SIMULATION OF TURBULENT STELLAR HYDRODYNAMICS

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SCIENTIFIC GOALS

We are interested in understanding the origin of the elements in the developing universe. 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. The products of nucleosynthesis are later expelled along with the outer envelopes of these stars, contributing to the gradual build-up of the chemical inventory that we find now in our solar system.

The H-ingestion events occur, for example, when a convection zone above a helium-burning shell reaches unprocessed hydrogen-helium gas above it in the asymptotic giant branch (AGB) stage of evolution of such stars. 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 critical to be able to quantitatively simulate convective boundary mixing between the hydrogen-helium gas and the helium-carbon mixture below it.

ACCOMPLISHMENTS TO DATE

The simulation of this process, if it is to yield accurate estimates of the elements that are produced, must be carried out in 3D. The entrainment of hydrogen-rich gas at the top of the convection zone is the result of complex, nonlinear shear instabilities that act against the stable stratification of the more buoyant hydrogen-rich gas. To accurately simulate this process we must resolve these unstable waves and also the thin layer in which the composition of the gas changes from the helium-carbon mixture of the convection zone to the hydrogen-helium mixture above. We require a fine grid and a numerical method capable of producing accurate results for modes that are only several cells in wavelength.

When the growing convection zone encounters the hydrogen-rich layers, it is deep in the sense that the ratio of the radii of its top and bottom boundaries is significant (i.e. about two or more). The depth of the convection zone implies that the convection cells that develop within it will be very large, so that only a few of the largest convection cells will fill the entire convection zone volume. Thus, we also require that our problem domain contain the entire convection zone, not just a small sector of it. Finally, we must carry the simulation through many turn-over times of the largest eddies in the convection zone so that entrainment of hydrogen-rich gas can, through burning of ingested hydrogen, react back on the flow to accelerate entrainment. This process is slow because the initial entrainment is small.

The above challenges to computation are met in this work by the combination of our PPMstar simulation code and the Blue Waters system. Our studies show that grids of $1{,}536^3$ cells are sufficient to deliver accurate simulation of the entrainment of hydrogen-rich gas at the top of the helium-shell flash-convection zone, using the piecewise-parabolic method (PPM) gas dynamics method and the piecewise-parabolic Boltzmann (PPB) advection scheme to follow the multi-fluid volume fraction. The result of this work-in-progress is that we have discovered a previously unknown global oscillation of shell hydrogen ingestion (GOSH). The GOSH is shown in Fig. 1. It causes the hydrogen ingestion rate to shoot up by as much as two orders of magnitude, with considerable impact on the evolutionary path of the star and on the synthesis of heavy nuclei that can be later expelled into the interstellar medium.

HOW BLUE WATERS PROJECT STAFF HELPED

Blue Waters staff assisted with improvements to the storage and I/O methods including reducing the number of writers and optimizing data location. They also adjusted the system resource manager to enable quick turn-around for large jobs for simulation and visualization and enabled generation of visualizations on the GPU nodes from data residing on the attached disk file system. This sped up the visual analysis of the computed results by nearly two orders of magnitude over previous practice.

WHY THE RESEARCH MATTERS

Recent astronomical observations have been revealing more and more fascinating information about the early era in the universe when stars and galaxies formed and began to produce the structure that we now see. Computer simulations of the development due to gravitational forces of such structure on very large scales are rapidly increasing our understanding of how the structure formed and evolved. The enrichment of the material in galaxies with the heavy elements that make possible planets like our own, as well as life, cannot be understood without the ability to simulate the processes leading to heavy element nucleosynthesis. These processes occur deep within stars and are mostly hidden from our view. The chains of events connecting these processes deep inside stars and their observable consequences are complex and can demand a fully 3D treatment in order to be properly simulated and understood. Our research focuses on brief but important stages of stellar evolution that 1D simulations indicate demand a 3D treatment. By studying these brief stages, we hope to improve our understanding of the chemical evolution of galaxies that creates the conditions that allow life to develop.

WHY BLUE WATERS

The hydrogen ingestion events that can affect nucleosynthesis in a star are brief, but not brief enough to be handled easily on a Track-2-class machine. We must simulate many turn-over times of convection cells whose size is a good fraction of the entire convection zone in order to accurately compute the hydrogen entrainment in the slow approach to the violent hydrogen combustion of the GOSH (see Fig. 1). The simulation in Fig. 1 illustrates why we need the power of Blue Waters for this research. The simulation shown there ran at 0.42 Pflop/s (10% to 11% of the peak 64-bit performance) on 443,232 cores, or about half the machine, for a sustained period of about four days with 26 time-step updates per second. It generated 1,362 data dumps, each consisting of 216 files for each of five variables, with one such dump of 1,080 files every three minutes, representing one minute of time for the simulated star. It would be possible to perform this simulation on a smaller system, but not in nearly so small a time. On Blue Waters, what would be a tremendous calculation extending over months or an entire year on another system took a week. Blue Waters entirely changed our concept of what is practical and what important research it is sensible to undertake.

PRE-PETASCALE PREPARATION

To prepare to take advantage of Blue Waters, we were fortunate to have the experience of designing a version of our code to run on the Cell processors in the Roadrunner machine at Los Alamos. Had we been unable to apply all our

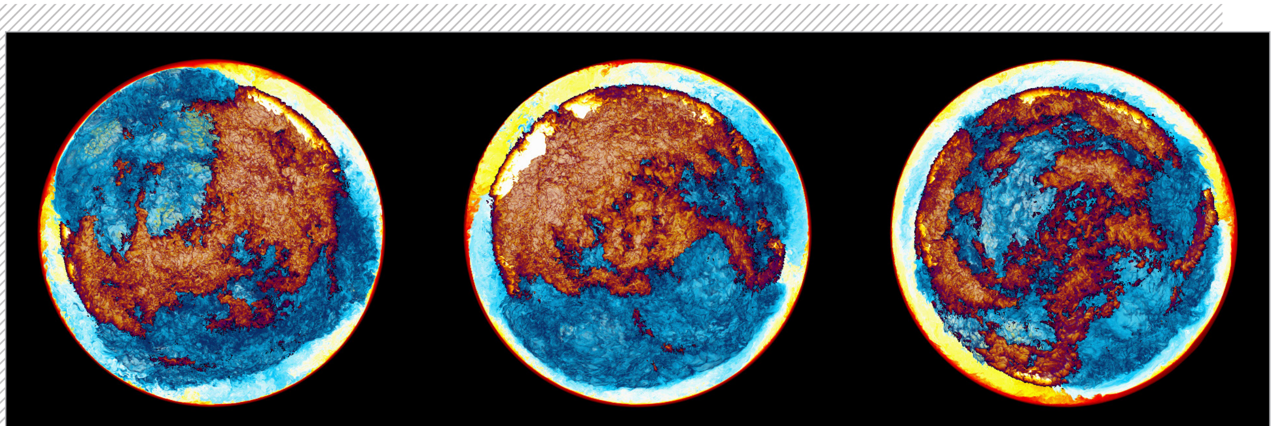

Figure 1. Here we see images from one half oscillation of the global mode for burning ingested hydrogen-rich gas. In each image we see a hemisphere of the central portion of the star in which the carbon-oxygen core and the carbon-helium gas of the convection zone above the helium burning shell have been made transparent. Concentrations of hydrogen ingested into the convection zone above the helium burning shell are visible, from high concentration to low, as red, yellow, white, aqua, and dark blue. The energy generation rate from burning the ingested hydrogen is represented by the red and yellow flame-like regions just inside the shell of higher hydrogen concentration in the upper portion of the convection zone. In the left-most image, we see a band of burning gas driving a wave of hydrogen ingestion toward the upper left side of the star, where in the center image a few minutes later this wave converges to produce a large hydrogen enrichment with rapid burning at its base. This in turn drives a wave of entrainment propagating around the star in the opposite direction, as seen in the right-most image.

lessons in code design from Cell and Roadrunner to other systems, this might not have been a fortunate experience at all. However, all of the extensive changes to our code that we made for Roadrunner—every one of them—carried over pretty much directly to Blue Waters. This was possible because we wrote automated code translator utilities to produce the very low-level code expressions the Cell processor required. After Roadrunner, we found running our codes on Blue Waters to simply be a delight. The code translation software we developed for Roadrunner is also proving very useful to us still. In a project we are just now beginning, we are extending that translation software to accommodate a new technique for generating from a single Fortran expression very high performance code for both Blue Waters' CPU and GPU nodes.

LOOKING FORWARD TO THE NEXT TRACK-1 SYSTEM

Heavy element synthesis in the brief events in stars we are studying, as well as when stars explode, provides insight into the creation of many fundamental elements needed for life, such as carbon and oxygen. The current calculations for hydrogen ingestion flashes such as the one shown in Fig. 1 are challenging because of the need to simulate the entire central region of the star for a significant period of time. Simulations of just one sector of the star miss the global oscillation that develops, and a simulation for a shorter time would miss the enormous increase in the hydrogen ingestion rate at late times in this process. Simulating the nuclear reactions and heavy element synthesis in much greater detail and fidelity and simulating a larger radial volume of the star will reduce the influence of boundary conditions we impose on the simulation while revealing the effects on the star's outer layers. Today, with the Blue Waters system, only a handful of such simulations in a year are feasible. Being able to investigate a wider variety of such events in stars of different masses and metal content is critical to a better understanding of how heavy elements form.

At present, we are simulating the details of unburned fuel ingestion into a single convection zone, its subsequent combustion, and effects of this process. However, in massive stars there can be evolutionary stages when the convection zones above two different nuclear burning shells are separated only by a relatively small amount of material. If ingestion of this material into the convection zone below causes the two burning shells and their convection zones to directly interact, the consequences could be quite unexpected. Such a situation is difficult to investigate at present because the time intervals over which the simulation would need to be carried out are too long. On a future Track-1 machine, one would expect to be able to simulate this sort of very complex and interesting event.

Looking further to the future, we would like to simulate stars under conditions in which their material is not entirely opaque to radiation. Then radiation transport must be simulated. Although this can be done using a number of simplifying assumptions, we anticipate that future Track-1 systems could make first-principles calculations of this sort practical. We would like to represent the radiation as a fluid in a 6D phase space, with the three usual spatial dimensions plus two angle dimensions and an energy dimension. In the last year we have experimented with an adaptation of the highly accurate moment-conserving advection scheme, PPB, which we use now to track different constituents of our fluid, to GPU devices like those in Blue Waters. The PPB method maps well to GPUs; the extra computing power then helps reduce the cost of a simulation in six dimensions. The high accuracy of the method helps also by enabling a very coarse grid of, for example, only 16 or 20 cells in each of the three new dimensions to be used. Such an approach could also prove useful in other problems, such as stellar dynamics of galaxies or in plasma physics applications, where a representation using a continuous fluid in a 6D phase space makes sense. We can try out such a new approach using Blue Waters' present GPU nodes. However, for such calculations to advance beyond the testing stage and, perhaps, one or two initial demonstration calculations, we would need a next-generation Track-1 system.

COMMUNITY IMPACT

In preparation for this project, we wrote automated code translator utilities that we have found to be very versatile and useful. It got us thinking much more deeply about how to write our codes to accommodate modern devices, and it also got us onto a path of development of code translators along with the codes themselves that continues to prove productive and effective. Blue Waters can also allow us to test new approaches to solving fluid problems in six dimensions in preparation for future Track-1 systems.

PUBLICATIONS

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