Type: Renewal LRAC

Title: 3-D Stellar Hydrodynamics of Convective Boundary Mixing and Shell Mergers in Massive Stars

Principal Investigator: Paul Woodward (University of Minnesota (UM))
Co-Investigators:

Field of Science: Stellar Astronomy and Astrophysics

Abstract:

We are using detailed 3-D stellar hydrodynamics simulations to improve our understanding and predictive capability of material mixing at the boundaries of convection zones in stars and of its consequences for stellar evolution and nucleosynthesis. Mixing length theory (MLT) enables us to model in 1D the effects of convection, an inherently 3-D process, so that we can evolve a model star through the millions or billions of years of its life in an affordable computation. The MLT description does very well in the main volume of a convection zone, but it has considerable diffi¬culty describing the flow near convective boundaries. This is where material from just outside a convec¬tion zone can become incorporated into it and then carried significant distances radially in the star. The material transported in this way can then participate in nuclear reactions that can alter the course of the star's evolution and/or alter significantly its production of heavy elements. Under special circumstances, such as the hydrogen ingestion flash, the energy release from burning fuel brought into a convection zone from the convective boundary can be so great that the local structure of the star is disrupted. To follow the behavior in such cases, we must perform 3-D simulations.

In our work, we identify brief intervals in the evolution of stars when convective boundary mixing can have very important consequences. By simulating the mixing and its effects in 3D for those brief intervals and using our results to inform the 1-D models that can be implemented in stellar evolution codes, we try to assure that the 3-D simulation work that we do has a maximum impact. We are focussing on massive stars, and in particular upon the interaction and possible merger of nuclear burning shells, with their associated convection zones, that are separated by only very thin layers of stably stratified material. A key point about these events is that the energy release from nuclear burning of convectively mixed fuels can have dramatic feedback into the hydrodynamic flow. This requires both high grid resolution as well as a sufficient number of nuclear species to simulate the hydro¬dynamic flow and the nuclear energy generation simultaneously with high accuracy. The outcomes of the resulting detailed 3-D simulations are used to validate 1-D mixing models and parameter values from first principles of multi¬fluid hydro-dynamics. For brief episodes, such as flash phenomena driven by unstable or overstable nuclear burning in 3D, we can hope to simulate the entire episode in 3D. How the star evolves through these brief convective-reactive episodes has a profound impact upon the abundances it produces. For massive stars, shell merger events shortly before the core collapses can affect the star's symmetry and hence its explodability. As participants of the NSF JINA-CEE Physics Frontier Center and of its successor project pending DoE approval, we explore the ramifications for nucleosynthesis of our simulations.

This project also involves using our detailed 3-D simulations of convective boundary mixing to improve 1-D convection models for use in 1-D stellar evloution codes, particularly by improving their treatment of convective penetration and convective boundary mixing. Our 3-D simulations also address the action of internal gravity waves excited at the convective boundary for material and angular momentum transport in

the stably stratified envelope above the convective boundary.

Type: Renewal LRAC

Title: First Applications of Enzo-E to Frontier Problems in Cosmology

Principal Investigator: Michael Norman (University of California San Diego (UCSD) (UC San Diego))
Co-Investigators: Brian O'Shea (Michigan State University (MSU)); Greg L. Bryan (Columbia University in the City of New York (Columbia University)); John Wise (Georgia Institute of Technology); James Bordner (University of California San Diego (UCSD) (UC San Diego))

Field of Science: Extragalactic Astronomy and Cosmology

Abstract:

Enzo-E is the newly developed extreme-scale fork of the popular Enzo AMR code for astrophysics and cosmology simulations. The four-institution Enzo-E collaboration requests Frontera resources for the first science applications of Enzo-E. Three independent subprojects will carry out frontier simulations of the birth of galaxies and supermassive black holes, the entrainment physics of galactic winds, and early chemical enrichment of the intergalactic medium by Population III and II stars.

Type: Renewal LRAC

Title: Multi-scale Dynamics of Kinetic Turbulence and Dynamo in Collisionless Astrophysical Plasmas

Principal Investigator: Matthew Kunz (Princeton University)
Co-Investigators: Muni Zhou (Princeton University); Jonathan Squire (University of Otago (Te Whare Wnanga o Otgo)); Archie Bott (Princeton University)

Field of Science: Astronomical Sciences

Abstract:

This Frontera renewal allocation request focuses on the multi-scale dynamics of kinetic turbulence and dynamo in collisionless space and astrophysical plasmas. We propose to study three applications of this physics in particular. First, we will elucidate the thermodynamic and electromagnetic consequences of imbalanced Alfvénic turbulence in a collisionless and multi-ion plasma, making a direct connection to several notable features discovered by Parker Solar Probe and other heliospheric spacecraft. Second, we will continue our investigations into the origin and amplification of cosmic magnetic fields, this time paying particular attention to how seed magnetic fields generated self-consistently by plasma-kinetic effects can be stretched and amplified explosively by turbulent motions. Finally, we will continue our pioneering study of kinetic turbulence in high-beta plasmas, emphasizing the interplay between microscale plasma physics and macroscale fluid dynamics and how it determines the differential heating of the plasma particles. This NSF-funded research makes use of our aggressively optimized, massively parallel, hybrid-kinetic particle-in-cell code Pegasus++. This code demonstrates excellent single-core performance and excellent weak scaling on Frontera, and has contributed to more than a dozen publications in a variety of high-profile journals. The continued application of this novel code to frontier topics in plasma astrophysics on leadership-class facilities opens up new pathways for understanding the heating and structure of the solar wind, the origin of cosmic magnetic fields, and the thermodynamic stability of the intracluster medium of galaxy clusters.

Type: Renewal LRAC

Title: Renewal: TACC Frontera and super resolution cosmological simulations of galaxies and quasars

Principal Investigator: Tiziana DiMatteo (Carnegie Mellon University (CMU))
Co-Investigators: Anson D'Aloisio (University of California Riverside (UCR)); Yueying Ni (Harvard University); Rupert Croft (Carnegie Mellon University (CMU)); Simeon Bird (University of California Riverside (UCR))

Field of Science: Extragalactic Astronomy and Cosmology

Abstract:

As telescopes become more powerful, data on galaxies, quasars and the matter in intergalactic space becomes both more detailed and wide-ranging. Our cosmological simulations must adapt, so that even with supercomputers we are forced to decide whether to maximize either resolution, or volume, or else compromise on both. With Frontera, we are in the midst of a program to overcome these limitations. We have been running a newly optimized version of our cosmological hydrodynamics code, MP-Gadget, successfully at extreme scale on Frontera. We have run "Astrid", the largest cosmological simulation ever to reach redshift z= 2.3, the era relevant for Webb Telescope observations. In concert we have developed methods that leverage techniques from the AI revolution, and make "super resolution" simulations possible. Our hybrid approach offloads compute-intensive parts of our simulations to Neural Networks (NN). With this renewal, we will extend Astrid to later times, expecting to reach the epoch of galaxy cluster formation, when dark energy starts to dominate the universe, at redshifts z~1. We will continue to develop our AI super resolution techniques, applying them to hydrodynamic simulations for the first time. With this combined approach we will address a variety of science topics including predicting gravitational waves from supermassive black hole mergers, gravitational lensing of intergalactic gas clouds, and properties of extreme galaxies and quasars at high resolution.

Type: Renewal LRAC

Title: STARFORGE: Simulating star formation with realistic physics and feedback

Principal Investigator: Michael Grudic (Carnegie Institution for Science (Carnegie Science))
Co-Investigators: David Guszejnov (University of Texas at Austin (UT) (UT Austin)); Anna Rosen (University of California San Diego (UCSD) (UC San Diego)); Stella Offner (University of Texas at Austin (UT) (UT Austin))

Field of Science: Astronomical Sciences

Abstract:

Numerical simulations of star-forming giant molecular clouds (GMCs) can serve as powerful virtual laboratories for studying the many different processes involved in star formation (SF), which are subject to considerable theoretical uncertainty. We will use the newly-developed STARFORGE framework to perform a large parameter study of SF simulations to account for essentially all physical mechanisms thought to be important in SF, including gravity, N-body dynamics, radiation, magnetic fields, cooling and chemistry, and all important stellar feedback mechanisms (jets, radiation, winds, and supernovae). These will be the most physically-realistic SF simulations to date, and will allow us to attack major open theoretical questions about SF physics (including the stellar initial mass function). We will also be able to disentangle the presently-uncertain effects of each mechanism, and to interpret ambiguous observational data.

Type: Renewal LRAC

Title: Long-term 3D Core-Collapse Supernova Simulations

Principal Investigator: Adam Burrows (Princeton University)
Co-Investigators: Adam Burrows (Princeton University); Matthew Coleman (Princeton University); Tianshu Wang (Princeton University)

Field of Science: Stellar Astronomy and Astrophysics

Abstract:

Complexity has paced progress on the multi-physics, multi-dimensional, and multi-decade puzzle of the mechanism of supernova explosions. However, modern theory, building on decades of progress with the multitude of issues, inputs, and physics questions, is on the cusp of breakthrough. State-of-the-art simulations from many groups now evince explosions via the neutrino mechanism with roughly the correct general character and properties. However, we have yet to achieve a comprehensive, credible, and detailed explanation of explosion energy, neutron-star mass, nucleosynthesis, and morphology across the progenitor continuum. This LRAC proposal has been constructed to 1) build on our recent palpable progress, 2) capture this pivotal moment in theoretical astrophysics when codes and resources are aligning, and 3) help erect a standard model for core-collapse supernova explosions.

Type: Renewal LRAC

Title: Numerical Simulations of Interstellar Turbulence

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

Field of Science: Extragalactic Astronomy and Cosmology

Abstract:

The main science theme for this LRAC 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: Renewal LRAC

Title: A Multi-Fidelity Cosmological Emulator in 11 Dimensions for the Roman Space Telescope

Principal Investigator: Simeon Bird (University of California Riverside (UCR))
Co-Investigators:

Field of Science: Extragalactic Astronomy and Cosmology

Abstract:

The main focus of this renewal will be to generate a multi-fidelity emulator in 11 dimensions for the Roman Space Telescope. Several hundred dark matter simulations with different cosmological parameters will be run to redshift zero using our newly improved gravity implementation. We will continue to improve our multi-fidelity emulator for Lyman alpha cosmology, from the previous LRAC by adding 1 extra high resolution simulation. Finally we will explore baryonic corrections to the power spectrum using small test simulations.

Type: Renewal LRAC

Title: Simulations of reconnection-powered flares in magnetospheres of magnetars, binary neutron stars and black holes.

Principal Investigator: Alexander Philippov (University of Maryland College Park (University of Maryland) (UM) (UMCP))
Co-Investigators: Bart Ripperda (Simons Foundation); Elias Most (Princeton University)

Field of Science: Astronomical Sciences

Abstract:

Event Horizon Telescope observations of polarized radio emission show that accretion flows around supermassive black holes (BHs) are likely to be in a particular scenario uncovered by general-relativistic magnetohydrodynamics (GRMHD) simulations, the magnetically arrested (MAD) state. The plasma accreting onto main EHT sources, black holes in our own galaxy, Sgr A*, and M87, is collisionless, which makes the simplifying assumptions of commonly employed GRMHD formally inapplicable. In this proposal, by directly comparing 2D kinetic models and fluid simulations, we will uncover whether fluid approximation leads to consistent results for MAD accretion flows. Violent reconnection might occur in merging BH--neutron star (NS) systems, where magnetic flux tubes connecting NS to the BH can undergo dynamic eruptions. Emission of coherent radio waves, and thus non-repeating fast radio bursts (FRBs), will likely be associated with current sheets formed during these events, necessitating the fully three-dimensional (3D) studies of transient NS-BH magnetospheres. In this proposal, using global simulations of these dynamic environments we will identify reconnection events. In addition, we will investigate their coherent emission using first-principles 3D kinetic simulations.

Type: Renewal LRAC

Title: Interplay of large-scale instabilities and kinetic plasma processes in relativistic jets and accretion disks of black holes

Principal Investigator: Gregory Werner (University of Colorado Boulder)
Co-Investigators: Yuran Chen (University of Colorado Boulder); Mitchell Begelman (University of Colorado); Vladimir Zhdankin (Center for Computational Astrophysics, Flatirons Institute); Dmitri Uzdensky (University of Colorado); Fabio Bacchini (University of Colorado Boulder)

Field of Science: Astronomical Sciences

Abstract:

A supermassive black hole (SMBH) lies at the center of most galaxies, exerting a powerful gravitational pull on surrounding matter. In many cases, an SMBH indirectly powers a bright, compact region--the Active Galactic Nucleus--which may be more luminous than the rest of the galaxy combined. An accretion disk of hot, ionized plasma typically swirls around the SMBH, prevented from falling directly into the black hole by its angular momentum. In the famous "black hole shadow" image taken by the Event Horizon Telescope (EHT), the bright ring surrounding the central black hole is produced by this accretion disk. It is believed that the magneto-rotational instability (MRI) drives turbulence in the plasma and creates a sort of friction that facilitates the accretion of matter onto the SMBH. This turbulence can heat and accelerate charged plasma particles to high energies, where they can emit observable radiation. In some cases, an SMBH and its accretion disk launch a collimated jet of relativistic plasma traveling hundreds of thousands of light years or more away from the SMBH. Magnetic fields generated in the accretion disk may become twisted around the jet like a coiled spring, in a field configuration called a magnetic pinch that is known to be unstable to kinking. A kink-unstable plasma column may undergo magnetic reconnection, a fundamental plasma process that rapidly converts magnetic energy to particle energy, potentially leading to observable radiation.

We propose to use first-principles particle-in-cell (PIC) simulations to study the destabilization of a plasma column (a magnetic Z-pinch) relevant to the extreme plasma environment surrounding black holes. A state-of-the-art supercomputer like Frontera is essential for simulating plasma processes operating from microphysical scales up to mesoscopic scales where energy is injected by astrophysical instabilities in accretion flows and jets of SMBHs. With Frontera, we can thus investigate the basic plasma processes responsible for converting the energy between gravitational, magnetic, kinetic, and ultimately observable electromagnetic forms.

Type: Renewal LRAC

Title: Comprehensive Constraints on Self Interacting Dark Matter

Principal Investigator: Thomas Quinn (University of Washington)
Co-Investigators: Ferah Munshi (George Mason University); Alyson Brooks (Rutgers University (State University of New Jersey))

Field of Science: Extragalactic Astronomy and Cosmology

Abstract:

There is robust observational evidence that structures ranging from dwarf galaxies to galaxy clusters are dominated by dark matter, yet we know almost nothing about its particle nature. The prevalent assumption in astrophysical modeling is
that it is ``cold'' and collisionless (Cold Dark Matter or CDM), yet particle physicists have emphasized that it is theoretically natural for dark matter to have self interactions (Self Interacting Dark Matter, or SIDM). The proposed work
will result in a suite of high resolution, state-of-the art simulations of galaxy formation within both a CDM and SIDM paradigm. The initial conditions for every galaxy run in CDM will be used to run the same galaxy within SIDM, for a direct comparison of the effect of the dark matter model. SIDM preserves the large-scale success of CDM, while opening up the possibility of altering the small scales in testable ways using galaxy observations. With this suite, we can either rule out the SIDM model, or establish it as a compelling alternative to CDM.

Type: Renewal LRAC

Title: Merging Supermassive Binary Black Holes: Electromagnetic Outputs, Jet Interaction and Recoils

Principal Investigator: Manuela Campanelli (Rochester Institute of Technology (RIT))
Co-Investigators: Scott Noble (National Aeronautics and Space Administration (NASA)); Yosef Zlochower (Rochester Institute of Technology (RIT))

Field of Science: Gravitational Physics; Astronomical Sciences

Abstract:

Accreting supermassive binary black holes (SMBHBs) are promising multimessenger sources because they strongly emit both gravitational (GW) and electromagnetic (EM) radiation. This project's goal is to simulate gas flow around a pair of merging SMBHBs with sufficient physical realism that they can support specific predictions about the EM radiation they should produce. Observers could then use these predictions to identify examples of this dramatic phenomenon.

We request here a new allocation of 3.4M node hours on Frontera to perform simulations of SMBHB systems as they approach merger, merge into a single black hole, and the entire system relaxes post-merger. To make these predictions credible, we will assume astrophysically realistic conditions and employ the full suite of physically relevant mechanisms: general relativity (including the dynamical spacetime of the merger), magnetohydrodynamics (MHD), and radiation processes (Compton scattering, photoionization-driven emission, etc.).

Over the past ten years, our collaboration (RIT, JHU and NASA GSFC) has built the knowledge base and computational methods needed to reach this goal, and we are now ready to take the final steps. We have built the complete simulation infrastructure to permit simulation of gas accretion that will allow us to efficiently evolve these simulations from the early-inspiral, merger and post-merger regimes.

With these tools, we will explore how EM signals depend upon the binary separation and black hole spins focusing on the period when the binary separation is small enough for relativistic effects to become important---including the climax, the merger proper. We will then simulate what happens to the gas surrounding the black holes during the subsequent post-merger relaxation phase. We will use our post-processing machinery to predict EM spectra and light curves throughout all these phases.

This work will be critical as we approach possible detection of GWs via pulsar timing array observations and, a few years later, via LISA. Our work may support detection of the LISA source population even before it is launched and will greatly improve the odds for detection of EM radiation associated with LISA events.

Type: Renewal LRAC

Title: Multi-scale GRMHD Modeling of Accretion and Jets

Principal Investigator: Alexander Tchekhovskoy (Northwestern University)
Co-Investigators: Jonatan Jacquemin (Northwestern University); Ore Gottlieb (Northwestern University)

Field of Science: Extragalactic Astronomy and Cosmology

Abstract:

Active galactic nuclei (AGN) jets are launched very close to the central black hole. Highly collimated, they propagate through the ambient medium. During this process, jets can dissipate their magnetic energy into non-thermal particles which then emit powerful multi-wavelength electromagnetic radiation and neutrinos. Meaningful interpretation of multi-messenger jet observations requires multi-scale modeling that self-consistently includes a wide range of physical processes acting on vastly different physical scales. However, due to the complexity of the problem, so far theoretical works of relativistic jets have studied separately the accretion physics and jet propagation. Highly idealized treatments of such tightly coupled physical processes limit the predictive power of the models. We propose to perform multi-scale jet simulations that connect accretion physics, fluid dynamics, and jet formation and propagation, to construct the first multi-scale model of black hole accretion, ejection, and interaction with ambient medium in AGN. Namely, we propose to perform the largest general relativistic magnetohydrodynamic (GRMHD) simulation of AGN accretion and jets to date, that extend from the black hole to the emission zone. We will achieve this goal using our new GPU-accelerated code H-AMR, which makes efficient use of Lonestar6's A100 GPUs and includes advanced features such as adaptive mesh refinement and adaptive time-stepping. This will allow us for the first time to attack this long-standing multi-scale problem from first principles.

Type: Renewal LRAC

Title: Heating and Particle Energization in Space and Astrophysical Plasmas

Principal Investigator: Jason TenBarge (Princeton University)
Co-Investigators: Gregory Howes (University of Iowa (UI)); James Juno (Princeton Plasma Physics Laboratory (PPPL)); Ammar Hakim (Princeton Plasma Physics Laboratory (PPPL))

Field of Science: Magnetospheric Physics; Solar Terrestrial Research

Abstract:

Understanding energy dissipation and entropy production in collisionless processes such as shocks, turbulence, and magnetic reconnection are grand challenge problems in plasma physics and have been the subject of study for many decades. A major unanswered question on this frontier is, how does a collisionless plasma transform bulk flow and electromagnetic energy into particle thermal energy? The development of a detailed understanding of shocks in plasmas has been a long standing goal of the broader scientific community, both as a fundamental physics process and because of its applicability to a wide variety of phenomena throughout the universe. Under one of the four high-level science goals in the 2013 NRC Heliophysics Decadal survey, "Discover and characterize fundamental processes that occur both within the heliosphere and throughout the universe," shocks are identified as ubiquitous phenomena responsible for transforming high energy flows into thermal energy and energetic particles. Many potential mechanisms have been proposed to perform the conversion between flow and thermal energy in a collisionless plasma, but the answer has been elusive. Understanding how shocks and turbulent magnetic reconnection operate is of primary importance to understand the Sun-Earth coupling, protecting manned missions and spacecraft from high energy particles, achieving inertial confinement fusion, and interpreting radiation observed from astrophysical plasmas, such as supernova remnants and astrophysical jets.

To improve our understanding of plasma heating and distribution function dynamics in weakly collisional plasmas, we propose to study the phase space dynamics and particle energization that occurs during shock reformation and kinetic instabilities that regulate both macro-scale properties as well as energy dissipation in shocks using fully kinetic, continuum Vlasov-Maxwell (VM) simulations. The simulation code, Gkeyll, to be employed in this endeavor leverages cutting-edge numerical techniques to model the particle distribution function evolution in greater detail than ever before. The Vlasov approach with a continuum velocity representation is free of restrictions imposed by reduced continuum and Lagrangian kinetic models often employed, e.g., gyrokinetics and particle-in-cell methods.

Type: Renewal LRAC

Title: Multi-scale, MHD-kinetic modeling of the solar wind and its interaction with the local interstellar medium

Principal Investigator: Nikolai Pogorelov (University of Alabama Huntsville (UAH))
Co-Investigators: FEDERICO FRATERNALE (University of Alabama Huntsville (UAH)); Vadim Roytershteyn (Space Science Institute)

Field of Science: Solar Terrestrial Research

Abstract:

The goal of this project is to investigate the solar wind (SW) flow and its interaction with the local interstellar medium (LISM). This investigation requires self-consistent solution of the fluid and kinetic equations. Accurate modeling of the solar wind flow is required for prediction of Space Weather, which is defined by the transients in the space environment traveling from the Sun, through the heliosphere, to Earth. In the recent decade, the difficult task of understanding and predicting violent solar eruptions and their terrestrial impacts has become a strategic national priority, as it affects the daily life of humans, including communication, transportation, power supplies, national defense, space travel, and more. The proposed multi-scale simulations will help analyze and interpret observational data from the major space missions, e.g., Voyagers, Interstellar Boundary Explorer (IBEX), New Horizons, Parker Solar Probe, Solar Orbiter, etc.

Frontera resources are a proper venue for our research because it involves not only computationally challenging, high-resolution, 3D solutions of turbulent MHD equations on adaptive grids, but also kinetic modeling of neutral atoms and nonthermal PUIs. Using leadership computing resources, such as Frontera, for the analysis of flows of partially ionized plasma that are characterized by multiple or highly localized scales and multiple processes, is expected to have a transformative impact on the Heliophysics, LISM physics, and plasma physics, in general. Space missions involved in this project have enormous publicity. The physical processes we are investigating are of importance well beyond the space physics alone and reveal themselves on a broad range of astrophysical and laboratory plasma physics problems. Besides the impact on modeling complex physical systems, we anticipate that our approach to computational resource management for complex codes utilizing multiple algorithm technologies will be a major advance on current approaches. The development of resource management technologies will be essential for all future modeling efforts that incorporate the diversity of scales and physical processes. It will allow us to promote the application of adaptive technologies to contemporary plasma physics problems through the development of publicly available packages suitable for multiple applications.

Type: Renewal LRAC

Title: NSF Convergence Accelerator Track E: Combining global high-resolution climate simulations with ocean biogeochemistry, fisheries and decision-making models to improve sustainable fisheries management under climate change

Principal Investigator: Ping Chang (Texas A&M University (TAMU))
Co-Investigators:

Field of Science: Climate Dynamics

Abstract:

Fish and shellfish populations are a vital source of protein for many of the world's people, and several of the largest are found along the eastern boundaries of the Pacific and Atlantic Oceans, where cold, deep water moves towards the surface, bringing nutrients that support both production by plants (phytoplankton) and the fish populations that feed on them. To ensure sustainability, fish and shellfish managers need information not only on the number of animals available at any given time, but also on potential future numbers, so that they can plan for such things as the number of fishing boats required or the size of seafood processing plants. Forecasting what will occur in such eastern boundary areas is difficult, however, because local winds rapidly change conditions. Adverse climate impacts, such as rising ocean temperatures and increasing acidity, are already affecting many coastal fishing-dependent communities, and such longer-term changes also have to be considered. The project aims to develop a decision support system, which uses the latest ocean models incorporating marine physics, chemistry and biology, to assist fish and shellfish managers in making their decisions. This is important as there are many stakeholders involved in harvesting fish and shellfish, who may have potentially conflicting interests. To this end, the research is aimed at integrating the outputs from the ocean models with a web-based decision support system that will help fisheries managers and industry make informed decisions to ensure that both the industry and its associated food production are sustainable. The investigators will work directly with the stakeholders to develop tools that are specifically able to meet their needs. The initial focus of the work is the California Current system along the U.S. west coast from California to Washington, which supports a local seafood industry valued annually at about $12 billion, with additional billions from catches landed by foreign boats in the U.S. If successful, the new tools should be extendable to other similar regions of the global ocean, thus increasing the value of the research. The project will provide training for students, including those from under-represented groups, in the use of the latest ocean models, as well as development opportunities for young faculty members at the participating institutions.

Climate change-driven adverse ocean impacts are already affecting many rural, coastal, fishing-dependent communities, and these adverse impacts will likely accelerate for the foreseeable future. Forecasting potential changes in eastern boundary upwelling systems has benefitted recently from improvements in the resolution of global Earth system models, so that the latest eddy-resolving models at 10 km ocean resolution have greatly reduced systematic errors relative to observations. This project aims to use these advancements to improve forecasts of the fisheries potential of the California Current Ecosystem and improve decision making by managers and other stakeholders. The project will couple the output from such a high-resolution model simulation with the Marine Biogeochemistry Library and Fisheries Size and Functional Type models, thus incorporating physics, chemistry and biology with

climate variability. The results will be integrated with a prototype, web-based decision support system, that uses mathematical decision analysis capabilities, to assist fisheries managers to model the complex, climate-related decision problems on which fisheries production depends. This is vital to ensure that the region can continue to support a sustainable fishery in the long term and the communities that depend on fishing for a living. In Phase 1, the project will develop a prototype of this linked decision system. The project will also develop a well-networked multidisciplinary team of modelers, social scientists, fisheries managers, economists, and industry and community stakeholders to advance convergence science and develop avenues for more sustainable fisheries under a changing climate. This team is essential for developing tools that are directly applicable to the needs of fishery stakeholders and will be fostered by meaningful communication between all groups throughout the project period. If successful, the model suite and decision support system should be extendable to other similar regions of the global ocean. Students and post-doctoral researchers, the next generation of scientists, will be trained in decision analysis and to use the most current high-resolution models. Furthermore, the project will provide valuable professional development opportunities for early career female Co-PIs involved in the program.

Type: Renewal LRAC

Title: LRAC: High resolution simulations of damage-producing supercell thunderstorms

Principal Investigator: Leigh Orf (University of Wisconsin Madison (UW Madison))
Co-Investigators:

Field of Science: Atmospheric Sciences

Abstract:

This request for Frontera supercomputer access is to simulate tornado-producing thunderstorms. By simulating these storms accurately in various environments and using different techniques, the physics of how the storms work is better understood. This new knowledge eventually filters its way into the operational realm where it aids forecasters in making better predictions during severe weather outbreaks. Better predictions result in fewer lives lost.

Type: Renewal LRAC

Title: Real-time Convection-Allowing Numerical Weather Prediction Model Ensembles for NOAA Testbeds Using FV3-LAM

Principal Investigator: Keith Brewster (University of Oklahoma (OU))
Co-Investigators: Jun Park (Univ. of Oklahoma); Nathan Snook (University of Oklahoma (OU))

Field of Science: Meteorology

Abstract:

The National Oceanic and Atmospheric Administration National Weather Service (NOAA NWS) Testbeds bring research and operational meteorologists together to evaluate, both subjectively and objectively, new tools for improving forecasts of high-impact weather events across the United States. Recently the NOAA NWS selected a new model to unify its weather modeling efforts across scales in the Unified Forecast System (UFS); the Finite Volume Cubed Sphere Limited Area Model (FV3-LAM) uses a numerical core originally developed for global scales so testing and development is needed to optimize the model for convection-allowing, and convection-resolving scales. The Center for Analysis and Prediction of Storms (CAPS) at the University of Oklahoma (OU) has, for several years, been testing high-resolution numerical weather prediction (NWP) with support from, and in collaboration with, the NOAA NWS Testbeds. This project extends that work by ramping high-resolution NWP ensembles toward Exascale in support of two NOAA Testbed experiments, the 2023 Hydrometeorology Testbed (HMT) Flash Flood and Intense Rainfall (FFaIR) experiment, and 2023-24 HMT Winter Weather Experiment (WWE). CAPS plans to produce 15-member high-resolution NWP ensembles using the FV3-LAM in support of these quasi-operational testbeds and as part of an effort to evaluate components of the FV3-LAM at these scales. As part of the experiments, CAPS will develop and test ensemble post-processing tools to produce ensemble consensus products, including a spatial-aligned ensemble mean algorithm and machine learning (ML training done on local OU resources), for improving forecasts of heavy snow and other high-impact winter weather in WWE and flash flooding and heavy rainfall in the FFaIR. The project will extend CAPS prior successful execution of FV3-LAM ensembles on TACC Stampede2 and Frontera and move toward the Exascale on Frontera by augmenting our ensemble with an additional forecast covering the entire North American Continent at 3-km grid spacing (about 3.7x CONUS grid points) and a trial member with 1-km grid spacing requiring approximately 27 times the computations of the current 3-km grid-spacing.

Type: Renewal LRAC

Title: LRAC: NextGen Space Weather Modeling Framework Using Data, Physics and Uncertainty Quantification

Principal Investigator: Gabor Toth (University of Michigan (UMich))
Co-Investigators:

Field of Science: Solar Terrestrial Research; Natural and Man-Made Hazard Mitigation

Abstract:

Space weather results from solar activity that can impact the space environment of the Earth and damage our technological systems as well as expose pilots and astronauts to harmful radiation. Extreme events could knock out the power grid with a recovery time of months and cause about $2 trillion damage. Much of the impacts can be avoided or mitigated by timely and reliable space weather forecast. The NextGen Space Weather Modeling Framework will employ computational models from the surface of the Sun to the surface of Earth in combination with assimilation of observational data to provide optimal probabilistic space weather forecasting. The model will run efficiently on the next generation of supercomputers to predict space weather about one day or more before the impact occurs. The project will concentrate on forecasting major space weather events generated by coronal mass ejections (CMEs).

Current space weather prediction employs first-principles and/or empirical models. While these provide useful information, their accuracy, reliability and forecast window need major improvements. Data assimilation has the potential to significantly improve model performance, as it has been successfully done in terrestrial weather forecast. To allow for the sparsity of satellite observations, however, a different data assimilation method will be employed. The new model will start from the Sun with an ensemble of simulations that span the uncertain observational and model parameters. Using real time and past observations, the model will strategically down-select to a high performing subset. Next, the down-selected ensemble will be extended by varying uncertain parameters and the simulation continued to the next data assimilation point. The final ensemble will provide a probabilistic forecast of the space weather impacts. While the concept is simple, finding the optimal algorithm that produces the best prediction with minimal uncertainty is a complex and very challenging task that requires developing, implementing and perfecting novel data assimilation and uncertainty quantification methods. To make these ensemble simulations run faster than real time, the most expensive parts of the model need to run efficiently on the current and future supercomputers, which employ graphical processing units (GPUs) in addition to the traditional multi-core CPUs. The main product of this project will be the Michigan Sun-To-Earth Model with Quantified Uncertainty and Data Assimilation (MSTEM-QUDA) that will be made available to the space physics community with an open source license.

Type: New LRAC

Title: Biophysical Modeling and Machine Learning for Gliomastomas

Principal Investigator: George Biros (University of Texas at Austin (UT) (UT Austin))
Co-Investigators:

Field of Science: Biological and Critical Systems

Abstract:

We request 120K Node Hours on Frontera-GPU, 22K Node Hours on Lonestar6-GPU. The Frontera-GPU allocation will be used for comparing a single-species to a multi-species tumor growth model. The Lonestar6-GPU allocation the generation of a large dataset of synthetic tumor-bearing images that will be used to train a machine learning model that can rapidly infer tumor model parameters from patient images. We will make this dataset publically available. Finally, we request 5K Node Hours/system on both Lonestar6 and Frontera CPU partitions for pre- and post-processing supporting workflows.

The aim of the project is to apply our recently developed computational tools to clinical medical images of glioblastoma patients. Glioblastoma is the most common and aggressive malignant adult brain tumor, with grim prognosis and heterogeneous molecular imaging profiles~\cite{Collins:1998}. The median overall survival of patients diagnosed with a glioblastoma is 14--16 months after standard-of-care treatment, or perhaps a bit longer with some emerging treatments. Although the main currently applicable treatment options (i.e., surgery, radiotherapy, chemotherapy) have expanded during the last 20 years, there is no substantial improvement in the overall survival rates. Major obstacles include the heterogeneity and aggressiveness of glioblastomas, the difficulties of patient stratification, the difficulties in designing personalized treatment, and the difficulty in the evaluation of first-line therapies. Examples of personalized treatment include localized radiation plans, radio-chemotherapy dosage, and timing of deliveries. For example, radiation can be directed precisely to the tumor, sparing the nearby healthy tissue and leading to better outcomes.

Type: Renewal LRAC

Title: Development of accurate, transferable and extensible deep neural network potentials for molecules and reactions

Principal Investigator: Olexandr Isayev (Carnegie Mellon University (CMU))
Co-Investigators: Adrian Roitberg (University of Florida)

Field of Science: Physical Chemistry

Abstract:

In the 2023 allocation period, we would like to concentrate on one specific application of ML potentials for reactive systems: development neural network-based reactive force field (NNRFF). This task requires a molecular potential with accurate description of bond-breaking process. At the same time, they require massive amounts of computing resources if solved with traditional quantum-chemical methods. Therefore, NNRFF represents very promising areas of application of highly accurate ML potentials.

Type: Renewal LRAC

Title: Multiscale Simulation and Modelling of Biomolecular Phenomena on Frontera

Principal Investigator: Gregory Voth (University of Chicago)
Co-Investigators:

Field of Science: Chemistry

Abstract:

The proposal aims to simulate a number of large-scale biomolecular systems of interest using petascale simulation methodologies with coarse grained (CG), all-atom (AA), and multiscale models. We focus on providing insight into molecular behavior at scales that are inaccessible to more detailed simulation techniques and not feasible to study experimentally. Several systems to be studied under this award include key steps in the retroviral replication process of HIV, the budding mechanisms of SARS-COV-2, and cytoskeletal protein networks (e.g. actin and microtubules). Computational resources for these studies will broadly impact and contribute to scientific discoveries in the fields of biophysics, molecular simulation, and virology.

Type: Renewal LRAC

Title: Atomic-Level Characterization of the Human Immunodeficiency Virus Type 1 Envelope Glycoprotein

Principal Investigator: Mahmoud Moradi (University of Arkansas Fayetteville)
Co-Investigators:

Field of Science: Biophysics; Physical Chemistry

Abstract:

We employ path-finding algorithms and enhanced sampling molecular dynamics (MD) simulations to characterize the activation and deactivation paths of Human Immunodeficiency Virus Type 1 (HIV-1) envelope glycoprotein (Env). This is a project for which the Frontera will be vital in obtaining enhanced sampling data to perform the path-finding calculations. we will focus on characterizing local and global conformational changes of the closed and open states of the Env trimer and determining the dynamic behavior of the glycoprotein trimer to find its activation and deactivation path using a combination of path-finding algorithms and free energy calculation methods. This LRAC project advances our understanding of conformational dynamics of HIV-1 envelope glycoprotein in an attempt to reveal crucial atomistic information about the molecular machinery of the virus.

Type: New LRAC

Title: Application of MD Simulations to Rationally Design PROTACs

Principal Investigator: Jin Wang (Baylor College of Medicine (BCM))
Co-Investigators:

Field of Science: Chemistry

Abstract:

A PROTAC is a heterobifunctional molecule that can bind both a targeted protein and an E3 ubiquitin ligase to facilitate the formation of a ternary complex, leading to ubiquitination and ultimate degradation of the target protein. Compared with oligonucleotide and CRISPR therapeutics that face in vivo delivery challenges, PROTACs are small molecule therapeutics that provide opportunities to achieve broadly applicable body-wide protein knockdown. However, the current design and development of PROTACs is highly empirical due to the complicated nature of the E3 ligase complex formed. We will apply MD simulations to understand the structure-activity relationship of PROTACs and validate the computational modeling with experimental data. Our ultimate goal for this project is to develop a rational computational approach for PROTAC development.

Type: New LRAC

Title: Uncovering the Protective Mechanisms of SARS-CoV-2 within a Respiratory Aerosol During Airborne Transmission

Principal Investigator: Rommie Amaro (University of California San Diego (UCSD) (UC San Diego))
Co-Investigators:

Field of Science: Chemistry

Abstract:

We request this allocation to simulate the atomically detailed SARS-CoV-2 virion inside a respiratory aerosol particle in order to understand the chemical and molecular determinants of aerosol transmissibility. The virus-containing aerosol particle is ~ 300nm in diameter and comprised of roughly one billion atoms, thus providing a bleeding-edge use case for all-atom molecular dynamics simulations. We seek to understand how mucins and other molecules (e.g., divalent cations) may provide a protective cage around the virus while suspended in aerosols. Due to the huge particle counts and GPU elements involved in the computing, this work requires access to the Leadership Class Computing Facilities for successful completion.

Type: Renewal LRAC

Title: Direct numerical simulation and analysis of turbulent pipe flow at high Reynolds numbers

Principal Investigator: Fazle Hussain (Texas Tech University (TTU))
Co-Investigators: Jie Yao (Texas Tech University (TTU)); Philipp Schlatter (KTH mechanics)

Field of Science: Fluid, Particulate, and Hydraulic Systems

Abstract:

The main objective of this project is to perform high-fidelity direct numerical simulation of turbulent pipe flow at relatively high Reynolds numbers (i.e., Re τ up to 10000). This work will not only be a complement to both the existing high-Re simulations of turbulent boundary layers and channel flows but also be critical for addressing some important issues/controversies revealed in recent high-Re turbulent pipe experiments, particularly, for example, the CICLoPE project and “Hi-Reff” at AIST, NMIJ. It will also be essential to enhance our understanding of turbulence physics at high Re’s, and to develop better turbulence models for industrial applications. During the past allocation periods, we successfully conducted systematical comparisons between two high-order DNS codes - NEK5000 and OPENPIPE - for Re τ up to 2000. We have also performed full-scale DNS of turbulent pipe flow at Reτ = 5200 using OPENPIPE. The new pipe data is extensively comparedwith other simulation data pertaining to pipes and channels, and the processed statistics data has been freely shared to the community. In addition, we have also started the simulation at Re τ = 10 4 – the largest Reynolds numbers considered for turbulent flows. During the coming allocation period, we enthusiastically request another 300000 SUs to finish the simulation for Re τ = 10 4 .

Type: Renewal LRAC

Title: Particulate Acceleration and Lagrangian Intermittency in Turbulence

Principal Investigator: Pui-kuen Yeung (Georgia Institute of Technology)
Co-Investigators: Michael Wilczek (University of Bayreuth, Germany); Katepalli Sreenivasan (New York University (NYU)); Shankar Subramaniam (Iowa State University (ISU))

Field of Science: Fluid, Particulate, and Hydraulic Systems

Abstract:

This project is aimed to advancing fundamental understanding of the phenomenon of intermittency in turbulent fluid flow, where intense but localized fluctuations of much practical consequence can occur. The work emphasizes the nature of flow physics seen from the perspective of an observer moving with the disorderly fluid motion. Numerical simulations on cutting-edge platforms based on exact equations of motion spanning a wide range of scales in time and space are the best means of providing the type of data required for new progress in the understanding and modeling of this complex phenomenon. Massive simulations coupled with advanced data analyses will be conducted using codes that scale very well up to at least 2048 nodes on Frontera. This work will bring together four highly accomplished investigators of complementary expertise, including a strong element of international collaboration.

Type: Renewal LRAC

Title: Direct Numerical Simulations of Transport in Turbulent Boundary Layers over Sediment Bed

Principal Investigator: Sourabh Vasant Apte (Oregon State University)
Co-Investigators:

Field of Science: Fluid, Particulate, and Hydraulic Systems

Abstract:

It is proposed to perform pore-resolved, direct numerical simulation (DNS) of turbulent boundary layer flow over a sediment bed with polydispersed particles. The main goal of these numerical experiments is to test the hypothesis that polydispersity and the resultant local variations in the permeability can significantly alter the structure and dynamics of turbulence over a porous sediment bed as compared to mono-dispersed particles. Poyldispersed particles can affect the effective roughness scale and hence the permeability of the sediment bed. However, no detailed experimental or numerical data are currently not available. {Last year, the main focus was on computations of momentum transport across the sediment-water interface (SWI) involving monodispersed particles over a range of Reynolds numbers representative of transitional and turbulent transport in aquatic systems. It is proposed to investigate both mass and momentum transport over polydispersed particles in a random arrangement in the next year and compare against monodispersed cases.

A Cartesian, co-located grid, second-order, finite volume based incompressible flow solver (CGS-FDM) developed around the principles of energy conservation will be employed for these simulations. and has been used on several Teragrid machines for several sediment-laden turbulent flow problems.

A large-scale 304K node-hrs on the new Frontera machine are requested. The code has shown good scalability and is in production mode for the past two years and resulted in several journal and conference publications. The reseach team involves Shashank Karra (a PhD student, planning to defend in February 2023), Daniel Fust (a new PhD student), and Dr. Xiaoliang He (a post-doctoral fellow, PNNL), and the PI.

Type: Renewal LRAC

Title: Reducing the Noise of Twin Supersonic Turbulent Jets

Principal Investigator: Daniel Bodony (University of Illinois Urbana-Champaign (UIUC) (University of Illinois) (U of I))
Co-Investigators:

Field of Science: Fluid, Particulate, and Hydraulic Systems

Abstract:

This is a proposal for LRAC project CTS20006 (originally titled ``Direct Numerical Simulation of Mach 6 Flow Over A 35 Degree Compression Ramp'' but updated to ``Reducing the Noise of Twin Supersonic Turbulent Jets'') to use Frontera to study very-high-speed, shock-laden and heated jets of relevance to twin-engined jets used by the US Navy. This proposal seeks first to study the turbulence contained within the twin jet, and the noise produced by it, for three temperature ratios. Then, using massively parallel eigenvalue analysis, develop an optimal jet noise reduction strategy based on eigenvalue movement concepts. Finally, the jet noise reduction is to be evaluated through matching controlled-jet simulations. If successful, the simulations will demonstrate the very first jet noise reduction strategy suitable for Naval tactical fighters. The jet nozzle geometry and flow conditions are guided by existing experimental data to enable validations at the lowest temperature ratio. We will use a high-order computational fluid dynamics code written by the PI that has shown readiness and excellent scalability on Frontera. We request 3,472,000 node-hours to support this project. Our first two years of Frontera access through the LRAC process were very successful and well documented.

Type: New LRAC

Title: Study of Linear Instabilities in Laminar Hypersonic Shock-wave/Boundary-Layer Interactions using Kinetic Methods

Principal Investigator: Deborah Levin (University of Illinois Urbana-Champaign (UIUC) (University of Illinois) (U of I))
Co-Investigators: Vassilios Theofilis (University of Liverpool)

Field of Science: Fluid, Particulate, and Hydraulic Systems

Abstract:

This proposal aims to understand shock structures, unsteadiness and possible three dimen- sional effects for shock-laminar boundary-layer interactions (SWBLI) for hypersonic flows in the near continuum flow regime with the use of particle-based Direct Simulation Monte Carlo (DSMC) methods that offers the highest fidelity. We seek to understand these mechanisms through the use of data-driven modal analysis techniques such as operator-based global sta- bility analysis tools that have been parallelized to process big data. To make efficient use of petascale facilities, we have developed an MPI-based solver known as Scalable Unstructured Gas-dynamics Adaptive mesh-Refinement (SUGAR-3D) and have applied it successfully to the type of computationally intensive simulations that are proposed here. This project follows up our Pathways project with the project number CTS22009 where we identified the transition mechanisms and shock interaction dynamics for a laminar separation bubble in a supersonic flow which will be detailed in Sec. III. In this project we aim to expand the investigation about shock dynamics and transition mechanisms related to the laminar separation bubbles to the hypersonic flight regime with the help of particle-based Direct Simulation Monte Carlo (DSMC) method which provides the highest fidelity for such flows. The research findings of this project will serve as a part of Ph.D. thesis of a graduate student, Irmak Taylan Karpuzcu, under the guidance of Prof. Deborah Levin at the University of Illinois at Urbana-Champaign. These findings will also serve as a part of Ph.D. thesis of a graduate student, Angelos Klothakis, under the guidance of Vassilis Theofilis at the University of Liverpool. The findings will be published in peer-reviewed journal papers. The two research groups have been collaborating in the past three years where students in both groups have learned about DSMC (Levin's field of expertise) and linear stability theory (Theofilis' area of expertise).

Type: Renewal LRAC

Title: First-principles Study of Interactions and Topological Effects in Condensed Matter Systems

Principal Investigator: Steven G. Louie (University of California Berkeley (UC Berkeley))
Co-Investigators: Marvin Cohen (University of California, Berkeley)

Field of Science: Condensed Matter Physics

Abstract:

This is a proposal for the renewal of Leadership Resource Allocation (LRAC). These resources will be used by our group to carry out theoretical calculations as part of a major research program in theoretical condensed matter physics funded by NSF grant DMR-1926004. Last year we were awarded 1.1M NHs and have already utilized 86% by now. We are very confident that we could fully use all our allocation asked before April. This year, we have several proposed projects that will rely on Frontera resources if granted, as will be detailed in the following sections.

Our group is actively engaged in research in the fields of theoretical condensed matter physics and materials science. Our research covers a broad range of materials, from bulk materials (metals, semiconductors, and insulators) to low-dimensional materials, such as two-dimensional (2D) crystals as well as organic and inorganic nanostructures. Phenomena of interest include moiré physics, optical properties, superconductivity, magnetism, and topological properties, etc. Particular emphasis is placed on accurate calculations including many-body effects related to physical observables. Our primary goal is to understand and predict materials properties at the most fundamental level using first principles (ab initio) quantum mechanical calculations. A variety of different computational approaches are used that require typically only the atomic numbers and structures as inputs. These first-principles methods have, in the past, resulted in excellent quantitative agreement with experiments and have predicted with good accuracy materials properties that were later verified experimentally. There are currently two principal investigators together with ten graduate students and postdoctoral researchers working on the projects described in this proposal. On many of these projects, we are collaborating with experimentalists or theorists from UC Berkeley and other institutions.

Based on the justifications given in Section 3, we request an allocation of 1,651,000 node hours (NHs) on Frontera spread over four major areas with 8 inter-related topics. We hope that it will be clear from our project descriptions and Progress Report that our requested allocation will be used productively and is a worthwhile investment by TACC. In this proposal, we ask for computational resources on Frontera, because it will enable us to effectively utilize our BerkeleyGW code and to investigate novel and interesting condensed matter systems from first principles. About 80% of the requested allocation will be used in time-dependent GW (TD-aGW) calculations, GW perturbation theory (GWPT) calculations, and GW & GW-BSE calculations. A typical job of these calculations on real materials would require 128 nodes with 20 hours wall time, and we expect to run thousands of these jobs on Frontera in the coming allocation year. The major motivation of our Frontera proposal is to understand complex condensed matter phenomena (e.g., exciton physics, twistronics, pump-probe phenomena, etc.) by using or

extending existing state-of-the-art first-principles methods. These Frontera resources are required in addition to the NERSC resources (Cori) to which we have access through the Lawrence Berkeley National Laboratory, the OLCF resources (Summit) through the INCITE program, as well as the ACCESS resources (Stampede2). Those non-Frontera resources will be employed for separate projects different from those of our requested Frontera resources. For example, our NERSC and Stampede2 resources will be used to develop new theories, methods, and general softwares to elucidate and predict excited-state phenomena in energyrelated materials. Our OLCF resources will be mainly focused on the development of GPU-accelerated first-principles methods, with which we can progressively scale up the problem size.

Type: Renewal LRAC

Title: Electron-Phonon Coupling in Correlated Quantum Materials

Principal Investigator: Yao Wang (Clemson University)
Co-Investigators:

Field of Science: Condensed Matter Physics

Abstract:

The coexisting electron correlations and electron-phonon coupling account for many novel phenomena in quantum materials. However, the theoretical study of systems with both interactions is limited in quantum many-body systems by existing theoretical tools. This LRAC project and the associated NSF grant aim to develop, extend, and apply advanced hybrid methods to explain and predict quantum phases driven by both interactions accurately. Equipped with these advanced methods, the production calculations will elucidate many important problems in quantum materials, including unconventional superconductivity, excited-state spectroscopy, and correlated 2D materials, and the Wigner crystal.

Type: Renewal LRAC

Title: Engineering electron-phonon interactions in functional materials

Principal Investigator: Feliciano Giustino (University of Texas at Austin (UT) (UT Austin))
Co-Investigators: Jon Lafuente Bartolome (University of Texas at Austin (UT) (UT Austin));
Sabyasachi Tiwari (University of Texas at Dallas (UTD) (UT Dallas))

Field of Science: Materials Research

Abstract:

The Center for Quantum Materials Engineering (CQME) at the University of Texas, Austin, utilizes state-of-the-art computational methods to model and design advanced functional materials at the atomic scale. The CQME leads the development of the EPW code, a core module of the Quantum ESPRESSO materials simulation suite, to investigate the effects of phonon-assisted quantum processes in electronic and energy materials. In our most recent strong scaling tests on Frontera, EPW achieved above 92% of the ideal parallel speedup on 2000 nodes. The aim of this project is to tackle fundamental questions in the physics of electron-phonon interactions, for example the polaron formation in oxides, phonon mediated optical absorption in materials for green energy applications, and the temperature-dependent carrier transport in two-dimensional semiconductors for ultra-low-power electronics. We will also employ this allocation to continue refactoring the EPW code and the SternheimerGW code in preparation for exascale computing. This research will lay the foundations for the rational design of emerging materials for energy and electronics applications.

Type: Renewal LRAC

Title: Classical Simulations of Planetary Materials with Quantum Accuracy

Principal Investigator: Ivan Oleynik (University of South Florida)
Co-Investigators: Stan Moore (Sandia National Laboratories); Mitchell Wood (Sandia National Laboratories); Aidan Thompson (Sandia National Laboratories); Anatoly Belonoshko (Royal Institute of Technolofy)

Field of Science: Materials Research

Abstract:

The major goal of this LRAC project is to perform predictive simulations to solve one of the outstanding problems in science of matter at extreme conditions – uncovering the behavior of planetary materials at extreme pressures and temperatures characteristic of the interiors of carbon-rich exoplanets, including solid-solid and solid-liquid phase transitions, metastability and phase transitions in amorphous and liquid states, and exploration of novel pathways for synthesis of long-sought-after high pressure phases.

The major science goal of 2022 LRAC allocation was to investigate the behavior of the amorphous carbon (a-C) at high pressure/temperature (high-PT) conditions including its range of its metastability, potential interconversion to diamond polytypes and supercooled liquid, equation of state (EOS) and shock compression pathways to synthesize bc8 phase from a-C precursors. The major science results include (1) the development of machine-learning model of a-C; (2) uncovering a-C phase diagram within a wide range of pressures (from 0 to 1.5 TPa) and temperatures (from 0 to 8,000 K) from quantum accurate, multi-million atom molecular dynamics (MD) simulations; (3) discovering atomic-scale mechanisms of a-C phase transformations to polycrystalline diamond, mixed liquid-solid phase; metastable carbon liquid and high-pressure bc8 crystalline phase of carbon at experimental time and length scales of dynamic compression experiments.

The 2023 LRAC allocation will be focused on (1) to investigate the kinetics effects in phase transformations to BC8 phase from nanocrystalline diamond and computational design of compressive pathways in support of upcoming experiments at National Ignition Facility (NIF) within NIF Discovery Science project led by the PI; (2) to investigate fundamental physics of diamond shock melting and refreezing and determine the effect of refreeze microstructure on modulating initially planar second shock in billion atom single and double shock simulations.

Type: Renewal LRAC

Title: Ab initio engineering of superconducting materials

Principal Investigator: Elena Margine (Binghamton University)
Co-Investigators: Alexey Kolmogorov (Binghamton University)

Field of Science: Materials Research

Abstract:

Advances in electronic structure methodology have made it possible to screen candidate synthesizable materials for a host of complex properties prior to experiment. Modeling of superconductivity, in particular, has come a long way from making rough estimates of the critical temperature to probing pairing mechanisms and resolving superconducting energy gaps. The primary scientific goals of this project are to continue our work on designing high-Tc phonon-mediated superconductors synthesizable at ambient pressure and assess the predictive capabilities of the new functionalities that are being implemented in EPW on various families of superconductors.

Type: New LRAC

Title: Large-scale atomistic simulation of hydrogen embrittlement and first-principles high throughput screening of quantum engineering materials

Principal Investigator: Ju Li (Massachusetts Institute of Technology (MIT))
Co-Investigators:

Field of Science: Materials Research

Abstract:

This is a combined project consisting of three sub-projects 1) large-scale atomistic simulations on hydrogen embrittlement problem, 2) development of reinforcement learning algorithms for long-timescale atomistic simulations, and 3) optical control over nuclear spins for quantum engineering materials.

Hydrogen Embrittlement (HE) has been a long-standing and notorious issue for many structural applications. A widely accepted argument for HE is that absorbed hydrogen can promote crack initiation and propagation at quite early stages of deformation, significantly reducing materials' ductility. The relatively mobile hydrogen atoms can actively interact with various defects, rendering HE a complex process that may involve multiscale mechanisms. Some widely discussed mechanisms include hydrogen enhanced localized plasticity (HELP), hydrogen enhanced decohesion (HEDE), the synergy of HELP and HEDE, metal hydride formation, and phase transformation etc. Experiments under certain conditions seem to lend support to some of the proposed mechanisms, but a convincing explanation of the whole puzzle is still lacking. In this sub-project, we will use large-scale atomistic simulations based on the latest Fe-H EAM interatomic potential (better H interactions with various defects in Fe), and develop experimentally relevant sample conditions for parametric studies on hydrogen mediated crack initiation/propagation processes.

Diffusion-related atomic movements are essential to microstructure evolution and deformation mechanisms in solids, where atomistic simulation provides a predictive tool to understand the microscopic process. However, diffusion processes typically involve an inaccessibly long time scale for direct molecular dynamics simulation. In this sub-project, we will develop a reinforcement learning-based kinetic Monte Carlo method that simulates diffusion time-scale processes while keeping an atomic-scale spatial resolution. The algorithm will take atomic configurations as states and diffusion movements as actions and employ a deep Q network learning method for energy minimization along the diffusion pathway. We will try to detect various diffusion mechanisms by applying this method to bulk and surface defect diffusion in commonly used metals. The goal of our work is to establish an automatic, self-learning scheme to study the defect diffusion mechanisms.

In the era of quantum engineering, nuclear spins are considered as ideal quantum information carriers due to their robustness against environmental perturbations and unparalleled coherence time exceeding minutes and hours even at room temperature. However, the control over nuclear spins poses a grand challenge. Traditionally, nuclear spins have been manipulated using nuclear magnetic resonance (NMR) techniques. Recently, other approaches for controlling nuclear spins at the microscopic/mesoscopic scale have been explored as well, using electron-nuclear spin interaction, microwave electric field, phonons/mechanical waves, etc. Of particular interest are optical approaches, which can be non-contact, ultra-strong, and ultrafast. However, the optical control over nuclear spins studied by now requires nearby unpaired electron spins as the media, which interacts with the optical photon via the orbital interaction and with the nuclear spin through the hyperfine interaction. The necessity of electron spins lead to limited applicability only in systems with non-zero electron spins and shortened nuclear spin coherence time. We

plan to use high throughput calculations to screen for material systems (both bulk crystals and defect systems) suitable for the optical control over nuclear spins, to be used in quantum engineering.

Type: New LRAC

Title: Development of Operational Global Ocean Circulation Models and Hurricane Induced Storm Surge and Compound Flood Models for the United States

Principal Investigator: Clinton N. Dawson (University of Texas at Austin (UT) (UT Austin))
Co-Investigators: Joannes Westerink (University of Notre Dame); Eirik Valseth (University of Texas at Austin (UT) (UT Austin))

Field of Science: Computational Mathematics

Abstract:

In this Frontera Leadership Resource Allocation, we have two distinctive goals for the development of and operation of mathematical models for i) hurricane induced coastal flooding and ii) global ocean circulation. Numerical mathematical models for hurricane induced flooding are critical for emergency national, state, and local decision makers, emergency managers, and first responders. This requires very high spatiotemporal resolution models of the coastal ocean, floodplain, and adjacent river basins along with significant computational power as supplied by Frontera. Thus, we will develop and validate extreme resolution models of the entire United States Gulf and Atlantic coasts. Secondly, we will run operational global circulation models for the United States National Oceanic and Atmospheric Administration (NOAA) on a daily basis to provide global tidal forecasts.

Type: Renewal LRAC

Title: Harnessing big satellite imagery, deep learning, and high-performance computing resources to map pan-Arctic permafrost thaw

Principal Investigator: Chandi Witharana (University of Connecticut (UCONN))
Co-Investigators: Amal Perera (University of Connecticut (UCONN)); Kenton McHenry (National Center for Supercomputing Applications); Anna Liljedahl (University of Alaska, Fairbanks); Rajitha Udawalpola (University of Connecticut (UCONN))

Field of Science: Earth Sciences

Abstract:

The central goal of our research is to map permafrost landforms, thaw disturbances, and human-built infrastructure in the Arctic using sub-meter resolution satellite imagery (acquired by the Maxar commercial sensors), which are freely accessible to the NSF's Polar Program funded Arctic research community via the Polar Geospatial Center (PGC) . Despite the free access to entire Maxar archive, derived pan-Arctic geospatial maps products from this big imagery data (> 2PB) are yet rare. We centered our mapping effort on a prominent and critical microtopographic feature called ice-wedge polygons (IWPs) in the permafrost tundra region of the Arctic. We have developed an operational-scale GeoAI pipeline (Mapping application Arctic Permafrost Land Environment – MAPLE), which is capable of automatically analyzing tens of thousands of commercial satellite imagery using deep learning (DL) convolutional neural net (CNN) algorithms and high performance (HPC) computing resources. MAPLE can semantically segment permafrost microtopographic features, e.g., ice-wedge polygons, which occur at sub-meter scale, from Maxar satellite imagery. Our pan-Arctic ice-wedge polygon map is the first demonstration of a series of geospatial map products (e.g., ice-wedge polygon trough network, retrogressive thaw slumps, and human-built infrastructure) that we envision to derive from Maxar satellite imagery. We are currently under the support of NSF's Office of Polar Programs awards (1927723, 1827872, 1927720) and includes the Navigating New Arctic initiative that is part of the NSF's 10 Big Ideas. MAPLE stands as the first Pan-Arctic scale demonstration of transforming a large volume of Maxar imagery into science-ready geospatial products. Our NSF funding has supported the MAPLE development and is also enabling the discovery and knowledge-generation from the imagery products. The LRAC award (Award #: DPP 20001) has been instrument for us to implement the MAPLE at pan-Arctic scale using a large volume of Maxar image scenes. Using Longhorn HPC resources, the MAPLE have been deployed at operational scale to map IWPs across the Arctic polygonal tundra under three phases; Phase 1: areas of high-probability for ground ice occurrence, Phase 2: areas of medium-probability for ground ice occurrence, and Phase 3: areas of low-probability for ground ice occurrence. We have completed the first pass of all phases. Based on the knowledge gained from the first iteration of this mapping exercise, we seek to pursue two aims during rest of the project cycle. Our first aim is to map IWPs using multi-temporal Maxar data. This will allow us to identify microtopographic transformation and thaw disturbances over time. The second aim is to extend MAPLE's capabilities to create a first pan-Arctic human-built infrastructure map using Maxar data. Ice-wedge polygon mapping operation involves over 30,000 satellite image scenes (>200 TB). In our first pass, we have mapped over 1 billion individual ice-wedge polygons across the Arctic. We have been immensely benefited from the LRAC Award # 20001. This award expires in March 2023. Despite the delays spawned from the pandemic (in early stages of the project) and cascading Postdoc hiring delays, we have been able to utilize resources granted from LRAC award productively. At the time of proposal writing, we have utilized almost all the resources from the initial allocation. The remaining resources

reflect (on Frontera & Lonestar6) to SU additions made available to us when phasing down Longhorn system end of last year. In total, we have ~ 6,000 unused SUs of on Frontera and Lonestar8 systems and 55TB on Ranch. Continued access to HPC resources through a renewal of current LRAC award is critical for us to us remaining node hours to advanced ongoing mapping activities and to create new geospatial maps products. To successfully complete proposed satellite imagery analysis tasks, it is vital for us to have one year renewal to our LRAC award until March, 2024. The resulting circumpolar ice-wedge polygon maps will advance our understanding of the complex and interlinked processes responsible for the evolution of the pan-Arctic ice-wedge polygon tundra landscape. Proposed new maps products, such as human-built infrastructure maps will advance our abilities to assess economic impacts of permafrost thaw in the Arctic.

Type: Renewal LRAC

Title: Simulating 4D subduction and continental evolution

Principal Investigator: Lijun Liu (University of Illinois Urbana-Champaign (UIUC) (University of Illinois) (U of I))
Co-Investigators:

Field of Science: Geophysics

Abstract:

Evolution of oceanic and continental lithosphere represents the backbone of plate tectonics. These two key tectonic components may evolve in cohort or in parallel. On one hand, oceanic subduction may directly influence the overriding continental lithosphere, and vice versa. On the other hand, continents, especially ancient cratons, may evolve largely independently from subduction. Given the vast amounts of complexities in these processes, geodynamic simulation with data assimilation stands as one of the most promising tools to advance understanding in these fundamental problems. We advocate the urgent need in constructing data-centric physical models that could link these theorical/numerical breakthroughs with the fast-increasing data acquisition effort through the amazing supercomputing platform of Frontera.

Type: Renewal LRAC

Title: (An)elastic global full-waveform inversion

Principal Investigator: Hatice Bozdag (Colorado School of Mines)
Co-Investigators: Daniel Peter (King Abdullah University of Science and Technology (KAUST))

Field of Science: Seismology

Abstract:

High-resolution seismic images are essential to understand the structure and thermochemical composition of the mantle to interpret its dynamics, which directly control surface processes such as earthquakes and volcanos. Seismic tomography is at a stage where further refinements require the use of full complexity of wave propagation. Taking advantage of 3D wave simulations adjoint tomography leads to pure data-driven seismic models by avoiding commonly used approximations and corrections in classical tomography. After the publication of the first-generation global adjoint models, which are elastic and transversely isotropic in the upper mantle, constructed based on traveltimes only, our goal is to construct a new global anelastic mantle model by the simultaneous inversion of anelastic and elastic parameters based on adjoint tomography using full waveforms including amplitude information as well. We will perform similar inversions for a continental-scale study in the Middle East which allow us to demonstrate different strategies and measurements in a faster way. Furthermore, we perform 3D global tests with our anelastic inversion setup and data coverage, where we directly demonstrate the resolution, parameter trade-off, and effect of different measurements and inversion strategies on the results. As anelasticity causes physical dispersion, accurate anelastic models also improve the resolution of elastic models, locating earthquakes and other seismic sources more accurately. The outcome of this project will lead to a much improved Earth model with drastically sharper mantle images attempting to answer long-standing questions on the origin of plumes and hotspots and the water content of the upper mantle.

Type: Renewal LRAC

Title: Global, Repeat, and High-Resolution Earth Surface Elevation Data Production for the Scientific Community

Principal Investigator: Claire Porter (University of Minnesota (UM))
Co-Investigators: James Klassen (University of Minnesota (UM)); Karen Tomko (Ohio State University (OSU)); Myoung-Jong Noh (Ohio State University (OSU)); Ian Howat (Ohio State University (OSU)); Erik Husby (University of Minnesota (UM))

Field of Science: Earth Sciences

Abstract:

The EarthDEM project extracts 2m-resolution digital elevation models (DEMs) from stereoscopic commercial satellite imagery to produce a worldwide series of time-dependant, high-resolution topographic observations over time. The datasets are also used to create seamless 2m-resolution mosaics that serve as foundation datasets for other analyses. This project seeks to address the long-standing need for high-resolution repeat topography outlined by the NRC Decadal Survey. While the 16-year archive of satellite imagery collections has been processed to DEMs, new satellite acquisitions offer the opportunity to add valuable recent data to deepen the temporal archive and fill in gaps where no data currently exist.

Type: New LRAC

Title: Mechanism of Ca2+-evoked synaptic vesicle fusion

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

Field of Science: Neuroscience Biology; Biophysics

Abstract:

The research described in this application is focused on elucidating the mechanism by which neurotransmitters are release at synapses through Ca2+-evoked synaptic vesicle fusion, a process that is crucial for interneuronal communication and hence for brain function. This mechanism has been extensively studied for three decades, yielding critical insights into the functions of the core components of the release machinery. Among these components, particularly critical are the SNAREs syntaxin-1, synaptobrevin and SNAP-25, which play a crucial role in membrane fusion by forming a tight SNARE complex that brings the membranes together. Fusion is accelerated by synaptotagmin-1, which acts as the Ca2+-sensor that trigger release. However, despite the enormous advances in this field, it is still highly unclear how the SNAREs induce membrane fusion and how the function of synaptotagmin-1 is coupled to render fusion extremely fast and Ca2+ dependent. This LRAC application proposes to perform multiple all-atom molecular dynamics (MD) simulations in the microsecond time scale to address these questions. The proposal builds on MD simulations that are being performed through a Pathways allocation on Frontera and have already yield critical mechanistic insights. The results of the proposed simulations will complement ongoing experimental studies in my laboratory. Together, the simulation and experimental results are expected to lead to a description of the mechanism of Ca2+-triggered synaptic vesicle fusion in atomic detail.

Type: Renewal LRAC

Title: Simulation & experiment to optimize force fields for accurate atomistic modeling of nucleic acids and computer-aided drug design

Principal Investigator: Thomas Cheatham (University of Utah)
Co-Investigators:

Field of Science: Organic and Macromolecular Chemistry

Abstract:

AMBER simulation on various bimolecular systems, focusing on RNA, is used to probe drug interaction, to assess and optimize force fields, and to better understand structure, dynamics and function.

Type: Renewal LRAC

Title: Multi-Resolution Simulations of Mesoscale Biological Systems

Principal Investigator: Aleksei Aksimentiev (University of Illinois Urbana-Champaign (UIUC) (University of Illinois) (U of I))
Co-Investigators:

Field of Science: Biophysics

Abstract:

This proposal requests an allocation on Frontera to carry out several pioneering simulations in the general area of molecular biophysics and biotechnology. In collaboration with the leading experimental labs, we will use Frontera to develop a single molecule reader of protein sequence, a game-changing protein characterization technology that promises to revolutionize proteomics. Armed with new structural data, we will build the most complete, up-to-date model of the nuclear pore complex, revealing the mechanical interplay between its structural elements and the transported molecular species. Building on our previous work that delivered the first all-atom structure of a complete, packaged virus particle, we will use Frontera to determine which physical phenomena govern the process of viral genome ejection.

Type: Renewal LRAC

Title: Renewal request for MCB20004: Petascale Integrative Approaches for de novo Protein Structure Prediction

Principal Investigator: Ken Dill (Stony Brook University (SUNY Stony Brook))
Co-Investigators: Sridip Parui (Stony Brook University (SUNY Stony Brook)); Christopher Foran (Stony Brook University (SUNY Stony Brook))

Field of Science: Biophysics

Abstract:

The living cell is a miniature factory of interacting molecular machines called proteins that underlie cellular functions by interacting with other proteins, DNA, and small molecules such as drugs. Their activity thus determines an organism's health and survival. Knowing the structure of proteins and having an understanding of the physical principles underlying their mechanisms are essential for advancing the field of molecular biology and for prospective drug discovery. We aim at developing and applying methods that use computational molecular physics (CMP) to understand biological systems. Molecular dynamics, a CMP method that we use here, provides a microscopic picture of proteins and their underlying mechanisms, including the thermodynamic and kinetic quantities that dictate behavior. When operational cycles of protein usually take tens of milliseconds, conventional MD with a powerful supercomputer could trace the dynamics up to microseconds. It is a daunting task of searching and sampling very high-dimensional, rugged energy landscapes to identify and characterize free-energy minima which can translate to a high computational cost. Our lab has developed MELD, which accelerates MD by orders of magnitude to find low free energy protein states and protein-ligand complexes.

Our Frontera allocation in 2022 was utilized to model large protein systems consisting of 100+ amino acids (AA), inherently containing a large conformational population, to compute the relative stability of physically relevant configurations and to explore their binding with ligands. All of that was made possible by integrating different types of data sources (crystallographic data, NMR data, knowledge-based information, etc.) with MELD x MD. We are requesting this renewal of our Leadership Resource Allocation on the Frontera supercomputer to continue the quest for multi-faceted development of our MELD x MD method for computational protein modeling. We believe our work will lead to a better understanding of the underlying mechanisms of the biological species responsible for diseases at the molecular level which will revolutionize the discovery of drug targets and the development of novel drugs. We therefore request 359,000 SUs to continue our research using Frontera's single-precision GPU partition.

Type: New LRAC

Title: Weighted ensemble rare-events sampling of complex biological processes

Principal Investigator: Lillian T. Chong (University of Pittsburgh (Pitt))
Co-Investigators: Arvind Ramanathan (Argonne National Laboratory (ANL)); Nicolas Frazee (University of Pittsburgh (Pitt))

Field of Science: Biophysics

Abstract:

We will investigate mechanisms of (i) an RNA-mediated phase separation process that is essential for the packaging of the coronavirus, and (ii) how drug candidates cross cellular membranes. As these processes occur on the ms-sec timescale, it would not be feasible to generate atomically detailed pathways of these processes using conventional simulations on typical computing resources. A combination of weighted ensemble rare-events sampling and Frontera supercomputing resources are essential for enabling the simulation of these processes.

Type: Renewal LRAC

Title: Hadron-Hadron scattering from lattice QCD

Principal Investigator: Colin Morningstar (Carnegie Mellon University (CMU))
Co-Investigators: Ben Hoerz (Intel Corp.); Andre Walker-Loud (Lawrence Berkeley National Laboratory (Berkeley Lab) (LBNL)); John Bulava (German Electron Synchrotron DESY); Andrew Hanlon (Brookhaven National Laboratory)

Field of Science: Nuclear Physics

Abstract:

A study of hadron-hadron scattering is proposed which will help us gain insight into the key physical mechanisms at work inside hadrons and nuclei. The proposed research lends support to current experiments, such as the GlueX experiment in Hall D at the Thomas Jefferson National Accelerator Facility, the Deep Underground Neutrino Experiment which will study neutrinos, an important elementary particle that permeates the universe, and proposed
neutrinoless double beta-decay experiments aimed at understanding if neutrinos are their own anti-particle, which if so, could help explain the abundance of matter over anti-matter in the universe.

Type: Renewal LRAC

Title: Research in Theoretical Hadronic Physics and Related Topics

Principal Investigator: Carl Carlson (William & Mary)
Co-Investigators: Christopher Monahan (William & Mary); David Richards (Jefferson Laboratory); Kostas Orginos (William & Mary)

Field of Science: Nuclear Physics

Abstract:

Lattice QCD enables a first-principles calculation of the properties of hadrons such as the pion and proton. This project studies the internal structure of the proton, the building block of everyday nuclear matter, in terms of the fundamental quarks and gluons of QCD. We have in the previous year successfully calculated and published work on quark and gluon parton distribution functions (PDFs), which give a useful one dimensional projected view of proton structure, and done so for both polarized and unpolarized cases. We will in the current year focus on calculating generalized parton distributions (GPDs) of quarks and gluons in a proton. These give a 3-dimensional picture of the proton, in both coordinate and momentum space. We will use new gauge configurations (the crucial structures underlying all lattice gauge theory calculations) at significantly finer spacings than have been available. This will allow more accuracy and lower systematic errors. Additionally, we will calculate the flavor structure of the proton sea, the so-called disconnected diagrams, which give important contributions to many processes, including affecting the gluon GPDs via mixing. The work is related to the experimental programs at Jefferson Lab, at RHIC, and at the future EIC.

Type: Renewal LRAC

Title: Emergent Phenomena and Ultrafast Dynamics of Nonequilibrium Correlated Systems

Principal Investigator: Cheng-Chien Chen (University of Alabama at Birmingham (UAB))
Co-Investigators:

Field of Science: Physics

Abstract:

The motion of elections through some materials can be highly correlated, such that the electrons behave as cars move in heavy traffic: they cannot maneuver freely and their motions are strongly influenced by others. These correlated electron materials often exhibit intriguing properties, such as unconventional superconductivity. Overcoming the knowledge gap in understanding electron correlation effects could open up revolutionary opportunities for future device applications. Here the PI will use the supercomputing capabilities at TACC to tackle the challenging problem of studying emergent phenomena and ultrafast dynamics of nonequilibrium correlated materials. Large-scale simulations will be performed for atomic-scale modeling, and the results will be compared directly to ultrafast spectroscopic measurements. The research topics address several of the 10 Big Ideas for Future NSF Investments and the Grand Challenges in Basic Energy Sciences, thereby having potential impacts on U.S. science leadership and energy-sustainable future.

Type: Renewal LRAC

Title: Precision Flavor Physics at the Intensity Frontier

Principal Investigator: Carleton DeTar (University of Utah)
Co-Investigators: Ruth Van de Water (Fermilab); Aida El Khadra (University of Illinois); Steven Gottlieb (Indiana University Bloomington)

Field of Science: Theoretical Physics

Abstract:

We request a renewal of our LRAC allocation on Frontera to make further progress with two multiyear projects aimed at searches for new particles and interactions beyond the Standard Model. This search requires close coordination between theory and experiment. As part of a worldwide campaign we seek clues in small discrepancies between experimental measurement and theoretical prediction. In this project we study two such measurements, namely, decays of the B and Bs mesons that contain a heavy b quark (heavy flavor) and determinations of the anomalous magnetic moment of the muon (light flavor). In both cases recent experimental measurements disagree with predictions of the current Standard Model of fundamental interactions. For the B meson the disgreements are at the level of two to three standard deviations. For the anomalous magnetic moment of the muon, currently at 4.2 standard deviations. These disagreements have prompted new experiments that will reduce, significantly, the measurement uncertainties. A parallel reduction in the uncertainty of the theoretical predictions is also needed. This project uses precise, ab initio methods of numerical lattice quantum chromodynamics and the power of Frontera to reduce the theoretical uncertainties.

Type: Renewal LRAC

Title: Large-scale simulations of lattice QCD with physical up, down, strange, and charm quarks

Principal Investigator: Martha Constantinou (Temple University)
Co-Investigators: Giannis Koutsou (The Cyprus Institute); Constantia Alexandrou (University of Cyprus and The Cyprus Institute)

Field of Science: Elementary Particle Physics

Abstract:

We propose the continuation of our LRAC project for large-scale simulation of the theory of the strong interactions, Quantum Chromodynamics (QCD), using a doublet of mass degenerate up and down quarks, a strange, and a charm quark (Nf=2+1+1) tuned to their physical mass values. For the upcoming allocation, we propose simulations using the twisted mass fermion formulation with a lattice spacing of a=0.05 fm, the smallest lattice spacing simulated with this action. Combined with the available ensembles at three larger lattice spacings also at the physical point, the simulation of this ensemble will enable a robust continuum extrapolation ($a \to 0$) of several key hadronic quantities. Specifically, we will consider nucleon observables that connect to the scientific program of the Electron Ion Collider (EIC), such as nucleon generalized parton distributions, thus providing input for the experiments being planned, as well as for the muon hadronic vacuum polarization being measured at Fermi Lab. With this ensemble we will be able to precisely investigate fundamental questions of nucleon structure, such as how the nucleon mass and spin arise from its constituent quarks and gluons, as well as the determination of its 3D structure through the computation of generalized parton distributions. Such science questions have been identified as high-priority by The National Academies of Sciences, Engineering, and Medicine (NAS) and will be directly targeted experimentally by EIC.

Type: Renewal LRAC

Title: Beyond Standard Model Physics with Neutron Electric Dipole Moment

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

Field of Science: Nuclear Physics

Abstract:

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

Type: New LRAC

Title: Numerical Relativity Simulations of Compact Binary Mergers

Principal Investigator: David Radice (Penn State University (PSU))
Co-Investigators: Peter Hammond (Penn State); Eduardo Gutierrez (Penn State University (PSU)); Alireza Rashti (Penn State University (PSU)); Pedro Espino (University of California Berkeley (UC Berkeley))

Field of Science: Gravitational Physics

Abstract:

Using our newly developed GR-Athena++ code, we will perform large-scale simulations of binary black hole and binary neutron star mergers. Our simulations of black hole binaries will have unprecedented resolution, allowing us to create a catalog of gravitational wave waveforms with sufficient accuracy for use in next-generation experiments such as LISA, the Einstein Telescope, and Cosmic Explorer. In addition, we will investigate the impact of magnetoturbulence and QCD phase transitions on the gravitational wave, electromagnetic, and high-energy neutrino signatures of binary neutron star mergers.

Type: New LRAC

Title: Light quark vacuum polarization at the physical point and contribution to the muon's anomalous magnetic moment

Principal Investigator: Thomas Blum (University of Connecticut (UCONN))
Co-Investigators: santiago peris (Autonomous University of Barcelona (Universitat Autnoma de Barcelona) (UAB)); Christopher Aubin (Fordham University); Maarten Golterman (San Francisco State University (SFSU))

Field of Science: Physics

Abstract:

The anomalous magnetic moment of the muon (or anomaly) represents one of the most precise experimental measurements ever made and provides an important opportunity to test the most fundamental laws of Nature, known as the Standard Model. The theory prediction for the muon anomaly, while as precise as experiment, disagrees by several standard deviations when certain data-driven methods are used to compute the contribution from quantum chromodynamics (QCD), the part of the Standard Model that describes the interactions between elementary quarks and gluons. On the other hand recent numerical simulations in lattice QCD show a smaller discrepancy between theory and experiment. In this work we carry out calculations on state-of-the-art lattices with large size and small lattice spacing to resolve the theory and confront experiment.