part of space exploration since the late 1990s, high power EP (>100 kW), such as Nuclear Electric Propulsion, remains largely a concept due to insufficient correlation between ground-test results versus in-flight performance and wear. This primarily stems from ground-based EP test facilities interacting with thruster operations. As such, ground test measurements cannot adequately represent in-space environment, performance, and lifetime, leading to significant uncertainties in predictions. One major challenge is the presence of contaminants from the facility walls interacting with the thruster through back sputtering, contaminant transport and redeposition. To reduce these effects of facility back-sputtering, graphitic structures have traditionally been used to line the walls of the testing chamber. Nevertheless, at high ion energies (high eV), even pyrolytic graphite undergoes significant sputtering. The dispersion of these back sputtered carbon species throughout the facility, and subsequent deposition on the carbon pole covers, center-mounted cathode, anode, and on boron nitride channels, leads to significant errors in EP thrusters' lifetime and performance assessments. Previously, we were awarded 82,500 node hours on Frontera to perform sputtering simulations of graphitic structures using molecular dynamics (MD) simulations with LAMMPS. We are about to exhaust these computational resources, and request 225,000 node hours on Frontera which would enable us to compute the sputtering yields, and differential profiles of primary carbon atom bombardment of carbon substrates to obtain the sputtering yield of secondary carbon atoms for upscaling the results to a Monte Carlo simulation model. The proposed research is currently supported by a NASA grant under the "Joint Advanced Propulsion Institute, a NASA Space Technology Research Institute".

Type: Renewal 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: Bill Poirier (Texas Tech University (ttu.edu))
Co-Investigators: Janos Sarka (Texas Tech University (ttu.edu))

Field of Science: Physical Chemistry

Abstract:
SwitchIT: Rovibrational Molecular Spectroscopy
SwitchIT: Pushing the Limits of computational Rovibrational Molecular Spectroscopy Simultaneously with Respect to System Size, Convergence Accuracy, and Number of Computed States
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, and the hydrogen exchange dynamics in a transition metal polyhydride complexes. This project is currently supported by two grants, the TTU/FAPESP SPRINT (2022/00338-0) and the PD142580, while the development of SwitchIT was supported until very recently by NSF (CHE-1665370) and the Robert A. Welch Foundation (D-1523).

Type: New PW

Title: Systematic Predictions for Dynamical Signatures of New Dark Matter Physics in Galaxies

Principal Investigator: Lina Necib (Massachusetts Institute of Technology (mit.edu))
Co-Investigators: Mariangela Lisanti (Princeton University)

Field of Science: Galactic Astronomy

Abstract:
Despite decades of work, we have yet to understand the fundamental particle nature of dark matter (DM), whose gravity governs the motions of stars in galaxies, galaxies in clusters, and the Uni- verse as a whole. Recent advances in particle physics theory, terrestrial experiments, astrophysical observations, and cosmological simulations of galaxy formation have combined to open up a promising new avenue for testing theories of DM: studying the dynamics of stars and gas in individual galaxies for clues to how they interact with the DM. Individual studies have produced important predictions for galaxy-scale signatures of specific classes of DM models, but a systematic effort to connect theoretically-motivated DM particle candidates to their astrophysical consequences at galaxy scales has been lacking. This project will focus on a specific type of DM called Self- Interacting DM (SIDM): We propose to simulate galaxies as they evolve, introducing a self-interaction component for the DM component. We will study the effect of such interaction on the details of galaxy formation, its shape, and particularly identifying for the first time core-collapse of SIDM. Such results will be compared with available data in order to further constrain DM properties, and potentially make a discovery.

Type: Renewal PW

Title: Elucidation of molecular mechanisms of beta-1 adrenergic receptor biased signaling via all-atom molecular dynamics simulations

Principal Investigator: Igor Vorobyov (University of California Davis (ucdavis.edu))
Co-Investigators: Surl Hee Ahn (University of California Davis (ucdavis.edu)); Vladimir Yarov-Yarovoy (University of California Davis (ucdavis.edu))

Field of Science: Biophysics

Abstract:
Sympathetic nervous system (SNS) stimulation of cardiac cells proceeds through activation of beta-adrenergic signaling pathway and can lead to deadly arrhythmias in diseased myocardium, e.g. in heart failure (HF) or myocardial infarction (MI). Beta-blocking drugs can prevent those arrhythmias but have different efficacies. Experimental studies by our collaborators discovered that beta-blocker carvedilol but not metoprolol can promote biased beta-1 adrenergic receptor signaling towards compartmentalized inhibitory G protein pathway causing potentially cardioprotective effect in HF condition. However, molecular mechanisms of this phenomenon are not clear. Therefore, we assembled a collaborative molecular modeling expert team to tackle this problem using combination of structural modeling and enhanced sampling atomistic molecular dynamics (MD) simulations with the follow-up validation by multi-scale functional kinetic modeling and cell biology experiments by our collaborators. This approach will allow to obtain atomic-level understand of state-specific drug interactions with the receptor and their effect on biased G protein activation. This will help to develop more efficient ways to treat arrhythmias, HF, MI and other cardiovascular disorders. This study has been made possible by recent availability of multiple experimental structures of beta-adrenergic receptor bound to different ligands and receptor's complexes with both stimulatory and inhibitory G protein as well as advances in de novo and homology structural modeling. Moreover, we will be using a state-of-the-art combined Gaussian accelerated MD (GaMD) – weighted ensemble (WE) approach for accurate estimation of state-specific receptor - ligand and G protein interaction kinetics and thermodynamics. We hypothesize that different ligands might have distinct receptor binding poses, conformational preferences and/or kinetics, which leads to their differential association with G protein subtypes. This is corroborated by our recent MD simulation study on dynamic interplay between beta-2 adrenergic receptor, its agonist norepinephrine (NE) and stimulatory G protein, which clearly identified alternative NE receptor binding sites and their connection with different G protein conformations. This study was published in PNAS (Han et al PNAS 2023, 120 (10): e2215916120) and partially used our previous Frontera Pathways allocation. The proposed follow-up study using enhanced sampling MD simulations is most suitable for TACC Frontera petascale CPU and GPU architecture.

Type: Renewal PW

Title: Swirl-stabilized hydrogen combustion numerical simulation

Principal Investigator: Paul PALIES (University of Tennessee Knoxville (utk.edu))
Co-Investigators: Gan Xiao (University of Tennessee Knoxville (utk.edu))

Field of Science: Science and Engineering Education

Abstract:
Future combustion propulsion systems may operate with hydrogen fuel in premixed regime with air to reduce the emission of NOx and eliminate those of CO2. Swirl-stabilized combustion of hydrogen/air flames operating in premixed regime is important both from a fundamental point of view and for technological relevance. Numerical simulations aiming at describing the physical phenomena of these complex flows are critical and very few detailed simulations exist. The present pathway renewal proposal is focusing on continuing some of these challenging and computationally demanding simulations on relevant cases prior to submitting in a near future a LRAC proposal. The research proposed in this renewal pathway proposal will focus on ignition and assessing flame speed models and evaluate selected existing models from literature directly on the numerical simulation data generated within this Frontera pathway allocation. The simulation data will be significantly post-processed and analyzed and the code further optimized

Type: Renewal PW

Title: A Systematic Study of How AGN Feedback Regulates the Black Hole Accretion in Early Protogalaxies

Principal Investigator: Kung-Yi Su (Harvard University (harvard.edu))
Co-Investigators:

Field of Science: Galactic Astronomy

Abstract:
AGN feedback plays a crucial role in the evolution of galaxies and black hole accretion. Observations have identified supermassive black holes (>>1e5 solar mass) associated with jetted AGN quasars at high redshifts (Z>4). However, it remains unclear whether stellar-mass or intermediate-mass black holes can grow rapidly enough to become supermassive black holes within a relatively short period, particularly considering the presence of AGN feedback. Most studies on AGN feedback and black hole accretion either employ galaxy-scale simulations or GRMHD simulations capable of resolving the accretion disk. The former case achieves a best resolution of ~0.1 pc, while the latter case has an outer boundary of up to 1000 times the gravitational radius. This discrepancy creates a significant gap of several orders of magnitude, making it challenging to connect the sub-grid models of black holes at the galaxy scale with the self-consistently launched jet in the black hole accretion disk.

To address this gap and investigate the impact of AGN feedback on black hole accretion, we propose using high-resolution hydrodynamic simulations of pc-scale boxes. This set of simulations will allow us to study the propagation of bubbles resulting from various forms of AGN feedback in the vicinity of black holes and their effects on the accretion of stellar-mass to intermediate-mass black holes in different environments. We will systematically vary parameters such as background gas density, temperature, turbulence, magnetic fields, angular momentum, black hole mass, feedback efficiency, and AGN feedback models.

Our proposed simulation will incorporate the most relevant processes to model the interplay between galaxy evolution and AGN feedback. This includes (1) the use of state-of-the-art hydrodynamic code, GIZMO, under the MFM model that combines the advantages of Lagrangian and Eulerian methods, (2) ray transfer for radiative feedback, (3) hyper-refinement around the black hole and jet propagation region to achieve higher resolution for resolving jet propagation and black hole accretion, and (4) the particle spawning method for more accurate jet modeling, capturing the physics of jets. These simulations will provide an extensive survey of every aspect of jet AGN feedback models in black hole accretion and cocoon/bubble propagation.

Type: New PW

Title: Screening proto-drugs against novel therapeutic targets for cancer

Principal Investigator: Bruce Beutler (University of Texas Southwestern Medical Center (utsouthwestern.edu))
Co-Investigators:

Field of Science: Molecular Biosciences

Abstract:
The goal of the proposed work, to be carried out using the Frontera supercomputing platform, is to identify lead small molecule proto-drugs that bind to novel therapeutic targets for development as treatments for leukemia and lymphoma. Current targeted cancer therapies achieve therapeutic effects but suffer from both mechanism-related and off-target toxicities and diminishing effectiveness due to selection for resistance mutations in the target. Moreover, genotoxic drugs (alkylating agents, DNA crosslinkers, topoisomerase inhibitors, microtubule disruptors, antagonists of folate metabolism, and others) continue to be the mainstay of chemotherapy despite their cytotoxic and in some cases mutagenic effects on non-malignant cells. We have sought new therapeutic targets for the treatment of cancer by screening for genetic suppression of otherwise inevitable cancer development and progression in mice. We identified several well-tolerated germline mutations that suppress two genetically-driven leukemia/lymphoma and lymphoproliferative diseases. With a Pathways Allocation on Frontera, we intend to virtually screen 403 million lead-like small molecule compounds for binding to a pharmacophore on each of three target proteins discovered in this manner. The results will form the foundation for development of new classes of leukemia/lymphoma chemotherapeutics with a large therapeutic index. We anticipate future work focused on targeting proteins for the treatment of solid tumors. We expect this work will lead to new targeted therapies for cancer.

Type: Renewal PW

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

Principal Investigator: Benjamin Cash (George Mason University (gmu.edu))
Co-Investigators: David Straus (George Mason University (gmu.edu)); Erik Swenson (George Mason University (gmu.edu)); Chulsu Shin (George Mason University (gmu.edu))

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. This project advances NOAA's newest Unified Forecast System (UFS), which is currently developed via a community approach. Our specific goals are to (1) improve the physical foundation of selected UFS model components with a focus on the representation of diabatic heating in the atmospheric model, (2) improve the coupling between the UFS atmosphere, land, ocean, sea ice, and ocean surface wave model components, and (3) perform scientific evaluations of prototype UFS S2S versions over subseasonal-to-seasonal (S2S) time scales and beyond

Type: New PW

Title: Investigate Atomistic Mechanism of Phase Transition and Plasticity in Silicon Nanostructures

Principal Investigator: Wei Gao (Texas A&M University (tamu.edu))
Co-Investigators:

Field of Science: Mechanics and Materials

Abstract:
Nanostructured silicon, such as nanoparticles, nanopillars, nanocubes and nanowires have been widely used for integrated circuits, micro and nano-electromechanical systems and photovoltaics due to the unique mechanical, optical and electrical properties. The knowledge generated in this research will be applied to improve the mechanical reliability of silicon nanodevices, to advance the machining of silicon materials, and to explore novel approaches for silicon phase engineering, thereby to advance national health, prosperity, and welfare. In addition, the machine learning approach will provide new and convenient tools for mechanicians to develop interatomic potentials with meaningful dataset that contains rich mechanics information of interest, in order to study the mechanics problems at the atomic scale with high fidelity. Meanwhile, the proposed research will be integrated into undergraduate and graduate educations.

Recent nanomechanical experiments have shown many unique and intriguing features of phase transitions in nanostructured silicon that are different from the bulk silicon in many aspects. However, the kinetic mechanism of phase nucleation and propagation at atomic scale remains unknown. The central research goal of this project is to quantitatively determine the roles of stress field, grain/phase boundaries and plastic deformation on the phase transition of silicon nanostructures, in order to close the gap between experiments and atomistic modeling. It is noted that there is no reliable interatomic potential to describe silicon phase transition, thus a novel mechanics-informed machine learning potential based on deep neuron network will be developed to fill the gap. The potential will be trained with the dataset containing stress dependent phase transition minimum energy paths, which can provide sufficient resolution to sample the energy landscape under high stress during phase transition. The phase transition will be investigated with a combined molecular dynamics simulation and finite deformation nudged elastic band method. The results generated in this project will be applied to understand the experiments in literatures and those conducted by the collaborators.

Type: New PW

Title: Improving beam quality in laser wakefield acceleration

Principal Investigator: Lance Labun (University of Texas at Austin (utexas.edu))
Co-Investigators: Miguel Gracia (University of Texas at Austin (utexas.edu)); Rahul Kumar (Princeton University (princeton.edu))

Field of Science: Atomic, Molecular, and Optical Physics

Abstract:

Laser wakefield accelators are promising high-gradient accelerators with the potential to reduce facility size by orders-of-magnitude, leading to cost reductions in both fundamental science projects and industrial-access projects. However, technical challenges with wakefield acceleration remain due to the stringent requirements of these applications on beam stability and control, narrow energy spread of the beam, emittance and brightness preservation. Building on two decades of experimental and simulation work, the group of Prof. Hegelich at UT Austin has found that introducing nanoparticles results in significant improvements in the electron beam energy, energy spread, and divergence compared with standard self-injection. To understand wakefield accelerator dynamics, we perform numerous large-scale particle-in-cell simulations, which provide the detailed information required to unpick the underlying processes. Our research objectives include optimizing electron beam emittance and energy spread by tailoring plasma density profile and laser pulse profile, investigating the effect of nanoparticles on electron beam equality, and conduct first-of-their-kind start-to-end simulations of a wakefield accelerator feeding into free-electron laser.

Type: New PW

Title: Reduced models for stellarator turbulence

Principal Investigator: Gabriele Merlo (University of Texas at Austin (utexas.edu))
Co-Investigators: Frank Jenko (Max Planck Institute for Plasma Physics (ipp.mpg.de)); Ionut-Gabriel Farcas (University of Texas at Austin (utexas.edu))

Field of Science: Physics

Abstract:
We propose to construct reduced models for plasma turbulence in the core of stellarators, exploiting the uncertainty quantification and sensitivity analysis framework we have
developed during previous Frontera cycles. Such reduced models are currently not available and could be extremely useful for profile prediction and for designing turbulence-optimized devices. In addition, the ensembles of high-fidelity evaluations used to construct our reduced model will result in a database of nonlinear simulations that can be used to construct more generic quasilinear models, akin to those widely adopted in the tokamak community.

Type: Renewal LSCP

Title: LSCP: NOAA UFS Coastal Applications Models Evaluation: Water Quantity (Renewal)

Principal Investigator: Saeed Moghimi (US National Oceanic and Atmospheric Administration (noaa.gov))
Co-Investigators:

Field of Science: Ocean Sciences

Abstract:
The UFS Coastal Applications Team (CAT) for Water Quantity (i.e. physical properties) is developing model evaluation recommendations for selecting NOAA's next-generation coupled coastal models. Under UFS CAT Water Quantity, plans were developed for three applications: (a) Total Water Level (TWL) prediction, (b) Risk reduction, and (c) Safe and efficient navigation. To guide the evaluation process three white papers by the modeling community were developed. Within each of these white papers, lists of model candidates appropriate for each application are suggested. The idea is to utilize NSF/TACC computational resources to provide an evaluation environment for performing the evaluation process. The evaluation criteria suggested within each white paper will be used to decide the eventual next generation model for the next generation coastal ocean modeling system for each of the suggested sub-applications. We anticipate a 3-years collaborative model evaluation process. The evaluation team contains: NOAA, agencies reps and university partners. Here is the list of NOAA and university partners.

NOAA collaborators:
- National Ocean Service (NOAA-NOS)
- National Weather Service (NOAA-NWS)
- Oceanic and Atmospheric Research (NOAA-OAR)

Academic collaborators:
- Georgia Tech (POC: Di Lorenzo and Haas)
- University of Maryland, College Park (POC: Kayo Ide)
- University of South Florida (POC: Yonggang Liu)
- Colorado School of Mines (POC: Eric Anderson)
- University of Hawaii (POC: Yong Wei and Vasily Titov at Pacific Marine Environment Laboratory or PMEL)
- University of North Florida (POC: Cigdem Akan)

Type: New LSCP

Title: First bank of Intermediate Mass-Ratio Binary Black Holes with Numerical Relativity

Principal Investigator: Carlos Lousto (Rochester Institute of Technology (rit.edu))
Co-Investigators: James Healy (Rochester Institute of Technology (rit.edu))

Field of Science: Gravitational Physics

Abstract:
The goal of this project is to model the gravitational waves signals from the late inspiral and merger of black hole binaries (BHB) with large mass ratios as well as in eccentric orbits. These studies will be based on full numerical simulations solving the highly nonlinear gravitational dynamics and computing waveforms from those binary systems.

Our studies have a wide range of applications, from direct parameter estimation of BBH signals, currently being detected by LIGO-Virgo-KAGRA, to predictions for the third generation of gravitational wave detectors and LISA space mission, leading to the modeling of astrophysical formation scenarios for those BHB sources.

Those astrophysical scenarios involve intermediate mass black holes (having hundreds to thousands solar masses) merging either with an stellar mass black hole or a supermassive one at the core of galaxies.

The plan of work here consists of 3 stages: i) Design of full Numerical Relativity simulations of 14 binaries with the large black hole spinning, for each mass-ratio q=1/16, 1/32, 1/64, with low eccentric e=0.0 orbits, to evolve for the last 15-20 orbits before merger ii) Same as before, but for eccentricities e=0.1, 0.2 to study alternative astrophysical formation scenarios. iii) Systematic exploration of convergence rates of the numerical simulations for each mass ratio and each eccentricity with additional lower and higher resolutions to evaluate errors of our standard simulations.

The number of simulations are thus 126 binary cases plus 18 convergence tests to total 144 numerical runs with an estimated 0.5M node hours required and completion within a calendar year.

Type: Renewal LSCP

Title: LSCP Support for the SolFER DRIVE Center

Principal Investigator: William Daughton (Los Alamos National Laboratory (lanl.gov))
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: New LSCP

Title: Core-Collapse Supernovae from Bounce to Breakout

Principal Investigator: David Vartanyan (University of California Berkeley (berkeley.edu))
Co-Investigators: Dan Kasen (U.C. Berkeley); Adam Burrows (Princeton University (princeton.edu)); Benny Tsz Ho Tsang (University of California Berkeley (berkeley.edu))

Field of Science: Stellar Astronomy and Astrophysics

Abstract:
The last decade of simulations has done much towards resolving the enigmatic core-collapse problem: how do massive stars explode at the end of their lifetimes? Detailed, multi-dimensional core-collapse supernovae (CCSNe) simulations - over the course of seconds - on a network of high-performance clusters around the world have shown the viability of the neutrino-heating mechanism, wherein energetic neutrinos released on gravitational collapse couple to the stellar mantle and unbind the star in a vibrant explosion.

The next decade promises a revolution in the number of observed supernovae events with upcoming all sky-survey, creating a divide between CCSNe observations and theoretical models. To bridge this gap, we propose a series of shock breakout simulations, continuing the early CCSNe simulations past seconds until hours, when the developing shock emerges from the stellar envelope. The models will predict the three-dimensional structure of a supernovae as well as the distribution and abundances of the ejecta nucleosynthesis. The results will then be ready for post-processing into light curve and spectral templates to compare with observations. The design of this project is by its nature a large-scale community collaboration: from modeling of stellar evolution, to CCSNe, to shock breakout and templates jointly with ongoing observational efforts.

Type: Renewal LSCP

Title: SCEC Earthquake Modeling, Ground Motion, and Hazard Simulations

Principal Investigator: Philip Maechling (University of Southern California (usc.edu))
Co-Investigators: Yifeng Cui (San Diego Supercomputer Center (sdsc.edu)); Yehuda Ben-Zion (University of Southern California (usc.edu)); Scott Callaghan (University of Southern California (usc.edu)); Bruce Shaw (Columbia University in the City of New York (columbia.edu))

Field of Science: Earth Sciences

Abstract:
The Southern/Statewide California Earthquake Center (SCEC) conducts and coordinates fundamental and applied research on earthquakes using California as its main natural laboratory. SCEC's research program relies on strong collaborations among researchers, and supports research and education in seismology, tectonic geodesy, earthquake geology, and computational science. SCEC is a leader in research that integrates science results into computational tools to support seismic hazard improvements. Empirical data are extremely limited for infrequent large earthquakes, and particularly sparse for near-fault ground motions that largely control the design of critical infrastructure. Physics-based earthquake and ground motion simulators present a practical solution to these issues. Given sufficient validation against observations, our datasets can supplement or replace the empirical datasets and provide guidance for probabilistic seismic hazard analyses (PSHA) for ground motion and probabilistic fault displacement hazard analyses (PFDHA). Our long term goals in the seismic hazard realm are to 1) increase the accuracy of earthquake, ground motion, and hazard simulations; 2) reduce uncertainties in seismic hazard models; and 3) broaden the usefulness of seismic simulations for engineering and preparedness applications. These objectives are only attainable through strong collaborative team work and require Frontera-enabled HPC capabilities.

Type: New LSCP

Title: High resolution simulations of past drought and climate extremes for model evaluation

Principal Investigator: Pedro Di Nezio (University of Texas at Austin (utexas.edu))
Co-Investigators: Timothy Shanahan (University of Texas at Austin (utexas.edu))

Field of Science: Climate Dynamics

Abstract:
Petascale systems like Frontera have made running climate models at higher resolution feasible, offering a path to improve the simulation of physical processes that are critical for predicting changes in the hydrological cycle and extreme weather. Here we propose a set of high resolution simulations of the Earth's past climate, focusing on two key intervals relevant to predicting future changes. Simulating climatic states that are radically different from today will allow us to validate the model against real-world data obtained from geological archives – so-called paleoclimate records. To do this we will simulate two of the best spatially resolved past climate intervals that are relevant to studying future changes in the hydrological cycle: the Holocene Thermal Maximum and Heinrich Stadial 1. Existing simulations with coarser resolution models are unable to simulate many of the changes evident in paleoclimate records from these intervals. Our hypothesis is that improved simulation of weather systems, topography, ocean circulation, and air-sea interactions in our high resolution simulations will produce better agreement with the paleoclimatic evidence. Our simulations will also leverage existing simulations of future changes performed with the same model by colleagues from Texas A&M and NCAR. Our model-data evaluation focusing on past changes will be key to evaluate underlying mechanisms involved in key regional responses. Output from the proposed simulations will help team members address scientific objectives of existing funded projects and will be widely shared with the climate community for multiple applications given the novelty and relevance of the proposed simulations.

Type: Renewal LSCP

Title: Gravitational Waves from Compact Binaries: Computational Contributions to LIGO

Principal Investigator: Saul A. Teukolsky (Cornell University (cornell.edu))
Co-Investigators: Vijay Varma (California Institute of Technology (caltech.edu)); Mark Scheel (California Institute of Technology (caltech.edu)); Aaron Zimmerman (University of Texas at Austin (utexas.edu)); Francois Foucart (University of New Hampshire (unh.edu)); Matthew Duez (Cornell University (cornell.edu)); Geoffrey Lovelace (California State University Fullerton (fullerton.edu)); Leo Stein (University of Mississippi (olemiss.edu)); Nils Deppe (California Institute of Technology (caltech.edu))

Field of Science: Gravitational Physics

Abstract:
Gravitational waves from the inspiral and merger of binaries with black holes and neutron stars are primary targets for gravitational wave detectors. Detectors such as LIGO rely on waveform models to extract science from the detected signals. Current models are becoming inadequate as the detector sensitivity improves. Surrogate models are a newer technique that can retain the accuracy of the underlying numerical solutions of Einstein's equations while interpolating to varying binary parameters. We propose to do a series of simulations to construct improved surrogate models that cover broader parameter ranges than our earlier surrogates. We will also add the waveforms we produce to our public waveform catalog so they may be used by others in gravitational wave data analysis. Simulations of binaries with one or two neutron stars are more challenging as one must also take into account the unknown structure of the matter in the neutron star. We will perform high-accuracy simulations of such systems using an improved equation of state compared with previous simulations. The high accuracy is crucial to extracting important physics from the detections.

Type: New PW

Title: Unveiling the mechanism of alpha-synuclein aggregation and prevention with small molecules using molecular dynamics

Principal Investigator: Surl Hee Ahn (University of California Davis (ucdavis.edu))
Co-Investigators:

Field of Science: Biophysics

Abstract:
alpha-synuclein is an intrinsically disordered protein (IDP) that is implicated in Parkinson's when it aggregates and forms insoluble fibrils. Due to lacking a stable, folded structure and rapidly undergoing various conformations, with experimental methods alone, it has been notoriously difficult to characterize alpha-synuclein and develop drugs against it. The mechanisms of alpha-synuclein aggregation, the structures of alpha-synuclein aggregates or "toxic" conformations, and alpha-synuclein aggregates' binding sites are still unknown. The long-term objective of this project is to use molecular dynamics (MD) simulations to predict atomic mechanisms of alpha-synuclein aggregation and understand how alpha-synuclein aggregation is blocked from specific small molecules that have experimentally shown to block aggregation.

Type: Renewal PW

Title: Advancing Predictive Capability of High-throughput Methods for Drug Discovery

Principal Investigator: Darrin York (Rutgers University (rutgers.edu))
Co-Investigators:

Field of Science: Chemistry; Physical Chemistry

Abstract:
This is a Pathways proposal to support our ongoing efforts that have received ongoing LRAC support (CHE20002), but due to an administrative error, we missed the renewal deadline for our LRAC renewal (which is now exhausted), and we were informed our best option was to submit an allocation request for Pathways. The long-term goal of our Frontera Leadership Resource Allocation (LRAC) proposal is to develop and apply new tools for accurate and precise high-throughput lead optimization (HTLO) for drug discovery. In the current allocation period, we tested performance-optimized protocols for benchmark free energy (FE) simulations of ligand-protein relative binding free energies (RBFEs) against select ligands and targets, as well as absolute (ASFE) and relative solvation free energies (RSFE) of select compounds. This produced a number of new insights, identified several critical barriers to progress, and led to the development, testing and publication of several new key innovations: 1) a powerful new framework for the design of optimized alchemical transformation pathways for robust alchemical free energy calculations, 2) a novel alchemical enhanced sampling (ACES) method for high-precision free energy simulations, and 3) robust workflow technology that integrates new GPU-accelerated free energy simulation and network-wide analysis tools. These advances helped to solve the precision problems in free energy predictions, enabling us to move on the the development of more accurate potentials. Toward that end, we have developed a first-generation Quantum Deep-Potential Interaction Energy (QDpi) model that is in the form of “QM/delta-MLP”: a machine learning potential (MLP) correction to a fast, approximate 3rd-order density-functional tight-binding quantum mechanical (QM) model. The method has been trained and tested and demonstrated to be highly accurate for conformational energies, intermolecular interactions, and changes in tautomer and protonation states. These have been integrated into the AMBER software package that has had a broad worldwide developer and user base for nearly 40 years (currently ~30,000). Herein, we submit a Pathways request to continue to advance the state of the art to achieve protein-ligand binding affinity predictions on libraries of compounds with chemical accuracy within hours using leadership-class GPU computing systems. Our research continues to be funded by the National Institutes of Health (NIH) (GM107485) and National Science Foundation (NSF) (2209718).