2023 INCITE Proposal Submission
Proposal

Title: Long term 3D simulations of core collapse supernovae
Principal Investigator: William Raphael Hix
Organization: Oak Ridge National Laboratory
Date/Time Generated: 6/17/2022 2:44:06 PM

Section 1: PI and Co-PI Information

Question #1

Principal Investigator: *The PI is responsible for the project and managing any resources awarded to the project. If your project has multiple investigators, list the PI in this section and add any Co-PIs in the following section.*

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Question #2

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Question #3

Institutional Contact: *For the PI's institution on the proposal, identify the agent who has the authority to review, negotiate, and sign the user agreement on behalf of that institution. The person who can* *commit an organization may be someone in the contracts or procurement department, legal, or if a university, the department head or Sponsored Research Office or Grants Department.*

Institutional Contact

Institutional Contact Name

Susan Ochs

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Section 2: Project Information

Question #1

Select the category that best describes your project.

Research Category

Physics: Astrophysics

Question #2

Please provide a project summary in two sentences that can be used to describe the impact of your project to the public (50 words maximum)

Project Summary

We plan long running models of core-collapse supernovae to examine their neutrino and gravitational wave signals for potential detection by current and future observatories. We will also examine the elemental production that occurs in supernova, especially the potential for elements heavier than iron to be made late in the explosion.

Section 3: Early Career Track

Question #1

Early Career

Starting in the INCITE 2022 year, INCITE is committing 10% of allocatable time to an [Early Career Track](#) in INCITE. The goal of the early career track is to encourage the next generation of high-performance computing researchers. Researchers within 10 years from earning their PhD (after December 31st 2012) may choose to apply. Projects will go through the regular INCITE Computational Readiness and Peer Review process, but the INCITE Management Committee will consider meritorious projects in the Early Career Track separately.

Who Can Apply*: Researchers less than 10 years out from their PhD that need LCF-level capabilities to advance their overall research plan and who have not been a previous INCITE PI.*

How to Apply:

In the regular application process, there will be a check-box to self-identify as early career.

- *The required CV should make eligibility clear.*
- *If awarded, how will this allocation fit into your overall research plan for the next 5 years?*

Projects will go through the regular INCITE review process. The INCITE Program is targeting at least 10% of allocatable time. When selecting the INCITE Career Track, PIs are not restricted to just competing in that track.

- *What is the Early Career Track?*
  - *The INCITE Program created the Early Career Track to encourage researchers establishing their research careers. INCITE will award at least 10% of allocatable time to meritorious projects.*
- *Will this increase my chances of receiving an award?*
  - *Potentially, this could increase chances of an award. Projects must still be deemed scientifically meritorious through the review process INCITE uses each year.*
- *What do I need to do to be considered on the Early Career Track?*
  - *In the application process, select 'Yes' at 'If you are within 10 years of your PhD, would you like to be considered in the Early Career Track?' You will need to write a paragraph about how the INCITE proposal fits into your 5-year research and career goals.*
- *What review criteria will be used for the Early Career Track?*
  - *The same criteria for computational readiness and scientific merit will be applied to projects in the Early Career Track as will be applied to projects in the traditional track. The different will be manifest in awards decisions by the INCITE management committee.*

Early Career Track

If you are within 10 years of your PhD, would you like to be considered in the Early Career Track? Choosing this does not reduce your chances of receiving an award.

No

If ‘yes’, what year was your PhD? If 'no' enter N/A

N/A

If ‘yes’, how will this allocation fit into your overall research plan for the next 5 years? If 'no' enter N/A.

N/A

Section 4: INCITE Allocation Request & Other Project Funding/Computing Resources

Question #1

OLCF Summit (IBM / AC922) Resource Request - 2023

Node Hours

709000

Storage (TB)

550

Off-Line Storage (TB)

1050

Question #2

OLCF Frontier (Cray Shasta) Resource Request – 2023

Question #3

OLCF Frontier (Cray Shasta) Resource Request – 2024

Question #4

OLCF Frontier (Cray Shasta) Resource Request – 2025

Question #5

ALCF Theta (Cray XC40) Resource Request - 2023

Question #6

ALCF Polaris Resource Request - 2023

Question #7

ALCF Polaris Resource Request - 2024

Question #8

ALCF Polaris Resource Request - 2025

Question #9

ALCF Aurora (Intel X^e) Resource Request – 2023

Question #10

ALCF Aurora (Intel X^e) Resource Request – 2024

Question #11

ALCF Aurora (Intel X^e) Resource Request – 2025

Question #12

List any funding this project receives from other funding agencies.

Funding Sources

Funding Source

DoE Nuclear Theory Program

Grant Number

KB0301020 FWP

Funding Source

DoE, NP & ASCR SciDAC program

Grant Number

N/A

Funding Source

NSF, Gravitational Physics Program

Grant Number

PHY-2110177

Funding Source

NSF, Nuclear Theory Program

Grant Number

PHY-1913531

Question #13

List any other high-performance computing allocations being received in support of this project.

Other High Performance Computing Resource Allocations

Resource

Cori and Perlmutter

Allocation Agency

National Energy Research Scientific Computing Center

Allocation

38200 node-hours

Allocation Year

2022

Section 5: Project Narrative and Supplemental Materials

Question #1

Using the templates provided here, please follow the [INCITE Proposal Preparation Instructions]to prepare your proposal. Elements needed include (1) Project Executive Summary, (2) Project Narrative, (3) Personnel Justification and Management Plan, (4) Milestone Table, (5) Publications Resulting from prior INCITE Awards (if appropriate), and (6) Biographical Sketches for the PI and all co-PI's. Concatenate all materials into a single PDF file. Prior to submission, it is strongly recommended that proposers review their proposals to ensure they comply with the proposal preparation instructions.

Concatenate all materials below into a single PDF file.

1. **Project Executive Summary (One Page Max)**
2. **Project Narrative (15 Pages Max)**
3. **Personnel Justification and Management Plan (1 Page Max)**
4. **Milestone Table**
5. **Publications resulting from prior INCITE Awards (if appropriate)**
6. **Biographical Sketches for the PI and all co-PI's.**

Package.pdf
The attachment is on the following page.

PROJECT EXECUTIVE SUMMARY

Title: Long term 3D simulations of core-collapse supernovae

PI and Co-PI(s): W. R. Hix, S. W. Bruenn, J. A. Harris, E. J. Lentz, & A. Mezzacappa

Applying Institution/Organization: Oak Ridge National Laboratory

Number of Processor Hours Requested: 709,000 Summit node-hours (2023)

Amount of Storage Requested: 950 TB

Executive Summary:

Core-collapse supernovae, the explosive final moments of massive stars, are complex, dynamic, multi-physics events yielding a bright and energetic explosion from the birth of a neutron star or black hole. The central engine of a core-collapse supernova generates rare transient signals in gravitational waves and neutrinos. The explosion creates and ejects many chemical elements, including the primary constituents of the Earth, dominating the production of elements from oxygen to iron throughout the Universe. The core-collapse supernova problem has been a computational challenge for several decades, and today we are entering an era where the well-resolved, symmetry-free, three-dimensional (3D) simulations with sufficient physical detail and coupling necessary to understand these complex stellar explosions and their byproducts are now possible. However, the number of extant 3D simulations with adequate physics is small and none have been run until the explosion matures more than a second after the proto-neutron star forms.

The 3D supernova simulations that we propose here to continue have two goals. First, we seek to understand the impact of stellar rotation on the explosion mechanism of core-collapse supernovae and the associated observables. Theses studies are especially concerned with formulating templates for terrestrial gravitational wave detectors, where models with even mild rotation can be significantly different from their non-rotating brethren. Templates such as these are necessary to enable notoriously low signal-to-noise detections of gravitational waves from these events. Second, we seek to understand the development of the proto-neutron star wind following the onset of explosion. This phase, where accretion onto the newly-formed neutron star comes to an end, makes critical contributions to the nucleosynthesis of supernovae, especially the heaviest elements. Models to date, using lower physical fidelity, suggest that this phase will be different in three dimensions than two dimensional simulations, highlighting the need for models of the highest physical fidelity to investigate this epoch in three dimensions. These simulations will be performed using our `Chimera` multi-physics supernova code. `Chimera` contains all of the relevant physics required for core-collapse supernova simulations, including transport of energy by neutrinos and the required neutrino–matter interactions, general relativity and self-gravity, nuclear burning and nuclear equations of state, and 3D fluid dynamics.

This proposal builds on our current (2021) INCITE award, where we are examining the differences between the core-collapse supernova mechanism and the observable consequences for a single massive stellar progenitor with 2 models, one with zero rotation and one with moderate rotation, over the first second. We will generate neutrino and gravitational wave signals from our simulations for comparison to observations, directly probing the explosion mechanism. Under this proposal, we plan to extend these two models into the epoch where the proto-neutron star wind develops, one or more seconds after the formation of the neutron star. Reaching the wind phase is a goal for the `Chimera` portion of the SciDAC-5 project, Exascale Nuclear Astrophysics for FRIB (ENAF), with the goal of understanding the contribution of proto-neutron star wind to p-process and/or r-process nucleosynthesis. Such studies are essential to guide the experimental efforts at the Facility for Rare Isotope Beams (FRIB), which came online this year. Only by extending our simulations until the explosion matures, and including detailed nuclear reaction networks in our simulations and post-processing data extracted by tracers, will we be able to recover detailed isotopic and elemental compositions of the material ejected by the supernova with sufficient fidelity to contribute to FRIB priorities. Recent studies suggest these compositions will be quite different from current nucleosynthesis models that omit the neutrino-driven, multidimensional nature of the explosion.

Project Narrative

1 Significance of Research and Relevance to DoE Mission

Core-collapse supernovae (CCSNe), the explosive final moments of the lives of massive stars, are complex, dynamic, multi-physics events coupling all four of the fundamental forces to produce one of Nature's most powerful explosions. Marking the birth of a neutron star (NS) or black hole (BH), the central engine of a CCSN also generates rare transient signals in gravitational waves and neutrinos while the explosion creates and/or ejects many chemical elements including the primary constituents of the Earth.

The mission of the DOE Office of Science's Nuclear Physics (NP) program is to discover, explore, and understand all forms of nuclear matter. CCSNe provide a unique laboratory for this exploration, ranging from the extremes of dense matter found in the newborn neutron star to the production of heavy elements – many at the edge of stability – formed in the event and in its immediate aftermath. ***In particular, the studies described in this proposal will directly support and guide the experimental efforts at the Facility for Rare Isotope Beams (FRIB), which recently opened, and similar facilities by helping to establish the sites of the r-process and p-process.***

Various forms of our assembled project team have been awarded more than half a billion cpu-hours via thirteen years of ALCC and INCITE allocations since 2007. These awards have enabled the world's most detailed multidimensional models of core-collapse supernovae to date (Lentz et al., 2015; Bruenn et al., 2013; Bruenn et al., 2016; Sandoval et al., 2021). They have also enabled research on the fundamental nature of nuclear matter at high density (Pais & Stone, 2012; Newton & Stone, 2009; Landfield et al., 2022), an important input to CCSNe models as well as one of the subjects that observations of CCSNe can hope to address. For example, during the developing explosion, the neutron star may grow too massive, transitioning to a black hole and quenching the development of the explosion. Such a transition is strongly dependent on the physics of nuclear matter.

In this proposal, we seek to connect this and other "microphysics" to the large-scale "macrophysics" of the collapse of massive stars in order to make predictions for terrestrial detectors, including the newly-opened channel of gravitational waves. Building on models begun under our INCITE 2021 award, under this proposal, we will investigate the development of a wind from the newly formed neutron star in these models, a likely site of the p-process and potential site of the weak r-process.

1.1 Core-Collapse Supernovae

The final act in the life of a massive ($M \gtrsim 8\ M_\odot$ [solar masses]) star is the sudden collapse of the stellar core to super-nuclear densities. Remarkably, the result of core collapse and the formation of a neutron star is the violent expulsion of the rest of the star, through the transfer of a modest portion of the $\sim 10^{46}$ J change in core gravitational binding energy to the outer parts of the star, producing a $\sim 10^{44}$ J explosion. Studying the CCSN mechanism requires understanding the dynamics of that energy transfer to connect pre-explosion stars with explosions and their observational consequences. Fifty years of study have not yet revealed a fully satisfactory understanding of the CCSN problem, but have revealed a set of physical, dimensional, and resolution requirements needed to transform our understanding of stellar explosions and their consequences. The simulations proposed here reflect that understanding of these requirements and are prepared to extend our understanding of the mechanism and its natural variation.

The core-collapse mechanism...: After several million years of evolution and nuclear energy release, a massive star's core is composed of iron and similar "iron-peak" elements from which no further nuclear energy can be released by fission or fusion. Outside the iron core are shells representative of previous burning stages— a silicon shell, oxygen shell, etc., out to a helium shell surrounded by an envelope of hydrogen. At the base of the silicon shell, nuclear burning continues, increasing the mass of the iron core below. When this mass reaches the limiting Chandrasekhar mass, the core starts to collapse.

During the collapse, the inner core will become opaque to neutrinos and surpass the density of atomic nuclei ($\gtrsim 2.5 \times 10^{14}$ g cm^{-3}), reaching densities where individual nuclei merge together into nuclear matter. At densities larger than nuclear density, the nuclear equation of state (EoS) 'stiffens' and the core rebounds like an over-compressed spring, launching a rebound, or *bounce*, shock from the newly formed neutron star (a proto-NS). The bounce shock, initially enclosing roughly half of the $\sim 1.2\ M_\odot$ iron core at a radius of ~ 10 km, progresses outward through the rest of the infalling core, heating and dissociating the infalling nuclei to free nucleons and radiating a tremendous burst of neutrinos. Thermal energy removed from the shocked material by neutrinos and nuclear dissociation halts the progress of the shock about 50 ms after it was launched, rendering it a standing accretion shock (SAS) with a radius of 100–200 km. In the SAS state, the inner regions of the star continue to collapse and accrete through the shock, dissociate, and settle on the proto-NS. Heating due to accretion onto the proto-NS drives the emission of neutrinos of all three flavors (ν_e, ν_μ, ν_τ) and their anti-particles ($\bar{\nu}_e$, $\bar{\nu}_\mu$, $\bar{\nu}_\tau$). Below the shock, but above the proto-NS, the absorption of ν_e and $\bar{\nu}_e$ by the free nucleons results in a 'gain region' of net heating. In this way, the proto-NS's gravitational binding energy is transferred to the envelope of the star. In spherically symmetric (1D) simulations, fluid elements advect through the gain region before they heat sufficiently to reverse their direction and drive an explosion, thus 1D simulations of iron core collapse, with few exceptions, end in the accretion of the entire star, a situation that can not match observations of CCSNe.

...and its multidimensional nature: Nature demands more than spherical symmetry. Two primary fluid instabilities alter the dynamics of the post-bounce stellar core in ways that ultimately require a symmetry-free 3D approach to fully and properly understand the mechanism of CCSNe and their observational consequences. First, neutrino heating at the base of the gain layer drives convective overturn. Second, the SAS is unstable to non-radial perturbations (the standing accretion shock instability, SASI). These instabilities lead to turbulence, shear flow, and other multidimensional effects. In the SASI, small perturbations of the shock from symmetry amplify initially in a simple back-and-forth 'sloshing' mode. As the amplitude of the oscillation grows, the distortion wave starts to interact with itself, forming indentations in the shock (shock triple-points). Deviations from axial symmetry will eventually tip the oscillation sideways into a spiral mode with counter-rotating flows. The SASI can grow the volume of the shocked region to aid neutrino heating; inject lateral (non-radial) kinetic energy; and focus the accretion into narrow (sometimes supersonic) streams that can deposit more intense accretion heating at the proto-NS, producing higher, localized, neutrino emission. Heating by neutrino absorption is stronger closer to the proto-NS and differential heating of the fluid creates convectively unstable (buoyant) material that transports energy upward where it can lift the shock and drive an explosion. Neutrino-driven convection differs from more familiar convective systems where material is repeatedly heated, rises, cools, and sinks. Particularly after the shock expansion (and the nascent explosion) starts, much of material experiences a 'once through' pattern of accretion onto the proto-NS (frequently in a focused stream), accretion heating produces enhanced emission of neutrinos; and strong absorption of neutrinos by some of the accreted fluid, lifting the fluid buoyantly, and with it the shock. Interestingly, the presence of strong convection inhibits the development of the SASI (Fernández, 2015; Fernández et al., 2014). This multidimensional 'buoyant engine' allows continuing accretion and growth of the explosion energy while the shock expands. It functioned well enough in our past axisymmetric (2D) simulations with `Chimera` (Bruenn et al., 2013; Bruenn et al., 2016), as well as ongoing 2D models, to generate robust $\sim 10^{44}$ J explosions consistent with the energies observed in Nature.

Role of rotation: All stars, including massive stars, are known to have some rotation remaining from the angular momentum of the parent molecular cloud. Rotation can alter the behavior of convection, cause mixing between composition shells, and change the stellar surface properties (cf. Heger et al., 2000; Hirschi et al., 2004). Treating rotation in spherically symmetric stellar evolution models, such as those commonly used to evolve to the pre-CCSN state, is difficult and directly impacted by the parameterizations of angular momentum transport used in the stellar evolution model. Unfortunately, 3D models of stellar evolution cover only minutes. Models of stellar evolution consistent with observed surface rotation suggest modest rotation rates in the final iron core with periods of 10s of seconds are common. When rotating cores collapse, centripetal forces can alter the structure of the gain region, making it larger and more bipolar (i.e., like 2D) and enhance the growth of explosions (cf. Nakamura et al., 2014). This is consonant with delay of explosions in our 3D non-rotating `Chimera` models until dominant plumes can form when compared to 2D models, where the imposed symmetry, and resulting inverse turbulent cascade, causes large plumes to develop rapidly (Lentz et al., 2015; Melson et al., 2015a; Vartanyan et al., 2019). Sufficiently rapid rotation of the core has the potential to amplify magnetic fields to strengths that dominate the dynamics and lead to exotica like magnetars and gamma-ray bursts, though we focus in this proposal on the more common, slower rotating stars.

Observable Consequences: The wide variety of physics at work in CCSN manifests in a number of distinct observable consequences.

Isotopic Production: CCSN are an important link in the story of our origins from the Big Bang to life on Earth. The ejecta of CCSNe include both elements synthesized during the million-years stellar lifetime that are released by the explosion, and elements synthesized in and by the CCSN buoyant engine. Models of CCSNe complete the theoretical story of the stellar life-cycle, linking the end state of stellar evolution theory with the inputs to supernova lightcurve and spectra computations that are compared to observed stars and supernovae. To reach the final, observable, ejecta state, the abundances of a multitude of isotopes must carefully and consistently tracked, including changes in abundance due to nuclear burning and neutrino interactions, in any material that may be ejected. Analysis of numerous tracer particles included in our proposed 3D self-consistent models of the neutrino-driven supernova engine will extend our understanding of the composition of CCSN ejecta across a range of initial conditions, an understanding developed in part from similar analysis of 2D CHIMERA models (Harris et al., 2017, 2022; Sieverding et al., 2018). Under this proposal, as we complete the models we started under our INCITE 2021 award, these particles will experience the development of a high entropy, neutrino-driven wind from the proto-NS. In order to better capture the conditions in the low density wind, we may add additional tracers particles over time at the PNS surface. Depending on the neutron-richness of the wind, determined by interactions with the flux of neutrinos and anti-neutrinos that permeate the region above the proto-NS, this wind may be a site of the p-process or the r-process. ***To date, no sophisticated 3D models have run to sufficient time to witness the development of the wind.***

Gravitational Waves: CCSNe produce strong gravitational wave (GW) emission that should be observable with Advanced LIGO at distances within our Galaxy. Comparison of GW detections with simulations can be used to infer significant information regarding the fluid flows at high densities and the equation of state of matter at those densities. The GW emission from CCSN is expected to be much smaller than from the BHBH mergers and NSNS merger that LIGO has already detected (Abbott et al., 2016a,b, 2017), except perhaps for rare cases of *rapidly* rotating progenitors. Nonetheless, the physics we could learn from a Galactic CCSN, with its accompanying neutrino and gravitational wave signals, compels us to push the frontier of gravitational wave prediction for such events forward. Members of our collaboration have already computed waveforms based on `Chimera` CCSN simulations (Yakunin et al., 2015; Mezzacappa et al., 2020; Mezzacappa et al., 2022) and have provided simulation data to the LIGO collaboration. With the extension of these models to late times, the complete GW signal can be provided.

Neutrinos: Almost all of the energy from CCSNe is radiated in the form of neutrinos. This emission is key to both the explosion mechanism itself and to many of the subsequent observables, including the nucleosynthesis. Several properties of neutrinos are now known, including the squared mass differences and vacuum mixing angles. But the detection of neutrinos from a Galactic CCSN could produce information regarding the neutrino mass hierarchy, their Dirac or Majorana nature, and the possibility of sterile states. As in the case of GWs, answering questions about the explosion mechanisms and fundamental neutrino physics will require reliable templates against which the low signal-to-noise observations can be matched. There are several large, underground neutrino detectors extant, e.g. Super-K (Ikeda et al., 2007) and IceCube (Abbasi et al., 2011), and others are planned in the near future (e.g. DUNE; Acciarri et al., 2016), increasing our confidence that a high-statistics CCSN neutrino signal will eventually be observed. Though some of the impact of matter-induced oscillations can be computed for CCSNe in post-processing, spatial and temporal instability in coherent flavor transformation must be computed dynamically. Importantly, we will be able to correlate the time structure and emission regions for GWs and neutrinos from our simulations, an aim impossible to achieve definitively without accurate neutrino transport computed on effectively GR spacetimes. We compute detailed signal predictions, including detector response, from `Chimera` (Messer et al., in prep.) via the Open Source SNOwGLoBES package.

2 Research Objectives And Milestones

The major scientific goals for our overall 3D core-collapse supernova modeling program are:

- to understand the nature of the core-collapse supernova mechanism across the range of stellar progenitors in symmetry-free 3D, in particular to understand the impact that the removal of imposed axisymmetry on the nature of the explosion mechanism; and
- to compute the observable consequences of these three-dimensional core-collapse supernovae – their explosion energies, compact remnants, nucleosynthesis in the ejecta, gravitational wave signatures, and neutrino signatures.

Achieving these goals will require a number of detailed simulations, run to extended times, spanning the variety of stars that may supernova; varying in progenitor mass, metallicity, rotation rates, initial magnetic fields, etc.

2.1 The current state of supernova simulation

Studies of the coupled, multi-physics, symmetry-free 3D nature of CCSNe in their full generality exceed the capabilites of even exascale machines. Therefore modern simulations resort to a variety of approximate approaches to CCSN physics. Neutrinos create non-local coupling in the fluid, transporting energy without fluid motion. The neutrinos are diffusive deep in the proto-NS and free streaming above the shock, but in the critical gain region, the neutrinos are out of equilibrium with the fluid. Heating is dependent on the neutrino flux and the shapes of the neutrino momentum and energy distributions, therefore transport methods must resolve both the transition from diffusion to free streaming and the neutrino energy spectra. In the proto-NS, mass is sufficiently concentrated that general relativity (GR) is very relevant. When computed using GR, the proto-NS is more compact and the emitted neutrinos have higher mean energies, which increases the neutrino heating rate in the gain region. The importance of GR and neutrino transport, including the detailed interactions with the fluid, have been demonstrated in detailed 1D simulations (cf., Lentz et al., 2012). The proto-NS consists of hot nuclear matter, strongly interacting nucleons at densities that exceed those in nuclei, conditions found in few other places in Nature. Outside the proto-NS is a mixture of free nucleons and bound nuclei in nuclear statistical equilibrium (NSE). At lower densities and temperatures (everything initially outside the iron core and in the expanding and cooling ejecta), NSE is inadequate and the non-equilibrium composition must be evolved with a network of thermonuclear reactions as the composition changes on timescales relevant to CCSNe. Often a small (14-species, α-network) nuclear reaction network is utilized to get appropriate energetics and thermodynamics for the lower density and temperature components of simulations and rough estimates of the nucleosynthesis. In some cases, this is supplemented by passive tracers that collect thermodynamic and neutrino exposure information for use with very large (5000-species) networks in post-processing computations to capture the fine details of supernova nucleosynthesis.

A large number of symmetry-free 3D simulations with accurate approximations to all physics and couplings, like those proposed here, are needed to sort out the uncertainties in the nature of the CCSN mechanism, point to the best approximate methods and account for the diversity of CCSN progenitors.

Multi-dimensional radiation hydrodynamics: The computational cost of neutrino transport in modeling the CCSN central engine, especially in multi-dimensional simulations, has led to the emergence (or re-emergence) of a number of less costly approximations for this essential physics. One often-used formulation is the neutrino "lightbulb" approximation, wherein the neutrino transport calculation in and around the proto-neutron star is replaced with a proscribed neutrino luminosity, which in turn determines the heating rate, with the neutrino heating and cooling parameterized independently (see, for example, Murphy & Burrows, 2008; Nordhaus et al., 2010; Hanke et al., 2012; Nordhaus et al., 2012; Wongwathanarat et al., 2013; Couch, 2013). A more sophisticated, but still approximate, neutrino transport method is the "leakage" scheme (Baron et al., 1985; Scheidegger et al., 2010; Ott et al., 2013; Couch & O'Connor, 2014). Leakage schemes use the local neutrino emission rate and the opaqueness of the overlying material to estimate the cooling rate and from that the neutrino luminosity and heating rate. A more recent development has been the Isotropic Diffusion Source Approximation (IDSA) which treats the neutrinos as part of either a trapped (fluid) phase or a free streaming phase, with the interconversion of the phases determined by the rate of diffusion (Liebendörfer et al., 2009; Suwa et al., 2013, 2016). While each of these approximations offers significant advantages in computational speed, useful for explorations of wide parameter spaces, they all lack the fully self-consistent feedback provided by complete transport methods. Ultimately, the validity of such approximations for the CCSN problem can only be established by comparison to self-consistent transport models, like the `Chimera` models we propose herein.

The leading neutrino radiation hydrodynamics (νRHD) codes have several features in common. Each tracks the evolution of electron neutrinos (ν_e), anti-neutrinos ($\bar{\nu}_e$) and typically at least one species of 'heavy-flavor' neutrinos (ν_x) with resolved spectra (at least 12 energy groups covering two decades in neutrino energy). The feedback between neutrino emission (cooling) and absorption (heating) is directly computed with the appropriate evolution of the neutrino spectrum. All of these codes have both 2D and 3D modes and simulations are somewhat costly in 2D and expensive in 3D. Results from several such codes have been published in recent years. Our `Chimera` code and the `Vertex` code of the Max Planck Institute in Garching (Germany) group ***implement the most complete physics*** and are relatively similar in methodology. They both feature ray-by-ray transport (nearly independent 1D transport solves for each solid-angle column); detailed neutrino–matter interactions; and a spherical GR correction to the gravity, hydrodynamics, and transport. Several new codes including `Fornax` (Skinner et al., 2016, 2019), FLASH with M1 transport (O'Connor & Couch, 2018b) and Zelmani with M1 transport (Roberts et al., 2016) have recently been developed. These use multidimensional transport with the M1 analytic moment closure, ***but are currently limited in their opacities and neutrino energy group couplings.***

The geometric limitations of the ray-by-ray method should be of concern as the intensity of the neutrino field is related to the emission features only directly below, notably hotspots from accretion streams striking the proto-NS. ***However, recent work (Glas et al., 2019) has show that the impact of the ray-by-ray approximation is fairly unimportant in 3D (unlike in 2D) as the accretion streams are broken into smaller and less coherent and sustained features and cannot sustain a reinforced excess angular heating contrast.*** (In axisymmetry, only two model configurations emerge — two polar plumes with an equatorial accretion stream or accretion on one pole with a plume on the opposite, leading to more persistent accretion features.) The geometric impact is even less relevant for the late, wind phase, where the the transport is largely radial, there are no accretion hotspots, and lateral advection inside the proto-NS is included in all ray-by-ray implementations.

The fidelity of neutrino transport and spectral evolution is particularly important to neutrino heating (cf. Müller et al., 2012; Lentz et al., 2012) and proto-NS cooling in the wind phase (Fischer et al., 2010). ***Of the 3D νRHD codes, only*** `Chimera` ***and*** `Vertex` ***have included full, direct energy coupling and ν-$\bar{\nu}$ coupling throughout their simulations. Omitting this dramatically reduces the computational costs for the other codes, at considerable cost in physical fidelity (Lentz et al., 2012).*** `Chimera` simulations in 3D have included the 20 energy groups needed to resolve the Fermi-energy surface, while other codes have used only 12–15 energy groups in 3D simulations. `Chimera` is also the only 3D code that evolves ν_x separately from their anti-neutrinos. Indeed, `Chimera` is the only code that has included full neutrino coupling of 4 energy-resolved neutrino species in *all* of our published 2D and 3D simulations. For this reason, `Chimera` is well positioned to handle the late, neutrino-driven wind phase that concludes our planned work under this proposal.

Progress: The first reasonably well-resolved (15,000 angular zones), self-consistent, 3D νRHD CCSN simulation with spectral transport (using `Vertex`; Hanke et al., 2013) had not yet exploded despite reaching the epoch where a 2D simulation using the same progenitor and the same code had already begun to explode. Continuation of that model and two additional simulations using lighter progenitors (11.2 and 15 $M_\odot$) were reported in Tamborra et al. (2013) without explosions. A 20 $M_\odot$ progenitor simulated with `Vertex` did explode (Melson et al., 2015a), but only after the strangeness content of free nucleons was increased (and, therefore, the dominant neutrino scattering opacity decreased) to the maximum level allowed by current experimental limits. Without this change, the same simulation did not explode, demonstrating that this model, and likely others, are near the threshold for explosions. Simulations showing the start of apparent explosions have been achieved at lower resolution (2000 and 8000 angular zones) with the Zeus+IDSA code by Takiwaki et al. (2012, 2014) and with grey (non-spectrally resolved, which overestimates neutrino heating) smoothed-particle hydrodynamics simulations (Fryer & Warren, 2002). We demonstrated a 3D explosion of a 15 $M_\odot$ progenitor with `Chimera` at 2-degree resolution (Lentz et al., 2015, Fig. 1), though it is delayed about 100 ms relative to 2D. Lower resolution models show further delay in the explosion (Lentz et al., in prep.). This followed an early `Chimera` attempt at 3D using ~11,000 angular zones (Bruenn et al., 2009).

With similar codes and resources, the `Chimera` and `Vertex` groups are continuing to compute new 3D models at the rate of a couple per year. Both `Chimera` and `Vertex` have generated 3D explosions from a low mass progenitor (9.6 $M_\odot$). These lightest progenitors have also been shown to explode in 1D (Melson et al., 2015b, Lentz et al., in prep.). Glas et al. (2019) demonstrated successful explosions beginning in a 9 $M_\odot$ progenitor at 300 ms after bounce, but a 20 $M_\odot$ progenitor failing to explode within 700 ms after bounce. A new set of `Chimera` 3D angular wedge models of varying resolution (Casanova et al., 2020, computed with DD allocation AST109 and ALCC allocation NPH108 with analysis begun under INCITE allocation AST106 at OLCF) extends similar light-bulb models by Radice et al. (2016), showing qualitative (Fig. 2) differences in the turbulent and accretion flows that demonstrate the need to adequately resolve the flows inside CCSN simulations. In 2019 and 2020, using INCITE allocation AST137, we continued 3D models for 10, 15 and 25 $M_\odot$ progenitors, originally started on Blue Waters under PRAC allocation ACI-1713750, with robust explosions beginning to develop ~ 0.5 seconds after bounce (Lentz, et al., in prep.).

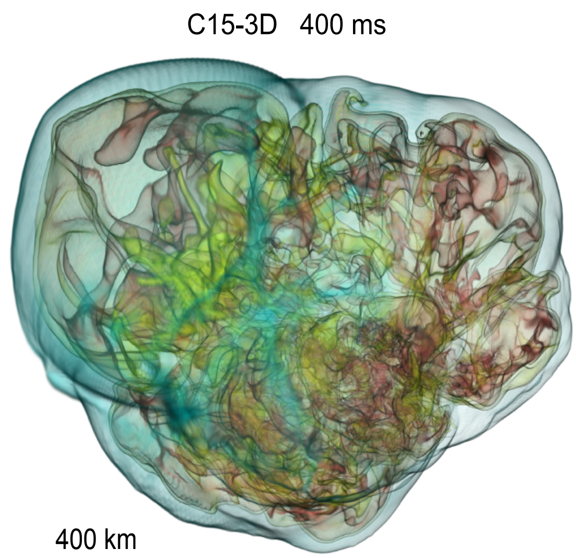

Figure 1: Volume rendering of entropy in an exploding `Chimera` 3D simulation (Lentz et al., 2015) coded light blue for low (shock), green for medium, and red/brown for high entropy material.

In recent years, `Chimera` and `Vertex` have been joined by additional high fidelity CCSN models. A number of `Fornax` models, from progenitors between 9 and 16 $M_\odot$, have demonstrated robust explosions developing within 0.5 seconds after bounce (Vartanyan et al., 2019; Burrows et al., 2019), although intriguingly a 13 $M_\odot$ progenitor does not develop an explosion in this timeframe. Meanwhile, models with FLASH for a 20 $M_\odot$ progenitor (O'Connor & Couch, 2018a) fail to explode within a half second, despite several perturbations to the initial model designed to mimic the effects of turbulence during shell burning. In contrast, models with Zelmani (Ott et al., 2018) exhibit rapid onset of the explosion (< 300 ms) for models based on 20, 27 and 40 $M_\odot$ progenitors, while a model for a 15 $M_\odot$ progenitor only begins to explode 500 ms after bounce, and a model for a 12 $M_\odot$ progenitor does not develop into an explosion over this timeframe. Clearly, the sparse sampling in progenitor space and seeming diversity of results between codes points to a need for additional modeling. ***Assessing the physics and variation in the CCSN mechanism will require multiple 3D νRHD***

models from multiple groups at good resolution and high physical fidelity.

CCSN models from rotating progenitors have a long history and have often been motivated as sources of GW signals — a key goal of this project. An early 2D νRHD model was the 2D MGFLD model of Burrows et al. (2007). Other 2D studies using leakage (Abdikamalov et al., 2014; Richers et al., 2017) with large numbers of models and IDSA (Suwa et al., 2010) have followed. Models in 3D utilizing light bulb (Kotake et al., 2011), leakage (Ott et al., 2012; Mösta et al., 2014; Nakamura et al., 2014; Mösta et al., 2015), and IDSA (Scheidegger et al., 2010; Takiwaki et al., 2016) neutrino approximations have followed. Many of these simulations are short in duration and focused on catching the prompt GW signal generated by core bounce. Of these, Nakamura et al. (2014) and Takiwaki et al. (2016) come the closest to what we propose, with the latter matching our planned resolution and the former having slightly more moderate rotation than we plan. Perhaps the best rotating models to date are those from the `Vertex` group (Summa et al., 2018), which examined a 15 $M_\odot$ progenitor with 5 variations in the imposed rotation rate as a function of radius. Only the highest rotation rate produced and explosion, but significant differences in the GW signal were calculated even for milder rotation rates (Andresen et al., 2019). ***However, the simulations we propose here represent a significant improvement in the treatment of neutrino physics, simulation duration, and resolution for CCSN simulations of the typical population of rotating massive stars.***

Under the aegis of our INCITE 2021 award, we began work on this campaign by starting two detailed, reasonably resolved (1.25-degree angular resolution), 3D CCSN simulations employing neutrino radiation hydrodynamics. Our aim, under this proposal, is to continue these models, a non-rotating 13 $M_\odot$ stellar progenitor (Model A) and a second 13 $M_\odot$ model with the core rotating $\approx$0.5 rad/s (Model B). These masses and rotation rates are typical of progenitors of massive stars that become CCSNe. Both simulations include $\mathcal{O}(10^5)$ tracer particles for nucleosynthetic post-processing. The approximate explosion energies and parts of the simulations needed for the primary phases of the neutrino and gravitational wave signals (up to 0.8–1.0 seconds) will be completed for Models A & B in 2022, at which points those signals can be analyzed and published. Under this proposal, we plan to extend the Models A & B to complete the development of the asymptotic explosion energy and simulate the development of the proto-NS wind, with an additional second of evolution.

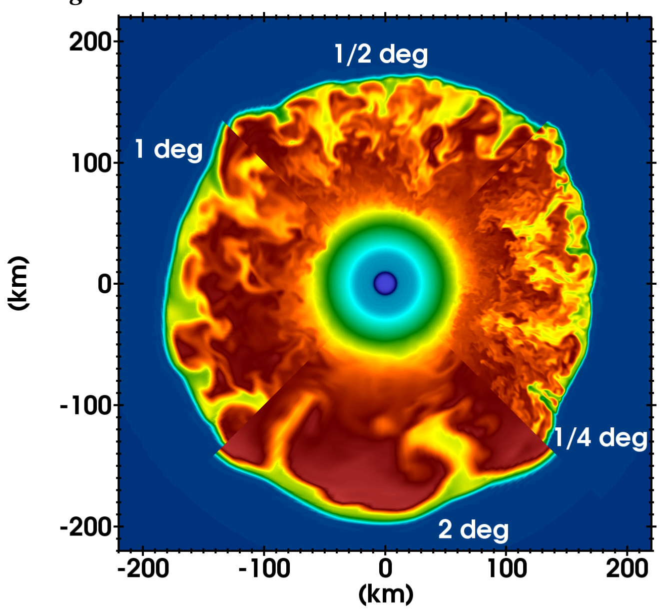

Figure 2: Entropy in `Chimera` simulations of stellar wedges (Casanova et al., 2020), showing the effect of increasing resolution on the turbulent flow. Blue to red represents low to high entropy material.

Detailed post-processing nucleosynthesis calculations of the ejecta will be carried out to determine its detailed composition. Because of their extended runtimes, the nucleosynthesis computed from Models A & B would represent the most complete CCSN nucleosynthesis calculations to date, making them a valuable resource for comparison to the results of more approximate models, including 2D `Chimera` models.

These 3D simulations will be supplemented by several dozen 2D `Chimera` simulations over the same period, computed with other resources, that will consist of systematic parameter studies of physical inputs, resolution, etc., and a wider range of stellar progenitors, providing the background against which 3D simulations will be compared. The results from this project will be disseminated primarily through journal publications (our usual practice is publication via *The Astrophysical Journal* and/or *Physical Review*). In addition, we will make observational signatures we generate from the simulations available via the `Chimera` website. Earlier results from 2D, non-rotating models are already available there.

2.2 Goals

Limits of axisymmetry: In recent years, detailed axisymmetric (2D) simulations have vastly improved our understanding of the CCSN mechanism. Simultaneously, numerous studies using simplified scenarios have examined the influence of full 3D dynamics. Each of these lacks a critical element: the 2D simulations contain consistent neutrino driving and feedbacks, but are artificially restricted to the axisymmetric behaviors of key hydrodynamic components like the SASI, convection, and turbulence. On the other hand, 3D parameterized simulations include the full hydrodynamic character, but omit important feedbacks that can lead to artificial physical conditions. Sorting out the question of dimensionality (3D v. 2D) raised by the lightbulb simulations can only be achieved with full νRHD simulations in 3D. All of our proposed simulations will contribute to this understanding and will help to resolve this question of dimensionality.

Variation in progenitors in 3D: Recent work by several groups using νRHD codes have explored the variation in CCSN properties over a range of masses and progenitors (Janka et al., 2012; Bruenn et al., 2013; Bruenn et al., 2016; Nakamura et al., 2015; Dolence et al., 2015; Suwa et al., 2016; Burrows et al., 2019, 2020). Variations with progenitor mass have been seen in 2D for basic properties (explosion success and strength, remnant mass, duration of explosion, relative strengths of instabilities), direct signals (gravitational waves, neutrino luminosity and spectra), and ejecta composition (amount of neutron-rich and proton-rich isotopes ejected, abundances). We have concluded a complementary, parallel campaign examining mass and initial composition in non-rotating progenitors in 3D simulation computed using PRAC and INCITE allocated resources (Lentz, et al. in prep.). The simulations proposed here are part of a campaign to examine a new parameter space in stellar progenitor: rotation. Our analysis will examine the variations in outcomes in 3D arising from rotation with an eye toward any differences in patterns and trends arising from dimensional difference. Under this proposal, we will extend promising rotating and non-rotating models, begun under INCITE 2021, to witness the development of the proto-NS wind and examine the dependence of the character of this wind (and its potential nucleosynthesis) on stellar characteristics like rotation rate and mass. This effort aligns with the CHIMERA portion of the ENAF collaboration proposed under SciDAC-5, seeking to understand the potential of the proto-NS wind to produce p-process or r-process nuclei in support of FRIB.

Direct signatures of core-collapse: Today, a CCSN in our Galaxy, or its nearest neighbors, would produce a strong and diagnostic neutrino signal in operational detectors, providing direct evidence from the inner engine of the CCSN mechanism. Gravitational waves (GW)–traveling disturbances in spacetime–produced by CCSNe should be detectable to about 10 kiloparsecs (the closer half of the Galaxy) with the Advanced LIGO detector currently in service. Gravitational waves are emitted with two polarizations, one of which is reduced to zero by the imposition of axisymmetry (2D). Both GW and neutrino signals can be altered by the changes in neutrino-driven convection, SASI, and other non-axisymmetric motions. As part of this work, we will generate and distribute GW and neutrino signals for each simulation that will have significant diagnostic power for the next Galactic CCSN and contribute to our understanding of fundamental physics like neutrino oscillations and the nature of spacetime. With our planned multi-second running times, gravitational waveforms from these CCSN models with rotating progenitors will be complete waveforms in the sense that they contain all phases of CCSN evolution: bounce, prompt convection, neutrino-driven convection/SASI, and explosion. Each of these phases provides important information about equations of states, hydrodynamics instabilities, shock expansion, etc. For the present, realistic simulations with rotating progenitors have been restricted by short simulation time (50–100 ms), concentrating on a bounce signal only. ***Our CCSN models with rotating progenitors will be the first that cover all phases of explosion (beyond 1 second), therefore, the gravitational waveforms from this model will be the most realistic available.***

Nucleosynthesis: Between elements created during the explosion and the ejection of elements synthesized during pre-supernova evolution, CCSNe make and release most of the elements that constitute rocky planets like Earth. CCSNe produce or release most of the O, Si, and other intermediate-mass elements; roughly half of the Fe, Ni and neighboring elements (mostly as short-lived ^{56}Ni). (Thermonuclear, or Type Ia, supernovae make the rest of these elements.) A key open question is the CCSN contribution to elements heavier than iron through the p- or r- processes. Understanding the elemental and isotopic production and release in CCSNe is an important aspect of our planned work. Nucleosynthetic yields for exploding massive stars have been traditionally computed by inducing a 1D explosion in a collapsed progenitor model with a proscribed energy for dozens to hundreds of progenitors. Such models lack the appropriate feedback with the mechanism, its multidimensionality, and the neutrinos.

The most basic configuration of `Chimera` uses an α-network (nuclei of even and equal neutron and proton numbers: ^{4}He,^{12}C–^{60}Zn) to track nuclear energy release and rough composition in the regions where nuclear statistical equilibrium (NSE) doesn't apply. In addition, this basic configuration also includes free neutrons, free protons and ^{56}Fe to follow the freezeout from NSE of matter that is not composed of equal numbers of neutrons and protons. ***This basic configuration of*** `Chimera` ***meets or exceeds the treatment of the nuclear composition from competing codes, but when used with larger reaction networks (see below),*** `Chimera`***'s treatment of the non-NSE regions is the most sophisticated of all CCSN codes.*** An α-network does an adequate job of estimating the total ejected mass for most of the species it covers, including radioactive ^{56}Ni, but can miss calculate the production of the radioactive tracer ^{44}Ti and other species of interest by an order of magnitude (Harris et al., 2017). Further, its facility to calculate the composition of proton-rich matter, which could lead to the production of the p-process, or neutron-rich matter, which could lead to the production of weak r-process, and other isotopes of interest to Galactic Chemical evolution, is very limited. To ameliorate this problem, `Chimera` also tracts passive Lagrangian tracer particles (in the 100s of thousands in 3D), which sample the thermodynamic conditions in each simulation. These thermodynamic histories can be used for post-processing calculations of the nuclear evolution with a nuclear reaction network using thousands of isotopes. However, these tracers results are not self-consistent and ignore the potentially important effects of mixing. We find that tracers are challenged to adequately resolve the low density regions in which ^{44}Ti and other rare isotopes are produced (Harris et al., 2017, 2022).

To improve on the basic configuration, we have run 2D and 3D simulations using a much more realistic 160 species network, including in a fully self-consistent fashion all of the products of explosive oxygen and silicon burning as well as normal freeze out from NSE and the dominant products of α-rich freeze out that can lead to the ν-p process and weak r-process. However, this more realistic network effectively doubles the total cost of a CPU-computed `Chimera` model, so it can not be employed in every case. We are pursuing two paths toward better nucleosynthesis. First, we are improving the efficiency of the network on GPUs. When complete, we expect to use a realistic network in all of our simulations for only a small increase in the total cost. Second, we have tested intermediate-sized networks, with 32 to 84 species, to find the most complete treatment of the nucleosynthesis that can be accommodated by a small increase in the overall cost of the model. For a 2D model at bounce, using a 32-species network increases the cost of the `Chimera` model by only 5-10%, but with two improvements over the standard α-network. First, larger networks achieve better accounting of the energy generation by the network due to the inclusion of important (α,p) reactions. Second, they improve the treatment of freeze-out from NSE in neutron-rich conditions by including a subset of recombination channels for free nucleons that also serve to link ^{56}Fe with other nuclei in the α-network. For Models A & B we have settled on a 52 species network, which consumes $\sim$15% of the runtime. *The detail and self-consistency of the nucleosynthetic yields produced by the direct computation and numerous tracer particles for these 3D models will surpass anything published to date for multidimensional simulations and are only approached by similar work we are preparing in 2D.*

Calibration of other models: The enormous cost of 3D νRHD CCSN simulations prevents the full coverage of the vast parameter space of CCSN progenitors which requires dozens to hundreds of models. Three-dimensional νRHD simulations can be used to build larger libraries in two ways. The first is to correct the outcomes of detailed, 2D νRHD CCSN simulations for biases, missing features, etc. This is critical since there are several well known differences between 2D and 3D simulations that may impact the explosion. The second will be to provide a training set against which to test cheaper, parameterized models for wide coverage of parameter space. *Our final goal will be to calibrate and correct our more extensive set of 2D simulations and to provide the information required to build better parameterizations.*

3 Computational Readiness

3.1 Code description

The name Chimera originates in its combination of three, separate, mature codes (Bruenn et al., 2020). The primary code modules evolve the stellar fluid dynamics (VH-1), the "ray-by-ray" neutrino transport (MGFLD-TRANS), and the thermonuclear kinetics (XNet). These three "heads" are augmented by a sophisticated equation of state for nuclear matter and a self-gravity solver capable of approximation to general-relativistic gravity.

Hydrodynamics are evolved using a dimensionally split, piecewise parabolic method (PPM) — a version of the publicly available astrophysics PPMLR hydrodynamics code VH-1. Self-gravity is computed via multipole expansion in spherical harmonics. Spherical symmetric corrections to gravity for GR replace the non-GR (Newtonian) monopole ($\ell = 0$) term.

As mentioned above, in the lower density regions outside the iron core, physical conditions require the use of a nuclear network to evolve the time-dependent abundances of nuclei. The nuclear network incorporated into Chimera is the publicly available nuclear network code XNet. XNet solves, for each non-equilibrium zone, a coupled system of non-linear ODEs (one for each nuclear species plus temperature) for the time evolution of the nuclear abundances. Where the nuclear time step is smaller than the hydrodynamic step, XNet will compute multiple sub-steps automatically to prevent the short reaction timescales in a few zones from severely restricting the global simulation time step. Previous Chimera simulations have largely used a 14-species α-network (^{4}He,^{12}C–^{60}Zn) network, but Models A & B utilize 52 species for the small network configuration. We also use at least 100,000 Lagrangian tracer particles to sample thermodynamic histories for post-processing nucleosynthesis with a 5000+ isotope network in XNet and other analyses.

Transport of neutrinos is computed as multi-(energy)-group angular moments of the neutrino distribution function in a diffusive approximation flux-limited to prevent aphysical (superluminal) 'diffusion' of neutrinos in semi-transparent and transparent regions (multi-group flux-limited diffusion, or MGFLD). The MGFLD equations – including local couplings between all energy groups (via scattering), neutrinos and anti-neutrinos (via pair emission processes), and to the local matter – are solved by Newton-Raphson iteration independently on each radial 'ray' using the ray-by-ray approximation. The neutrino–matter interactions are a modern set that include scattering on electrons and free nucleons with energy exchange, emission and absorption on free nucleons and an ensemble of nuclei in NSE, and neutrino–anti-neutrino pair emission from nucleon-nucleon bremsstrahlung and $e^{+}e^{-}$-annihilation.

The spherical coordinates used in Chimera are natural for the CCSN problem given the centrally concentrated, and round, proto-NS and the ray-by-ray approximation. Using spherical coordinates allows a better resolution of the radial structure of the proto-NS and helps limit error in the gravitational binding energy, which is the ultimate energy source of the explosions. Orienting the primary computational domains along the radial direction results in similar conditions on each process for the most expensive computational elements (transport and nuclear burning) and natural load balancing of the computational work. Spherical coordinates come at the price of restricted lateral zone sizes (and time steps) from coordinate convergence at the center and the pole. The center in Chimera (and similar codes) has been treated spherically, which suppresses non-radial motions in the inner core (few km) of the spherical proto-NS and relieves the simulation of the time step restrictions from the non-radial zone widths inside the spherical region. The convergence of the grid at the poles ($\theta = 0, \pi$) is the other limiting factor (the time step restricting length for the zone closest to the pole is $\Delta\ell = R\,\Delta\phi\,\sin\theta_c$).

Some previous 3D models with Chimera have utilized the pole-free, overset 'Yin-Yang' grid (Kageyama &

Sato, 2004) to avoid the pole-induced time step restrictions, but this grid is subject to minor mass conservation issues in the flow of matter across the boundary between meshes that are exacerbated by rotating flows, a concern for the rotating models in this project. As an alternative, we have implemented a 'cell merging' or 'derefinement' scheme in the θ and ϕ directions that merges progressively larger numbers of cells together during the ϕ-sweep for areas closer to the poles and θ-sweep closer to the center, such that the merged cells remain roughly 'square'. We then remap the coarse cells back to the fine base grid before computation is performed in other (directionally-split) directions. The 'cell-merged' grid is conservative by construction and avoids the ~10% simulation time communicate penalty between grids in our prior Yin-Yang models.

Computing a 3D model of a core-collapse supernova at reasonable resolution in longitude and latitude (1.5–2-degree; similar to the resolution of many 2D simulations; ~15,000–25,000 angular zones, or 'rays') and radial resolution (several hundred radial zones) results in simulation time steps of ~0.5 μs. For a total time to explosion of about 1–3 second, this leads to roughly 2–6 million time steps. When each solid angle element is distributed to a separate MPI-rank, `Chimera` can complete a few thousand time steps per hour (~2 ms of supernova time) for a full simulation time of ~1000 hours. This results in a simulation cost of $\sim 10^7$ CPU-core-hours for a single simulation, which is typical for all leading 3D CCSN codes. For Summit and this proposal, we have chosen to use 41,472 angular zones, or rays, (1.25-degree resolution on the cell-merged grid) with two rays per rank on each core with 7 ranks sharing a GPU. We will continuing tuning the CPU threading and GPU performance described below.

3.2 Use of Resources Requested

In Year 1, we will continue the non-rotating (Model A) and rotating (Model B; ≈0.5 rad/s) progenitor of 13 $M_\odot$ begin on Summit under our INCITE 2021 award for another second and into the wind phase. These rotation rates are typical values of rotation seen in pre-collapse stellar evolution models. All runs will be computed using a grid of 144×288 angular zones (41,472 rays using 20,736 ranks, packed 42 ranks per node onto 494 Summit nodes) with the cell-merged grid. We have developed a cost model for `Chimera` on Summit using the data from the scaling runs in §3.4, the first second of these models, and an equivalent 2D run from which we can count the number of hydrodynamic steps, $N_{\rm hyd} = 3.5$ M, and transport steps, $N_{\rm trans} = 1.0$ M, over the targeted additional second. Unlike previous models with `Chimera`, where the time step was set by the angular zone widths in the last resolved shell outside the spherical core, with the merged cell grid, the relevant length scale is fixed at δR_c, the thickness of the first zone outside the single spherical central zone (radius 1 km) given the optimal cell merging. Thus the minimal CFL time step is equal to the radial CFL time step of the second (and most restrictive) zone. Given the time step for $\delta R_c \approx 200$ m in the shell atop the 1-km central spherical zone, we set our base level of the proposed models at $N_{\rm hyd} = 3.5$ M. The total time for a simulation models as

$$t_{\rm sim} = N_{\rm hyd} * \left(\frac{200\rm m}{\delta R_c}\right) * \left(c_{\rm hyd} + c_{\rm nuc}\right) + N_{\rm trans} * c_{\rm trans} + N_{\rm HDF} * c_{\rm HDF} \quad (1)$$

where the number of HDF5 writes, $N_{\rm HDF}$, is one every 500 steps for checkpointing and 5000 per simulated second for analysis at $c_{\rm HDF} = 2.4$ s per write, transport cost, $c_{\rm trans} = 0.49$ s per step on the GPU, nuclear burning cost, $c_{\rm nuc} = 0.12$ s per step, and hydrodynamics, gravity, and internal communications, $c_{\rm hyd}$, is 0.46 s per step in the current runs. The resulting run time is 708 hours per model (350,000 Summit node-hours) for the additional second.

Thus for the two models we propose in Year 1, we request ***700,000 Summit node-hours (2023)***.

3.3 Computational Approach

Operator splitting (solving physics components separately, rather than simultaneously) and *dimensional splitting* (solving equations separately for the three spatial dimensions: r, θ, ϕ) are the key themes to `Chimera`'s computational approach to the multi-dimensional supernova problem.

Fluid motion (hydrodynamics) is solved using the piecewise parabolic method (PPM) to solve 1D Riemann problems explicitly in each direction. For the radial direction (r), the grid moves to track mean fluid motion and appropriately resolve features like shocks and the steep density gradient at the edge of the proto-NS. Self-gravity is computed via multipole expansion in spherical harmonics with a global reduction to gather the coefficients needed by each processor to compute the gravitational force and potential.

In the lower density regions in the outer parts of the simulation domain, physical conditions require the use of a nuclear reaction network to solve for the time-dependent abundances of nuclei. The incorporated nuclear network, XNet, solves a system of coupled non-linear ODEs (one for each nuclear species plus temperature) for the time evolution of the nuclear abundances independently for each zone. The system of equations is integrated in time by either the backward Euler method or backward differentiation formula (“Gear") methods. Where the nuclear time step is smaller than the hydrodynamic step, XNet will compute multiple sub-steps automatically to prevent the short reaction timescales in a few zones from severely restricting the global simulation time step. We also advect passive Lagrangian tracer particles in the code to use in post-processing nucleosynthesis and other analyses.

Transport of neutrinos is computed as multi-(energy)-group angular moments of the neutrino distribution function in a diffusive approximation flux-limited to prevent aphysical (superluminal) ‘diffusion’ of neutrinos in semi-transparent and transparent regions (multi-group flux-limited diffusion, or MGFLD). The MGFLD equations are coupled integro-partial differential equations. The left (or transport) side of the MGFLD equations include spatial and energy partial derivatives, while the right (or collision integral) side includes local couplings between all energy groups (via scattering), neutrinos and anti-neutrinos (via pair emission processes), and to the local electron abundance ($\mathrm{Y_e}$, via emission and absorption). Note the local electron abundance ($\mathrm{Y_e}$) is equal to the local proton abundance and hence a measure of the neutron-richness or isospin of the fluid. The MGFLD equations are solved by Newton-Raphson iteration. The resulting Jacobian has a block tri-diagonal structure. The off-diagonal blocks are themselves diagonal and contain only the discretized radial derivative terms. (Our use of the ‘ray-by-ray’ approximation in the transport removes the pairs of off-diagonal blocks that would be created by the omitted θ- and ϕ-derivatives and the inter-process communication that they would require.) The dense diagonal blocks include all of the local couplings from the collision integral. There are 81 unknowns (20 energy groups each for 4 species of neutrinos plus the $\mathrm{Y_e}$) in each block and $\sim$700 blocks (one for each radial zone). The linear system from the Newton-Raphson iteration is solved by the stabalized biconjugate gradient method using an ADI-like preconditioner (D’Azevedo et al., 2005). Preconditioners include the inverse of the dense blocks and the solution of the 81 tridiagonal (spatial) systems constructed, one for each unknown.

Neutrino-matter interactions (opacities) are interpolated from tables in $(\rho, T, \mathrm{Y_e})$ and terms from the collision integral are computed for each Newton-Raphson iteration. The tables are built on-the-fly and stored independently by each MPI process, eliminating the prior cost of generating an independent mini-table for each zone.

Libraries: `Chimera` uses only a handful of libraries. `LAPACK` is used to perform the dense block linear solves in the transport and network computations. For restart/checkpoint/analysis I/O, we use parallel HDF5, where we write collectively to a low-integer number of files (typically, 4-12 per restart dump). The GPU work also requires CUDA Runtime math libraries (e.g., cuBLAS and cuSPARSE), and we have been developing new GPU solvers using customized versions of MAGMA routines. Data analysis and visualization also requires several Python libraries (`h5py`, `numpy`, `matplotlib`, `scipy`, `yt`, etc.).

Domain decomposition with MPI: The primary sub-domain found in `Chimera` is a ‘ray’— a thin domain that spans the entirety of one dimension but is only one zone wide in the other dimensions. All of the dimensionally split work is done on independent rays in each of the directions (r, θ, ϕ). To pass data to and from the native radial-ray orientation of `Chimera` for computing along the angular dimensions, we use a system of sub-communicators. Sub-communcators are constructed by taking a group of MPI tasks that cover the full domain in r and one of the angular dimensions (θ, for example) while covering the same narrow extent in the other angular dimension (ϕ, as thin a one zone). Data within this 'slab' of zones is transposed by `MPI_AllToAll` on a sub-communicator for that 'slab' that consists of $\mathcal{O}(100)$ tasks, with a similar number of independent sub-communicators to cover the entire problem domain. After the required computations are computed in the angular dimension (θ this example) the data is transposed back to the original radial orientation by a second `MPI_AllToAll` on the same group of sub-communicators. A similarly constructed, but different, set of sub-communicators is required for the other angular dimension (ϕ), and a pair of such transposes are required for each of our $\mathcal{O}(10^6)$ time steps. All-to-all time is kept manageable by the small size and independence of the sub-communicators. Advection of the tracer particles requires a `MPI_AllToAllV` (the distribution of particles is not uniform and varies) within the 'slab' of the tracer position into each direction during each time step. Time step determination, conservation monitoring, and the computation of 1D average values for computing radial grid motion require global reductions (some with broadcasts of computed consequences) during each time step. The scalable MPI design for `Chimera` remains viable after 10 years with only a few minor tweaks required to scale to $\mathcal{O}(10^5)$ cores. Typically we have placed a single radial ray on each MPI task (~700 zones), however recent work to broaden the implementation of threads is permitting effective replacement of on-node MPI with OpenMP.

Threading with OpenMP: Our threading efforts have concentrated on the two components that represent the largest computational effort: the neutrino transport and the nuclear network (in the case of larger networks), with the near-term goal of bringing more computational elements to bear on the smallest MPI-only domains to reduce the time to solution. We have replaced some on-node MPI parallelism with OpenMP, which has allowed sharing of previously replicated resources and reduces communication loads. Threading of the nuclear network in `Chimera` was completed in 2012 and shows good efficiency (3.6 speed-up for 4 cores/MPI rank). A dozen 2D simulations and one 3D simulation using the larger, threaded network have been completed. The 'ADI-like' linear solver used by the neutrino transport is fully threaded and shows similar speed-ups. We have also threaded the rest of the transport sector to good effect. We have implemented threading for the lateral 'sweeps' (θ and ϕ) and are working to build nested threading in the intensive parts of the radial sweep to replace on-node MPI.

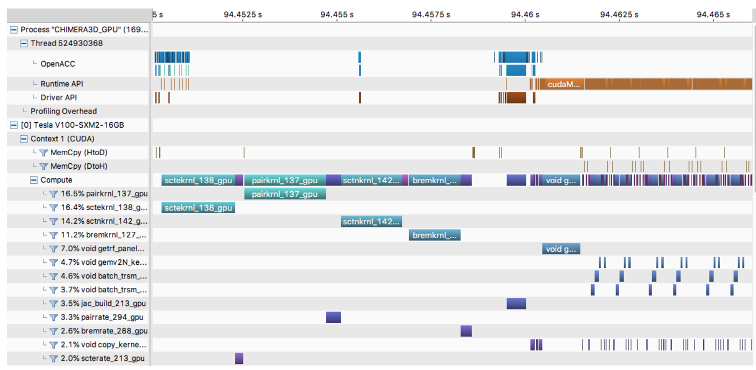

Figure 3: GPU executation trace from NVIDIA Visual Profiler for one neutrino transport Newton-Raphson iteration including opacity interpolation, Jacobian build, and BiCGSTAB linear solver.

GPU usage: The neutrino transport has been nearly fully implemented on the GPU, and we achieve ~5x speedup in the total transport cost with the GPU on Summit relative to the CPU-only threaded implementation. We show in Fig. 3 the GPU execution trace for a single Newton-Raphson iteration of the neutrino transport generated from the NVIDIA Visual Profiler. This consists of three computationally intensive parts: (1) interpolation of the neutrino opacities, (2) construction of the Jacobian, and (3) a linear solve (node-local BiCGSTAB). The interpolation (1) and Jacobian (2) sectors were ported with OpenACC and could see more benefit with additional tuning. We're particularly interested in exploring the use of asynchronous CUDA streams to overlap each of the distinct opacity interpolations ('sctekrnl', 'pairkrnl', 'sctnkrnl', and 'bremkrnl' in Fig. 3). To solve the linear system (3), we rewrote the ADI solver, using a combination of cuBLAS, cuSPARSE, and MAGMA routines. The profile shows very little time of the iteration not being spent using the GPU. Some small number of data copies between the CPU and GPU are needed for scalars used to decide execution paths (e.g. iteration convergence), but otherwise all of the GPU kernels are enqueued and launched asynchronously. All of the computation is performed via GPU library routines with very little data transfer between the CPU and GPU needed until the solution vector is copied at the end of the solve.

Batched interfaces were particularly helpful for the LU decomposition (`cublasDgetrfBatched`), triangular back-substitution (`cublasDgetrsBatched`), tridiagonal solve (`cusparseDgtsv2StridedBatch`), and matrix–vector multiplications (`cublasDgemmStridedBatched`, `magmablas_dlascl2`). For the nuclear network, we have restructured the internals of XNet (Harris, 2015) to batch multiple zones together, even when they require different numbers of Newton-Raphson iterations or time steps to solve. We have implemented this scheme on the GPU with OpenACC and cuBLAS for the batched linear solve (LU + back-substitution). For 160-species networks, the batched GPU version of XNet gives a ∼3x speedup over the CPU-alone. Integration of this version into `Chimera` required some modification to the interface routine to handle the batched solution of the network, but this work is complete. We have already obtained more than an order of magnitude performance improvement in the equation of state calculations in a separate microphysics mini-app (WeakLib) for the ExaStar project as part of ECP. We will be able to incorporate continuing improvements to WeakLib prior to the beginning of the INCITE allocation by updating existing WeakLib interfaces in `Chimera`.

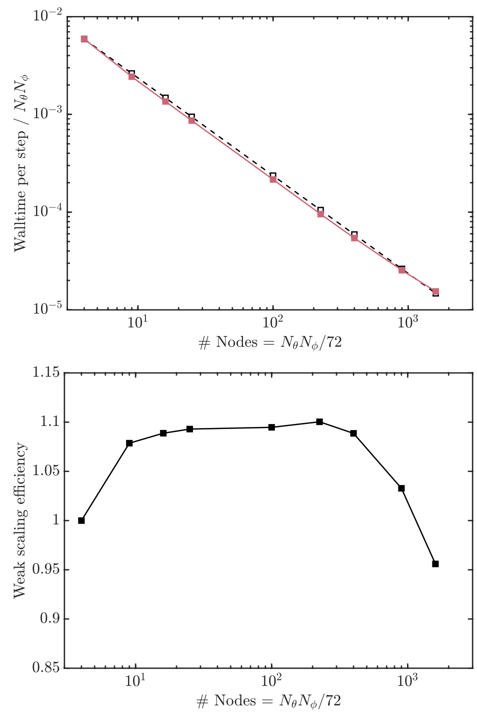

Figure 4: a) Weak scaling runtime per ray and b) Weak scaling efficiency for `Chimera` on Summit up to 1,600 nodes (67,200 CPU cores, 9,600 GPUs), keeping the number of radial rays per MPI rank fixed by increasing angular resolution with the number of nodes. Super ideal scaling explained in §3.4.

Workflow: A single `Chimera` simulation consists of about 700 hours of wall clock time and therefore 50–150 individual jobs. Automated restart from the correct restart file is accomplished by inserting a simple resubmission command into the batch script. To optimize the throughput, we will bundle pairs of runs together into a single 988-node job, but if needed we can run each of them separately by cutting the load on each rank in half, doubling the number of nodes used. We plan to run the first pair of models in the first five months of each year and the second in the second five months with the remaining portion of the year for post-run analyses. We use a system of our own creation called Bellerophon (Lingerfelt et al., 2011, 2014) to manage the conversion of output to suitable formats (`xdmf`), for imaging via `matplotlib`, trigger analyses, and to ship images and line plots to an off-site server for display in a Java client for live monitoring by our team. Bellerophon was developed by our team to manage and present information about project components, including plotting, imaging, animation, automated regression testing, and data management. The main offline processing tool is the *Chimera Analysis Tool* (`C.A.T.`) that uses the same MPI parallel structures to read and analyze `Chimera` data in parallel and extract tracer particle data. Archiving of the data (including the tracer particle and analysis files) is done manually to HPSS at intervals driven by the sweeping policy. Post-processing of nucleosynthesis is done with larger networks using a standalone version of the XNet nuclear network code incorporated into `Chimera`.

I/O and storage requirements: The primary I/O is the restart files (which also serve as checkpoint and analysis files), written typically at ∼0.2 ms intervals during the course of the simulation. These 44 GB file sets contain all of the data needed for restart and some additional information for analysis purposes. About 12 sets are written each hour with a total cost of a few percent of the total simulation depending on the current status of the scratch file system — about 5–600 GB/hr. Shortly after generation, each restart file will be read by the visualization system, at least one analysis tool, and then copied to HPSS. About 220 TB will be required for each CCSN second simulated. Some, or all, of this data may be extracted from storage for custom visualization and newly added analyses during, or after, the simulation. There will be approximately 450 TB from the part of Models A & B run under INCITE 2021 to which we will need continued access under this proposal. To this we will add 450 TB of aggregate new storage for the proposed simulations. Six months to a year after the completion of each simulation (once primary analysis and publication of the simulation is finished) the data can be thinned to about 10–20% of the original size and retained for several years for any analyses comparing to future simulations including those of other groups. We will make processed data, including tracer trajectories, available (off-site) with publication of results.

3.4 Parallel Performance

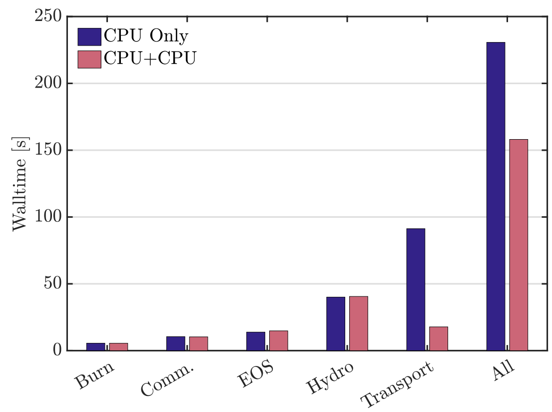

Figure 5: Runtime comparisons from 900 node run for various `Chimera` components using CPU-only and with GPU (transport only).

Plotted in Fig. 4 is the measured weak scaling with `Chimera` on Summit. For this test, we evolve a 3D CCSN model with identical physics to that of the proposed INCITE simulations for 100 timesteps in 3D spherical polar geometry, restarting from a rotated 1D simulation at 30 ms after core-bounce. Though the computational cost of the various physics components will change as the simulation evolves, this time was chosen as a reasonable representation of the overall cost profile for a fully evolved simulation. We establish a baseline performance with 4 nodes using $N_r = 720$ radial zones, $N_\theta = 12$ polar zones, and $N_\phi = 24$ azimuthal zones ($N_\theta N_\phi = 288$ radial rays) and linearly scale the angular resolution with increasing node count up to 1,600 nodes ($N_\theta = 240$, $N_\phi = 480$), keeping the number of radial rays per MPI rank fixed. The improvement over ideal scaling clearly seen in Fig. 4b is a result of the neutrino transport calculation requiring many more linear solver iterations for the large timestep permitted by the CFL condition for large angular zones at low resolution (all of the simulations above 16 nodes have roughly the same number of iterations). Each node was configured with 6 MPI ranks per GPU, using CUDA MPS to concurrently schedule work on the GPU from each MPI rank. We also found some small benefit to using 2 hardware threads (SMT2) per MPI rank via OpenMP over other hardware threading options.

We demonstrate our use of the GPUs for 900 nodes of Summit in Fig. 5. Efforts to improve the performance of `Chimera` with GPUs to this point have focused on the neutrino transport module that has historically been the computational bottleneck for `Chimera` and CCSN simulations in general. We obtain a ~5x speedup of the transport solver (~1.5x for all of `Chimera`) relative to multi-core threading alone by using a combination of OpenACC, cuBLAS, cuSPARSE, and MAGMA to offload the computation to the GPU. This has effectively removed neutrino transport as a bottleneck for `Chimera` and we are now focusing on improvements to other sectors of the code.

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M. A. Skinner, A. Burrows & J. C. Dolence (2016), *Should One Use the Ray-by-Ray Approximation in Core-collapse Supernova Simulations?*, *ApJ*, **831** 81.

M. A. Skinner, J. C. Dolence, A. Burrows, D. Radice & D. Vartanyan (2019), *FORNAX: A Flexible Code for Multiphysics Astrophysical Simulations*, *ApJS*, **241** 7.

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Y. Suwa, S. Yamada, T. Takiwaki & K. Kotake (2016), *The Criterion of Supernova Explosion Revisited: The Mass Accretion History*, *ApJ*, **816** 43.

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T. Takiwaki, K. Kotake & Y. Suwa (2016), *Three-dimensional simulations of rapidly rotating core-collapse supernovae: finding a neutrino-powered explosion aided by non-axisymmetric flows*, *MNRAS*, **461** L112–L116.

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Team Description

- PI Hix will be responsible for management of the INCITE allocation and the 3D simulations this will enable, implementing the decisions made by the team. He is Group Leader for the Theoretical Physics Group at ORNL and the chief architect of XNet. He provides high-performance computing expertise and has a long history of work on the core-collapse problem. He will be responsible for producing post-processed analyses of the nucleosynthesis produced in the 3D simulations.
- Co-PI Bruenn is the principal developer of MGFLD and chief architect of CHIMERA. He will provide direct help with the analysis of the 3D simulations.
- Co-PI Harris has been instrumental in the transition of CHIMERA to utilize GPUs, having worked on porting XNet and the neutrion transport to use hardware accelerators. He continues efforts to improve our GPu usage and will also contribute to the post-processed analyses of the nucleosynthesis produced in the 3D simulations.
- Co-PI Lentz is a principal developer of CHIMERA, having been responsible in recent years for the development of the Yin-Yang and merged cell grids. He will contribute expertise on the code and will run many of the post-processing analyses, enabled by the CHIMERA Analysis Tool (CAT) he has developed. He will run the 3D simulations.
- Co-PI Mezzacappa will manage the implementation of improved general relativity in CHIMERA, contributing his expertise on neutrino transport, gravitational wave signatures, and general relativity. He will oversee with GW and neutrino signature analyses.

Management Plan

Scientific management of the CHIMERA project is driven by consensus among the senior project personnel. Our principal management vehicle is weekly conference calls, where progress is discussed and future directions are decided. The simulations enabled by this INCITE proposal will be among the principal scientific fruits of the CHIMERA effort, and thus will receive attention from the entire team.

Project Milestones: Detailed Schedule; Year 1

Milestone	Details	Dates
(1) Extend Models A & B to asymptotic explosion and neutrino wind phase **A:** non-rotating 13 $M_{\odot}$ simulation **B:** moderately-rotating 13 $M_{\odot}$ simulation	**Resources:** Summit **Node hours:** 700,000 **Filesystem storage (TB and dates):** 450 TB total, January – May **Archival storage (TB and dates):** 900 TB total **Software Application:** `Chimera` **Tasks:** Run additional 1000 ms of explosion evolution each for models A & B **Dependencies:** INCITE 2021/2022	June 1, 2023
(2) Calculate GW signature template for Models A & B Calculate neutrino signatures for Models A & B	**Resources:** Andes **Node hours:** 2000 **Filesystem storage (TB and dates):** 520 TB, June – July **Archival storage (TB and dates):** None **Software Application:** `C.A.T.`, analysis codes **Tasks:** GW & neutrino signatures and other analyses for Models A & B **Dependencies:** (1)	August 1, 2023
(3) Nucleosynthesis analysis for Models A & B	**Resouces:** Summit **Node hours:** 6,000 **Filesystem storage (TB and dates):** 40 TB total , June – August **Archival storage (TB and dates):** 40 TB total **Software Application:** XNet, `C.A.T.` **Tasks:** Process tracer particles with large nuclear network for models A & B Perform other analyses on models A & B **Dependencies:** (1)	Sept. 1, 2023
(4) Wind analysis for Models A & B	**Resouces:** Summit **Node hours:** 3,000 **Filesystem storage (TB and dates):** 10 TB total, September – October **Archival storage (TB and dates):** 10 TB total **Software Application:** XNet, `C.A.T.` **Tasks:** Process tracer particles added to the wind with large nuclear network for models A & B **Dependencies:** (1)	Nov. 1, 2023

Publications Resulting From Prior Incite Awards

1. A. Mezzacappa, P. Marronetti, R. E. Landfield, E. J. Lentz, W. R. Hix, J. A. Harris, S. W. Bruenn, J. M. Blondin, O. E. B. Messer, J. Casanova & L. L. Kronzer (2022), *Core Collapse Supernova Gravitational Wave Emission for Progenitors of 9.6, 15, and 25 $M_{\odot}$*, *Phys. Rev. D*, **submitted**
2. M. A. Sandoval, W. R. Hix, O. E. B. Messer, E. J. Lentz & J. A. Harris (2021), *Three-dimensional Core-collapse Supernova Simulations with 160 Isotopic Species Evolved to Shock Breakout*, *ApJ*, **921** 113, doi: 10.3847/1538-4357/ac1d49, arxiv:2106.01389
3. A. Mezzacappa, P. Marronetti, R. E. Landfield, E. J. Lentz, K. N. Yakunin, S. W. Bruenn, W. R. Hix, O. B. Messer, E. Endeve, J. M. Blondin & J. A. Harris (2020), *Gravitational-wave signal of a core-collapse supernova explosion of a 15$M_{\odot}$ star*, *Phys. Rev. D*, **102** 023027, doi: 10.1103/physrevd.102.023027
4. J. Casanova, E. Endeve, E. J. Lentz, O. E. B. Messer, W. R. Hix, J. A. Harris & S. W. Bruenn (2020), *On the character of turbulent-like flows in self-consistent models of core-collapse supernovae*, *Phys. Scr.*, **95** 064005, doi: 10.1088/1402-4896/ab7dd1, arxiv:2004.02055
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7. W. R. Hix, E. J. Lentz, S. W. Bruenn, A. Mezzacappa, O. E. B. Messer, E. Endeve, J. M. Blondin, J. A. Harris, P. Marronetti & K. N. Yakunin (2016), *The Multi-dimensional Character of Core-collapse Supernovae*, *Acta Physica Polonica B*, **47** 645
8. S. W. Bruenn, E. J. Lentz, W. R. Hix, A. Mezzacappa, J. A. Harris, O. E. B. Messer, E. Endeve, J. M. Blondin, M. A. Chertkow, E. J. Lingerfelt, P. Marronetti & K. N. Yakunin (2016), *The Development of Explosions in Axisymmetric Ab Initio Core-collapse Supernova Simulations of 12-25 $M_{\odot}$ Stars*, *The Astrophysical Journal*, **818** 123
9. H. Pais & J. R. Stone (2012), *Exploring the Nuclear Pasta Phase in Core-Collapse Supernova Matter*, *Phys. Rev. Lett.*, **109** 151101, doi: 10.1103/PhysRevLett.109.151101
10. K. N. Yakunin, A. Mezzacappa, P. Marronetti, S. Yoshida, S. W. Bruenn, W. R. Hix, E. J. Lentz, O. E. B. Messer, J. A. Harris, E. Endeve, J. M. Blondin & E. J. Lingerfelt (2015), *Gravitational wave signatures of ab initio two-dimensional core-collapse supernova explosion models for* $12-25M_{\odot}$ *stars*, *Phys. Rev. D*, **92** 084040
11. E. J. Lentz, S. W. Bruenn, W. R. Hix, A. Mezzacappa, O. E. B. Messer, E. Endeve, J. M. Blondin, J. A. Harris, P. Marronetti & K. N. Yakunin (2015), *Three-Dimensional Core-Collapse Supernova Simulated Using a 15 $M_{\odot}$ Progenitor*, *The Astrophysical Journal Letters*, **807** L31
12. J. A. Harris, W. R. Hix, M. A. Chertkow, S. W. Bruenn, E. J. Lentz, O. E. B. Messer, A. Mezzacappa, J. M. Blondin, P. Marronetti & K. N. Yakunin (2014), *Advancing Nucleosynthesis in Self-consistent, Multidimensional Models of Core-Collapse Supernovae*, in *Nuclei in the Cosmos (NIC XIII)*
13. W. R. Hix, J. A. Harris, E. J. Lentz, S. W. Bruenn, M. A. Chertkow, O. E. B. Messer, A. Mezzacappa, E. Endeve, J. M. Blondin, P. Marronetti & K. N. Yakunin (2014), *Multidimensional simulations of core-collapse supernovae and implications for nucleosynthesis*, in *Nuclei in the Cosmos (NIC XIII)*
14. E. Lingerfelt, O. E. B. Messer, S. Desai, C. Holt & E. Lentz (2014), *Near Real-time Data Analysis of Core-Collapse Supernova Simulations with Bellerophon*, *Procedia Computer Science*, **29** 1504 – 1514, 2014 International Conference on Computational Science, doi: 10.1016/j.procs.2014.05.136
15. W. R. Hix, E. J. Lentz, E. Endeve, M. Baird, M. Chertkow, J. Harris, O. E. B. Messer,

A. Mezzacappa, S. Bruenn & J. M. Blondin (2014), *Essential ingredients in core-collapse supernovae*, *AIP Advances*, **4** 041013
16. S. W. Bruenn, A. Mezzacappa, W. R. Hix, E. J. Lentz, O. E. B. Messer, E. J. Lingerfelt, J. M. Blondin, E. Endeve, P. Marronetti & K. N. Yakunin (2013), *Axisymmetric Ab Initio Core-Collapse Supernova Simulations of 12-25 $M_\odot$ Stars*, *ApJ*, **767** L6
17. K. N. Yakunin, P. Marronetti, A. Mezzacappa, S. W. Bruenn, C.-T. Lee, M. A. Chertkow, W. R. Hix, J. M. Blondin, E. J. Lentz, O. E. B. Messer & S. Yoshida (2010), *Gravitational waves from core collapse supernovae*, *Classical and Quantum Gravity*, **27** 194005
18. W. G. Newton & J. R. Stone (2009), *Modeling nuclear "pasta" and the transition to uniform nuclear matter with the 3D Skyrme-Hartree-Fock method at finite temperature: Core-collapse supernovae*, *Phys. Rev. C*, **79** 055801, doi: 10.1103/PhysRevC.79.055801
19. C. Y. Cardall, R. D. Budiardja, E. Endeve & A. Mezzacappa (2014), *GENASIS: General Astrophysical Simulation System. I. Refinable Mesh and Nonrelativistic Hydrodynamics*, *The Astrophysical Journal Supplement Series*, **210** 17
20. E. Endeve, C. Y. Cardall, R. D. Budiardja, A. Mezzacappa & J. M. Blondin (2013), *Turbulence and magnetic field amplification from spiral SASI modes in core-collapse supernovae*, *Physica Scripta*, **2013** 014022
21. E. Endeve, C. Y. Cardall, R. D. Budiardja, S. W. Beck, A. Bejnood, R. J. Toedte, A. Mezzacappa & J. M. Blondin (2012), *Turbulent Magnetic Field Amplification from Spiral SASI Modes: Implications for Core-collapse Supernovae and Proto-neutron Star Magnetization*, *The Astrophysical Journal*, **751** 26
22. A. Mezzacappa, E. J. Lentz, S. W. Bruenn, W. R. Hix, O. E. B. Messer, E. Endeve, J. M. Blondin, J. A. Harris, P. Marronetti, K. N. Yakunin & E. J. Lingerfelt (2015b), *A Three-Dimensional Neutrino-Driven Core Collapse Supernova Explosion of a 15 $M_\odot$ Star*, in *Astronomical Society of the Pacific Conference Series*, N. V. Pogorelov, E. Audit & G. P. Zank, eds., *Astronomical Society of the Pacific Conference Series*, vol. 498, 108
23. A. Mezzacappa, S. W. Bruenn, E. J. Lentz, W. R. Hix, O. E. Bronson Messer, J. A. Harris, E. J. Lingerfelt, E. Endeve, K. N. Yakunin, J. M. Blondin & P. Marronetti (2015a), *Two- and Three-Dimensional Multi-Physics Simulations of Core Collapse Supernovae: A Brief Status Report and Summary of Results from the 'Oak Ridge' Group*, in *8th International Conference of Numerical Modeling of Space Plasma Flows (ASTRONUM 2013)*, *Astronomical Society of the Pacific Conference Series*, vol. 488, 102
24. S. W. Bruenn, A. Mezzacappa, W. R. Hix, J. M. Blondin, P. Marronetti, O. E. B. Messer, C. J. Dirk & S. Yoshida (2009a), *2D and 3D core-collapse supernovae simulation results obtained with the CHIMERA code*, *Journal of Physics: Conference Series*, **180** 012018
25. S. W. Bruenn, A. Mezzacappa, W. R. Hix, J. M. Blondin, P. Marronetti, O. E. B. Messer, C. J. Dirk & S. Yoshida (2009b), *Mechanisms of Core-Collapse Supernovae & Simulation Results from the CHIMERA Code*, in *Probing Stellar Populations Out To The Distant Universe: Cefalu 2008*, G. Giobbi, A. Tornambe, G. Raimondo, M. Limongi, L. A. Antonelli, N. Menci & E. Brocato, eds. (AIP), 593–601
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27. A. Mezzacappa, S. W. Bruenn, J. M. Blondin, W. R. Hix & O. E. B. Messer (2007), *Ascertaining the Core Collapse Supernova Mechanism: An Emerging Picture?*, in *The Multicolored Landscape of Compact Objects and Their Explosive Origins*, T. di Salvo, G. L. Israel, L. Piersant, L. Burderi, G. Matt, A. Tornambe & M. T. Menna, eds., *American Institute of Physics Conference Series*, vol. 924, 234–242

28. A. Mezzacappa, J. M. Blondin, O. E. B. Messer & S. W. Bruenn (2006), *Core Collapse Supernovae: Modeling Requirements and Surprises*, in *Origin of Matter and Evolution of Galaxies*, S. Kubono, W. Aoki, T. Kajino, T. Motobayashi & K. Nomoto, eds., *American Institute of Physics Conference Series*, vol. 847, 179–189, doi: 10.1063/1.2234400

NAME: Eric J. Lentz

POSITION TITLE & INSTITUTION: Research Assistant Professor, University of Tennessee

A. PROFESSIONAL PREPARATION - (see PAPPG Chapter II.C.2.f.(i)(a))

INSTITUTION	LOCATION	MAJOR/AREA OF STUDY	DEGREE (if applicable)	YEAR (YYYY)
University of Maryland	College Park, MD	Mathematics	BS	1989
University of Maryland	College Park, MD	Physics, with Honors, & Astronomy	BS	1989
Harvard University	Cambridge, MA	Astronomy	AM	1991
Harvard University	Cambridge, MA	Astronomy	PhD	1995
University of Texas	Austin, TX	Astronomy	Post-doc	1997
University of Tennessee	Knoxville, TN	Physics & Astronomy	Post-doc	2000

B. APPOINTMENTS - (see PAPPG Chapter II.C.2.f.(i)(b))

From - To	Position Title, Organization and Location
2021-present	Group Leader for Theoretical & Computational Physics, Oak Ridge National Laboratory (ORNL), Physics Division, Oak Ridge , TN
2020 - present	Group Leader for Nuclear Structure & Nuclear Astrophysics, Oak Ridge National Laboratory (ORNL), Physics Division, Oak Ridge , TN
2015 - present	Joint Faculty Professor, University of Tennessee (UTK), Department of Physics and Astronomy, Knoxville, TN (50% appointment)
2010 - present	Joint Faculty Appointment (50%), ORNL, Physics Division, Oak Ridge, TN
2004 - present	R&D Staff, ORNL, Physics Division, Oak Ridge, TN
2012 - 2020	Group Leader for Theoretical Physics, ORNL, Physics Division, Oak Ridge, TN
2010 - 2015	Joint Faculty Associate Professor, UTK Depart. of Physics and Astronomy, Knoxville, TN (50% appointment)
2006 - 2010	Adjunct Associate Professor, UTK, Depart. of Physics and Astronomy, Knoxville, TN
2004 - 2006	Adjunct Assistant Professor, UTK Depart. of Physics and Astronomy, Knoxville, TN
2000 - 2004	Research Assistant Professor, UTK, Depart.of Physics and Astronomy, Knoxville, TN
1997 - 2000	Postdoctoral Research Associate, UTK, Depart. of Physics and Astronomy,
1995 - 1997	Knoxville, TN
1990 - 1995	Postdoctoral Fellow, University of Texas, Department of Astronomy, Austin, TX
1990 - 1994	Research Assistant, Harvard University, Department of Astronomy, Cambridge, MA
1990 - 1991	NASA Graduate Student Researchers Program Fellow, Harvard University, Cambridge, MA
	Teaching Fellow, Harvard University, Department of Astronomy, Cambridge, MA

C. PRODUCTS - (see PAPPG Chapter II.C.2.f.(i)(c)) Products Most Closely Related to the Proposed Project

1. M. A. Sandoval, W. R. Hix, O. E. B. Messer, E. J. Lentz, and J. A. Harris, Three-dimensional Core-collapse Supernova Simulations with 160 Isotopic Species Evolved to Shock Breakout (2021) The Astrophysical Journal 921 : 10.3847/1538-4357/ac1d49

2. K. A. Chipps, P. Adsley, M. Couder, W. R. Hix, Z. Meisel, and K. Schmidt, Evaluation of experimental constraints on the 44Ti(α ,p)47V reaction cross section relevant for supernovae (2020) Physical Review C 102 : 10.1103/PhysRevC.102.035806

3. S. W. Bruenn, J. M. Blondin, W. R. Hix, E. J. Lentz, O. E. B. Messer, A. Mezzacappa, E. Endeve, J. A. Harris, P. Marronetti, R. D. Budiardja, M. A. Chertkow, and C.-T. Lee, CHIMERA: A Massively Parallel Code for Core-collapse Supernova Simulations (2020) The Astrophysical Journal Supplement Series 248 : 10.3847/1538-4365/ab7aff

4. W. R. Hix, J. A. Harris, E. J. Lentz, S. Bruenn, O. E. Bronson Messer, and A. Mezzacappa, Learning About Nucleosynthesis from Multi-dimensional Simulations of Core-Collapse Supernovae (2019) Nuclei in the Cosmos XV 219 : 10.1007/978-3-030-13876-9_19

5. R. Surman, G. C. McLaughlin, M. Ruffert, H.-T. Janka, and W. R. Hix, r-Process Nucleosynthesis in Hot Accretion Disk Flows from Black Hole-Neutron Star Mergers (2008) The Astrophysical Journal 679 : 10.1086/589507

Other Significant Products, Whether or Not Related to the Proposed Project

1. H. Schatz, Z. Meisel, E. F. Brown, S. S. Gupta, G. W. Hitt, W. R. Hix, R. Jain, R. Lau, P. Möller, W.-J. Ong, P. S. Shternin, Y. Xu, and M. Wiescher, The Impact of Neutron Transfer Reactions on the Heating and Cooling of Accreted Neutron Star Crusts (2022) The Astrophysical Journal 925 205 : 10.3847/1538-4357/ac4271

2. A. Mezzacappa, P. Marronetti, R. E. Landfield, E. J. Lentz, K. N. Yakunin, S. W. Bruenn, W. R. Hix, O. E. B. Messer, E. Endeve, J. M. Blondin, and J. A. Harris, Gravitational-wave signal of a core-collapse supernova explosion of a 15 M star (2020) Physical Review D 102 023027 : 10.1103/PhysRevD.102.023027

3. S. Starrfield, M. Bose, C. Iliadis, W. R. Hix, C. E. Woodward, and R. M. Wagner, Carbon-Oxygen Classical Novae Are Galactic ⁷Li Producers as well as Potential Supernova Ia Progenitors (2020) The Astrophysical Journal 895 70 : 10.3847/1538-4357/ab8d23

4. A. Sieverding, G. Martínez Pinedo, K. Langanke, J. A. Harris, and W. R. Hix, The ν process in the innermost supernova ejecta (2018) European Physical Journal Web of Conferences 165 01045 : 10.1051/epjconf/201716501045

5. J. A. Harris, W. R. Hix, M. A. Chertkow, C. T. Lee, E. J. Lentz, and O. E. B. Messer, Implications for Post-processing Nucleosynthesis of Core-collapse Supernova Models with Lagrangian Particles (2017) The Astrophysical Journal 843 2 : 10.3847/1538-4357/aa76de

D. SYNERGISTIC ACTIVITIES - (see PAPPG Chapter II.C.2.f.(i)(d))

1. Supervisor of graduate and undergraduate research, Department of Physics and Astronomy, University of Tennessee at Knoxville, (1999-present)

2. Lead Developer of XNet, a widely used astrophysical thermonuclear reaction network code (1995-present)

3. Co-Developer, CHIMERA core-collapse supernova code (1999-present)

NAME: Eric J. Lentz

POSITION TITLE & INSTITUTION: Research Assistant Professor, University of Tennessee

A. PROFESSIONAL PREPARATION - (see PAPPG Chapter II.C.2.f.(i)(a))

INSTITUTION	LOCATION	MAJOR/AREA OF STUDY	DEGREE (if applicable)	YEAR (YYYY)
University of Maryland	College Park, MD	Mathematics	BS	1989
University of Maryland	College Park, MD	Physics, with Honors, & Astronomy	BS	1989
Harvard University	Cambridge, MA	Astronomy	AM	1991
Harvard University	Cambridge, MA	Astronomy	PhD	1995
University of Texas	Austin, TX	Astronomy	Post-doc	1997
University of Tennessee	Knoxville, TN	Physics & Astronomy	Post-doc	2000

B. APPOINTMENTS - (see PAPPG Chapter II.C.2.f.(i)(b))

From - To	Position Title, Organization and Location
2021-present	Group Leader for Theoretical & Computational Physics, Oak Ridge National Laboratory (ORNL), Physics Division, Oak Ridge , TN
2020 - present	Group Leader for Nuclear Structure & Nuclear Astrophysics, Oak Ridge National Laboratory (ORNL), Physics Division, Oak Ridge , TN
2015 - present	Joint Faculty Professor, University of Tennessee (UTK), Department of Physics and Astronomy, Knoxville, TN (50% appointment)
2010 - present	Joint Faculty Appointment (50%), ORNL, Physics Division, Oak Ridge, TN
2004 - present	R&D Staff, ORNL, Physics Division, Oak Ridge, TN
2012 - 2020	Group Leader for Theoretical Physics, ORNL, Physics Division, Oak Ridge, TN
2010 - 2015	Joint Faculty Associate Professor, UTK Depart. of Physics and Astronomy, Knoxville, TN (50% appointment)
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1997 - 2000	Postdoctoral Research Associate, UTK, Depart. of Physics and Astronomy, Knoxville, TN
1995 - 1997	Postdoctoral Fellow, University of Texas, Department of Astronomy, Austin, TX
1990 - 1995	Research Assistant, Harvard University, Department of Astronomy, Cambridge, MA
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Harvard University	Cambridge, MA	Astronomy	AM	1991
Harvard University	Cambridge, MA	Astronomy	PhD	1995
University of Texas	Austin, TX	Astronomy	Post-doc	1997
University of Tennessee	Knoxville, TN	Physics & Astronomy	Post-doc	2000

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Section 6: Software Applications and Packages

Question #1

Please list any software packages used by the project, and indicate if they are on open source or export controlled.

Application Packages

Package Name

CHIMERA

Indicate whether Open Source or Export Controlled.

Open Source

Section 7: Wrap-Up Questions

Question #1

National Security Decision Directive (NSDD) 189 defines Fundamental Research as "basic and applied research in science and engineering, the results of which ordinarily are published and shared broadly within the scientific community, as distinguished from proprietary research and from industrial development, design, production, and product utilization, the results of which ordinarily are restricted for proprietary or national security reasons." Publicly Available Information is defined as information obtainable free of charge (other than minor shipping or copying fees) and without restriction, which is available via the internet, journal publications, textbooks, articles, newspapers, magazines, etc.

The INCITE program distinguishes between the generation of proprietary information (deemed a proprietary project) and the use of proprietary information as input. In the latter, the project may be considered as Fundamental Research or nonproprietary under the terms of the nonproprietary user agreement. Proprietary information, including computer codes and data, brought into the LCF for use by the project - but not for generation of new intellectual property, etc., using the facility resources - may be protected under a nonproprietary user agreement.

Proprietary Information

Are the proposed project and its intended outcome considered Fundamental Research or Publicly Available Information?

Yes

Will the proposed project use proprietary information, intellectual property, or licensing?

No

Will the proposed project generate proprietary information, intellectual property, or licensing as the result of the work being proposed?

If the response is Yes, please contact the INCITE manager, INCITE@doeleadershipcomputing.org, prior to submittal to discuss the INCITE policy on proprietary work.

No

Question #2

The following questions are provided to determine whether research associated with an INCITE proposal may be export controlled. Responding to these questions can facilitate - but not substitute for - any export control review required for this proposal.

PIs are responsible for knowing whether their project uses or generates sensitive or restricted information. Department of Energy systems contain only data related to scientific research and do not contain personally identifiable information. Therefore, you should answer "Yes" if your project uses or generates data that fall under the Privacy Act of 1974 U.S.C. 552a. Use of high-performance computing resources to store, manipulate, or remotely access any national security information is prohibited. This includes, but is not limited to, classified information, unclassified controlled nuclear information (UCNI); naval nuclear propulsion information (NNPI); and the design or development of nuclear, biological, or chemical weapons or of any weapons of mass destruction. For more information contact the Office of Domestic and International Energy Policy, Department of Energy, Washington DC 20585, 202-586-9211.

Export Control

Does this project use or generate sensitive or restricted information?

No

Does the proposed project involve any of the following areas?

i. Military, space craft, satellites, missiles, and associated hardware, software or technical data

ii. Nuclear reactors and components, nuclear material enrichment equipment, components (Trigger List) and associated hardware, software or technical data

iii. Encryption above 128 bit software (source and object code)

iv. Weapons of mass destruction or their precursors (nuclear, chemical and biological)

No

Does the proposed project involve International Traffic in Arms Regulations (ITAR)?

No

Question #3

The following questions deal with health data. PIs are responsible for knowing if their project uses any health data and if that data is protected. Note that certain health data may fall both within these questions as well as be considered sensitive as per question #2. Questions regarding these answers to these questions should be directed to the centers or program manager prior to submission.

Health Data

Will this project use health data?

No

Will this project use human health data?

No

Will this project use Protected Health Information (PHI)?

No

Question #4

The PI and designated Project Manager agree to the following:

Monitor Agreement

I certify that the information provided herein contains no proprietary or export control material and is correct to the best of my knowledge.

Yes

I agree to provide periodic updates of research accomplishments and to

acknowledge INCITE and the LCF in publications resulting from an INCITE award.

Yes

I agree to monitor the usage associated with an INCITE award to ensure that usage is only for the project being described herein and that all U. S. Export Controls are complied with.

Yes

I understand that the INCITE program reserves the right to periodically redistribute allocations from underutilized projects.

Yes

Section 8: Outreach and Suggested Reviewers

Question #1

By what sources (colleagues, web sites, email notices, other) have you heard about the INCITE program? This information will help refine our outreach efforts.

Outreach

Question #2

Suggested Reviewers

Section 9: Testbed Resources

Question #1

The ALCF and OLCF have test bed resources for new technologies, details below. If you would like access to these resources to support the work in this proposal, please provide the information below. (1 Page Limit)

The OLCF Quantum Computing User Program is designed to enable research by providing a broad spectrum of user access to the best available quantum computing systems, evaluate technology by monitoring the breadth and performance of early quantum computing applications, and Engage the quantum computing community and support the growth of the quantum information science ecosystems. More information can be found here: https://www.olcf.ornl.gov/olcf-resources/compute-systems/quantum-computing-user-program/quantum-computing-user-support-documentation.

The ALCF AI Testbed provides access to next-generation of AI-accelerator machines to enable evaluation of both hardware and workflows. Current hardware available includes Cerebras C-2, Graphcore MK1, Groq, Habana Gaudi, and SambaNova Dataflow. New hardware is regularly acquired as it becomes available. Up to date information can be found here: https://www.alcf.anl.gov/alcf-ai-testbed.

Describe the experiments you would be interested in performing, resources required, and their relationship to the current proposal. Please note, these are smaller experimental resources and a large amount of resources are not available. Instead, these resources are to explore the possibilities for these technologies might innovate future work. This request does not contribute to the 15-page proposal limit.

QC:AI interest.pdf
The attachment is on the following page.

At present, the CHIMERA team has no interest in Quantum computing or AI-accelerator systems.