Research Interests Michael A. Zingale

I am interested in modeling thermonuclear explosions over a wide range of length scales in astrophysical environments. The physics of nuclear burning under extreme conditions is key to providing an understanding of supernovae, classical novae, and X-ray bursts. My research involves the use of computational fluid dynamics and parallel computing. In the past few years, I have focused on mainly on Type Ia supernova (SNe Ia) flame instabilities, but have also studied multidimensional aspects of type I X-ray bursts and mixing in Type II supernovae. At present, I am applying two large simulation codes to my research, each with their own strengths. The first code stems from a collaboration I initiated with the Center for Computational Science and Engineering (CCSE) group at Lawrence Berkeley Laboratory. We are applying their adaptive-mesh, low Mach number terrestrial combustion code to flames in SNe Ia [1, 2, 3]. The low Mach number formulation frees us from the severe timestep constraints demanded by sound waves. The second code, FLASH [4], is an adaptive mesh, parallel, compressible hydrodynamics code developed at the Flash Center/University of Chicago, where I was a graduate student and one of its original developers. This code is very well suited to problems with strong shocks and large ranges of spatial scales, and has been used as the basis for my work on X-ray bursts [10, 11, 12] and mixing in Type II SNe. In a limited time, I feel that I have already made major contributions in each of these areas.

Flame Instabilities in Type Ia Supernovae

Type Ia supernovae are believed to result from the thermonuclear explosion of a Chandrasekhar mass white dwarf. Modeling and observations demand that the burning begin as a subsonic deflagration at one or more points near the center of the star. This flame must accelerate considerably, up to one third the sound speed, in order to account for the observed nucleosynthetic yields, spectra, and energies [6]. There is some speculation that it may transition to a detonation [8], but large scale simulations suggest that a deflagration alone can produce an explosion [5, 9]. Observations suggest that SNe Ia are 'nor-

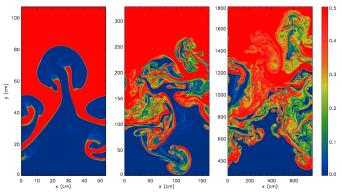


Figure 1: Carbon mass fraction for 1.5×10^7 g cm⁻³, 10^7 g cm⁻³, 6.67×10^6 g cm⁻³ flames showing the transition from the flamelet to distributed burning regime.

malizable' standard candles, and they have had an incredible impact on cosmology [7].

A detailed understanding of the explosion is still missing, however. The range of length scales in this problem span 12 orders of magnitude—from a flame thinner than a sheet of paper to a star the size of the earth. This puts a fully resolved calculation of the entire explosion well out of reach of even today's massively parallel computers. I have choosen to focus on the small scale physics, fully resolving the flame, and applying what we learn about the combustion processes on the small scales to building subgrid models, that will allow us to simulate the full stellar explosion.

The dominant acceleration mechanism in this context is the Rayleigh-Taylor (R-T) instability. The cool fuel ahead of the flame is in pressure equilibrium with the hot, less dense ash behind it. This configuration is R-T unstable. These flames are very subsonic, with a Mach number of $\sim O(10^{-3})$ or less, putting them out of reach of fully compressible algorithms. Through our collaboration with the CCSE group, we have performed direct numerical simulations of these R-T unstable flames over a relevant range of densities. We find that if the burning is fast enough, it can burn away small perturbations before they have a chance to grow, a process called 'fire-polishing'. This sets a small scale cutoff to the growth of the reactive R-T instability. At densities

Recently, we have extended these calculations to three dimensions (see Figure 2). Here, in addition to the dynamics of the R-T instability, turbulence takes a greater role. This simulation is very high resolution, an effective grid of $512 \times 512 \times 1024$, and again we resolve the burning structure of the flame. At this density, the flame thickness, the fire-polishing scale, and the smallest scale where turbulent eddies can perturb the flame before burning away (the Gibson scale) are all about equal. As Figure 2 shows, the flame is initially disturbed by the R-T instability, and fire polishing prevents the wrinkling on the smallest scales. As the flame evolves, turbulence from the large scales cascades down to scales on the order of the flame thickness itself, thoroughly wrinkling it. This calculation was featured in the

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highlighted by the NERSC computer center at SC 2004.

around 10^7 g cm⁻³, the flame is proposed to transition from the flamelet regime, characterized by a well defined separation of fuel and ash, to the distributed burning regime [8], where small scale turbulence and instabilities can rip the flame apart, directly mixing fuel and ash. We have performed the first multidimensional (2-d) simulations of this transition [3] and have concluded, contrary to speculations in the literature, that a transition to detonation at this point appears unlikely. Figure 1 shows the carbon mass fraction for the R-T unstable flame at three different densities. At the lowest density, 6.67×10^6 g cm⁻³, the reactions are peaked in small pockets and the flame surface is not very well defined—the hallmark of the distributed burning regime. At the highest density, 1.5×10^7 g cm⁻³, the flame looks much more laminar and it is easy to trace out a well-defined flame surface. In all cases, significant acceleration (up to six times laminar) is observed, limited only by the size of our domain. In these simulations, we resolve the thermal structure of the flame—no flame model is required. This ensures that we model the true dynamics of the flame, including its response to stretch and strain by the flow.

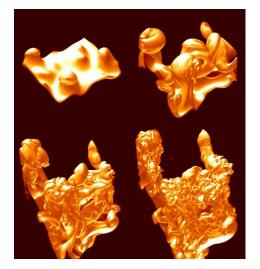


Figure 2: 3-d R-T unstable flame at several times showing the transition to turbulence.

A critical piece of the SNe Ia puzzle is understanding how the ignition proceeds. It is thought to begin with one or many hot bubbles forming near the center of the convecting white dwarf. If these bubbles can burn quicker than they cool by expansion, a flame is born. A first principles calculation of buoyantly rising reacting bubbles has never been done previously—either in the astrophysical or combustion literature. We can approach the problem again using the low Mach number hydrodynamics formulation and resolving the flame structure. We pick a density of 1.5×10^7 g cm⁻³, much lower than the ignition actually occurs at, so that we can resolve all of the interesting length scales. Since this flame is in the flamelet regime, where ignition occurs, the qualitative features

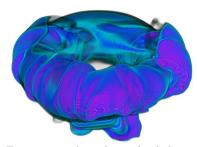


Figure 3: A 3-d resolved burning floating bubble, after it has deformed into a torus.

of the calculation carry over to the true ignition densities and much larger length scales through a self-similar scaling. Figure 3 shows a volume rendering, from a 3-d calculation, of the ash after drag has deformed the initially spherical bubble into a torus. Hydrodynamic instabilities begin to wrinkle this torus. We hope to continue this calculation far enough to see the ash grow by many times its initial mass. We are most interested in seeing whether the instabilities become large enough to fragment the bubble and learning, in detail, how the burning spreads.

Type I X-ray Bursts and Type II Supernovae Mixing

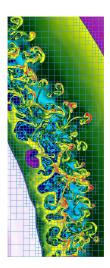


Figure 4: FLASH calculation of mixing in Type II SNe.

I also enjoy working on type I X-ray bursts—the ignition of H/He or He in the accreted envelope of a neutron star. Simulating a type I X-ray burst in multi-dimensions is very difficult. The burning is subsonic, making fully explicit timestepping algorithms ill-suited. My first approach was looking at detonations through the burning layer [11], but this is rather unphysical, as it requires extraordinarily high densities. Trying to maintain hydrostatic equilibrium in FLASH led to modifications to the PPM algorithm [10] which help greatly. Attempts to model a subsonic deflagration have met with difficulty in the ignition process, especially localized ignition without rotation [12]. Understanding the ignition of these bursts is a problem I would like to return to.

Another problem of interest to me is the late stages of Type II supernovae, where the outward propagating shock runs through composition gradients left from the previous stages of burning, prompting mixing through the R-T instability (see Figure 4). I have spent some time working on improving the resolution of previous studies, using adaptive mesh refinement, pushing to earlier times in the post-bounce evolution, and plan to compare 2- and 3-d. These results can also provide a better model of the mixing for use in 1-d stellar evolution codes.

Future Research Directions

In the short term, I wish to continue my studies of small-scale flame dynamics. There are still a lot of important questions regarding flame physics in SNe Ia. For example, how does the flame propagate transverse to gravity? We expect there to be a large amount of shear across the flame interface. It is naïve to expect it to propagate at the same speed transverse to gravity as it does against gravity, via the R-T instability, but this is what most current flame models assume. Studies of flames propagating in sheared flows will let us formulate a model for the directional dependence of the flame speed.

In the future, I would like to continue toward large scale simulations on SNe Ia, working up from the small scales. I have come to appreciate that choosing the proper algorithm is the most important part of multidimensional modeling of SNe Ia and X-ray bursts. Resolved simulations of the reactive R-T instability would not be possible without a low Mach number formulation of the Navier-Stokes equations. Fully compressible hydrodynamics codes, popular in the astrophysics community, simple cannot do the problem. The productivity gained from exploring alternate hydrodynamics algorithms is enormous. I wish to apply what I've learned about these methods to the development of a code tuned toward large scale simulations of the SNe Ia explosions. Such a code would also be applicable to type Ia X-ray bursts. I will draw on my experiences as one of the developers of FLASH, a $\sim 500,000$ line simulation code, to work on this next generation supernova code. Being a developer of FLASH has taught me how to work in a large, distributed development group, as well as the importance of regular testing, version control, and regular code validation, so you have confidence in your results. Even with the best of codes, all of these simulations require large computers. Both of the 3-d simulations described above contained over 100 million computational zones, generated several terabytes of data, and required 256–512 processors and several weeks to run.

The trickiest part of the large scale simulations is the development of a flame model that can treat the subgrid scale physics. There are two methods of representing an unresolved flame in a large-eddy simulation that are in wide use today, level-sets and thickened flame methods. What is missing from their application is a validation against direct numerical simulations in the astrophysical environment. I am starting to do comparisons of different flame models against the fully resolved calculations we have already performed, matching the parameters of the calculation as close as possible, but using the flame model to move the flame instead of fully resolving it. Such validation of flame models against resolved calculations has never been done in the astrophysics community, and it is an important step in producing reliable supernova models. Current flame models do not include all the details of the flame physics, especially the directional dependence of the flame speed and the flame's response to stretch. We are also the only group presently able to perform multidimensional simulations in the distributed burning regime without a flame model. It is here that the last 10-20% of the supernova's energy is released. Missing these details could mean the difference between a successful explosion and a failed one. It is my hope that in a year, we will have enough confidence in a flame model, from this validation, to apply it to the full star.

There are a lot of outstanding questions regarding the SNe Ia explosion mechanism—how many points does the ignition begin at? Is a deflagration to detonation transition necessary? Are there nucleosynthetic signatures resulting from these differing modes of explosion that can be used to constrain the models? Working up from the small scales where we can understand the flame physics, toward the large scales, and building on what we have learned previously can help answer these questions. This will be the focus of my next few years of research.

Movies of these simulations and further information can be found at http://www.ucolick.org/~zingale/.

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