3-D SIMULATIONS OF I-PROCESS NUCLEOSYNTHESIS IN THE EARLY UNIVERSE

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EXECUTIVE SUMMARY

We are exploiting the scale and speed of Blue Waters to enable 3-D simulations of brief events in the advanced evolution of stars that can have profound impacts upon their production of heavy elements. We are focusing on hydrogen ingestion flash events, because these have been identified as potential sites for the origin of observed, strongly anomalous abundance signatures in stars that formed in the early universe. In this second year of our three-year project, we have simulated H-ingestion in a very low metallicity giant star formed in the early universe. Our results reveal an unstable, global oscillatory burning of the ingested hydrogen which gives rise to quite different behavior than was anticipated from the earlier 1-D modeling of this hydrogen-ingestion flash phenomenon. We are also building simplified models of this behavior and are restructuring our PPMstar simulation code to accurately handle more challenging cases such as nuclear burning shell mergers in massive stars.

INTRODUCTION

We are interested in understanding the origin of the elements in the developing universe. The elements heavier than hydrogen and helium were manufactured within stars and later expelled into the interstellar gas to become incorporated in later generations of stars and planets. The first generations of stars played a particularly important role. The late stages of evolution of these stars can be strongly affected by hydrogen ingestion events. These events occur, for example, when a convection zone above a helium burning shell in the asymptotic giant branch (AGB) stage of evolution of such stars reaches up to unprocessed hydrogen-helium gas above it. This gas is lighter than the helium and carbon mixture of such a helium shell flash convection zone, and therefore is more buoyant. It resists being entrained into the gas of the convection zone, yet can nevertheless be dragged downward as the result of a process we call convective boundary mixing. In order to understand the H-ingestion flashes, as well as the evolution of many other types of stars, such as the pre-supernova evolution of stars that eventually explode, it is critically important to be able to quantitatively simulate this convective boundary mixing. Neutrons produced in H-ingestion flash events are captured by trace concentrations of heavy elements in the gas to build up an entire series of progressively heavier nuclei. This material can ultimately be expelled from the star along with its outer envelope as it forms a planetary nebula.

METHODS & RESULTS

Despite the relative brevity of these H-ingestion flash events in the lives of stars, simulating this entire process, even on Blue Waters, is a challenge. In the top two images in the figure, we see results for a very low metallicity AGB star of the early universe simulated on a grid of 3.6 billion cells for over 9 million time steps on 0.44 million processor cores of Blue Waters running at about 0.41 Pflop/s. The simulated time interval is nearly 2 days in the life of the star, but in order to follow this star through the flash we increased the driving helium burning luminosity by a factor of about 30 to more quickly traverse a long, slow initial ingestion period leading up to the flash itself. In the top-left image, rapid burning of locally ingested hydrogen-rich gas has

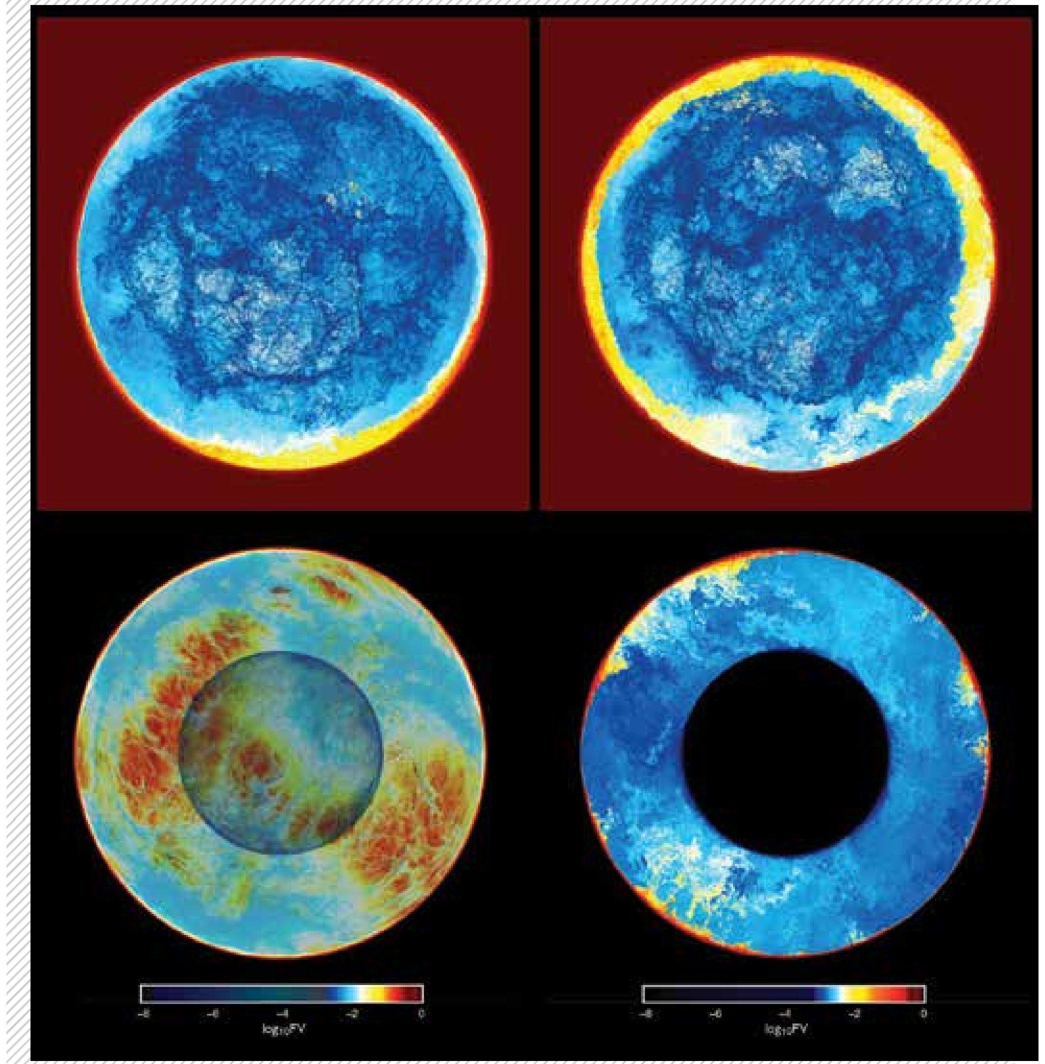

FIGURE 1: In the top 2 images the process of entrainment of hydrogen-rich gas into the helium shell flash convection zone of a very low metallicity star and the development of the Global Oscillation of Shell Hydrogen ingestion (GOSH) is shown. The front half of the star has been cut away, and the central degenerate carbon-oxygen core, which will ultimately become a white dwarf star, has been made transparent. Only mixtures of the helium and carbon gas of the convection zone with entrained hydrogen-helium gas from above it are made visible in this volume rendering. Concentrations of entrained gas from large to small range in color from red (1.6x10-2) to yellow (1x10-3), white (1.6x10-4), aqua (2.5x10-5), and finally dark blue (3x10-6). In the bottom pair of images, we see a similar display, but with a different mapping of concentration to color that is shown, for a study of entrainment of gas from above the convection zone caused by oxygen burning in a massive star (see Jones et al. 2016).

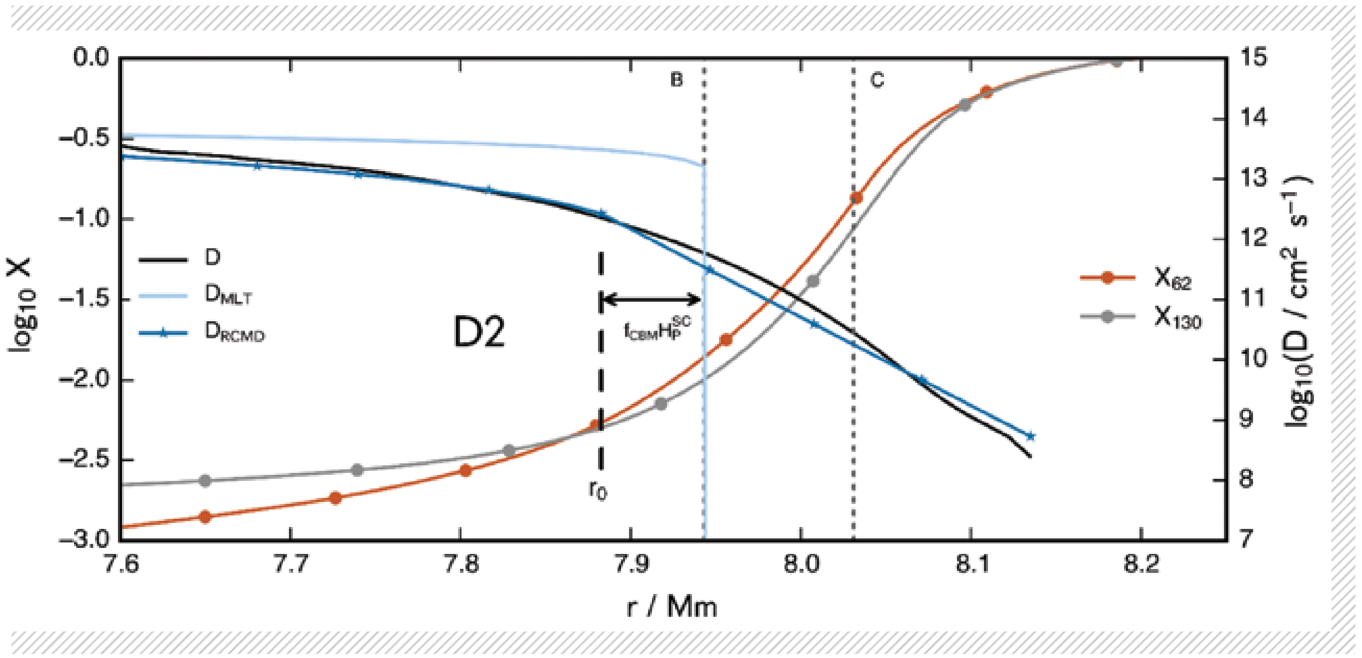

FIGURE 2: An analysis of this oxygen shell entrainment simulation in terms of 1-D stellar evolution code requirements for approximating the process in 1D. The solid black line shows an effective diffusion coefficient that produces the spherically averaged result of the 3-D simulation, the light blue line gives the diffusion coefficient as derived from standard mixing length theory, and the darker blue line gives the result for a revised 1-D model that our work recommends.

created a high pressure at the bottom right of this hemisphere of the star that is driving pressure waves outward around the star, peeling off a layer of newly entrained hydrogen-rich material as they go. About 6 minutes later, in the top-right image, these waves have reached all the way around the star, where burning of the newly entrained material will produce a new pressure wave racing back in the other direction, setting off a growing global oscillation of shell hydrogen ingestion, (GOSH). Working with a case that evolves more rapidly, a study of the oxygen burning shell in a massive star, shown in the middle of the figure, we find that a simplified model of convective mixing previously used in 1-D stellar evolution calculations by our collaborator, Falk Herwig, produces a good representation of the 1-D averaged behavior if we use the correct coefficients for the model, as shown at the bottom of the figure. In the coming year we will experiment with a 1D-3D simulation approach in which we use 3-D simulations performed at fairly widely spaced time intervals to determine the proper model coefficients that enable a 1-D stellar evolution approach to carry the simulation to the threshold of truly 3-D behavior, where we must proceed without the help of the 1-D model.

Our team is now working intensely to restructure our code completely, so that it can serve us well for the next decade. The design of the new code explicitly counts upon the very large numbers of simultaneous threads that must execute on the nodes of modern machines. These are exploited in a new approach to dynamic load balancing both on the node and over the machine interconnect. Our stellar hydrodynamics problems do not require many grid refinement levels, and therefore we are able to introduce simplifications into our design for just three such levels that will enable our runs to scale with high efficiency to over 10,000 nodes, even on machines whose nodes support many more simultaneous threads than the present Blue Waters.

WHY BLUE WATERS

3-D simulations like the ones shown here, made possible by the sustained petaflops computing capability of Blue Waters, allow us to explore and understand phases of stellar evolution that are very long in duration compared to a stellar explosion, but are nevertheless very short compared to those behaviors which are well approximated by 1-D stellar evolution codes. With the insights provided by these simulations, we are building new 1-D models and 1D-3D computational techniques that will allow us to follow stars through these stages of their lives with greater confidence.

NEXT GENERATION WORK

One challenging goal of our present code developments is to enable the accurate simulation at affordable cost of the merger of two nuclear burning shells initially separated by a convection zone above which is a thin stable layer before the next burning shell begins. On a future Track-1 system, we would like to follow a massive star through multiple hydrogen ingestion and shell merger events to the point just before its core collapses and a supernova explosion results.

PUBLICATIONS AND DATA SETS

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