Type: New LSCP

Title: Multi-scale Modeling of Accretion and Jets

Principal Investigator: Alexander Tchekhovskoy (Northwestern University)
Co-Investigators:

Field of Science: Extragalactic Astronomy and Cosmology

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. This will allow us for the first time to attack this long-standing multi-scale problem from first principles. Additionally, we also propose to attack jet-ambient medium interaction in the context of mysterious Fast Blue Optical Transients (FBOTs) using the power of Frontera CPUs.

Type: Renewal LSCP

Title: SCEC Earthquake Modeling, Ground Motion, and Hazard Simulations

Principal Investigator: Christine Goulet (University of Southern California (USC))
Co-Investigators: Bruce Shaw (Columbia University in the City of New York (Columbia University)); Scott Callaghan (University of Southern California (USC)); Yehuda Ben-Zion (University of Southern California (USC))

Field of Science: Earth Sciences

Abstract:
The Southern California Earthquake Center (SCEC) conducts and coordinates fundamental and applied research on earthquakes using southern California (SoCal) as its main natural laboratory. SCEC's research program is investigator-driven, relies on strong collaboration among researchers, and supports research and education in seismology, tectonic geodesy, earthquake geology, and computational science. SCEC is a leader in research that integrates science results into computational tools to support seismic hazard improvements. Empirical data are extremely limited for infrequent large earthquakes, and particularly sparse for near-fault ground motions that largely control the design of critical infrastructure. Physics-based earthquake and ground motion simulators present a practical solution to these issues. Given sufficient validation against observations, our datasets can supplement or replace the empirical datasets and provide guidance for probabilistic seismic hazard analyses (PSHA) for ground motion and probabilistic fault displacement hazard analyses (PFDHA). Our long term goals in the seismic hazard realm are to 1) increase the accuracy of earthquake, ground motion, and hazard simulations; 2) reduce uncertainties; and 3) broaden the usefulness of seismic simulation software tools for engineering and preparedness applications. These objectives are only attainable through strong collaborative team work and require Frontera-enabled HPC capabilities.

Type: New PW

Title: A Systematic Study of How AGN Feedback Regulates the Black Hole Accretion in Early Protogalaxies

Principal Investigator: Kung-Yi Su (Columbia University in the City of New York (Columbia University))
Co-Investigators:

Field of Science: Galactic Astronomy

Abstract:
AGN feedback is critical in galaxy evolution and the black hole accretions. Observations find supermassive black holes (>>1e5 solar mass) at high-redshift (Z>4) with jetted AGN quasars. It is unclear whether a stellar-massive to intermediate-mass black hole can grow and become a supermassive black hole within such a relatively short period of time, in particular, with the presence of AGN feedback. Most studies in AGN feedback and black hole accretions either utilize galaxy scale simulations or GRMHD simulations that can resolve the accretion disk. The finest resolution of the former case is at best ~0.1 pc, while the outer boundary of the latter case is at most 1000 times the gravitational radius. The discrepancy creates a several order of magnitude gap in between, making it hard to connect the sub-grid models of black holes at galaxy scale from the self-consistently launched jet in black hole accretion disk scale.

To study the effect of AGN feedback on black hole accretion and also to fill in the gap in the two kinds of simulations above, we propose to utilize high-resolution hydrodynamic simulations of pc-scale boxes. We will utilize the set of simulations to study the propagation of bubbles resulting from various forms of AGN feedback in black hole vicinity and its effect on black hole accretion onto stellar-mass to intermediate-mass black holes in a different environment. We will systematically vary the background gas density, temperature, angular momentum, black hole mass, feedback efficiency, and AGN feedback models. The proposed simulation will incorporate the most relevant processes for modeling the interplay of galaxies evolution and AGN feedback, including (1) state-of-the-art hydrodynamic code, GIZMO, under the MFM model that combines the advantages of Lagrangian and Eulerian methods, (2) ray transfer for radiative feedback (3) the hyper-refinement around the black hole and around the jet propagation region for higher resolution resolving jet propagation and black hole accretion, and (4) the particle spawning method for jet modeling to more accurately capture the jet physics. This set of simulations will enable the most extensive survey of every aspect of jet AGN feedback models in black hole accretion and cocoon/bubble propagation.

Type: Renewal 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 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. Built on the results of previous allocation, we plan to perform full 3D simulations of Alfven wave parametric instabiltities, with the hope of addressing perpendicular wave dynamics which are critically important as suggested by experiments. The simulation study is a vital part of our project funded by the NSF/DOE Partnership in Basic Plasma Science and Engineering.

Type: Renewal PW

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

Principal Investigator: Graeme Henkelman (University of Texas at Austin (UT) (UT 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 and catalysis, 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: 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. The Frontera-enabled computational work that was conducted in the first year has produced a plethora of exciting preliminary data and resulted in three peer-reviewed publications. We plan to expand our work on the application of computational and machine learning techniques with an emphasis on big data analysis of mechanisms of photochemical transformations and specific interactions of substrates and photocatalysts.

Type: New PW

Title: Study of Linear Instabilities in Laminar Supersonic Shock-wave/Boundary-Layer Interactions using Kinetic Methods

Principal Investigator: Deborah Levin (University of Illinois Urbana-Champaign (UIUC) (University of Illinois) (U of I))
Co-Investigators: Vassilios Theofilis (University of Liverpool)

Field of Science: Fluid, Particulate, and Hydraulic Systems

Abstract:
This proposal aims to understand shock structures, unsteadiness and possible three dimensional effects for shock- laminar boundary-layer interactions (SWBLI) for supersonic flows in the near continuum flow regime with the use of particle-based Direct Simulation Monte Carlo (DSMC) methods that offers the highest fidelity. We seek to understand these mechanisms through the use of data-driven modal analysis techniques such as operator-based global stability analysis tools that have been parallelized to process big data. To make efficient use of petascale facilities, we have developed an MPI-based solver known as Scalable Unstructured Gas-dynamics Adaptive mesh-Refinement (SUGAR) and have applied it successfully to the type of computationally intensive simulations that are proposed here. Our primary goals for this project, as outlined in Sec. II, will serve as a part of Ph.D. thesis of a graduate student, Irmak Taylan Karpuzcu, under the guidance of Prof. Deborah Levin at the University of Illinois at Urbana-Champaign. These goals will also serve as a part of Ph.D. thesis of a graduate student, Angelos Klothakis, under the guidance of Vassilis Theofilis at the University of Liverpool. The findings will be published in peer-reviewed journal papers. The two research groups have been collaborating in the past three years where students in both groups have learned about DSMC (Levin's field of expertise) and linear stability theory (Theofilis' area of expertise).

Type: New PW

Title: Scalable hierarchical CFD solvers for future exascale architectures

Principal Investigator: Juan Alonso (Stanford University)
Co-Investigators:

Field of Science: Fluid, Particulate, and Hydraulic Systems

Abstract:
The thousand-fold increase in computational capabilities expected over the next decade will change the way in which both engineering and scientific discovery are pursued. But we will only be able to achieve such new methods of scientific inquiry if we are able to harness the power of future supercomputers for, among other areas, complex Navier-Stokes computations of turbulent fluid flow using scalable preconditioners and solvers that do not exist today. Our proposed work will focus on the following key ingredients and research questions relating solver technology that we have been developing recently:
-Assess performance and scalability of a class of preconditioners based on low-rank compression and hierarchical matrices embedded into a nested dissection and multifrontal elimination based approach.
-Assess performance and scalability of pipelined s-step communication-hiding and communication-reducing strategies for iterative Krylov solvers.
-Demonstrate the performance and scalability of these new preconditioned solvers using the task-based runtime environment TaskTorrent.
-Demonstrate our solver strategies in the SU2 DG-FEM higher-order solver for LES and WMLES solutions and demonstrate applicability of our solver to higher order problems ($p > 3$) that represent an advancement over the state of the art.
-Demonstrate large-scale system algorithmic scalability in $O(N \log^p N)$, and guaranteed convergence of iterative methods in $O(1)$ steps with $O(N \log^p N)$ preconditioner cost.

The outcome of this effort will be an assessment of the scalability and performance of such hierarchically-preconditioned solvers and improvements to the solvers to enable scaling to very large numbers of processors.

Type: New PW

Title: Engineering of molecular probes using active learning to sense per- and polyfluoroalkyl substances (PFAS) in water

Principal Investigator: Siva Dasetty (University of Chicago)
Co-Investigators:

Field of Science: Mathematical Sciences

Abstract:
Per- and polyfluoroalkyl substances (PFAS) contamination in water is a pressing global problem because of their high persistence and detrimental effects on the environment. Birth defects, cancer, and alterations to immune system are some of the example health effects in humans induced by PFAS exposure. There are more than 4700 variants of PFAS, which are mostly molecules containing at least one fully fluorinated methyl or methylene carbon group. In this work, we develop an integrated computational and experimental framework to tackle PFAS contamination in water by engineering molecular probes to sense PFAS. For navigating the vast chemical space of molecular probes efficiently, we take assistance from machine learning (ML). We use all-atom molecular dynamics (MD) simulations and enhanced sampling methods to evaluate the effectiveness of optimal probes identified by ML. Each simulation system comprises a target contaminant variant or an interferent and a probe molecule solvated in water with a net total of ~15000 to 55000 atoms. With ML assistance, we expect to simulate ~10% (~385 probes) of our initial search space of molecular probes comprising linear molecular probes.

From our benchmark study with Frontera startup allocations, we estimate ~12,000 GPU node hours and ~153,000 CPU node hours are needed to study a total of ~100 systems. Through the pathways allocations, we plan to use the requested node hours for running the all-atom MD simulations and enhanced sampling of our systems using singularity containers of GROMACS 2018.6 patched with PLUMED 2.5.2. To analyze the collected simulation data (~80 GB per system) using GROMACS tools and Python, we plan to mainly use the CPU nodes. The results from our computational work will be validated using rigorous experiments and subsequently will be applied to design efficient and effective sensors to detect PFAS in water. In addition, we expect our results to reveal novel understanding of design rules of probe molecules to sense PFAS in water and in developing technologies to remediate PFAS from water.

Type: Renewal PW

Title: Computational Infrastructure for Geodynamics - Community Code Scaling

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

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: Renewal PW

Title: Enhanced sampling molecular dynamics simulations to elucidate molecular determinants of pro-arrhythmic proclivities of beta blocking drugs

Principal Investigator: Igor Vorobyov (University of California Davis (UCD) (UC Davis))
Co-Investigators: Vladimir Yarov-Yarovoy (University of California Davis (UCD) (UC Davis)); Colleen Clancy (University of California, Davis)

Field of Science: Biophysics

Abstract:
Sympathetic stimulation of cardiac β adrenergic receptors (βAR) is essential for controlling heart rhythm and vascular tone. Beta-blockers downregulate their activity and thus reduce heart rate, lower blood pressure, and prevent arrhythmias. However, these drugs are capable of binding to cardiac ion channels such as voltage-gated potassium channel Kv11.1 encoded by the human Ether-à-go-go-Related Gene (hERG), a notorious drug anti-target. Drug-induced hERG blockade is clinically manifested as a prolongation of QT interval on the ECG, associated with increased arrhythmogenic risk. However, not all hERG blocking drugs cause arrhythmia. We seek to understand how the combination of hERG and beta-block alters pro-arrhythmia risks by examining the underlying molecular mechanisms of these interactions via molecular dynamics (MD) simulations. Our approach is based on a multi-target extension of a recently published multiscale computational pipeline capable of distinguishing cardiac safe and pro-arrhythmic drugs based on their chemical structure, which used kinetics of hERG – drug interactions from atomistic simulations as functional model parameters (Yang et al Circulation Research 2020; 126:947–964). We will demonstrate it here on the example of the anti-arrhythmic and beta-blocking drugs sotalol, propranolol and metoprolol, which have different cardiac safety profiles possibly resulting from stereospecific affinities for βARs as well as off-target cardiac ion channel binding. Previously, we performed all-atom MD simulations of d- and l-sotalol interactions with the open-state model of the hERG channel and used the resultant affinities and rates as parameters for the multi-scale functional kinetic models of cardiac arrhythmia (DeMarco et al Journal of Molecular and Cellular Cardiology 2021; 158:163-177). In this proposed study we will extend this work to probe sotalol and other beta-blocking drug interactions with new structural models of the inactivated state of the hERG channel as well as different conformational states of the β1AR for a more accurate predictions of pro-arrhythmia risks. Enhanced sampling MD simulations on TACC Frontera petascale architecture and Longhorn GPUs are most suitable for performing a crucial atomic-scale component of our multiscale in silico pipeline for predictive cardiac safety pharmacology.

Type: New PW

Title: Computational investigations on RNA liquid–liquid phase separation and single-stranded DNA folding

Principal Investigator: Devarajan Thirumalai (University of Texas at Austin (UT) (UT Austin))
Co-Investigators:

Field of Science: Biophysics

Abstract:
We have extensively used the Frontera pathway allocations to carry out theoretical/computational research on various aspects of nucleosome structure and dynamics, chromosome organization, glassy materials, as well as self-assembly of RNA repeats. Through this proposal we are requesting new allocations for continuing our research on RNA repeat assembly, and to initiate new research projects on the structural transition of RNA and the effect of ions on single-stranded DNA folding.

Type: New PW

Title: Advanced Signal Processing and Machine Learning to Detect RNA Tails on DNA using 2D Nanopore Sensor

Principal Investigator: Jean-Pierre Leburton (University of Illinois Urbana-Champaign (UIUC) (University of Illinois) (U of I))
Co-Investigators:

Field of Science: Biophysics

Abstract:
In this research, we will conduct an extensive investigation using molecular dynamics and device engineering to demonstrate the capabilities of 2D material membranes with nanopores to sequence DNA structures with RNA tails. The sensing technique will include the calculation of both ionic blocking currents and electronic currents along 2D membranes caused by the modified DNA structures during their translocation through the nanopore. Furthermore, advanced signal processing and machine learning will be employed to undermine the effect of noise and obtain a reliable signal which can prove to be revolutionary in this field. To successfully carry out the intended goals of this project, we estimate our usage to be around 202,428 node-hours in CPUs and 1,775 node-hours in GPUs in Frontera Pathway.

Type: New PW

Title: Sputtering of Graphitic Structures for Lifetime Estimates of Space Propulsion System

Principal Investigator: Huck Beng Chew (University of Illinois Urbana-Champaign (UIUC) (University of Illinois) (U of I))
Co-Investigators:

Field of Science: Mechanics and Materials

Abstract:
The need for an efficient, high-thrust space propulsion system to augment or replace traditional chemical propulsion systems is of great national importance, and is paramount to advancing space supremacy of the United States. One of the candidate propulsion system for NASA's Artemis program and human space flight missions on Mars is the Hall Thruster, which is a high power electric propulsion (EP) system. Even though EP has been an integral part of space exploration since the late 1990s, high power EP (>100 kW), such as Nuclear Electric Propulsion, remains largely a concept due to insufficient correlation between ground-test results versus in-flight performance and wear. This primarily stems from ground-based EP test facilities interacting with thruster operations. As such, ground test measurements cannot adequately represent in-space environment, performance, and lifetime, leading to significant uncertainties in predictions. One major challenge is the presence of contaminants from the facility walls interacting with the thruster through back sputtering, contaminant transport and redeposition. To reduce these effects of facility back-sputtering, graphitic structures have traditionally been used to line the walls of the testing chamber. Nevertheless, at high ion energies (high eV), even pyrolytic graphite undergoes significant sputtering. The dispersion of these back sputtered carbon species throughout the facility, and subsequent deposition on the carbon pole covers, center-mounted cathode, anode, and on boron nitride channels, leads to significant errors in EP thrusters' lifetime and performance assessments. Here we seek to quantify how the presence of carbon contaminants affect the boron-nitride thruster chamber sputter properties, and in turn the failure lifetime of the EP thruster using molecular dynamics (MD) simulations performed with LAMMPS. The requested 250,000 node hours of allocation on Frontera will enable us to quantify the sputtering rates of graphitic structures across the range of ion energies relevant in the ground-based EP test facility. The proposed research is currently supported by a NASA grant under the "Joint Advanced Propulsion Institute, a NASA Space Technology Research Institute".

Type: New PW

Title: Merging Magnetized Neutron Stars with Neutrino Transport

Principal Investigator: Steven Liebling (Long Island University)
Co-Investigators:

Field of Science: Gravitational Physics

Abstract:
We have created a distributed, adaptive mesh code, MHDuet, to solve the fully nonlinear, general relativistic, magnetohydrodynamics equations with an approximate neutrino scheme to model the merger of two magnetized neutron stars. This code incorporates large eddy simulation (LES) techniques that has been shown convergent in the magnetic field amplification at merger from the Kelvin-Helmholtz instability. The proposed simulations serve to understand the multimessenger signals observed by gravitational wave (GW) observatories and conventional, electromagnetic (EM) telescopes. Such simulations are critical to extracting science from the wide spectrum of observations of GW170817, a neutron star binary merger that was observed in 2017 in both GW and EM bands, as well as future multimessenger observations. Our code relies on LLNL's SAMRAI infrastructure to achieve good scaling on large machines, and our testing with a start-up allocation on frontera demonstrated weak scaling at 87\% efficiency up to at least 512 nodes (28,672 processes). With the proposed simulations, we anticipate addressing two important astrophysical questions: (1) What are the implications for understanding GW170817 when one uses LES to help resolve the magnetic field amplification during the merger of two neutron stars in conjunction with neutrino transport scheme? (2) To what extent do our MHDuet results agree with the results of other codes for the GW170817 system to better constrain our uncertainties in the parameters of that and future observations?

Type: New PW

Title: Computational contributions for the next-generational gravitational wave detectors

Principal Investigator: Milinda Fernando (University of Texas at Austin (UT) (UT Austin))
Co-Investigators: Hari Sundar (University of Utah)

Field of Science: Gravitational Physics

Abstract:
Existing codes for Numerical relativity and relativistic magnetohydrodynamics do not scale well on modern heterogeneous clusters and this is a major impediment to scientific progress in these areas. In recent work, we have developed a highly scalable adaptive numerical relativity framework, Dendro-GR. The framework provides a flexible high-level interface for numerical relativity using problem description using a Symbolic interface in symbolic python. The problem is then automatically discretized and architecture-specific code is automatically generated. We currently support distributed memory parallelism via MPI, shared memory parallelism via OpenMP, SIMD vectorization using `avx2` and `avx512`, and support for Nvidia GPUs using CUDA. We have demonstrated the excellent scalability of our framework and the code generation capabilities on TACC's Frontera supercomputing using up to 229K cores. In this work, we are requesting a pathways allocation to shed light on unexplored parameter configurations for the binary black hole problem. We specifically target to perform, black hole binary mass ratios 16, 32, and 64 with precession spin configurations. These simulations will be used to tune low-cost surrogate models which is essential for gravitational wave detection.

Type: New PW

Title: Swirl-stabilized hydrogen combustion numerical simulation

Principal Investigator: Paul PALIES (University of Tennessee Knoxville (UT Knoxville))
Co-Investigators: Gan Xiao (University of Tennessee Knoxville (UT Knoxville))

Field of Science: Science and Engineering Education

Abstract:
Future combustion propulsion systems may operate with hydrogen fuel in premixed regime with air to reduce the emission of NOx and eliminate those of CO2. Swirl-stabilized combustion of hydrogen/air flames operating in premixed regime is important both from a fundamental point of view and for technological relevance. Numerical simulations aiming at describing the physical phenomena of these complex flows are critical and very few detailed simulations exist. The present pathway proposal is focusing on conducting some of these challenging and computationally demanding simulations on relevant cases prior to submitting in a near future a LRAC proposal. The research proposed in this pathway proposal will focus on several aspects such as assessing flame speed models and evaluate selected existing models from literature directly on the numerical simulation data generated within this Frontera pathway allocation. The simulation data will be significantly post-processed and analyzed and the code further optimized.