Research Statement

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My research activities center around

- Stellar Evolution, accented with 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 specific examples from this portfolio of research activities that are in the recent past, current, or coming to fruition in the near future.

Software Infrastructure - MESA

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, and is designed to accommodate present and future multi-core and multi-thread architectures in mind. 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. MESA's domain of applicability continues to grow, with recent extensions enabling users to model oscillations, rotation, and explosions. Recent innovations allow for user plugins and bit-for-bit consistent results across all supported platforms.

I have been with the MESA project since inception (~2004) and I am one of the principal drivers alongside Bill Paxton and Lars Bildsten. The MESA project was publicly launched in 2011 and since that time 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 prototype cloud resource for education, MESA-Web. See `http://mesa.sourceforge.net`.

The three MESA instrument papers, which describe major new software and science capabilities, have been cited ≃1000 times and has a current citation rate of ≃300/year (all citation data from SAO/NASA ADS). The papers that cite MESA have generated ≃ 10,835 citations, for a radius-of-influence multiplicative factor of ≃ 10, which suggests MESA helps generate citations to papers the astrophysics community values. More specifically, MESA I [Paxton et al. 2011] is one the 15 most cited astronomy/astrophysics papers published in 2011. MESA II [Paxton et al. 2013] 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 [Paxton et al. 2015] is one of the 25 most cited astronomy/astrophysics papers published in 2015. 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 additional capabilities to enable new science motivated by observational breakthroughs include supernova light curves, co-process nuclear burning, the red edge of instability strips and automatic instability strip delineation, flame propagation, and MESA-Web. MESA IV (2017) is also in active preparation.

Software Infrastructure - FLASH

The FLASH solve 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 , Multimaterial 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., and a built-in unit test framework can be run nightly on multiple platforms for verification. See `http://flash.uchicago.edu`.

The first bare-knuckles version of FLASH (version 0.0) was created by Kevin Olson (he had the adaptive mesh and his hands on the keyboard), Bruce Fryxell (he had the hydro), and me (had the local physics) in late 1998 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 (had the gravity) and Mike Zingale (had the viz and all-purpose skills) added critical capabilities. Jonathan Dursi and Alan Calder made key contributions and gave the original development team its critical mass for Fryxell et al. [2000].

FLASH was allowed to fork, meaning there are multiple customized version of FLASH in the wild - Bob's FLASH, Sally's FLASH, etc. Near future additional capabilities to enable new massive star supernova science include a port of my TORCH software instrument – a general nuclear reaction network solver – into Sean Couch's FLASH framework, possibly with GPU accelerators.

Nuclear Reactions - STARLIB

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.

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.

My colleagues Christian Iliadis, Art Champange, Alain Coc, Anne Sallaska and I are continuously updating STARLIB (see `http://starlib.physics.unc.edu`), a next-generation compilation of thermonuclear reaction rates, that provides the necessary probability density functions [Sallaska et al. 2013]. One approach we pioneered is the use of Monte Carlo based reaction rates. 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. The Monte Carlo-based method of estimating reaction rates is limited, in its present formulation , to nuclear reactions that are dominated by resonant contributions to the total rate.

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. We are actively developing a framework that incorporates robust parameter estimation, systematic effects, and non-Gaussian uncertainties in a consistent manner.

We are initially applying this new approach to the d(p,γ)^{3}He, ^{3}He(^{3}He,2p)^{4}He, and ^{3}He(α,γ)^{7}Be reactions, important for deuterium burning, solar neutrinos, and big bang nucleosynthesis. These are the first Bayesian informed nuclear reaction rates, will be included in the next version of STARLIB, and I am anticipating publication in late 2016.

Stellar Evolution - White Dwarfs

My undergraduate Carl Fields (now a grad student at MSU with Sean Couch), postdocs Rob Farmer and Ilka Petterman, colleague Christian Iliadis, and I recently 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 [Fields et al. 2016]. 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. Relative to the arithmetic mean value, we found 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 fractions of ^{12}C, ^{16}O, and ^{22}Ne. Uncertainties in the experimental ^{12}C$(\alpha,\gamma)^{16}$O, triple-α, and ^{14}N$(p,\gamma)^{15}$O reaction rates dominated these variations. We also considered a grid of 1 to 6 $M_\odot$ models evolved from the pre main-sequence to the final white dwarf to probe the sensitivity of the initial-final mass relation to experimental uncertainties in the hydrogen and helium reaction rates.

By early 2017 I anticipate completing a new investigation that uses the same Monte Carlo full stellar evolution model framework applied to Pop III and Pop I massive star models across representative masses.

Stellar Evolution - Super AGB Stars

Super-asymptotic giant branch (SAGB) stars are characterized by the development of a degenerate carbon-oxygen (CO) core and the subsequent ignition of off-center carbon fusion within it. Stellar evolution calculations show that this occurs in stars that have zero-age main sequence (ZAMS) masses ≈ 7-11 $M_\odot$, with this mass range depending on the metallicity and the efficiency of mixing at convective boundaries. Carbon ignition initially occurs as an off-center flash, but after one or more of these flashes, a self-sustaining carbon-burning front can develop. This "flame" propagates towards the center of the star extremely sub-sonically, as heat from the burning front is conducted inward. The heat from the burning also drives a convective zone above the burning front, and in the quasi-steady-state, the energy released by carbon fusion is balanced by energy losses via neutrino cooling in this convective zone. As the carbon-burning flame propagates to the center, it leaves behind oxygen-neon (ONe) ashes. This process creates the core that will become a massive ONe WD or collapse to a neutron star, powering an electron-capture supernova.

However, the presence of additional mixing near the flame can lead to its disruption, preventing carbon burning from reaching the center. There are at least two physical processes that may play a role in this region: (1) mixing driven by the thermohaline-unstable configuration of the hot ONe ash on top of the cooler CO fuel and (2) mixing driven by the presence of a convective zone above the flame via convective overshoot. With a thermohaline diffusion coefficient informed by multi-dimensional hydrodynamics simulations, several groups have recently concluded that thermohaline mixing was not sufficient to disrupt the flame. However, they did find that sufficient convective boundary mixing – using a model of exponential overshooting – disrupted the flame, preventing carbon burning from reaching the center. This led to the production of "hybrid C/O/Ne" WDs, in which a CO core is overlaid by an ONe mantle. Several groups have begun to model the explosions that would originate from objects with this configuration.

My postdoc Rob Farmer, (then) undergraduate Carl Fields and I recently drove an exploration of the properties of carbon burning in SAGB stars with ≃ 3000 MESA models [Farmer et al. 2015]. The location of first carbon ignition, quenching location of the flame, angular frequency of the rotating carbon core, and carbon core mass were studied as a function of the ZAMS mass, initial rotation rate, and mixing parameters such as convective overshoot, semiconvection, thermohaline and angular momentum transport. We found carbon burning in SAGB models are not a strong function of the initial rotation profile, but indeed are a sensitive function of the overshoot parameter. We analytically derived an approximate ignition density, $\rho_{ign} \approx 2.1 \times 10^6$ g cm^{-3}, to predict the location of first carbon ignition in models that ignite carbon off-center. For zero overshoot, $f_{\rm ov}$=0.0, our models in the ZAMS mass range ≈ 8.9–11 $M_\odot$ showed off-center carbon ignition. For canonical amounts of exponential overshooting, $f_{\rm ov}$=0.016, the off-center carbon ignition range shifted to ≈ 7.2–8.8 $M_\odot$. Only systems with $f_{\rm ov} \geq 0.01$ and ZAMS mass ≈ 7.2-8.0 $M_\odot$ show carbon burning is quenched a significant distance from the center. These results suggested a careful assessment of overshoot modeling approximations on claims of producing "hybrid C/O/Ne" WDs.

My Berkeley colleagues Daniel Lecoanet, Josiah Schwab, Eliot Quataert, and I are studying 3D simulations of an idealized model of a convectively-bounded carbon flame. These simulations allow us to measure the enhanced mixing due to convective overshoot, and to determine if the thermal diffusivity is of order the turbulent diffusivity, which would mix ash into the fuel and quench the flame. The simulations are in the Boussinesq approximation with a Brunt-Väisälä frequency profile motivated by the above [Farmer et al. 2015] MESA models. In all of our preliminary simulations, the height at which the turbulent diffusivity is of order the thermal diffusivity is well outside the region near the peak of the buoyancy frequency that MESA simulations 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 is due to a simple physical principle: convective plumes must overcome a huge buoyancy barrier to reach the flame. As a result, we are tentatively concluding that convection provides insufficient mixing to disrupt a carbon flame and that "hybrid C/O/Ne" WDs are unlikely to be a typical product of stellar evolution. I anticipate this new research to reach fruition by early 2017.

White Dwarf Supernova

Within the single-degenerate paradigm, my colleagues and I have explored propagation of nuclear flames (reaction-diffusion tool, Stan Woosley, 1994); carbon detonations in 2D and 3D (FLASH, Mike Zingale); metallicity effects on variations in the peak luminosity (pen and paper, Ed Brown, 2003); ignition conditions (FLASH, Jonathan Dursi, 2006); how the neutron-rich isotope 22Ne changes the speed of laminar flames (reaction network, David Chamulak, Ed Brown, 2007); changes in the electron fraction during the simmering phase (reaction network, David Chamulak, Ed Brown, 2008); changes in ^{56}Ni from the expansion phase and ^{22}Ne (FLASH, Dean Townsley, Alan Calder, 2009); the effects of the deflagration to detonation transition density on the production of ^{56}Ni (FLASH; Aaron Jackson, Alan Calder, 2010); correlations between the peak brightness and the age of the progenitor stellar population (FLASH, Brendan Krueger, Aaron Jackson, 2012); metallicity effects silicon group elements ejected (pen and paper, Soma De, 2014); and most recently potential spectroscopic signatures of the metallicity of the progenitor (radiative transfer, Miles Broxton, Daan van Rossum, 2016).

In the near future, I anticipate early 2017, my colleagues Pranav Dave, Rahul Kashyap, Robert Fisher and I will complete a new study within the single-degenerate paradigm on a specific object. Specifically, Suzaku X-ray spectra of SNR 3C 397 indicate enhanced stable iron-group element abundances of Ni, Mn, Cr, and Fe. We seek to address key questions about the progenitor of 3C 397 by computing nucleosynthetic yields from a suite of FLASH models. Varying the progenitor white dwarf internal structure, composition, ignition and explosion mechanisms, we are searching for the best match to the observed iron-peak elements of 3C 397 through the central density, initial carbon abundance in offset ignition models. Our preliminary results favor higher densities and lower carbon abundances that are commonly considered in the literature, yet still produce enough ^{56}Ni to be consistent with a Branch normal supernova Type Ia. In contrast to 1D models of 3C 397 that suggest a large super-solar metallicity for the white dwarf progenitor, we appear to be finding the best agreement to the observations in our 2D models with a sub-solar metallicity progenitor.

I'm pleased that my early 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 (SNSPH, Cody Raskin, Evan Scannapieco, 2009, 2010); a comprehensive survey of white dwarf binary mergers (SNSPH, Cody Raskin, Evan Scannapieco, 2010); combining population synthesis and explosion models with radiation-hydrodynamics light-curve models (StarTrack, Chris Fryer, Ashley Ruiter, 2010); and head-on collisions (FLASH, Themis Athanassiadou, Wendy Hawley, 2012) lays the groundwork for my near future investigations.

One example of that near future research is the investigation of ^{55}Mn yields from double-degenerate models. For if ^{55}Mn is underproduced relative to solar in even the the highest mass double white dwarf collisions, then there cannot be a single degenerate channel accounting for the majority of Type Ia supernova. If instead white dwarf collisions produce significant ^{55}Mn, then this deflects argument being made in the community for the necessity of a single degenerate channel. I am presently gearing up with my former student and now colleague Cody Raskin 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.

Massive Star Supernova

My colleagues Sean Couch, Manos Chatzopoulos, Dave Arnett and I recently presented 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 [Couch et al. 2015]. We captured the development of strong convection driven by violent silicon burning in the shell surrounding the iron core with FLASH simulations that used Cartesian coordinates coupled with adaptive mesh refinement in one octant of the full 3D sphere. We concentrated on the final three minutes in a 15 $M_\odot$ star evolved initially in 1D with MESA.This timescale captured ~8 eddy turnover times of the convection in the silicon region and the synthesis of 0.2 $M_\odot$ of iron. We found 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 kilometers per second and the largest eddies being roughly the full width of the silicon shell. We then examined the impact of such physically-realistic 3D initial conditions on the core-collapse supernova mechanism using 3D FLASH Newtonian simulations including a multispecies neutrino leakage scheme that includes charged current heating and pre-bounce deleptonization. We found the enhanced post-shock turbulence resulting from 3D progenitor structure aids successful explosions – primarily due to the attendant turbulent pressures that aid shock expansion. 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. We were forced to make approximations to the nuclear network making this pioneering effort only a first step toward accurate, self-consistent 3D stellar evolution models of the end states of massive stars.

Following up an aspect related to the effort above, my colleagues Manos Chatzopoulos, Sean Couch, Dave Arnett and I studied the effects of rotation on convective carbon, oxygen, and silicon shell burning during the late stages of evolution in a 20 $M_\odot$ star [Chatzopoulos et al. 2016]. We constructed MESA models both with no rotation and with an initial rigid rotation of 50% of critical. At different points during the evolution, we mapped the 1D MESA models into 2D FLASH simulations and followed the multidimensional evolution for many convective turnover times until a quasi-steady state wss reached. We characterized the strength and scale of convective motions via decomposition of the momentum density into vector spherical harmonics. We found that rotation influences the total power in solenoidal modes, with a slightly larger impact for carbon and oxygen shell burning than for silicon shell burning. We also found that including $\sim 50\%$ of critical rotation in the MESA models has a significant impact on the character of multidimensional convection, but adding only modest amounts of rotation to a MESA mode lhad little impact on the character of resulting convection. Since the spatial scale and strength of convection present at the point of core collapse directly influence the supernova mechanism, our results suggested that rotation could play an important role in setting the stage for non-spherical progenitor structure and the subsequent massive stellar explosions.

Intrigued by the MESA + FLASH results above, my postdoc Rob Farmer and I are currently exploring the variation in single star 15 –30 $M_\odot$ pre-supernova MESA models due to changes in the number of isotopes in a fully-coupled nuclear reaction network and adjustments in the mass resolution. Within this two-dimensional plane we plan to quantitatively detail the range of core masses at various stages of evolution, mass locations of the main nuclear burning shells, electron fraction profiles, mass fraction profiles, burning lifetimes, stellar lifetimes, and compactness parameter at core-collapse for models with and without mass loss. Up to carbon burning we generally find in our preliminary models that 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 are finding that the choice of mass resolution dominates the variations in the structure of the intermediate convection zone and secondary convection zone during core and shell hydrogen burning respectively, where we are finding a minimum mass resolution of ≈ 0.01 $M_\odot$ is necessary to achieve convergence in the helium core mass at the $\approx 5\%$ level. On the other hand, at the onset of core-collapse the tentative models suggest $\approx 30\%$ variations in the central electron fraction and mass locations of the main nuclear burning shells, a minimum of ≈ 127 isotopes is needed to attain convergence of these values at the $\approx 10\%$ level. I anticipate this new research effort to reach fruition by early 2017.

In October 2016 I agreed/contracted with Princeton University Press to produce a pragmatic graduate level opus on stellar evolution with my co-authors Rich Townsend, Lars Bildsten, and Bill Paxton I suspect parts of this forthcoming monograph will be influenced by some of the research described above.

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

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