Low Mach Number Modeling of Stratified Flows

Ann Almgren, John Bell, Andrew Nonaka and Michael Zingale

Abstract Low Mach number equation sets approximate the equations of motion of a compressible fluid by filtering out the sound waves, which allows the system to evolve on the advective rather than the acoustic time scale. Depending on the degree of approximation, low Mach number models retain some subset of possible compressible effects. In this paper we give an overview of low Mach number methods for modeling stratified flows arising in astrophysics and atmospheric science as well as low Mach number reacting flows. We discuss how elements from the different fields are combined to form MAESTRO, a code for modeling low Mach number stratified flows with general equations of state, reactions and time-varying stratification.

1 Introduction

Physical phenomena encompassing a wide range of length and time scales occur in a large number of fluid dynamical areas. In the atmosphere, for example, we want to understand flows on the scale of local regions, continents, or the entire globe. In astrophysics we want to understand not only how the nuclear energy release from thin flame fronts may unbind a star, resulting in a dramatic supernova, but also how the

A. Almgren (⊠) · J. Bell · A. Nonaka Lawrence Berkeley National Laboratory, Berkeley, CA, USA e-mail: ASAlmgren@lbl.gov

J. Bell e-mail: JBBell@lbl.gov

A. Nonaka e-mail: AJNonaka@lbl.gov

M. Zingale Stony Brook University, Stony Brook, NY, USA e-mail: Michael.Zingale@stonybrook.edu large-scale convective flows that precede the explosion lead to ignition. In laboratoryscale turbulent combustion, we need to understand not only the detailed chemistry of how the flame burns, but also how it influences and responds to the turbulent flow around it. In principle these scenarios can all be modeled using the equations of motion that govern compressible reacting fluids. Even with today's (and tomorrow's) supercomputers, however, in each of these areas there are phenomena for which simulating all the fluid dynamical scales of these problems over the time periods of interest is beyond our reach. For many of these problems, our understanding of the flow does not require tracking the acoustic waves that carry relatively little energy and travel much faster than the fluid itself.

We are interested in numerical methods that can accurately model the phenomena of interest but are not limited by needing to resolve the acoustic time scale. One approach is to advance the acoustic signal in time with an implicit time discretization or to treat the acoustic signal explicitly yet separately from the rest of the flow, for example as used in cloud modeling in [41] and [22], respectively. Another approach is to modify the governing equations so that acoustic waves are no longer supported by the equations. In this paper we explore the latter approach for low Mach number flows, i.e. flows for which we can exploit the separation of scales that occurs when the Mach number, M (the ratio of the fluid velocity to the sound speed), is much less than unity. Physically, one can think of the solution to a low Mach number model as supporting infinitely fast acoustic equilibration rather than finite-velocity acoustic wave propagation. Mathematically, this is manifest in the addition of a constraint on the velocity field to the system of otherwise hyperbolic evolution equations. This velocity constraint can be translated into an elliptic equation for pressure that expresses the equilibration process. Because the time step in explicit discretization schemes for a low Mach number system is limited by the fluid velocity and not by the sound speed, these methods often gain several orders of magnitude in computational efficiency over traditional compressible approaches.

Fundamental to the traditional low Mach number approach is that we can decompose the pressure as

$$p(\mathbf{x},t) = p_0 + p'(\mathbf{x},t)$$

where p_0 is the ambient thermodynamic (or "reference" or "background") pressure, and p' is the perturbational pressure, where $p'/p_0 \sim \mathcal{O}(M^2)$. For small-scale reacting flows in an open environment, p_0 reduces to a constant in space and time; in a closed combustion chamber, $p_0 = p_0(t)$. For reacting, stratified flow on a larger scale, p_0 is a function of both the radius (distance from the center of the star for stellar applications, or elevation in the atmospheric case) and time, when large-scale net heating/cooling is present.

2 Background

The simplest low Mach number model is expressed by the incompressible Navier-Stokes equations for a constant density fluid. This can be generalized to variable density incompressible flow, in which the density varies spatially across the domain but the density of an individual fluid element does not change over time. Low Mach number models for chemical combustion [10, 31, 40] and nuclear burning [6] incorporate large compressibility effects due to chemical/nuclear reactions and thermal processes with a spatially constant background pressure. The Boussinesg approximation [8] includes a heating-induced buoyancy term in the momentum equation but requires that the flow itself be incompressible. The anelastic equations (see, e.g., [4, 5, 14, 20, 27–29, 37, 44] for atmospheric flows, and [18, 19, 26] for astrophysical flows; see also the references in [9]), capture volumetric expansion due to motion relative to a stratified background in addition to buoyancy due to deviation of the local state from the background state, and have been widely used in modeling of atmospheric and astrophysical flows. The pseudo-incompressible (PI) approximation, introduced by [12, 13] and rigorously derived using low Mach number asymptotics by [7], generalizes anelastic models by allowing larger variations in density and temperature in response to localized heat release, but is restricted to an ideal gas equation of state. A low Mach number model for astrophysical flows [1-3, 35, 46], implemented in a code named MAESTRO, has generalized the pseudo-incompressible approximation to more general equations of state for use in astrophysical modeling, and has extended its applicability by allowing time variation of the background stratification to accommodate an expanding stellar atmosphere. Recently, a modification of the momentum equation to improve the accuracy of the buoyancy term in the low Mach number equation set was proposed, in a general form by [21], and then by [43] using an alternate derivation based on Lagrangian analysis.

3 Fully Compressible Equations for Stratified Flow

The fully compressible (FC) equations for a reacting multicomponent gas in the presence of gravity, neglecting Coriolis terms, viscosity, thermal and species diffusion, and weak nuclear interactions, can be written in conservation form as

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho U) = 0, \tag{1}$$

$$\frac{\partial(\rho h)}{\partial t} + \nabla \cdot (\rho U h) = \frac{Dp}{Dt} - \rho \sum_{k} q_k \dot{\omega_k}, \tag{2}$$

$$\frac{\partial(\rho U)}{\partial t} + \nabla \cdot (\rho U U) + \nabla p = -\rho g \mathbf{e}_r,\tag{3}$$

$$\frac{\partial(\rho X_k)}{\partial t} + \nabla \cdot (\rho U X_k) = \rho \dot{\omega_k},\tag{4}$$

where ρ , U, p and h are the density, velocity, pressure and enthalpy (per unit mass), respectively, and g is the gravitational acceleration in the direction of \mathbf{e}_r , the unit vector in the radial direction. The species are represented by their mass fractions, X_k , along with their associated production rates, $\dot{\omega}_k$, and specific binding energies, q_k . The equation of state can be written in a general form as $p = \hat{p} (\rho, T, X_k)$ or $\rho = \hat{\rho} (p, T, X_k)$ where T is the temperature.

Still allowing the fluid to be fully compressible, we can define a hydrostatic base state pressure, $p_0(r, t)$, and corresponding base state density, $\rho_0(r, t)$ such that $\nabla p_0 \equiv -\rho_0 g \mathbf{e}_r$. We define the deviation from the reference value, $p' = p - p_0$, but make no assumptions about the size of the deviation. Then, with no approximation, Eq. (3) can be written instead as

$$\frac{\partial(\rho U)}{\partial t} + \nabla \cdot (\rho U U) + \nabla p' = -\rho' g \mathbf{e}_r,\tag{5}$$

where $\rho' \equiv \rho - \rho_0$. Even though we have decomposed the variables into reference state values and perturbational values, no assumptions about the magnitude of the perturbations have been made at this point, and the perturbational form is algebraically equivalent to the non-perturbational form.

4 Low Mach Number Approach

The methodology developed for low Mach number modeling of astrophysical flows, and implemented in a code named MAESTRO [1–3, 35, 46], represents the synthesis of ideas from three separate fields into a new algorithmic approach. First, the anelastic and pseudo-incompressible approximations, first derived in the context of atmospheric science, suggest how to filter sound waves for environments in which the background stratification due to gravity plays a significant role in the dynamics. These approximations differ from those in incompressible and low Mach number combustion modeling in that the background pressure and density are in hydrostatic equilibrium rather than spatially constant. Second, methods developed for low Mach number combustion inform how to incorporate local expansion effects due to reactions and thermal diffusion in a low Mach number setting. Finally, formulation of the equation of state, reaction networks, and other thermodynamical characterizations of stellar material require detailed astrophysical expertise. Contributions from all three fields were used to devise a method that

- captures the same large-scale motions as the fully compressible equations
- allows for local expansion due to reactions, thermal diffusion, and compositional mixing
- allows for local expansion due to movement relative to background stratification
- allows the background state to evolve in time in response to large-scale heating and/or mixing

- does not require an ideal gas equation of state
- removes acoustic wave propagation.

Low Mach number equations in all settings are typically derived by first expanding all of the variables asymptotically in the Mach number, M, which is assumed to be small. Using standard asymptotic techniques, one can show that in the momentum equations we retain the zeroth order terms of velocity and density, but the zeroth order term of the pressure gradient must be either zero or, in the case of stratified flows, balanced by the hydrostatic gravitational forcing. The dynamic component of the pressure gradient must be $O(M^2)$; this is typically translated into writing the pressure, p, as $p = p_0 + p'$, where p_0 is the background pressure, p' is the dynamic pressure, and $p'/p_0 \sim O(M^2)$. Standard techniques would also dictate that the density variation from ambient must be small at all times or the buoyancy term would lead to too strong an acceleration. A slightly more general approach, outlined in [2], replaces the restriction on the magnitude of the buoyancy term itself by a restriction on the effect of the buoyancy term, namely the magnitude of the velocity itself.

The fundamental approximation made in the the low Mach number equations is that the compressible pressure can be approximated by the background pressure in the equation of state. This differs from earlier derivations of similar equations (e.g, the anelastic approximation) which required that density and temperature variations from the ambient be small in order to ensure the pressure perturbation be small; here we require only that the pressure perturbation itself be small. In the low Mach number system, then, we write the equation of state in a general form as $p_0 = \hat{p} (\rho, T, X_k)$ or $\rho = \hat{\rho} (p_0, T, X_k)$.

To model a full star, for example, we would start by defining a radial background state in hydrostatic equilibrium. In practice, this profile would come from a onedimensional stellar evolution code, which provides us with a model in hydrostatic balance. Thus our base state satisfies

$$\frac{\partial p_0(r,t)}{\partial r} = -\rho_0(r,t)g(r,t),\tag{6}$$

where g(r, t) can be computed from $\rho_0(r, t)$ as

$$g(r,t) = \frac{GM_{\text{encl}}(r,t)}{r^2}$$
(7)

with the mass enclosed within a radius r defined as

$$M_{\rm encl}(r,t) = 4\pi \int_0^r \rho_0(r',t) r'^2 dr'.$$
 (8)

Here *G* is the gravitational constant. For modeling the earth's atmosphere, one can remove the time dependence of ρ_0 and p_0 , and consider *g* to be spatially and temporally constant.

Given the base state, standard asymptotic analysis yields the following system of equations:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (U\rho) = 0, \tag{9}$$

$$\frac{\partial(\rho h)}{\partial t} + \nabla \cdot (U\rho h) = \frac{Dp_0}{Dt} - \rho \sum_{k} q_k \dot{\omega_k}, \tag{10}$$

$$\frac{\partial U}{\partial t} + U \cdot \nabla U = -\frac{1}{\rho} \nabla p' - \frac{\rho'}{\rho} g \mathbf{e}_r, \tag{11}$$

$$\frac{\partial(\rho X_k)}{\partial t} + \nabla \cdot (\rho U X_k) = \rho \dot{\omega_k}.$$
(12)

The first and second equations are unchanged from the fully compressible versions with the exception that p is replaced by p_0 in the enthalpy evolution equation. The only source terms in the velocity evolution equation (21) are due to the dynamic pressure and the buoyancy. However, if one asymptotically examines not the difference between the solution and the base state, but the difference between the solution to the low Mach number system and the solution to the compressible system, one finds a correction to the buoyancy term of the form,

$$\left(\frac{\rho_0}{\rho^2} \frac{\partial \rho}{\partial p_0} \bigg|_{s} p'\right) g \mathbf{e}_r,\tag{13}$$

where the derivative is taken at constant entropy, s, so that the velocity equation now has the form

$$\frac{\partial U}{\partial t} + U \cdot \nabla U = -\frac{1}{\rho} \nabla p' - \frac{1}{\rho} \left(\rho' + \frac{\rho_0}{\rho} \left. \frac{\partial \rho}{\partial p_0} \right|_s p' \right) g \mathbf{e}_r.$$
(14)

This additional term, which can be viewed as modifying the density appearing in the buoyancy term to have a correction due to the perturbational pressure, was introduced first in [21] and then in [43]; both demonstrated that the inclusion of this term enables the system to conserve a low Mach number form of total energy. This modified system yields a solution that is closer to the solution to the fully compressible system of equations than the original low Mach number system.

The more fundamental change in the structure of the system of equations results from replacing the pressure in the equation of state by the background pressure. Differentiating the equation of state along particle paths then converts the algebraic equation of state into a constraint on the divergence of the velocity. Differentiating $p_0 = \hat{p}(\rho, T, X_k)$ along particle paths and rearranging terms yields

$$-\nabla \cdot U = \frac{1}{\rho} \frac{D\rho}{Dt} = \frac{1}{\rho p_{\rho}} \left(\frac{Dp_0}{Dt} - p_T \frac{DT}{Dt} - \sum_k p_{X_k} \dot{\omega_k} \right), \tag{15}$$

with $p_{\rho} = \partial p / \partial \rho|_{X_k,T}$, $p_{X_k} = \partial p / \partial X_k|_{T,\rho,(X_j, j \neq k)}$, and $p_T = \partial p / \partial T|_{\rho,X_k}$. Expanding and simplifying this expression as in [1] results in

$$\nabla \cdot U + \frac{1}{\Gamma_1 p_0} \left(\frac{\partial p_0}{\partial t} + U \cdot \nabla p_0 \right) = -\sigma \sum_k \xi_k \dot{\omega}_k + \frac{1}{\rho p_\rho} \sum_k p_{X_k} \dot{\omega}_k - \sigma \sum_k q_k \dot{\omega}_k \equiv S,$$
(16)

where $\xi_k \equiv \partial h / \partial X_k|_{T, p, (X_j, j \neq k)}, \Gamma_1 \equiv d(\log p) / d(\log \rho)|_s$. and

$$\sigma = \frac{p_T}{\rho c_p p_{\rho}},\tag{17}$$

which, for a gamma law gas, reduces to $\sigma = 1/(c_p T)$. We see that the first two terms in *S* capture the effect of compositional changes, while the third represents heat release from the reactions. If we now allow Γ_1 to be replaced by its lateral average, $\overline{\Gamma}_1(r, t)$, then, as shown in [2], $\nabla \cdot U + (1/(\overline{\Gamma}_1 p_0))U \cdot \nabla p_0$ can be rewritten as $(1/\beta_0)\nabla \cdot (\beta_0 U)$ where

$$\beta_0(r,t) = \beta(0,t) \exp\left(\int_0^r \frac{1}{(\overline{\Gamma}_1 p_0)} \frac{\partial p_0}{\partial r'} dr'\right).$$
(18)

Thus we can write the constraint as

$$\nabla \cdot (\beta_0 U) = \beta_0 \left(S - \frac{1}{\overline{\Gamma}_1 p_0} \frac{\partial p_0}{\partial t} \right), \tag{19}$$

which allows us to use a variable density projection method analogous to that used to solve the incompressible Navier-Stokes equations. This constraint on the velocity field controls the degree to which the fluid can expand, forcing the evolution of the thermodynamic quantities to be consistent with the equation of state. It is the presence of $\beta_0 \neq 1$ that allows the fluid to expand as it rises; the magnitude of *S* determines the degree to which the fluid expands due to heat release and compositional changes.

The resulting Poisson equation for p', in the absence of the additional term, (13), in the velocity evolution equation, can be written

$$\nabla \cdot \left(\frac{\beta_0}{\rho} \nabla p'\right) = RHS, \tag{20}$$

where RHS includes the divergence of the advective terms as well as *S* and the time derivative of p_0 . With the substitution of $\overline{\Gamma}_1$ for Γ_1 , it was shown in [43] that the velocity evolution equation with the additional term, (13), can be written as

$$\frac{\partial U}{\partial t} + U \cdot \nabla U = -\frac{\beta_0}{\rho} \nabla \left(\frac{p'}{\beta_0}\right) - \rho' g \mathbf{e}_r,\tag{21}$$

instead of (14). This results in a Poisson equation for the perturbational pressure in the form

$$\nabla \cdot \left(\frac{\beta_0^2}{\rho} \nabla \frac{p'}{\beta_0}\right) = RHS.$$
(22)

For simulations of full stars where the background stratification varies with both radius and time, we must evolve the base state pressure and density in time in response to large scale heating and convection while retaining hydrostatic equilibrium. The velocity field used to update the density includes a local component, \tilde{U} , which accounts for localized convective and compressibility effects, and a base state component, w_0 , which accounts for large-scale equilibration of the atmosphere. We can calculate w_0 by deriving a one-dimensional expression for the divergence of w_0 , containing terms representing the average of S, and integrating that expression in the radial direction. Once we have advanced the density field, we can compute the new base state density as the average stratification, and compute the new base state pressure using hydrostatic equilibrium. Details are given in [35].

5 Numerical Approach

Low Mach number formulations replace the compressible flow equations with a constrained system of partial differential equations similar in structure to the incompressible Navier-Stokes equations. A number of projection-type methods have been developed to simulate incompressible and other low Mach number flows using a time step based on the fluid velocity and not the sound speed. Projection methods are fractional step schemes in which the solution is first advanced using a lagged approximation to the constraint, then, in a second step, a projection is applied to enforce the constraint. To solve the low Mach number equations for astrophysics in the MAESTRO code, we use an explicit second-order upwind discretization for advection, and Strang splitting to incorporate the contributions of reactions to the species and enthalpy. The projection step solves a second-order, self-adjoint, variablecoefficient elliptic equation for an update to the perturbational pressure, which is then used to correct the velocity. To include the base state evolution, in the predictor step we use an estimate of the expansion term, S, to compute a preliminary solution at the new time level, and in the corrector step we use the results from the predictor step to compute a more accurate expansion term, and compute the final solution at the new time level. The resulting algorithm advances the fluid evolution equations using a time step constrained by the fluid velocity rather than the acoustic wave speed, resulting in a significant increase in efficiency over traditional fully compressible methods.

We have implemented the entire low Mach number algorithm in MAESTRO in an adaptive mesh refinement (AMR) framework. Our approach to AMR uses a nested

hierarchy of logically rectangular grids with successively finer grids at higher levels. The key difference between our method and most block-structured AMR methods stems from the presence of a one-dimensional base state whose time evolution is coupled to that of the full solution. The algorithm does not subcycle in time, i.e., the solution at all levels is advanced with the same time step. Complete details are available in [35].

6 Case Study: Type Ia Supernovae

Type Ia supernovae (SNe Ia) are important distance indicators in cosmology, responsible for the discovery of the acceleration of the expansion of the Universe. They are also important sites of nucleosynthesis, making half of the iron in our galaxy. Despite their great importance, there are major uncertainties in the theoretical understanding of SNe Ia, even as to what progenitor systems give rise to these explosions. One of the theoretically favored models is the explosion of a carbon/oxygen white dwarf (a compact star about the volume of Earth weighing roughly 1.4 solar masses, the Chandrasekhar limit) which accretes mass from a stellar companion. As its mass grows, the central temperature increases and carbon fusion reactions begin, driving convection throughout the white dwarf interior. This convection, during which heated parcels of fluid buoyantly rise away from the center and cool as they expand, can last for centuries [45]. Eventually the reactions proceed so vigorously that the hot parcels do not cool fast enough and a thermonuclear burning front (flame) is formed. This burning front propagates through the white dwarf in seconds, converting the majority of carbon and oxygen into heavy elements [including silicon, iron, and nickel (Ni)], releasing enough energy to unbind the star. The brightness of the event depends on how much radioactive ⁵⁶Ni is produced, and this in turn depends on how complete the burning is, the composition of the white dwarf, and at what densities it occurs (see e.g. [23, 42]). While there are great uncertainties in all phases of this picture, a critical uncertainty is the nature of the convection preceding ignition, and how that affects ignition of the first flame. Computationally it has been shown that variations in the location of the ignition lead to great differences in the explosion outcome [15, 30, 34, 39]. We conducted a computational study of this convective phase preceding explosion using MAESTRO.

In order to model convection in the (roughly) spherical self-gravitating white dwarf, the core algorithm in MAESTRO, which solves the low Mach number equations on a Cartesian grid, was modified to allow the base state to vary in the radial direction, which is not aligned with any of the coordinate axes [46]. In addition, we used AMR in order to focus spatial refinement on the regions of most intense heating where ignition was most likely to occur. This required a novel spatial mapping technique between the time-evolving one-dimensional radial base state and the hierarchical Cartesian mesh [35]. The procedure to expand the base state in response to large-scale heating is also considerably more complex for a self-gravitating fluid in a spherical geometry.

In a series of three papers [36, 46, 48] we presented results from a suite of simulations of the last few hours of convection preceding ignition. Once a burning front ignited we ended each simulation. However, by running many simulations and looking at the spatial and temporal distribution of "failed" hotspots (plumes that approached the ignition temperature but cooled before actually igniting) we built up statistics on the likelihood of ignition at a given radius from the center. Our major findings were:

- A strong jet-like feature dominates the outward-moving convective flow. This is similar to the dipole feature reported in previous studies [24], but more collimated and with a rapidly changing direction.
- Ignition most likely occurs at a single location, not multiple distinct locations all at once.
- Although the strongest heating occurs at the center of the star, ignition itself is most likely off-center, with a typical radius of 75 km from the center.
- The turbulent field in the convective layer follows Kolmogorov scaling with a smaller turbulent intensity and larger integral scale than assumed in previous works.
- The turbulent field is likely too weak to affect the initial flame propagation.

Figure 1 shows a snapshot of the convective region in the star. We see that a strong outflow feature (colored red) dominates the flow, and that the nuclear energy generation is strongly peaked toward the center of the star.

7 Future Work

MAESTRO in its current form can be used for a variety of astrophysical applications beyond that of modeling the Chandrasekhar-mass progenitor of SNe Ia. To date, MAESTRO has been used to study the sub-Chandra progenitor model for SNe Ia (in which burning begins in an accreted helium layer on the surface of a white dwarf) [47], core convection in massive stars [16, 17], and X-ray bursts [32]. MAESTRO simulation results have also provided the initial conditions for fully compressible simulations of the explosion phase of SNe Ia, as in [33]. Potential future applications include classical novae, proto-neutron star cooling, and convection in exoplanetary interiors.

Modeling warm, moist, non-precipitating flows in the earth's atmosphere with MAESTRO is easily achieved by assuming constant gravity, neglecting base state expansion, and including an appropriate equation of state for moist microphysics. A representation of phase change that is suitably accurate at the larger time steps of a low Mach number model must be used; see [11] for a discussion of the role of the time step in the accuracy of moist compressible models. An alternative, pseudo-incompressible, model for moist flows has been developed by [38].

Future developments of the MAESTRO code include the extension of the base state to include long-wavelength lateral variation. For future stellar modeling, we plan



Fig. 1 Snapshot of the convection region in a white dwarf seconds before a supernova explosion. The *red* and *blue* contours show the radial velocity field (*red* is outflow, *blue* is inflow) and the *yellow* to *green* to *purple* contours show the nuclear energy generation rate. The radius of this region is \sim 1000 km. Figure adopted from [36]

to include rotation of the star, which generates additional terms in the momentum equation as well as breaking the spherical symmetry of the base state. Finally, following recent studies in [25] of a generalized anelastic model compared to a standard anelastic model for moist flows, we plan to investigate further issues about the potential role of the pressure perturbation in the thermodynamics for both astrophysical and atmospheric applications.

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