Type: New PW
Title: GPU-Accelerated Computing for Solving Partial Differential Equations using Nodal Discontinuous Galerkin Methods

Principal Investigator: Lizy John (University of Texas at Austin)
Co-Investigators:

Field of Science: Advanced Scientific Computing

Abstract:
Typical seismic surveys can cover hundreds of square kilometers and can generate hunderds of terabytes of data. This vast amount of data will be used to find the optimum model of the Earth's subsurface that can best match the observed data. This problem is called full-wavefield inversion (FWI) which is a family of partial differential equations (PDE)-constrained optimization problems. The Nodal Discontinuous Galerkin is one of the methods to find the optimum solutions for such PDE optimization problems. The whole problem is then discritized both in time (in the form of time steps) and in space (in the form of mesh).

Currently, the PDE solver software for this problem is built in C++ and make uses of p4est library to distribute the meshes to all MPI-capable nodes to distribute the computation jobs across all CPUs. Although it is already capable to use multiple CPUs in multiple nodes, the runtime of the solver is still not acceptable. Increasing the fidelity and resolution of the model will increase the runtime evenmore. By looking at the problem itself, the computation algorithm used in the solver, and the nature of the data that is processed, we have found large number of parallelism that can be exploited to accelerate the solver. This large number of parallelism can be mapped into GPUs which have thousands of compute units and thus potentially can speed up the computation significantly over CPUs only implementation. We are currently developing the solver that can use GPUs for its computation as a part of our research.

Type: New PW
Title: Pedestrian Dynamics-Based Analysis of Infection Propagation Through Air Travel

Principal Investigator: Ashok Srinivasan (n/a)
Co-Investigators:

Field of Science: Advanced Scientific Computing

Abstract:
The goal of our project is to develop a novel cyberinfrastructure to simulate the movement of people in order to understand how movement patterns influence transmission of infections at local as well as global scales. A central focus of our cyberinfrastructure will be on enabling fundamental scientific advances in decision making contexts, such as estimating the effectiveness of alternative policy choices and the global impact of local decisions in mitigating epidemic risk. This requires providing tools to enable robust scientific analysis in the presence of real-world constraints, such as uncertainty in data. With this broad goal in mind, we specifically target the spread of infectious diseases during air travel as an initial domain. This will be extended to other domains – such as disaster shelters and theme parks – through community contributions.

Type: New PW

Title: Investigating the final assembly of the inner solar system with GPU acceleration

Principal Investigator: Matthew Clement (Carnegie Institution of Washington)

Co-Investigators:

Field of Science: Planetary Astronomy

Abstract:

Our solar system is the most observationally constrained planetary system known, and understanding its rich dynamical history will help us characterize the prevalence of, and requirements for solar system analogs and habitable planets around other stars. Our proposed research will involve using numerical simulations to study the formation of the four terrestrial planets: Mercury, Venus, Earth and Mars. In particular, successful terrestrial planet formation models must provide an explanation for the inner solar system's peculiar mass distribution. Models of the Sun's primordial gaseous nebula generally predict that the inner planets' building blocks originated from a uniform radial distribution of solids. However, Mars is about an order of magnitude less massive than Earth and Venus, and the total mass in the modern asteroid belt is estimated to only be ~0.0005 Earth masses. Multiple dynamical models (e.g.: the ``Grand Tack'' hypothesis, low-mass asteroid belt model and Early Instability scenario) have offered explanations for the solar system's curious mass distribution. However, until recently, it has been difficult to definitively rule out one model, in favor of another. Our project will utilize a new, GPU accelerated N-body algorithm to scrutinize simulated systems against geological constraints from the Apollo missions, and the modern asteroid belt's well-characterized orbital structure.

Type: New PW
Title: Exploring the Physical Ingredients of Star Formation with Simulations

Principal Investigator: Michael Grudic (Northwestern University)
Co-Investigators: Claude-André Faucher-Giguère (Northwestern University); Stella Offner (University of Texas at Austin); David Guszejnov (University of Texas at Austin)

Field of Science: Astronomical Sciences

Abstract:
Numerical simulations of star formation in giant molecular clouds (GMCs) are an essential tool for understanding the roles of different physics in star formation. We will perform a new suite of suite of MHD simulations following the formation of individual stars in GMCs with the GIZMO code. These simulations will explore the effects of feedback physics upon star formation in GMCs, initially including accretion-powered jets and radiation, and eventually fusion-powered stellar winds, radiation, and supernovae.

Type: New PW
Title: Numerical Simulations of Interstellar Turbulence

Principal Investigator: Alexei Kritsuk (University of California, San Diego)
Co-Investigators:

Field of Science: Galactic Astronomy

Abstract:
The main science theme for this Pathways allocation request for compute time on Frontera is a study of the energy cycle in the interstellar medium of disk-like galaxies, namely how the energy injected by stellar feedback and gravitational instabilities at the scale comparable to the disk scale height cascades to larger and smaller scales, shaping the structure of interstellar filaments and regulating star formation. High resolution simulations of compressible turbulence in three dimensions will be carried out to break ground for advanced galactic disk simulations that would capture generation of interstellar turbulence self-consistently for the first time. Simulations of multiphase magnetized interstellar turbulence will yield realistic maps of galactic foreground dust emission at radio frequencies. These simulations will paint a detailed picture of the polarized emission of dust grains in our Galaxy, which is known to interfere with measurements of the cosmic microwave background (CMB). They will contribute to an ongoing effort to more fully understand how dust affects the appearance of the CMB, helping to inform the design of future CMB experiments.

Type: New PW
Title: MPM: Towards a peta-scale simulation of landslide hazards

Principal Investigator: Krishna Kumar (University of Texas at Austin)
Co-Investigators: Ellen Rathje (University of Texas at Austin)

Field of Science: Natural and Man-Made Hazard Mitigation

Abstract:
Among the various natural hazards, landslides are the most widespread and damaging, causing billions of dollars in damages to life and infrastructure. The first-ever geological-scale landslide simulation with billions of particles offers insights on the initiation and evolution of geohazards at realistic stresses and geometric intricacies. Exploiting the petascale capabilities of the CB-Geo MPM code, the mechanism leading to the long run-out of Sea-front landslide is assessed by analyzing the combined influence of different triggering factors, such as earthquake-induced shaking, fault rupture, progressive failure sequence. The pioneering attempt at geological-scale hazard modeling will redefine the field of natural hazard management.

Type: New PW

Title: Future Application, Programming Model, and Runtime Research for OpenSHMEM

Principal Investigator: Jonathan Grossman (Rice University)
Co-Investigators: Vivek Sarkar (Georgia Institute of Technology); Howard Pritchard (LANL); Tony Curtis (SBU)

Field of Science: Software Systems

Abstract:
This project focuses on research and software development in future applications, programming models, and runtimes for the OpenSHMEM community. OpenSHMEM is a distributed programming system for writing scalable parallel applications on large supercomputers. OpenSHMEM's Partitioned Global Address Space (PGAS) programming model makes it a perfect fit for irregular, large scale applications where fine grain communication is common. OpenSHMEM is commonly applied in graph processing, data analytics, and scientific simulation. Our research team performs work with OpenSHMEM, including: (1) evaluating and experimenting with new application areas, (2) performing research and development in to novel extensions to OpenSHMEM and OpenSHMEM implementations, and (3) developing tools and libraries on top of OpenSHMEM for use by others.

Type: New PW

Title: Numerical simulations of plasma based flowsusing heterogeneous computational strategies.

Principal Investigator: Deborah Levin (University of Illinois)
Co-Investigators:

Field of Science: Fluid, Particulate, and Hydraulic Systems

Abstract:
High fidelity numerical plasma modeling has been a key aspect for predicting physics in plasma. Using Frontera we plan to conduct a series of numerical studies on a variety of plasma based flows such as space-plasma surface interactions, and beam neutralization for plume plasma. A GPU based code, CHAOS, has been developed during our previous compute resources, and it showed a 85% strong scaling on the Bluewaters system. This code will again be used for high-fidelity plasma modeling on new set of problems. Given a huge range of length and time-scales in plasma based flows, a parallel computing architecture, such as Frontera, is necessary for their self-consistent numerical modeling.

Type: New PW
Title: Structure and Dynamics of Highly Turbulent Premixed Combustion

Principal Investigator: Peter Hamlington (University of Colorado)
Co-Investigators: Samuel Whitman (University of Colorado Boulder); Shashank Yellapantula (National Renewable Energy Laboratory); Michael Meehan (University of Colorado)

Field of Science: Fluid, Particulate, and Hydraulic Systems

Abstract:
Direct numerical simulations (DNS) of practically relevant premixed flame configurations will be performed across a range of conditions, including high turbulence intensities. Highly turbulent premixed flames are a relatively unexplored terra incognita in combustion research, and much of the current knowledge in this regime has been obtained from DNS of idealized configurations using relatively simple chemical models. To improve understanding of realistic systems, however, new DNS with more sophisticated chemical kinetics modeling is now required for practically relevant configurations where, for example, secondary flows, shear, swirl, and walls are important. Through a carefully planned campaign of new DNS enabled by adaptive mesh refinement (AMR), the science team will use the Pathways allocation on Frontera to address two fundamental research questions: (i) How does high intensity turbulence affect premixed flame structure, dynamics, and chemical pathways? and (ii) How do flame properties depend on configuration and operating conditions? Insights obtained by answering these questions will allow refinement of prevailing theories, including those encompassed in classical regime diagrams, as well as provide physics-based guidance on improvements to reduced-order chemical kinetics and turbulence models for simulations of practical systems.

Type: New PW
Title: Predicting orientation-dependent plastic events in amorphous solids via deep learning

Principal Investigator: Evan Ma (Johns Hopkins University)
Co-Investigators:

Field of Science: Materials Research

Abstract:
Structure-property relationship is a central tenet of materials science and of glass research. For metallic glasses, the amorphous nature of their internal structure poses major challenges, to a quantitative correlation of the (local) atomic configurations with their properties (i.e., responses to stimuli such as temperature and stress). This project will demonstrate that the static information of atomic position can be used to predict the orientation-dependent stress-driven plastic events in both 2D and 3D amorphous solids using state-of-the-art deep learning algorithms. This is expected to improve our understanding of the unusual structural and mechanical heterogeneity inherent to the seemingly homogeneous amorphous solid and thus push the boundary of materials science.

Type: New PW

Title: Prediction of functional defect properties in materials for clean energy and brain-inspired information processing

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

Field of Science: Materials Research

Abstract:

Abstract. Here, we request a research allocation on Frontera supercomputer for the prediction of functional defect properties in materials for clean energy and brain-inspired information processing. We mainly focus on two research topics: (1) search of novel superprotonic solid-state conductors, and (2) investigation of the Al2O3|Al interface structure for designing superior hydrogen permeation barriers. These projects require massive density functional theory (DFT) calculations, namely (1) ab initio molecular dynamics (AIMD) simulations of proton conductivity, and (2) DFT-based Monte Carlo (MC) simulations to assess atomic-scale structure of Al2O3|Al interface. We expect that information obtained using ab initio modeling will help to identify the most promising material combinations and guide our experimental studies for non-volatile memory devices and hydrogen permeation barriers. In our calculations, we will primarily exploit VASP computational package designed to run on high-performance parallel supercomputers. Based on our scaling test, we kindly request a total of 147,653 SUs on Frontera CPU nodes.

Type: New PW

Title: Advanced machine learning force field development for linear alkoxy dehydrogenation on Cu-based catalysts

Principal Investigator: Boris Kozinsky (Harvard University)
Co-Investigators:

Field of Science: Materials Research, Chemistry

Abstract:
Highly efficient catalysis is the key to sustainable chemical production. In the laboratory of Material Intelligence Research, we use advanced machine learning algorithms with atomistic simulations to develop bottom-up material design principles. In this proposal, we plan to develop machine learning force fields for alkoxy dehydrogenation on Cu catalysts. The fast and accurate force fields will be employed in accelerated molecular dynamics simulations over a long time scale that cannot be reached with traditional ab initio calculations. This study will help us to elucidate the role of dynamical effect in catalytic reactions and find possible knobs to improve catalytic activity.

Type: New PW
Title: Predictive Simulations of Phase Transitions in Dynamically Compressed Silicon

Principal Investigator: Ivan Oleynik (University of South Florida)
Co-Investigators: Anatoly Belonoshko (University of South Florida)

Field of Science: Materials Research

Abstract:
The overarching goal of this Frontera Pathway project is to perform predictive simulations to make significant scientific advances in solving one of the outstanding problems in high-energy-density (HED) condensed matter and materials physics – uncovering fundamental atomic-scale mechanisms and kinetics of phase transitions under dynamic compression in prototypical elemental silicon.

Our scientific goals are:
(1) To perform very accurate quantum molecular dynamics (QMD) simulations of free energies, and phase diagrams within a wide range of pressures and temperatures.

(2) To devise machine learned quantum-accurate SNAP interatomic potential to accurately describe phases and dynamics of Si at extreme conditions and perform atomistic simulations of shock-induced phase transitions in experimental space-strain-rate domain;

(3) To guide experiments by focusing on the most interesting predictions and to perform comprehensive comparison of simulation and experimental results validating theoretical predictions.

Our research plan includes the following Thrusts:

Thrust 1: First-principles MD simulations of silicon phase diagram

Thrust 2: High-fidelity machine learned SNAP interatomic potential

Thrust 3: Large-scale MD simulations of shock-induced phase transitions in silicon

Type: New PW

Title: Mini-Protein Binder Design

Principal Investigator: David Baker (University of Washinton)

Co-Investigators:

Field of Science: Biochemistry and Molecular Structure and Function

Abstract:

The recent global outbreak of coronavirus (SARS-Cov2) has highlighted the need for therapeutic-driven pandemic preparedness. We at the Institute for Protein have developed software tools to quickly create new protein drug candidates which act by binding to a specific target protein. Leveraging modern biochemical practices, we can screen 100,000 designed proteins for binding at once. Generating these 100,000 proteins requires sampling billions of possibilities and enormous amounts of compute time. With the help of Frontera, we will be able to design new drugs and hone our techniques to be able to respond at a moments notice when the world needs to stop an infection.

Type: New PW

Title: Computational and Theoretical Studies on DNA Folding, Eukaryotic Chromosomes, and Glassy Materials

Principal Investigator: Devarajan Thirumalai (University of Texas at Austin)

Co-Investigators:

Field of Science: Biophysics

Abstract:

The group of Prof. Thirumalai is interested in adopting a variety of computational and theoretical methods to understand dynamic and structural properties of biomacromolecules, cancer cells, and glassy materials. With the allocated time, we aim to carry out full atomic simulation of DNA wrapping, develop coarse-grained models for eukaryotic chromosomes, and investigate the glassy dynamics of polymeric materials.

Type: New PW
Title: Exploration of Energy Landscapes of Protein Folding and Amyloid Formation

Principal Investigator: Ulrich Hansmann (University of Oklahoma)
Co-Investigators:

Field of Science: Biochemistry and Molecular Structure and Function

Abstract:
Proteins are the driving force behind many of the vital processes of organic life. Hence, for potential medical, biological or chemical application it is important to understand the variables that regulate and control their working. However, the relationship between a protein's function-determining three-dimensional structure and its governing amino acid sequence is only partially understood. We have proposed to overcome the bottlenecks that have hold back computational studies of this problem by a variant of Hamiltonian replica exchange, named replica exchange with tunneling (RET). In the present project we propose to extend this technique to studies of fold-switching proteins and the formation, conversion and propagation of amyloids, implicated in various illnesses including Alzheimer's disease.

Type: New PW

Title: Multiscale Modeling of Blood Circulation and Tumor Extravasation of Nanomaterials for Targeted Drug Delivery

Principal Investigator: Ying Li (University of Connecticut)
Co-Investigators:

Field of Science: Biophysics

Abstract:
Through nanomedicine significant methods are emerging to deliver drug molecules directly into diseased areas for cancer treatment. Targeted drug delivery is one of the most promising approaches which relies on nanoparticles (NPs) that carry and release drugs. The therapeutic efficacy of NP-based drug carriers is determined by the proper concentration of drug molecules at the lesion site. NPs need to be delivered directly to the diseased tissues while minimizing their uptake by other tissues, thereby reducing the potential harm to healthy tissue. Therefore, the design of these NPs and hence the efficacy of the targeted drug delivery could be significantly improved by understanding how the drugs carried by NPs are transported and dispersed in human body. We request computing time on Frontera resources for multiscale modeling of blood circulation of NPs and their tumor extravasation behaviors. We will use a hybrid molecular dynamics (MD) and Lattice Boltzmann (LB) method, implemented in LAMMPS, for proposed computational research. LB method is used to solve the fluid flow dynamics and a coarse-grained MD model is employed to capture the dynamics of red blood cells and NPs. These two solvers are coupled together by immersed boundary method. We request a total of 250,000 SUs on Frontera. The proposed simulations include: (a) explore how the size, shape, surface and stiffness of NPs will affect their transport and near wall adhesion within blood flow; (b) explore how the size, shape, surface and stiffness of NPs will affect their tumor extravasation. The simulation results will provide guidance in design of efficient nanomaterials that optimally accumulate within diseased tissue, thus providing better imaging sensitivity, therapeutic efficacy and lower toxicity.

Type: New PW
Title: Plasma Dynamics and Particle Acceleration in 3D Relativistic Magnetic Reconnection

Principal Investigator: Fan Guo (Los Alamos National Laboratory)
Co-Investigators: Patrick Kilian (Los Alamos National Lab); Xiaocan Li (University of Alabama in Huntsville); Yi-Hsin Liu (Dartmouth College)

Field of Science: Physics

Abstract:
Magnetic reconnection is a fundamental plasma process that allows rapid changes of magnetic field topology and the conversion of magnetic energy into plasma kinetic energy. In high-energy astrophysical systems such as pulsar wind nebulae and relativistic jets from gamma-ray bursters and black holes, it is expected that the magnetization parameter σ, the ratio of the magnetic energy density and plasma energy (i.e., enthalpy) density, can be much larger than unity and therefore the Alfvén speed is close to the speed of the light c. There has been a strong surge of interests on relativistic reconnection over the past five years in plasma astrophysics, but the rich physics of collisionless reconnection and its associated particle acceleration in the relativistic regime remain less studied compared to the non-relativistic counterparts. Magnetic reconnection in a realistic system is often accompanied with the magnetic field shear and shear flows. This setting is more general and likely the more common situation where most reconnection takes places, for instance, in the solar corona, solar winds, and astrophysical accretion disks and jets how the effect of special relativity, among other effects, influences the dynamics of reconnection in the strongly magnetized astrophysical plasmas under these conditions is largely unknown. Our proposed research is to use fully kinetic simulations to understand kinetic physics and particle acceleration in relativistic magnetic reconnection in more realistic configurations and physical conditions. The primary goal of this project is to identify the fundamental effects caused by special relativity under the presence of a guide field.

Type: New LSCP
Title: Understanding the Global Behavior of Core-Collapse Supernovae

Principal Investigator: David Vartanyan (University of California, Berkeley)
Co-Investigators: Aaron Skinner (Lawrence Livermore National Laboratory); Hiroki Nagakura (Princeton University); Joshua Dolence (Los Alamos National Laboratory); Adam Burrows (Princeton University)

Field of Science: Stellar Astronomy and Astrophysics

Abstract:
Core-collapse supernovae herald the death of massive stars and the birth of neutron stars. During this violent process, a combination of high-density nuclear physics, multi-dimensional hydrodynamics, radiation transport, and neutrino physics determines the final seconds of a star's life. Despite the early attempts in the 1960s to understand core-collapse supernovae, the explosion mechanism - thought to involve the detailed neutrino physics of the stellar interior - still remains poorly understood. Detailed long-term, three-dimensional calculations proving this paradigm are lacking, but are essential if we are ever to understand this problem. Current advances in computational capabilities and the availability of HPC resources, together with improvements in nuclear theory, provide a golden opportunity to tackle this long-standing problem with renewed vigor.

Using our new state-of-the-art, highly-scalable, 3D, multi-group, radiation-hydrodynamics code FORNAX we developed and tested over the last four years, we propose to conduct multiple three-dimensional radiation/hydrodynamic simulations to help resolve this fifty-year-old problem in nuclear astrophysics. Our thesis is that going to fully 3D neutrino radiation-hydrodynamics using the state-of-the-art FORNAX computational capability and employing the best neutrino and nuclear physics may together be the keys to demonstrating and understanding the generic core-collapse supernova explosion mechanism. We propose a series of detailed 3D simulations of a broad host of stellar progenitors carried out to late time, until the explosion diagnostics saturate, to resolve the core-collapse supernovae problem. Such an endeavor will additionally inform future high-energy experiments and observational efforts, as well as guide nuclear theory at these extreme conditions.

Viewed as a nuclear physics laboratory, core-collapse supernovae produce the highest densities of matter and energy in the modern universe. These vigorous explosions also are responsible for seeding most of the elements in Nature. The neutrino and gravitational wave signalsthey emit carry information about the high-density nuclear equation of state. Thus, supernovae probe the same sort of physics as FRIB, JLAB, ATLAS, and low-energy runs at RHIC, FAIR (GSI/Darmstadt), SHINE (CERN) and NICA (Dubna).

A resolution of the core-collapse supernova problem would benefit ongoing efforts of observers and instrument designers in the U.S. and around the world engaged in projects to determine the origin of the elements, measure gravitational waves (LIGO), and interpret laboratory nuclear reaction rate measurements in light of stellar nucleosynthesis.

Type: New LSCP

Title: Advancing Computational Methods to Understand the Dynamics of Ejection, Accretion, Winds and Jets in Neutron Star Mergers

Principal Investigator: Manuela Campanelli (Rochester Institute of Technology)
Co-Investigators: Yosef Zlochower (Rochester Institute of Technology); Julian Krolik (Johns Hopkins University); Scott Noble (National Aeronautics and Space Administration)

Field of Science: Astronomical Sciences, Gravitational Physics

Abstract:
The recent observations of a binary neutron star merger using both gravitational wave interferometers as well as electromagnetic telescopes across the full spectrum have initiated the age of multimessenger astronomy and astrophysics.

This proposal is to request an LSCP allocation of 2.3MSU on Frontera to support research in multimessenger astrophysics performed by a collaborative group of more than 15 researchers across 4 US institutions (RIT, NASA-GSFC, UWV, JHU) and another dozen or so at universities around the world, brought together under a NASA Theory and Computational Astrophysics Network (TCAN). Our network, comprising numerous experts in the fields of theoretical and computational astrophysics, is poised to complement these observational successes with simulations of binary neutron star and black-hole/neutron star performed with greater self-consistency and more complete physics than any previous work. We will track coalescences from the approach to merger, trough the merger itself, and collapse of the merged remnant. This portion will be seamlessly linked to the ejection of matter, formation of disks, jet-launching and propagation through surrounding matter, and initiation of outflows from the disk.

In this proposal, we request time on Frontera to run four simulations, their topics carefully chosen to both be relevant to observed examples and illustrate the sensitivity of the outcomes to system parameters. We list six simulations, of which we will select four, so that we can adjust flexibly if the scientific context changes during the 2 1/2 year duration of this allocation. These include two of the observed LIGO binary neutron star mergers, GW170817 and GW190425, and binaries with different total mass and mass ratio such that the merged neutron star remnant collapses to a black hole. In each case, we will calculate detailed electromagnetic and neutrino fluxes as well as characterize the evolution of the magnetic fields, including the launching of jets and other outflows from the nascent remnant. We may also simulate a black hole-neutron star merger, allowing us to disentangle the two leading sources of multimessenger transients based on their observed properties. Finally, we may explore the merger of two neutron stars with skewed magnetic fields, a largely unexplored scenario.

Type: New LSCP

Title: The Frontera-Event Horizon Telescope Partnership

Principal Investigator: Chi-kwan Chan (University of Arizona)

Co-Investigators: Feryal Ozel (University of Arizona); Ramesh Narayan (Harvard University); Dimitrios Psaltis; Charles Gammie

Field of Science: Astronomical Sciences

Abstract:

This Frontera Large-Scale Community Partnerships (LSCP) proposal seeks three years of computation resources to support the science utilization of the Event Horizon Telescope (EHT). The EHT is an international collaboration of over 200 researchers that captured the first horizon-scale resolution images of a black hole. Its science objectives include understanding accretion processes and jet launching mechanisms around black holes, as well as testing Einstein's general theory of relativity in strong field regimes and deepening our understanding of the properties of spacetime. As a result, a significant number of U.S.-based EHT members work on theoretical research and simulations of black holes with strong computation needs. The proposed LSCP allocation will support the EHT to achieve its science objectives by carrying out state-of-the-art numerical simulations; building, maintaining, and releasing the most complete black hole accretion simulation libraries; enabling EHT researchers to model, interpret, and understand its current and future observation results; advancing the forefront of black hole astrophysics research in the U.S.; and helping the EHT to design its next generation observations in order to place tighter constraints on Einstein's general theory of relativity.

Type: Renewal LSCP
Title: SCEC Earthquake Modeling, Ground Motion, and Hazard Simulations

Principal Investigator: Christine Goulet (University of Southern California)
Co-Investigators: Yehuda Ben-Zion (SCEC/USC); Bruce Shaw (Columbia University); Scott Callaghan (University of Southern California)

Field of Science: Earth Sciences

Abstract:
SCEC conducts and coordinates fundamental and applied research on earthquakes using southern California (SoCal) as its main natural laboratory. SCEC's research program is investigator-driven, relies on strong collaboration among researchers and supports core research and education in seismology, tectonic geodesy, earthquake geology, and computational science. SCEC is a leader in research that integrates science results and new technologies into broad impact products to improve seismic hazard assessment. Our long term goals in the seismic hazard realm are to 1) increase the accuracy of our earthquake, ground motion and hazard simulations; 2) reduce uncertainties; and 3) broaden the usefulness of our seismic simulation software tools for engineering and preparedness applications. These objectives are only attainable through strong collaborative team work and require leadership-class HPC capabilities such as those from Frontera.

With the 2020 allocations, we will perform research on earthquake catalog simulation (using RSQSim), fault dynamics (SORD), and complete large-scale high-frequency ground motion simulations (EDGE, 3D-EWP) that include material nonlinearity and topography. In addition, we will implement recently vetted models into CyberShake, including a new high-frequency seismogram module, and integrate synthetic earthquake catalogs from RSQSim in lieu of traditional earthquake rupture forecasts.

Type: New LSCP
Title: IceCube Computing on Frontera

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

Field of Science: Physics

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

Principal Investigator: Kenneth Bloom (University of Nebraska at Lincoln)
Co-Investigators: Tulika Bose (University of Wisconsin)

Field of Science: Elementary Particle Physics

Abstract:
The Compact Muon Solenoid (CMS) is one of the two general-purpose particle physics detectors at the Large Hadron Collider (LHC). The CMS Collaboration co-discovered the Higgs boson in 2012, has provided constraints on many models of new physics, and has made many precise measurements of the properties of known particles. 955 scientific papers have been submitted to date. The collaboration is now actively analyzing data recorded during 2016-18, with an emphasis on searches for dark matter and supersymmetric particles and measurements of the properties of the Higgs boson, while also preparing for the next data run that will commence in 2021. The prompt delivery of scientific results depends on the availability of computing resources that are capable of performing extensive simulations of physics processes in short amounts of time. The full suite of CMS physics measurements requires the simulation of billions of proton-proton collision events, including both processes that would arise from new, speculative physics models and those that arise from standard model processes that would be the background to the new physics. We propose to use Frontera for the simulation of about 1.9B collision events during the year that commences on July 1, 2020. Not only will this provide about 5% of the simulations needed during this year for the work of the global collaboration in performing dozens of physics measurements, it will also allow us to demonstrate the use of Frontera resources at very large scales in preparation for meeting the needs of CMS at the planned High Luminosity LHC.

Type: New LSCP

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

Principal Investigator: Saul A. Teukolsky (Cornell University)

Co-Investigators: Geoffrey Lovelace (Cal State Fullerton); Aaron Zimmerman (University of Texas at Austin); Matthew Duez (Washington State University); Francois Foucart (University of New Hampshire); Mark Scheel (California Institute of Technology)

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 LSCP
Title: Discovery and Measurement at the Energy Frontier with the ATLAS Detector at the CERN Large Hadron Collider

Principal Investigator: Robert Gardner (University of Chicago)
Co-Investigators:

Field of Science: Elementary Particle Physics

Abstract:
After discovering the Higgs boson in 2012 and exploring its properties in subsequent years, the ATLAS experiment at the CERN Large Hadron Collider is now searching for evidence of new physics phenomena at the energy frontier. Prior to its shutdown at the end of 2018 (the end of Run 2), the LHC had an extraordinary year delivering 10 billion proton-proton collisions events, its largest dataset to date, which continues to be analyzed by the collaboration. To achieve its full physics potential, ATLAS will use the CPU resources of Frontera to accelerate the pace of discovery.