Type: Renewal LRAC

Title: Machine learning accelerated reduced models for complex fluids

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

Field of Science: Advanced Scientific Computing

Abstract:

We request 210K 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: 3-D Stellar Hydrodynamics of Convective Boundary Mixing and Shell Mergers in Massive Stars

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

Field of Science: Stellar Astronomy and Astrophysics

Abstract:

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 (UCSD) (UC San Diego))
Co-Investigators: James Bordner (University of California San Diego (UCSD) (UC San Diego)); John Wise (Georgia Institute of Technology); Greg L. Bryan (Columbia University); Brian O'Shea (Michigan State University (MSU))

Field of Science: Extragalactic Astronomy and Cosmology

Abstract:

This request will support our 4 institution team which is applying the Enzo and Enzo-E hydrodynamic cosmolog code to the formation of first and second generation stars, the first galaxies, and radiative mixing layers in the multiphase interstellar medium of galaxies.

Type: Renewal LRAC

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

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

Field of Science: Astronomical Sciences

Abstract:

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

Type: Renewal LRAC

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

Principal Investigator: Michael Grudic (Carnegie Institution for Science (Carnegie Science))
Co-Investigators: David Guszejnov (University of Texas at Austin (UT) (UT Austin)); Stella Offner (University of Texas at Austin (UT) (UT Austin)); Anna Rosen (Center for Astrophysics Harvard & Smithsonian (CfA))

Field of Science: Astronomical Sciences

Abstract:

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

Type: Renewal LRAC

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

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

Field of Science: Stellar Astronomy and Astrophysics

Abstract:

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

Type: Renewal LRAC

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

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

Field of Science: Extragalactic Astronomy and Cosmology

Abstract:

This renewal will continue to improve our emulator for Lyman alpha cosmology, generated with the current LRAC. We will perform further MP-Gadget simulations, including baryonic physics, to improve overall interpolation accuracy. We will extend our coverage to higher redshift using a few high resolution simulations and our recently developed multi-fidelity modelling technique. Results will be compared to upcoming data from the Dark Energy Spectroscopic Instrument and will be used for constraining cosmological parameters.

Type: Renewal LRAC

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

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

Field of Science: Astronomical Sciences

Abstract:

Event Horizon Telescope observations show that the accretion flows around supermassive black holes are likely to be in a particular scenario, the magnetically arrested state. Episodic magnetic reconnection in this state was conjectured to power observed multi-wavelength flares. In this proposal we will use a combination of first-principles large-scale numerical simulations to test this hypothesis. Reconnection can also occur in merging neutron star-black hole binaries, and we will investigate whether it can give rise to observable electromagnetic precursors prior to the gravitational-wave signals.

Type: Renewal LRAC

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

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

Field of Science: Extragalactic Astronomy and Cosmology

Abstract:

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

Type: Renewal LRAC

Title: Comprehensive Constraints on Self Interacting Dark Matter

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

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: New LRAC

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

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

Field of Science: Astronomical Sciences

Abstract:

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

We propose to use first-principles particle-in-cell (PIC) simulations to study these fundamental plasma processes--magnetic reconnection and MRI-driven 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 mesoscopic scales where energy is injected by astrophysical instabilities in accretion flows and jets of SMBHs. With Frontera, we can thus investigate the basic plasma processes responsible for converting the energy between gravitational, magnetic, kinetic, and ultimately observable electromagnetic forms.

Type: New LRAC

Title: Numerical Simulations of Interstellar Turbulence

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

Field of Science: Extragalactic Astronomy and Cosmology

Abstract:

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

Type: Renewal LRAC

Title: Heating and Particle Energization in Space and Astrophysical Plasmas

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

Field of Science: Magnetospheric Physics; Solar Terrestrial Research

Abstract:

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

To improve our understanding of plasma heating and distribution function dynamics in weakly collisional plasmas, we propose to study kinetic instabilities that regulate both macro-scale properties as well as energy dissipation in shocks, and large-scale, high resolution turbulence 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 (UAH))
Co-Investigators: Vadim Roytershteyn (Unknown Institution)

Field of Science: Solar Terrestrial Research

Abstract:

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

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

Type: Renewal LRAC

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

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

Field of Science: Climate Dynamics

Abstract:

Climate change-driven adverse ocean impacts are already affecting many rural, coastal, fishing-dependent communities, and these adverse impacts will likely accelerate for the foreseeable future. Forecasting potential changes in eastern boundary upwelling systems has benefitted recently from improvements in the resolution of global Earth system models, so that the latest eddy-resolving models at 10 km ocean resolution have greatly reduced systematic errors relative to observations. This project aims to use these advancements to improve forecasts of the fisheries potential of the California Current Ecosystem and improve decision making by managers and other stakeholders. The project will couple the output from such a high-resolution model simulation with the Marine Biogeochemistry Library and Fisheries Size and Functional Type models, thus integrating physics, chemistry and biology with climate variability. The results will be combined with a web-based decision support system, named as Sustainable Blue, that uses mathematical decision analysis capabilities, to assist fisheries managers to model the complex, climate-related decision problems on which fisheries production depends. This is vital to ensure that the region can continue to support a sustainable fishery in the long term and the communities that depend on fishing for a living. The project will also develop a well-networked multidisciplinary team of modelers, social scientists, fisheries managers, economists, and industry and community stakeholders to advance convergence science and develop avenues for more sustainable fisheries under a changing climate. This team is essential for developing tools that are directly applicable to the needs of fishery stakeholders and will be fostered by meaningful communication between all groups throughout the project period. If successful, the model suite and decision support system should be extendable to other similar regions of the global ocean. Students and post-doctoral researchers, the next generation of scientists, will be trained in decision analysis and to use the most current high-resolution models. Furthermore, the project will provide valuable professional development opportunities for early career female Co-PIs involved in the program.

This computational proposal is to support this research effort by providing high-resolution climate predictions for the development of the Sustainable Blue decision support system that combines high-resolution climate predictions with local knowledge, fisheries management policy, and decision-making tools to provide the necessary information for fisheries management and other decision-makers in response to changing climatic conditions

Type: Renewal LRAC

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

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

Field of Science: Atmospheric Sciences

Abstract:

Supercell thunderstorms, long-lived rotating storms that are prolific producers of the most powerful tornadoes, remain the target of active observational, theoretical, and numerical research. Tornadoes cause annual loss of life across the world, but primarily in the United States where these storms are the most common. An overarching goal of our team's cloud modeling work on NSF sponsored supercomputers such as Blue Waters and Frontera is to improve tornado forecasts such that appropriate lead time is available for people in the path of these storms to take shelter. A more immediate, specific goal of our research is to resolve and identify important, potentially unknown, features within supercells that are related to the life cycles of tornadoes and above anvil cirrus plumes, and to identify flow features (identifiable on radar or satellite imagery) that skillfully predict tornado behavior.

Type: New LRAC

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

Principal Investigator: Keith Brewster (University of Oklahoma (OU))
Co-Investigators: Nathan Snook (University of Oklahoma (OU)); Tim Supinie (University of Oklahoma (OU))

Field of Science: Meteorology

Abstract:

The National Oceanic and Atmospheric Administration National Weather Service (NOAA NWS) Testbeds bring research and operational meteorologists together to evaluate, both subjectively and objectively, new tools for improving forecasts of high-impact weather events across the United States. Recently the NOAA NWS selected a new model to unify its weather modeling efforts across scales in the Unified Forecast System (UFS); the Finite Volume Cubed Sphere Limited Area Model (FV3-LAM) uses a numerical core originally developed for global scales so testing and development is needed to optimize the model for convection-allowing, and convection-resolving scales. The Center for Analysis and Prediction of Storms (CAPS) at the University of Oklahoma (OU) has, for several years, been testing high-resolution numerical weather prediction (NWP) with support from, and in collaboration with, the NOAA NWS Testbeds. This project extends that work by ramping high-resolution NWP ensembles toward Exascale in support of three NOAA Testbed experiments, the 2022 Hazardous Weather Testbed (HWT) Spring Forecasting Experiment (SFE), the 2022 Hydrometeorology Testbed (HMT) Flash Flood and Intense Rainfall (FFaIR) experiment, and 2022-23 HMT Winter Weather Experiment (WWE). CAPS plans to produce 5- to 15-member high-resolution NWP ensembles using the FV3-LAM in support of these quasi-operational testbeds and as part of an effort to evaluate components of the FV3-LAM at these scales. As part of the experiments, CAPS will develop and test ensemble post-processing tools, including a spatial-aligned mean and machine learning, for improving forecasts of heavy snow and other high-impact winter weather in WWE and flash flooding and heavy rainfall in the FFaIR. The project will extend CAPS prior successful execution of FV3-LAM ensembles on TACC Stampede2 and Frontera and move toward the Exascale on Frontera by augmenting our ensemble with an additional forecast covering the entire North American Continent at 3-km grid spacing (about 3.7x CONUS grid points) and a trial member with 1-km grid spacing requiring approximately 27 times the computations of the current 3-km grid-spacing.

Type: Renewal LRAC

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

Principal Investigator: Ivan Soltesz (University of California Irvine (UCI))
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 (State University of New Jersey))
Co-Investigators:

Field of Science: Chemistry

Abstract:

The long-term goal of this Frontera Leadership Resource Allocation (LRAC) proposal is to develop a novel computational high-throughput lead optimization (HTLO) pipeline to accelerate drug discovery. We were grateful to have been awarded 320,237 Longhorn Node-hours in the current allocation, which we effectively will have used up (90% used with 2.5 months remaining). In the current allocation period, we applied performance optimized protocols for benchmark free energy (FE) simulations of ligand-protein relative binding free energies (RBFEs) using the GAFF and GAFF2 force fields against select ligands and targets within an established “gold-standard” drug discovery dataset, as well as absolute (ASFE) and relative solvation free energies (RSFE) of select compounds in the FreeSolv database. This produced a number of new insights, identified several critical barriers to progress, and led to the development, testing and publication of several new key innovations: 1) a powerful new framework for the design of optimized alchemical transformation pathways, 2) a novel alchemical enhanced sampling (ACES) method for free energy simulations, and 3) robust workflow technology that integrates new GPU-accelerated free energy simulation and network-wide analysis tools. These have been integrated into the AMBER software package that has had a broad worldwide developer and user base for nearly 40 years (currently ~30,000). Herein, we submit a renewal allocation proposal request to continue to advance 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 (CMU))
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 ANI 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: Renewal LRAC

Title: Multiscale Simulation and Modelling of Biomolecular Phenomena on Frontera

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

Field of Science: Chemistry

Abstract:

The proposal aims to simulate a number of large-scale biomolecular systems of interest using petascale simulation methodologies with coarse grained (CG), all-atom (AA), and multiscale models. We focus on providing insight into molecular behavior at scales that are inaccessible to more detailed simulation techniques and not feasible to study experimentally. Several systems to be studied under this award include key steps in the retroviral replication process of HIV, including protein aggregation at cell membranes, and cytoskeletal protein networks (e.g. actin and microtubules).

Type: Renewal LRAC

Title: Conformational Free Energy Landscape of Spike Protein in SARS-CoV-1 and SARS-CoV-2 Variants

Principal Investigator: Mahmoud Moradi (University of Arkansas Fayetteville)
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. Emerging SARS-CoV-2 variants also have their most significant differences within this protein. 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 spike protein of SARS-CoV-1 and 2 variants 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 seven 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 different variants of SARS-CoV-2 and pave the way to develop universal vaccines and therapeutics for COVID-19.

Type: Renewal LRAC

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

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

Field of Science: Fluid, Particulate, and Hydraulic Systems

Abstract:

The main objective of this project is to perform high fidelity The direct numerical simulation of turbulent pipe flow at relatively high Reynolds numbers (i.e.Re_{τ}up to 10000). This work will not only be a complement to both the existing high-Re simulations of turbulent boundary layers and channel flows, but also be critical for addressing some important issues/controversies revealed in recent high-Re turbulent pipe experiments, particularly,for example, the CICLoPE project and “Hi-Reff” at AIST, NMIJ. It will also be essential to enhance our understanding of turbulence physics at high Re’s, and to develop better turbulence models for industrial applications. During last allocation periods, we have conducted systematical comparison between two high-order DNS codes - NEK5000 and OPENPIPE - for Re_{τ} up to 2000. In addition, we have also performed full-scale DNS of turbulent pipe flow at Re_{τ}= 5200 using OPENPIPE. The new pipe data is extensively compared with other simulation data pertaining to pipes and channels. During the coming allocation period, we enthusiastically request 0.5 Million SUs to aggressively and decisively conduct production runs for Re_{τ}= 10000

Type: Renewal LRAC

Title: Particulate Transport in Turbulence

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

Field of Science: Fluid, Particulate, and Hydraulic Systems

Abstract:

This project is aimed to advanced understanding, and hence the ability to model, transport of small particles in with inertial and density-mismatch when carried in a turbulent fluid flow. State-of-the-art numerical simulations scaling efficiently to 2048 nodes (and likely beyond) on Frontera followed by very detailed data analyses will be performed to examine how high local concentrations may build up as a result of the process of backward dispersion which requires large collections of time histories along the particle trajectories. The work will also provide new insights on various mechanisms and indicators of preferential concentration of inertial particles through extracting data not readily available or often neglected for expediency for past work in the field. The proposed simulations will be at record resolution and accuracy as well as particle count exceeding 1 billion.

Type: Renewal LRAC

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

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

Field of Science: Fluid, Particulate, and Hydraulic Systems

Abstract:

It is proposed to perform pore-resolved, direct numerical simulation (DNS) of turbulent boundary layer flow over a sediment bed with polydispersed particles. The main goal of these numerical experiments is to test the hypothesis that 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. Last year, the focus was on computations involving monodispersed particles whereas it is proposed to investigate flow over polydispersed particles in random arrangement in the next year. A Cartesian, co-located grid, second-order, finite volume based incompressible flow solver (CGS-FDM) developed around the principles of energy conservation will be employed for these simulations. and has been used on several Teragrid machines for several sediment-laden turbulent flow problems.

A large-scale 442K node-hrs on the new Frontera machine are requested. The code has shown good scalability and is in production mode for the past year. The reseach team involves Shashank Karra (a PhD student, OSU), Xiaoliang He (a post-doctoral fellow, PNNL), and the PI.

Type: New LRAC

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

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

Field of Science: Fluid, Particulate, and Hydraulic Systems

Abstract:

This is a renewal proposal for LRAC project CTS20006 to continue to use Frontera to study hypersonic fluid-thermal-structure interaction (FTSI). This renewal proposal seeks to add ablation into 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 with a thermal protection system. 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 and the resultant boundary layer is modulated by ablation. 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 ablative and thermo-mechanical finite element solvers through a parallelized C++ interface. We request 4,500,000 node-hours to support this project. Our first year of Frontera access was very successful and well documented. In our second year of Frontera usage we grew our physical model complexity but production runs were significantly impacted by COVID-19. Our Frontera-supported simulations continue to highlight 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.

Type: Renewal LRAC

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

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

Field of Science: Condensed Matter Physics

Abstract:

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: 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, which have promising usage in superconducting electric grids, quantum information devices, batteries, and photovoltaic 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 accurately explain and predict quantum phases driven by both interactions. Equipped with these advanced methods, the production calculations will elucidate many essential quantum-material problems, including unconventional superconductivity, excitonic insulator, excited-state spectroscopy and dynamics, metal-to-insulator transition, correlated 2D materials, and the Wigner crystal.

Type: Renewal LRAC

Title: Engineering electron-phonon interactions in functional materials

Principal Investigator: Feliciano Giustino (University of Texas at Austin (UT) (UT Austin))
Co-Investigators: Jon Lafuente Bartolome (University of Texas at Austin (UT) (UT Austin))

Field of Science: Materials Research

Abstract:

The Center for Quantum Materials Engineering (CQME) at the University of Texas, Austin, utilizes state-of-the-art computational methods to model and design advanced functional materials at the atomic scale. The CQME leads the development of the EPW code, a core module of the Quantum ESPRESSO materials simulation suite, to investigate the effects of phonon-assisted quantum processes in electronic and energy materials. In our most recent strong scaling tests on Frontera (01/2022), EPW achieved 92% of the ideal parallel speedup on 2000 nodes. The aim of this project is to tackle fundamental questions in the physics of electron-phonon interactions, such as for example the polaron formation and dynamics in metal halide perovskites for solar light harvesting, and the temperature-dependent carrier transport in wide-gap semiconductors for power electronics. We will also employ this allocation to continue refactoring the EPW code in preparation for exascale computing. This research will lay the foundations for the rational design of emerging materials for energy and electronics applications.

Type: Renewal LRAC

Title: Classical Simulations of Planetary Materials with Quantum Accuracy

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

Field of Science: Materials Research

Abstract:

The major goal of this LRAC allocation project is to perform predictive simulations to solve one of the outstanding problems in science of matter at extreme conditions – fundamental understanding of solid-solid and solid-liquid phase transitions at extreme pressures and temperatures in planetary materials. The research objectives include: (1) studies of solid-solid and solid-liquid phase transitions at conditions of the interior of carbon-rich exoplanets; (2) investigation of metastability and phase transitions in amorphous carbon (a-C) at high-PT conditions of dynamic compression experiments; (3) exploration of novel pathways for synthesis of long-sought-after BC8 high pressure phase of carbon; (4) development of quantum accurate SNAP potentials for classical simulations of planetary materials with quantum accuracy.

Type: New LRAC

Title: Flow-induced configurational microphase separation and crystallization in polydisperse entangled polyethylene under planar elongational flow

Principal Investigator: Bamin Khomami (University of Tennessee Knoxville (UT Knoxville))
Co-Investigators: Mohammad Hadi Nafar Sefiddashti (University of Tennessee Knoxville (UT Knoxville))

Field of Science: Materials Research

Abstract:

Polymer and polymer matrix composites play an essential role in many industries ranging from consumer goods to terrestrial and extraterrestrial vehicular transport. A significant portion of these polymeric based products are produced by manipulating the microstructure of highly entangled polymer chains in the molten liquid state. Hence, fundamental understanding of the intricate flow/microstructure coupling, which to a great extent determines the final product properties, is paramount in rational design of processes used to manufacture polymer-based products. Liquid state processing techniques for net shape manufacturing of polymeric products make use of a variety of flows with shear and/or extension dominated kinematics. Hence, strong flows, namely, extensionally dominant flows are a vital component of many efficient and cost-effective liquid polymer processing techniques due to their ability to manipulate effectively macromolecular configuration and the entanglement network topology. However, the description of the elongational flow of polymeric fluids has proven to be a difficult challenge. Many theories have been proposed to explain the microstructural responses of these complex liquids under flow, but each invariably diverged from experiments at high strain rates. Recent evidence suggests that part of the reason for these divergences is that most flow models track bulk-average properties that can approximate the collective dynamics of the individual molecules. In recent studies, we have observed via nonequilibrium molecular dynamics (NEMD) simulations of monodisperse entangled polyethylene (PE) liquids that a remarkable dynamical response occurs in elongational flows, namely, configurational microphase separation occurs at intermediate extension rates, wherein the simulation cell is composed of distinct local regions of either highly stretched or coiled macromolecules. These two states produce a bimodal distribution function of the fractional extension within the Wi range wherein the coil-stretch hysteresis is evident. At high extension rates, the system undergoes a flow-induced crystallization at temperatures approximately 50 K higher than the quiescent melting point of PE.

The implications of this phenomenon have significant ramifications on liquid-state processing of highly entangled melts in strong flows. However, commercially processed polymers are polydisperse due the significant limitations of synthesis technique to produce bulk quantities of monodisperse polymers. To that end, we propose to study the influence of polydispersity on the aforementioned novel flow induced phenomena using extremely large scale (millions of particles) NEMD simulations. Specifically, a prototypical polydisperse polyethylene melt with a polydispersity index of 1.8 and entanglement density of approximately 25 will be used to develop a mechanistic understanding of the influence of polydispersity on flow-induced configurational phase separation and crystallization. Of particular interest is the quantification phase transition and flow-induced crystallization kinetics using novel thermodynamic based techniques developed recently by our research group.

The advances made from this study will contribute to bridging the gap between academic research and industrial practice in polymer manufacturing, which still relies heavily on empirical models that lack

robustness and contain process-specific empiricism. The proposed research will provide fundamental knowledge of the individual and collective chain dynamics that are crucial to a complete understanding of strong flows that occur in polymer processing operations, ultimately leading to more predictive models for industrial processes. Another broader impact is that the extensive NEMD simulation data produced in this study will be archived in the PolyHub warehouse and made available to any research group that requests it. This will allow scientists worldwide to share in the accumulation of knowledge that will result from this unprecedented series of simulations and aid the development of a new fundamental understanding of the flow behavior of polymeric liquids.

Type: New LRAC

Title: Ab initio engineering of superconducting materials

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

Field of Science: Materials Research

Abstract:

Advances in electronic structure methodology have made it possible to screen candidate synthesizable materials for a host of complex properties prior to experiment. Modeling of superconductivity, in particular, has come a long way from making rough estimates of the critical temperature to probing pairing mechanisms and resolving superconducting energy gaps. The primary scientific goals of this project are: (1) screen a large chemical space for synthesizable superconductors with high critical temperature using machine learning-based structure prediction methods, (2) perform superconductivity calculations using the anisotropic Eliashberg theory on the most promising candidates identified from the evolutionary search, and (3) develop, test and benchmark new functionalities that will be implemented in the open-source EPW code.

Type: Renewal LRAC

Title: Simulating realistic subduction and lithosphere deformation

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

Field of Science: Geophysics

Abstract:

An overarching question of modern geosciences is how the deep Earth operates and influences surface tectonics. Although significant progress has been made along many individual lines of geophysical research toward understanding deep Earth structures and subduction dynamics, major gaps exist due to the parallel development of these research disciplines. We suggest that an urgent need is the construction of data-centric physical models that could link the theorical/numerical breakthroughs in geodynamic modeling with the fast-increasing data acquisition effort. This represents a promising way forward where major advancements in understanding the mantle-surface dynamic coupling could be effectively achieved.

Type: Renewal LRAC

Title: (An)elastic global full-waveform inversion

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

Field of Science: Seismology

Abstract:

High-resolution seismic images are essential to understand the structure and thermochemical composition of the mantle to interpret its dynamics, which directly control surface processes such as earthquakes and volcanos. Seismic tomography is at a stage where further refinements require the use of full physics of wave propagation. Taking advantage of 3D wave simulations adjoint tomography leads to pure data-driven seismic models by avoiding commonly used approximations and corrections in classical tomography. After the publication of the first-generation global adjoint models, which are elastic and transversely isotropic in the upper mantle, constructed based on traveltimes only, our goal is to construct a new global anelastic mantle model by the simultaneous inversion of anelastic and elastic parameters based on adjoint tomography using full waveforms including amplitude information as well. Furthermore, we will perform 3D global tests with our anelastic inversion setup and data coverage, where we will directly demonstrate the resolution, parameter trade-off, and effect of different measurements and inversion strategies on the results. As anelasticity causes physical dispersion, accurate anelastic models also improve the resolution of elastic models, locating earthquakes and other seismic sources more accurately. The outcome of this project will lead to a much improved Earth model with drastically sharper mantle images attempting to answer long-standing questions on the origin of plumes and hotspots and the water content of the upper mantle. We request 2,650,000 Frontera CLX SUs to perform the proposed project.

Type: New LRAC

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

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

Field of Science: Earth Sciences

Abstract:

The EarthDEM project extracts 2m-resolution digital elevation models (DEMs) from stereoscopic commercial satellite imagery to produce a worldwide series of time-dependant, high-resolution topographic observations over time. The datasets are also used to create seamless 2m-resolution mosaics that serve as foundation datasets for other analyses. This project seeks to address the long-standing need for high-resolution repeat topography outlined by the NRC Decadal Survey. While the 10-year archive of satellite imagery collections has been processed to DEMs, new satellite acquisitions offer the opportunity to add valuable recent data to deepen the temporal archive and fill in gaps where no data currently exist.

Type: Renewal LRAC

Title: Emergent Phenomena and Ultrafast Dynamics of Nonequilibrium Correlated Systems

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

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:

Field of Science: Biophysics

Abstract:

Protein states and their actions characterize cellular pathways and interactions in biochemistry. We aim at developing and applying computational methods that use physical principles to understand biological systems. Physical approaches such as the molecular dynamics methods that we use here provide detailed understanding of protein systems, including thermodynamic and kinetic quantities that dictate behavior. Proteins are large biomolecular systems, and hence, the bottleneck in modeling them is the vast space of different conformations and their corresponding energies, making it prohibitively difficult to explore the numerous possible states using high resolution MD to find the low free energy states. Our lab has developed MELD, which accelerates high resolution MD by orders of magnitude to find the thermodynamically stable states of proteins and of protein ligand complexes. We have utilized our Frontera allocation in 2021 to model larger protein systems, explore multi-protein associations and protein-ligand binding. All of that was made possible by integrating different types of data sources (depending on the problem at hand) with MELD x MD.

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: Biophysics; Cross-Disciplinary Activities; Theoretical Physics

Abstract:

The proposed research is focused on two subfamilies of neutral solute transporters, aquaglyceroporins [aquaporin (AQP) 3, 7, 9 or 10] and glucose transporters (GLUTs). These proteins tirelessly perform the mundane chores of transporting water, energy, and nutrients across the cellular membrane, which are essential in human physiology and relevant in various diseases including obesity, De Vivo disease, and cancer. The goals are to fill several knowledge gaps in the cell- and transporter-specific details that are fundamental in understanding how these molecular machineries operate and useful in finding ways to modulate them for improving human health. Here are two examples. First, a paradox to resolve. Aquaglyceroporins are high affinity facilitators as evidenced in glycerols bound in all of the available crystal structures: Escherichia coli GlpF in 2000, Plasmodium falciparum PfAQP in 2008, AQP10 in 2018, and AQP7 in 2020. How does a high-affinity facilitator (AQP3/7/9/10 or GlpF or PfAQP) carry out unsaturated transport of its substrate? Knowing how this protein operates in its cell-specific membrane environments will lead to new possibilities of modulating a physiologically/pathologically essential process for lipid homeostasis. Second, a challenge to the current literature. Do the passive uniporters (all GLUTs except GLUT13) and the active symporters and antiporters all operate in the same mode regardless of the passive-vs.-active nature of a transporter or the cell-specific membrane environments it is in, as we are taught in Physiology? Now, we have the necessary supercomputing power and the crystal structures to quantify the cell-specific characteristics of a GLUT from the statistical mechanics of multi-million jiggling-and-wiggling atoms constituting the protein and the cell membrane, producing new insights in the research of energy transport. In the upcoming year (4/1/2022 to 3/31/2023), the systems of our research will be all-atom models of neutral solute carrier proteins (GlpF, AQP10, GLUT1 etc.) constituted into cell membranes. This research is to increase the knowledge of two types of transporter proteins: aquaglyceroporins and glucose transporters. The knowledge gained from this research will lead to new ways to modulate these biological machineries for better human health.

Type: Renewal LRAC

Title: How membrane properties control enveloped viral entry

Principal Investigator: Peter Kasson (University of Virginia)
Co-Investigators:

Field of Science: Biophysics

Abstract:

Enveloped viruses infect cells via a process of membrane fusion. The properties of the viral and cellular membranes have been shown experimentally to affect both overall viral infectivity and likely the mechanism of entry, but a detailed molecular understanding has thus far been lacking. This project uses detailed molecular dynamics simulations of multiple enveloped viruses (influenza and HIV) to understand how membrane properties control viral infection and how this might be manipulated for therapeutic effect.

Type: Renewal LRAC

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

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

Field of Science: Organic and Macromolecular Chemistry

Abstract:

Our understanding of the role of nucleic acids in biology is ever-expanding. Critical to nucleic acids function and biology is not only their structure, but their dynamics, since the structures of nucleic acids are very sensitive to their environment of solvent, ions and other biomolecules. Experimentally, studying flexible nucleic acid systems and their binding processes is challenging. Simulation, with sufficient conformational sampling and accurate force fields, can characterize nucleic acid structure and dynamics. What if we could accurately model molecular interactions such as ligand binding, intercalation, and accurately capture the complete and dynamic conformational ensemble? This would allow unbiased understanding of binding processes of interacting biomolecules, enable optimization of lead compounds targeting RNA, and better understanding of nucleic acid function. Thanks to advances in the GPUs and the optimized codes that run on them, it turns out we can simulate these processes in unbiased simulations. This includes the spontaneous intercalation of ethidium to DNA duplexes, characterization of the minor groove and intercalative properties of various copper ligand complexes, the observation of the formation of known low population Hoogsteen base pairs in DNA duplexes, and recently the unbiased and spontaneous binding of active COVID-19 inhibitors to the experimentally measured site of various tRNA initiators in the anticodon stem loop.

Type: Renewal LRAC

Title: Molecular architecture of paracellular ion transport barriers

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

Field of Science: Biophysics

Abstract:

This proposal requests an allocation on Frontera to carry out several pioneering simulations that will answer fundamental questions about the structural organization and biological function of exceptionally important biomolecular systems. Building on our previous work that delivered the first all-atom structure of a complete, packaged virus particle, we will use Frontera to determine which physical phenomena govern the process of viral genome ejection into a host cell. For this purpose, we will develop a liposome cell mimetic -- a reduced-scale computational model of a living biological cell that makes all-atom molecular dynamics simulations of in vivo biological processes possible without compromising the complexity of a real biological environment. Starting with a complete all-atom model of a Dengue virus constructed using our last year allocation, we will determine how the structure of the Dengue virus changes when it enters the host cell and how such structural changes promote virus disassembly and fusion with the cell membrane. Finally, we will complete our landmark study of biomolecular transport through the nuclear pore complex by determining the role that proteins known to assist transport of larger cargoes play in modulating the structure and visco-elastic properties of the disordered protein mesh that serves as a gatekeeper of nuclear transport.

Type: Renewal 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 (UCSB))
Co-Investigators: PRITAM GANGULY (University of California Santa Barbara (UCSB))

Field of Science: Biophysics

Abstract:

This LRAC renewal focuses on two scientific problems: 1) The self-assembly of Alzheimer's disease-related disordered proteins and 2) The mechanism by which osmolyte mixtures stabilize proteins. Project 1: Extracellular deposition of Aβ plaques in the brain is the hallmark for the pathogenesis of Alzheimer's disease. Small peptide amyloid-inhibitors have emerged in recent years as a possible therapeutic treatment of Alzheimer's disease. The human innate immune peptide Cathelicidin LL-37, which is a known antimicrobial protein ubiquitous in human tissues, has been found to bind to protein Aβ and modulate its fibrillization. Using enhanced-sampling replica-exchange molecular dynamics (REMD) simulations, we will probe the mechanism by which LL-37 modulates Aβ aggregation. The atomistic level insights gained from this study will be key for the therapeutic development of peptide-based amyloid inhibitors. Project 2: In response to high osmotic pressure, many marine organisms 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 protein-denaturation, and how different osmoprotectants can act competitively or synergistically is poorly understood. Using 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.

Type: Renewal LRAC

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

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

Field of Science: Biochemistry and Molecular Structure and Function

Abstract:
\section*{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 molecular mechanisms involved in 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 simulte the full model of SARS-CoV-2 envelope, at an atomistic level, both under control conditions and in the presence of commonly used disinfectants, alcohol and soap. Simulations aim at characterizing the main site of action (protein or lipid) and the mechanism by which these chemicals completely neutralize the virus. The result can shed light on the structural elements stabilizing the virus and are of potential use when rationally designing novel strategies against the viral infection.

Type: New LRAC

Title: Three-Dimensional Geodynamic Models of Subduction Initiation

Principal Investigator: Michael Gurnis (California Institute of Technology (Caltech))
Co-Investigators:

Field of Science: Marine Geology and Geophysics

Abstract:

We are developing a new generation of dynamic models of subduction initiation – the last remaining unsolved component of plate tectonic theory. The largest changes in the forces of plate tectonics occur during this critical phase of plate evolution. We will exploit recent advances in computational methods that allow the time-dependent solution of visco-elasto-plastic problems in three dimensions. A Lagrangian integration point finite element method will allow tracking of fault nucleation, fault evolution, and thermo-chemical convection. The time to address this problem is ideal -- coming on the heels of major observational efforts made from deep-sea drilling and high-resolution seismic imaging that provide key constraints on the process of subduction initiation. During the year, we will specifically compute on Frontera two classes of models – time-dependent and instantaneous – that are constrained by well-observed New Zealand subduction initiation while addressing the question “how much energy is dissipated when a new subduction zone forms.”

Type: Renewal LRAC

Title: Kinetic characterization of 3D magnetic reconnection

Principal Investigator: Shan Wang (University of Maryland College Park (University of Maryland) (UM) (UMCP))
Co-Investigators: Brandon Burkholder (University of Maryland Baltimore County (UMBC)); Wei Xiang Jonathan Ng (University of Maryland College Park (University of Maryland) (UM) (UMCP)); Li-Jen Chen (NASA Goddard Space Flight Center)

Field of Science: Physics

Abstract:

We propose to perform simulations on Frontera to study magnetic reconnection, focusing on the 3D effects and the kinetic aspects. In the past two years, we have investigated in detail the lower-hybrid wave properties and the associated wave-particle interactions during 3D reconnection with symmetric upstream conditions. We also studied the ion-ion beam instability that resembles the situation at the Earth's foreshock. The parameter scan using 1D simulations is performed to reveal the regimes where different modes of the instability dominates, and we analyzed how the field grows and how ions are decelerated/accelerated. The 2D simulation shows the occurrence of magnetic reconnection inside the wave field. In addition, we start to use the global simulation to study solar wind-magnetosphere coupling through magnetic reconnection. For the upcoming allocation period, we plan to continue and advance the aspects of research. We request for 270k SU on Frontera and request to maintain the 160T storage on Ranch.

Type: Renewal LRAC

Title: Simulations of Extreme and Eccentric Binary Black Hole Mergers

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

Field of Science: Gravitational Physics

Abstract:

The goal of this project is to model the gravitational waves signals from the late inspiral and merger of black hole binaries (BHB) with large mass ratios as well as in eccentric orbits. These studies will be based on full numerical simulations solving the highly nonlinear gravitational dynamics and computing waveforms from those binary systems.

Our studies have a wide range of applications, from direct parameter estimation of BBH signals, currently being detected by LIGO-Virgo, to predictions for the third generation of gravitational wave detectors and LISA space mission, leading to the modeling of astrophysical formation scenarios for those BHB sources.

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

The plan of work here consists of 3 stages: i) Design full Numerical Relativity simulations of non-spinning, mass-ratio q=1/2, 1/4, eccentric e=0.1-1.0, binary configurations to evolve for the last 20 orbits before merger ii) Same as before, but for aligned / counteraligned spins (of the large hole) S/m^2=+/-0.9 configurations to evolve for up to the last 40 orbits before merger and obtain full waveforms from the Numerical Relativity simulations. iii) Systematic exploration of the large mass ratio binaries from 15:1 to 128:1 cases with the large black hole possibly spinning S/m^2=0,+/-0.9, and configurations to evolve for the last 20 orbits before merger to obtain full waveforms and to study its numerical convergence with 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 for Plasma Physics (Max-Planck-Institut fr Plasmaphysik) (IPP))
Co-Investigators: Gabriele Merlo (University of Texas at Austin (UT) (UT Austin))

Field of Science: Theoretical Physics

Abstract:

This project is a continuation of the Frontera allocation awarded for the first and second LRAC cycles (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 in conjunction with modern uncertainty quantification techniques to address outstanding open questions related to the influence of plasma shaping, in particular negative triangularity δ, on plasma confinement.

Type: Renewal LRAC

Title: Hadron-Hadron scattering from lattice QCD

Principal Investigator: Colin Morningstar (Carnegie Mellon University (CMU))
Co-Investigators: Andrew Hanlon (Brookhaven National Laboratory); John Bulava (Unknown Institution); Andre Walker-Loud (Lawrence Berkeley National Laboratory (Berkeley Lab) (LBNL)); Ben Hoerz (Johannes Gutenberg University of Mainz (University of Mainz) (Johannes Gutenberg-Universitt Mainz))

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: Kostas Orginos (William & Mary); David Richards (Jefferson Laboratory); Christopher Monahan (William & Mary)

Field of Science: Nuclear Physics

Abstract:

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

Type: Renewal LRAC

Title: Precision Flavor Physics at the Intensity Frontier

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

Field of Science: Theoretical Physics

Abstract:

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

Type: Renewal LRAC

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

Principal Investigator: Martha Constantinou (Temple University)
Co-Investigators: Constantia Alexandrou (University of Cyprus and The Cyprus Institute); Giannis Koutsou (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 tuned to their physical mass values. For the continuation of our LRAC project, we target simulations using the twisted mass fermion formulation with a lattice spacing of a=0.07 fm and a spatial volume of (7.8 fm) cubed. The simulation will be the largest volume ever simulated with this action and being at the physical point will allow for the calculation 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.

Type: New LRAC

Title: Beyond Standard Model Physics with Neutron Electric Dipole Moment

Principal Investigator: Keh-Fei Liu (University of Kentucky (UK))
Co-Investigators: Andre Walker-Loud (Lawrence Berkeley National Laboratory (Berkeley Lab) (LBNL)); Andrei Alexandru (George Washington University); Frank Lee (George Washington University); Terrence Draper (University of Kentucky)

Field of Science: Nuclear Physics

Abstract:

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

Type: New LRAC

Title: Mergers of spinning supermassive binary black holes in gaseous environments and their electromagnetic signatures

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

Field of Science: Gravitational Physics; Astronomical Sciences

Abstract:

A team from the Rochester Institute of Technology, NASA Goddard Space Flight Center, Johns Hopkins University, and their collaborators, propose to perform realistic simulations of gas surrounding supermassive binary black holes mergers, enabling prediction of photon spectral and timing signatures of these binary black holes.

Accreting supermassive binary black holes (SMBHBs) are potential multi-messenger sources because they emit both gravitational wave and electromagnetic radiation. It is the goal of this project to combine astrophysical knowledge about the environments of SMBHBs with detailed physical simulations of gas flows in the immediate neighborhoods of these binaries, and explicit computation of the time-dependent spacetimes in which the gas is placed, in order to predict the light observers would see to identify them. Over the past ten years, our group has built the knowledge base and computational methods needed to reach this goal, and we are now ready to take the final steps. We have built a ``multipatch" simulation infrastructure to permit the simulation of gas accretion in the approach to merger; to avoid prohibitive computational cost in the long inspiral stage of the process, it is necessary both to compute the changing spacetime by means of post-Newtonian and other sorts of perturbative approximations and to create simulation tools permitting separate treatment of subregions within the binary environment. We also have built a new code framework that will allow us to efficiently perform these simulations into the merger regime.

Finally our post-processing tools allows us to transform fluid simulation data into predictions of photon radiation, accounting for the principal radiation mechanisms, opacities, and photon propagation through dynamical spacetimes.

Here, we propose to use the TACC's Frontera system, to study how the accretion from a surrounding circumbinary disk is apportioned between the members of the supermassive black hole binary as a function of the black hole spin, and how this may change when the separation becomes small enough for relativistic effects to become important. Mass transfer from one member of the binary to the other may play an especially interesting role. We will then simulate what happens to the gas surrounding the black holes during the merger proper and the subsequent relaxation phase. Our plan it to use our post-processing machinery to predict EM spectra and light curves throughout all these phases.

This allocation will allow us to identify the most distinctive features of the photon emission associated with a SMBHB and how they may change over time; the clearest spectral signatures to distinguish merging black holes against the background of stellar light from their host galaxies or from single supermassive black hole systems,

and the radiation produced in jets arising from SMBHBs.

This project will be a stepping stone to enable current and future observational campaigns to recognize the transient EM signals of supermassive black hole mergers, events that both emit enormous amounts of energy in gravitational waves and strongly influence the cosmological evolution of the supermassive black hole population.
Creating such a capability is a prime goal of the new field of multimessenger astronomy.