Type: New PW

Title: Large Scale Immersed Multiphysics Simulations

Principal Investigator: Aditya Balu (Iowa State University (ISU))
Co-Investigators: Ming-Chen Hsu (University of Texas at Austin (UT) (UT Austin)); Baskar Ganapathysubramanian (Iowa State University (ISU)); Adarsh Krishnamurthy (Iowa State University)

Field of Science: Advanced Scientific Computing

Abstract:

This request seeks computing allocation to support three major thrusts with current funding from different federal agencies:

Thrust 1: Large Scale Multi-physics Simulations of Aircraft Buffeting:
The first research thrust is to obtain accurate large-scale multi-physics simulation results for complex flow phenomena around aircraft and its structural loads under buffeting. we will deploy a high-fidelity computational fluid--structure interaction (FSI) framework to predict the aeroelastic loads and the fatigue life due to buffeting phenomena of a full-scale Boeing P-8A Poseidon aircraft stabilizer.

Thrust 2: Field-scale Agricultural Simulations:
Along with accurately performing simulations for flow over complex geometry, we also focus on field-scale massive simulations with multiple complex objects in each scenario. We will deploy field-scale digital twins for performing analysis to make decisions about physiological, agronomic, and genetic conditions of the crops to improve yield for better economically and environmentally sustainability.

Thrust 3: Physics-aware Generative Design for Inertial Particles:
In the final thrust, we will perform large-scale distributed deep learning for physics-aware generative design using immersed methods for precise and passive manipulation of inertial particles in microscale flow channels.

These research thrusts answer transformative scientific questions that need large-scale computing resources. TACC Frontera would be an important asset for making progress towards achieving our goals in these projects.

Type: New PW

Title: Computational Study of Astrophysical Plasmas

Principal Investigator: Kenichi Nishikawa (Alabama A&M University (AAMU))
Co-Investigators: Yosuke Mizuno (Shanghai Jiao Tong University); Yosuke Mizuno (Goethe University Frankfurt); Nicholas MacDonald (Max-Planck-Institut für Radioastronomie,); Martin Pohl (Universit¨at Potsdam); Kouichi Hirotani (Academia Sinica, Institute of Astronomy & Astrophysics); Ioana Dutan (Institute of Space Science); Michael Watson (Lipscomb University); Athina Meli (North Carolina Agricultural and Technical State University (NCAT) (A&T)); Jacek Niemiec (Institute of Nuclear Physics Polish Academy of Sciences); Christoph Koehn (Technical University of Denmark (Danmarks Tekniske Universitet))

Field of Science: Extragalactic Astronomy and Cosmology

Abstract:

Astrophysical jets are dynamically magnetized plasma flows that are launched most likely in regions where the Poynting flux (magnetic field energy) dominates over the particle flux. We will investigate how the Poynting flux of relativistic jets dissipates into kinetic energy to rapidly accelerate particles by studying the interaction of the particles with the surrounding plasma environment on the microscopic scales, using particle-in-cell (PIC) simulations. We will also generate synthetic spectra by our simulated relativistic jets, polarization images through radiative transfer, particle accelera- tion related to electric discharges and the dynamics of black holes. Our research team employs new computational tools to investigate the important topics of magnetic reconnection, nonlinearly gener- ated turbulence, and associated particle acceleration in collisionless astrophysical relativistic plasmas. Simulations of relativistic jets injected into ambient plasmas with helical (toroidal) magnetic fields have demonstrated possible signatures of magnetic reconnection and nonlinearly generated turbu- lence. Based on our promising and published results using Comet, Bridges and Pleiades, this research project will further explore relativistic particle acceleration associated with magnetic reconnection in jets with helical magnetic fields including turbulence using Frontera. There is a need to explore these processes in more realistic environments, with the best computer power. Therefore, our proposed systematic study will simulate these physical processes in a much more realistic astrophysical context and will elucidate the important factors leading to reconnection and particle acceleration in active galactic nuclei and gamma-ray burst jets. In this research effort, we will analyze the evolution of jets through the use of our extensive visualization tools which help isolate locations of reconnection and its associated phenomena such as particle acceleration. Our initial simulation results and published work show complicated structures of jet evolution due to combined kinetic and kink-like instabilities in the relativistic jets containing helical magnetic fields. The magnetic field structures generated by kinetic and kink-like instabilities determine where and when reconnection occurs. More computational power using Frontera will help our team to make further progress in our simulations. Often explosive in nature, magnetic reconnection enables the rapid release of magnetic energy stored in the jets. Our overall goal is to integrate interdisciplinary scientific aspects to study basic plasma physics and the- oretical astrophysics and to develop new numerical methods to simulate the microphysical processes responsible for reconnection, turbulence, and high-energy particle acceleration. At Alabama A&M University (AAMU) we will educate students through this research. We will create animations of the 3D evolution of relativistic jets with kinetic processes, and present them not only at scientific meetings but also use them for AAMU student outreach, public outreach activities, high school outreach, and presentations at the Space and Rocket Center, and Planetarium in Huntsville.

Type: New PW

Title: First-Principles Simulations of Electrocatalytic Kinetics of Single Metal Atom in Nitrogen Doped Graphene

Principal Investigator: Yuanyue Liu (University of Texas at Austin (UT) (UT Austin))
Co-Investigators:

Field of Science: Chemistry

Abstract:

Single metal atom in nitrogen doped graphene is a promising catalyst for a variety of electrochemical reactions in aqueous solution, while there is limited atomic level understanding about the catalytic kinetics. Conventional first-principles simulations often overlook the complexities such as the dynamical surface charge and hydrogen bonding, and are usually limited to thermodynamics. We recently developed a model enabling effective simulation of electrochemical kinetics at solid-water interface. Here we propose to apply this model to elucidate the catalytic mechanism of single metal atom anchored on nitrogen doped graphene for oxygen reduction reaction, and discover better catalyst. To accomplish these goals, we request 235,200 node hours. This project is supported by two NSF grants (#1900039 and # 2029442).

Type: New PW

Title: Deformation of Reactive Surfaces in Stirred Turbulence

Principal Investigator: Fabrizio Bisetti (University of Texas at Austin (UT) (UT Austin))
Co-Investigators:

Field of Science: Fluid, Particulate, and Hydraulic Systems

Abstract:

Understanding underlying mechanisms controlling turbulence-interface interactions is crucial in a variety of practical applications. We seek a better understanding of Reynolds number effects on the propagation of the flame surface, attempting to extend our power law scaling hypothesis obtained from spherical turbulent flames in decaying isotropic turbulence, to a system which presents practically relevant turbulence conditions. Under the support of an NSF award, this new system, the von Kármán swirling flow, is being investigated numerically by the PI’s group, alongside collaborative experimental studies. We seek to expand our existing database of von Kármán swirling flow simulations from the previous allocation cycles to higher Reynolds numbers, to maintain synergy with our experimental collaborators, as well as focusing on regimes of practical relevance. The simulations will be run through a code which has been used on numerous high performance computing platforms with up to 22 B grid points and 130,000 processors. The code displays excellent strong and weak scaling capabilities upto 32,768 processors on the Stampede2 supercomputer, which shares architectural similarities to Frontera at the processor level. To support this work, 250,000 SU on Frontera, and 25 TB on Ranch are requested.

Type: New PW

Title: Compressibility Effects in Turbulence Flows of Non-Ideal Fluids

Principal Investigator: Sanjiva Lele (Stanford University)
Co-Investigators:

Field of Science: Fluid, Particulate, and Hydraulic Systems

Abstract:

This research is primarily motivated by the need for fundamental understanding of turbulence at extreme thermodynamic states for development of modern thermal energy and power systems. The proposed work studies the fundamental dynamics of the compressible turbulent flows involving thermodynamically complex fluids. A set of direct numerical simulations of compressible isotropic turbulence and homogeneous shear turbulence will be conducted at high Reynolds number and a wide range of turbulent Mach numbers. An validated equation of state for non-ideal fluids is incorporated to capture non-classical thermodynamic behavior. The effects of fluid properties under different working conditions and the coupled effects of the compressibility will be systematically investigated. All the computation configurations, data, and related results will be well documented and available to the public.

Type: New PW

Title: Large Eddy Simulation for Novel Wave Energy Converter

Principal Investigator: Yingchen Yang (University of Texas Rio Grande Valley)
Co-Investigators:

Field of Science: Fluid, Particulate, and Hydraulic Systems

Abstract:

Although wind wave energy harvesting is still in its infancy, it has proven to be a promising method of renewable energy against other common sources, such as solar panels or wind turbines. Wave energy has the advantage of both having a higher predictability and lower intermittency than both solar power and wind power, as waves are always present and tides can be predicted with ease. Another advantage that wave energy holds over its competitors is its considerably higher power density in comparison, which makes it a very promising technology. Additionally, waves have very little energy loss despite long distances travelled. WEC also require less hazardous materials to be built in contrast to solar panels, this makes them more beneficial in terms of net environmental impact. However, the issue of current WEC technologies lies in their dependence on the resonance principle to harvest energy.

These WEC are designed and manufactured taking into consideration the average of the wave frequencies of the coastline they will be installed in. However, this is not an accurate enough approach. The wind waves are unpredictable and unsteady, so relying on the resonance principle does not make it possible for them to work at their highest efficiency.

We propose a lift-type rotor based on unidirectional motion that can work for the entire range of wave frequencies and oscillations. Our simulation will validate the design of this rotor using Computational Fluid Dynamics (CFD) simulations using OpenFOAM, an open source CFD solver. We will be studying the energy transfer from the waves to the WEC, which calls for a good resolution of the turbulent eddies at the fluid-solid interface since they carry a lot of the energy of the wave. For this purpose, we will use the Large Eddy Simulation (LES) to properly study the turbulence encountered by the WEC rotor. Additional differential equations will be used to study the energy transfer process between the rotating unidirectional WEC and the energy it interacts with. The simulation will be on a 3-D water-air domain using multiphase solvers to have the air drive the ocean waves, which will then drive the rotor we propose, as it would in a real-life set up. The proposed rotor is designed using two sets of NACA 0021 hydrofoils installed in a Wells turbine and Darrieus turbine. These turbine structures are meant to deal with vertical and horizontal flows, respectively, which would help our WEC design deal with incoming waves omnidirectionally.

The simulation will also be implemented to corroborate experimental results obtained using a wave tank with a model of the rotor installed built to scale, whereas the simulation will have the geometry at full scale.

We hope that our numerical and experimental results can help validate our proposed WEC design and that they can help provide more focus on this advanced technology that still has a lot of potential for the renewable energy sector.

Type: New PW

Title: Reproducible preprocessing of open neuroimaging data

Principal Investigator: Russell Poldrack (Stanford University)
Co-Investigators: Christopher Markiewicz (Stanford University)

Field of Science: Behavioral and Neural Sciences

Abstract:

Brain imaging techniques, particularly magnetic resonance imaging (MRI), have provided growing insight into the ways that the structure and function of the brain give rise to the human mind, and the ways in which brain functions go awry in mental health disorders. These data are increasingly shared in an open manner, which greatly benefits the scientific community. However, the variability in processing of these data across different groups has the potential to reduce reproducibility of research results. We propose to use a set of well-established tools for quality control and preprocessing of functional magnetic resonance imaging datasets to consistently preprocess all of the more than 350 relevant datasets in the OpenNeuro data archive. This will provide a broad group of researchers with analysis-ready data, enabling the pursuit of a wide range of neuroscientific questions.

Type: Renewal PW

Title: First-principles Study on Strongly Correlated and Energy Storage Materials

Principal Investigator: Xin Li (Harvard University)
Co-Investigators:

Field of Science: Materials Research

Abstract:

Energy storage plays a crucial part in the clean energy revolution of the twenty-first century. Advanced electrochemical energy storage technologies are essential to any future implementation of broad-base clean energy. Material design methodologies are needed that synergistically consider the performance, safety, and cost of new energy storage materials. These issues can be addressed by computational search and design of advanced new battery electrode and electrolyte materials for improved performance, controlled interface reaction and reduced cost [1–4]. High-throughput computational simulations are not only less expensive and time-consuming as compared to experiments, but also efficient to test new ideas in the materials design schema. Such computational approaches are an ideal guide for the experimental discovery of new functional materials. At the Li laboratory at Harvard University, computation and experiment are merged under this principle. The main research goal of this proposal is to develop the material understanding and design needed to supply Li lab experimentalists with the strategic guidance to recognize practical next-generation superconductive and energy storage materials.

Type: Renewal PW

Title: Flow-induced configurational microphase separation and crystallization in entangled polymers in 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:

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 at enelongational 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 Wi range wherein the coil-stretch hysteresis is evident. We propose to study this startling phenomenon behavior using 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. We further quantify phase transition and flow-induced crystallization kinetics for this entangled liquid well above its quiescent melting temperature.

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 chain dynamics that are crucial to a complete understanding of the in homogeneous 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 new fundamental understanding of the flow behavior of polymeric liquids.

Type: New PW

Title: High Fidelity Hurricane Storm Surge and Ocean Modeling

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

Field of Science: Computational Mathematics

Abstract:

The first goal of this Pathways allocation is the verification and development of new finite element meshes to be used in operational forecasting and prediction of hurricane storm surge on the Louisiana-Texas coast. This requires the computation of storm surge forecasts of extraordinary resolution within a time scale of 1 to 1.5 hours to provide critical information to emergency managers and decision makers. The verification will be performed using the advanced circulation (ADCIRC) model by comparing the results of computations using the current operational forecasting mesh, the new proposed meshes, and available elevation gauge data for past hurricanes. A secondary goal is oil spill source location detection for disaster-mediated oil spills using the ADCIRC model and the Lagrangian Particle Tracking code PYthon Ocean PArticle TRAcking (PYOPATRA).

Type: Renewal PW

Title: Mini-Protein Binder Frontera Pathways Application

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

Field of Science: Biochemistry and Molecular Structure and Function

Abstract:

The coronavirus (SARS-CoV-2) pandemic has highlighted the need for therapeutic-driven pandemic preparedness. We at the Institute for Protein have developed software tools to quickly create new protein drug candidates, but these require massive amounts of compute time. A recent publication from our lab demonstrates what we can do with this pipeline. In this paper, we created small proteins (<65 amino acids) that bind with picomolar affinity to the surface of the virus, neutralizing it. These antiviral proteins are currently progressing through preclinical testing and may someday be on the market to fight COVID-19. With additional time on Frontera, we can continue to develop our tools to be ready to stop the next pandemic before it takes hold and to create useful protein therapeutics for other diseases along the way.

Type: Renewal PW

Title: Mechanism of Ca2+-evoked synaptic vesicle fusion

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

Field of Science: Neuroscience Biology; Biophysics

Abstract:

The mechanism of neurotransmitter release by Ca2+-evoked synaptic vesicle fusion has been extensively studied for three decades, yielding critical insights into the functions of the core components of the release machinery. The SNAREs syntaxin-1, synaptobrevin and SNAP-25 play a critical role in membrane fusion by forming a tight SNARE complex that brings the membranes together, and synaptotagmin-1 acts as the Ca2+-sensor that trigger release. However, the mechanism of membrane fusion remains highly unclear. This application proposes to perform all-atom molecular dynamics simulations in the microsecond time scale to investigate how the SNAREs and synaptotagmin-1 cooperate to trigger fast, Ca2+-dependent membrane fusion.

Type: New PW

Title: Large-scale structure prediction and classification of virulence factors in marine pathogens

Principal Investigator: Richard Schaeffer (University of Texas Southwestern Medical Center (UTSW) (UT Southwestern))
Co-Investigators:

Field of Science: Biochemistry and Molecular Structure and Function

Abstract:

The virulence of pathogens is moderated in part by effector proteins and secretion systems that can be transferred between organisms within an environment. The complex evolutionary history of these proteins can complicate identification of their function and identification of pathogenic and pandemic strains. We propose to use recently developed structural prediction tools as a method for characterization of known effectors and identification of novel effectors.

Type: New PW

Title: Mechanisms of the Sliding Clamp Loader Complex

Principal Investigator: Brian Kelch (University of Massachusetts Medical School (UMMS) (UMass Worcester))
Co-Investigators:

Field of Science: Molecular Biosciences

Abstract:

We are interested in the dynamics of the sliding clamp loading process. Towards this goal we have several aims, including characterizing the dynamics the sliding clamp/clamp loader complex, which we have captured at many stages of the sliding clamp loading process, and characterizing the transitions between these states.

Type: Renewal PW

Title: R-Matrix with Time Dependence Calculations for Ultrafast Atomic Processes in Strong Laser Fields

Principal Investigator: Kathryn Hamilton (Drake University)
Co-Investigators: Klaus Bartschat (Drake University)

Field of Science: Atomic, Molecular, and Optical Physics

Abstract:

The study of both electron- and photon-driven processes in atoms could have many wide-ranging applications, not only in the field of atomic, molecular, and optical physics, but also in astrophysics, plasma physics, and further afield in chemistry and biology. We propose to use two different ab-initio R-Matrix methods to explore such phenomena: the B-Spline atomic R-Matrix code (BSR) and the R-Matrix with Time Dependence (RMT) method. Possible avenues of investigation include the study spin-orbit interaction in a time dependent manner, electron scattering from helium and rubidium, and novel techniques for the measurement of attosecond photoionization delays.

Type: Renewal PW

Title: Renewal for PHY20032: First-principles study of many-body interactions and excited-state properties in two-dimensional systems

Principal Investigator: Diana Qiu (Yale University)
Co-Investigators:

Field of Science: Condensed Matter Physics

Abstract:

Two-dimensional (2D) materials are the subject of significant ongoing research for technological applications in electronics, optoelectronics, valleytronics, and energy. Under optical excitation, 2D materials in general exhibit strong electron-hole interactions due to the strong spatial variations in the screening of the Coulomb interaction, as well as reduced total screening and electronic confinement resulting from the dimensionality reduction. It is thus very important to accurately calculate and thoroughly understand the many-electron properties of 2D materials for developing devices based on such materials. Our group is actively focused on studying the effect of many-body interactions on the excited state properties of materials in reduced dimensions and complex functional materials. Particular emphasis is placed on engineering optical excitations of 2D materials by inducing and controlling structural/chemical defects, aiming to provide an understanding of fundamental processes such as charge/energy transfer between heterointerfaces and guidelines for designing 2D systems for technological applications. Our group is also engaged in developing high-performance first-principles quantum physics methods based on the GW-Bethe-Salpeter-Equation (BSE) approach to calculate many-electron interaction effects for a broad range of material systems with a current focus on novel efficient algorithms for solving the BSE including non-uniform spatial sampling schemes, finite momentum excitons, time-dependent approaches, and electron-hole interactions in core-level spectra. Two specific research topics will be investigated on the renewed Frontera Pathway allocation. In the first project, we will use the GW-BSE method to study how optical excitations and valley-selectivity in monolayer transition metal dichalcogenides (TMDs) can be tuned by proximity effects from the adsorption of chiral molecules and induction of structural defects. In the second project, we will apply a new many-body downfolding approach for calculating exciton effects on core-level excitations to the study X-ray absorption spectra of monolayer TMDs, where exciton effects are expected to be large.

Type: Renewal PW

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

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

Field of Science: Gravitational Physics

Abstract:

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

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

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

Type: New PW

Title: Neutron Electric Dipole Moment from Lattice QCD

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

Title: Pushing the Boundaries of Quantum Circuit Simulation

Principal Investigator: Brian La Cour (The University of Texas at Austin)
Co-Investigators: Brajesh Gupt (The University of Texas at Austin)

Field of Science: Physics

Abstract:

The capabilities of quantum computing devices are beginning to rival that of current high performance systems. An important challenge now is the ability to validate the results of quantum computations and assess whether a computational advantage has been demonstrated. Under this project we will investigate the classical simulation of quantum circuits with a large number of qubits (> 45) and a comparably large circuit depth, representing the most challenging computational problems. A successful demonstration of this capability will enable research into physical phenomena that are currently out of reach of numerical simulation.