Theoretical and Computational Astrophysics Networks Program
Abstracts of Selected Proposals
(NNH20ZDA001N-TCAN)

Below are the abstracts of proposals selected for funding for the Theoretical and Computational Astrophysics Networks Program (TCAN). Principal Investigator (PI) name, institution, and proposal title are also included. Twenty-two proposals (22) were received in response to this opportunity. On September 29, 2020, four (4) proposals were selected for funding.

Nickolay Gnedin/University Of Chicago
Simulating Cosmic Reionization Beyond the Current State-of-the-Art

The reionization of the all-pervading intergalactic medium - the transformation of cold neutral hydrogen into a highly ionized warm plasma - marks a turning point in the history of structure formation in the Universe. The details of this process reflect the nature of the first astrophysical sources of radiation and heating, the power-spectrum of density fluctuations on small scales, the thermodynamics and chemistry of cosmic baryons, the star formation and black hole accretion history, and a complex network of poorly understood feedback mechanisms. These outstanding issues represent crucial missing links in galaxy formation and cosmology research. A number of unprecedented datasets from new space- and ground-based facilities are poised to revolutionize our understanding of the dawn of galaxies in the next decade, and promise an era of precision reionization studies. In particular, the large wavelength coverage, unique sensitivity, and different spectroscopic and imaging capabilities of the James Webb Space Telescope (JWST) will allow the discovery of star-forming galaxies out to redshift 15, the tracing of the evolution of the cosmic star-formation rate density to the earliest cosmic times, the measurement of the evolving fraction of Lyman-alpha emitting galaxies (LAEs), and will provide tight constraints on both the reionization history and the contribution of different sources to the ionizing photon budget of the Universe.

The critical challenge in leveraging next generation capabilities remains the lack of sufficiently realistic and detailed theoretical modeling tools to predict and interpret new observations. This program seeks to address that challenge and to develop a theoretical and computational support for the anticipated observational breakthroughs. Our two main objectives are to (1) develop a physical understanding of the process of cosmic reionization on large scales and of the connection between galaxies and the surrounding IGM and (2) provide detailed predictions and elaborate modeling that will enable and guide the interpretation of high-redshift data from JWST observations. We describe in this proposal a two-tier suite of state-of-the-art numerical simulations with up to 500 billion cells that incorporate realistic baryonic physics and self-consistently couple RT calculations with cosmological hydrodynamics over an almost million-fold range of spatial scales.

This program will focus here on core reionization science, i.e. the ionization and reheating of intergalactic hydrogen and the properties of early UV sources. In order to be most useful to future observational studies, we put heavy emphasis on the potential observables at the end of reionization process - a scientific area where the synergy between JWST and both the existing large samples of high redshift quasars and future observations from 30-meter-class telescopes is expected to lead to the most significant discoveries in the very near future.

Software development efforts will include developing a radiative transfer module into the GPU-accelerated massively parallel Computational Hydrodynamics On Parallel Architectures (Cholla) code to model the IGM via cosmological simulations and developing Machine Learning pipelines for matching diverse properties of simulated galaxies (such as stellar masses, star formation rates, ionizing luminosities, etc) to their host dark matter halos, with all developed codes to be made publicly available to the community.

Our team is composed of researchers from three major US institutions who have a proven track record in computational astrophysics and have pioneered many of the ideas, techniques, and developments of modern reionization/IGM studies. We seek to capitalize on our complementary expertise and strengths and create a synergistic, coordinated program addressing a fundamental issue in theoretical and computational astrophysics.

Wladimir Lyra/New Mexico State University

Dynamical instabilities in the aid of planet formation in circumstellar disks

The dynamical state of the protoplanetary disk is the fundamental canvas on which the planet formation narrative is etched. Among the many steps in the planet formation process, there is perhaps no step as least well understood as the formation of planetesimals, bodies approximately 1-100 km in size that comprise the building blocks of fully fledged planets. The current favored model for planetesimal formation, the streaming instability, whereby inward-drifting grains spontaneously form gravitationally bound clumps of pebbles, is known to work only for solid-to-gas ratios above that of the ISM. Large scale structures in disk turbulence may provide the route towards such initial concentrations, such as has been shown in models of disk turbulence induced via the magnetorotational instability (MRI). However, recent years have seen the MRI mechanism being replaced by a number of hydrodynamic and low-ionization magnetohydrodynamic processes that generate turbulence in such disks and produce large scale structures that often drastically differ from those produced via the MRI.

Given these results, and the recent realization that turbulence may actually hinder planetesimal formation (depending on the initial pebble size) it is crucial that we understand the role of turbulence on the streaming instability. As such, the primary goal of this proposal is to investigate and characterize the interplay between these dynamical processes, their synergy with the streaming instability, and the outcome of this synergy on planetesimal formation. We will run a series of independent high-resolution 3D models (typical resolution 768x256x2048 mesh points in spherical coordinates) tailored to the regions where the instabilities are expected to be active. We will model the instabilities in isolation, as well as the transition region between them. Each model will contain (1) the conditions for the instabilities, (2) adequate dynamical range, (3) Lagrangian particles to model the grains, (4) conditions for the streaming instability, and (5) particle gravity to produce planetesimals. The proposed work will solve the long-standing issue of the robustness of planetesimal and thus planet formation, specifically for the most realistic (ISM) dust-to-gas ratios of 0.01, by examining the synergy between dynamical instabilities and the streaming instability.

Molly Peeples/Space Telescope Science Institute
Gas and Galaxies Across Cosmic Time with Enzo-E

Galaxies grow and evolve by exchanging gas with the diffuse cosmic web in a grand cycle that is mediated by their “circumgalactic medium” (CGM). NASA's operating astrophysics missions, most especially the Hubble and Chandra “Great Observatories,” have shown that these components cannot be understood in isolation, but must be pieced together as a whole to explain how galaxies evolve to have the diverse shapes, sizes, chemical abundances, and spins that these telescopes observe. In the next five years, NASA will commission two new flagship observatories---the James Webb Space Telescope (2021) and the Nancy Grace Roman Space Telescope (2025)---that will revolutionize studies of galaxy evolution. Webb will push galaxy studies all the way back into the cosmic Dark Ages, and Roman will deploy Hubble-like resolution over huge fields to survey cosmological volumes. A key consequence of these advances is that the current frontier for theoretical galaxy formation studies lies where our ability to simulate galaxies encompasses a full treatment of the CGM-galaxy connection, high spatial and mass resolution, and cosmological volumes.

Our proposed TCAN will commission Enzo-E, a new simulation code that is optimized to meet this challenge. Over the last three years, a sub-group of our proposed network has pioneered new techniques for simulating galaxies and their gas at unprecedented resolution, while another sub-group has rebuilt the underlying simulation code Enzo-E from the ground up to run efficiently on exascale supercomputers. We propose to combine these efforts into an interwoven program to explore the gas-galaxy connection over cosmic time using a suite of entirely new, high-resolution, full-physics cosmological hydrodynamic simulations uniquely situated to model the diffuse gas between galaxies and its role in forming galaxies. Enzo-E is uniquely suited for modeling small-scale structure of diffuse gas while simultaneously reaching large volumes; our program will add to Enzo-E the new physical modules needed to address forthcoming data from NASA facilities.

Our TCAN will: (1) commission the new Enzo-E simulation code with full physics modules and verify its performance on state-of-the-art computing facilities, (2) create a suite of highly resolved production simulations targeted at interpreting the observations of galaxies that will be collected by Webb and Roman, as well as their predecessors, (3) generate and publicly release a suite of high-fidelity simulated data products matching up with the key observational data products, and (4) support four PhD dissertations and significant amounts of software development for delivering to the community open-source software for Enzo-E itself and associated analysis codes. When added to new observational data, our efforts will follow the formation of galaxies in conjunction with their gas, trace the dispersion of heavy elements, track the reionization of the Universe, and uncover the seeds of cosmic structure.

Daniel Proga/University Of Nevada, Las Vegas

Global Models of Accretion and Outflows in Astrophysical Disks: A new DAWN (Disk Accretion & Winds Network)

The standard model of accretion disks developed in the 1970s cannot account for the observed spectral features of disk-accreting systems such as excess thermal emission (e.g. the ‘big blue bump’ in active galactic nuclei), non-thermal X-ray emission, and broad emission and absorption lines. Moreover, the model does not account for either magnetically-driven or radiation-driven outflows known to always accompany optically thick, geometrically thin accretion disks. In the past decade, algorithms have been developed to solve the equations of radiation-magnetohydrodynamics (rad-MHD), making it possible to understand the coupled dynamics of accretion flows and outflows from first principles using a single model. However, in order to enable realistic calculations of disks and winds, these algorithms must be extended to include frequency-dependent radiation transport (to properly model Compton cooling), photoionization and non-LTE effects (to compute the net heating/cooling rates and opacities correctly), and the radiation force on spectral lines in a three-dimensional turbulent flow.

Our network proposes to carry out these tasks by collaborating on the development of numerical tools for coupled disk-wind dynamics. To facilitate testing the new models that will result against observations, we also propose to build sophisticated spectral diagnostic tools capable of producing synthetic spectra from our models. Both components require calculating the ionization balance to varying degrees of accuracy, which will be done by interfacing the XSTAR atomic database withthe rad-MHD code Athena++. We will apply these new models of radiatively efficient accretion disks to four different systems: active galactic nuclei, cataclysmic variables, X-ray binaries,and FU-Orionis systems. This project is very relevant to past, present, and future NASA facilities (e.g., the HST, Chandra, NuSTAR, and finally JWST and XRISM). Our network will consist of five institutions: UNLV, IAS, UVa, NASA/GSFC, and the CCAat the Flatiron Institute. It will support collaborative research by graduate students, postdocs,and senior personnel. We plan a winter school on accretion disks and winds at UNLVfor students and postdocs outside the network, as well as a summer school on computational astrophysics at the IAS for URM students.