Type: New PW

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

Principal Investigator: Michael Boylan-Kolchin (University of Texas at 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 (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: Misaligned Accretion Disk Simulations for Interpreting Event Horizon Telescope Black Hole Images and Movies

Principal Investigator: Jason Dexter (University of Colorado)
Co-Investigators:

Field of Science: Astronomical Sciences

Abstract:
We propose to expand the existing Event Horizon Telescope library of numerical simulations of gas falling onto black holes to incorporate self-consistent heating of the electrons and misalignment between the infalling gas and black hole spin. Misalignment results in Lense-Thirring precession and shocks, which can greatly influence the gas motions and provide extra heating. Incorporating self-consistent heating of the radiating electrons improves the predictive power of the resulting black hole images and movies. Exploring movies from high resolution, long duration misaligned simulations, we will study possible alignment mechanisms to determine whether the Galactic center black hole, Sgr A*, or the supermassive black hole in M87 might be fed by a tilted disk. Within the EHT, we will study the image shapes and sizes to see whether they are compatible with observations, and use them to infer the black hole mass and spin of target sources.

Type: New PW

Title: A Numerical Investigation of Fracture in Transitional Metal Dichalcogenides

Principal Investigator: Horacio Espinosa (Northwestern University)
Co-Investigators:

Field of Science: Mechanics and Materials

Abstract:
Transition metal dichalcogenides, a family of two-dimensional materials, have shown unique optical, electrical, and thermal properties that enable emergent applications in batteries, solar cells, electronics, and sensors. In all these applications, failure by fracture is a major concern. Under this project, the aim is to advance the fundamental knowledge of failure in transition metal dichalcogenides, and to establish robust experimental and computational protocols that are applicable to similar studies on other nanomaterials.

Type: Renewal PW

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

Principal Investigator: Jonathan Grossman (Rice University)
Co-Investigators:

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: Renewal PW

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

Principal Investigator: Fan Guo (Los Alamos National Laboratory)
Co-Investigators:

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: Renewal 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:
We propose the use of advanced sampling techniques to study the folding and association of various proteins, either implicated in diseases or being drug candidates.

Type: Renewal PW

Title: Advanced machine learning force field development for heterogeneous catalysis

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

Field of Science: Chemistry; Materials Research

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 to model the structural evolution of catalysts under reaction conditions, which cannot be easily resolved in experiments. This study will help us elucidate important intermediate structures that govern catalytic reactions and find possible knobs to improve catalytic activity.

Type: New PW

Title: Direct numerical simulation of the atomization of a planar liquid jet assisted by co-flowing turbulent gas streams

Principal Investigator: Yue Ling (Baylor University)
Co-Investigators: Gretar Trggvason (Johns Hopkins University)

Field of Science: Interfacial, Transport, and Separations Processes

Abstract:
Rigorous modeling and simulation of atomization that can precisely predict droplet size distributions and dynamics characteristics are essential to many spray applications such as combustion engines, spray cooling, and pathogen spreading by respiratory droplets. The air-blast atomization is an effective way to produce fine sprays compared to other fuel injection techniques and has been widely used gas turbine engines. A fundamental barrier that limits the predictive capability of atomization simulation in practical applications lies at the lack of comprehensive understanding on the fine details of inlet conditions on atomization. \cite{Jiang_2020a}. Traditionally, research on atomization and sprays relies primarily on experiment. However, high-level details of atomization are difficult to measure even with the advanced diagnostic techniques. DNS which can provide full temporal evolution of turbulence and interfaces is thus an important alternative approach for atomization investigation. The intellectual merit of the proposed project is to advance the understanding of inlet gas turbulence on airblast atomization through direct numerical simulations. The simulation results can be used to understand the interplay of different scales, as in direct numerical simulations of single phase turbulence, and also to provide the ground truth needed to develop and validate coarse models that are suitable for predictions of industrial systems. The results of the proposed simulations will contribute to the large databases required to develop data-driven models.

Type: New PW

Title: Study of ligand binding to proteins and nucleic acids by polarizable molecular dynamics simulations

Principal Investigator: Pengyu Ren (University of Texas at Austin)
Co-Investigators:

Field of Science: Biophysics

Abstract:
Protein-ligand binding is an integral part of many biological processes. Currently, the most reliable method for predicting protein-ligand binding is molecular dynamics (MD) simulations using physics-based models. There have been significant improvements in the accuracy of physics-based models. However, challenges remain for some important systems, especially those involving charged ligands or receptors, such as ion channels, metalloproteins and nucleic acids. It has been shown that the AMOEBA polarizable force field achieves superior accuracy for charged ligands, such as calcium and phosphate. This allocation will allow us to systematically study the binding of various ligands to common protein and nucleic acids using the AMOEBA force field. This will improve our understanding of the roles of electrostatics and polarization in ligand recognition and facilitate future application of polarizable force fields in basic and applied research.

Type: New PW

Title: Calculation of Electron Collisions with Molecular Targets using the Convergent Close-Coupling Method

Principal Investigator: Barry Schneider (National Institute of Standards and Technology)
Co-Investigators: Dmitri Fursa (Curtin University); Igor Bray (Curtin University)

Field of Science: Atomic, Molecular, and Optical Physics

Abstract:
This project is designed to produce high-quality and comprehensive data describing the collisions of electrons with molecules using the Convergent Close Coupling Method. The cross sections are much needed in a range of applications, particularly fusion. The major computational thrust, is to extend present approaches to computing state-specific ro-vibrational cross sections that go beyond what is known as the fixed-nuclei approximation (FNA).

Type: Renewal 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:
We have extensively used Frontera GPU and CPU pathway allocations for conducting various researches regarding structural and dynamic properties of DNAs, chromatins, cancer cells, and glassy materials. As an extension of our previous Frontera pathway projects, we aim to specifically
focus on two research topics, (1) investigation of molecular mechanism of salt-induced disassembly of nucleosome and (2) seeking universal RFOT (random first-order transition) features of glassy materials.

Type: Renewal 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:
We request a renewal of our 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 and LAMMPS computational packages designed to run on high-performance parallel supercomputers. Based on our scaling test, we kindly request a total of 143,660 SUs on Frontera CPU nodes.

Type: Renewal 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. 1045 scientific papers have been submitted to date. We request a renewal of our allocation on Frontera to continue our large-scale simulations of proton collisions, with an allocation sufficiently large to generate nearly 2B events, which would be about 5\% of the total simulated data set planned by CMS for the year beginning April 1, 2021. This effort 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: Renewal 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); Charles Gammie (University of Illinois)

Field of Science: Astronomical Sciences

Abstract:
This progress report is for renewing the Frontera Large-Scale Community Partnership (LSCP) allocation entitled "the Frontera-Event Horizon Telescope Partnership" for its second year. We seek computation resources to continually 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. This LSCP allocation has been the EHT's main computation resource since last year and has been supporting the EHT to achieve its science objectives. We have used this LSCP for 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: 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.

Type: Renewal LSCP

Title: IceCube Computing on Frontera

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

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: New LSCP

Title: Simulating New Physics on Cosmological Scales: The Feedback In Realistic Environments (FIRE) Project

Principal Investigator: Philip Hopkins (California Institute of Technology)
Co-Investigators: Jorge Moreno (Pomona College); Dusan Keres (UC San Diego); Robyn Sanderson (Columbia University); Sarah Loebman (University of California, Davis); Michael Boylan-Kolchin (University of Texas at Austin); Lina Necib (Massachusetts Institute of Technology); Daniel Angles-Alcazar (Northwestern University); Coral Wheeler (California Institute of Technology); Christopher Hayward (California Institute of Technology); Andrew Wetzel (University of California, Davis); Claude-Andre Faucher-Giguere (Northwestern University); Eliot Quataert (University of California, Berkeley)

Field of Science: Extragalactic Astronomy and Cosmology

Abstract:
The most important fundamental and unsolved problems in our understanding of the large-scale structure of the Universe, the origins of galaxies and stars, and the nature of dark matter revolve around the interplay between wildly non-linear, dynamical processes on small and large scales. While gravity acts "top down" to drive structure formation and collapse material into galaxies, stars and black holes, those stars and accreting black holes (in the form of quasars) emit copious radiation and drive winds from their vicinity, and massive stars explode as supernovae. These processes feed back on the large-scale environment to drive galactic outflows and completely re-shape the environment, subsequent generations of star and black hole formation, and the dark matter structure around galaxies. Our Feedback In Realistic Environments (FIRE) collaboration represents a theory network across astrophysical institutions combining expertise in a variety of crucial fields: stellar evolution, high-energy astrophysics, interstellar plasma physics, black hole accretion, star formation, cosmology and large-scale structure, in order to synthesize the crucial physics into a new generation of simulations that can capture many of these processes in a fully-cosmological context for the first time. The simulations proposed will allow us to explore and constrain the fundamental physics shaping these phenomena, make new predictions for a host of new astrophysical observations and facilities, and develop new understanding of the behaviors of the Universe on a tremendous range of scales.

Type: Renewal LSCP

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

Principal Investigator: Saul A. Teukolsky (Cornell University)
Co-Investigators: Mark Scheel (California Institute of Technology); Aaron Zimmerman (University of Texas at Austin); Francois Foucart (University of New Hampshire); Matthew Duez (Washington State University); Geoffrey Lovelace (California State University, Fullerton)

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.