Type: New PW
Title: Frontera Pathways Allocation Proposal: Cyberinfrastructure for GeoSciFramework and Big Data Innovation

Principal Investigator: Scott Baker (UNAVCO Corporation)
Co-Investigators:

Field of Science: Earth Sciences

Abstract:
GeoSciFramework is an innovative approach to geophysical research and hazard early warning that looks at the world with a fly's eye perspective from thousands of harmonized high-rate real-time GNSS, seismic, pressure and other geophysical sensors. These sensor data continuously stream into an integrated framework that includes satellite radar time series generated across the globe. Machine learning algorithms and spatio-temporal analyses will be trained in this multi-data environment and informed by physical models, to enable instant recognition that a tsunamigenic earthquake has occurred, or to identify longer term subtle motions of the earth's surface on previously unrealized scales. This approach is extensible to not just detection and characterization of earthquakes but also to the onset of other geophysical signals like slow-slip events or magmatic intrusion, expanding the potential for new scientific discoveries. Development of these spatio-temporal datasets for machine learning requires HPC resources such as those available through Frontera and XSEDE.

Type: New PW
Title: Computational Infrastructure for Geodynamics - Community Code Scaling

Principal Investigator: Lorraine Hwang (Computational Infrastructure for Geodynamics, UC Davis)
Co-Investigators: Hiroaki Matsui (University of California, Davis); Timo Heister (Clemson University)

Field of Science: Geophysics

Abstract:
The Computational Infrastructure for Geodynamics (CIG) is an NSF-funded organization dedicated to developing, providing, and maintaining 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 and the deformation of the lithosphere, and in the generation of the geodynamo.

Type: New PW
Title: Dynamics of Aquaporin Membrane Junctions

Principal Investigator: Liang Xu (University of Texas at San Antonio)
Co-Investigators:

Field of Science: Biophysics

Abstract:
The aquaporins (AQPs) are a family of integral membrane proteins that facilitate water transport across the plasma membranes of cells in all form of life. Aquaglyceroporins, a subset of AQPs, also facilitate the passive transport of glycerol and other small solutes such as urea and carbon dioxide. The AQPs are involved in many biological functions and modulation of AQP function may have important physiological implications. With support from the current TACC computing resources, we have performed extensive in silico studies on the water/glycerol conduction in various AQPs, and computed their binding affinity using the newly developed method in our lab. In this project, we focus on AQP0 and AQP4, which also play a role in cell adhesion by forming membrane junctions. The formation of membrane junctions appears to convert AQP0 and AQP4 from a water channel to a pure adhesion protein. However, the underlying mechanism is not well understood. Furthermore, it remains elusive how the terminal domain of AQP0 and AQP4 regulate the formation of stable junctions. With access to the powerful computational capabilities provided by Frontera, we are now able to model and simulate these large systems (~0.64 million atoms at least) comprising double-layered 2D crystals in adjoining membranes. The dynamics of membrane junctions formed by AQP0 and AQP4 will be characterized in near physiological environment using the high-performance parallel simulation packages. Results emerged from this project will provide molecular insights into the interactions between junction-forming units that potentially attenuate the water permeability and membrane adhesion.

Type: New PW
Title: Mechanism of Ca2+-evoked synaptic vesicle fusion

Principal Investigator: Jose Rizo-Rey (University of Texas Southwestern Medical Center)
Co-Investigators:

Field of Science: Neuroscience Biology; Biophysics

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

Type: New PW
Title: Pathways Proposal: Protein Stability in Mixed Osmolyte Conditions and the Self-assembly of the Tau Protein

Principal Investigator: Joan-Emma Shea (University of California, Santa Barbara)
Co-Investigators: PRITAM GANGULY (University of California, Santa Barbara)

Field of Science: Biophysics

Abstract:
This pathways proposal focuses on two scientific problems: 1) the mechanism by which osmolyte mixtures stabilize proteins, and 2) the early stages of aggregation of the tau protein. Both projects require extensive computational resources as they require an enhanced sampling molecular dynamics protocol involving multiple processors and long simulations times (on the order of 500 - 1000 ns per replica) for convergence. The pathways grant will enable us to optimize the simulation protocol for the two systems studied on Frontera, with the aim of scaling up to larger simulations in the context of an LRAC grant.

Type: New PW

Title: Develop A Data-driven Approach To The Mechanics of Nanoscale Interfibrillar Interface in Collagen

Principal Investigator: Dong Qian (University of Texas at Dallas)
Co-Investigators: Yang Wang (University of Texas at Dallas)

Field of Science: Mechanics and Materials

Abstract:
The overall objective of this PATHWAYS allocation request is to utilize this resource to establish and implement a data-driven approach to investigate the mechanics of the nanoscale interfibrillar interface in collagen. The proposed data-driven computational approach is motivated by the significant challenge in experimentally characterizing the mechanical properties of this nanoscale bio-interface, as well as the overwhelming number of metastable configurations of the noncollagenous interfibrillar interface in the form of OC/OPN composite. As such, this allocation request is aimed at developing and implementing a data-driven approach to understand the structure-property relation that is responsible for the mechanical properties of the nanoscale collagen interfibrillar interface by combining machine learning with statistical analysis.

Type: New PW
Title: Large-scale simulation of quantum computers with realistic noise models

Principal Investigator: Gian Giacomo Guerreschi (Intel Corporation)
Co-Investigators: Nicolas Sawaya (Intel Corporation)

Field of Science: Physics

Abstract:
Quantum computers will allow the research community to solve problems and simulate systems that are intractable on quantum computers. However, one of the most stubborn barriers to building a useful quantum computer is the effect of environmental noise. In order to mitigate the errors introduced by noise and decoherence, it is essential to develop realistic models and apply them to the study of scaled-up quantum algorithms. We propose to use a mix of quantum simulation methods in order to parametrize a set of realistic noise models: computationally expensive simulations based on the density-matrix representation provide the ground truth to be approximated with more scalable approaches based on state vectors. Once learned, we will apply the noise model to large-scale simulations of quantum algorithms up to 34 qubits, well outside the regime reachable with density-matrix simulators. The results of this study will be useful for (a) understanding the robustness to noise of short-term quantum algorithms, and (b) demonstrating that simulations can be tailored on realistic noise, possibly device specific.

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

Principal Investigator: Kristina Launey (Louisiana State University)
Co-Investigators: Daniel Langr (Czech Technical University in Prague); Tomas Dytrych (Louisiana State University)

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: New PW

Title: R-Matrix with Time Dependence Calculations for Ultrafast Atomic Processes in Strong Laser Fields

Principal Investigator: Kathryn Hamilton (Drake University)
Co-Investigators: Klaus Bartschat (Drake University)

Field of Science: Atomic, Molecular, and Optical Physics

Abstract:
Accurately determining the response of matter to short bursts of high-intensity light could have many wide-ranging applications, not only in the field of physics but also in chemistry and biology. We propose to use the ab-initio R-matrix with Time Dependence (RMT) method to explore the influence of ultrashort, intense laser pulses on general multi-electron atomic systems. Possible avenues of investigation include the study spin-orbit interaction in a time dependent manner, and the effect of laser ellipticity on the population of excited states.

Type: New PW
Title: Studies In Theoretical Astrophysics and General Relativity

Principal Investigator: Stuart Shapiro (University of Illinois at Urbana-Champaign)
Co-Investigators: Antonios Tsokaros (University of Illinois at Urbana-Champaign)

Field of Science: Stellar Astronomy and Astrophysics

Abstract:
We request a Frontera allocation to tackle several large-scale, long-standing, unsolved problems in theoretical astrophysics and numerical relativity. We numerically solve the Einstein field equations coupled to the relativistic magnetohydrodynamic equations to simulate the inspiral and merger of binary compact objects (COs), as well as isolated COs, in full general relativity. These include binary black holes (BHBHs), both in vacuum and surrounded by magnetized disks, binary neutron stars (NSNSs), binary black hole-neutron stars (BHNSs), ergostars, and supermassive stars. We are interested in the study of gravitational and electromagnetic radiation generated from these sources (``multimessenger astronomy''). Our numerical studies address fundamental
questions dealing with strong-field gravitation and focus on problems that are motivated by present and future observations of gravitational waves by aLIGO/VIRGO, GEO, KAGRA, PTAs, LISA, and other laser interferometers now
operating or under development. Our simulations also model promising gamma-ray burst sources (GRBs) observed by NASA satellites such as SWIFT, INTEGRAL and FERMI,
X-ray sources observed by NICER, CHANDRA, and XMM-Newton, and optical and infrared sources observed by the HST, NuSTAR and PanSTARRS telescopes. A successful completion of this research that is supported by grants from the National Science Foundation (NSF) and the National Aeronautics and Space Agency (NASA) will only be possible
if our team acquires the necessary computational resources to do so.

Type: New LSCP
Title: Neutron Electric Dipole Moment from Lattice QCD

Principal Investigator: Keh-Fei Liu (University of Kentucky)
Co-Investigators: Frank Lee (George Washington University); Andrei Alexandru (George Washington University); Terrence Draper (University of Kentucky)

Field of Science: Nuclear Physics

Abstract:
Why does the Universe have many more particles than antiparticles? At the beginning of the Universe, there should be equal numbers of particles and antiparticles. One of the necessary conditions for the antiparticles to disappear is the charge and parity (CP) symmetry breaking. The standard model does not explain this. There should be another source. This is the motivation for experiments to detect neutron electric dipole moment (nEDM) which would signal the CP-violation. We propose to calculate the nEDM as induced by the \theta term with lattice gauge Monte Carlo approach to solving quantum chromodynamics (QCD) and help explain and understand the experiments when the nEDM is discovered.