Type: Renewal PW

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

Principal Investigator: Falk Amelung (U of Miami)
Co-Investigators:

Field of Science: Geophysics

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: Renewal PW

Title: Using multiscale mantle convection modeling to understand the physics of plate boundary evolution and tectonic surface deformation

Principal Investigator: Thorsten Becker (University of Texas at Austin (UT) (UT Austin))
Co-Investigators: Antoniette Greta Grima (University of Glasgow)

Field of Science: Geophysics

Abstract:
Plate tectonics is the surface expression of mantle convection. However, some of the processes involved, such as those that allow subduction, i.e., deformation and recycling of the oceanic lithosphere, remain poorly understood. Related questions have broad implications, from the evolution of terrestrial planets to understanding seismic hazard. We continue to seek to better understand the dynamics of plate boundaries, from earthquakes to global tectonics scales, using medium and large-scale computations.

One particular focus is on tectonic inheritance, where material behavior shows hysteresis, as seen in strain localization at plate boundaries and dormant zones of weakness within plates. The origin of these sutures is often associated with earlier subduction, e.g., leading to orogeny as in the western US. Unraveling such mantle convection – overriding plate interactions is important for understanding planetary evolution. A key missing piece in our understanding of plate boundaries is how those arise from mantle convection, and what role strain localization and damage memory play.
With the resources available through Frontera we seek to continue to analyze large-scale, 3-D spherical, time-evolving models of mantle convection exploring a number of processes consistently for the first time (e.g., Figs. 1 and 2). We seek renewal of our allocation to build on initial results arising from efforts empowered by Frontera resources. Products include five papers in high impact journals, including Nature Geoscience and Geophysical Research Letters, and capacity building includes training of a Ph.D. student about to graduate and move on to a computational post-doc at a government lab.

Type: New PW

Title: Multi-scale Analysis of Congo Basin Precipitation: Understanding the Regional Rainfall Climatology and the Potential for Change

Principal Investigator: Kerry Cook (University of Texas at Austin (UT) (UT Austin))
Co-Investigators: Edward Vizy (University of Texas at Austin (UT) (UT Austin))

Field of Science: Atmospheric Sciences

Abstract:
The Congo Basin rain forest is known around the world for its biodiversity and rich cultural heritage. But the rains that provide water resources to the people and ecosystems of the forest are understudied and fundamental aspects of their behavior have not been fully documented. One challenge to understanding rainfall in the basin is lack of observations, as economic hardship and political instability have hampered development of weather observing networks. Another challenge is that much of the rainfall comes from mesoscale convective systems (MCSs), intense propagating thunderstorms like the ones seen over the central US in summer, which are difficult to observe in detail.

Research performed under this project seeks to characterize the rain-bearing weather systems of the Congo Basin, including their seasonality, connections to the large-scale atmospheric circulation, moisture distribution, and the extent to which evaporation and transpiration from the vegetated land surface serves as a moisture source for rainfall. The work takes advantage of recent datasets that make up for the lack of ground-based observations through satellites and global atmospheric data assimilation systems. The datasets have high enough resolution to track MCSs and determine their formation regions, propagation paths, total contribution to precipitation, and interaction with the large-scale environment.

Further research is conducted using the Weather Research and Forecasting (WRF) model, a regional model which can capture MCS dynamics. Here WRF is applied in a triply nested configuration over Central Africa with boundary forcing from reanalysis products, which ensure that the large-scale features of the simulations mimic their real-world counterparts. In some simulations the boundary forcing is modified to represent the effects of future climate change based on output from global climate models. The impact of simulated future precipitation change on the rain forest is assessed using a Potential Vegetation Model.

The work is of societal as well as scientific interest given the vulnerable population of the region and its importance as a biodiversity hotspot.

Type: Renewal PW

Title: Interfacial turbulence modeling in environmental flows

Principal Investigator: Marcelo Garcia (University of Illinois Urbana-Champaign (UIUC) (University of Illinois) (U of I))
Co-Investigators:

Field of Science: Interfacial, Transport, and Separations Processes; Fluid, Particulate, and Hydraulic Systems

Abstract:
The purpose of this proposal is to apply for a Pathways allocation on Frontera's Cascade Lake (CLX) computational system, which is one of the world's top-ranked supercomputing resources. This project involves the study of interfacial turbulence in two fundamental problems observed in environmental flows: the buoyancy force-driven mixing layer and turbulent hyporheic boundary layer flows. The first case will help us understand how density effects amplify the mixing efficiency by several orders of magnitude in the mixing process, while the second case will help us gain insight into how pollutants in bottom sediments are entrained and transported in a water body. Both studies will be the first of their kind to simulate multiple fluid dynamics processes in a scaled-down environmental flow domain using high-performance computing models. The observations and theories resulting from this work will be widely used in different environmental flow applications without the need to make simplifying assumptions like those found in previous theoretical works.

Type: Renewal PW

Title: Advanced simulations of train derailments to assess the tank cars conditional probability of release

Principal Investigator: Paolo Gardoni (University of Illinois Urbana-Champaign (UIUC) (University of Illinois) (U of I))
Co-Investigators:

Field of Science: Mechanical and Structural Systems

Abstract:
The release of hazardous materials following the derailment of freight trains can have devastating effects on the surrounding environment. It also represents a serious concern for the well-being and health of the affected communities. As such, it is important to improve the derailment performance and safety of new tank cars carrying hazardous materials. One significant challenge in introducing new tank designs is the lack of satisfactory empirical or testing data on its accident safety, typically quantified in terms of the conditional probability of release (CPR). The CPR provides insight into tank car resistance against the release of hazardous materials in the event of a derailment. As such, high-fidelity derailment models are needed to simulate the accident performance of these tank cars and determine associated performance measures. This project aims to quantitatively assess the conditional probability of release (CPR) of tank cars during derailments. By using our advanced Finite Element (FE) train derailment model, we plan to conduct a series of computationally-demanding accident simulations to capture the variability in the existing derailment mechanisms, site and derailment conditions, and train characteristics. These input variables will be determined through a full-fledged experimental design.

Type: Renewal PW

Title: High-performance computational approach to improve cardiac interventional predictability

Principal Investigator: Vijay Govindarajan (University of Texas Health Science Center at Houston)
Co-Investigators:

Field of Science: Advanced Scientific Computing

Abstract:
The main goal of the cardiovascular system is to efficiently drive, control, and maintain systemic and pulmonary blood flow. The form and function of the cardiovascular system is shaped by blood flow during its development. The goal of the patient's heart team (a multidisciplinary team including cardiologists and surgeons providing evidence-based care) is to achieve an efficient hemodynamics post-surgery that is close to its normal physiological state. The ultimate goal of our research is to develop and utilize advanced engineering and high-performance computational approaches to provide quantitative insights and predictive capabilities to the patient's heart team to better understand the implications of cardiovascular disease and help improve surgical predictability.

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 PW

Title: Structure and Dynamics of Highly Turbulent Premixed Combustion

Principal Investigator: Peter Hamlington (University of Colorado Boulder)
Co-Investigators:

Field of Science: Fluid, Particulate, and Hydraulic Systems

Abstract:
Highly turbulent premixed flames are found in a range of engineering and natural systems, including engines, gas turbines, and even supernova explosions. Much of the current knowledge in this area has been obtained from numerical simulations of idealized configurations using relatively simple chemical models. To address the need for greater realism, this project will use advanced computational tools and more sophisticated chemical modeling to study the characteristics and behaviors of highly turbulent premixed flames in practically relevant configurations. Ultimately, physical insights resulting from this project will enable more accurate simulations of advanced energy systems. This research will make use of adaptive mesh refinement (AMR) for overcoming the computational cost of simulating more complex practical configurations, including those where secondary flows, shear, swirl, and walls are important. Using AMR, new direct numerical simulations will be performed, and the resulting datasets will be examined using Lagrangian and scale-dependent diagnostics. In addition to refining theories and models of highly turbulent combustion, the proposed project will impact the broader combustion community by publicly sharing data and statistics from each of the simulations, as well as all analysis codes and diagnostic tools.

Type: New PW

Title: Research and development of methods for many-body electronic structure theory and applications in FHI-aims

Principal Investigator: Uthpala Herath (Duke University)
Co-Investigators: Volker Blum (Duke University)

Field of Science: Materials Research

Abstract:
In this proposal, we request a Frontera Pathways allocation to perform electronic structure calculations on a series of semiconductors, hybrid organic-inorganic perovskites and chalcogenides with the aim of obtaining a deeper understanding of their internal chemical mechanisms which have profound impacts on optoelectronics and photovoltaics applications. The allocation will aid in progressing the computational segments of several NSF and DOE funded projects. The allocation will also support code development efforts to implement periodic GW calculations with spin-orbit coupling, which is an essential methodology for studying heavy element materials. The scope of the calculations will encompass Kohn-Sham density functional theory (DFT) and the GW approximation along with semilocal and hybrid spin-orbit coupled DFT. This proposal requests a total of 50,060 SU's on Frontera CPU nodes and 1,500 SU's on Frontera GPU nodes.

Type: Renewal PW

Title: Flow-induced configurational microphase separation and crystallization in polydisperse entangled polyethylene under planar elongational flow

Principal Investigator: Bamin Khomami (University of Tennessee Knoxville (UT Knoxville))
Co-Investigators: Mahdi Boudaghi (University of Tennessee Knoxville (UT Knoxville))

Field of Science: Fluid, Particulate, and Hydraulic Systems; Materials Research

Abstract:
Polymer and polymer matrix composites play an essential role in many industries ranging from consumer goods to terrestrial and extraterrestrial vehicular transport. A significant portion of these polymeric based products are produced by manipulating the microstructure of highly entangled polymer chains in the molten liquid state. Hence, fundamental understanding of the intricate flow/microstructure coupling, which to a great extent determines the final product properties, is paramount in rational design of processes used to manufacture polymer-based products. Liquid state processing techniques for net shape manufacturing of polymeric products make use of a variety of flows with shear and/or extension dominated kinematics. Hence, strong flows, namely, extensionally dominant flows are a vital component of many efficient and cost-effective liquid polymer processing techniques due to their ability to manipulate effectively macromolecular configuration and the entanglement network topology. However, the description of the elongational flow of polymeric fluids has proven to be a difficult challenge. Many theories have been proposed to explain the microstructural responses of these complex liquids under flow, but each invariably diverged from experiments at high strain rates. Recent evidence suggests that part of the reason for these divergences is that most flow models track bulk-average properties that can approximate the collective dynamics of the individual molecules. In recent studies, we have observed via nonequilibrium molecular dynamics (NEMD) simulations of monodisperse entangled polyethylene (PE) liquids that a remarkable dynamical response occurs in elongational flows, namely, configurational microphase separation occurs at intermediate extension rates, wherein the simulation cell is composed of distinct local regions of either highly stretched or coiled macromolecules. These two states produce a bimodal distribution function of the fractional extension within the Wi range wherein the coil-stretch hysteresis is evident. At high extension rates, the system undergoes a flow-induced crystallization at temperatures approximately 50 K higher than the quiescent melting point of PE.

The implications of this phenomenon have significant ramifications on liquid-state processing of highly entangled melts in strong flows. However, commercially processed polymers are polydisperse due the significant limitations of synthesis technique to produce bulk quantities of monodisperse polymers. To that end, we propose to study the influence of polydispersity on the aforementioned novel flow induced phenomena using extremely large scale (millions of particles) NEMD simulations. Specifically, a prototypical polydisperse polyethylene melt with a polydispersity index of 1.8 and entanglement density of approximately 25 will be used to develop a mechanistic understanding of the influence of polydispersity on flow-induced configurational phase separation and crystallization. Of particular interest is the quantification phase transition and flow-induced crystallization kinetics using novel thermodynamic based techniques developed recently by our research group.

The advances made from this study will contribute to bridging the gap between academic research and industrial practice in polymer manufacturing, which still relies heavily on empirical models that lack robustness and contain process-specific empiricism. The proposed research will provide fundamental

knowledge of the individual and collective chain dynamics that are crucial to a complete understanding of strong flows that occur in polymer processing operations, ultimately leading to more predictive models for industrial processes. Another broader impact is that the extensive NEMD simulation data produced in this study will be archived in the PolyHub warehouse and made available to any research group that requests it. This will allow scientists worldwide to share in the accumulation of knowledge that will result from this unprecedented series of simulations and aid the development of a new fundamental understanding of the flow behavior of polymeric liquids.

Type: Renewal PW

Title: Ab initio nuclear structure and reactions for light to medium-mass nuclei

Principal Investigator: Kristina Launey (Louisiana State University (LSU))
Co-Investigators: Grigor Sargsyan (Lawrence Livermore National Laboratory); Daniel Langr (Czech Technical University in Prague (esk vysok uen technick v Praze)); Tomas Dytrych (Louisiana State University (LSU))

Field of Science: Nuclear Physics

Abstract:
The recent advent of radioactive beam facilities has enabled exotic-nuclei measurements, based on collisions of nuclei and their reactions. To predict inaccessible nuclei, these reactions must be well understood and modeled. However, exact solutions exist up to about five particles. The objective of this program is to expand dramatically the capabilities of nuclear reaction theory, by providing input to reaction simulations that is anchored in first principles but also can accommodate heavier nuclei and enhanced deformation by exploiting symmetries known to dominate in nuclei. This can help address the origin of elements and neutrino properties, two of the biggest challenges in physics today, and will have a wider impact since nuclear energy and national security research has similar needs. Future leaders (postdocs and students) will be trained in low-energy nuclear science and petascale computing, while preparing a web-database for research and educational purposes. The overarching goal is to learn from and inform experiments at radioactive beam facilities, and to predict properties of experimentally inaccessible nuclei that are key to advancing our knowledge about astrophysical processes and neutrino physics. The program targets to improve reaction modeling, by constructing the effective interaction between a target and a projectile from first principles (historically, referred to as an optical potential and fitted to experimental data), and thus to account for the challenging microscopic structure of the participating nuclei. As these interactions are an essential input to numerous reaction models that are currently in use, the new developments will serve as an important tool in a broad spectrum of studies.

Type: Renewal PW

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

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

Field of Science: Magnetospheric Physics

Abstract:
The dawn-dusk extent of magnetic reconnection in Earth's magnetotail determines the magnetic energy release rate during geomagnetic substorms. In this project, we will study whether magnetic reconnection will spread, increase its extent, or stay localized. The proposed work will explore the 3D nature of magnetic reconnection in kinetic plasmas.

Type: Renewal PW

Title: An accelerated path to a Negative Triangularity tokamak reactor using first principle models

Principal Investigator: Alessandro Marinoni (Massachusetts Institute of Technology (MIT))
Co-Investigators: Federico Halpern (General Atomics)

Field of Science: Physics

Abstract:
The main research priority of Fusion Energy Science is to develop controlled nuclear fusion as an economically viable and environmentally sustainable energy source. The leading candidate for operations in future magnetically controlled reactors is a regime called H-mode, which provides the level of energy and particle confinement necessary to self-sustain thermonuclear reactions by employing an Edge Transport Barrier (ETB), a narrow layer near the plasma edge where the radial pressure profile increases rapidly thanks to turbulence suppression by large flow radial gradients.
Plasma operation in the H-mode regime is intrinsically characterized by contrasting requirements. More specifically, while the energy flux flowing from the core to the edge needs to be large enough for the plasma to maintain an ETB, a large fraction of it must be radiatively dissipated outside the confined region before being convected to the vessel in order to preserve Plasma Facing Components (PFCs). Additionally, the H-mode regime requires active controllers to suppress or mitigate Edge Localized Modes (ELMs), uncontrolled bursting instabilities generated by the large pressure gradients that developing ETBs, and widen the footprint of the energy flux convected to PFCs. While intense research is being pursued worldwide to overcome these issues, a satisfactory solution is still to be found.
Recent experiments on the DIII-D tokamak demonstrated what could be an revolutionary solution alternative to the H-mode regime. Confinement levels typical of H-mode plasmas have been obtained without ETBs thanks to a significant modification of the cross sectional shape of the plasma. Known as Negative Triangularity, this configuration significantly increases the ETB power threshold while substantially reducing turbulence across most of the plasma thus enabling high pressure levels to be obtained.
The absence of an ETB reconciles the afore-mentioned contrasting requirements for operation and eliminates the need for complex active controllers, thus potentially greatly accelerating successful operation in future reactors.
By combining state-of-the-art gyro-kinetic and fluid codes for core and edge turbulence, respectively, we aim at self consistently predict the core performance of a fusion reactor at negative triangularity and its impact on PFCs. The numerical tools to be employed have been recently optimized for HPC and include the most sophisticated physics models available. The use of first principle models is necessary in view of the fact that all reduced models currently available in the fusion community have not been calibrated in this novel plasma shape and are therefore unreliable. As a consequence, new calibration data that extend the applicability of reduced models will be generated in this work.

Type: New PW

Title: Exploring Entanglement in Ab Initio Calculations of Atomic Nuclei

Principal Investigator: Alexis Mercenne (Louisiana State University (LSU))
Co-Investigators:

Field of Science: Nuclear Physics

Abstract:
Accurately modeling atomic nuclei is crucial for understanding fundamental symmetries in nature and processes such as fusion and fission. Ab initio approaches and petascale computing have enabled physically relevant nuclear calculations with superior efficacy. However, quantifying entanglement in these calculations can reveal insights into emergent symmetries in nuclei and pave the way for merging ab initio techniques with quantum information. This study aims to quantify entanglement in ab initio calculations and open up new perspectives on the efficacy of symmetries, deepening our understanding of heavy and exotic nuclear species.

Type: New PW

Title: Predictive Excited-State Calculations for Solids using Many Body Perturbation Theory Based and Optimally Tuned Range Separated Hybrid Functionals

Principal Investigator: Jeffrey Neaton (University of California Berkeley (UC Berkeley))
Co-Investigators: Marina Filip (University of Oxford)

Field of Science: Condensed Matter Physics

Abstract:
The overarching goal of this project is to develop a robust framework to predict quasiparticle band gaps and band structures for chemically and structurally heterogeneous semiconductors and insulators using DFT and the generalized Kohn-Sham DFT formalism. Our efforts are centered on new computational frameworks that make use of our recently developed Wannier Optimally Tuned Screened Range Separated Hybrid (WOT-SRSH) functionals, both as a stand alone approach and as a starting point for ab initio many-body perturbation theory calculations. We use these frameworks to perform calculations of excited state properties, including electron-phonon interactions, for complex materials systems. In this one year allocation we have carefully planned a set of interconnected projects in three main categories of systems: (1) 3D heterogeneous bulk crystals including halide double perovskites and transition metal oxides, (2) van der Waals layered semiconductors and (3) surfaces and systems including point defects. The common goal of these projects is to extend the range and types of materials studied within the WOT-SRSH framework, to understand both the potential and the limitations of our methodology, and to advance the overall understanding of the excited state properties of these important materials classes.

Type: New PW

Title: Studies of Circumbinary Accretion onto Supermassive Black Hole Binaries in Full General Relativity

Principal Investigator: Vasileios Paschalidis (University of Arizona (U of A))
Co-Investigators: Jane Bright (University of Arizona (U of A))

Field of Science: Gravitational Physics

Abstract:
Investigating accreting supermassive binary black holes is extremely timely because they are promising multimessenger sources with gravitational waves and because they are the targets of multiple current and future sky surveys such as Pan-STARRS1, Pan-STARRS and LSST.
Existing observations identify such supermassive binary black hole through periodicities in the lightcurves of active galactic nuclei (AGN). The usual assumption is that periodicities in the accretion flow onto the binary power these lightcurve periodicities. However, we recently discovered that when minidisks form onto each black hole individually the variability of the accretion flow is appreciably decreased. Larger minidisks are expected to form at larger separations (more relevant for current sky surveys), therefore it is crucial to study if the variability of the accretion flow decreases even further for binaries at wider orbital separation. In this work we will perform simulations of magnetized circumbinary accretion onto black holes at unprecedented orbital separations to study how the accretion flow variability is affected when larger minidisks are allowed to form around each black hole in order to apply our simulations to binary black hole AGN observations. Our studies will reveal correlations between the expected gravitational wave and electromagnetic signals from these systems. Frontera is crucial to enable the proposed work.

Type: New PW

Title: Therapeutic Peptides Design for COVID-19 Treatment Using High-Performance Computing at TACC

Principal Investigator: Baofu Qiao (City University of New York (CUNY))
Co-Investigators: Yong Wei (High Point University); Tao Wei (Howard University)

Field of Science: Biophysics

Abstract:
Neutralizing peptides are highly promising for drug design. Nevertheless, the design of therapeutic peptides is highly challenging owing to the lack of the fundamental understanding of protein-peptide interactions. With the HPC resources at TACC, we are aiming to explore the protein-peptide interactions for SARS-CoV-2 spike protein to rationalize the design of neutralizing peptide.

Type: Renewal PW

Title: Frontera Pathways Renewal: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: Liam Scarlett (Curtin University); Dmitri Fursa (Curtin University); Igor Bray (Curtin University)

Field of Science: Atomic, Molecular, and Optical Physics

Abstract:
Electrons, and positrons interact with other atoms and molecules in very complex ways. The overall goal of this renewal proposal is to continue to develop and apply the most sophisticated numerical and computational techniques to enable accurate calculations of the collision cross sections of electrons with simple molecular targets. At a fundamental level, the interactions between these systems lead to energy exchanges resulting in excitation, ionization, and breakup of the systems which are often only understood after high level and complex calculations. At the more applied level, the data that one derives from the calculations is required for the modeling of astrophysical and fusion plasmas, atmospheric modeling, the etching of microelectronic chips, to a better understanding of many lighting devices and in other emerging quantum technologies. There is no shortage of applications that benefit from a quantitative understanding of the underlying atomic and molecular processes under consideration in the current proposal.

Type: Renewal PW

Title: Studies In Theoretical Astrophysics and General Relativity

Principal Investigator: Stuart L. Shapiro (University of Illinois Urbana-Champaign (UIUC) (University of Illinois) (U of I))
Co-Investigators: Antonios Tsokaros (University of Illinois Urbana-Champaign (UIUC) (University of Illinois) (U of I)); Milton Ruiz (University of Illinois Urbana-Champaign (UIUC) (University of Illinois) (U of I))

Field of Science: Gravitational Physics

Abstract:
We numerically solve the General Relativity field equations coupled to both the relativistic magnetohydrodynamic equations and those of radiation trans- port. Our goal to simulate prominent sources of gravitational waves such as neutron stars (NSs), black holes (BHs), and accretion disks, in isolation or in binary systems. We also model the electromagnetic radiation from these sources to solidify their role as “multimessenger astron- omy”sources. Our numerical studies address fundamental questions dealing with strong-field gravitation and focus on problems that are motivated by current and future observations of gravitational waves by aLIGO/VIRGO, GEO, KAGRA, Pulsar Timing Arrays, LISA/DECIGO, and other laser interferometers now operating or under development.

Type: Renewal PW

Title: BioPathways: Computational studies of novel microbial membrane exporter proteins

Principal Investigator: Hedieh Torabifard (University of Texas at Dallas (UTD) (UT Dallas))
Co-Investigators:

Field of Science: Chemistry; Biochemistry and Molecular Structure and Function

Abstract:
CLC F is a transmembrane antiporter that export F- ions when F- intracellular concentration approaches toxic level. ICLC F exports F- and import H+ via a bifurcated pathway. Our preliminary data shed light on these ions movement along the pathway, explained the high F- selectivity compared to HF, and identified the contributing residues in F- export. These preliminary results were presented in ACS-national meeting in August 2022 in Chicago, and are currently under review in the Journal of Chemical Information and Modeling, and are available in bioRxive. In the proposed research. we built upon our preliminary data and proposed to apply advanced computational modeling to investigate the predicted mutants, the proton import, and the selectivity against other solutes. Additionally, we will perform virtual screening on large-scale small molecules libraries to find promising inhibitors to prevent the F- export. The time allocation by the Pathways mechanism will enable us to investigate these unique and interesting proteins with the hope of finding a novel target for developing effective antibiotics.

Type: Renewal PW

Title: Seamless coupled hydrologic-hydrodynamic simulations using a next-generation community model

Principal Investigator: Joseph Zhang (Virginia Institute of Marine Science (VIMS))
Co-Investigators: Charles Seaton (Columbia River Inter-Tribal Fish Commission (CRITFC))

Field of Science: Earth Sciences

Abstract:
Continuing on our successes made possible with previous Frontera allocation (EAR21010) and to accommodate greatly increased demand from several on-going funded projects, we request a Pathway allocation on NSF's leadership computing capabilities for science and engineering (Frontera). The software we use is the world's first bona fide compound flooding modeling framework, and the simulations planned using the allocation will significantly advance the frontiers of knowledge in the realm of nonlinear compound flooding and related safe navigation studies. The impact from this effort will be widely felt because (1) we are testing one new NOAA pre-operational forecast, based on the model for the Pacific basin; (2) we need to conduct shadow forecast for NOAA's operational forecast STOFS3D-Atlantic for US Atlantic & Gulf coasts; (3) we are starting the simulation campaign with thousands of simulations for the funded EPA project; (4) we serve a large and diverse community world-wide with the open-source community code.