Type: New PW

Title: Boundary-Layer Stability and Control for Hypersonic Problems

Principal Investigator: Helen Reed (Texas A&M University)
Co-Investigators:

Field of Science: Fluid, Particulate, and Hydraulic Systems

Abstract:
The Computational Stability and Transition (CST) Laboratory within the Texas A&M Department of Aerospace Engineering is a computational lab focused on investigating boundary-layer laminar to turbulent transition for a range of different aerospace problems. Studying the transition phenomenon is critical for a number of reasons: Increasing the length of laminar flow on an aircraft can decrease drag, reducing fuel consumption, thus lowering emissions. Controlling the laminar-to-turbulent transition process can lead to better dynamics for aircraft since turbulent flow over control surfaces can stay attached at larger deflection angles, leading to higher maneuverability. At very high speeds (Mach 5+), understanding transition is critical, as turbulent heat loading on a vehicle can become 10X that seen for laminar flow, and thus turbulent flow can destroy a vehicle if not properly understood.
The CST lab uses high performance research computational fluid dynamics (CFD) codes to create highly resolved laminar solutions on which to perform stability analysis. In particular, NASA's Data Line Parallel Relaxation (DPLR) and OVERFLOW CFD codes are used to solve the Navier-Stokes equations in order to generate flowfields at hypersonic speeds over general geometries of interest. Several in-house stability codes are used to study the stability of boundary layers such as the Linear/Nonlinear Parabolized Stability Equations (LPSE/NPSE) and/or Spatial biGlobal (SBG). Due to the sensitivity of stability analysis, very highly resolved simulations that regularly exceed 200+ million cells are needed to accurately model the transition process. Due to the very large simulation requirements along with the Export-Controlled nature of these CFD codes, Frontera is the ideal supercomputer for this class of CFD problems.

Type: Renewal LSCP

Title: Understanding the Global Behavior of Core-Collapse Supernovae

Principal Investigator: Matthew Coleman (Princeton University)
Co-Investigators: Christopher White (Princeton University); Aaron Skinner (Lawrence Livermore National Laboratory); David Vartanyan (University of California, Berkeley); Adam Burrows (Princeton University)

Field of Science: Stellar Astronomy and Astrophysics

Abstract:
Core-collapse supernovae herald the death of massive stars and the birth of neutron stars. During this violent process, a combination of high-density nuclear physics, multi-dimensional hydrodynamics, radiation transport, and neutrino physics determines the final seconds of a star's life. Despite the early attempts in the 1960s to understand core-collapse supernovae, the explosion mechanism - thought to involve the detailed neutrino physics of the stellar interior - still remains poorly understood. Detailed long-term, three-dimensional calculations proving this paradigm are lacking, but are essential if we are ever to understand this problem. Current advances in computational capabilities and the availability of HPC resources, together with improvements in nuclear theory, provide a golden opportunity to tackle this long-standing problem with renewed vigor.

Using our new state-of-the-art, highly-scalable, 3D, multi-group, radiation-hydrodynamics code FORNAX we developed and tested over the last four years, we propose to conduct multiple three-dimensional radiation/hydrodynamic simulations to help resolve this fifty-year-old problem in nuclear astrophysics. Our thesis is that going to fully 3D neutrino radiation-hydrodynamics using the state-of-the-art FORNAX computational capability and employing the best neutrino and nuclear physics may together be the keys to demonstrating and understanding the generic core-collapse supernova explosion mechanism. We propose a series of detailed 3D simulations utilizing a broad range of micro-physics configurations (e.g. equations of state, many body calculations) out to late time, until the explosion diagnostics saturate, to resolve the effects of micro-physical uncertainty in the core-collapse supernovae problem. Such an endeavor will additionally inform future high-energy experiments and observational efforts, as well as guide nuclear theory at these extreme conditions.

Viewed as a nuclear physics laboratory, core-collapse supernovae produce the highest densities of matter and energy in the modern universe. These vigorous explosions also are responsible for seeding most of the elements in Nature. The neutrino and gravitational wave signals they emit carry information about the high-density nuclear equation of state. Thus, supernovae probe the same sort of physics as FRIB, JLAB, ATLAS, and low-energy runs at RHIC, FAIR (GSI/Darmstadt), SHINE (CERN) and NICA (Dubna).

A resolution of the core-collapse supernova problem would benefit ongoing efforts of observers and instrument designers in the U.S. and around the world engaged in projects to determine the origin of the elements, measure gravitational waves (LIGO), and interpret laboratory nuclear reaction rate measurements in light of stellar nucleosynthesis.

Type: Renewal PW

Title: Real-time High Resolution Ensemble Numerical Weather Forecasts Using FV3-LAM for NOAA Testbeds - Ramping Toward Exascale

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

Field of Science: Meteorology

Abstract:
The Center for Analysis and Prediction of Storms (CAPS) at the University of Oklahoma (OU) has, for several years, been testing high-resolution numerical weather prediction (NWP) with support from, and in collaboration with, the National Oceanic and Atmospheric Administration National Weather Service (NOAA NWS) Testbeds. The NOAA NWS Testbeds bring research and operational meteorologists together to evaluate, both subjectively and objectively, new tools for improving forecasts of high-impact weather events across the Contiguous United States (CONUS). This project extends that work by ramping high-resolution NWP ensembles toward Exascale in support of the Hydrometeorology Testbed (HMT) Winter Weather Experiment (WWE) 2020-21 and the HMT Flash Flood and Intense Rainfall (FFaIR) experiment. CAPS plans to produce a 15-member high-resolution NWP ensemble in support of the these quasi-operational testbeds as part of a project to develop and extend NOAA's next-generation Unified Forecasting System (UFS) in a high-resolution regional weather configuration, the Finite Volume Cubed Sphere Limited Area Model (FV3-LAM). This model is part of the emerging NWS Unified Forecasting System (UFS) that CAPS is helping to develop and trial. As part of the experiments, CAPS will develop and test ensemble post-processing tools, including a spatial-aligned mean and machine learning, for improving forecasts of heavy snow and other high-impact winter weather in WWE and flash flooding and heavy rainfall in the FFaIR. The project will extend CAPS prior successful execution of FV3-LAM (formerly known as SAR-FV3) ensembles on large scale XSEDE resources (TACC Stampede2) and move toward the Exascale on Frontera by augmenting our previous ensemble with 5 additional members covering the entire North American Continent at 3-km grid spacing (about 3.7x CONUS grid points) and a trial member with 1-km grid spacing requiring approximately 27 times the computations of the current 3-km grid-spacing.

Type: New PW

Title: Understanding the partitioning of surface-active material in aged marine aerosols

Principal Investigator: Rommie Amaro (University of California, San Diego)
Co-Investigators:

Field of Science: Chemistry

Abstract:
Marine atmospheric aerosols make up a significant portion of the planetary aerosol budget but represent one of the largest sources of uncertainty in current climate models. Recent developments in the collection and characterization of nascent sea spray aerosols (SSA) have led to a greater understanding of their chemical components and size distributions, as well as the physical mechanics of bubble production and bubble bursting that lead to the transfer of organic and biological material from the ocean to the atmosphere. However, due to significant limitations in single particle analysis instrumentation, there is still an incomplete understanding of individual SSA chemical composition and morphology and how this directly influences the climate-relevant properties of SSA. In 2019, as part of the NSF CAICE CCI, we received a generous allocation on Blue Waters, which we used to initiate our study of large-scale model marine aerosols. Using many types of experimental data, determined through CAICE labs, we used tools in the Amaro lab to develop 3D molecular-level whole SSA particle models. These models mimic the composition of ‘real world’ SSA particles and provide a radical change in approach to many current studies at the molecular scale, which utilize lipid and fatty acid monolayers to explore structural dynamics of SSA constituents. By utilizing our data-centric methods to model these SSAs, we have provided the first glimpses into the detailed time-dependent dynamics of nascent SSA. In this proposal we seek to extend on our paradigm-shifting work by simulating secondary marine aerosols, to explore how the aging process affects these particles and the chemical reactions occurring at their surface.