Type: Renewal PW

Title: Forming Globular Clusters in Fully Cosmological Simulations of Galaxy Formation

Principal Investigator: Michael Boylan-Kolchin (University of Texas at Austin (UT) (UT Austin))
Co-Investigators:

Field of Science: Astronomical Sciences

Abstract:
The formation and evolution of globular clusters is one of the oldest topics in Astronomy, yet many aspects remain poorly understood. We request Frontera time to run a suite of cosmological simulations with the well-established GIZMO code. The purpose of these simulations is to study the evolution of globular clusters at high redshift, and their tidal evolution within the galactic environments. In order to accomplish this goal, we will run two sets of simulations: one suite of fully-hydrodynamic simulations at extremely high resolution (0.1 pc) to capture the formation of globular clusters, and a separate suite of high-resolution (18 pc) dark-matter-only runs with embedded disk potentials in order to track small dark matter halos to the present day and understand how the halos in which GCs grow are disrupted over time. These results will then be combined in order to give us a holistic picture of how many globular cluster survive to the present day, and to give robust predictions for how the disrupted globular cluster contribute to the growth of the stellar halo, and formation of the stellar streams. Owing to the high resolution necessary to both simulate the formation of globular clusters and to track their host dark matter halos from the early Universe to the present day, we need the computing power of Frontera. We estimate that 244,420 SUs will be sufficient to meet our goals.

Type: New 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, the world top-ranked supercomputing resources. This project includes the study of interfacial turbulence on two fundamental problems observed in environmental flows: the buoyancy force driven mixing layer and particle embedded wall boundary layer. 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 the insight about how pollutants in bottom sediments are entrained and transported in a water body. Both studies will be first of their kind to simulate multiple fluid dynamics process 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: New 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 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. Using Frontera high-performance computing environment, we will determine the clinical applicability of our workflow toward improving surgical predictability of 1) Heart Valve (mitral and aortic) and 2) Fontan surgery for single ventricle disease using retrospective patient data.

Type: New PW

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

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

Field of Science: Geophysics

Abstract:
Plate tectonics is the surface expression of thermo-chemical mantle convection. However, the physical interactions that allow the deformation, subduction and recycling of the lithosphere are poorly understood. Understanding these interactions has implications from the long-term evolution of terrestrial planets to seismic hazard. A key missing link in our understanding lies in how the bulk behavior of plate boundaries is embedded within convection, and the role of damage memory and hysteresis in their establishment, longevity and long term deformation. With the computational resources available through Frontera we can now access large-scale, high-resolution, 3-D, time-evolving models of mantle convection that can self-consistently capture key ingredients such as the development of transform faults, orogenesis and overriding plate deformation through the use of a visco-plastic-elastic damage rheology.

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: 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:
A novel, first principle approach to evaluate the feasibility of a tokamak fusion reactor at Negative Triangularity (NT) is proposed. The study aims at predicting the maximum core fusion performance with a self-consistent edge solution compatible with damage threshold to Plasma Facing Components (PFC).

Negative Triangularity is a revolutionary configuration alternative to the H-mode regime, which is the current leading candidate for operations in future fusion reactors. Thanks to a significant reduction of the turbulence at play, NT plasmas achieve similar confinement levels as H-mode discharges without the need for narrow insulating layers near the plasma edge known as pedestals. As such, NT plasmas naturally avoid wall damaging ELM instabilities and reduce both impurity content and heat flux to PFCs.

The numerical tools to be employed implement highly sophisticated turbulence models and were extensively optimized for leadership-class computational systems. The use of first principle models is necessary in view of the fact that all reduced models currently available in the fusion community were calibrated for standard regimes, which makes them unreliable in this novel configuration. This research will further result in new calibration data that will be used to extend the applicability of transport models based on reduced physics and fast neural-networks.

The predictions resulting from this project will remedy for the paucity of data in this novel regime, thereby providing researchers with confinement scalings without having to carry out long and expensive experiments in large scale devices.

Type: New PW

Title: Scalable Graph Machine Learning and Graph Pattern Mining

Principal Investigator: Arvind Mithal (Massachusetts Institute of Technology)
Co-Investigators: Xuhao Chen (Massachusetts Institute of Technology)

Field of Science: Distributed and Parallel Processing, Vectorization

Abstract:
We request computing time and disk space on Frontera, to support research into developing our large-scale graph machine learning and graph pattern mining systems. Specifically, we aim to support large-scale (1) graph neural network (GNN) training and (2) graph pattern mining (GPM) in graph databases, both on the multi-CPU and multi-GPU platform. Previously, with support from NSF, Samsung and IBM (§1), we have developed: (1) GraFboost [42] a flash-based hardware accelerator for out-of-core analytics of multi-terabyte graphs, and DeepGalois [32], a distributed framework for graph neural networks targeting the multi-CPU and multi-GPU platform; (2) Pangolin [14] and Sandslash [13], two programming systems for graph pattern mining that simplifies programming and also runs efficiently on CPU and GPU; (3) FlexMiner [15], a dedicated hardware accelerator for graph pattern mining that keeps the same programming interface as Pangolin but further improves performance by an order of magnitude. Our work has been published in various top tier conferences such as VLDB, ISCA, MICRO, ICS, etc.

Our proposed work (§2) includes developing (1) a locality-aware training algorithm for GNN, and (2) a highly scalable GPM system. We plan to evaluate our GNN and GPM systems using the Frontera resources requested in this proposal (§3): we will use Frontera CPUs and GPUs to develop, test, and run scaling experiments on our proposed systems, and compare the performance with prior systems (§4).

Type: Renewal PW

Title: Towards Robust Atmospheric Retrievals for Cloudy L Dwarfs: Tests on Sonora Spectra

Principal Investigator: Caroline Morley (University of Texas at Austin (UT) (UT Austin))
Co-Investigators: Melanie Rowland (University of Texas at Austin (UT) (UT Austin))

Field of Science: Astronomical Sciences

Abstract:
Retrieving atmospheric properties from spectra is the only method through which properties of brown dwarf and exoplanet atmospheres can be determined since in situ measurements are impossible at astronomical distances. Retrieval frameworks are computationally expensive, but this process can be accelerated through the use of graphics processing units (GPUs) in the calculation of the millions of model atmospheres generated in a retrieval framework. But to date, retrieval frameworks with clouds have not been robustly verified for accuracy despite the fact that clouds are abundant in cooling brown dwarfs and exoplanets. Before we can incorporate the more complex physics governing cloud formation into retrieval frameworks for cloudy L dwarf atmospheres, we must first test a number of assumptions regarding thermal structure and chemical abundances on synthetic brown dwarf spectra for which we know ground-truth values.

Type: Renewal PW

Title: Advancing understanding of aerosol-cloud feedback using the world's first global climate model with explicit boundary layer turbulence

Principal Investigator: Michael Pritchard (University of California Irvine (UCI))
Co-Investigators: Peter Blossey (University of Washington)

Field of Science: Atmospheric Sciences

Abstract:
Overview:
Ultraparameterization (UP) is a new global climate modeling approach that explicitly simulates the turbulent air motions that create most low-lying clouds, rather than relying on uncertain parameterized representations that have driven large uncertainties in the sensitivity of global and regional climate change to CO2 increase. In each climate model grid column, a cloud-resolving model (CRM) is embedded with a grid spacing of about 250 m horizontally by 20 m vertically, representing a significant refinement of the resolution of standard cloud superparameterization. UP will be coupled to a model of aerosol evolution (UP-AER) to provide a simulation of the interaction between aerosols and low-lying clouds better grounded in fundamental physics than in conventional climate models, which will be comprehensively tested against a diversity of observations. Novel software engineering (a 'CRM Orchestrator') will upgrade UP-AER to efficiently use computers with many more processors than at present to enable multiyear simulations, and to use embedded cloud-resolving models with geographically variable meshes and more grid points that more realistically simulate all relevant cloud regimes.

Intellectual Merit:
The interaction of aerosols and clouds (through processes such as cloud droplet nucleation, aerosol scavenging by precipitation, and mixed phase microphysics) is tied to local air motions much smaller than the grid cell of any climate model. UP's embedded CRM is a more fundamental solution to representing such interactions than even a sophisticated parameterization of subgrid process variability could hope to achieve. By engineering UP to use a larger grid spacing in regions of persistent deep cumulus convection and smaller grid spacing in regions dominated by boundary-layer cloud, and to use three-dimensional rather than two-dimensional grids, all turbulent cloud types and their interaction with aerosol will be better simulated, including removing a bias in current UP of too little coastal stratocumulus. The result is a more credible, comprehensible global model of cloud-aerosol-climate interaction.

Broader Impacts:
UP-AER is complementary to the global models used today for comprehensive climate change modeling. UP-AER will contribute to a more reliable estimate of the effect of anthropogenic aerosol perturbations on clouds, a key uncertainty in interpreting the historical record of climate change and in projecting future global and regional patterns of climate change in support of societal decision-making. Meanwhile, our technical work addresses a challenge in the national transition to the manycore supercomputing paradigm, which has proved difficult for climate simulation to exploit. This will enhance national expertise in high performance computing and climate model development.

Type: Renewal PW

Title: Studies In Theoretical Astrophysics and General Relativity

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

Field of Science: Gravitational Physics

Abstract:
We request a renewal of our current Frontera allocation AST20025 to continue our multi- year effort to tackle several large-scale, long-standing, unsolved problems in theoretical astro- physics and numerical relativity. We numerically solve the Einstein field equations coupled to the relativistic magnetohydrodynamic equations and the equations of radiation transport to simulate neutron stars (NSs), black holes (BHs), and accretion disks, in isolation or in binary systems. 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 cur- rent and future observations of gravitational waves by aLIGO/VIRGO, GEO, KAGRA, Pulsar Timing Arrays, LISA/DECIGO, and other laser interferometers now operating or under devel- opment. Of particular interest in the latter category are the Einstein Telescope and the Cosmic Explorer. Our simulations also model promising gamma-ray burst sources (GRBs) observed by NASA satellites such as INTEGRAL and FERMI, X-ray sources observed by NICER, CHAN- DRA, and XMM-Newton, and optical and infrared sources observed by the HST, NuSTAR and PanSTARRS telescopes. This research is supported by grants from the National Science Foundation (NSF) and the National Aeronautics and Space Agency (NASA).

Type: Renewal LSCP

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

Principal Investigator: Saul A. Teukolsky (Cornell University)
Co-Investigators: Leo Stein (University of Mississippi (Ole Miss)); Nils Deppe (Caltech); Geoffrey Lovelace (California State University Fullerton); Matthew Duez (Cornell University); Francois Foucart (University of New Hampshire (UNH)); Aaron Zimmerman (University of Texas at Austin (UT) (UT Austin)); Mark Scheel (California Institute of Technology (Caltech))

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 paramaters. 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: 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: CHRISTOPHER SIMMONS (University of Texas at Dallas (UTD) (UT Dallas))

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

Abstract:
Fluoride ion (F^-) is a natural xenobiotic that inhibits two essential enzymes for microorganisms' survival. However, many bacterial species have developed membrane transport proteins to export F^- from the cytoplasm and to decrease its concentration below the toxic level. The unique and unusual properties of these F^- exporters (known as "Fluc" ion channels) and their potential as novel targets for antibiotics call for further investigations. I plan to study Fluc, and to uncover the details about its molecular structure, dynamics, energetics, and mechanism. This proposal is designed based on the preliminary data obtained from MD simulations using time allocation awarded by Pathways mechanism last year. These preliminary data was presented in ACS-SWRM 2021, and TACC Symposium 2021 and has evolved into new specific aims. The pathways grant will enable me to accomplish these new aims using their powerful computational resources and move toward exploring larger biological systems in the context of an LRAC grant.

Type: New PW

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

Principal Investigator: David Vanderbilt (Rutgers University (State University of New Jersey))
Co-Investigators: Kristjan Haule (Rutgers University); David Vanderbilt (Rutgers University (State University of New Jersey)); Subhasish Mandal (Rutgers University (State University of New Jersey))

Field of Science: Condensed Matter Physics

Abstract:
Materials are often loosely categorized into weakly and strongly correlated systems depending on the strength of electron-electron correlation. Materials with strong electronic correlations have magnetic, optical
and transport properties that are interesting for materials design, and useful in technological applications. While density functional theory (DFT) or DFT+U methods give quite accurate results for structural parameters
in most materials, qualitative predictions of excited state properties usually requires beyond DFT methods such as the GW approximation, the dynamical mean field theory (DMFT), or, hybrid functionals. Various methods going beyond density-functional theory have been developed to describe the electronic structure of correlated materials, but it is unclear 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. The existing materials databases, constructed in response to materials genome initiative, are built almost exclusively by DFT engines, and are thus very often making incorrect predictions in correlated materials. In this proposal
we want to test the readiness and performance of beyond-DFT methods by testing them on a training set of materials which are both weakly and strongly correlated. Our database for beyond-DFT methods, called JARVIS-Beyond DFT is hosted at NIST. The goal of this proposal allocation request is to continue testing the set of beyond-DFT ab initio methods (hybrid functionals, DFT+DMFT, and GW), and build up a database of spectral functions and optical properties, and their comparison to available experiments. This
allocation request is intended to continue the seed support to develop a culture of data-sharing in the spirit of
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: 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 two new NOAA pre-operational forecasts based on the model for US Atlantic & Gulf coasts and Pacific basin; (2) we serve a large and diverse community world-wide with the open-source community code.