Research Statement

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My research activities focus on

- Stellar Evolution, accented by Modules for Experiments for Stellar Astrophysics (MESA)
- Supernovae, with emphasis on their progenitor evolution, explosion, and nucleosynthesis
- Cosmic chemical evolution, the evolution of every isotope at every point in spacetime
- Astrobiology, the synthesis and delivery of bioessential elements to habitable systems
- Gamma-ray astronomy, particularly from radioactive isotopes
- Stellar thermodynamics and nuclear reactions
- Software infrastructure for sustained innovation
- High performance computing and next-generation internet
- Digital toolsets for online education at scale

Below I discuss a few examples from this portfolio that are in the recent past, current, or coming to fruition in the near future.

Software Infrastructure - MESA, FLASH, and NSF SI2

The MESA (Modules for Experiments in Stellar Astrophysics) software instrument solves the 1D fully coupled structure and composition equations governing stellar evolution. It is based on an implicit finite volume scheme with adaptive mesh refinement and sophisticated timestep controls; state-of-the-art modules provide equation of state, opacity, nuclear reaction rates, element diffusion, boundary conditions, convection, angular momentum transport, and changes to the mass of the star. MESA is an open source library that employs contemporary numerical approaches, supports shared memory parallelism based on OpenMP, is designed to accommodate present and future multi-core and multi-thread architectures, and provides hooks to allow user customization without the need to modify the source code. MESA combines composable, interoperable, robust, efficient, thread-safe numerical and physics modules for provenance-capable simulations of a wide range of stellar evolution scenarios ranging from giant planets to low mass single stars to massive star binaries relevant to interpreting LIGO's recent discoveries of gravitational waves.

I am one of the principals of the MESA project. Launched in 2011, MESA 1) has attracted over 900 registered users world-wide; 2) has witnessed over 10,000 downloads of the source; 3) has distributed over 12,000 archived and searchable posts on community discussions; 4) provides a Software Development Kit to build MESA across a variety of platforms; 5) delivers an annual Summer School program that now has over 200 graduates; 6) hosts a web-portal for the community to share analysis tools and build provenance; 7) offers a cloud resource for education, MESA-Web.

The four MESA instrument papers, which describe major new science and software capabilities, have been cited $\simeq$1600 times and has a current citation rate of $\simeq$500/year (all citation data from SAO/NASA ADS). Papers that cite papers that use MESA have generated $\simeq$ 10,835 citations, for a radius-of-influence multiplicative factor of $\simeq$ 10, which suggests MESA generates papers the larger astrophysics community values. More specifically, MESA I is one the 10 most cited astronomy/astrophysics papers published in 2011. MESA II is one of the 15 most cited astronomy/astrophysics papers published in 2013 and was one of 15 "high-impact" papers highlighted by the American Astronomical Society at the 2015 International Astronomy Union triennial meeting. MESA III is one of the 15 most cited astronomy/astrophysics papers published in 2015. MESA IV has ben submitted and is under review. The aggregate of these citation metrics suggest that MESA provides a crucial resource to the stellar community, has had a significant impact within and beyond the stellar community, and is on its way to becoming the world standard for evolving stars – accounting for about 1/2 of all stellar models in the literature.

Near future new capabilities in MESA to enable new science motivated by observational breakthroughs include supernova light curves, co-process nuclear burning, the red edge of instability strips, automatic instability strip delineation, flame propagation, and Type Ia supernova models.

I suspect that Rich Townsend (UW Madison), Lars Bildsten (UCSB), Bill Paxton (UCSB), and I will generate a new, outside-the-box, graduate level textbook on Stellar Evolution with MESA within the next few years.

The FLASH software instrument solves the three-dimensional Eulerian magnetohydrodynamics equations with adaptive-mesh refinement for general astrophysical problems. The architecture allows arbitrarily interoperable modules to co-exist and interchange with each other. Examples of physics modules include 1) Hydrodynamics: Unsplit PPM and WENO, Split PPM, Two Temperature + Radiation; 2) Magnetohydrodynamics: Unsplit Staggered Mesh, Split 8 wave ; 3) Equation of State: Ideal gas; Ionized plasma with arbitraty degreees of degeneracy and relativity , Multi-material gamma law; 4) Radiation Transfer: Multigroup Flux-limited Diffusion; 5) Diffusion and Conduction: Implicit with Adaptive Mesh Refinement; 6) Laser Energy Deposition: Geometric Optics with Inverse Brensstrahlung 7) Opacity: Constant, Multimaterial Tabular; 8) Particle Tracers: Massive, Sink, Charged; 9) Nuclear Burning; 10) Gravity: Constant; Point Mass, Planar, Self Gravity; 11) Magnetic Resistivity, Conductivity; 12) Primordial Chemistry. User plugins exist for customization without the need to modify the source.

I am one of the original developers of FLASH. The first bare-knuckles version, version 0.0, was created in 1998 by Kevin Olson (he had the adaptive mesh package and his hands on the keyboard), Bruce Fryxell (he had the hydro package and was on Kevin's right), and me (I had the local physics packages and was on Kevin's left) in the Laboratory for Astrophysics and Space Research building at the University of Chicago where Kevin and I shared an office. We had some nifty SGI O2 desktop computers at the time! Shortly thereafter Paul Ricker (he had the gravity package) and Mike Zingale (he had the visualization package and all-purpose skills) added critical capabilities. Jonathan Dursi and Alan Calder made key contributions and gave the development team a critical mass.

Near future new capabilities in FLASH to enable new massive star supernova science include a port of my general nuclear reaction network solver into Sean Couch's version of FLASH. With a bit of fortune, our 2018 NSF proposal will see funding to help move this along.

I was the Chair and PI for the 2015, 2016, and 2018 NSF SI2 PI Workshop. In this role I drove, from inception to final report, a meeting for about 150 PIs with various NSF awards for software infrastructure. I might do it again in 2019 or 2020.

Nuclear Astrophysics - JINA-CEE, STARLIB, ^{12}C(α,γ), and B-Fields

Thermonuclear reaction rates are at the heart of nuclear astrophysics. They are essential for for energy generation and element synthesis from the big bang to stars. The growing volume of new, precision astronomical data motivates the community's expressed need for assessing the impact of the uncertainties in nuclear reaction rates.

The Joint Institute for Nuclear Astrophysics - Center for the Evolution of the Elements (JINA-CEE) is an NSF Physics Frontier Center headquartered at Michican State University. JINA-CEE brings together nuclear experimentalists, nuclear theorists, astronomers, theoretical astrophysicists, and computational physicists in a unique cross-disciplinary research network that enables rapid communication and coordination across field boundaries and connects research at new accelerator facilities, observatories, and numerical simulations in new ways.

I am a Co-PI of JINA-CEE, along with Hendrik Schatz (MSU), Michael Wiescher (Notre Dame), Sanjay Reddy (UW), and Tim beers (Notre Dame). My primary role is to lead and organize the theoretical and computational efforts of the Major Activity "Rise of the Elements in the First Billion Years". The NSF site review for JINA-CEE went really well, a home run actually, and I strongly suspect that we will re-compete as a Physics Frontier Center in 2020.

STARLIB is a next-generation compilation of thermonuclear reaction rates that, for the first time, provides the probability density functions needed to rigoursly assess the experimental and theoretical uncertainties in a reaction rate. In the past, compiling reaction rates without uncertainties was standard practice in part because the additional resources needed to explore the impacts of the reaction rate uncertainties in stellar models was computationally prohibitive, and in part because it was unclear how to proceed in evaluating a limited number of stellar models in a statistically rigorous manner. To produce realistic nucleosynthesis and stellar structure that can match the new observations it is necessary for stellar models to access a reaction rate library that incorporates probability density functions for each reaction rate at a given temperature.

One approach my colleagues and I pioneered is the use of Monte Carlo based techniques. All of the measured nuclear physics properties entering into a reaction rate calculation are randomly sampled according to their individual probability density functions. The sampling is repeated many times and thus provides a Monte Carlo reaction rate probability density. The associated cumulative distribution is used to derive reaction rate uncertainties with a quantifiable coverage probability.

A new approach we are exploring is using Bayesian probability theory for calculating the non-resonant reaction rates (i.e., astrophysical S-factors that vary smoothly with energy). The advantages of this approach are manifold. First, the Bayesian approach yields directly the quantity of interest, i.e., the reaction rate probability density function. These rates can be easily implemented, together with the Monte Carlo-based rates for resonant reactions discussed above, into the STARLIB rate library. Second, the Bayesian model provides a more consistent method for extracting information from measured data, even in ill-conditioned situations, compared to traditional statistics. I am actively helping to develop a framework that incorporates robust parameter estimation, systematic effects, and non-Gaussian uncertainties in a consistent manner.

While nearly all models of different nucleosynthesis environments are affected by the production of carbon and oxygen, a key ingredient, the precise determination of the $^{12}C(\alpha,\gamma)^{16}O$ reaction rate has long remained elusive. This is owed to the reaction's inaccessibility, both experimentally and theoretically. Nuclear theory has struggled to calculate this reaction rate because the cross section is produced through different underlying nuclear mechanisms. Isospin selection rules suppress the E1 component of the ground state cross section, creating a unique situation where the E1 and E2 contributions are of nearly equal amplitudes. Experimentally there have also been great challenges. Measurements have been pushed to the limits of state-of-the-art techniques, often developed for just these measurements. The data have been plagued by uncharacterized uncertainties, often the result of the novel measurement techniques that have made the different results challenging to reconcile.

However, the situation has markedly improved in recent years, and the desired level of uncertainty 10% may be in sight. In a 2017 Review of Modern Physics article that I co-authored with Richard DeBoer, Michael Wiescher and other, the current understanding of this critical reaction is summarized. The emphasis is placed primarily on the experimental work and interpretation of the reaction data, but discussions of the theory and astrophysics are also pursued. The main goal of the review is to summarize and clarify the current understanding of the reaction and then point the way forward to an improved determination of the reaction rate.

Nuclei have magnetic moments. In a strong enough magnetic field their interaction shifts the nuclear binding energy, hence modifies the zero B-field statistical equilibrium distribution of nuclei in hot environments. In 2018 my colleagues Ashley Ruiter and Ivo Seintenzahl and I are exploring this exciting new concept of "magnetic NSE" in core-collapse supernova and merging neutron star scenarios. As far as I am aware, this has never been calculated in detail.

Stellar Evolution - White Dwarfs, Massive Stars, and Pop III with JWST

My former undergraduate student Carl Fields (now a grad student at MSU with Sean Couch), postdocs Rob Farmer, Bill Wolf, and Ilka Petterman have undertaken a program aimed at assessing the impact of known uncertainties in stellar evolution models. I'll highlight a few of these efforts.

For example, in Fields et al 2016 we investigated properties of carbon-oxygen white dwarfs with respect to the composite uncertainties in the reaction rates using MESA and the probability density functions in STARLIB. *These are the first Monte Carlo stellar evolution studies that use complete stellar models.* Focusing on 3 $M_{\odot}$ models evolved from the pre main-sequence to the first thermal pulse, we surveyed the remnant core mass, composition, and structure properties as a function of 26 STARLIB reaction rates covering hydrogen and helium burning using a Principal Component Analysis and Spearman Rank-Order Correlation. We determined the width of the 95% confidence interval for the core mass at the first thermal pulse, stellar age, central temperature, density and electron fraction, and core mass composition. We also explored the sensitivity of the initial-to-final mass relation to experimental uncertainties in the hydrogen and helium reaction rates.

As another example, in Farmer et al 2015 we explored carbon burning in Super-Asymptotic Giant Branch (SAGB) stars, which are stars that straddle the boundary between those whose final fate is a white dwarf and those whose final fate is a neutron star or black hole. The location of carbon ignition and quenching location of the flame (if any), were studied as a function of the initial mass, rotation rate, and mixing parameters. We found rotation to be a minor factor, while overshoot mixing is a major factor. For zero overshoot, models with $\approx$ 8.9–11 $M_{\odot}$ showed off-center carbon ignition. For canonical amounts of exponential overshooting, the off-center carbon ignition range shifted to $\approx$ 7.2–8.8 $M_{\odot}$. Only systems with mass $\approx$ 7.2-8.0 $M_{\odot}$ show carbon burning is quenched a significant distance from the center. These results suggested a careful assessment of modeling approximations on recent claims of producing "hybrid C/O/Ne" white dwarfs.

Lecoanet et al (2106) followed up by stydying these SAGB convectively-bounded carbon flames with idiealized 3D simulations. These simulations allowed measurement of the enhanced mixing due to convective overshoot, which would mix ash into the fuel and quench the flame. The location where the turbulent diffusivity is of order the thermal diffusivity is well outside the region of peak buoyancy frequency that MESA models show must be mixed in order to stall the flame. Moreover, this height shifts away from the flame front as either the Rayleigh number or Lewis number increase towards more realistic stellar values. The lack of mixing by convection is due to a simple physical principle: convective plumes must overcome a huge buoyancy barrier to reach the flame. We concluded that convection provides insufficient mixing to disrupt a carbon flame and that "hybrid C/O/Ne' white dwarfs are unlikely to be a typical product of stellar evolution.

Farmer et al 2016 broke new ground by exploring the variation in single star 15-30 $M_{\odot}$, non-rotating, solar metallicity, pre-supernova MESA models due to changes in the number of isotopes in a fully-coupled nuclear reaction network and mass resolution. We quantitatively detail numerous physical properties with and without mass losss. Up to carbon burning we generally find mass resolution has a larger impact on the variations than the number of isotopes, while the number of isotopes plays a more significant role in determining the span of the variations for neon, oxygen and silicon burning. We find a minimum mass resolution of $\approx$0.01 $M_\odot$ is necessary to achieve convergence in the helium core mass at the $\approx$5% level. At the onset of core-collapse we find $\approx$30% variations in the central electron fraction and mass locations of the main nuclear burning shells, a minimum of $\approx$127 isotopes is needed to attain convergence of these values at the $\approx$10% level.

In Fields et al 2018 we explored properties of core-collapse supernova progenitors with respect to the composite uncertainties in the thermonuclear reaction rates by coupling the reaction rate probability density functions provided by the STARLIB reaction rate library with MESA stellar models. We evolve 1000 15 $M_\odot$ models from the pre main-sequence to core O-depletion at solar and subsolar metallicities for a total of 2000 Monte Carlo stellar models. For each stellar model, we independently and simultaneously sample 665 thermonuclear reaction rates and use them in a MESA in situ reaction network that follows 127 isotopes from ^{1}H to ^{64}Zn. With this framework we survey the core mass, burning lifetime, composition, and structural properties at five different evolutionary epochs. At each epoch we measure the probability distribution function of the variations of each property and calculate Spearman Rank-Order Correlation coefficients for each sampled reaction rate to identify which reaction rate has the largest impact on the variations on each property. We find that uncertainties in ^{14}N$(p,\gamma)^{15}$O, triple-α, ^{12}C$(\alpha,\gamma)^{16}$O, ^{12}C(^{12}C,p)^{23}Na, ^{12}C(^{16}O,p)^{27}Al, ^{16}O(^{16}O,n)^{31}S, ^{16}O(^{16}O,p)^{31}P, and ^{16}O(^{16}O,α)^{28}Si reaction rates dominate the variations of the properties surveyed. We find that variations induced by uncertainties in nuclear reaction rates grow with each passing phase of evolution, and at core H-, He-depletion are of comparable magnitude to the variations induced by choices of mass resolution and network resolution. However, at core C-, Ne-, and O-depletion, the reaction rate uncertainties can dominate the variation causing uncertainty in various properties of the stellar model in the evolution towards iron core-collapse.

Most of my immediate attention in 2018 will be spent finishing up a tome with my ASU colleagure Rogier Windhorst on the observability of individual Population III stars and their stellar-mass black hole accretion disks through cluster caustic transits.

In this work we summarize panchromatic Extragalactic Background Light data to place upper limits on the integrated near-infrared surface brightness that may come from Population III stars and possible accretion disks around their stellar-mass black holes in the epoch of First Light, broadly taken from z$\simeq$7–17. We outline the physical properties of zero metallicity Population III stars from MESA stellar evolution models through helium-depletion and of BH accretion disks at z$\gtrsim$7. We assume that second-generation non-zero metallicity stars can form at higher multiplicity, so that black hole accretion disks may be fed by Roche-lobe overflow from lower-mass companions. We use these near-infrared surface brightness constraints to calculate the number of caustic transits behind lensing clusters that the James Webb Space Telescope and the next generation ground-based telescopes may observe for both Population III stars and their black hole accretion disks.

Supernova - White Dwarf and Massive Stars

Within the single-degenerate paradigm, my colleagues and I have explored propagation of nuclear flames; carbon detonations in 2D and 3D; metallicity effects on variations in the peak luminosity; carbon ignition conditions; how the neutron-rich isotope 22Ne changes the speed of laminar flames; changes in the electron fraction during the simmering phase; changes in ^{56}Ni from the expansion phase and ^{22}Ne; the effects of the deflagration to detonation transition density on the production of ^{56}Ni; correlations between the peak brightness and the age of the progenitor stellar population; metallicity effects on silicon group elements ejected; and most recently potential spectroscopic signatures of the metallicity of the progenitor.

I'm pleased that my forays into merging and colliding white dwarfs with my students and colleagues helped bring about the present day resurgence in the double-degenerate paradigm for Type Ia supernova. This body of research collisions between two white dwarfs; white dwarf binary mergers; and combining population synthesis and explosion models with radiation-hydrodynamics light-curve models.

For example, in Martínez-Rodríguez et al 2017, we report on a new method to determine ejecta neutronization using Ca and S lines in the X-ray spectra of Type Ia supernova remnants. Applying this method to *Suzaku* data of Tycho, Kepler, 3C 397 and G337.2-0.7 in the Milky Way, and N103B in the Large Magellanic Cloud, we find that the neutronization of the ejecta in N103B is comparable to that of Tycho and Kepler, which suggests that progenitor metallicity is not the only source of neutronization in Type Ia supernova. We then use a grid of explosion models to infer the metallicities of the stellar progenitors of our supernova remnants. For 3C 397, G337.2-0.7, and N103B we find that progenitor metallicity may not be the only source of neutronization. Although the relationship between ejecta neutronization and progenitor metallicity is subject to uncertainties stemming from the ^{12}C+^{16}O reaction rate, our main results are not sensitive to these details.

Near future research on Type Ia supernova includes is an investigation of ^{55}Mn yields from double-degenerate models. If ^{55}Mn is underproduced relative to solar in even the highest mass double white dwarf collisions, then there cannot be a single degenerate channel accounting for the majority of Type Ia supernova. If collisions produce significant ^{55}Mn, then this deflects argumenst being made in the community for the necessity of a single degenerate channel. I am gearing up to explore double white dwarf collisions with a more detailed nuclear reaction network than the simple α-chain reaction network used in *all* previous studies, including our own.

In 2015 my colleagues Sean Couch, Manos Chatzopoulos, Dave Arnett and I pioneered the first 3D simulation of the final minutes of iron core growth in a massive star, up to and including the point of core gravitational instability and collapse. We capture the development of strong convection driven by violent Si burning in the shell surrounding the iron core. This convective burning builds the iron core to its critical mass and collapse ensues, driven by electron capture and photodisintegration. The non-spherical structure and motion generated by 3D convection is substantial at the point of collapse, with convective speeds of several hundreds of km s^{-1}. We examine the impact of such physically-realistic 3D initial conditions on the core-collapse supernova mechanism using 3D simulations including multispecies neutrino leakage and find that the enhanced post-shock turbulence resulting from 3D progenitor structure aids successful explosions. We concluded that non-spherical progenitor structure should not be ignored, and should have a significant and favorable impact on the likelihood for neutrino-driven explosions. In order to make simulating the 3D collapse of an iron core feasible, we were forced to make approximations to the nuclear network making this effort only a first step toward accurate, self-consistent 3D stellar evolution models of the end states of massive stars.

Introductory astronomy texts stress that massive stars are the element factories that produce most of the periodic table of the elements. Yet, the most advanced 3D massive star explosion simulations to date rely on at most 21 isotopes, and usually more like 13 isotopes, to predict the nuclear energy generation rate and explosive nucleosynthesis. I emphasize that explosive nucleosynthesis in massive stars has essentially only ever been done in 1D with artificial explosions. The yawning gap between element factories and 13 isotopes in 3D simulations is due, in part, by choosing to invest the ever increasing compute capabilities into spatial resolution rather than the number of isotopes. In a new project with Sean Couch and Carl Fields we will take the world-leading step of providing the community with a more encompassing and detailed view of massive star element factories.

We will use a set of well developed computational tools in concert with fundamental theoretical considerations and strong connections with observations to address how

- non-spherical 3D pre-supernova massive stars evolve over their final few minutes
- aspherical progenitors impact the nucleosynthesis from 3D explosion simulations
- 3D explosive nucleosynthesis compares to 1D explosive yields
- 3D explosive structures and yields compare to young supernova remnants

Massive star models will be evolved with MESA from the pre-main sequence to the onset of shell silicon-burning. The 1D profiles will then be mapped into the 3D FLASH simulation tool. We will then carry out the first study of the 3D evolution to core-collapse collapse using a nuclear reaction network large enough ($\simeq$ 100 isotopes) to directly simulate silicon shell burning and iron core neutronization. These presupernova structures will then be exploded in 3D with FLASH and in 1D with MESA. The stellar structure profiles and explosive nucleosynthesis of the 3D simulations and 1D models will be compared with each other, and to key radionuclide and stable element diagnostics observed in supernova remnants such as Cas A, SN 1987A, Puppis A, 3C 58, and the Crab Nebula. I anticipate this super exciting new research effort will reach fruition in 2019.

This is not a complete description of my research activities, but it is enough for now.

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