NUMERICAL SIMULATIONS OF MULTI-SCALE ASTROPHYSICAL PROBLEMS:
THE EXAMPLE OF TYPE Ia SUPERNOVAE

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Vastly different time and length scales are a common problem in numerical simulations of astrophysical phenomena. Here, we present an approach to numerical modeling of such objects on the example of Type Ia supernova simulations. The evolution towards the explosion proceeds on much longer time scales than the explosion process itself. The physical length scales relevant in the explosion process cover 11 orders of magnitude and turbulent effects dominate the physical mechanism. Despite these challenges, three-dimensional simulations of Type Ia supernova explosions have recently become possible and pave the way to a better understanding of these important astrophysical objects.

Keywords: Type Ia supernovae, Numerical techniques, Hydrodynamics, Turbulence

1. Introduction

Astrophysics naturally features problems on large scales, which often can be addressed with the methods of hydrodynamics. The number of particles is huge and the interactions are in many cases (with the important exception of gravity) short-ranged. This allows the description of the systems in terms of thermodynamical variables. From the formation of planets to the evolution of large-scale structure in the Universe, hydrodynamical methods have been successfully applied to astrophysical problems on various spatial scales.

Astrophysical problems usually challenge numerical techniques and computational resources due to their pronounced multi-scale character. Physical processes take place on vastly different time scales. Moreover, the range of spatial scales involved is typically far beyond the capabilities of to-
day’s supercomputers. Therefore, approximations and numerical modeling are inevitable.

Here, we will discuss the a typical astrophysical scenario – the thermonuclear explosion of a white dwarf (WD) star which is believed to give rise to a Type Ia supernova (SN Ia) explosion. A comprehensive treatment of this scenario would involve the modeling of the formation of the progenitor system, its stellar evolution, its approach to the explosive state, the ignition of the explosion, the explosion stage itself, and the evolution of the remnant. But we are far from dealing with problems of such complexity. The different stages of the evolution of the system are characterized by very different timescales and distinct physical mechanisms. For instance, the stellar evolution of the progenitor system may take more than a billion years while the actual explosion takes place on a timescale of seconds. Therefore, different methods are applied to address these stages. Stellar evolution is usually treated in hydrostatic approaches, the evolution towards the ignition of the thermonuclear explosion takes about a century and needs special hydrodynamical approximations, while the explosion process is modelled via a combination of hydrodynamics, turbulence modelling and treatment of nuclear reactions.

2. Astrophysical Model

The favored astrophysical model of SNe Ia is the thermonuclear explosion of a WD star composed of carbon and oxygen.\textsuperscript{1,2} This end stage of stellar evolution for intermediate and low-mass stars is stabilized by the pressure of a degenerate electron gas, because after nuclear burning of hydrogen and helium it fails to trigger carbon and oxygen burning. A WD is a compact object which would be eternally stable, cool off, and disappear from observations. However, since many stars live in binary systems, it is possible that it accrets material from its companion. There exists a limiting mass for stability of a degenerate object like a carbon/oxygen WD (the Chandrasekhar mass $\sim 1.38M_\odot$) beyond which it becomes unstable to gravitational collapse. Approaching the Chandrasekhar mass, the density in the core of the WD reaches values that eventually trigger carbon fusion reactions.

This leads to about a century of convective burning. Finally, however, a thermonuclear runaway occurs and gives rise to the formation of a burning front, usually called a thermonuclear flame. This flame propagates outward burning most of the material of the star and leading to an explosion – a process that occurs on timescales of seconds.

Hydrodynamics allows for two distinct modes of flame propagation.\textsuperscript{3}
While in a subsonic deflagration the flame is mediated by the thermal conduction of the degenerate electrons, a supersonic detonation is driven by shock waves. Observational constraints rule out a prompt detonation for SNe Ia and the flame must therefore start out in the slow deflagration mode. The flame propagation has to compete with the expansion of the star due to the nuclear energy release. Once the dilution due to expansion has lowered the fuel density below a certain threshold, no further burning is possible. The energy release up to this point needs to be sufficient to gravitationally unbind the WD star and to lead to a powerful explosion. This is only possible if the propagation velocity of the deflagration flame is accelerated far beyond the speed of a simple planar flame (the so-called laminar burning speed).

It turns out that this can be achieved by the interaction of the flame with turbulence. This turbulence is generic to the scenario. Burning from the center of the star outward, the flame leaves light and hot nuclear ashes below dense and cold fuel. This inverse density stratification in the gravitational field of the WD is buoyancy unstable. Consequently, burning bubbles form and float towards the surface. Shear flows at the interfaces of these bubbles lead to the generation of turbulent eddies. By wrinkling the flame these increase its surface and the net burning rate is enhanced. Thus, the flame accelerates. Whether this acceleration suffices to yield the strongest SNe Ia observed, is currently debated. It has been hypothesized that a transition of the flame propagation from subsonic deflagration to supersonic detonation in later stages of the explosion may occur and provide an the ultimate speed-up of the flame.

3. Challenges

The astrophysical scenario of SNe Ia described in the previous section obviously poses great challenges numerical modeling. Many of the problems found here are typical for a broad range of astrophysical phenomena. The contrast between the time scales of the actual explosion to that of the ignition process (let alone the stellar evolution of the progenitor) is only part of the scale-problem. The spatial scale ranges in the explosion as well as in the pre-ignition phase are huge. Both processes are dominated by turbulence effects with integral scales not much below the radius of the star (∼2000 km). A typical Reynolds number is as high as $10^{14}$ and consequently the Kolmogorov scale is less than a millimeter. Turbulence effects with Reynolds numbers far beyond anything occurring on Earth are common in astrophysics. The scales of the objects and typical velocities are huge but at the
same time the viscosities of astrophysical fluids are not extraordinarily high. This indicates that neither a full temporal nor spatial resolution in a single numerical approach is possible. Therefore the problems are usually broken down into sub-problems which can be treated with specific approximations and numerical techniques. Moreover, astrophysical equations of state are often more complex than those found under terrestrial conditions and are in some cases not even well-known.

4. Governing Equations

Hydrodynamical problems in astrophysics can often be treated with the Euler equations with gravity as external force which have to be augmented by a description of nuclear reactions and an appropriate astrophysical equation of state. This set of equations is obtained when reaction and diffusive transport phenomena are neglected:

\[
\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{v}), \tag{1}
\]

\[
\frac{\partial \mathbf{v}}{\partial t} = -(\mathbf{v} \nabla) \cdot \mathbf{v} - \frac{\nabla p}{\rho} + \nabla \Phi, \tag{2}
\]

\[
\frac{\partial \rho e_{\text{tot}}}{\partial t} = -\nabla \cdot (\rho e_{\text{tot}} \mathbf{v}) - \nabla (\rho \mathbf{v} \cdot \mathbf{v}) + \rho \mathbf{v} \cdot \nabla \Phi + \rho S, \tag{3}
\]

\[
\frac{\partial \rho X_i}{\partial t} = -\nabla \cdot (\rho X_i \mathbf{v}) + r_{X_i}, \tag{4}
\]

\[r_{X_i} = f(\rho, T, X_i), \tag{5}\]

\[p = f_{\text{EOS}}(\rho, e_{\text{int}}, X_i), \tag{6}\]

\[T = f_{\text{EOS}}(\rho, e_{\text{int}}, X_i), \tag{7}\]

\[S = f(r), \tag{8}\]

\[\Delta \Phi = 4\pi G\rho. \tag{9}\]

Mass density, velocity, pressure, total energy, internal energy, mass fraction of species \(i\), temperature, reaction rates, chemical source term, and gravitational potential are denoted by \(\rho\), \(\mathbf{v}\), \(p\), \(e_{\text{tot}}\), \(e_{\text{int}}\), \(X_i\), \(T\), \(r\), \(S\), and \(\Phi\), respectively. Index \(i\) runs over \(1 \ldots N\), where \(N\) is the number of species contained in the reacting mixture.

The equation of state is indicated by \(f_{\text{EOS}}\). For astrophysical objects matter may occur under extreme conditions and the equation of state may differ significantly from that of terrestrial matter. This is the case for our example as the equation of state of the WD star is dominated by an arbitrarily relativistic an degenerate electron gas. The nuclei form an ideal
gas of nuclei, and radiation and electron-positron pair creation/annihilation contribute to the equation of state as well.

In many cases effects like heat conduction and diffusion play a major role. In principle this holds for the example considered here, too. On the smallest scales, the flame is mediated by the heat conduction of the degenerate electrons. However, these scales cannot be resolved in full-star simulations and the treatment of flame propagation we will discuss below parametrizes it in a way such that the above set of equations is sufficient to describe the astrophysical scenario.

5. Modeling approaches

Different methods for modeling the hydrodynamics make different approximations and are suitable to certain sub-problems or simplifications of the problems. First and pioneering approaches to simulate SNe Ia, for instance, assumed spherical symmetry. These neglect instabilities and turbulence effects, which have to be parametrized in such simulations, but they allow for efficient Lagrangian discretization schemes. Consistency and independence of artificial parameters can, however, only be reached in multi-dimensional simulations. Eulerian discretizations are preferred here.

Depending on the time scales of the physical phenomena under considerations, certain simplifications can be made to the hydrodynamical equations. While in the explosion simulations usually the set of equations spelled out above is applied, the pre-ignition convection and ignition processes, as well as the propagation of deflagration flames on small scales, are strongly subsonic phenomena. The magnitude of steps allowed in the numerical simulations is set by the fastest motions that contribute to the mechanism. Therefore, for subsonic phenomena it would be an overkill (and in some cases it would also be numerically unstable) to follow sound waves. Therefore these are filtered out in anelastic and low-Mach number approaches applied specifically to the pre-ignition and ignition phase of thermonuclear supernovae. Allowing for much larger time steps than the sound crossing time over a computational grid cell, such approaches facilitate the numerical study of phenomena taking place on time scales of minutes and hours. These approaches are described in detail elsewhere and will focus on the traditional implementation of hydrodynamical processes below.

The problem of spatial scales is approached in two strategies. While off-line small-scale simulations of otherwise unresolved phenomena test the assumptions of large-scale models, these in turn rely on models for unresolved effects. The outstanding challenge in the latter is the description
of turbulence effects and a promising strategy for addressing these in astrophysical simulations is the application of subgrid-scale turbulence models. Since in SNe Ia the propagation of the deflagration flame is dominated by turbulence effects, such models are applied here and an example will be discussed below.

The nucleosynthesis in astrophysical events is a rich phenomenon which can involve hundreds of isotopes and reactions between them. While it is possible to run extended nuclear reaction networks concurrently with one-dimensional astrophysical simulations, they are prohibitively expensive in three-dimensional approaches. Therefore, such simulations usually apply greatly simplified treatments of nuclear reactions in order to approximate the energy release. In this way the dynamical effects of nuclear burning can be treated without large errors. However, in order to compare the results of astrophysical simulations with observables such as spectra and light curves\(^a\) (the only way to validate astrophysical models), details of the chemical structure of the object are to be known. One approach to this issue is to advect a number of tracer particles with the hydrodynamical simulation which record the evolution of the thermodynamical conditions, and to feed this information into extended nuclear reaction networks in a postprocessing step.\(^{17,18}\)

6. Numerical Methods

There exists a large number of standard techniques for solving the Euler equations in hydrodynamical simulations. In astrophysics, a widely used finite-volume approach that discretizes the integral form of the equations, is the piecewise parabolic method\(^{19,20}\) – based on a higher-order Godunov scheme.

The selection of the geometry of the computational grid needs special consideration. Although spherical coordinates seem best suited for many astrophysical objects featuring an average spherical symmetry, these are afflicted with coordinate singularities. Therefore, currently there seems to be a trend towards Cartesian set-ups.

The challenge of incorporating phenomena that occur on scales unresolved in simulations has to be addressed by modeling. For the example of large-scale SN Ia simulations this applies to the propagation of the thermonuclear flame and to turbulence. As described above, both are connected.

\(^a\)the temporal evolution of the luminosity of the event, usually restricted to a range of wavelengths set by an observational filter
For modeling turbulence on unresolved scales, a Large Eddy Simulation (LES) ansatz is chosen. Flow properties on resolved scales are used to determine closure relations for a balance equation of the turbulent velocity $q$ at the grid scale.\(^{21}\)

The structure profiles of a thermonuclear flame at high and intermediate fuel densities extent typically over less than a centimeter. These scales cannot be resolved in simulations capturing the evolution of the entire WD star (radius 2000 km and expanding). Therefore, in these simulations, the flame is treated as a mathematical discontinuity separating the nuclear fuel from the ashes. A numerical technique to represent the propagation of this discontinuity is the level set method.\(^{22,23}\) It associates the flame surface $\Gamma(t)$ with the zero level set of function $G$:

$$\Gamma(t) := \{ r | G(r, t) = 0 \}.$$ 

For numerical convenience, we require $G$ to be a signed distance function to the flame front, $|\nabla G| \equiv 1$ with $G < 0$ in the fuel and $G > 0$ in the ashes. The equation of motion is then given by

$$\frac{\partial G}{\partial t} = (v_u n + s_u) |\nabla G|.$$ 

Here, $v_u$ is the fluid velocity ahead of the flame, $s_u$ is the effective flame propagation velocity with respect to the fuel, and $n = -\nabla G / |\nabla G|$ is the normal to the flame front. This equation ensures that the zero level set (i.e. the flame) moves in normal direction to the flame surface due to burning and additionally the flame is advected with the fluid flow. The burning speed $s_u$ has to be provided externally in this approach since the burning microphysics is not resolved. While the flame propagation proceeds with the well-known laminar flame speed in the very first stages of the explosion, it quickly gets accelerated by interaction with turbulence. By virtue of the implemented subgrid-scale model the turbulent burning speed of the flame can easily be determined. In the turbulent combustion regime that holds in most parts of the supernova explosion, it is directly proportional to the turbulent velocity fluctuations. This is the way in which the multidimensional LES approach to flame propagation in thermonuclear supernovae avoids tunable parameters in the description of flame propagation.

In order to take the expansion of the WD into account in the simulation, one has to adapt the computational grid accordingly. One option is adaptive mesh refinement, which, however, suffers from the usually volume-filling turbulent flame structure. Therefore, a refinement all over the domain would be necessary and the gain in efficiency from this method is marginal. An
alternative is to use a computational grid with variable cell sizes. This grid can be constructed to track the expansion of the star\textsuperscript{24} or the propagation of the flame inside it (or both\textsuperscript{25}).

7. Three-dimensional Type Ia supernova simulations

Applying the techniques discussed above, three-dimensional simulations of deflagration thermonuclear burning can be performed\textsuperscript{6,21,26} (the incorporation of a delayed detonation stage is also possible with slight modifications of the methods\textsuperscript{27}). The goals of such simulations is to determine whether an explosion of the WD can be achieved in the model and whether the characteristics of such an explosion meet observational constraints. As a direct link from the simulation of the pre-ignition convection studies and the flame ignition simulations to the explosion models is still lacking, the flame ignition is introduced by hand in configurations motivated by off-line studies\textsuperscript{10,28,29}.

To illustrate the typical flame evolution in deflagration SN Ia models, the full-star model presented by\textsuperscript{26} shall be described here. The flame was ignited in a number of randomly distributing spherical flame kernels around the center of the WD. This resulted in a foamy structure slightly misaligned with the center of the WD (shown in Fig. 1). Such multi-spot ignition models are motivated by the strongly turbulent convective carbon burning phase preceding the ignition (but alternatives such as asymmetric off-center ignitions have also been considered). Starting from this initial flame configuration, the evolution of the flame front in the explosion process is illustrated by snapshots of the $G = 0$ isosurface at $t = 0.3\, \text{s}$ and $t = 0.6\, \text{s}$ in Fig. 1. The development of the flame shape from ignition to $t = 0.3\, \text{s}$ is characterized by the formation of the well-known “mushroom-like” structures resulting from buoyancy. This is especially well visible for the bubbles that were detached from the bulk of the initial flame. But also the perturbed parts of the flame closer to the center develop nonlinear Rayleigh-Taylor features. During the following flame evolution, inner structures of smaller scales catch up with the outer “mushrooms” and the initially separated structures merge forming a more closed configuration (see snapshot at $t = 0.6\, \text{s}$ of Fig. 1). This is a result of the large-scale flame advection in the turbulent flow, burning, and the expansion of the ashes. After about 2 s self-propagation of the flame due to burning has terminated in the model. The subsequent evolution is characterized by the approach to homologous (self-similar) expansion. The resulting density structure at the end of the simulation is shown in the $t = 10\, \text{s}$ snapshot of Fig. 1.
Fig. 1. Snapshots from a full-star SN Ia simulation starting from a multi-spot ignition scenario. The density is volume rendered indicating the extend of the WD star and the isosurface corresponds to the thermonuclear flame. The last snapshot corresponds to the end of the simulation and is not on scale with the earlier snapshots.

The goal of such simulations is to construct a valid model for SNe Ia which meets the constraints from nearby well-observed objects. Such models can then be used to test and refine the methods that are used to calibrate cosmological distance measurements based on SN Ia observations,\textsuperscript{30} which pioneered the new cosmological standard model with an accelerated expansion of the Universe\textsuperscript{31,32} pointing to a dominant new “dark” energy form.
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