Large-scale simulations of buoyancy-driven turbulent nuclear burning

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Abstract. An critical uncertainty in modeling thermonuclear supernovae is the degree of enhancement of the burning rate by turbulence during the subsonic burning (deflagration) phase. As turbulent combustion in the laboratory is still an active area of research, this remains a challenging problem. A unique feature of turbulent combustion in supernovae is that the driving of the turbulence arises from the strong buoyancy of the burned material. We discuss the large-scale fully three dimensional studies under way. These studies have the goals of characterizing the essential length scales of flame surface structure and thereby developing specific requirements that models of small-scale structure must meet. We discuss some preliminary results of our study concerning the scale-dependence of flame surface structure.

1. Introduction
A fundamental challenge in our understanding of reactive flows is the process by which turbulence wrinkles a combustive flame front, thereby increasing its surface area and effective flame speed. By determining the amount of matter burnt in the initial deflagration phase, and the amount of pre-expansion in the white dwarf progenitor, the process of turbulent combustion plays a central role in our understanding of the explosion mechanism of Type Ia supernovae.

Models of the deflagration phase of Type Ia supernovae typically begin with the ignition of a flame bubble near the center of the progenitor white dwarf. The hot, less dense nuclear ash buoyantly drives the bubble upward through the progenitor. Once the bubble exceeds the fire-polishing scale \( \lambda_{fp} \approx 4\pi S_l^2/Ag \) \cite{1}, where \( S_l \) is the laminar flame speed, \( g \) is the gravity and \( A = (\rho_2 - \rho_1)/(\rho_2 + \rho_1) \) is the density contrast, the Sharp-Wheeler growth timescale on the scale of the bubble becomes shorter than the laminar flame crossing time, causing the bubble to become Rayleigh-Taylor unstable and to become turbulent. The turbulent driving on the scale of the bubble establishes the integral scale of the turbulent flow as essentially the bubble radius. On smaller scales, the Gibson scale (defined as the scale at which the flame-crossing timescale is equal to the local eddy turnover time) may possibly establish a lower cutoff to the scales on which the flame surface can be effectively wrinkled. According to this picture, scales intermediate between the flame bubble radius and the Gibson scale are in the inertial regime. Almost immediately after ignition, a substantial inertial range opens up between the
flame bubble radius and the fire-polishing scale; *turbulent burning is the dominant reaction mechanism throughout.*

For laboratory combustion, researchers have made some progress in understanding the fundamental physics of turbulent, premixed combustion using a wide variety of theoretical techniques. These techniques can be broadly divided into three classes citepPoinVeyn05, in order of increasing computational cost: Reynolds averaged Navier Stokes (RANS) methods, large eddy simulation (LES) methods, and direct numerical simulation (DNS). Within each of these classes there generally exist several methods that can even make different assumptions about the best way to characterize (or parameterize) turbulent combustion, for example, enhanced flame speed or enhanced flame area. It is important to note that no universal model exists, and existing models have been shown to not necessarily apply in all circumstances. For example, a model that performs satisfactorily in free flow may not work at all well near an igniter or in shear flow near a wall. At the coarsest level of approximation, RANS models resolve only the largest-scale features of the flow and rely on models to describe all the effects of turbulence. While RANS models are generally the most well tested and therefore have the best-understood characterizations, they are limited to steady-state flows and thus cannot be used directly in the inherently nonsteady supernova. At the next-coarsest level of approximation, LES methods resolve some portion of the turbulent cascade itself and use subgrid models to treat the effects of scales beneath the grid scale. In some cases, it has proven valid to forego an explicit model for subgrid effects and instead depend on the corresponding effects of numerical techniques to provide a suitable implicit substitute, leading to implicit LES (ILES) methods [2]. At the highest level of accuracy, DNS fully resolves all scales of interest. DNS simulations require no subgrid model, relying directly on microscopic physical principles instead, making them powerful techniques to verify other RANS or LES turbulent combustion models. The high Reynolds numbers (∼10^{14}) and likely importance of magnetohydrodynamic effects in the ionized plasma at the smallest scales make informative, true DNS in the stellar context essentially impossible. Hybrid ILES-DNS schemes that resolve the smallest scales of interaction between the flow and burning front are the best available direct verification tests [3; 4].

The physical thickness of the carbon burning stage of the nuclear flame front in the deflagration phase of a Type Ia supernova is 10^{-5} to 10^{4} cm for the densities of interest and is therefore unresolvable in full-star simulations, which typically have linear resolution of several 10^{5} cm. Consequently, the flame front must be modeled in some LES fashion. To date, two primary numerical methodologies have been applied to studies of white dwarf deflagration. One is an LES-level set method, in which the turbulence is treated in an LES model, and the location of the flame front is calculated based on the value of a smooth field defined on the grid and propagated with an advection equation in addition to the hydrodynamics [5]. This method has undergone some evolution ([6] being the most recent) and has been used to study the effect of turbulence on the nuclear burning rate [7] and in many simulations of the deflagration phase of Type Ia supernovae [8–11]. The other method, which is currently implemented in the FLASH code, is an ILES-thickened flame model, in which the turbulent velocity field is treated in an ILES approach, and the flame front is propagated by using an advection-diffusion-reaction (ADR) equation [12]. The ILES/ADR method has been applied to a number of scientific problems, including buoyancy-driven turbulent burning [13], and 2D and 3D simulations of Type Ia models [14–17]. Both of these methods characterize the effects of turbulence on the combustion via an enhanced front propagation speed.

Despite this progress in the development of theoretical and numerical techniques to treat turbulent combustion, a number of key outstanding questions remain, including the following: How does buoyancy-driven turbulent nuclear combustion in a stratified medium differ from turbulent nuclear combustion in a homogeneous isotropic turbulent background? Is it possible to describe the burning rate of a turbulent flame by a single characteristic turbulent timescale?
If so, what scale dominates the flow – the largest integral scale, the smallest Kolmogorov scale, or some intermediate scale? If it is not possible to describe the turbulent burning rate with a single scale, how can we accurately model the large dynamic range involved in a realistic turbulent combustion flow?

2. Simulation Configuration

Our simulation setup is designed to test the effects of buoyancy and the turbulence that it generates on structure of the flame surface, and therefore the burning rate. (Higher-density) fuel is placed above (lower-density) ash in hydrostatic equilibrium in a square cross-section vertical channel whose dimension in the directions transverse to gravity is $L$ (see figure 1). This type of configuration originated with [18], has been used in several studies of buoyancy-driven turbulent burning since, and is similar to many studies of the Rayleigh-Taylor instability; see, for example, [19]. Our implementation is described in detail in [20]. Our simulation is periodic in the transverse direction, closed at the bottom of the channel, and open at the top. The total channel height is much larger than the size of the burning region but still small compared to the pressure scale height. As burning progresses, the expanded ash will force unburned fuel out of the top of the box as the burning surface, which is localized, moves up the channel. We used the 3.0 version of the hydrodynamics code FLASH [21], which implements the Piecewise Parabolic Method for fully compressible, inviscid hydrodynamics with a fully ionized degenerate plasma equation of state on an adaptively block-refined mesh. Simulations of the Rayleigh-Taylor instability with this code have been compared to experiments [22] and a variety of other codes [19]. The reaction, and therefore energy release, is represented by a progress variable, $\phi$, which is zero in the fuel and one in the ash. The burning front is propagated by using an advection-reaction-diffusion scheme [23] with a Kolmogorov Petrovski Piskunov reaction term with the sharpening modification discussed in [15]. The flame width is $\delta \approx 4\Delta$, where $\Delta$ is the grid resolution.

Figure 1. (a) Diagram of simulation configuration for studying a buoyantly-unstable flame front. (b) The flame surface in the fully-developed, self-regulated state. (c) Volume rendering of vorticity magnitude (seconds$^{-1}$).
3. Metrics for turbulent burning
The complexity of turbulent burning itself and that of the methods used to model it, along with the breadth of work under way on this topic, leads us to consider a variety of metrics to characterize properties of the combustion. Of foremost interest is the scale dependence of the flame surface structure, in particular, determination of the smallest scale of flame surface structure. A quantitative description of this scale dependence is essential for model development in the LES framework, in which a model for subgrid structure must integrate properly with resolved structures. As discussed above, it has been found that in certain circumstances an implicit subgrid model may prove sufficient for many characteristics of the combustion. Our large-scale simulations will demonstrate whether this continues to hold at nontrivial Reynolds number as well as giving a wide enough range in resolution to understand why such an ILES approach seems to work and therefore help to quantify its domain of validity. We are using two approaches to measurement of surface structure. The first, described in the next section, uses counts of surface-covering boxes of varying size to quantify the fractal dimension of the flame surface. The second approach will use direct smoothing of the progress variable field to measure the contributions to the total flame surface area which arise from various scales in the flow.

In addition to metrics addressing the flame surface directly, we are applying the most insightful methods available to study the creation, evolution, and decay of the turbulence resulting from buoyancy. This approach is especially important for supernova simulations, as the morphology of the turbulence field is likely to have the largest impact on the spreading of the flame through the star. The nonstationary and nonisotropic nature of our flow makes application of the traditional turbulence workhorse, the energy spectrum, difficult to interpret. For this reason we have come to depend more heavily on structure functions that can be defined appropriately under lateral symmetry. Additionally we are using the ability of the FLASH code to include passive Lagrangian tracer particles in order to measure the Lagrangian structure functions. We expect these to be particularly insightful, as we have found that the turbulence has a markedly different character before and behind the flame surface (see figure 1c).

4. Fractal dimension of the flame surface
As a final point we give brief details about one the techniques being used to measure flame surface characteristics. The burning rate of a flame front depends upon its surface area and is thus sensitive to its complexity (curvature on different scales). Fractal analysis methods provide a measure of the amount of structure in a curve or surface at different length scales and can help our understanding of the evolution and propagation of the flame front [24].

To this end, we have implemented a box counting algorithm in which the simulation domain is divided into a contiguous grid of cubic boxes of width $w$; those boxes that straddle the flame surface are counted to provide a measure of the surface area at this scale. Over some range of $w$, we can define a fractal (Minkowski-Bouligand) dimension $p$ such that the number of boxes $N_w \propto w^{-p}$ as $p = -d \log N_w/d \log w$. For a smooth surface, $p \approx 2$, owing to the topological dimension of the surface. If the surface has a rough, complex structure on these scales, $p > 2$.

We find that the flame surface does not have a fixed value of $p$ for all scales, and shows significant time-variation. We can determine an effective dimension $p_l$ for a scale $l$ based on $N_w$ for values of $w$ about $l$. As anticipated, we find that $p_l \approx 2$ for small $l$. By determining the range of $l$ for which $p_l$ deviates significantly from 2, as a function of flame speed, we can inform our choice of models for flame propagation.

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