Type: Renewal
Title: Structural and Mechanical Analysis of Biological Condensates Using a Computational Microscope

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

Field of Science: Biophysics

Abstract:
Only ten years ago, the inner volume of a biological cell was thought to be a well-mixed collection of biomolecules suspended in a soup-like environment that allows biomolecules to roam freely by diffusion. Recent experiments, however, suggest a much more complex organization of the intracellular volumes, where both diffusion and active transport of biomolecules are restricted and regulated in response to specific biochemical signals by means that are yet to be identified. One such mode of regulation is liquid-liquid phase separation, where biomolecules of a particular kind condense into liquid droplets, forming a membraneless organelle. It is, however, not at all clear what forces drive the formation of such condensates, how target biomolecules are recruited into the condensates, or how the condensates dissolve after fulfilling their function. Using Frontera, this project will obtain the first microscopic models of biological condensates and use the computational model to answer the most pressing questions regarding the nature of physical interactions that govern the condensate's behavior. Building on our preliminary work that demonstrated feasibility of a dual-resolution approach to modeling the structure and dynamics of the condensate, we will determine the role of RNA in regulating the properties of the condensate, the physical mechanisms that amplify the effect of single point mutations and characterize the transport of the condensate's components in and out of the nucleus. The quantitative information derived from these pioneering simulations will be used to obtain a mechanistic interpretation of single-molecule and live cell experiments, greatly enhancing our knowledge about the biological states of matter.

Type: New
Title: Fundamental Studies in Nanomechanics: Optofluidics and Molecular Electronics

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

Field of Science: Materials Research

Abstract:
Ab initio and molecular simulations are widely used 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 two interrelated problems using quantum and molecular computational tools. First, we will investigate the electronic and optical transport properties in carbon nanotubes. In the second problem, our goal is to obtain better electronic and molecular materials for nanoelectronics through studying the formation of heterogeneous nanowire connections between graphene nanoribbons.

Type: Renewal
Title: Coarse-grained Molecular Dynamics Simulations of Bulk Heterojunction Organic Solar Cells

Principal Investigator: Ganesh Balasubramanian (Lehigh University)
Co-Investigators:

Field of Science: Design and Computer-Integrated Engineering

Abstract:
The research project explores the role of processing conditions on the structure, property and performance of quasi-random nanostructured materials. We consider the bulk heterojunction (BHJ) of organic solar cells as our testbed and use the widely employed polymer-fullerene mixtures as sample materials for the investigation. The computational thrust of the project focuses on understanding the processing-structure correlation using large-scale coarse-grained molecular dynamics simulations.

Type: New
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:
Hypersonic vehicles have high temperature, shock-laden turbulent air flowing adjacent to thermo-mechanically compliant surfaces. The intense pressure and heat loads cause the vehicle to deform, heat up, and ultimately change its aerodynamic performance, propulsive efficiency, and controllability. Engineering models for this fluid-structure interaction do not exist. Through direct numerical simulation we will study the interaction of a Mach 6 flow with a 35 degree compression ramp, 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 disturbance free, as would be found in flight, and when 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 Python interface. The total resource request for this project is 5,000,000 node hours.

Type: New
Title: Simulated Inside and Out: the Milky Way Galaxy at Unprecedented Resolution

Principal Investigator: Alyson Brooks (Rutgers University)
Co-Investigators: Jessica Werk (University of Washington); Jillian Bellovary (Queensborough Community College); Charlotte Christensen (Grinnell College); Andrew Pontzen (University College London); Thomas Quinn (University of Washington)

Field of Science: Extragalactic Astronomy and Cosmology

Abstract:
Galaxies are systems of gas, stars, and dark matter interacting across vast scales over billions of years. Our Milky Way contains billions of stars, a halo of hot gas, stars, and dark matter extending 10 times further than its disk, dozens of orbiting dwarf satellites, and a supermassive black hole (SMBH) at its center. These components all act on each other, creating a complex interplay across cosmic time. We propose a series of simulations that will further our understanding of how the stars, gas, and SMBHs both in the central galaxy and the surrounding satellites and halo co-evolve. These simulations of galaxies similar to our own Milky Way will be run at unprecedented resolution, with a state-of-the art simulation code, ChaNGa, using cutting edge models for the physics of star formation, black hole evolution, and energy output ("feedback") from massive stars and SMBHs. This suite of simulations will both provide essential, testable predictions for next generation telescopes on Earth and in space, as well as acting as a legacy dataset that can be studied for years to come to help understand a myriad of different phenomena in the evolution of galaxies and their constituent parts. Only with world-class compute facilities like Frontera, combined with the advances that our collaboration has made in the accuracy, fidelity, and performance of our simulation code, can simulations at this scale be run.

Type: New
Title: Supermassive Black Hole Approaching Merger: Accretion Dynamics, Jets and Electromagnetic Signals

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

Field of Science: Gravitational Physics, Astronomical Sciences

Abstract:
Essentially every good-sized galaxy contains a supermassive black hole in its center; because galaxies merge from time to time, it is expected that recently merged galaxies hold two large black holes, which eventually form a bound pair and some time later merge. Because supermassive black hole binaries can often accumulate sizable quantities of gas, they should be bright electromagnetically for a significant time before they merge. Until an orbiting gravitational wave observatory is operational, the best way to discover such systems is by the photons they emit. Therefore this demands having specific features to search for.

A team of researchers from the Rochester Institute of Technology (RIT), NASA Goddard Space Flight Center (GSFC), Johns Hopkins University (JHU), and their international collaborators propose to use the TACC's Frontera system to perform the first realistic simulations of gas surrounding supermassive binary black holes ``en route'' to merger, enabling prediction of photon spectral and timing signatures of these binary black holes.

Over the past ten years, the group has built the knowledge base and computational methods needed to reach this goal, and we are now ready to take the final steps. Under current NSF funding, we have completed the development of a ``multipatch'' simulation infrastructure to permit simulation of gas accretion in the approach to merger; to avoid prohibitive computational cost, 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 have also built post-processing tools 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 spin and mass-ratio, 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.

This allocation will allow us to identify of the most distinctive features of the photon emission associated with SMBBHs approaching merger: the bands in which the most electromagnetic power emerges 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, and also separate them from AGN; and the radiation produced in jets.

This project will be a stepping stone to enabled LSST and other similar surveys 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.

Type: Renewal
Title: Research in Theoretical Hadronic Physics and Related Topics

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

Field of Science: Nuclear Physics

Abstract:
Lattice QCD enable 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 extend our previous studies of the quark structure of pions and protons to that of gluons, and embark on program of 3D imaging of hadrons. The work is related to the experimental programs at Jefferson Lab, RHIC, and at a future EIC.

Type: Renewal
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: New
Title: Simulation and experiment to optimize force fields for accurate atomistic modeling of RNA

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

Field of Science: Molecular Biosciences

Abstract:
RNA molecules are dynamic, their structures are very sensitive to their environment (of solvent, ions and other biomolecules), and interactions that stabilize particular conformations are subtle and varied. Despite significant advances in the simulations and continuous improvement in the available and emerging force fields, RNA is proving extremely challenging to accurately model at the atomistic level in the absence of experimental data. For relatively regular structures, such as duplexes, the recent AMBER force fields perform remarkably well. For example, microsecond+ ensemble molecular dynamics (MD) simulations of the Dickerson DNA dodecamer converge to structures less than 0.5 Å from the highest resolution NMR averaged structures (PDB 1NAJ) neglecting the terminal base pairs. Here, minor discrepancies in the (over) stacking, hydrogen bonding, and varied inter- and intra- molecular interactions do not significantly affect the structure since the regular stacked helical structure largely buries the Watson-Crick hydrogen bonds, although such force field discrepancies could lead to inaccurate base pair opening times, melting temperatures, and stability. However, many of the most interesting and functional structures observed in RNA are not pure duplex and involve specific stabilizing interactions that are much more sensitive to the balance of forces between water, ions, and the RNA atoms. Slight misbalance in any of the inter- or intra-molecular interactions can lead to over-stabilization of anomalous structure. Over the past few years, we were able to demonstrate convergence in independent molecular dynamics simulations of RNA and DNA ranging from dinucleotides and tetranucleotides to RNA tetraloops and DNA dumbbells and helices. This Frontera allocation proposal is based on our recent NIH 4-year renewal of GM081411 which aims to test, validate and improve the available and emerging force fields for nucleic acids on a variety of tractable model systems (tetranucleotides, DNA dumbbells, and RNA tetraloops) and also assess larger nucleic acid structures that are dynamic (i.e. they populate multiple conformations).

Type: New
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

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
Title: Emergent Phenomena and Ultrafast Dynamics of Nonequilibrium Correlated Systems

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

Field of Science: Physics

Abstract:
The motion of elections through some materials can be highly correlated, such that the electrons behave as cars move in heavy traffic; they cannot maneuver freely and their motions are strongly influenced by others. These correlated electron materials often exhibit intriguing properties, such as metal-insulator transitions and unconventional superconductivity. Overcoming the knowledge gap in understanding electron correlation effects could open up revolutionary opportunities for novel transistor and ultrafast device applications. In this proposal, 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 to state-of-the-art 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 also having potential impacts on U.S. science leadership and energy-sustainable future.

Type: Renewal
Title: Precision Flavor Physics at the Intensity Frontier

Principal Investigator: Carleton DeTar (University of Utah)
Co-Investigators: Alejandro Vaquero (University of Utah); Maria Gamiz (University of Granada); William Jay (Fermilab); Zechariah Gelzer (University of Illinois); Ethan Neil (University of Colorado); Aida El Khadra (University of Illinois); Steven Gottlieb (Indiana University)

Field of Science: Elementary Particle 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. These disgreements are at the level of two to three standard deviations and 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
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
Title: Super-resolution cosmological simulations of galaxies and black holes

Principal Investigator: Tiziana DiMatteo (Carnegie Mellon University)
Co-Investigators: Yin Li (University of Tokyo); Yu Feng (University of California, Berkeley); Yueying Ni (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: Renewal
Title: Fundamental studies of compressible turbulence and turbulent mixing

Principal Investigator: Diego Donzis (Texas A&M University)
Co-Investigators:

Field of Science: Fluid, Particulate, and Hydraulic Systems

Abstract:
The purpose of this proposal is to renew our Leadership Resource Allocation on Frontera, the new NSF leadership-class computing resource. The allocation will allow us to study mixing in compressible turbulence using direct numerical simulations (DNS) to reach conditions not possible before and will thus provide data at unprecedented levels of realism in a data-scarce field. The simulations will be at sufficiently high Reynolds numbers to permit the investigation, for the first time, of inertial range dynamics of the velocity as well as the scalar fields, providing data to further our understanding of mixing processes in compressible flows. The level of details we will be able to study from the proposed simulations will provide enough data to answer long-standing and new questions, including the nature of the inertial range for the two components of the velocity field, the scalar field, the nature of small-scale fluctuations, and deep concepts of up-to-now-elusive universal scaling laws. The size and characteristics of Frontera will also allow us to explore single-precision computing for computation-intense sections of the code, as well as a new algorithmic approach based on asynchrony which could potentially mitigate all bottlenecks expected at extreme scales. Funding for this work comes from NSF, DOD, and internal university funds. Data generated from this simulations will be made available to the scientific community.

Type: New
Title: Large-Scale Computational Screening on Leadership Resources to Assess the Estrogenic Potential of Environmental Chemicals

Principal Investigator: Emilio Gallicchio (City University of New York)
Co-Investigators: Lauren Wickstrom (BMCC of CUNY)

Field of Science: Molecular Biosciences

Abstract:
We request an allocation through the Leadership Computing Allocation (LRAC) program to conduct a large-scale binding free energy screening of a library of ~200 potential xenoestrogen toxins. The proposed study, one of the largest ever conducted of this type, will result in a better understanding of the damaging action of these chemicals and will assess the feasibility of the computational screening of environmental pollutants using modern molecular simulation tools on Leadership National Computing Resources. The merits of the proposed request rest on the scientific and biomedical impact of the proposed study and on the opportunity to assess the feasibility of the use of national high performance computing facilities for the computational characterization of toxins. The PIs are qualified to conduct the research and are current users of XSEDE systems. The methodology on which the proposed study is based is well established and the molecular simulation software is already deployed and in current use on XSEDE systems. The scientific and software aspects of the project are supported by an NSF CAREER grant (NSF 1750511 to E.G.). The project will involve a team of undergraduate and graduate students who will help with the set up, management, and analysis of the molecular simulations and will be exposed to interdisciplinary computational research on leadership resources. The results of the study will be disseminated through news bulletins, scientific conferences and peer-reviewed journal articles.

Type: New
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
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 13 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 origin and formation of star clusters, and the effects of radiation on galaxy formation during the epoch of reionization. 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
Title: Direct numerical simulation and analysis of turbulent pipe flow at high Reynolds numbers

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

Field of Science: Fluid, Particulate, and Hydraulic Systems

Abstract:
Pipe flows are frequently encountered in a variety of environmental, technological, and even biological applications. Typical examples of pipe flows can be found in urban drainage systems, transport of natural gas or oil in the energy sector, or the flow of blood in arteries and veins. Accordingly, the understanding of flow physics in pipes has a direct and substantial impact on everyday life, and adequate knowledge of such flow problems will help in finding scientific methods to control phenomena, like heat and mass transfer. Of particular importance in flows delimited by solid walls is the near-wall region in which a large fraction of the drag stems from velocity fluctuations in a thin boundary layer adjacent to the walls. Near-wall turbulent structures primarily scale on the so-called viscous length scale, which becomes very small as Reynolds number (Re) increases. However, according to recent experimental studies, large and very large-scale motions with lengths of 5R up to 20R are found in high-Re turbulent pipe flows (R being the radius). These structures, being strongest in the outer region, extend across the entire shear region and even leave their footprint quite close to the wall. These large-scale, very energetic motions play an important role in the heat, mass, and momentum transportation.
Compared to other canonical cases, such as the plane channels and spatially evolving boundary layers, pipe flow is the easiest realizable in experiments. However, due to numerical difficulties related to the cylindrical coordinates and the corresponding numerical singularity arising along the axis, it is the only canonical flow case that has not yet been thoroughly studied using direct numerical simulation (DNS). It is very timely to obtain a high-fidelity numerical database for fully-developed turbulent pipe flow that is well-validated with both experiments and other canonical flow simulations. The main objective of this project is to perform DNS of turbulent pipe flow at relatively high Reynolds numbers (i.e. Re_τ up to 5000) using an accurate and efficient spectral-element code Nek5000. The proposed simulation requires the use of massively parallel computational resources, which perfectly fit the multi-petascale computing capabilities offered by Frontera. This work will not only be a complement to both the existing high-Re simulations of turbulent boundary layer 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. 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.

Type: Renewal
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:
In this project, we aim to enhance the accuracy, improve the design, and extend the applicability of the recently suggested ANI-11 deep neural network potential for molecular simulations on modern architectures. Apart from other similar efforts in quantum chemistry and materials science, this neural network potential was shown to be transferable across different chemical environments, generalizing to the density-functional theory (DFT) level of accuracy on a large dataset of organic molecules while being six orders of magnitude faster. Yet, the DFT level of accuracy is often insufficient for many realistic simulations of chemical, biochemical, and material applications. We suggest to replace the DFT-based training with a more accurate, but also much more computationally demanding wavefunction-based training, leveraging the NSF leadership computational resources and our expertise in accurate electronic structure methods. Two students working on this project are supported by NSF MolSSI software fellowships.

Type: New
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. Experiments have shown that membrane properties can control fusion outcomes, but it remains unknown whether changes at the membrane alter protein organization or affect the lipid intermediates and mechanism of fusion itself. We have performed molecular dynamics simulation of fusion by influenza hemagglutinin assemblies, showing how these assemblies manipulate the membrane to achieve viral entry. This project seeks to understand how changes to the membrane affect this process using multi-scale ensemble molecular dynamics simulation. It will yield a molecular-level understanding of how changes to membrane composition and properties control viral fusion and infection.

Type: Renewal
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 build an atomic model of tight junction networks at cellular level and investigate its transport properties computationally.

Type: New
Title: Configurational microphase separation in entangled polymers in elongational flow

Principal Investigator: Bamin Khomami (University of Tennessee, Knoxville)
Co-Investigators:

Field of Science: Materials Research

Abstract:
The description of 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 experiment 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 have effectively dynamical phenomena of the individual molecules. In recent studies, we have observed via nonequilibrium molecular dynamics (NEMD) simulations of moderately-entangled polyethylene liquids that a remarkable dynamical response occurs in elongational flows: configurational microphase separation, wherein the simulation cell is composed of distinct local regions that are composed mostly of either highly stretched or coiled macromolecules. These two states produce a bimodal distribution function of the fractional extension within the extension rate range wherein the coil stretch hysteresis is evident. We propose to study this startling phenomenon behavior extremely large scale (millions of particles) NEMD simulations of a polyethylene liquid with 30 entanglements per chain, and to use the knowledge gained to develop a mechanistic understanding configurational phase separation.

Type: New
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); Eliot Quataert (University of California, Berkeley); Jonathan Squire (University of Otago)

Field of Science: Astronomical Sciences

Abstract:
The transport of energy and momentum and the heating of plasma particles by waves and turbulence are key ingredients in many problems at the frontiers of heliospheric and astrophysics research. This includes the heating and acceleration of the solar wind; the observational appearance of black-hole accretion flows on event-horizon scales; and the properties of the hot, diffuse plasmas that fill dark-matter halos. 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. In pursuit of addressing this issue, we plan to carry out a series of ground-breaking hybrid-kinetic simulations to address the fundamental physics of plasma waves, turbulence, and dynamo in weakly collisional, magnetized, high-beta plasmas. Our group has previously shown that, in this regime, deviations from local thermodynamic equilibrium (i.e., pressure anisotropies) and the instabilities they excite (firehose, mirror, ion-cyclotron) can dramatically change the properties of waves and turbulence from those predicted by fluid (i.e., magnetohydrodynamic) and linear kinetic theories, with surprising consequences for magnetic-field amplification, turbulent transport, and particle heating. This DOE-, NSF-, and NASA-funded work makes use of a new version of our hybrid-kinetic particle-in-cell code (Pegasus++). The old version of the code (Pegasus) had facilitated several discoveries and pioneering results, including the evolution and saturation of firehose and mirror instabilities, the properties of kinetic magnetorotational turbulence in a collisionless accretion disk, and the “interruption” of Alfvén waves in high-beta plasmas (all of which have been featured in Physical Review Letters). Our new code retains the old code’s essential algorithms, but has been aggressively optimized for use on KNL architectures. It demonstrates excellent single-core performance, and excellent weak scaling on Frontera. The application of these novel computational algorithms to frontier topics in plasma astrophysics on leadership-class facilities opens up new possibilities for understanding the evolution of cosmic magnetic fields, black-hole accretion flows, and fundamental plasma turbulence of relevance to the near-Earth solar wind.

Type: New
Title: The Final Minutes of a Massive Star

Principal Investigator: Eric Lentz (University of Tennessee, Knoxville)
Co-Investigators: W Hix (university of tennesee)

Field of Science: Astronomical Sciences

Abstract:
We propose to model the final minutes of a massive star in 3D and compute from the state of that model when it collapses the core collapse supernova that follows. We seek to understand how multidimensional effects impact the final state of collapsing massive stars and the supernova that follows.

Type: New
Title: Formulation of a general collisional-radiative model to study nonequilibrium flows

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

Field of Science: Fluid, Particulate, and Hydraulic Systems

Abstract:
Hypersonic Edney type shock-wave/boundary layer interaction (SWBLI) flows are characterized by complex multi-length scale features that include the triple point, flow separation, shear layer, and lambda shocklets. These features lead to a complex shock system which is characterized by the thermal nonequilibrium, low frequency unsteadiness of the separation bubble, potential growth of the Kelvin-Helmholtz (KH) instability, and the amplification of input disturbances that pass through the SWBLI system. The particle based Direct Simulation Monte Carlo (DSMC) method is an good candidate to simulate such flows because it provides a solution to the Boltzmann transport equation. The latter is valid even in strong shock regions where the continuum assumptions inherent in the derivation of Navier-Stokes equations fail. As a consequence, the velocity and temperature slip, thermochemical nonequilibrium, and the accurate dynamic evolution of flow features are natural outcomes of the time accurate DSMC method. For three dimensional complex flows, however, the use of DSMC requires peta-scale computations arising from the need to simulate a large number of particles to satisfy numerical requirements. Therefore, to solve such computationally demanding cases in an efficient manner, we have developed an in-house code, Scalable Unstructured Gas-dynamics Adaptive mesh-Refinement (SUGAR), that scales demonstrably well on thousands of cores even for the challenging flow over a double wedge. The code takes advantage of adaptive mesh refinement (AMR)/Octree grids to model multi-scale physics, a robust cut-cell method to simulate complex geometries, Morton based domain partitioning, and novel data communication strategies that make use of Message Passing Interface (MPI) to harness the computational power of modern computing architectures for parallel computing. In our previous work, a hypersonic flow of molecular nitrogen over a double wedge at a freestream Knudsen number of 0.00324 was simulated for 0.4 ms using 20,000 Intel Xeon E5-2699v3 Haswell processors on DoD HPC's Topaz and NSF's Bluewaters cluster with 26 billion particles and 2 billion collision cells, where the flow was found to be unsteady. In this work, we are applying the SUGAR code to investigate the self-excited spanwise homogeneous perturbations arising in this SWBLI system by imposing spanwise periodic boundaries. Strong thermal nonequilibrium exists downstream of the Mach 7 detached (bow) shock generated due to the upper wedge surface. Global linear instability mechanisms are expected to make the pre-computed 2-D base flow potentially unstable under self-excited, spanwise periodic perturbations. Goertler-type vortices are also expected to form due to curved streamlines in the presence of a strong recirculation region. Our specific intent is to assess the growth rates of unstable modes, the wavelength, location, and the origin of spanwise periodic flow structures, and the characteristic frequencies present in this interaction. To simulate such demanding cases, the Cascade Lake configuration on Frontera is particularly attractive because of the larger RAM of 192 GB per node and availability of large nodes per queue.

Type: New
Title: Computational Studies of Transition Metal-Catalyzed Reactions

Principal Investigator: Peng Liu (University of Pittsburgh)
Co-Investigators:

Field of Science: Organic and Macromolecular Chemistry

Abstract:
Large-scale quantum mechanical calculations will be performed to study transition metal catalyzed reactions that are widely used to synthesize functionalized organic compounds, biologically active molecules, and polymer materials. These computational studies will elucidate detailed reaction mechanisms, factors that control reactivity and selectivity, as well as predictive models to computationally screen and design new catalytic systems with improved efficiency. We have established extensive collaborations with more than 30 synthetic organic chemistry groups, where our computational results and predictions are used to explain experimental results and guide the rational design and development of novel catalytic reactions.

Type: New
Title: Simulating realistic subduction and lithosphere deformation

Principal Investigator: Lijun Liu (University of Illinois at Urbana-Champaign)
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 make 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, resulting in 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
Title: First-principles Study of Interactions and Topological Effects in Condensed Matter Systems

Principal Investigator: Steven 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, TD-aGW) 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: New
Title: Binary black hole simulations with eccentricity 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:
We will perform full numerical relativity simulations of spinning binary black holes in eccentric orbits to compare to assess errors and match to integrations of the third and a half post-Newtonian equations of motion for a fully generic binary black hole system, allowing both for non-circular orbits, and for one or both of the black holes to spin, in any orientation. Using the second post-Newtonian order expression beyond the leading order quadrupole formula, the RIT group studied the gravitational waveforms produced from such systems. The results are validated by comparing to Taylor T4 in the aligned-spin circular cases, and the additional effects and modulations introduced by the eccentricity and the spins are analyzed. We will use the framework to evaluate the evolution of eccentricity, and trace its contributions to source terms corresponding to the different definitions. Finally, we discuss how this direct integration equations-of-motion code calibrated with strategically places numerical relativity simulations may be relevant to existing and upcoming gravitational wave detectors, such as LIGO and LISA, showing fully generic, precessing, eccentric gravitational waveforms from a fiducial binary system with the orbital plane and spin precession, and the eccentricity reduction.

Type: New
Title: Hadron-hadron scattering from lattice QCD

Principal Investigator: Colin Morningstar (Carnegie Mellon University)
Co-Investigators: Andrew Hanlon (n/a); John Bulava (University of Southern Denmark); Ben Hoerz (Lawrence Berkeley National Laboratory); Andre Walker-Loud (Lawrence Berkeley 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: New
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 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
Title: Simulations of damage-producing supercell thunderstorms at very high resolution

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

Field of Science: Atmospheric Sciences

Abstract:
Supercell thunderstorms are long-lived, often violent storms that produce large hail, strong winds and tornadoes. The strongest tornadoes, those ranked EF4/5 on the Enhanced Fujita scale, are produced from supercells. In this proposal we extend previous work that began on the Blue Waters supercomputer and more recently has been conducted on TACC's Frontera supercomputer. Work is split between two main projects: Simulating supercells that produce devastating tornadoes, and simulating supercells that produce above-anvil cirrus plumes (AACPs), features researchers have recently identified on satellite imagery that have been correlated with especially strong storms, and hence could serve as a forecasting tool for operational meteorologists. Both 30-m resolution EF5 producing supereclls and 50-m resolution supercells producing AACPs have been successfully simulated on Frontera with an existing early-user allocation. In addition to 30-m and 50-m simulations, one 10-m simulation is proposed to attempt to reproduce prior results on Blue Waters and to pave the way for future 10-m simulations on Frontera in new environments. Finally, we request a small amount of additional time to conduct analysis and visualization of simulation data on Frontera with proven tools used regularly by the PI and his collaborators.

Type: New
Title: Investigating electormagnetic precursors to neutron star merger gravitational wave events

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

Field of Science: Astronomical Sciences

Abstract:
Electromagnetic precursors emitted prior to the merger of two neutron stars promise an exciting new window into the fundamental properties of neutron star binaries. Establishment of the properties and observability of these events requires large scale numerical simulations of electrodynamics and particle dynamics in curved-space time. With this project we will perform large-scale electrodynamic and kinetic plasma simulations of magnetospheres of binary neutron stars and calculate their emission signatures. These calculations are very timely as they will allow to help planning the observational search of such precursor signals to gravitational wave events.

Type: New
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:
Flows of partially ionized plasma are frequently characterized by the presence of both thermal and nonthermal
populations of ions. This occurs, e.~g., in the outer heliosphere -- the part of the heliosphere beyond ~ 5~AU whose properties are determined by the solar wind (SW) interaction with the local interstellar medium (LISM).
Simulation of the SW--LISM interaction problem with data-driven boundary conditions, requires the application of adaptive mesh refinement technologies and petascale supercomputers. Supported by the NSF ITR, NSF/DOE, and various NASA projects, we have implemented these
in our Multi-Scale FLUid-Kinetic Simulation Suite (MS-FLUKSS). To couple kinetic and fluid space/time scales, we also use a fully kinetic, particle-in-cell (PIC) code, VPIC, and a highly accurate Vlasov code, Spectral Plasma Solver (SPS).

The objective of this proposal is to take advantage of the new possibilities provided by the NSF's Leadership Resource Allocation (LRAC) program to perform numerical modeling of a number of fundamental and challenging space physics problems described below. All our codes have demonstrated excellent performance on Frontera and other petascale computers, including Blue Waters. All our codes have been ported to Frontera and demonstrated an outstanding performance. Simulations on Frontera will help us understand and interpret observations in a way previously unthinkable because of the limitations in both physical models and computing power. Reciprocally, due to the diversity of our numerical and memory handling approaches, our codes will serve as ideal stress tests for Frontera and may help identify issues with compilers and hardware which affect the productivity of the system.

We request a supplement to our current NSF PRAC project to address the following scientific problems.

1. Nonthermal, pickup ions (PUIs) are of importance to understand the global structure of the heliosphere. They also play a major role in the birth of energetic neutral atoms (ENAs) measured in different energy bands by the Interstellar Boundary Explorer (IBEX) mission. We have implemented an innovative approach to add them to our code, which self-consistently solves the MHD equations for the ion-electron mixture, the pressure and continuity equations for co-moving PUIs, and the Boltzmann equation for the neutral atom transport. This approach is based on imposing boundary conditions onto PUIs crossing the heliospheric termination shock. We will i) perform full-PIC simulations of the termination shock crossing by PUIs and ii) use the output of our kinetic simulations in the MHD-kinetic model of SW--LISM interaction, which will make it possible, for the first time, to obtain a realistic, self-consistent distribution of ENAs in the IBEX energy range.

2. We will perform spectral Vlasov simulations of the evolution of the PUI distribution function in the LISM immediately after the heliopause. These PUIs give birth to ENAs that
are the major contribution to the IBEX ribbon -- a narrow stripe of enhanced ENA flux on full sky maps --

a fascinating discovery of IBEX.

3. We will perform simulations of the SW flow driven by the cornal boundary conditions and compare our simulation results with the Parker Solar Probe measurements.
We will also investigate the shocks born in the SW as they propagate through the LISM.

From the plasma physics perspective, we will extract the fundamental physics of plasma-neutral flows accompanied by the interaction with energetic particles. This will not only allow us to acquire a transformative knowledge on physical processes occurring in the heliosphere, but also extract important information about the LISM properties. The self-consistent coupling of disparate regimes, each governed by distinct physical processes, is a challenge that will be addressed by a new generation of our computational models.

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

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

Field of Science: Nuclear Physics

Abstract:
Hadrons are the bound states of quarks held together by gluons, particles mediating the strong nuclear force. The mass of the quark compounds cannot be understood by only summing its constituent masses. In addition a dynamic contribution introduced by the strong force has to be considered. The observed hadron mass hierarchy remains a mystery to date. Simulating detector setups on Frontera, we intend to determine an optimized set of instrumentation to experimentally address the hadron mass puzzle with the future COMPASS++/AMBER experiment to run at CERN after 2021. Using Frontera, we will also complete the 2015-2018 COMPASS measurement campaigns to unravel the transverse hadron structure in momentum and position space, and the origin of proton spin.

Type: New
Title: QM/MM studies of ibrutinib covalent kinase inhibitor

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

Field of Science: Biophysics

Abstract:
Though molecular mechanical (MM) force fields are based on quantum mechanical (QM) calculations and experimental observations, only QM allows a complete and accurate understanding of many biochemical processes, particularly those that involve chemical reactions and charge redistribution. However, even with the advanced hardware technology available today, the computational cost of studying nanosecond-long dynamics of entire systems solely via QM methodologies is usually prohibitive. A common way to circumvent this cost barrier is to confine the QM treatment to a subregion of a system and include the effects of the surrounding system through an MM treatment, a strategy generally referred to as a hybrid "QM/MM". NAMD, a widely used software package for molecular dynamics (MD) simulations of large biomolecular systems, supports QM/MM calculations together with a large array of enhanced sampling, free energy perturbation, multiple copy algorithms (MCAs), and string reaction pathway methodologies. By virtue of its scalability, NAMD has become the computational engine of choice to study complex biomolecular systems on supercomputers. In this renewal application for 3,950,000 SUs on Frontera, we propose to use the QM/MM feature of NAMD with the string method to determine the chemical reaction pathway leading to the covalent binding of the anti-cancer drug Ibrutinib to Bruton's tyrosine kinase (BTK).

Type: Renewal
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: New
Title: Multi-scale Modeling of Accretion and Jets in Active Galactic Nuclei

Principal Investigator: Alexander Tchekhovskoy (Northwestern University)
Co-Investigators: Matthew Liska (Harvard-Smithsonian Center for Astrophysics)

Field of Science: Astronomical Sciences

Abstract:
Active galactic nuclei (AGN) jets are launched very close to the central black hole. Highly collimated, they propagate through the ambient medium. During this process, jets can dissipate their magnetic energy into non-thermal particles which then emit powerful multi-wavelength electromagnetic radiation and neutrinos. Meaningful interpretation of multi-messenger jet observations requires multi-scale modeling that self-consistently includes a wide range of physical processes acting on vastly different physical scales. However, due to the complexity of the problem, so far theoretical works of relativistic jets have studied separately the accretion physics and jet propagation. Highly idealized treatments of such tightly coupled physical processes limit the predictive power of the models. We propose to perform multi-scale jet simulations that connect accretion physics, fluid dynamics, and jet formation and propagation, to construct the first multi-scale model of black hole accretion, ejection, and interaction with ambient medium in AGN. Namely, we propose to perform the largest general relativistic magnetohydrodynamic (GRMHD) simulation of AGN accretion and jets to date, that extend from the black hole to the emission zone. We will achieve this goal using our new GPU-accelerated code H-AMR, which makes efficient use of Longhorn's V100 GPUs and includes advanced features such as adaptive mesh refinement and adaptive time-stepping. Together with a "moving window" technique, this will allow us for the first time to attack this long-standing multi-scale problem from first principles.

Type: New
Title: Heating and Particle Energization in Quasi-Perpendicular Shocks

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

Field of Science: Magnetospheric Physics

Abstract:
Collisionless shocks are a grand challenge problem in plasma physics and have been the subject of study for more than six decades. A major unanswered question on this frontier is, how does a collisionless plasma transform flow 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 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: New
Title: PRE-EVENTS Multiscale Space Weather Modeling

Principal Investigator: Gabor Toth (University of Michigan)
Co-Investigators: Ward Manchester (University of Michigan); Bart van der Holst (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
Title: DMREF: 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://www.ctcms.nist.gov/~knc6/JVASP.html), and freely available for public.

Type: New
Title: Enhanced sampling atomistic simulations for predictive multi-scale modeling safety pharmacology pipeline

Principal Investigator: Igor Vorobyov (University of California, Davis)
Co-Investigators: Kevin DeMarco (University of California, Davis); Colleen Clancy (University of California, Davis)

Field of Science: Biophysics

Abstract:
Heart rhythm disturbances originating from unwanted drug interactions with cardiac proteins is a serious regulatory concern for drugs on the market and in the development often leading to their withdrawal. They have been linked to a blockade of the potassium ion current through the cardiac ion channel protein KV11.1, encoded by the human ether-a-go-go related gene (hERG). This leads to the prolongation of the QT interval on the ECG, sometimes causing potentially deadly arrhythmias. However, not all hERG blocking and QT prolonging drugs cause arrhythmia. We have developed a multi-scale computational pipeline from atomic to cell and tissue scales, which let us assess drug arrhythmogenic propensity from its chemical structure. Using all-atom molecular dynamics (MD) simulations in our previous supercomputer allocations we informed functional protein, cell and tissue scale models that were able to confirm emergent pro-arrhythmia proclivities of two drugs: high-risk dofetilide and low-risk moxifloxacin. However, we encountered with issues related to an efficient sampling of the drug conformation in the hERG pore, which could limit our model accuracy and predictive potential. Additionally, we need to take into account how drug binding affects channel gating equilibrium Moreover, many hERG blocking drugs are known to bind to other protein targets, especially cardiac sodium and calcium voltage-gated ion channels, NaV1.5 and CaV1.2, respectively, which is known to potentially ameliorate drug's arrhythmogenic activities. Enhanced sampling MD simulations using Hamiltonian replica exchange umbrella sampling as well as string method with a swarm of trajectories on TACC Frontera petascale architecture will help us elucidate thermodynamics and kinetics of state-dependent drug binding to hERG, NaV1.5, CaV1.2, which will be used as an integral component of the predictive multi-scale computational models of drug proclivity for arrhythmogenesis.

Type: Renewal
Title: Multiscale Simulation and Modelling of Biomolecular Phenomena on Frontera

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

Field of Science: Chemistry

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

Type: New
Title: Kinetic characterization of 3D magnetic reconnection

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

Field of Science: Physics

Abstract:
Magnetic reconnection is one of the most important processes in plasmas, where impulsive energy conversion from electromagnetic fields to plasmas takes place. Most of the past reconnection studies are for two-dimensional (2D) laminar current sheets. A few recent studies suggest that three-dimensional (3D) reconnection enhances particle mixing and energization, and the variation in the 3rd dimension allows the generation of additional waves such as the lower-hybrid waves. Reconnection is also reported to occur in the highly turbulent shock transition region. We propose to use particle-in-cell simulations starting from a laminar equilibrium current sheet and from unstable particle distributions with homogeneous fields to study 3D reconnection. We will study (1) the effect of lower-hybrid waves during symmetric reconnection, (2) ion heating during symmetric reconnection, and (3) reconnection born out of the ion instabilities at the shock transition region. By investigating the field structures, particle velocity distribution functions, and particle trajectories, we will advance the understanding of the plasma energization in 3D reconnection from the kinetic level. We request resource to perform 3D particle-in-cell simulations using the VPIC code, and the cost is estimated to be 2.23M SU.

Type: New
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: Kenton McHenry (National Center for Supercomputing Applications); Anna Liljedahl (University of Alaska, Fairbanks); Md Abul Ehsan Bhuiyan (University of Connecticut)

Field of Science: Polar Programs

Abstract:
Permafrost is ground that remain below zero degree Celsius for at least two consecutive summers and it underlays about 25% of the land in the Northern Hemisphere. Vast portions of the near-surface permafrost is both ice- and carbon rich, which, combined with the rapidly warming climate, creates risks to the global climate through the release of greenhouse gases as the permafrost carbon thaws and risks to local and national security as the ice-rich permafrost degrades with subsequent slumping of the ground. Thawing of ice-rich permafrost can be documented using satellite imagery due to surface disturbances, such as landslides and the development of new ponds and channels. The entire Arctic has been imaged down to 31 cm resolution by commercial satellite sensors on average four times in the last six years, accumulating over 2 PB of 'big' pan-Arctic image data that is currently stored at the Polar Geospatial Center. The uses of this imagery are so far limited to field reconnaissance and local-scale remote sensing analysis despite the transformational potentials of this imagery to observe, monitor, and document thawing of ice-rich permafrost in fine details and across large regions. Localized field and remote sensing studies across the Arctic has shown rapid and dramatic thaw in recent decades. Canada, and Russia collectively harbor approximately 5 million km2 of tundra. Producing maps of ice-rich permafrost and permafrost thaw features across the pan-Arctic requires automated analysis of thousands of commercial satellite images. Such an effort requires sophisticated computational approaches that automates image interpretation with an efficient use of high-performance computing (HPC) resources. In this project, we will combine big imagery, deep learning, and HPC to navigate the first very high resolution circumpolar permafrost mapping effort. Our first mapping effort will identify ice-wedge polygons that are typical surface features found in ice-rich permafrost. The resulting map will advance our understanding how the Arctic land surface processes is responding to a warming climate and, therefore, inform national security decisions as well as refine the role that the Arctic tundra plays in the global climate system. Access to the final product by the general public will be made possible through a recent $3M NSF award that will develop an online visualization platform, the Permafrost Discovery Gateway, to enable discovery and knowledge-generation from big imagery products.

Type: New
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 diffi¬culty describing the flow near convective boundaries. This is where material from just outside a convec¬tion zone can become incorporated into it and then carried significant distances radially in the star. The material transported in this way can then participate in nuclear reactions that can alter the course of the star's evolution and/or alter significantly its production of heavy elements. Under special circumstances, such as the hydrogen ingestion flash, the energy release from burning fuel brought into a convection zone from the convective boundary can be so great that the local structure of the star is disrupted [1,2,8,20-25]. 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 consequ¬ences. 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 (see for example [1,2]), 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 [8,10,25]. For massive stars, shell merger events shortly before the core collapses can affect the star's symmetry and hence its explodability [3,24,26]. As participants of the NSF JINA-CEE Physics Frontier Center we explore the ramifications for nucleosynthesis of our simula¬tions.

Type: Renewal
Title: A high-resolution study of intermittency in turbulent mixing using multiple independent simulations

Principal Investigator: Pui-kuen Yeung (Georgia Institute of Technology)
Co-Investigators: Katepalli Sreenivasan (New York University)

Field of Science: Fluid, Particulate, and Hydraulic Systems

Abstract:
This project is directed at a study of important aspects of the mixing of substa
nces and entities in a turbulent fluid flow, especially concerning questions whe
re state-of-the-art computational science methods can achieve the greatest impact. A series of simulations based on exact equations will be performed to study the characteristics of intermittency or intense but localized fluctuations in temperature or concentration fields transported in the flow. A key objective is to clarify the effects of numerical and sampling limitations at large problem sizes in a pragmatic and informative manner. A multiple independent simulations approach is used which greatly facilitates the task of obtaining crucial new insights from the largest simulations possible which are nevertheless constrained by resources available.

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

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

Field of Science: Chemistry

Abstract:
This Leadership Resource Allocation (LRAC) proposal aims to address a current major barrier to progress in drug discovery: the lack of predictive computational methods to identify and optimize potent drugs. We propose a novel computational high-throughput computational lead optimization pipeline to accelerate drug discovery through computer-aided drug design. Our strategy involves integration of novel computational tools that can be used for the accurate and robust prediction of binding affinities of entire libraries of compounds in order to facilitate lead refinement and optimization. The ultimate goal of this project is to advance the state of the art in alchemical free energy simulations so as to be able to achieve binding affinity predictions on libraries of compounds with chemical accuracy within hours using leadership-class GPU computing systems.