Type: Renewal PW

Title: Computational Study of Astrophysical Plasmas

Principal Investigator: Kenichi Nishikawa (Alabama A&M University (AAMU))
Co-Investigators: Jacek Niemiec (Institute of Nuclear Physics · Department of Mathematical Physics and Theoretical Astrophysics); Christoph Koehn (Technical University of Denmark (Danmarks Tekniske Universitet)); Athina Meli (North Carolina Agricultural and Technical State University (NCAT) (A&T)); Michael Watson (Lipscomb University); Kouichi Hirotani (Academia Sinica, Institute of Astronomy & Astrophysics); Nicholas MacDonald (Max-Planck-Institut für Radioastronomie,); Yosuke Mizuno (Goethe University Frankfurt); Yosuke Mizuno (Shanghai Jiao Tong University); Ioana Dutan (Astronomical Institute of the Romanian Academy (Institutul Astronomic al Academiei Romne))

Field of Science: Extragalactic Astronomy and Cosmology

Abstract:

Active Galactic Nuclei and Gamma-ray Bursts are hosts of astrophysical relativistic jets where intensive particle (cosmic-ray) acceleration occurs via various mechanisms. Astrophysical jets are dynamically magnetized plasma flows that are launched most likely in regions where the Poynting (magnetic field energy) flux dominates over the particle flux. We will investigate how the Poynting flux of relativistic jets dissipates into kinetic energy to accelerate particles rapidly by studying the interaction of the particles with the immediate plasma environment on the microscopic scales. We will also investigate synthetic spectra emitted from relativistic jets, polarity images through radiative transfer, particle acceleration related to electric discharges and the dynamics of black holes. It has recently been shown with our Particle-in-Cell (PIC) simulations that relativistic jets of different particle components (electron-ion, electron-proton or electron-positron) excite instabilities which drive particle acceleration. This proposed project will aim to employ advanced computational tools to investigate complex astrophysical phenomena involving propagating relativistic jets which interact with their environment in order to study potential acceleration mechanisms. Our research team employs new computational tools to investigate the important topics of magnetic reconnection, nonlinearly generated turbulence, and associated particle acceleration in collisionless astrophysical relativistic plasmas. Simulations of relativistic jets injected into ambient plasmas with helical (toroidal) magnetic fields have demonstrated possible signatures of magnetic reconnection and nonlinearly generated turbulence. Based on our promising and published results using Comet, Bridges and Pleiades, and very recently Frontera as well, this research project will further explore relativistic particle acceleration associated with magnetic reconnection in jets with helical magnetic fields including non-linearly generated turbulence and other research topics using Frontera. There is a need to explore these processes in more realistic environments, with the best computer power.

Therefore, our aimed systematic study in a much more realistic astrophysical context will elucidate the important processes and mechanisms of reconnection and particle acceleration in active galactic nuclei and gamma-ray burst jets. In this research effort, we will analyze the evolution of jets through the use of our extensive visualization tools which provide the location of reconnection and its associated phenomena such as particle acceleration. Our simulation results and published work show complicated structures of jet

evolution due to combined kinetic and kink-like instabilities in the relativistic jets containing helical magnetic fields.

The magnetic field structures generated by kinetic and kink-like instabilities determine where and when reconnection occurs. More computational power using Frontera will help our team to make further progresses with our simulations. Often explosive in nature, magnetic reconnection enables the rapid release of magnetic energy stored in the jets. Our overall goal is to integrate interdisciplinary scientific aspects to

study basic plasma physics and theoretical astrophysics and to develop new numerical methods to simulate the microphysical processes responsible for reconnection, turbulence, and high-energy particle acceleration. The proposed research approach is unique and more realistic. This research will provide new insights on relativistic jet physics, on the associated particle acceleration, and will ultimately assist into understanding better the origin and the acceleration of very high energy cosmic-rays, and the emission from relativistic sources. It has also the potential to developing new numerical methods to tackle the microphysical plasma processes. On human capital this project will (1)}engage students in interdisciplinary research; (2) inspire students to think of more ways to apply their physics knowledge and interdisciplinary skills to promote societal benefit; (3) improve the student enrollment in a physics program at two HBCU Universities (NCAT and AAMU), therefore contribute to diversity in the physics community. Animations of the 3D evolution of relativistic jets with kinetic processes will be created, and be presented, not only at public and university scientific and technology meetings but also use them for public outreach, high school outreach with presentations at the NCA&T Planetarium in Greensboro and the Space and Rocket Center, and Planetarium in Huntsville.

Type: New PW

Title: Kinetic simulations of collisionless shocks: large scale shocks evolution and particle acceleration

Principal Investigator: Anatoly Spitkovsky (Princeton University)
Co-Investigators: Vladimir Zekovic (Princeton University)

Field of Science: Astronomical Sciences

Abstract:

Collisionless shocks are thought to be nature's most efficient particle accelerators. Driven by exploding stars observed as supernovae (SNe) and their remnants (SNRs), or by gamma-ray bursts (GRBs) and the jets of active galactic nuclei (AGNs), collisionless shocks are capable of producing the highest-energy cosmic rays (CRs). To understand the acceleration of CRs at collisionless shocks, considerable effort is being put into both, numerical simulations and analytic modeling. Although the analytic models have an advantage over simulations because of their simplicity, they entirely depend on the prescribed mechanism of generation of magnetic turbulence.

Conversely, results from recent kinetic simulations of high Mach number shocks indicate that the short large amplitude magnetic structures (SLAMS) can significantly alter the shock processes. Quasi-stationarity in the interplay between the evolution of the upstream plasma turbulence and particle acceleration is challenging to achieve with kinetic simulations. Tracing the entire shock evolution is limited by the available computational resources.

To understand the role of SLAMS in the shock evolution and particle acceleration, we propose to run kinetic simulations of non-relativistic collisionless shocks using a massively-parallel and multi-dimensional relativistic Particle-In-Cell (PIC) code, Tristan-MP. Motivated by our recent findings about SLAMS, we will investigate the following topics:

1) SLAMS formation and their influence on the structure of evolving shocks where accelerated CRs are being injected at the shock location,

2) injection and acceleration of ions and electrons at high Mach number shocks with the developed upstream turbulence.

This campaign will provide an unprecedented understanding of the non-linear and non-thermal phenomenology of a wide range of astrophysical objects such as SNRs, galaxy clusters, radio SNe, AGNs, and GRBs. It will contribute shock acceleration efficiency measurements to bridge the scale gap between simulations and observations.

Type: New PW

Title: Fundamental and Applied Studies of Turbulent Flow Phenomena in the Environment Computational Research Proposal

Principal Investigator: Marco Giometto (Columbia University in the City of New York (Columbia University))
Co-Investigators: Atharva Sathe (Columbia University in the City of New York (Columbia University))

Field of Science: Meteorology

Abstract:

Land-atmosphere exchange processes have a direct impact on weather and climate variability, thus affecting human health, water resource management, ecological and hydrological processes and their concomitant services. Turbulent flow phenomena play a major role in governing the exchange of energy, momentum and mass between the earth and the atmosphere. Motivated by the need to better predict weather and dispersion processes where people live, the past decades have seen substantial efforts devoted to the study of turbulence within and above urban canopies, but the current knowledge still lags behind the actual needs. The vast majority of studies have relied on the open channel flow over arrays of surface-mounted cuboids setup to study these flow systems, which is a convenient surrogate of the urban boundary layer. This approach proved useful to advance the current understanding of how surface morphology affects turbulence statistics, but because these simulations are an approximation of reality, special care is often required in the setup of the computational model, in order to obtain a faithful representation of the desired physical processes. Many-a-times, findings are not in agreement with well established theories, experimental results, and with results from related numerical investigations. This is often the result of a poorly designed computational domain. Oftentimes, the choice of the numerical domain is influenced by a need to accommodate repeating units of surface patterns within the bounds of the domain, which results in arbitrary domain size with different aspect ratios. With this study, we aim to provide a set of recommendations that will help researchers tailor the domain size to their specific application, which will balance the predictive accuracy and computational cost of the simulations. Specifically, we aim at analyzing the impact of three length scales associated with the numerical domain on turbulent flow statistics.

Type: Renewal PW

Title: Machine-Learning-accelerated regional-scale inverse modeling of landslide hazards

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

Field of Science: Advanced Scientific Computing

Abstract:

Landslides cause billions of dollars in damages and thousands of casualties every year, the majority of which are associated with long run-out distances. The Graph Network Simulator (GNS) accelerated regional-scale inverse modeling of landslide hazards will be the first method to extract material properties using inverse analysis at a regional-scale, which has been impossible prior to this work. The GNS surrogate can reasonably predict the complex flow dynamics at orders of magnitude faster than current numerical simulators. GNS is also generalizable and supports upscaling, which allows us to train the model on high-resolution small-scale trajectories and then use the trained GNS to predict regional-scale landslide simulations. Regional-scale visualization is challenging. We employ a GNS oracle to identify critical regions in the simulations, before the occur, and use in situ visualization in MPM to render regional- scale dynamics. By providing advanced, realistic in situ visualization and rendering of geo-hazards, officials would have a more visceral sense of the potential danger for loss and take actions to mitigate it.

Type: New PW

Title: Acoustic Pulsation for Heat Transfer Enhancement in Roughened Heat Exchangers

Principal Investigator: Iman Rahbari (University of Southern California (USC))
Co-Investigators:

Field of Science: Thermal Systems

Abstract:

The demand for high power-density compact propulsion systems has been steadily increasing in the past few decades and the advent of hybrid and electric power generation systems has only intensified the need for more efficient, and high-capacity, compact heat exchangers. There are several approaches to improve the thermal capacity of the current heat exchangers. One recent technique, is using the acoustic pulsations, where under specific conditions, improves the heat transfer on flat surfaces while adding minimal drag penalties. The other technique involves incorporating ribs in the flow passage which can dramatically increase the heat exchange rate, however, introduces significant pressure drag losses in the system, due to large recirculation bubbles, acting as a heat shield, created by the rib in the passage.

The present project has two main objectives. The first objective focuses on using Large-Eddy Simulations to assess the mechanism of flow-generated noise over an open cavity to create the acoustic pulsation required for heat transfer enhancement in a passage. The second section is geared towards improving the heat transfer in flow over a ribbed surface by applying acoustic pulsations. The optimal frequency and location for applying the acoustic excitation is determined via a three-step methodology based on the Linearized Navier-Stokes Equations. Large-Eddy Simulations will be used to study the flow field, with and without the excitations, to assess the effectivity of the control mechanism.

Finally, the results in all cases will be compared against the lower-fidelity Reynolds Averaged Navier-Stokes (RANS) simulations to determine these model's accuracy in such complex flow configurations. A database with the post-processed LES and RANS results will be created and released publicly.

Type: New PW

Title: Coupled Interaction of High-Speed Boundary Layer Transition and Ablation

Principal Investigator: Christoph Brehm (University of Maryland College Park (University of Maryland) (UM) (UMCP))
Co-Investigators:

Field of Science: Fluid, Particulate, and Hydraulic Systems

Abstract:

Performance of hypersonic flight vehicles is intricately dependent on several physical mechanisms such as the process of boundary layer transition, the effects of roughness on the transition process, the ablation of the surface, interaction of shocks, chemical reactions, etc. that are encountered in the extreme conditions associated with hypersonic flight. The accurate prediction of these relevant phenomena is extremely important to reduce design margins and system uncertainties to provide optimal design parameters for these systems. The proposed research effort aims to tackle the challenges associated with hypersonic flight using high-fidelity numerical simulations to investigate the effects of roughness on the different stages of boundary layer transition. First of its kind fully-coupled simulations will also be performed to analyze the characteristics of boundary layer transition with an ablative surface.

Type: Renewal PW

Title: Prediction of functional defect properties in materials for clean energy applications

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

Field of Science: Materials Research

Abstract:

This project continues and expands our previous project with Frontera allocation. Our group, the Laboratory for Electrochemical Interfaces at the Massachusetts Institute of Technology, conducts significant computational and experimental work devoted to 1) applying electrochemical methods to achieve superconducting state, 2) improving the durability and performance of solid oxide fuel cells (SOFCs), and 3) designing fast proton conductors for the SOFC and electrochemical random-access memory (ECRAM) devices. The requested Frontera allocation will support the computational team working on the proposed projects. In our calculations, we will primarily exploit first-principles VASP and Quantum ESPRESSO packages, as well as LAMMPS code.

Type: Renewal PW

Title: First-Principles Studies of Excited-State Phenomena in Quasi-Two-Dimensional Materials

Principal Investigator: Felipe Jornada (Stanford University)
Co-Investigators:

Field of Science: Materials Research

Abstract:

This is a renewal proposal for a Pathways allocation at Frontera. These resources will be used to explore new domains of research and scale our current computational methodologies in thefield of computational materials science. Our proposal utilizes parameter-free methods and massively parallel computer calculations to understand the excited-state properties of novel 2D materials. We are particularly interested in understanding the interplay between structural properties and electronic and optical excitations in such 2D systems. Specifically, our proposal addresses the general trends arising when two monolayer materials are stacked on top of each other, forming moiré potentials that localize electrons and excitons. We also seek to understand the role of lattice vibrations (phonons) in the scattering of excitons in such systems. Finally, we also seek to understand the nature of magnetic defects in 2D materials, and their experimental signature. Alltogether, our proposal addresses challenging scientific problems which have not yet been accessible with the level of prediction possible with state-of-the-art first-principles computational approaches. It also addresses emerging questions in the field of atomically thin materials, and has the possibility of impacting future photovoltaic materials and quantum science.

Type: New PW

Title: Coupling between phonons and correlated electronic excitations from first-principles GW-based approaches

Principal Investigator: Zhenglu Li (University of Southern California (USC))
Co-Investigators:

Field of Science: Materials Research; Condensed Matter Physics

Abstract:

Interaction between electrons and phonons, i.e., electron-phonon (e-ph) coupling, plays a dominant role in a wide spectrum of phenomena in condensed matter physics and materials physics, such as phonon-mediated superconductivity, charge-density wave, electrical and thermal transport, phonon-assisted optical absorption, to name a few. Predictive first-principles, or ab initio, computation for accurate descriptions of e-ph coupling provides significant insights and understanding in relevant novel phenomena and new physics. Major computational challenges arise 1) when studying e-ph coupling in complex materials where many-electron correlation effects become strong, and 2) when correlated multiparticle excitations such as excitons couple to phonons, particularly in the nonequilibrium fashion. The standard and most prevalent first-principles approaches – typically based on the density functional theory (DFT) – often fail to accurately capture the correlation effects in e-ph coupling and the excitonic (correlated electron-hole) effects in both equilibrium and nonequilibrium.

This Pathways proposal addresses the challenges mentioned above using advanced GW-based methodologies that capture the many-electron correlation effects beyond DFT. This proposal focuses on 1) applications of the cutting-edge GWPT method to study e-ph coupling in several strongly correlated materials at the many-electron level, and 2) the development of the new ab initio time-dependent adiabatic GW with electron-phonon coupling methodology, including its implementation and validations.

Type: New PW

Title: Scalable tools for high-frequency wave-propagation with applications in optical fiber modeling

Principal Investigator: Leszek Demkowicz (University of Texas at Austin (UT) (UT Austin))
Co-Investigators: Stefan Henneking (University of Texas at Austin (UT) (UT Austin))

Field of Science: Computational Mathematics

Abstract:

We request 103,000 service units (SUs) to support our NSF-funded project on simulation of optical fiber amplifiers and development of the supporting hp3D finite element library and advanced solvers. Optical fiber amplifiers are of interest in a number of applications including telecommunications, manufacturing, medicine, and military defense; however, power scaling of fiber amplifiers is limited by a complex trade-space of nonlinear effects that arise during high-power operation. Modeling and simulation can inform the design of increasingly performant fiber amplifiers, but accurate and reliable simulation of high-power operation has proved challenging for prevalent models. As part of our NSF Office of Advanced Cyberinfrastructure funded project, we are working to develop versatile and verifiably accurate computational tools for simulation of nonlinear effects in optical fiber amplifiers. The computational tools developed in this work enable large-scale simulation of high-fidelity models that can be used in the fundamental study of fiber nonlinearities and for quantifying the limitations of prevalent models.

The requested allocation will support high-fidelity simulation of nonlinear effects in optical fiber amplifiers, establishment of benchmarks to verify simplified fiber models, and continued development of tools for optical fiber modeling. We anticipate a number of broader impacts from this project: (1) High-fidelity modeling of limiting phenomena in optical fibers will provide insight into limitations of lower fidelity models and help advance fiber-optic technology; and (2) Tools developed in this project will enable simulation of high-frequency wave-propagation at an unprecedented scale; additional applications of these tools include RF-heating in tokamak devices for nuclear fusion research, seismic inversion for resource exploration, and nondestructive testing of reusable structures.

Type: New PW

Title: Development of a Viscous Numerical Model for Predicting Unsteady Turbulent Flow over Propellers

Principal Investigator: Spyridon Kinnas (University of Texas at Austin (UT) (UT Austin))
Co-Investigators:

Field of Science: Engineering Infrastructure Development

Abstract:

A viscous vorticity numerical solver for predicting 3-D turbulent flows around hydrofoils and propellers will be developed. The proposed numerical solver has been parallelized using MPI/OpenMP hybrid strategy. The presented method will be applied on three geometries: a 3-D hydrofoil between slip walls, a 3-D rectangular wing and a propeller. Experiments will be carried out with respect to grid independence tests, time-step independence tests and parameter studies. The estimated total computational plan is 180,000 SU.

Type: Renewal PW

Title: Mini-Protein Binder Frontera Pathways Application

Principal Investigator: David Baker (University of Washington)
Co-Investigators:

Field of Science: Biochemistry and Molecular Structure and Function

Abstract:

Access to the Frontera system has allowed us to rapidly develop a series of mini-protein binders to a variety of natural protein targets. These designed binders may serve as starting points for future therapeutics and diagnostics. To date, potent mini-protein therapeutics have been developed for the SARS-CoV-2 virus, MERS coronavirus, and Influenza Group B2 virus. Additionally, binders have been designed and experimentally characterized for 23 different cellular receptors which will have immediate applications for targeted cancer therapeutics as well as therapeutics that function by activating or deactivating these receptors.

Type: Renewal 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:

As the time-scales on which we can observe electron behavior steadily decrease, there is a great need for theoretical support, and also prediction, for the growing number of ultrafast experiments that have become possible. These experiments are very challenging, and without theoretical comparison it is hard to rule out systematic errors with confidence. Furthermore, theoretical guidance is often used to focus the parameter space in which to actually perform the measurements. While calculations on supercomputers are undoubtedly expensive, the benefits of carrying them out in advance of the measurements for a range of experimental parameters can be very beneficial when compared to the cost associated with beamtime, for example, on an X-ray Free-Electron Laser (XFEL). In this Pathways award we seek to perform large-scale calculations which will help to quantify how important semi-relativistic effects are when determining the response of atoms to laser light, explore novel schemes to measure the time-delay associated with ionizing an electron, and compute cross-sections for electron collisions with singly-ionized neon.

Type: Renewal PW

Title: Renewal for "Shedding light on light dark matter candidates in strong gravity environments"

Principal Investigator: Thomas Helfer (Johns Hopkins University)
Co-Investigators: Emanuele Berti (Johns Hopkins University)

Field of Science: Gravitational Physics

Abstract:

Gravitational waves (GWs) were first predicted by Einstein in 1916 as a consequence of general relativity. Their recent detection by the LIGO and Virgo observatories has opened up a new window on the Universe. This window led to new probes of the nature of black holes (BHs) and to a wealth of astrophysical findings, challenging our understanding of stellar evolution and binary population models. However, one of the most exciting and as yet unrealized prospects is to use GWs to shed light on the nature of the dark matter (DM) component of the Universe's energy budget. In the absence of direct couplings between DM and baryonic matter, this may be the only way to probe fundamental characteristics of DM - i.e. mass, spin and strength of self-interactions. With WIMPs proving elusive in direct detection experiments, there has been a resurgence in interest in other DM candidates, particularly those with lower masses ($m < eV$). Promising alternatives include the QCD axion, axion-like particles (ALPs) motivated by string theory compactifications, and ``dark photons''. At low masses, the high occupation numbers of the DM in halos implies a bosonic particle, and also admits a description of the DM fluid as a classical field obeying wave-like equations.

In this project we aim to use state of the art numerical relativity (NR) simulations to better understand the DM environment around BHs and identify distinct GW signatures particular to this light, wave-like DM. In particular, we focus on addressing the following specific questions:
- Can environmental effects or self-interaction in the DM fluid destabilize the superradiant instability of light particles (described further below), leading to GW bursts or other observable consequences?
-Does the dynamical formation of DM spikes occur for light DM candidates during an astrophysical collapse to a BH, and might these environments have an impact on the the binary merger signal?
This work is relevant for both LIGO/Virgo/KAGRA searches and for the upcoming LISA mission. Earth- and space-based detectors will probe different BH masses, and therefore also different DM masses.

A secondary goal of this pathways allocation is to test the limits of our open source NR code, GRChombo, at scale, for larger problem sizes.

Type: New PW

Title: The pathway to heavy quarkonium thermalization – Open quantum systems with the quantum trajectories method

Principal Investigator: Michael Strickland (Kent State University)
Co-Investigators:

Field of Science: Nuclear Physics

Abstract:

The strong suppression of bound states of heavy quarks and anti-quarks in relativistic heavy-ion collisions is a smoking gun for the production of a deconfined quark-gluon plasma (QGP). The experimental effort to produce and study the QGP is one of the most important international high energy physics efforts in decades, with experiments taking place both in US at Brookhaven National Laboratory and in Europe at CERN. Recently, there has been a paradigm shift in our understanding of the suppression of such state based on the application of effective field theory (EFT) methods and the framework of open quantum systems (OQS). Within this context it is now possible to make experimentally verifiable predictions for the level of suppression at various collision energies, with the EFT+OQS methods providing an excellent description of the data. Despite this phenomenological success, an open question remains as to what is the precise time scale for thermalization of bottomonium (b and bar quark bound states) is. Unfortunately, this time scale is much longer than the lifetime of the QGP formed in relativistic heavy-ion collisions and, as a result, in order to carry out numerical studies of this question, a significant amount of computing time is required. Luckily, the codes necessary for this investigation are already written and released as public open-source packages. We are now at the stage where we can fully leverage existing large scale computing facilities in order to answer this question definitively.

Type: New PW

Title: Numerical Relativity simulations for strong-field tests of gravity

Principal Investigator: Helvi Witek (University of Illinois Urbana-Champaign (UIUC) (University of Illinois) (U of I))
Co-Investigators: Alexandru Dima (University of Illinois Urbana-Champaign (UIUC) (University of Illinois) (U of I))

Field of Science: Gravitational Physics

Abstract:

The first direct observation of a gravitational wave (GW) emitted by a merging black hole (BH) binary by NSF's Laser Interferometer Gravitational Wave Observatory (LIGO) in 2015 [1] marked the beginning of a new era of astronomy. Heralded as the "discovery of the century," it opened up an unprecedented discovery space in astronomy, gravitational physics, cosmology and quantum gravity and was rewarded with the Nobel Prize in 2017. Since then, more than 90 GW events from colliding BHs or neutron stars have been de- tected. These observations allow us to decode the sources' fundamental properties, such as their masses and spins, determine their cosmological origin and, of particular interest to this project, provide a unique avenue for probing Einstein's theory of General Relativity (GR) in a regime inaccessible via other tests.

In this project we will perform numerical relativity simulations of single and binary BHs in quadratic gravity. We will perform a comprehensive parameter study that forms the foundation for future beyond-GR waveform catalogs and theory-specific tests of gravity. BHs in these theories have a richer phenomenology than their counterparts in GR, as they acquire scalar charges or "hair". Placed in a binary, these charges produce scalar radiation – much like oscillating electric charges produce electromagnetic radiation. We will then utilise these simulations to develop the very first model of the scalar mode, a fundamental prediction in several classes of beyond-GR theories and absent in GR. After the scalar mode, we will extend the work to tensorial modes.

Type: Renewal 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 (RIT))
Co-Investigators: Scott Noble (National Aeronautics and Space Administration (NASA)); Julian Krolik (Johns Hopkins University); Yosef Zlochower (Rochester Institute of Technology (RIT))

Field of Science: Gravitational Physics; Astronomical Sciences

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: Data-driven, biologically constrained computational models of in-vivo and in-vitro neural information processing

Principal Investigator: Mattia Gazzola (University of Illinois Urbana-Champaign (UIUC) (University of Illinois) (U of I))
Co-Investigators: Ivan Soltesz (University of California Irvine (UCI))

Field of Science: Neuroscience Biology

Abstract:

Computational biophysical models of neural circuits provide effective tools to study the neurophysiological correlates of information processing in the brain. However, there are often significant gaps in the physiological, morphological and anatomical data of brain regions, which then make it difficult to quantify to what degree models represent the biological system.

We aim to reduce this gap by validating large-scale simulation of \invitro{} (grown in the lab) living neural networks, which are highly accessible experimentally, and specific brain regions for which extensive characterizations exist. Supported by an NSF Expedition in Computing (\#2123781) on the development of \invitro{} neural computing substrates, and by an NIH BRAIN initiative (\#U19-NS104590) on hippocampal information processing, we plan to develop biophysically realistic neural models and use them to investigate the complex dynamics of millions of connected neural elements and explore their information processing capabilities.

Type: Renewal LSCP

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

Principal Investigator: Tulika Bose (University of Wisconsin Madison (UW Madison))
Co-Investigators: Tulika Bose (University of Wisconsin Madison (UW Madison)); Mia Liu (Purdue University)

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. 1070 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 standard pp collision events, which would be about 4% of the total simulated data set planned by CMS for the year beginning March 1, 2023. 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.