Type: New LRAC

Title: Machine learning accelerated reduced models for complex fluids

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

Field of Science: Advanced Scientific Computing

Abstract:
We request 410K service units to support research in machine learning accelerated reduced-order models of complex fluids flows for predictive simulations. Such flows describe numerous phenomena in biophysics, industrial processes, and medicine. Our focus in this project are red blood cells flows. The methodology is applicable to many other types of deformable particles. Examples include blood flow in small vessels, intra- and extra-cellular flows, flows in medical and industrial micro/nanofluidic devices, polymer flows, and amorphous materials. Simulations of complex flows are extremely challenging because they involve nonlocal hydrodynamic interactions, moving interfaces, near collisions, nonlinear interface mechanics, long-time horizons, and multiple time and space scales without clear scale separation. Despite the formidable challenges, tremendous advances in algorithms and their high-performance computing implementations nave enabled solutions of problems of unprecedented scale and complexity. Given such high costs, tasks like uncertainty quantification, parameter estimation, and design/control remain out of reach for complex fluids problems.

To deliver 1000X speedups over existing methods we propose deep learning algorithms that generalize to unseen data because they do not entirely substitute the simulation: instead, they are used in an operator splitting fashion within with a low-resolution simulation. We anticipate a number of broader impacts from the proposed project. (1) The generic complex fluid solvers developed in this project, will impact a broad spectrum of disciplines in sciences and engineering; (2) The multiscale modeling algorithms developed in this project will impact many other problems which are characterized by an evolving microstructure.

Type: Renewal LRAC

Title: The role of low collisionality in compressible, magnetized turbulence

Principal Investigator: Philipp Grete (Michigan State University)
Co-Investigators:

Field of Science: Astronomical Sciences

Abstract:

While our understanding of incompressible hydrodynamic turbulence has significantly advanced over the past decades, many critical questions in the realm of compressible magnetohydrodynamic (MHD) turbulence remain unanswered, particularly in the weakly collisional regime. This regime is of particular interest in astrophysics, where processes on a huge variety of scales are either governed or at least influenced by MHD turbulence and by anisotropic transport processes. Examples include energy transport in the solar convection zone, the interstellar medium with its star-forming molecular clouds, and the intergalactic and circumgalactic media, which offer crucial clues to galaxy formation. The behavior of weakly collisional, magnetized turbulence is also crucial to understanding the physics of high energy density plasma physics experiments such as Z-pinches and tokamaks. In all of these circumstances, modern computational models are typically unable to resolve the MHD turbulent cascade, and thus the predictive power of even the most advanced simulations are severely constrained.

One of the most important aspects of MHD turbulence is the transport of energy across spatial scales. Many uncertainties exist regarding the energy dynamics of MHD turbulence, including the existence of a universal turbulent cascade, the amplification of magnetic fields from small-scale turbulent motion, the behavior of the inverse cascade (i.e., the transfer of energy from smaller to large scales via magnetic fields), and dissipative and anisotropic transport processes. The primary reason for uncertainty in key quantities in magnetized turbulence is due to lack of numerical resolution and computational resources.

With this LRAC allocation we will execute the highest-resolution calculations of weakly compressible MHD turbulence using anisotropic transport ever achieved, fully resolving the MHD turbulent cascade and probing the energetics of both driven and decaying turbulence in great detail. We will perform subsonic ($M_s = 0.5$) simulations at $3{,}072^3$ cell resolution with an adiabatic equation of state, a realistic plasma cooling function, and anisotropic viscosity and thermal conductivity whose properties depend on the local magnetic field direction. Physical parameters will be chosen to be relevant to a range of astrophysical phenomena, focusing primarily on the intergalactic, circumgalactic, and intracluster media. These simulations, in combination with novel compressible shell-to-shell energy transfer analysis techniques pioneered by our collaboration, will address critical questions relating to the universality of the energy cascade in weakly collisional magnetized turbulence, the dissipation of energy in such turbulence, and the amplification of magnetic fields in small-scale dynamos.

The successful completion and analysis of these calculations will have substantial consequences for our understanding of magnetized, weakly compressible turbulence in the weakly collisional regime. Perhaps most importantly, it will contribute to the theoretical understanding of the energy cascade in this regime, and to the development of appropriate models for its behavior in astrophysical situations. This will be important for the development of subgrid models in simulations of cosmological structure formation and circumgalactic, intergalactic, and intracluster media that cannot fully resolve turbulence, and more

generally in the treatment of subgrid models in large eddy simulations of magnetized turbulence for a wide range of astrophysical applications.

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)
Co-Investigators:

Field of Science: Stellar Astronomy and Astrophysics

Abstract:
As set out in our funded NSF proposal, 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 difficulty describing the flow near convective boundaries. This is where material from just outside a convection 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 focusing 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 hydrodynamic 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 multifluid hydrodynamics. 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 we explore the ramifications for nucleosynthesis of our simulations.

Type: Renewal LRAC

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

Principal Investigator: Michael Norman (University of California, San Diego)
Co-Investigators: Brian O'Shea (Michigan State University); Greg L. Bryan (Columbia University); John Wise (Georgia Institute of Technology); James Bordner (University of California, 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. Five independent subprojects will carry out frontier simulations of the birth of galaxies and supermassive black holes, the physics of galactic winds, and the cosmic evolution of the intergalactic/circumgalactic medium.

Type: Renewal LRAC

Title: Rotational and Convective Instability and Transport in Collisionless Astrophysical Plasmas

Principal Investigator: Matthew Kunz (Princeton University)
Co-Investigators: Lev Arzamasskiy (Princeton University); Jonathan Squire (University of Otago); Eliot Quataert (University of California, Berkeley); Archie Bott (Princeton University)

Field of Science: Astronomical Sciences

Abstract:
The transport of energy and momentum by instabilities and turbulence are key ingredients in many problems at the frontiers of astrophysics research. Despite a decades-old appreciation for the influence of cosmic magnetism on the evolution of astrophysical systems and an ever-ripening interest in the impact of plasma-kinetic microphysics on "fluid" macrophysics, the community still lacks a rigorous and accurate means of incorporating this physics into large-scale astrophysical and cosmological simulations. This proposal represents a renewal of our pursuit to address this issue, now focusing on the transport of angular momentum and of heat in collisionless, magnetized astrophysical plasmas. Namely, we plan to carry out a series of ground-breaking hybrid-kinetic simulations of rotational and convective instability and turbulence, in which deviations from local thermodynamic equilibrium and the microscale kinetic instabilities they excite play a crucial role in influencing the macroscale evolution. This NSF-, DOE-, and NASA-funded work 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. The continued application of this novel code to frontier topics in plasma astrophysics on leadership-class facilities opens up new pathways for understanding the evolution of cosmic magnetic fields and their influence on the stability of and transport in the intracluster medium of galaxy clusters and low-luminosity black-hole accretion flows.

Type: Renewal LRAC

Title: Testing Fundamentally New Physics in Galaxies

Principal Investigator: Philip Hopkins (California Institute of Technology)
Co-Investigators:

Field of Science: Extragalactic Astronomy and Cosmology

Abstract:
This proposal will support a program to understand the origin and nature of galaxies, using massively-parallel simulations that follow the birth and evolution of galaxies and stars from the very early Universe into the present day. The simulations will model the origins, evolution, internal structure, and observable properties of galaxies ranging in size from the smallest observed ``dwarf'' galaxies (with just a few thousand stars) to the Milky Way and Andromeda (the ``Local Group'') and the most massive ``giant'' galaxies. Deep and fundamental questions remain unsolved in this area, including simply "How did we get from the Big Bang to the Milky Way?" As well as "Why did the Universe form so few stars [compared to its total mass]?", "Why did stars form where and when they did?," and "How can we use galaxies to probe the fundamental nature of dark matter?" At the heart of these issues lies the fact that stars, once they form, are not passive actors within a galaxy: the shine, and emit tremendous amounts of energy in the form of light (radiation), stellar winds, and (sometimes) supernova explosions. This energy can blow material out of the galaxy entirely and completely alter the evolutionary history of galaxies. But these processes remain poorly understood, in large part because they (a) couple very small and very large scales in the Universe, so require simulations with enormous dynamic range to model them, and (b) involve a diverse range of physics including (but not limited to) gravity, fluid dynamics, magnetic fields, conduction and viscosity, radiation-matter interactions, interstellar chemistry, relativistic plasma physics, black hole formation, and stellar evolution. The simulations proposed here will incorporate all of these processes into the highest-resolution simulations yet run, to allow us to address these questions for the first time at the level of detail needed to make observable predictions.

A wealth of exciting new observational projects promise to revolutionize our understanding of galaxy and star formation: from the LSST and Gaia measuring Milky Way stellar populations in game-changing detail, to the James Webb Space Telescope probing galaxies during cosmic ``first light,'' while the Hubble telescope identifies the long-``missing'' mass in the medium around galaxies. The cosmological hydrodynamic simulations we propose will be the most powerful tools to make detailed predictions and leverage these transformative observations. The simulations will support the Feedback In Realistic Environments (FIRE) project, a network of theorists at 14 institutions, including several NSF postdoctoral and graduate student fellows: this collaboration has developed new, fully-cosmological simulations of galaxy formation that explicitly follow the physics above. This proposal will push the frontiers of galaxy modeling into the next generation on all key fronts: physics, numerical accuracy, and dynamic range. This will provide new predictions for the structure of dark matter in the faintest galaxies, the origin and dynamics of outflows and the baryon cycle, the multi-phase nature of the medium around galaxy and galactic ``cold flows,'' the formation and growth of super-massive black holes, the origin of the heavy elements in the Universe, and the interactions between radiation and relativistic particles in space plasmas. The simulations will also directly support a program where non-astronomy high school students and undergraduates are involved directly in generating visualizations of simulations for planetarium shows, while high school teachers are trained to use the simulation data directly via interactive tools to

build in-classroom demonstrations and videos illustrating key curriculum topics. These programs have recently provided visualizations for planetaria, television shows, and nationally-distributed feature films. Our simulation code is also public and used by multiple groups in non-astronomy fields (in fluid dynamics, in particular); all new development of hydrodynamics algorithms and massively-parallel optimizations will be integrated into the public code for wider use.

Type: New LRAC

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

Principal Investigator: Michael Grudic (Northwestern University)
Co-Investigators: Anna Rosen (Harvard-Smithsonian Center for Astrophysics); Stella Offner (University of Texas at Austin); David Guszejnov (University of Texas at 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, which are subject to considerable theoretical uncertainty. We will use the newly-developed STARFORGE framework to perform a large parameter study of star formation simulations to account for essentially all physical mechanisms thought to be important in star formation, 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 star formation simulations to date. They will allow us to attack major open theoretical questions about star formation physics, to disentangle the presently-uncertain effects of each mechanism, and to interpret ambiguous observational data.

Type: New LRAC

Title: Multi-Dimensional, Multi-Physics Resolution of Core Collapse Supernova

Principal Investigator: David Vartanyan (University of California, Berkeley)
Co-Investigators: Joshua Dolence (Los Alamos National Laboratory); Matthew Coleman (Princeton University); Adam Burrows (Princeton University)

Field of Science: Stellar Astronomy and Astrophysics

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

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

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

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

Type: New LRAC

Title: Numerical Simulations of Interstellar Turbulence

Principal Investigator: Alexei Kritsuk (University of California, 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: New LRAC

Title: Cosmological Constraints from the Lyman-alpha Forest with Baryonic Modelling

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

Field of Science: Extragalactic Astronomy and Cosmology

Abstract:
The NSF's Dark Energy Spectroscopic Instrument (DESI) has just started a vast new survey of the Universe, and will measure the spectra of 35 million galaxies and quasars over the next five years. With this data we will be able to observe intergalactic physics in amazing detail. To understand these processes (such as the intergalactic Lyman-alpha forest) however requires theoretical modeling using simulations that are qualitatively more powerful than have been used
before. We will perform 50 simulations with different cosmological initial conditions, varying 8 parameters in total. Our simulation suite will be the first of its kind to include baryonic physics.

Type: New LRAC

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

Principal Investigator: Alexander Philippov (Princeton University)
Co-Investigators: Bart Ripperda (Simons Foundation, Flatiron Institute); Elias Most (Princeton University)

Field of Science: Astronomical Sciences

Abstract:
Fast Radio Bursts (FRBs) are transient radio phenomena with millisecond duration. While their precise origin is still unknown, several models have been investigated, including those connecting to magnetar flares. With the very recent observation of an FRB-like event associated with a galactic magnetar, the study of flares in magnetospheres of magnetars has become an even more important topic of current research in high-energy astrophysics. This particular event also featured and X-ray afterglow, for the first time enabling the study of multi-wavelength signals associated with FRBs and pointing to a likely importance of magnetic reconnection. Other scenarios for non-repeating FRBs included flares powered by the gravitational collapse of neutron stars into rotating black holes. Building upon our previous LRAC study of magnetic flares in binary neutron stars, we will investigate flares in relativistic magnetospheres of compact objects using global force-free simulations, as well as study their X-ray signals using first-principles kinetic simulations of radiative reconnection.

Type: New LRAC

Title: Magnetic reconnection and turbulence in extreme plasmas: jets and accretion flows of supermassive black holes

Principal Investigator: Gregory Werner (University of Colorado)
Co-Investigators: Mitchell Begelman (University of Colorado); Yuran Chen (University of Colorado Boulder); Dmitri Uzdensky (University of Colorado); Fabio Bacchini (University of Colorado); Vladimir Zhdankin (Princeton University)

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 generally 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. 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 these fundamental plasma processes---magnetic reconnection and turbulence---in 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 macroscopic scales large enough to allow extrapolation of understanding to astronomically-large accretion flows and jets of SMBHs. With Frontera, we can thus connect observed radiation to the basic plasma processes responsible for converting the energy between gravitational, magnetic, kinetic, and ultimately observable electromagnetic forms.

Type: Renewal LRAC

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

Principal Investigator: Tiziana DiMatteo (Carnegie Mellon University)
Co-Investigators: Yueying Ni (Carnegie Mellon University); Rupert Croft (Carnegie Mellon University); Simeon Bird (University of California-Riverside)

Field of Science: Extragalactic Astronomy and Cosmology

Abstract:
As telescopes and satellites become more powerful, observational data on galaxies, quasars and the matter in intergalactic space becomes more detailed, and covers a greater range of epochs and environments in the Universe. Our cosmological simulations must also become more detailed and more wide ranging in order to make predictions and test the effects of different physical processes and different dark matter candidates. We propose to use TACC Frontera to develop a new framework for cosmological simulations of galaxy formation.
In concert with the new technology we propose to merge deep learning with cosmological codes. We will combine expertise and existing super-scalable codes for petascale-plus cosmological hydrodynamic simulations with Machine Learning techniques to effectively create models on the scale of the observable Universe that incorporate information from higher resolution models of individual galaxies. This hybrid approach which will imply offloading our simulations to neural networks and other ML algorithms will enable us to predict quasar, supermassive black hole and galaxy properties in a way which is statistically identical to full hydrodynamic models but with a significant speed up.

Type: New LRAC

Title: Comprehensive Constraints on Self Interacting Dark Matter

Principal Investigator: Thomas Quinn (University of Washington)
Co-Investigators: Alexie Leauthaud (UCSC); Ferah Munshi (University of Oklahoma); Alyson Brooks (Rutgers University)

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: PRE-EVENTS Multiscale Space Weather Modeling

Principal Investigator: Gabor Toth (University of Michigan)
Co-Investigators: Bart van der Holst (University of Michigan); Ward Manchester (University of Michigan)

Field of Science: Solar Terrestrial Research

Abstract:
The goal of our PRE-EVENTS project is to predict extreme space weather events and their impact on Earth's environment by employing novel and unprecedented computational simulation techniques. We model solar eruptions from the solar corona to Earth's magnetosphere and determine the magnetospheric response from the global to the small kinetic scales. Our goal is to provide improved prediction of space weather as well as reliable assessment of the impacts of extreme events, in other words, estimate the consequences of worst-case scenarios.

Major space weather events are caused by large-scale expulsions of magnetized plasma from the Sun known as coronal mass ejections (CMEs) that typically travel to Earth in one to three days. These eruptions occur frequently, as often as several times per day during solar maximum, and cause geomagnetic storms by triggering sudden reconfigurations of the magnetosphere by magnetic reconnection. Extreme space weather events are caused by the most energetic CMEs, which drive sudden and extensive changes in the Earth's magnetic field producing among other effects, large-scale electric impulses that can melt transformers and cause cascading blackouts. The potential impact of such an event could far exceed even the largest hurricane or earthquake at the national level. Being able to predict extreme space weather is a challenging task, which requires both accurate simulations of CME structures when they reach Earth and the response of the magnetosphere.

The magnetic reconnection process that lies at the heart of space weather events depends on the magnetic field carried by the coronal mass ejection as well as on the plasma processes happening at small kinetic scales. Strong dayside magnetopause reconnection is expected when the solar wind carries southward pointing interplanetary magnetic field (negative IMF BZ). Reconnection in the magnetotail can be either triggered by changes in the solar wind and IMF, or spontaneously. These events result in magnetic storms producing rapid changes in the magnetic and electric fields. Accurate modeling of magnetic storms therefore requires prediction of the interplanetary magnetic field of CMEs and an accurate model for the reconnection process that happens on small scales.

Our research addresses both of these crucial issues by employing a complex multi-scale space weather model. The Space Weather Modeling Framework (SWMF) integrates and couples several first-principles based numerical models extending from the solar surface to the solar corona, the heliosphere, the outer magnetosphere, the inner magnetosphere, the radiation belts and the ionosphere.

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); James Juno (University of Maryland, College Park); Ammar Hakim (Princeton University)

Field of Science: Magnetospheric Physics

Abstract:
Understanding energy dissipation and entropy production in collisionless processes such as shocks 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 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 kinetic quasi-perpendicular shocks using fully kinetic 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)
Co-Investigators: Vadim Roytershteyn (n/a)

Field of Science: Solar Terrestrial Research

Abstract:
Developing deeper understanding of the physical processes operating in the heliosphere, the “local neighborhood” of the Sun in the universe, is of great importance for predicting space weather at Earth and other planets, which is necessary to mitigate possible consequences of hazardous space events that can harm humans and spacecraft. Interaction of the solar wind with the local interstellar medium plays a crucial role in shaping the boundary of the heliopshere and provides a fascinating natural laboratory where a multitude of physical phenomena not accessible in Earth-bound laboratories play an important role. Among them are shocks and turbulence in large-scale space and astrophysical plasma, as well as interplay between phenomena operating on small scales (e.g. magnetic reconnection and kinetic and fluid instabilities) and large-scale behavior of the astrophysical plasmas. This project addresses the fundamental physical processes accompanying the solar wind-interstellar medium interaction: acceleration of ions at shocks waves, penetration of the interstellar material into the heliosphere, generation of turbulence, etc. Proposed numerical simulations connect micro- and macro-scales, open new avenues in software development and data management, and help interpret observational data from multiple space missions, such as Advances Composition Explorer (ACE), Interstellar Boundary Explorer (IBEX), New Horizons, Parker Solar Probe, Solar Orbiter, Ulysses, Voyager 1 and 2, as well as Interstellar Mapping and Acceleration Probe (IMAP), scheduled for launch in 2024.

Type: Renewal LRAC

Title: Understanding and Predicting Climate Extremes Using a Global High-Resolution Earth System Model

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

Field of Science: Climate Dynamics

Abstract:
Due to the extremely high computing power needs and associated costs, the current generation of global climate models used for the Intergovernmental Panel on Climate Change (IPCC) (https://www.ipcc.ch) assessment report can only be run at low-resolution that excludes many small-scale climate phenomena in the simulations, including climate extremes such as tropical cyclones in the atmosphere and fronts and eddies in the ocean. As such, large uncertainties exist in our understanding of the trends and variability of climate extremes. And yet, the impact of these small-scale climate extremes on societies, economies, and ecosystems is enormous and long lasting. There is an urgent need to develop a comprehensive understanding of how increasing resolutions in the IPCC-class climate models can improve the ability of the models to simulate and predict climate extremes at regional and finer scales. The computing resources provided by Frontera at TACC allow us to directly address this urgent need. By leveraging the knowledge that we have gained from our ongoing NSF-funded project using a high-resolution regional modeling approach and other related projects, we propose to expand our knowledge base of high-resolution climate modeling by carrying out an unprecedented large ensemble of global climate simulations at a high spatial resolution that explicitly permit tropical cyclones and ocean fronts and eddies in the model. With the previous year's allocation on Frontera we have already made significant progress in this research effort. Not only have we completed the porting and optimization of a high-resolution Earth system model on Frontera, but we have also completed a set of two century-long, fully coupled, high-resolution climate simulations for the High-Resolution Model Intercomparison Project (https://collab.knmi.nl/project/highresmip/) endorsed by the IPCC. The results show significant improvement of climate extreme simulations by the high-resolution model than its low-resolution counterpart. In this renewal project, we propose to carry out a large ensemble of high-resolution climate prediction experiments to advance our understanding of the benefit of high-resolution in prediction of climate extremes.

Type: Renewal LRAC

Title: High resolution simulations of damage-producing supercell thunderstorms (Renewal)

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

Field of Science: Atmospheric Sciences

Abstract:
Supercell thunderstorms are long-lived, often violent storms that can produce devastating tornadoes. The understanding and prediction of these storms and the processes that involve tornadoes within them is a high priority for forecasters and research scientists. Currently, forecasters are unable to predict tornado behavior (onset, path, width, strength, and longevity) with any skill, and the false alarm rate for tornado warnings remains at about 70%, underscoring the fact that the processes that differentiate tornado occurrence from tornado failure remain elusive. Frontera resources are requested in order to conduct a wide variety of supercell simulations in different environments run at different resolutions. A large amount of lower resolution simulations in different environments will be conducted, with a selected set of environments from these simulations being run at tornado-resolving resolution (30 m). A single 10 m simulation, already begun, will be continued in order to most accurately capture the small scale flow features associated with tornado behavior.

Type: New LRAC

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

Principal Investigator: Gabor Toth (University of Michigan)
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: Renewal LRAC

Title: Data-driven, biologically constrained biophysical computational model of the hippocampal network at full scale

Principal Investigator: Ivan Soltesz (Stanford University)
Co-Investigators:

Field of Science: Neuroscience Biology

Abstract:
We propose to study how the hippocampal formation in the brain generates sharp-wave-ripples, which are events in the brain that are thought to represent replay of episodic memory sequences and are required for subsequent memory recall; as part of this effort, we are constructing the first full-scale computational model of the hippocampus, in order to provide insight into the dynamical properties of hippocampal networks that produce the feature selectivity and specific oscillatory patterns in neural ensembles that encode location information and generate episodic memory traces.

Type: Renewal LRAC

Title: Advancing Predictive Capability of High-throughput Methods for Drug Discovery

Principal Investigator: Darrin York (Rutgers University)
Co-Investigators:

Field of Science: Chemistry

Abstract:
Our original Frontera Leadership Resource Allocation (LRAC) proposal aimed at developing a novel computational high-throughput lead optimization (HTLO) pipeline to accelerate drug discovery through computer-aided drug design, and had three primary research objectives: 1) Develop performance-optimized protocols for benchmark quality ligand binding free energies, 2) Apply optimized protocols to benchmark
performance of GAFF and GAFF2 against "gold-standard" drug discovery dataset, and create key data infrastructure for reference potential "book-ending" methods, and 3) Use data infrastructure to develop and test performance-optimized protocols for accurate "book-ending" free energy methods that enable rapid development and assessment of new force fields for drug design.

We leveraged our current Frontera LRAC allocation to make several new methodological developments within the AMBER software (some of which are already made available in AMBER20) that led a total of 6 publications in the calendar year 2020. Key highlights of our work in the past year include a fruitful academia-industry collaboration with the company Silicon Therapeutics to develop several new features and performance enhancements for drug discovery that has led to three publications in 2020 and the release of the AMBER Drug Discovery Boost Package as a patch upgrade to
AMBER20.

Herein, we submit a renewal allocation proposal request to continue and extend our allocation on Frontera to support our research objectives in drug discovery that have the overarching aim of advancing the state of the art to achieve protein-ligand binding affinity predictions on libraries of compounds with chemical accuracy within hours using leadership-class GPU computing systems. Our research continues to be funded by a National Institutes of Health (NIH) grant (GM107485).

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)
Co-Investigators: Adrian Roitberg (University of Florida)

Field of Science: Physical Chemistry

Abstract:
Increased access to better computer hardware has made the generation of vast databases of molecular properties computed with high-level quantum mechanical methods a reality. With recent advances in machine learning methodologies, computational chemists and physicists have been searching for ways to extract physical insight from and improve upon these large databases. In our proposed research we aim to contribute to the field of machine-learned potential development. We will develop and use new ways to search chemical space for the generation of information-rich and diverse data sets of non-optimized molecules and energies for training machine-learned potentials. As part of this effort, we will improve our existing methods ANAKIN-ME and AIMNet, and develop algorithms for generating machine-learned potentials to increase accuracy and universality.

Through these improvements, we aim to continue the development of extensible and transferable deep learned potentials. Such potentials will bridge the gap between the speed of classical force fields and the accuracy and universality of quantum mechanical methods. This research will help lead to breakthroughs in a broad number of communities interested in in-silico experimentation by providing innovative and modern tools to the scientific community.

Type: New LRAC

Title: Characterizing Differential Dynamic Behavior of Glycosylated Spike proteins of SARS Coronaviruses 1 and 2

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

Field of Science: Biophysics; Physical Chemistry

Abstract:
Coronavirus spike protein, which binds to the same human receptor in both SARS coronaviruses 1 and 2 (SARS-CoV-1 and SARS-CoV-2), has been implied to be a potential source of the differential transmissibility of SARS-CoV-1 and 2, the causes of 2003 SARS epidemic and the ongoing COVID-19 pandemic. However, the mechanistic details of spike protein binding to its human receptor remain elusive at the molecular level. Here, we employ all-atom molecular dynamics (MD) simulations of SARS-CoV-1 and 2 spike proteins in conjunction with multi-copy path-finding algorithms and free energy calculations to determine the differential dynamic behavior of prefusion, glycosylated spike protein structure of the SARS-CoV-1 and three different variants of SARS_CoV-2 with different transmissibility levels. In particular, we are interested in the energetics and kinetics of large-scale conformational changes of the spike protein associated with the activation process, a step that occurs prior to the binding of spike protein to the human receptor. The mechanistic details associated with the spike protein activation could help us understand, at least partly, the differential behavior of SARS-CoV-1 and three different variants of SARS-CoV-2.

Type: Renewal LRAC

Title: Direct Numerical Simulation of Mach 6 Flow Over A 35 Degree Compression Ramp

Principal Investigator: Daniel Bodony (University of Illinois)
Co-Investigators:

Field of Science: Fluid, Particulate, and Hydraulic Systems

Abstract:
This is a renewal proposal for LRAC project CTS20006 (``Direct Numerical Simulation of Mach 6 Flow Over A 35 Degree Compression Ramp'') to continue to use Frontera to study hypersonic fluid-thermal-structure interaction (FTSI). Our first year of Frontera access was very successful and well documented. It also highlighted how little the hypersonics community understands its ground wind tunnels and the impact tunnel-specific features have on the interpretation and modeling of physical phenomena. Our renewal proposal seeks to complete our study of the FTSI of a compliant panel embedded in a 35 degree compression ramp and exposed to a uniform Mach 6 flow, a configuration that models a hypersonic vehicle's deflected control surface and which was experimentally tested at NASA Langley. Our specific objective is to predict the thermal-mechanical response of a compliant panel embedded in the ramp when the incoming flow is exposed to the freestream disturbances found in the experiment. We will use a high-order computational fluid dynamics code written by the PI that has shown readiness and excellent scalability on Frontera and that is coupled to a thermo-mechanical finite element solver through a parallelized C++ interface. We request 5,000,000 node-hours to support this project.

Type: Renewal LRAC

Title: Extreme events and particle dynamics in high Reynolds number turbulence

Principal Investigator: Pui-kuen Yeung (Georgia Institute of Technology)
Co-Investigators: Shankar Subramaniam (Iowa State University)

Field of Science: Fluid, Particulate, and Hydraulic Systems

Abstract:
This LRAC allocation will support a high-resolution study of turbulence focusing on the connection between extreme fluctuations and the dynamics of small particles, such as airborne disease agents transmitted by liquid droplets enclosing microscopic viral particles, that are transported by turbulent fluid flow. Extreme fluctuations in space, accessible only through such very large simulations, are expected to directly affect the acceleration and trajectories of these particles. Concentration of such particles by turbulent structures can thus be predicted, which can inform protocols to prevent or reduce disease transmission.

Type: New LRAC

Title: Study of Linear Global Instability of Three- Dimensional Hypersonic Shock/Laminar Separation Bubble Interaction using DSMC

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

Field of Science: Fluid, Particulate, and Hydraulic Systems

Abstract:
The goal of the proposed work is to understand the global linear instability mechanism of hypersonic laminar shock-wave/boundary-layer interactions (SBLI) at near-continuum flow regimes corresponding to altitudes of 55-70~km with the use of a high-fidelity, kinetic Direct Simulation Monte Carlo (DSMC) method.
To make efficient use of petascale facilities, we have developed an MPI-based solver known as Scalable Unstructured Gas-dynamics Adaptive mesh-Refinement (SUGAR) and demonstrated it to successfully to simulate a compute-intensive Mach 7 flow of nitrogen over a 30°-55° double-wedge using partially the FRONTERA leadership resource award (LRAC) granted for Yr 2020-2021 (CTS20001).
The exciting results from this simulation include the presence of spanwise-periodic flow structures in not only the separated region, as has already been seen in a multitude of experiments and numerical simulations, but also in the internal structure of the separation shock, as we have shown for the first time.
In the proposed work, we intend to investigate the coupling between the internal structure of the separation shock and a three-dimensional laminar separation bubble generated over canonical compression surfaces at hypersonic conditions.
We would also like to apply our newly-developed anisotropic conservation equation (ACE) formulation that improves upon traditional compressible Navier-Stokes equations (NSE) for linear instability analysis to predict whether hypersonic two-dimensional base flows over compression surfaces computed using DSMC are unstable to self-excited, small-amplitude, spanwise-homogeneous perturbations.

Type: New 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. The main goal of these numerical experiments is to test the hypothesis that structure and dynamics of turbulence over a porous sediment bed can be significantly different than that over an impermeable, rough wall. Bed permeability decreases anisotropy in the near-bed turbulence as compared to flow over an impermeable, rough wall and thus can alter momentum and mass transport across the sediment-water interface by influencing the sweep-burst cycle in turbulent boundary layers. The flow solver has been used for large-scale simulations on Teragrid machines (Lonestar, Comet, Stampede, Stampede2) for almost ten years wherein simulations were performed on about 150M CVs and up to 1500 processors for different particle-laden turbulent flow problems. Two NSF projects (one funded, one pending) and a graduate student internship at PNNL are based on large-scale computations proposed here.
For the above multiyear projects, a large-scale request of about {556,000 NODE-hrs} on the Frontera machine is planned for the LRAC solicitation.

Type: New LRAC

Title: Large-eddy simulations of solar PV arrays for higher system efficiency through enhanced convection

Principal Investigator: Marc Calaf (University of Utah)
Co-Investigators: Todd Harman (University of Utah)

Field of Science: Thermal Systems

Abstract:
This project aims to develop new solar photovoltaic (PV) module- and system-scale designs that increase the convective heat transfer coefficient of solar arrays by at least 40%, reducing the operating temperature of the solar PV panels, and leading to a boost of the annual energy yield by at least 5%. By achieving this goal, it is foreseen that we will further be able to decrease solar panel degradation by +0.3%/year, reducing the LCOE by 2.9-4.5 cent/kWh. This work consists of an experimental component based on scaled wind tunnel measurements, and a computational component that aims to model the atmospheric flow around solar modules within a solar farm. The computational resources allocated through this project will facilitate the execution of the latter component.

Type: Renewal LRAC

Title: Fundamental Studies in Nanomechanics: Optofluidics and Molecular Electronics

Principal Investigator: Narayana Aluru (University of Illinois at Urbana-Champaign)
Co-Investigators:

Field of Science: Mechanics and Materials

Abstract:
Ab initio and molecular simulations are widely used as predictive computational tools in emergent nanotechnology applications as they provide detailed physical insights at the atomistic scale in a wide range of scientific fields including energy, biophysics, and materials science. In this proposal, we aim to investigate interdisciplinary nanomechanics problems using quantum and molecular computational tools.

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)
Co-Investigators: Marvin Cohen (University of California, Berkeley)

Field of Science: Condensed Matter Physics

Abstract:
The primary goal of our group is to understand and predict materials properties at the most fundamental level using first-principles quantum-mechanical calculations. To achieve this goal, we take into consideration various interactions among quasiparticles and collective excitations in condensed matter systems (e.g., electron-electron interactions, electron-phonon interactions, exciton-photon interactions, etc.), as well as topological effects underlying the exotic electronic structure. A variety of different computational approaches (GW, GW-BSE, GWPT) are used that require only the atomic numbers and positions as inputs. These first-principles methods have, in the past, resulted in excellent quantitative agreement with experiment and have predicted with good accuracy materials properties that were later verified experimentally. Here, we propose to combine the multi-petascale computing capability of Frontera and our expertise in the first-principles study of condensed matter systems. With our recent implementation of GPU support in our massively parallel workhorse application -- BerkeleyGW, we are now ready to explore interactions and topological effects in condensed matter systems at unprecedented scale and with state-of-the-art efficiency.

Type: Renewal LRAC

Title: Spectral function database of correlated materials from first principles

Principal Investigator: David Vanderbilt (Rutgers University)
Co-Investigators: Subhasish Mandal (Rutgers University)

Field of Science: Condensed Matter Physics

Abstract:
Materials with strong electronic correlations have magnetic, optical and transport properties that are interesting for materials design, and useful in technological applications. While density functional theory (DFT) or DFT+U methods give quite accurate results for structural parameters in most materials, qualitative predictions of excited state properties usually requires beyond DFT methods such as the GW approximation, the dynamical mean field theory (DMFT), or, hybrid functionals. It is equally important to test these beyond-DFT methods for weakly correlated materials, in which DFT performs quite well. The existing materials databases, constructed in response to materials genome initiative, are built almost exclusively by DFT engines, and are thus very often making incorrect predictions in correlated materials. In this proposal we want to test the readiness and performance of beyond-DFT methods by testing them on a training set of materials which are both weakly and strongly correlated. There are several issues in using beyond DFT methods. One is the relative complexity of these methods, which are not so well tested, and many times do not have user-friendly interfaces. Our team includes world experts in beyond-DFT methods, which will allow us to overcome this difficulty. The second is the computational expense, which can increase dramatically for some materials. We carefully selected the set of materials, which should be representative, and still be computationally manageable in petascale computing facilities. The goal of this proposal allocation request is to test the set of beyond-DFT ab initio methods (hybrid functionals, DFT+DMFT, and GW), and build up a database of spectral functions and optical properties, and their comparison to available experiments. The database is now hosted at NIST (https://jarvis.nist.gov/jarvisbdft/) and freely available for public.

This allocation renewal request is intended to continue the seed support to develop a culture of data-sharing in the spirit of Materials Genome Initiative that will enable data-driven or data-intensive approaches to accelerate the discovery of 2D materials, their understanding, and related devices. Our Frontera project was initiated in 2019 in connection with a 2018 DMR-2D Data Framework supplement that funded a consortium of three collaborative NSF DMREF projects: 1629059 (Rutgers) + 1629079 (Tennessee); 1629346 (Rutgers) + 1629260 (Minnesota) + 1629477 (Penn State) + 1629457 (UCLA). The funding for this consortium is channeled via the Rutgers DMREF 1629059.

Type: New 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: New LRAC

Title: Engineering electron-phonon interactions in functional materials

Principal Investigator: Feliciano Giustino (University of Texas at Austin)
Co-Investigators: Joshua Leveillee (University of Texas at Austin)

Field of Science: Materials Research

Abstract:
The Center for Quantum Materials Design (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 solids and nanostructures. Full-system runs of the EPW code on Frontera with nearly 90% of the ideal speedup have been demonstrated during the 2020 Texascale Days. The aim of this project is to address some grand challenges in atomic-scale calculations of the transport, optical, and superconducting properties of advanced materials. We will use EPW to explore carrier transport in topological semimetals, gate-tunable superconductivity in superconducting semiconductors, electron hydrodynamics in two-dimensional materials, and light emission from halide perovskites. Throughout this project, we will continue to improve EPW in preparation for exascale computing.

Type: New 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:
Recent exciting discoveries of thousands of exoplanets beyond our solar system raised important questions about diversity of planetary systems, structure, evolution and physical state of the planetary materials subjected to extreme pressures and temperatures. The advent of powerful laser compressions and X-ray free electron laser diffraction experiments allows to recreate such conditions in the laboratory and to study exotic physics of planetary materials at extreme PT conditions with atomic resolution. However, a lack of predictive simulations of dynamic materials behavior at micrometer and nanosecond length and time scales substantially limits the discovery science return from these sophisticated but very expensive experiments.

This LRAC allocation project will advance the frontiers of classical molecular dynamics (MD) simulations by developing and applying machine-learning Spectral Neighbor Analysis Potentials (SNAP) to perform quantum-accurate predictive simulations of major exoplanetary material SiO_2 subjected to terapascal pressures (P) and temperatures (T) up 100,000 K characteristic of exoplanetary interiors. The project leverages recent breakthrough made by the PI's group – the revolutionary capability of SNAP to dramatically extend the time and length scales in quantum-accurate large-scale MD simulations by running extreme-scale calculations on the fastest HPC systems in the world.

Our overarching goals are (1) to extend SNAP to two-element materials by developing chem-SNAP to accurately describe novel fundamental physics of phase transformations at multi-Mbar pressures and multi-kK temperatures using a comprehensive set of first-principles quantum MD (QMD) training data; (2) to perform predictive simulations of dynamic compression of SiO_2 to uncover novel physics of solid-solid and solid-liquid phase transitions including appearance of novel metastable states, incongruent melting, kinematic frustration, and nucleation of new phases in intermediate liquid-like phase; (3) to devise a joint simulation and experimental program to conduct chem-SNAP MD simulations with quantum accuracy hand-in-hand with dynamic compression experiments of our collaborators while guiding experiments to focus on the most interesting predictions and promising leads and performing a comprehensive validation of our simulations.

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)
Co-Investigators: Rajitha Udawalpola (University of Connecticut); Anna Liljedahl (University of Alaska, Fairbanks); Kenton McHenry (National Center for Supercomputing Applications)

Field of Science: Earth Sciences

Abstract:
Warming climate has been radically changing the Arctic permafrost landscapes. Our understanding on spatiotemporal continuity of permafrost disturbances is yet constrained to local scales. The tundra region plays a major role in moderating the global climate system and, most urgently, through the release of potent greenhouse gases as permafrost thaws. However, the climate and land surface models that are used to assess this permafrost-carbon climate feedback are operating at spatial resolutions of several km's at best, while the footprint of field observations range from 0.1 to 100's of meters. Accordingly, a long-term challenge to the Arctic earth science community has been the linkage of the coarse climate models and the fine-scale observations. Sub-meter resolution commercial satellite imagery and advances in computing can now be merged to finally obtain a watching-eye over a large remote region that is experiencing rapid change including permafrost degradation. We are in the process of creating the first circumpolar ice-wedge polygon map based on very high spatial resolution (VHSR) commercial satellite imagery. We have developed an imagery-enabled pipeline (Mapping Application for Arctic Permafrost Land Environments – MAPLE) to automatically analyze large volumes of VHSR imagery using deep learning (DL) convolutional neural net algorithms. The ice-wedge polygon model is the first in what we envision a series of very high resolution permafrost thaw feature map products aimed for the broader science and public stakeholder communities. We are currently working under two projects funded by NSF's Office of Polar Programs (Award #s: 1720875, 1722572, 1927872, 1927723, 1927729), and includes the Navigating New Arctic initiative that is part of NSF's 10 Big Ideas. Our NSF funding has supported the model development and is also enabling the discovery and knowledge-generation from the imagery products, while also establishing a workflow for big imagery remote sensing analyses that apply advanced image analytics. The final map product is of great interest to the Arctic science and the climate modeling community as well as national and international stakeholders involved in the planning and management of infrastructure in a rapidly changing Arctic landscape.

Type: Renewal LRAC

Title: Simulating realistic subduction and lithosphere deformation

Principal Investigator: Lijun Liu (University of Illinois)
Co-Investigators:

Field of Science: Geophysics

Abstract:
How plate tectonics have shaped the Earth's surface geology (such as mountain building, basin formation, landscape evolution, volcanic activities and earthquakes) remains a fundamental question in geosciences. Key to this question is the uncertain variation in the style and dynamics of subduction, a process when cold oceanic plates recycle into the Earth's warm interior. In this proposal, we plan to study the causes and consequences of flat-slab subduction (i.e., down-going plates travel sub-horizontally beneath the lithosphere before sinking into the mantle) that has found to be greatly affecting the evolution of continents. This problem has been traditionally difficult to understand due to the many complexities and unknowns involved. Fortunately, the recent progress in geophysical data acquisition and high performance computing makes it possible to tackle this important geodynamic problem by building sophisticated physical models using various techniques of data assimilation. Using our previous experience on constructing both forward and inverse data-oriented models (similar to how weather prediction works), we will explore the subduction history in South America, North America and East Asia, where multiple flat-slab epochs have likely occurred and shaped the unique geology surrounding the Pacific Ocean. Results from this project will help to better understand not only basic earth evolution but also formation of natural hazards and resources.

Type: New LRAC

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

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

Field of Science: Geophysics

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

Type: New 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 & 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 physics of wave propagation. Adjoint tomography efficiently takes advantage of 3D wave simulations leading 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 only traveltimes, our goal is to construct a new global anelastic mantle model by the simultaneous inversion of anelastic and elastic parameters based on adjoin tomography including amplitudes of waveforms. Furthermore, we aim to finalize our ongoing azimuthally-anisotropic global adjoint model with the requested allocation. As anelasticity also causes physical dispersion, accurate anelastic models also allows for locating earthquakes and other seismic sources more accurately. This will result in 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. We request 3,250,000 Frontera CLX SUs to perform the proposed project.

Type: Renewal LRAC

Title: Emergent Phenomena and Ultrafast Dynamics of Nonequilibrium Correlated Systems

Principal Investigator: Cheng-Chien Chen (University of Alabama at Birmingham)
Co-Investigators: CHIA MIN LIN (University of Alabama at Birmingham); WEI-CHIH CHEN (University of Alabama at Birmingham)

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: Petascale Integrative Approaches for de novo Protein Structure Prediction

Principal Investigator: Ken Dill (Laufer Center, Stony Brook University)
Co-Investigators: Emiliano Brini (Stony Brook University)

Field of Science: Biophysics

Abstract:
We propose to use Molecular Dynamics (MD) simulations on Frontera's leadership class computational resources to understand the physical principles underlying protein actions in biology. Physics is needed for free energies, driving forces, binding affinities, motions and mechanisms. The computational challenge is the exploration of very high-dimensional rugged landscapes to find global optima; it is computationally very costly even with supercomputing. To tackle this limitation we developed MELD, a tool that leverages external information to accelerate physics based MD, importantly preserving the Boltzmann distribution properties. MELD is now making tractable problems that were prohibitive before. Our research focuses on predicting protein structures and interactions with other proteins and small molecules. This has direct application in drug discovery and drug formulation.

Type: Renewal LRAC

Title: Large-Scale All-Atom Simulations of Neutral-Solute Transporters in Cell-Like Environments

Principal Investigator: Liao Chen (University of Texas at San Antonio)
Co-Investigators:

Field of Science: Theoretical Physics; Biophysics; Cross-Disciplinary Activities

Abstract:
The state-of-the-art high-performance computing enables researchers to simulate the motions of millions of atoms interacting with one another. Now it is feasible to produce quantitative predictions of biological functions of a protein that are “deterministic” out of the atomistic interactions and motions that are stochastic in nature. In this project, the researchers propose to study the functions of several neutral-solute transporters/carriers, aquaporins (AQPs) and glucose transporters (GLUTs), that are fundamental to biology in general and to human physiology in specific. They will build the transporters and their biological environments from atoms up, simulate their stochastic dynamics, and elucidate their deterministic functional behaviors under various controllable conditions. Specifically, they aim to conduct full investigations of several water-glycerol channels--- aquaglyceroporins (especially, E. coli GlpF vs. human AQP3) and one neutral solute carrier (human GLUT1) by conducting very large-scale simulations of the all-atom models of these channel/transporter proteins. With the PI’s C++ modules for hybrid molecular dynamics (MD) integrated with the NAMD 2.13 source code, they will be able to take full advantage of the well-tested highly scalable MD engine, the high-resolution protein structures, the mature CHARMM force field parameters etc. They will harness the massively parallel computing power afforded by Frontera to solve several outstanding questions about these biological machineries in a quantitatively predictive manner.

Type: Renewal LRAC

Title: QM/MM studies of ibrutinib covalent kinase inhibitor

Principal Investigator: Benoit Roux (University of Chicago)
Co-Investigators:

Field of Science: Biochemistry and Molecular Structure and Function

Abstract:
Protein kinases is an important class of signaling enzymes implicated in numerous pathologies including cancer. These proteins are key therapeutic targets, and discovering kinase-specific inhibitors is an intensely pursued topic within the pharmaceutical industry. To optimize specificity and potency, there is increased interest in inhibitor molecules that bind covalently to their kinase target. The binding of covalent inhibitors involve multiple reactive steps that need to be treated theoretically within a Quantum Mechanical (QM) framework. Our long-term objective is to develop a general computational approach to investigate the formation of covalent linkages (reversible or irreversible) between a ligand and a target protein. Specifically, we seek to explain the specificity and reactivity of a known anti-cancer drug (ibrutinib), which binds covalently and irreversibly to a cysteine residue in the active site of Bruton's tyrosine kinase (BTK). To investigate whether the complete reaction takes place in separate steps or a single complex concerted step, we will determine the reaction pathway using the string method with swarms-of-trajectories.

Type: Renewal LRAC

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

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

Field of Science: Organic and Macromolecular Chemistry

Abstract:
The Cheatham lab will continue to apply the AMBER suite of biomolecular simulation and analysis tools to study nucleic acids and proteins and their interactions with ligands and continue assess, validate, optimize and improve force fields for RNA.

Type: Renewal LRAC

Title: Molecular architecture of paracellular ion transport barriers

Principal Investigator: Fatemeh Khalili (University of Illinois at Chicago)
Co-Investigators:

Field of Science: Biophysics

Abstract:
Permeation of water, ions and small molecules through the space between adjacent cells is controlled by macromolecular protein structures known as tight junctions. Tight junctions seal the paracellular space and act as barriers that limit the diffusion of molecules down their electrochemical gradient. Claudins are one of the major components of tight junctions and play a key role in determining paracellular permeability. Little is known about the assembly of claudins and the architecture of tight junction pores. We have recently build an atomic model of claudin pores and have verified its function using molecular dynamics simulations. However, the architecture of tight junctions at cellular level is still unknown. In this project, we use MD simulations to investigate mechanical properties of tight junction strands and their morphology computationally.

Type: Renewal LRAC

Title: Multi-Resolution Simulations of Mesoscale Biological Systems

Principal Investigator: Aleksei Aksimentiev (University of Illinois)
Co-Investigators:

Field of Science: Biophysics

Abstract:
This proposal requests an allocation on Frontera to carry our several pioneering simulations that will answer fundamental questions about the structural organization and biological function of exceptionally important biomolecular systems. Using a multi-resolution simulation approach, we will determine the microscopic structure of an mRNA vaccine delivery particle, informing future vaccine development efforts on physical interactions affecting shelf life and setting the stage for full-scale simulation of the vaccine delivery process. Building on our successful reconstruction of the structure of a bacteriophage virus genome, we will assemble and simulate a complete all-atom model of the Dengue virus, which may reveal new pharmaceutical targets and, methodologically, advance us a step closer to building complete molecular models of other medically-relevant RNA viruses, such as Influenza and SARS-Cov-2. Our landmark all-atom simulation of a nuclear pore complex in an in vivo-like environment will determine the global arrangement of disordered proteins mesh that serve as the key barrier to nuclear transit, uncovering how these proteins collectively interact with transport factors, which are known to ferry larger cargo. Having previously developed a model of a biological condensate, we will now apply the model to reveal how a polymerase is recruited into the membraneless organelle where it is activated for transcription.

Type: New LRAC

Title: Conformational Stability of Folded Proteins and Aggregation of Disordered Proteins under Cellular Solution Conditions

Principal Investigator: Joan-Emma Shea (University of California, Santa Barbara)
Co-Investigators: PRITAM GANGULY (University of California, Santa Barbara)

Field of Science: Biophysics

Abstract:
This LRAC grant focuses on two scientific problems: 1) the mechanism by which osmolyte mixtures stabilize proteins, and 2) the early stages of aggregation of intrinsically disordered proteins implicated in Alzheimer's disease. Project 1: In response to high osmotic pressure, many marine organisms accumulate urea, a protein-denaturant. To counteract the deleterious effects of urea, these organisms also accumulate a variety of small organic molecules, collectively termed protein-protective osmolytes or osmoprotectants, which stabilize the functional structures of cellular proteins. The mechanisms by which osmoprotectants counteract urea-induced denaturation, and how different osmoprotectants can act competitively or synergistically is poorly understood. Using enhanced-sampling replica-exchange molecular dynamics (REMD) simulations, we will investigate the molecular mechanisms responsible for the protein-protective properties of two of the most common osmoprotectants, trimethylamine N-oxide and glycine betaine, under mixed solvent conditions. Project 2: The formation of intraneuronal neurofibrillary tangles of Tau protein and extracellular deposits of amyloid-beta plaques in the brain are hallmark of Alzheimer’s disease. Using REMD simulations, we will probe the early stages of aggregation of Tau fragments belonging to the microtubule binding domain of the Tau protein. We will also investigate the mechanism by which the human innate immune peptide Cathelicidin LL-37, an amyloid inhibitor, modulates the early-stage oligomerization of amyloid beta.

Type: New LRAC

Title: Investigating the Complete SARS-CoV-2 Envelope Using Atomistic Simulations

Principal Investigator: Emad Tajkhorshid (University of Illinois)
Co-Investigators:

Field of Science: Biochemistry and Molecular Structure and Function

Abstract:
The pandemic caused by SARS-CoV-2 virus has resulted in huge impacts on our lives and our societies, calling for immediate attention of the entire scientific community to extensively study the viral infection at all levels and to pave the way for developing novel therapeutics against the virus. To that end, understanding the molecular details of the SARS-CoV-2 viral envelope structure, which is the most relevant part of the virus when interacting with and infecting human cells, is of paramount importance. The primary objective of this application is to develop the most complete structure for the SARS-CoV-2 envelope and to describe, at an atomistic level, its dynamics.This is an absolutely necessary step towards enabling rational molecular approaches towards developing novel diagnostic tools and therapeutic means against the viral infection. The computational approach proposed here parallels and complements ongoing extensive experimental effort in structural biology with the same goal, namely developing the full-scale model of the whole virus.

Three structural proteins (S, M, and E) compose the envelope of SARS-CoV-2, with the S protein playing a key role in initial contact and fusion with the host cell, thereby initiating the infection. The prime focus of the majority of computational researchers has been on studying the dynamics of S protein (either separately or together with the human receptor) by simulating its homo-trimeric form in isolation, i.e., outside the context of the whole envelope. A major milestone in our project is to construct a complete atomistic SARS-CoV-2 envelope with a realistic spatial scale and accurate density. This project leverages advanced computational techniques developed in our lab over the past few years specifically for modeling and simulation of cell-scale membrane systems. We utilize structural data from different experimental sources (e.g., cryo-EM and NMR), as well as employ template and machine learning-based modeling methods and MD simulations.

The resulting integrative model of the complete SARS-CoV-2 envelope will be then simulated using our program NAMD (tested for billion-atom, cell-scale models) to describe in situ dynamics and interaction of the envelope proteins. The resulting atomic-level models will allow for next-generation drug design approaches through small molecule docking and screening performed on a complete viral envelope. We envision that the resulting model and the simulation trajectory will pave the way for the next natural steps in modeling the viral infection, namely, developing a full virus model (with nucleic acids), and studying the initial encounter of the virus with a host cell.

Type: Renewal LRAC

Title: Unraveling Hadron Mass and Quark Structure with COMPASS and COMPASS++/AMBER

Principal Investigator: Caroline Riedl (University of Illinois at Urbana-Champaign)
Co-Investigators: Matthias Perdekamp (University of Illinois); Riccardo Longo (University of Illinois); Vincent Andrieux (University of Illinois)

Field of Science: Nuclear Physics

Abstract:
We study transverse degrees of freedom of quarks and gluons in the nucleon by analyzing data from the particle-physics experiment COMPASS at CERN. Our work aims to fully characterize the interior quark structure of the proton and to understand the dynamics of quark-gluon interactions in Quantum Chromo Dynamics. In addition we will carry out simulations guiding the development of new instrumentation for the future COMPASS++/AMBER experimental facility at CERN. AMBER measurements will investigate the differences in the dynamic mass generation through QCD interactions in pions, kaons and protons and aim to explain the wide spectrum of hadron masses observed in nature. In summary the work will create a detailed understanding of the quark structure of hadrons and of the generation of the large nuclear masses observed in nature.

Type: Renewal LRAC

Title: Kinetic characterization of 3D magnetic reconnection

Principal Investigator: Shan Wang (University of Maryland)
Co-Investigators: Li-Jen Chen (NASA Goddard Space Flight Center); Wei Xiang Jonathan Ng (University of Maryland)

Field of Science: Physics

Abstract:
We request to renew the project PHY20005 for the upcoming allocation year starting on 4/1/2021. The project is to study 3D kinetics in 3D magnetic reconnection, including (1) lower-hybrid waves, (2) ion heating, and (3) reconnection in ion instabilities in the shock transition region. In the current year, we performed 2D and 3D simulations of reconnection starting from the Harris current sheet. The ongoing analyses show that the 3D system develops various types of fluctuations along the current direction that may or may not have response of ions. The 1D and 2D simulations of ion instabilities show the development of magnetic field pulsations, resembling the structures in observations. The studies have led to 3 publications (and at least 2 in preparation) and a new grant. In the upcoming year, we propose to perform additional 2D Harris sheet simulations, 3D simulations of localized structures, and 2D simulations of ion instabilities, to further study the proposed objectives. We request 360,000 SUs computation time on Frontera, and 400TB disk space on Ranch.

Type: Renewal LRAC

Title: Eccentric binary black hole simulations for LIGO observations

Principal Investigator: Carlos Lousto (Rochester Institute of Technology)
Co-Investigators: James Healy (Rochester Institute of Technology)

Field of Science: Gravitational Physics

Abstract:
Three body encounters and accretion effects can lead to highly eccentric binaries, with residual eccentricity surviving down to merger, and these eccentric binaries may have very interesting Gravitational Waves signals that cannot be adequately modeled using quasicircular approximations.

The goal of this project is to model the gravitational waves signals associated with eccentric BHB late inspiral and mergers. These studies will be based on full numerical evolutions of the binary to study the dynamics and waveforms of precessing quasicircular and eccentric binaries in the merger phase, and evaluate its impact on LIGO-Virgo parameter estimations.

The plan of work consists of 3 stages: i) Design full Numerical Relativity simulations (3 resolutions) of non-spinning, mass-ratio $q=1$, eccentric $e\sim0.5$, binary configurations to evolve for the last 20 orbits before merger ii) Same as before, but for aligned spin (of large hole); Design of aligned spinning large black hole, $S/m^2=0.9$, mass ratio $q=1/2$, eccentric $e\sim0.5$, binary configurations to evolve for the last 40 orbits before merger and obtain full waveforms for the Numerical Relativity simulations (3 resolutions). iii) Same as above, but for miss-aligned spin (large hole); Design miss-aligned spinning large black hole, $S/m^2=0.9$, mass ratio $q=1/4$, eccentric $e\sim0.5$, binary configuration to evolve for the last 80 orbits before merger to obtain waveforms for the corresponding Numerical Relativity simulations (3 resolutions).

Type: Renewal LRAC

Title: Grid-based gyrokinetic simulations for studying confinement properties of negative triangularity tokamaks

Principal Investigator: Frank Jenko (Max Planck Institute of Plasma Physics)
Co-Investigators: Gabriele Merlo (University of Texas at Austin)

Field of Science: Theoretical Physics

Abstract:
This project is a continuation of a Frontera allocation awarded for the first LRAC cycle (PHY20008), targeting gyrokinetic simulations of turbulent transport in magnetic confinement fusion plasmas. One of the world-leading codes used for this purpose, GENE, will be employed to address outstanding open questions related to the influence of plasma shaping, namely negative triangularity δ, on plasma confinement. We plan to continue our ongoing investigations by looking, in particular, at a pair of discharges in the DIII-D tokamak, which indicate that $\delta < 0$ might be a very appealing candidate regime for future fusion power plants. Global simulations will be performed to investigate the near-edge region, which is know to be a crucial element in setting the overall confinement properties. A dedicated set of runs will be devoted to quantify the importance of multiscale interactions, which have been identified as potentially relevant in the first cycle.

Type: Renewal LRAC

Title: Hadron-Hadron scattering from lattice QCD

Principal Investigator: Colin Morningstar (Carnegie Mellon University)
Co-Investigators: Ben Hoerz (Lawrence Berkeley National Laboratory); Andre Walker-Loud (Lawrence Berkeley National Laboratory); John Bulava (n/a); 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 (College of William and 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 pion, the lightest hadron, and of the proton, the building block of everyday nuclear matter, in terms of the fundamental quarks and gluons of QCD. In the current year, we will generate new gauge configurations (the crucial structures underlying all lattice gauge theory calculations) at significantly finer spacings than presently available. This will allow more accuracy and lower systematic errors. We will use the new, and existing gauge configurations to calculate generalized parton distributions (GPDs) of quarks and gluons in a proton. GPDs give a 3-dimensional picture of the proton, in both coordinate and momentum space. 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 by mixing. The work is related to the experimental programs at Jefferson Lab, at RHIC, and at the future EIC.

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)

Field of Science: Theoretical Physics

Abstract:
The search for new particles and interactions lies at the heart of high energy physics research, and requires close coordination between theory and experiment. Searches at the "intensity frontier" 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. The disgreements are at the level of two to three standard deviations. These disagreements have prompted new experiments that will reduce, significantly, the measurement uncertainties. A parallel reduction in the uncertainty of the theoretical prediction 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: New 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 a large-scale simulation of the theory of the strong interactions, Quantum Chromodynamics (QCD), using a doublet of degenerate up and down quarks, a strange and a charm quark (Nf=2+1+1) tuned to their physical mass values. We target simulations using the twisted mass fermion formulation with a lattice spacing of a~0.06 fm, the smallest ever simulated using this discretization of the QCD action. The simulation will allow for a first continuum limit study directly at the physical point of key nucleon observables of relevance to the scientific program of the Electron Ion Collider (EIC), thus providing input and helping interpret results of the experiments being planned at the EIC. Quantities that will be targeted using these simulations are connected to 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 and tomography through the computation of parton distribution functions and 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. A similar effort from theory is imperative, and is the main objective of this proposal.

Type: New LRAC

Title: Ab initio nuclear structure and reactions for light to medium-mass nuclei

Principal Investigator: Kristina Launey (Louisiana State University)
Co-Investigators: Daniel Langr (Czech Technical University in Prague); Tomas Dytrych (Louisiana State University)

Field of Science: Nuclear Physics

Abstract:
The recent advent of radioactive beam facilities has enabled exotic-nuclei measurements, based on collisions of nuclei and their reactions. To predict inaccessible nuclei, these reactions must be well understood and modeled. However, exact solutions exist up to about five particles. The objective of this program is to expand dramatically the capabilities of nuclear reaction theory, by providing input to reaction simulations that is anchored in first principles but also can accommodate heavier nuclei and enhanced deformation by exploiting symmetries known to dominate in nuclei. This can help address the origin of elements and neutrino properties, two of the biggest challenges in physics today, and will have a wider impact since nuclear energy and national security research has similar needs. Future leaders (postdocs and students) will be trained in low-energy nuclear science and petascale computing, while preparing a web-database for research and educational purposes. The overarching goal is to learn from and inform experiments at radioactive beam facilities, and to predict properties of experimentally inaccessible nuclei that are key to advancing our knowledge about astrophysical processes and neutrino physics. The program targets to improve reaction modeling, by constructing the effective interaction between a target and a projectile from first principles (historically, referred to as an optical potential and fitted to experimental data), and thus to account for the challenging microscopic structure of the participating nuclei. As these interactions are an essential input to numerous reaction models that are currently in use, the new developments will serve as an important tool in a broad spectrum of studies.

Type: New LRAC

Title: An accelerated path to a Negative Triangularity tokamak reactor using first principle models

Principal Investigator: Alessandro Marinoni (Massachusetts Institute of Technology)
Co-Investigators: Federico Halpern (n/a)

Field of Science: Physics

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

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

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

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

Type: New LRAC

Title: Nuclear Physics from the Standard Model

Principal Investigator: Phiala Shanahan (Massachusetts Institute of Technology)
Co-Investigators: Assumpta Parreno (University of Barcelona); Zohreh Davoudi (University of Maryland); Michael Wagman (Fermi National Accelerator Laboratory); William Detmold (Massachusetts Institute of Technology)

Field of Science: Nuclear Physics

Abstract:
Understanding the physics of atomic nuclei, which make up more than 99% of the visible matter in the universe, is central to understanding the world around us. Particularly important are the questions: How does the complex structure of a nucleus arise from the dynamics of the quarks and gluons described by the Standard Model which, along with gravity, is our current description of Nature? How do nuclei interact with each other, and with other Standard Model particles? How can new physics beyond the Standard Model be discovered using nuclear isotopes as targets? The Lattice Quantum Chromodynamics calculations proposed in this project will address parts of these broad questions and further elucidate the nuclear realm.
In particular, through computations of the spectroscopy of light nuclei we will be able to demonstrate that nuclei can be understood directly from the Standard Model of particle physics. Calculations of scalar matrix elements will provide constraints critical to the interpretation of direct experimental searches for dark matter, and studies of axial currents will enable theory predictions of weak processes including the cross-section for the low-energy pp-fusion process that powers the Sun. This proposal is submitted by the Nuclear Physics from Lattice QCD (NPLQCD) collaboration, which has led the development of lattice QCD for nuclear physics over the last decade. This project will build on the previous work to reach a new milestone: the first time that calculations of nuclear structure with controlled systematic uncertainties have been achieved from QCD. The results will directly impact priorities of the U.S. nuclear physics community as stated in the Nuclear Science Advisory Council long range plan.