Type: Renewal   PW

Title: Predicting orientation-dependent plastic events in amorphous solids via deep learning

Principal Investigator: Michael Falk (Johns Hopkins University)
Co-Investigators:

Field of Science: Materials Research

Abstract:
In our recent work [Fan and Ma, Nat. Commun. 12, 1506 (2021)], we developed a new deep learning framework – a novel structure representation we refer to as the spatial density map (SDM) that can be used to provide atomisitic data to a convolutional neural network (CNN). Using this framework we have achieved unprecedented accuracy for identifying atoms in amorphous solids with a high propensity for shear transformation solely from their static structure. We now plan to use the developed deep learning models to present evidence of correlation between initial static structure and shear band locations in simulated metallic glasses. This is an essential step towards formulating robust theories of failure modes in amorphous solids. Then we will use some examples to demonstrate that our new deep learning framework can achieve high-fidelity prediction of rotation-invariant properties, which are more common in both amorphous and crystalline materials. This will be of interest broadly in many disciplines, including physics, chemistry, biology, and materials science. Furthermore, we will train a deep learning model to identify complex crystal structures locally in atomistic simulations, which is necessary for the study of phase transition behavior and deformation mechanism of complex intermetallics like Laves phases.

Type: New   PW

Title: Parametric Instabilities of Alfven Waves

Principal Investigator: Xiangrong Fu (New Mexico Consortium)
Co-Investigators:

Field of Science: Solar Terrestrial Research

Abstract:
Alfven waves are of fundamental importance in magnetized plasmas. In this study, we plan to carry out 3D large-scale plasma simulations of the Alfven wave dynamics in low-beta environments. The results will advance our understanding of nonlinear behaviors of Alfven waves, especially the parametric instabilities, which can lead to development of turbulence and energization of charged particles in laboratory, space, and astrophysical plasmas. The simulation study is a vital part of our project funded by the NSF/DOE Partnership in Basic Plasma Science and Engineering.

Type: New   PW

Title: Formation and Evolution of the Local Group of Galaxies

Principal Investigator: Oleg Gnedin (University of Michigan)
Co-Investigators:

Field of Science: Astronomical Sciences

Abstract:
We request computing time on Frontera and storage on Ranch. We have developed a new approach to modeling star formation in cosmological simulations by simultaneously following the formation of star clusters and their feedback on the parent molecular cloud. Using a powerful adaptive-mesh-refinement code ART, we will test the implementation of star formation and stellar feedback on the scale of parsecs, in addition to the global galaxy properties on the scale of kiloparsecs. We will run a suite simulations of the Local Group volume. These simulations will produce a rich data set that will be used to interpret observations of Galactic star clusters and stellar halo. We will investigate the chemical evolution of the stellar populations and the origin of the galactic mass-metallicity relation. We will also analyze the age-metallicity distribution of globular clusters.

Type: Renewal   PW

Title: Structure and Dynamics of Highly Turbulent Premixed Combustion

Principal Investigator: Peter Hamlington (University of Colorado)
Co-Investigators:

Field of Science: Fluid, Particulate, and Hydraulic Systems

Abstract:
Highly turbulent premixed flames are found in a range of engineering and natural systems, including engines, gas turbines, and even supernova explosions. Much of the current knowledge in this area has been obtained from numerical simulations of idealized configurations using relatively simple chemical models. To address the need for greater realism, this project will use advanced computational tools and more sophisticated chemical modeling to study the characteristics and behaviors of highly turbulent premixed flames in practically relevant configurations. Ultimately, physical insights resulting from this project will enable more accurate simulations of advanced energy systems. This research will make use of adaptive mesh refinement (AMR) for overcoming the computational cost of simulating more complex practical configurations, including those where secondary flows, shear, swirl, and walls are important. Using AMR, new direct numerical simulations will be performed, and the resulting datasets will be examined using Lagrangian and scale-dependent diagnostics. In addition to refining theories and models of highly turbulent combustion, the proposed project will impact the broader combustion community by publicly sharing data and statistics from each of the simulations, as well as all analysis codes and diagnostic tools.

Type: New   PW

Title: Modeling Materials for Energy Conversion and Storage over Experimental Timescales

Principal Investigator: Graeme Henkelman (University of Texas at Austin)
Co-Investigators:

Field of Science: Chemistry

Abstract:
One of the most significant challenges for the computational understanding of current materials and the design of new materials for energy storage and conversion is the limitation in accessible time scales. A direct simulation of atomic motion is limited to picoseconds when the forces and energies are based upon density functional theory (DFT) calculations. The relevant timescale for the function of batteries and fuel cells, however, are on a human timescale of second to minutes. In this proposal we will use the adaptive kinetic Monte Carlo (AKMC) method with DFT codes to model novel materials that can function as electrolytes and electrodes in rechargeable batteries, which can accelerate and select reactions of interest. The parallel resources offered by the TACC program will allow us to explore the potential energy surface around stable states and determine the mechanism and rates of possible reaction mechanisms. We have, and will continue over the duration of this project, to develop the EON code which manages the individual calculations that identify saddle points on the potential landscape which correspond to each possible reaction mechanism and collects the information to evolve the system over timescales set by the elementary reaction mechanisms. Importantly, this methodology does not require intuition (or bias!) from the user so that reaction pathways are determined automatically and can be surprising and complex, if that is the nature of the potential energy landscape. We show, in this proposal that we will be able to efficiently use the TACC resources for these calculations. This project will also enable us to accomplish the goals set out in our NSF funded projects to improve the efficiency of our computational methods as well as model diffusion in battery and fuel cell materials.

Type: Renewal   PW

Title: Computational Infrastructure for Geodynamics - Community Code Scaling

Principal Investigator: Lorraine Hwang (Computational Infrastructure for Geodynamics, UC Davis)
Co-Investigators: Timo Heister (Clemson University); Rene Gassmoeller (University of Florida); Hiroaki Matsui (University of California, Davis); Arushi Saxena (University of Florida)

Field of Science: Geophysics

Abstract:
The Computational Infrastructure for Geodynamics (CIG) is an NSF-funded organization dedicated to developing, providing, and maintaining a suite of high-quality, open-source software packages that are widely used in the geosciences to simulate the dynamics of the solid earth. An important mission of CIG is the development of computational capabilities in the scientific community we serve, particularly the use of modern numerical methods, software development methodologies, and high performance computing facilities. To achieve this goal, we aim to further the scalability of codes used in simulating the fluid flow in the Earth's mantle, the deformation of the lithosphere, and in the generation of the geodynamo with the goal of running large 3D simulations in studying the dynamics of the Earth's interior.

Type: New   PW

Title: Structure elucidation of novel molecular substances via machine learning and nuclear magnetic resonance spectroscopy

Principal Investigator: Eric Jonas (University of Chicago)
Co-Investigators:

Field of Science: Chemistry

Abstract:
Small molecules are of vital importance in chemistry, biology, and society, but determining the structure of new molecules continues to be a challenge. Currently, spectroscopic techniques are used that require considerable human effort to interpret. Here we propose building on our recent success in automating this analysis for carbon nuclear magnetic resonance (NMR) spectroscopy to the more challenging proton NMR, which offers a significantly higher signal-to-noise ratio. We do this using ML and AI techniques developed in our research group, requesting both CPU time (for data generation) and GPU time (for scaling and development of novel models).

Type: New   PW

Title: Development of Mechanistic Models of New Photocatalytic Systems with Predictive Capabilities for Efficient Organic Photocatalysis

Principal Investigator: Oleg Larionov (University of Texas at San Antonio)
Co-Investigators:

Field of Science: Organic and Macromolecular Chemistry

Abstract:
Recent advances in organic photocatalysis have led to transformative changes in organic synthesis, yet the development of new photocatalytic systems has been slow and is typically achieved through empirical structure-reactivity studies, while the understanding of underlying mechanistic principles of the photocatalytic activities is lacking. We have recently developed new photocatalysts that enable the activation of strong chemical bonds by harnessing the energy of visible light. Given the synthetic importance of the chemical transformations that are facilitated by the new photocatalysts and the mechanistic novelty of the photocatalysis modes, it is important to develop accurate mechanistic models that account for the observed catalytic activities and allow for prediction of new and more active catalysts. In this study, we will perform a detailed computational analysis of the mechanistic parameters of the new photocatalysts and develop accurate predictive models of the photocatalytic systems, merging high-level TD-DFT calculations of excited states, multivariate linear regression, and machine learning techniques as a part of our combined experimental and computational NSF-funded study (CHE-2102646, PI: Oleg Larionov). The development of the new approaches to modeling and prediction of photocatalytic activities is expected to enable the discovery of a wide range of currently unknown photocatalysts based on a systematic and mechanism-guided merger of quantum mechanics, statistical analysis, and machine learning, resulting in transformative advances in our understanding of complex chemical systems and improvements in the public access to medicines, agrochemicals, and new materials through previously unknown photocatalytic chemical reactions.

Type: New   PW

Title: Elucidating Structural Roles of Cardiac Disease-associated Mutations in Voltage-gated Sodium Channel Nav1.5

Principal Investigator: Jing Li (University of Mississippi)
Co-Investigators:

Field of Science: Biophysics

Abstract:
As one of the most widely distributed types of ion channels, voltage-gated sodium (Nav) channels initiate action potentials and serve a central role in electrical excitability. More than 1000 mutations in human Nav channels have been linked to various excitability disorders in heart, muscle, and brain. For instance, genetic disruption of the activation and inactivation of Nav1.5 channel has been identified as one of the major causes of various cardiac disorders, such as type 3 long QT syndrome (LQT3) and Brugada syndrome (BrS). Inspired by the great physiological/biomedical significance of Nav channels, our group seeks to study the underlying molecular mechanisms of disorders with Nav-channel dysfunction as leading causes. Although great progresses have been made very recently in structural biology of Nav channels, there are many key mechanistic aspects that remain unclear for their function and dysfunction. This proposal focuses on the activation and inactivation transition of the voltage-sensing domain (VSD) in Nav1.5 channel, and aims to illuminate the molecular effects of cardiac disorder-associated mutations in the context of structural transition. Molecular dynamics (MD) simulations will be performed to characterize the activation/inactivation transition between structural states, and structural perturbations induced by mutations on the transition. Then 2-dimensional potential of mean force (2D PMF) will be calculated for the free energy landscape to quantify the mutational alteration on the thermodynamics/kinetics among functional states. This computational study will provide structural and dynamical insights for the mutational effects, and to achieve a deeper understanding of the molecular mechanism of sodium channelopathies, which will also bring more selective treatments for this physiologically critical drug target.

This is an intensive computing project with extended MD simulations and large-scale free energy (2D PMF) calculation. Especially the free energy calculation requiring at least 240 nodes per job in present proposal cannot be performed on our other supercomputing resources, thus, we expect this study to greatly benefit from supercomputer Frontera.

Type: New   PW

Title: ryujin - towards robust and efficient computation of supersonic hyperbolic flow at large and small scales

Principal Investigator: Matthias Maier (Texas A&M University)
Co-Investigators: Jean-Luc Guermond (Texas A&M University)

Field of Science: Computational Mathematics

Abstract:
The objective of this project is to develop the high-performance hydrodynamics solver ryujin (https://github.com/conservation-laws/ryujin, C++, MIT license). This code is based on the open-source finite element library deal.II (https://github.com/dealii/dealii, C++, LGPL-2.1+ license). We are currently developing ryujin into a general hydrodynamics framework to solve PDEs with dominant hyperbolic structures (e.g., compressible Navier-Stokes equations, compressible Euler equations, Euler-Poisson, or Euler-Maxwell equations) and with strong, physics inspired, point-wise stability properties. The algorithms used in ryujin are provably robust, i.e. the computations are guaranteed to satisfy physical bounds under appropriate time step restriction without invoking any ad-hoc tuning parameters or ad-hoc slope limiting techniques. We have demonstrated on 3D hydrodynamics simulations that, in its current version, ryujin can efficiently handle 85 billion spatial degrees of freedom on up to 100,000 cores.

The TACC Pathways allocation will be used to pursue a number of fundamental R&D directions aiming at improving the performance of ryujin: (i) we will dramatically improve the scalability and the compute kernel efficiency of ryujin; (ii) we will implement an Euler-Poisson and Euler-Maxwell module; (iii) we will validate the new developments by performing a series of large scale 3D computations. We expect that the above improvements will allow ryujin to run efficiently over several millions of MPI ranks.

Type: New   PW

Title: Towards Robust Atmospheric Retrievals for Cloudy L Dwarfs: Tests on T Dwarf
Spectra

Principal Investigator: Caroline Morley (University of Texas at Austin)
Co-Investigators: Melanie Rowland (University of Texas at Austin)

Field of Science: Astronomical Sciences

Abstract:
Retrieving atmospheric properties from spectra is the only method through which properties of brown
dwarf and exoplanet atmospheres can be determined since in situ measurements are impossible at
astronomical distances. Retrieval frameworks are computationally expensive, but this process can be
accelerated through the use of graphics processing units (GPUs) in the calculation of the millions of
model atmospheres generated in a retrieval framework. But to date, retrieval frameworks with clouds
have not been robustly verified for accuracy despite the fact that clouds are abundant in cooling brown
dwarfs and exoplanets. Before we can incorporate the more complex physics governing cloud formation
into retrieval frameworks for cloudy L dwarf atmospheres, we must first test a number of assumptions
regarding thermal structure, chemical equilibrium, and uniform chemical abundances on the more
straightforward and relatively cloud-free T dwarf emission spectra.

Type: Renewal   PW

Title: Studies In Theoretical Astrophysics and General Relativity

Principal Investigator: Stuart Shapiro (University of Illinois at Urbana-Champaign)
Co-Investigators: Antonios Tsokaros (University of Illinois); Milton Ruiz (University of Illinois)

Field of Science: Gravitational Physics

Abstract:
We request a renewal of our current Frontera allocation AST20025 to continue our multi-year effort to tackle several large-scale, long-standing, unsolved problems in theoretical astrophysics and numerical relativity. We numerically solve the Einstein field equations coupled to the relativistic magnetohydrodynamic equations to simulate neutron stars (NSs), black holes (BHs), and accretion disks, in isolation or in binary systems. We are interested in the study of gravitational and electromagnetic radiation generated from these sources ("multimessenger astronomy"); our numerical studies address fundamental questions dealing with strong-field gravitation and focus on problems that are motivated by current and future observations of gravitational waves by aLIGO/VIRGO, GEO, KAGRA, Pulsar Timing Arrays, LISA/DECIGO, the Einstein telescope, and other laser interferometers now operating or under development. Our simulations also model promising gamma-ray burst sources (GRBs) observed by NASA satellites such as, INTEGRAL, SWIFT, and FERMI, X-ray sources observed by NICER, CHANDRA, and XMM-Newton, and optical and infrared sources observed by the HST, NuSTAR and PanSTARRS telescopes. This research is supported by grants from the National Science Foundation (NSF) and the National Aeronautics and Space Agency (NASA).

Type: Renewal   PW

Title: Enhanced sampling molecular dynamics simulations for a multi-scale personalized safety medicine pipeline

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

Field of Science: Biophysics

Abstract:
Cardiac arrhythmias arising from unintended drug interactions have been linked to a blockade of the potassium ion current through the ion channel protein Kv11.1, encoded by the human Ether-à-go-go-Related Gene (hERG). They present a serious regulatory concern for drug candidates and even drugs already on the market often leading to their abandonment or withdrawal.   A drug-induced hERG channel blockade may lead to the prolongation of the QT interval on the ECG, sometimes resulting in potentially deadly arrhythmias. However, not all hERG channel blocking and QT prolonging drugs are arrhythmogenic. Our recently developed multi-scale computational safety pharmacology pipeline lets us assess arrhythmogenic propensities of various drugs from their chemical structures. Enhanced sampling all-atom molecular dynamics (MD) simulations of hERG – drug interactions are used to estimate parameters for functional kinetic protein, cell and tissue scale models that can detect emergent drug's pro-arrhythmia proclivity. We recently successfully applied these models to assess arrhythmogenicity of two drugs: high-risk dofetilide and low-risk moxifloxacin (Yang et al Circulation Research 2020; 126:947–964) with al-atom MD simulations on multiple HPC resources including those at TACC playing a key role in these efforts. In the proposed study we plan to expand our efforts and investigate how hERG mutations, associated with genetic cardiovascular abnormalities and/or altered channel gating may affect state-dependent drug binding and thus their pro-arrhythmia proclivities. We will also investigate how sex hormones and their derivatives affect drug-induced hERG channel blockade. Female sex is an independent risk factor for drug-induced cardiac arrhythmias, and our experimental collaborators observed an acute cooperative effect of drug and sex hormone blockade of hERG channel conduction. These simulations will be essential for designing in silico safety medicine pipeline, which will take into account patient's sex and genotype to predict a personalized drug's arrhythmogenic risk. Enhanced sampling MD simulations on TACC Frontera petascale architecture and Longhorn GPUs are most suitable for performing a crucial atomic-scale component of this pipeline.

Type: New   PW

Title: Seamless coupled hydrologic-hydrodynamic simulations using a next-generation community model

Principal Investigator: Joseph Zhang (College of William and Mary)
Co-Investigators: Charles Seaton (Columbia River Inter-Tribal Fish Commission)

Field of Science: Earth Sciences

Abstract:
Continuing on our successes made possible with previous XSEDE allocations (TG-OCE130032; CDA21001) and to accommodate the increased demand from several recently funded projects, we request a Pathway allocation on NSF's leadership computing capabilities for science and engineering (Frontera). The software we use is the world's first bona fide compound flooding modeling framework, and the simulations planned using the allocation will significantly advance the frontiers of knowledge in the realm of nonlinear compound flooding studies. The impact from this effort will be widely felt because (1) we are testing operational forecasts based on the model for US Atlantic and Gulf coasts; (2) we serve a large and diverse community world-wide.