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RESEARCH ARTICLE

A conservative, thermodynamically consistent numerical approach for low Mach number combustion. I. Single-level integration.

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We present a numerical approach for low Mach number combustion that conserves both mass and energy while remaining on the equation of state to a desired tolerance. We present both unconfined and confined cases, where in the latter the ambient pressure changes over time. Our overall scheme is a projection method for the velocity coupled to a multi-implicit spectral deferred corrections (SDC) approach to integrate the mass and energy equations. The iterative nature of SDC methods allows us to naturally incorporate a series of volume discrepancy corrections that lead to additional mass and energy influx/outflux in each finite volume cell in order to satisfy the equation of state. The method is second order, and satisfies the equation of state to a desired tolerance with increasing iterations. Motivated by experimental results, we test our algorithm on hydrogen flames with detailed kinetics. We examine the morphology of expanding cylindrical flames in high-pressure environments for confined and unconfined cases.

Keywords: low Mach number combustion, detailed chemistry and kinetics, thermodynamic pressure, confined domains, spectral deferred corrections

1. Introduction

Low Mach number numerical simulation methodology provides a valuable tool for efficiently modelling reacting flow with detailed kinetics and transport; see [1–8] for a variety of recent studies. Low Mach number models are derived from fully compressible equations using low Mach number asymptotics [9, 10] and do not include acoustic wave propagation, allowing for much larger time steps based on an advective CFL condition. Central to the low Mach number approximation is a decomposition of the pressure into a background ambient pressure plus a perturbational pressure that is order Mach number squared. The ambient pressure represents the thermodynamic state of the fluid. The perturbational pressure does not effect the thermodynamic state of the fluid. Asymptotic analysis shows that for small systems, the ambient pressure is spatially constant. For unconfined systems, the ambient pressure is constant in time whereas for confined systems, the ambient pressure is a function of time that is determined by the thermodynamic processes within the domain. (We note that for large-scale atmospheric or stellar environments with density stratification, the ambient pressure can vary with height and time [11, 12].)

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In the low Mach number system, the thermodynamic pressure is expressed in terms of the species masses and energy using an equation of state (EOS). The evolution of the mass and energy are constrained by the thermodynamic pressure, which ideally matches the ambient pressure. The perturbational pressure provides the mechanism for enforcing the constraint; it modifies the velocity field so that the combination of advection, diffusion, and reaction of the thermodynamic state leads to a thermodynamic pressure that matches the ambient pressure. Typically, in low Mach number systems, the constraint is recast as a divergence constraint on the velocity field, which is obtained by taking the Lagrangian derivative of the EOS. Analytically, this divergence constraint guarantees that the conservative evolution of mass and energy is thermodynamically consistent with the ambient pressure. However, in numerical simulations this is not true and the thermodynamic pressure will drift from the ambient pressure except in special cases (e.g., for a linear EOS). There are a number of choices for how to deal with this drift. One approach is to forego conservation and redefine either the mass or energy at the end of the integration step using the EOS and the ambient pressure. This approach has been used by many, and has been extended to adaptive meshes, and higher-order discretisations [13–18]. Another approach is to maintain conservation of mass and energy, and add a lagged correction term to the divergence constraint [19–21]. These methods are referred to as “volume discrepancy” approaches since they allow for additional mass and energy influx/outflux in each finite-volume cell to balance diffusion and reactions to maintain thermodynamic consistency. This correction term does not exactly preserve the EOS, but is able to control the drift to a modest degree.

Here we present a new volume discrepancy approach that iteratively modifies the constraint within a time step, so that we can reduce the thermodynamic drift to an arbitrary tolerance while maintaining conservation of mass and energy. Our overall temporal integration strategy is based on second-order projection methodology [22, 23] that extends Chorin’s approach for incompressible flow [24]. The distinguishing feature of our algorithm is the mass and energy integration, which uses a new multi-implicit spectral deferred correction (SDC) scheme. SDC algorithms, originally introduced by Dutt et al. [25] for ordinary differential equations, are a class of numerical methods that represent the solution as an integral in time and iteratively solve a series of correction equations to reduce the error. Bourlioux et al. [26, 27] introduced a multi-implicit SDC approach for advection-diffusion-reaction systems where advection terms are evaluated explicitly, reaction and diffusion terms treated implicitly, and different time steps are used for each process. Recently, we introduced a multi-implicit SDC algorithm for low Mach number reacting flow [20] and demonstrated increased efficiency and accuracy over Strang splitting. In this approach, we used an explicit discretisation for advection, a semi-implicit discretisation for diffusion, and a variable-order BDF scheme (VODE) [28] for reactions. We have also developed a fourth-order one-dimensional multi-implicit SDC algorithm using a backward Euler discretisation for reactions that incorporates an iterative volume discrepancy algorithm to reduce the thermodynamic drift [21].

In this paper, we present an improved version of the algorithm in [20], where we leverage the iterative nature of the scheme to compute a series of volume discrepancy correction terms, where in each iteration we more accurately enforce the EOS. Two iterations is sufficient for second-order accuracy, but we demonstrate that we can reduce the thermodynamic drift to a desired tolerance with increasing iterations. We also present the modifications required for confined domains, where the ambient pressure is a function of time. A general prescription for modelling ambient pressure changes was presented in seminal works that derived the low

Mach number equations [9, 10]. Here, we propose an iterative volume discrepancy approach that allows us to iteratively update the ambient pressure while satisfying the EOS and preserving conservation.

2. Model Equations

In the low Mach number regime, the characteristic fluid velocity is small compared to the sound speed (typically the Mach number is $M = U/c \sim \mathcal{O}(0.1)$ or smaller), and the effect of acoustic wave propagation is unimportant to the overall dynamics of the system. In a low Mach number numerical method, acoustic wave propagation is mathematically removed from the equations of motion, allowing for a time step based on an advective CFL condition. Thus, this approach leads to a $\sim 1/M$ increase in the allowable time step over an explicit compressible approach, if the time step is limited by advective transport. Note that a low Mach number method does not enforce that the Mach number remain small, but rather is suitable for flows in this regime.

In this paper, we use the low Mach number equation set from [19, 20], which is based on the model for low Mach number combustion introduced by Rehm and Baum [9] and rigorously derived from an asymptotic analysis by Majda and Sethian [10]. We consider a gaseous mixture ignoring Soret and Dufour effects, and assume a mixture model for species diffusion [29, 30]. The resulting equations are a set of partial differential equations for mass, momentum, and energy representing coupled advection, diffusion, and reaction processes that are closed by an EOS (here we use an ideal gas). We note that the ideal gas assumption is not central to the success of the method we propose, but does allow us to express the algorithm and subsequent examples more concretely.

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

$$p(\mathbf{x}, t) = p_0(t) + \pi(\mathbf{x}, t), \tag{1}$$

where p_0 is the ambient pressure and π is a perturbational pressure field satisfying $\pi/p_0 \sim \mathcal{O}(M^2)$. The evolution of the system is constrained so that the thermodynamic state of the fluid is consistent with the ambient pressure p_0. The perturbational pressure π controls the evolution of the velocity to preserve spatial homogeneity of the thermodynamic state of the fluid.

Using the notation in [19, 20], the evolution equations for the thermodynamic variables, $(\rho, \mathbf{Y}, h)$, are instantiations of mass and energy conservation:

$$\frac{\partial(\rho Y_m)}{\partial t} = -\nabla \cdot (\mathbf{U}\rho Y_m) - \nabla \cdot \mathbf{\Gamma}_m + \dot{\omega}_m, \tag{2}$$

$$\frac{\partial(\rho h)}{\partial t} = -\nabla \cdot (\mathbf{U}\rho h) + \frac{Dp_0}{Dt} + \nabla \cdot \frac{\lambda}{c_p}\nabla h + \sum_m \nabla \cdot h_m \left(\rho\mathcal{D}_m - \frac{\lambda}{c_p}\right)\nabla Y_m, \tag{3}$$

where ρ is the density, Y_m is the species m mass fraction with $\mathbf{Y}$ the vector of all mass fractions, $\mathcal{D}_m(\mathbf{Y}, T)$ are the species mixture-averaged diffusion coefficients, $\mathbf{\Gamma}_m \equiv -\rho\mathcal{D}_m\nabla Y_m$ are the species diffusion fluxes, $T = T(\rho, \mathbf{Y}, h)$ is the temperature, $\dot{\omega}_m(\mathbf{Y}, T)$ is the production rate for ρY_m due to chemical reactions, $h = \sum_m Y_m h_m$ is the enthalpy with $h_m = h_m(T)$ the enthalpy of species m, $\lambda(\mathbf{Y}, T)$ is the thermal conductivity, and $c_p = \sum_m Y_m dh_m/dT$ is the specific heat at constant pressure. Our definition of enthalpy includes the standard enthalpy of formation, so there is no net change to h due to reactions. Summing the species equations and noting that $\sum_m Y_m = 1$ and $\sum_m \dot{\omega}_m = 0$, we see that (2) implies the continuity equation,

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\mathbf{U}\rho). \tag{4}$$

A property of multicomponent diffusive transport is that the species diffusion fluxes, $\boldsymbol{\Gamma}_m$, must sum to zero in order to conserve total mass. For mixture models such as the one considered here that property is not satisfied in general. To conserve mass, these fluxes must be modified so that they sum to zero. We use the "conservation diffusion velocity" approach described in [19] to correct $\boldsymbol{\Gamma}_m$. Also, whenever $\boldsymbol{\Gamma}_m$ is evaluated implicitly (as is done in the implicit diffusion discretisations for Y_m), we first solve the implicit system, conservatively correct $\boldsymbol{\Gamma}_m$, and then modify the time-advanced values of Y_m to be consistent with the corrected fluxes. These modifications will be noted in the algorithm descriptions below.

The evolution equation for velocity is a form of conservation of momentum:

$$\rho \left(\frac{\partial \mathbf{U}}{\partial t} + \mathbf{U} \cdot \nabla \mathbf{U} \right) = -\nabla \pi + \nabla \cdot \boldsymbol{\tau}, \tag{5}$$

with stress tensor

$$\boldsymbol{\tau} = \mu \left[\nabla \mathbf{U} + (\nabla \mathbf{U})^T - \frac{2}{3} \boldsymbol{\mathcal{I}} (\nabla \cdot \mathbf{U}) \right], \tag{6}$$

where $\mu(\mathbf{Y}, T)$ is the viscosity and $\boldsymbol{\mathcal{I}}$ is the identity tensor.

The system is closed by specifying the EOS. Here we use the ideal gas EOS,

$$p_{\text{therm}} = \rho \mathcal{R} T \sum_m \frac{Y_m}{W_m}, \tag{7}$$

where $\mathcal{R}$ is the universal gas constant and W_m is the molecular weight of species m. In the low Mach number model, the thermodynamic pressure computed from the species masses and the energy using the EOS, p_{therm}, ideally is equal to the prescribed ambient pressure, p_0.

Equations (2), (3), (5) subject to (7) (with p_0 instead of p_{therm}) form the system that we would like to solve. Rather than directly attacking this system of constrained differential algebraic equations, we use a standard approach of recasting the EOS (7) as a divergence constraint on the velocity field. To do this, we differentiate the EOS in the Lagrangian frame of the moving fluid,

$$\frac{Dp}{Dt} = \frac{\partial p}{\partial \rho} \frac{D\rho}{Dt} + \frac{\partial p}{\partial T} \frac{DT}{Dt} + \sum_m \frac{\partial p}{\partial Y_m} \frac{DY_m}{Dt}, \tag{8}$$

Using continuity (4), taking the partial derivatives of (7) and rearranging terms, we rewrite (8) as

$$\nabla \cdot \mathbf{U} = \left(-\frac{1}{p} \frac{Dp}{Dt} + \frac{1}{T} \frac{DT}{Dt} + \frac{W}{W_m} \frac{DY_m}{Dt} \right), \tag{9}$$

where $W = (\sum_m Y_m / W_m)^{-1}$ is the mixture-averaged molecular weight. For open domains we replace p with the constraint ambient pressure, p_0. Next, we substitute in the evolution equations for temperature (converted from the enthalpy equation; see equation (12) in [19]), and species (2) to obtain the constraint

$$\nabla \cdot \mathbf{U} = \frac{1}{\rho c_p T}\left(\nabla \cdot \lambda \nabla T - \sum_m \mathbf{\Gamma}_m \cdot \nabla h_m\right) \\ -\frac{1}{\rho}\sum_m \frac{W}{W_m}\nabla \cdot \mathbf{\Gamma}_m + \frac{1}{\rho}\sum_m\left(\frac{W}{W_m} - \frac{h_m}{c_p T}\right)\dot{\omega}_m \equiv S, \tag{10}$$

Altogether, this approach leads to instantaneous acoustic equilibration while retaining local compressibility effects due to reactions, mass diffusion, and thermal diffusion. Analytically, this velocity field guarantees that the conservative evolution of mass and energy is thermodynamically consistent with the ambient pressure.

3. Volume Discrepancy

In our time-advancement scheme, as part of the computation of the advective fluxes for mass and energy we apply a projection operator to compute advection velocities at cell faces that discretely satisfy the divergence constraint (10). In our derivation of the constraint, we reformulated (8) as (9) by substituting in the evolution equations for temperature, species, and density while assuming the pressure is constant. Thus, the resulting velocity field corresponds analytically to the velocity required so that the advective fluxes of mass and energy lead to constant thermodynamic pressure. Numerically this is not the case, and the solution drifts from the EOS. The key observation in volume discrepancy approaches is that we can replace the derivative of pressure in (9) with local numerical values that specify how we wish the local thermodynamic pressure to change over a time step to account for the numerical drift. After numerical integration over a time step, for a given cell if the thermodynamic pressure is too low, the net flux into the cell needs to be increased; if it is too high, the net flux needs to be decreased.

Before proceeding to the iterative scheme, it is important to note that in general, the mass and energy are not in thermodynamic equilibrium at the beginning of a time step, so we define a correction term, χ, to the right-hand-side of the velocity constraint based on the local corrections required in each cell to be used in the first SDC iteration,

$$\chi = \frac{1}{p^n_{\text{therm}}}\frac{p^n_{\text{therm}} - p_0}{\Delta t}. \tag{11}$$

Again, this correction can be derived by considering (9) and the fact that we are adding an additional term to the right-hand-side with the intent of changing the thermodynamic pressure locally in each cell.

Next we perform a series of SDC correction steps, each iteratively updating the time-advanced solution. At the end of each SDC iteration, we increment χ based on the latest thermodynamic pressure, where the superscript (k) denotes the time-advanced solution after the k^{th} SDC iterate,

$$\chi := \chi + \frac{1}{p^{(k)}_{\text{therm}}}\frac{p^{(k)}_{\text{therm}} - p_0}{\Delta t}. \tag{12}$$

This correction term is used in the projection operator to compute the updated advection velocities in the next iteration.

In our previous work [20], we only included the initial volume discrepancy correction using the state at t^n and did not iteratively modify χ. Here, we modify χ with each SDC iteration, which effectively drives the deviation of the thermodynamic pressure from the ambient pressure to zero with increasing iteration count. A similar technique is used in our our fourth-order approach for one-dimensional low Mach number combustion [21]. The full implementation details for our scheme are given in Section 5.

4. Confined Domain Ambient Pressure

In our previous work, we have considered unconfined domains where the ambient pressure is constant in time. For confined domain systems this is not the case. The mathematical formulation describing how the ambient pressure evolves over time was originally derived in [9, 10]. Here we summarize this results, and describe how to incorporate a volume discrepancy approach so that the thermodynamic variables evolve in a consistent manner. In the derivation of (10) we assumed p_0 was constant. If p_0 is a function of time, we restore the pressure derivative term so the constraint becomes,

$$\nabla \cdot \mathbf{U} + \theta \frac{dp_0}{dt} = S \tag{13}$$

where $\theta \equiv 1/(\Gamma_1 p_0)$, with $\Gamma_1 = \partial \ln(p)/\partial \ln(\rho)|_s$ is the first adiabatic exponent. We note that here, unlike in the work of Majda and Sethian [10], Γ_1 depends on composition and is not a constant. A detailed derivation of θ can be found in Appendix A of [31]. The unknowns in (13) are $\mathbf{U}$ and dp_0/dt. We can rewrite this equation as follows:

$$\nabla \cdot \mathbf{U} + (\bar{\theta} + \delta\theta) \frac{dp_0}{dt} = \bar{S} + \delta S, \tag{14}$$

where $\bar{\theta}$ and $\bar{S}$ are the mean values of θ and S over the domain, and $\delta\theta$ and δS are perturbations off the mean that, by definition, integrate to zero over the domain. Thus, $S = \bar{S} + \delta S$ and $\theta = \bar{\theta} + \delta\theta$. By the divergence theorem $\int \nabla \cdot \mathbf{U}\, dV = 0$ in a closed domain, since the normal velocity is equal to zero on the entire domain boundary. Furthermore, p_0 is only a function of time. These observations allow us to decompose changes in the thermodynamic state into an evolution equation for p_0

$$\bar{\theta} \frac{dp_0}{dt} = \bar{S}. \tag{15}$$

and a velocity constraint,

$$\nabla \cdot \mathbf{U} = \delta S - \delta\theta \frac{dp_0}{dt} \tag{16}$$

$$= \delta S - \delta\theta \frac{\bar{S}}{\bar{\theta}}. \tag{17}$$

We can again use χ to remain on the equation of state, but we need to split $\chi = \bar{\chi} + \delta\chi$ into mean and perturbational components in order to form a solvable system for dp_0/dt and $\mathbf{U}$. The full details are described in the time-advancement scheme below.

5. Numerical Algorithm

Our overall temporal integration strategy uses the projection method framework discussed in Day and Bell [19], which is based on second-order extensions [22, 23] of Chorin's algorithm for incompressible flow [24]. We use an explicit discretisation for the convective terms and a semi-implicit treatment of momentum diffusion to create a provisional update to the velocity field. The velocity field is projected onto the space satisfying the divergence condition (10) for open domains or (17) for closed domains while simultaneously updating the perturbational pressure, π. Within this framework, we incorporate a new temporal integration scheme for the mass and energy. Our approach is based on the multi-implicit SDC approach originally presented in [26, 27] for reacting gas dynamics, and later extended to low Mach number combustion in [20]. We refer the reader to Sections 3.1 and 3.2 in [20] for an overview on SDC methods, and on how the multi-implicit formulation can be applied to the mass and energy evolution. To summarize, we couple advection, diffusion, and reaction by iteratively re-integrating each physical process using lagged source terms representing the effects of the other physical processes. We use a second-order explicit Godunov scheme for advection, a semi-implicit discretisation of diffusion, and a high-order stiff chemical kinetics solver (VODE) [28] for reactions. The source terms are carefully constructed in a way that reduces splitting error as the number of iterations increase.

The algorithm in this paper differs from [20] in three ways. The first change is that rather than perform a predictor and a series of corrector steps, we have re-factored our algorithm to require only a series of notationally identical corrector steps. This is a simplification of the algorithm that still preserves the convergence properties of SDC methods. Second, our volume discrepancy approach for maintaining the equation of state requires iteratively recomputing the advective velocities used to construct mass and energy fluxes, as outlined in Section 3. Third, we present the modifications required to track the ambient pressure change while maintaining the equation of state for confined domains, as outlined in Section 4.

We use a finite-volume, Cartesian grid approach with constant grid spacing, where $\mathbf{U}$, ρ, $\mathbf{Y}$, h, and T represent cell averages at integer indexed time levels t^n, whereas π is defined at nodal point-values at half time levels, $t^{n-1/2}$. We wish to advance the species (2), enthalpy (3), and momentum (5) in time subject to constraint (10). The thermodynamic variable advance is a series of SDC corrector steps. We use the superscript "(k)" notation to denote the time-advanced solution at t^{n+1} after the k^{th} iterate. When we denote the right-hand-side of the constraint, S, and also transport coefficients with a superscript "n", "(k)", "$n+1$", etc., it is understood that they are computed directly from the corresponding thermodynamic variables.

Given the complete state at t^n (and pressure $\pi^{n-1/2}$), here are the steps to advance the solution by Δt to t^{n+1}:

Step 1: (*Compute unconstrained advection velocities*) Use a second-order Godunov procedure to predict a time-centered velocity, $\mathbf{U}^{n+1/2,*}$, on cell faces. This procedure is identical to the algorithm described in detail in Section 2.1 of [32] for computing normal velocities on cell faces. The provisional field, $\mathbf{U}^{n+1/2,*}$, represents a normal velocity on cell faces analogous to a MAC-type staggered grid discretisation of the Navier-Stokes equations (see [33], for example). However,

$\mathbf{U}^{n+1/2,*}$ fails to satisfy the divergence constraint (10).

Step 2: (*Initialize time-advanced thermodynamic variables*) We set the initial estimate for the thermodynamic variables at t^{n+1} equal to the state at t^n, i.e., $(\rho h, \rho\mathbf{Y})^{(k=0)} = (\rho h, \rho\mathbf{Y})^n$. Also, set the first estimate for the updated ambient pressure in the same way, $p_0^{(k=0)} = p_0^n$. We will loop over **Steps 3** and **4** to iteratively update this estimate. We also initialize the volume discrepancy correction to $\chi^{n+1/2,(k=0)} = 0$ and will iteratively increment this correction term.

Next, we loop over **Step 3** and **Step 4** from $k = 1, k_{\max}$ as follows:

Step 3: (*Compute constrained advection velocities*) Update χ using the current estimate for the time-advanced state,

$$\chi^{n+1/2,(k)} = \chi^{n+1/2,(k-1)} + \frac{1}{p_{\mathrm{therm}}^{(k-1)}} \frac{p_{\mathrm{therm}}^{(k-1)} - p_0^{(k-1)}}{\Delta t}. \tag{18}$$

Again, note that in the first iteration ($k = 1$), all quantities with a $(k-1)$ superscript are copies of the state from t^n. Next we define a time-centered right-hand-side for the constraint equation (noting that we include χ in the right-hand-side) along with a time-centered θ,

$$S^{n+1/2,(k)} = \left(\frac{S^n + S^{(k-1)}}{2} + \chi^{n+1/2,(k)} \right), \tag{19}$$

$$\theta^{n+1/2,(k)} = \frac{\theta^n + \theta^{(k-1)}}{2}. \tag{20}$$

We want to solve the following constraint equation for the velocity and the time-derivative of the ambient pressure,

$$\nabla \cdot \mathbf{U}^{n+1/2,(k)} + \theta^{n+1/2,(k)} \left(\frac{dp_0}{dt} \right)^{(k)} = S^{n+1/2,(k)} \tag{21}$$

For unconfined domains, we set $(dp_0/dt)^{(k)} = 0$, and define $S_{\mathrm{eff}}^{n+1/2,(k)} = S^{n+1/2,(k)}$. For confined domains, we split θ and S into average and perturbational quantities,

$$\nabla \cdot \mathbf{U}^{n+1/2,(k)} + (\bar{\theta}^{n+1/2,(k)} + \delta\theta^{n+1/2,(k)}) \left(\frac{dp_0}{dt} \right)^{(k)} = \bar{S}^{n+1/2,(k)} + \delta S^{n+1/2,(k)}. \tag{22}$$

In order for this system to be solvable, we set the spatially constant terms equal to each other,

$$\left(\frac{dp_0}{dt} \right)^{(k)} = \frac{\bar{S}^{n+1/2,(k)}}{\bar{\theta}^{n+1/2,(k)}}, \tag{23}$$

and define a pressure update using this derivative,

$$p_0^{(k)} = p_0^n + \Delta t \left(\frac{dp_0}{dt} \right)^{(k)}. \tag{24}$$

The velocity is now subject to the following constraint, noting that by construction the terms on the right-hand-side integrate to zero over the domain,

$$\nabla \cdot \mathbf{U}^{n+1/2,(k)} = \delta S^{n+1/2,(k)} - \delta\theta^{n+1/2,(k)} \left(\frac{dp_0}{dt}\right)^{(k)} \equiv S_{\mathrm{eff}}^{n+1/2,(k)}. \tag{25}$$

For both confined and unconfined domains, we apply a discrete projection by first solving the elliptic equation,

$$D^{\mathrm{F}\to\mathrm{C}} \frac{1}{\rho^n} G^{\mathrm{C}\to\mathrm{F}} \phi^{(k)} = D^{\mathrm{F}\to\mathrm{C}} \mathbf{U}^{n+1/2,*} - S_{\mathrm{eff}}^{n+1/2,(k)}, \tag{26}$$

for a cell-averaged $\phi^{(k)}$, where $D^{\mathrm{F}\to\mathrm{C}}$ represents a cell-averaged divergence of face-averaged data, and $G^{\mathrm{C}\to\mathrm{F}}$ represents a face-averaged gradient of cell-averaged data, and ρ^n is computed on cell faces using arithmetic averaging from neighboring cells. The solution, $\phi^{(k)}$, is then used to define face-centered velocities that satisfy the constraint,

$$\mathbf{U}^{n+1/2,(k)} = \mathbf{U}^{n+1/2,*} - \frac{1}{\rho^n} G^{\mathrm{C}\to\mathrm{F}} \phi^{(k)}. \tag{27}$$

Thus, $\mathbf{U}^{n+1/2,(k)}$ is a second-order accurate, staggered grid vector field at $t^{n+1/2}$ that discretely satisfies the constraint (10), and is used for computing the time-explicit advective fluxes for ρh, and $\rho \mathbf{Y}$, and time-explicit convective term for $\mathbf{U}$.

Step 4: (*Advance thermodynamic variables*) There are several sub-steps involved in integrating $(\rho\mathbf{Y}, \rho h)$ over the full time step to obtain an updated estimate of the time-advanced state.

Step 4a: (*Advection step*) We use a standard unsplit multidimensional Godunov scheme [34, 35] using upwinding based on the constrained MAC velocity field, $\mathbf{U}^{n+1/2,(k)}$, to compute face-centered, time-centered edge states for mass and energy, $(\rho\mathbf{Y}, \rho h)^{n+1/2,(k)}$. This procedure is also described in detail in Section 2.1 of [32]. Note that the equations of motion (2) and (3) have the general form,

$$\frac{\partial(\rho Y_m)}{\partial t} + \nabla \cdot (\mathbf{U}\rho Y_m) = \mathcal{R}_{\rho Y_m} \tag{28}$$

$$\frac{\partial(\rho h)}{\partial t} + \nabla \cdot (\mathbf{U}\rho h) = \mathcal{R}_{\rho h}. \tag{29}$$

In the Godunov scheme, the forcing terms, $\mathcal{R}_{\rho Y_m}$ and $\mathcal{R}_{\rho h}$, are explicitly evaluated from the t^n state, except for the time derivative of the ambient pressure, where we use (23), and for the reaction term in the mass equations, where we use lagged estimates of the integral of $\dot{\omega}_m$ over the time step.

The face-centered, time-centered velocities and scalars are used to construct advective flux divergences that are used in subsequent steps to solve for mass and enthalpy diffusion implicitly, as well as part of the source term in the reaction integration.

We can now integrate total density over Δt to advance ρ^n to $\rho^{(k)}$ using

$$\rho^{(k)} = \rho^n - \Delta t \nabla \cdot (\mathbf{U}\rho)^{n+1/2,(k)}. \tag{30}$$

Step 4b: (*Mass diffusion correction equation.*) Compute conservatively corrected versions of $\mathbf{\Gamma}_m^{(k-1)} = -\rho^{(k-1)}\mathcal{D}_m^{(k-1)}\nabla Y_m^{(k-1)}$. Then, following the multi-implicit SDC approach, compute provisional, time-advanced species mass fractions, $Y_{m,\mathrm{AD}}^{(k)}$, by solving a backward Euler type correction equation,

$$\begin{aligned}\frac{\rho^{(k)}Y_{m,\mathrm{AD}}^{(k)} - (\rho Y_m)^n}{\Delta t} &= -\nabla\cdot(\mathbf{U}\rho Y_m)^{n+1/2,(k)} \\ &+\nabla\cdot\rho^{(k-1)}\mathcal{D}_m^{(k-1)}\nabla Y_{m,\mathrm{AD}}^{(k)} - \frac{1}{2}\nabla\cdot\left(\mathbf{\Gamma}_m^n - \mathbf{\Gamma}_m^{(k-1)}\right) + I_{R,\rho Y_m}^{(k-1)}. \qquad (31)\end{aligned}$$

Note that $I_{R,\rho Y_m}^{(k-1)}$ is the effect of the chemistry, defined iteratively in equation (36). In the first SDC iteration, we use the final value from the previous time step. Each of the species equations is implicit, requiring a linear solve for $Y_{m,\mathrm{AD}}^{(k)}$.

Next, compute conservatively corrected versions of iteratively-lagged species fluxes, $\mathbf{\Gamma}_{m,\mathrm{AD}}^{(k)} = -\rho^{(k-1)}\mathcal{D}_m^{(k-1)}\nabla Y_{m,\mathrm{AD}}^{(k)}$ and define an effective contribution of advection-diffusion to the update of ρY_m,

$$Q_{\rho Y_m}^{(k)} = -\nabla\cdot(\mathbf{U}\rho Y_m)^{n+1/2,(k)} - \nabla\cdot\mathbf{\Gamma}_{m,\mathrm{AD}}^{(k)} - \frac{1}{2}\nabla\cdot\left(\mathbf{\Gamma}_m^n - \mathbf{\Gamma}_m^{(k-1)}\right). \qquad (32)$$

Step 4c: (*Enthalpy diffusion correction equation.*) Following the multi-implicit SDC approach, compute a provisional, time-advanced enthalpy, $h_{\mathrm{AD}}^{(k)}$, by solving a backward Euler type correction equation,

$$\begin{aligned}\frac{\rho^{(k)}h_{\mathrm{AD}}^{(k)} - (\rho h)^n}{\Delta t} &= -\nabla\cdot(\mathbf{U}\rho h)^{n+1/2,(k)} + \left(\frac{dp_0}{dt}\right)^{(k)} \\ &+\nabla\cdot\frac{\lambda^{(k-1)}}{c_p^{(k-1)}}\nabla h_{\mathrm{AD}}^{(k)} + \frac{1}{2}\left(\nabla\cdot\frac{\lambda^n}{c_p^n}\nabla h^n - \nabla\cdot\frac{\lambda^{(k-1)}}{c_p^{(k-1)}}\nabla h^{(k-1)}\right) \\ &-\frac{1}{2}\sum_m\nabla\cdot\left[h_m^n\left(\mathbf{\Gamma}_m^n + \frac{\lambda^n}{c_p^n}\nabla Y_m^n\right) + h_m^{(k-1)}\left(\mathbf{\Gamma}_m^{(k-1)} + \frac{\lambda^{(k-1)}}{c_p^{(k-1)}}\nabla Y_m^{(k-1)}\right)\right]. \\ &\qquad (33)\end{aligned}$$

The enthalpy term is implicit, requiring a linear solve for $h_{\mathrm{AD}}^{(k)}$, whereas the species enthalpy terms, h_m, are discretized with a trapezoidal rule using iteratively lagged, time-advanced values of h_m in order to avoid a more computationally expensive linear system. Once we have computed $h_{\mathrm{AD}}^{(k)}$, we define $Q_{\rho h}^{(k)}$ as the evaluation of the right-hand side of (33), which represents an effective contribution of advection-diffusion to the update of ρh.

Step 4d: (*Chemistry integration.*) Use the VODE [28] package to integrate species (2) and enthalpy (3) over Δt to advance $(\rho\mathbf{Y}, \rho h)^n$ to $(\rho\mathbf{Y}, \rho h)^{(k)}$ using the advection/diffusion source terms, $Q_{\rho Y_m}^{(k)}$ and $Q_{\rho h}^{(k)}$ (defined in **Step 4b** and **4c**):

$$\frac{\partial(\rho Y_m)}{\partial t} = Q_{\rho Y_m}^{(k)} + \dot{\omega}_m(\mathbf{Y}, T). \qquad (34)$$

$$\frac{\partial(\rho h)}{\partial t} = Q_{\rho h}^{(k)}. \qquad (35)$$

After the integration is complete, we compute the effect of reactions in the evolution of ρY_m in the VODE integration by defining

$$I_{R,\rho Y_m}^{(k)} = \frac{(\rho Y_m)^{(k)} - (\rho Y_m)^n}{\Delta t} - Q_{\rho Y_m}^{(k)}. \tag{36}$$

If $k < k_{\max}$, set $k = k+1$ and return to **Step 3**. Otherwise, the time-advancement of the thermodynamic variables is complete, and set the new-time thermodynamic variables using $(\rho Y_m, \rho h, p_0)^{n+1} = (\rho Y_m, \rho h, p_0)^{(k)}$.

Step 5: (*Advance the velocity*) Next, we compute a provisional time-advanced, cell-averaged velocity field, $\mathbf{U}^{n+1,*}$ using the lagged pressure gradient, by solving

$$\rho^{n+1/2}\left(\frac{\mathbf{U}^{n+1,*} - \mathbf{U}^n}{\Delta t} + \mathbf{U}^{(k_{\max}),n+1/2} \cdot \nabla \mathbf{U}^{n+1/2}\right) = \frac{1}{2}\left(\nabla \cdot \boldsymbol{\tau}^n + \nabla \cdot \boldsymbol{\tau}^{n+1,*}\right) - \nabla \pi^{n-1/2}, \tag{37}$$

where $\boldsymbol{\tau}^{n+1,*} = \mu^{n+1}[\nabla \mathbf{U}^{n+1,*} + (\nabla \mathbf{U}^{n+1,*})^T - \frac{2}{3}\boldsymbol{\mathcal{I}} S^{n+1}]$ and $\rho^{n+1/2} = (\rho^n + \rho^{n+1})/2$. This is a semi-implicit discretisation for $\mathbf{U}^{n+1,*}$, requiring a linear solve. The face-centered, time-centered velocity in the convective term, $\mathbf{U}^{n+1/2}$, is computed using the same algorithm used for the face-centered, time-centered mass and energy. At this point, the intermediate cell-centered, new-time velocity field $\mathbf{U}^{n+1,*}$ does not satisfy the constraint (10). Hence, we apply an approximate projection to decompose $\mathbf{U}^{n+1,*}$ into an update of the perturbational pressure field and the final new-time velocity, $\mathbf{U}^{n+1}$. In particular, we solve

$$L^{\mathrm{N}\to\mathrm{N}}\phi^{\mathrm{N}} = D^{\mathrm{C}\to\mathrm{N}}\left(\mathbf{U}^{n+1,*} + \frac{\Delta t}{\rho^{n+1/2}} G^{\mathrm{N}\to\mathrm{C}}\pi^{n-1/2}\right) - S_{\mathrm{eff}}^{n+1} \tag{38}$$

for nodal values of ϕ^{N}. Here, $L^{\mathrm{N}\to\mathrm{N}}$ represents a nodal Laplacian of nodal data, computed using the standard bilinear finite-element approximation to $\nabla \cdot (1/\rho^{n+1/2})\nabla$. Also, $D^{\mathrm{C}\to\mathrm{N}}$ is a discrete second-order operator that approximates the divergence at nodes from cell-averaged data and $G^{\mathrm{N}\to\mathrm{C}}$ approximates a cell-averaged gradient from nodal data. For open chambers, $S_{\mathrm{eff}}^{n+1} = S^{n+1}$. For closed chambers, we do not need to compute an update to p_0 in this step since we have already computed a new ambient pressure that is consistent with thermodynamic processes. In order to address solvability issues, following our splitting of θ and S into average and perturbational quantities used in the MAC projection (see equation (17)), we have

$$S_{\mathrm{eff}}^{n+1} = \delta S^{n+1} - \delta\theta^{n+1}\frac{\bar{S}^{n+1}}{\bar{\theta}^{n+1}}. \tag{39}$$

Also note that there is no χ correction in this projection since these velocities are not directly used to compute the advection terms for the thermodynamic variables. Equation (38) requires nodal values of S_{eff}^{n+1}, which we obtain by averaging the neighboring cell-averaged values. Finally, we determine the new-time cell-averaged velocity field using

$$\mathbf{U}^{n+1} = \mathbf{U}^{n+1,*} - \frac{\Delta t}{\rho^{n+1/2}} G^{\mathrm{N}\to\mathrm{C}}(\phi^{\mathrm{N}} - \pi^{n-1/2}), \tag{40}$$

and the new time-centered pressure using $\pi^{n+1/2} = \phi^{\mathrm{N}}$. This completes the description of the time-advancement algorithm.

6. Results

Here we illustrate the behavior of the new algorithms on hydrogen flames. For the simulations we use the H_2/O_2 kinetic model of Burke et al. [36]. We examine the performance of our algorithm using premixed hydrogen flames in one and two dimensions. First, we examine the convergence rates and thermodynamic consistency of our algorithm for both confined and unconfined domains. Second, motivated by experiments [37, 38], we examine the morphology of expanding cylindrical flames in high-pressure environments for confined and unconfined cases.

6.1 Convergence and Thermodynamic Consistency

The initial conditions are obtained by interpolating from a frame-shifted, refined steady 798-point, one-dimensional premixed flame solution computed using the PREMIX code at 10 atm pressure and an equivalence ratio of 0.4. The computational domain has length 0.75 cm. Refer to Figure 1 for the initial configuration of the reactants, products, and temperature, as well as the final temperature profiles for the unconfined and confined cases. We divide the domain into 512, 1024, and 2048 computational cells, and use time steps of $\Delta t = 50$, 25, and 12.5 μs, respectively. These time steps correspond to an advective CFL of $\sigma \sim 0.2$ for the unconfined case, and $\sigma \sim 0.1$ for the confined case (since the maximum velocity is smaller). We evolve the flame for 2.5 ms to allow the initial data to relax on the coarse grid, and allow the flame to propagate a non-trivial distance through the domain. We perform each simulation using 2, 3, 4, and 8 SDC iterations for both the unconfined and confined cases. For the confined case, we use adiabatic, no-slip boundary conditions. As seen in Figure 1, for the confined case the flame propagates more slowly with an increased temperature in the burned region; we will explore this in more detail in our two-dimensional calculations.

In Table 1, we report convergence rates using 2 SDC iterations for the unconfined and confined domain cases for velocity and key thermodynamic variables based on the L_1 norm of errors over the entire domain. For the confined case, we also include the convergence rate of the time-evolving ambient pressure, which rises from 10 atm to approximately 10.6 atm in the course of this simulation. We see second-order convergence in each variable. We also performed the same convergence test using 3, 4, and 8 SDC iterations and as expected, we achieve second-order convergence in each variable. Even though the order of accuracy of the method does not improve, the L_1 norm of the errors in each variable for the finest simulations with 8 iterations are $\sim 40\%$ smaller than the 2 iteration simulations. This is expected since additional SDC iterations will decrease the splitting error between physical processes [26, 27]. Also, we demonstrate that additional SDC iterations decreases the thermodynamic drift. In particular, in Figures 2 and 3, we show the effect of increasing number of SDC iterations on the thermodynamic drift for the 2048 zone simulation. We observe a significant decrease in drift with each iteration. For the unconfined case, the L_1 (and L_∞) norm of the drift decreases by a factor of 9.0 (7.6) when increasing the iterations from 2 to 3, and then decreases by another factor of 7.1 (6.1) when increasing the iterations from 3 to 4. By 8 iterations, the maximum drift is 0.05 Pa. For the confined case, the L_1 (and L_∞) norm of the drift decreases by a factor of 8.8 (7.5) when increasing the iterations from 2 to 3, and then decreases by another factor of 6.0 (4.8) when increasing the iterations from 3 to 4. By 8 iterations, the maximum drift is 0.06 Pa. We conclude that 2 SDC iterations is sufficient for second-order accuracy, however there are still gains to be had from performing additional SDC iterations from a thermodynamic consistency

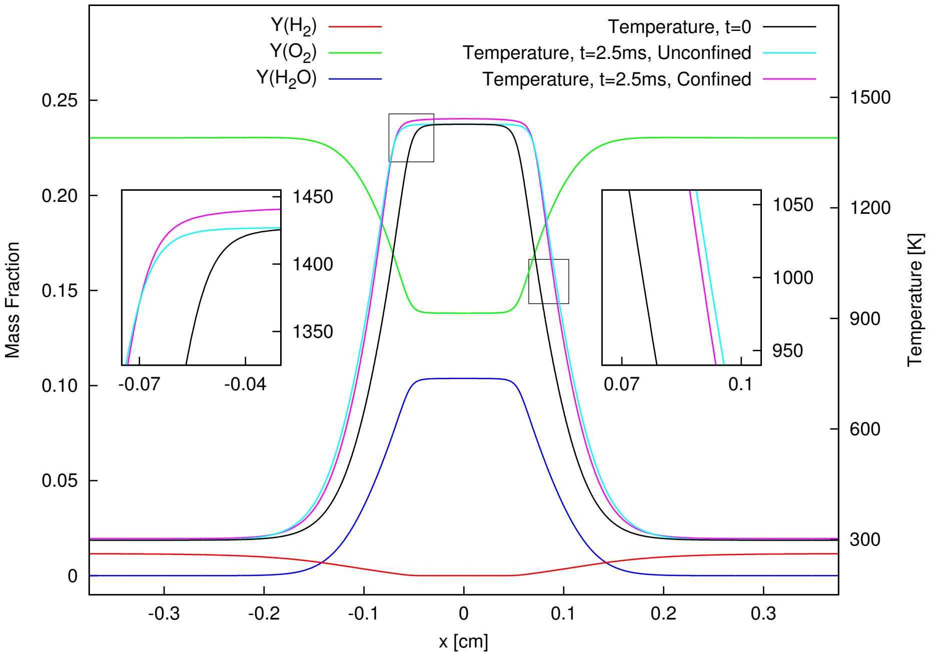

Figure 1. Initial profiles of the primary reactants, product, and temperature for a one-dimensional premixed hydrogen flame. Also shown is the final ($t = 2.5$ ms) temperature profile for unconfined and confined cases. We highlight two regions of the flame to illustrate the temperature increase in the burned region (left) and the differences in flame front propagation (right) for the confined and unconfined cases.

standpoint.

Table 1. Convergence rates in L_1 for a premixed hydrogen flame for the confined and unconfined cases using 2 SDC iterations. We observe second-order convergence for all variables, including the time-dependent ambient pressure for the confined case.

	Unconfined	Confined
$Y(\mathrm{H})$	1.80	1.79
$Y(\mathrm{H_2})$	3.13	2.85
$Y(\mathrm{O})$	1.92	1.89
$Y(\mathrm{OH})$	2.06	2.02
$Y(\mathrm{H_2O})$	2.40	2.20
$Y(\mathrm{O_2})$	2.33	2.25
$Y(\mathrm{HO_2})$	2.05	2.14
$Y(\mathrm{H_2O_2})$	2.16	2.11
$Y(\mathrm{N_2})$	2.88	2.83
ρ	2.20	2.29
h	2.24	2.24
T	2.23	2.18
U	2.15	2.14
p_0		3.19

6.2 Cylindrical Flames

We now perform more detailed calculations of the surface morphology of expanding cylindrical hydrogen flames in high-pressure environments. Our simulations are based on studies in [37, 38]. We defer more detailed, three-dimensional, adaptive mesh refinement (AMR) simulations to our next paper where we describe the

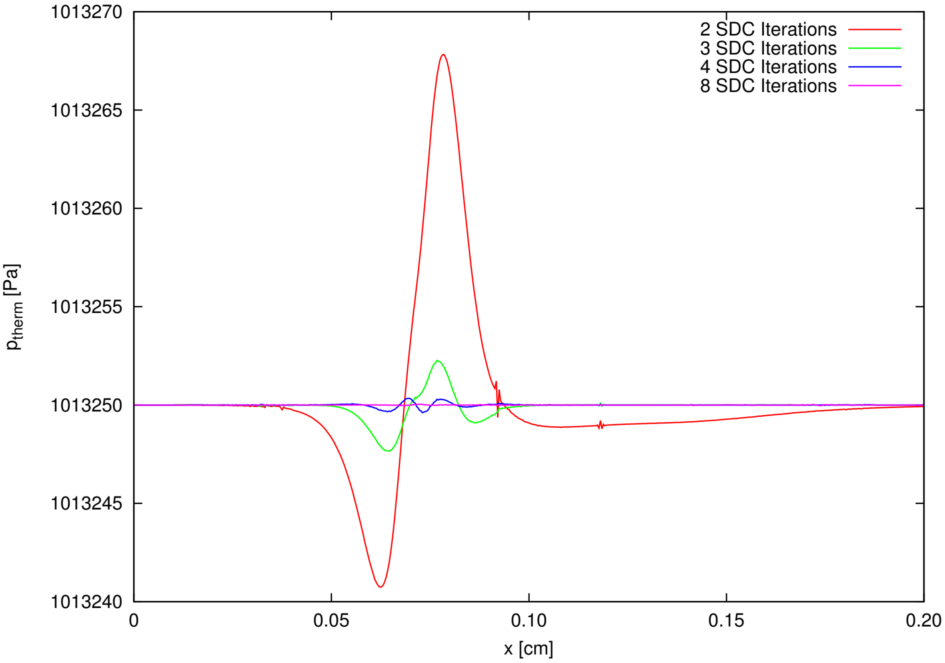

Figure 2. Thermodynamic pressure for the unconfined case at the final time using 2, 3, 4, and 8 SDC iterations. As the number of SDC iterations increases, the thermodynamic drift is greatly reduced.

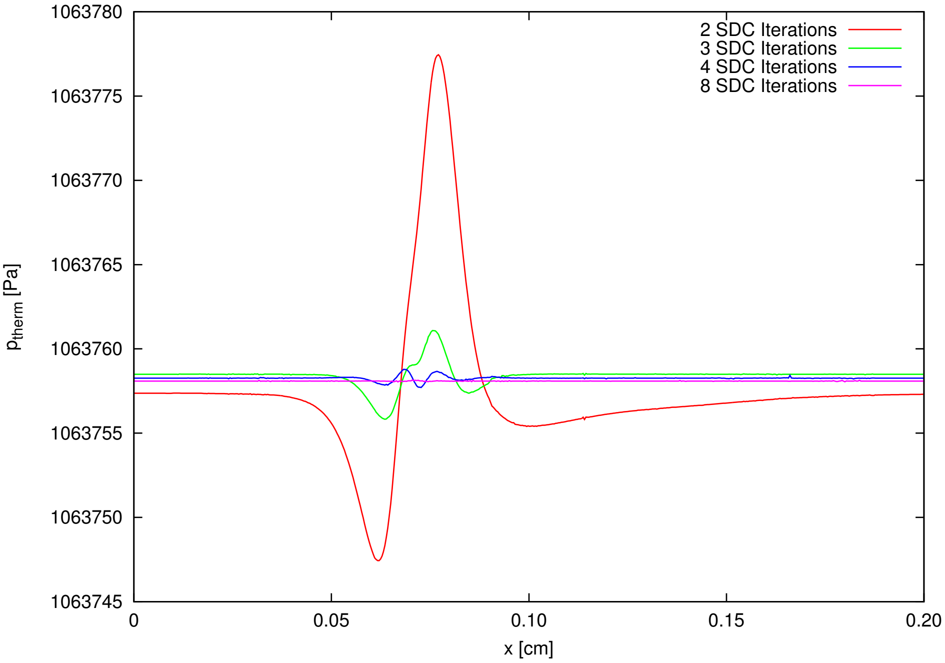

Figure 3. Thermodynamic pressure for the confined case at the final time using 2, 3, 4, and 8 SDC iterations. We note that the algorithm is able to capture the $\sim 5\%$ rise in ambient pressure while simultaneously reducing the thermodynamic drift with increasing iteration count.

modifications required to perform AMR. Here we perform confined and unconfined simulation and compare the results.

The two-dimensional simulation domain is 3 cm square with 2048^2 computational zones. Thus our spatial resolution matches the coarsest resolution used in the convergence study above. We use the same PREMIX solution used in the convergence study to initialize the domain, and radially map the solution with an angle-dependent three-mode sinusoidal perturbation. The time step changes over the simulation so that in each step it respects an advective CFL number of $\sigma = 0.2$, so a typical time step is $\sim 20\mu$s, noting that the flame accelerates over time. We use 3 SDC iterations to control the thermodynamic drift.

In Figures 4 and 5 we show temperature profiles of the initial configuration, as well as profiles at $t = 20, 40, 50$, and 60 ms (for both cases), as well as $t = 70, 80$ and 100 ms for the confined case. We halt the open domain simulation shortly after $t = 60$ ms since the flame front passes through the domain boundary. We note that for the first 50 ms, the flame morphology looks qualitatively very similar. By 60 ms, the unconfined flame has expanded to a noticeably larger fraction of the domain. This can be more clearly seen in Figure 6, which shows a horizontal profile of the density field about the center of the domain in the initial data, and at $t = 60$ ms.

We see in the confined case that by $t = 100$ ms, the flame has expanded to cover nearly the entire the computational domain, and the maximum temperature in the burnt region has increased from $\sim$ 1400 K (at $t = 0$), to $\sim$ 1700 K (at $t = 60$ ms) to $\sim$ 2100 K (at $t = 100$ ms). In Figure 7, we plot the maximum temperature as a function of time for both simulations, as well as the fuel temperature for the confined case, which rises from 298 K to 475 K over the course of the simulation due to the ambient pressure and fuel density increase. Also included in Figure 7 is a plot of the ambient pressure as a function of time for the confined case, which rises from 10 atm to 54 atm.

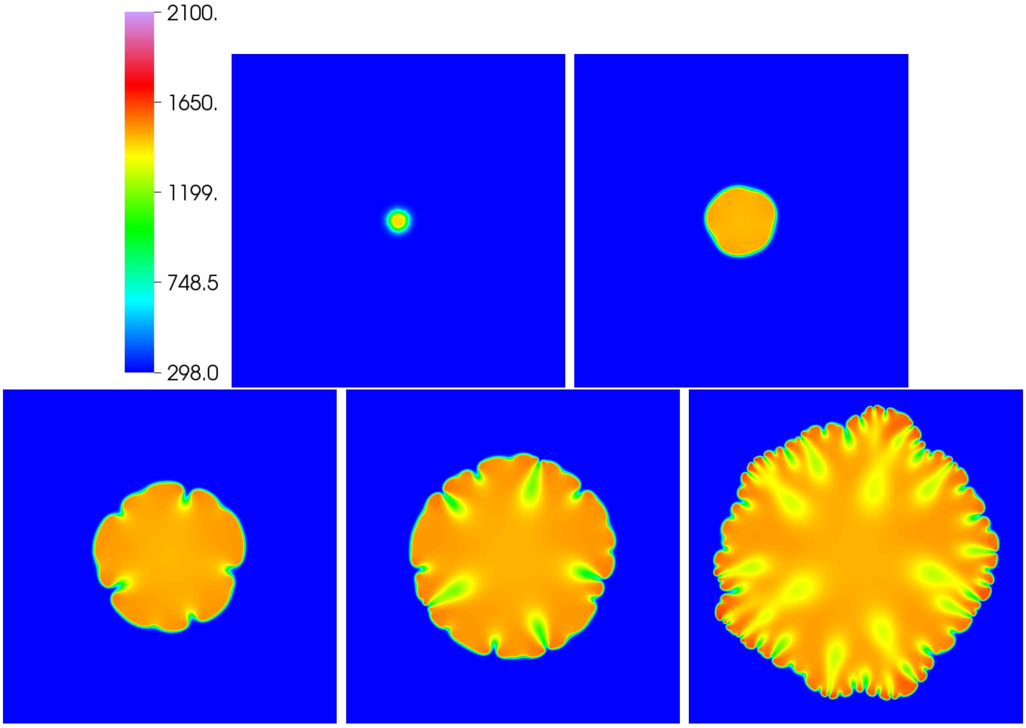

Figure 4. Temperature profiles of an unconfined premixed hydrogen flame at $t = 0, 20, 40, 50$, and 60 ms. Comparing directly to the first five frames in Figure 5, we see that the size of the burned region is noticeably larger.

In Figure 8 we plot the mass of H_2O product as a function of time for both simulations. Despite the difference in the size of the burnt region at $t = 60$ ms, the amount of H_2O is very similar, as seen in the figure inset. At $t = 60$ the confined simulation has produced 6.2% more H_2O than the unconfined case. At earlier times, the amount of H_2O produced is (relatively) closer, with a 1.9% difference at $t = 40$ ms and a 0.7% difference at $t = 20$ ms.

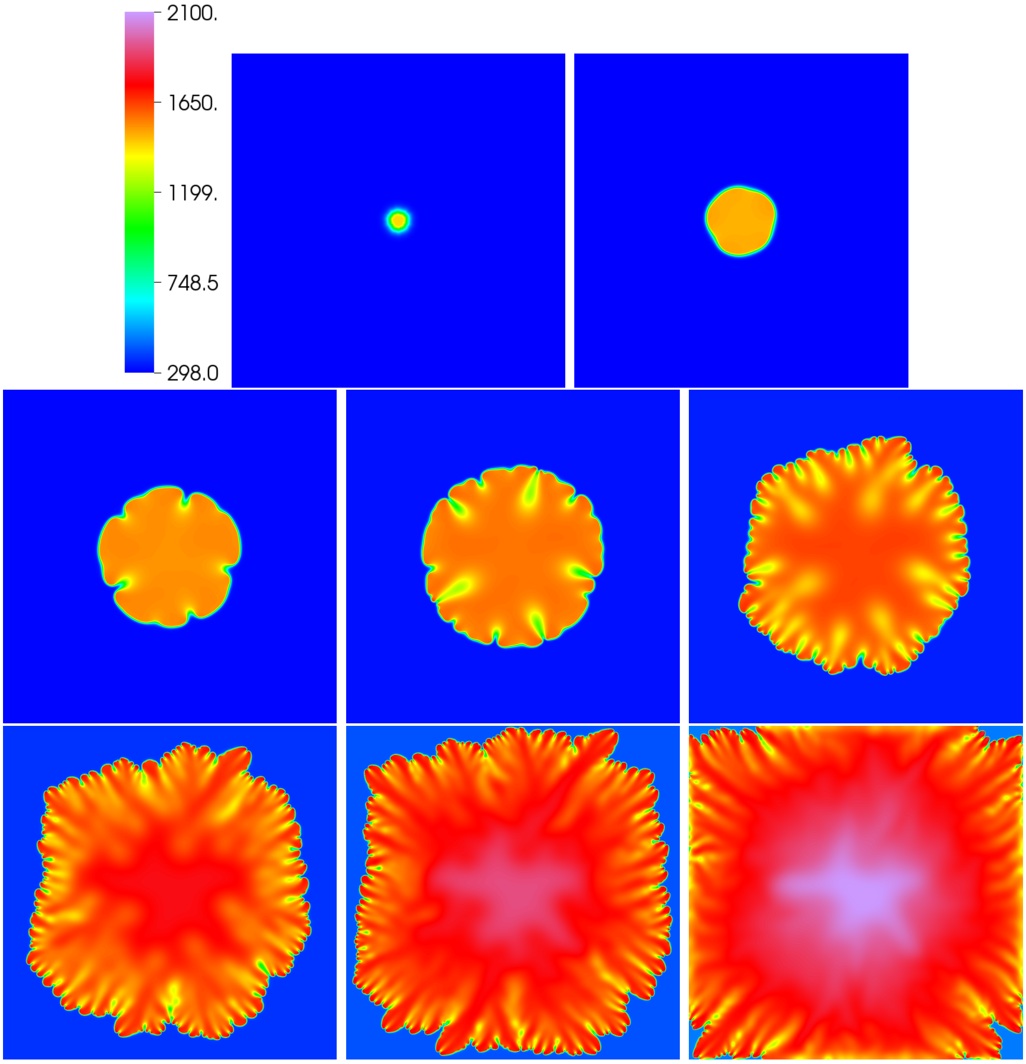

Figure 5. Temperature profiles of a confined premixed hydrogen flame at $t = 0, 20, 40, 50, 60, 70, 80$, and 100 ms.

7. Conclusions

We have developed an iterative scheme for evolving thermodynamic variables in a fully conservative manner while staying consistent with the EOS. The method naturally fits into an iterative SDC methodology. We have also developed a model for handling ambient pressure changes in confined domains. We have shown that two SDC iterations is sufficient for second-order accuracy, and that additional iterations greatly reduce the thermodynamic drift. We have also shown that our methodology is useful for studying multi-dimensional flames under realistic experimental conditions.

In the next paper we will extend our simulation methodology to utilize AMR. There are at least three issues associated AMR. First, we need to re-factor the algorithm to use the net fluxes of mass, energy, and momentum when posed in an SDC correction form in the mulitlevel synchronization steps, as opposed to the using the net fluxes in the Strang splitting formulation used in [19]. Second, in the original AMR approach, the multilevel synchronization steps did nothing to ensure that the solution either stayed on, or was driven toward the EOS. We can implement an iterative volume discrepancy algorithm in the multilevel synchronization steps to reduce the drift everywhere, but particularly near the coarse-fine inter-

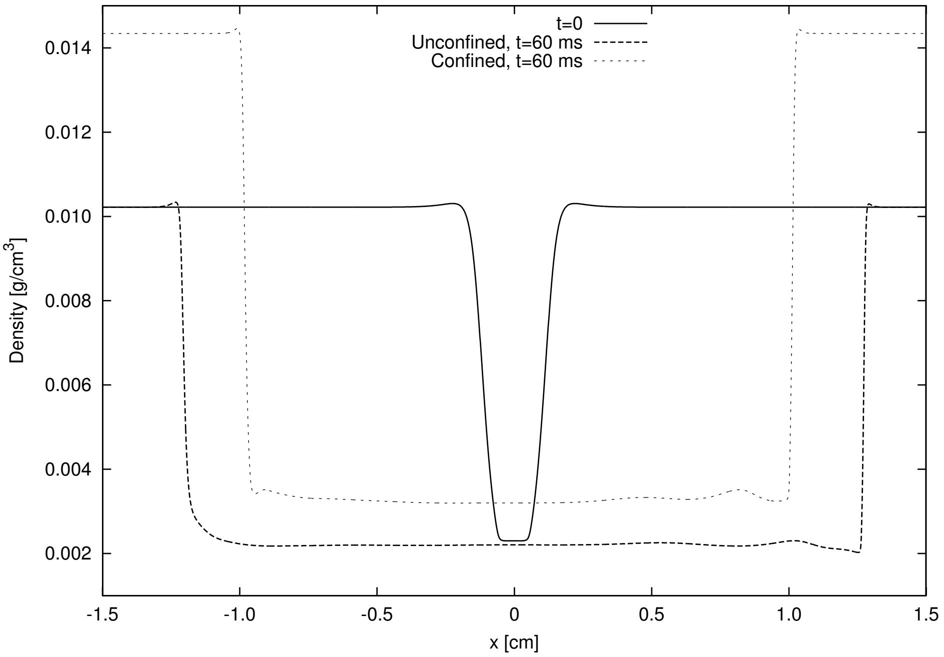

Figure 6. Horizontal profiles of density in the initial configuration, and at $t = 60$ ms for the unconfined and confined cases.

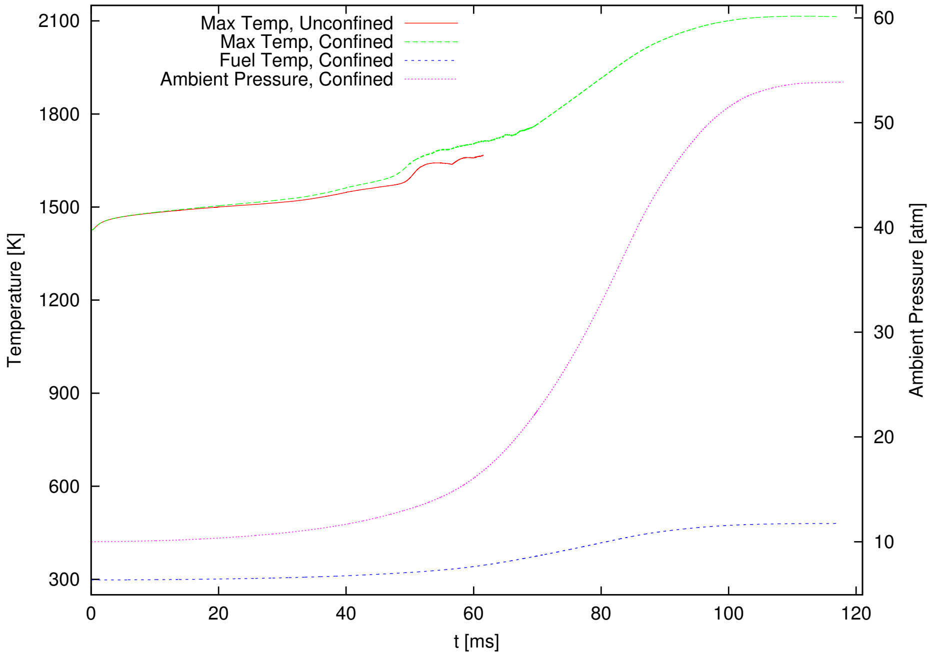

Figure 7. Maximum temperature as a function of time for the unconfined and confined cases. We also show the temperature of the fuel for the confined case as a function of time. We also show the ambient pressure as a function of time for the confined case.

face where synchronizing the coarse and fine fluxes often causes numerical drift. Third, we need to develop methodology for advancing and synchronizing the ambient pressure across levels of refinement in a subcycling adaptive framework. There is a question about how to represent the trajectory of p_0 over time, given that the different AMR levels are advanced, typically, at different time steps, and how to form synchronization equations that drive the solution toward the constraint while

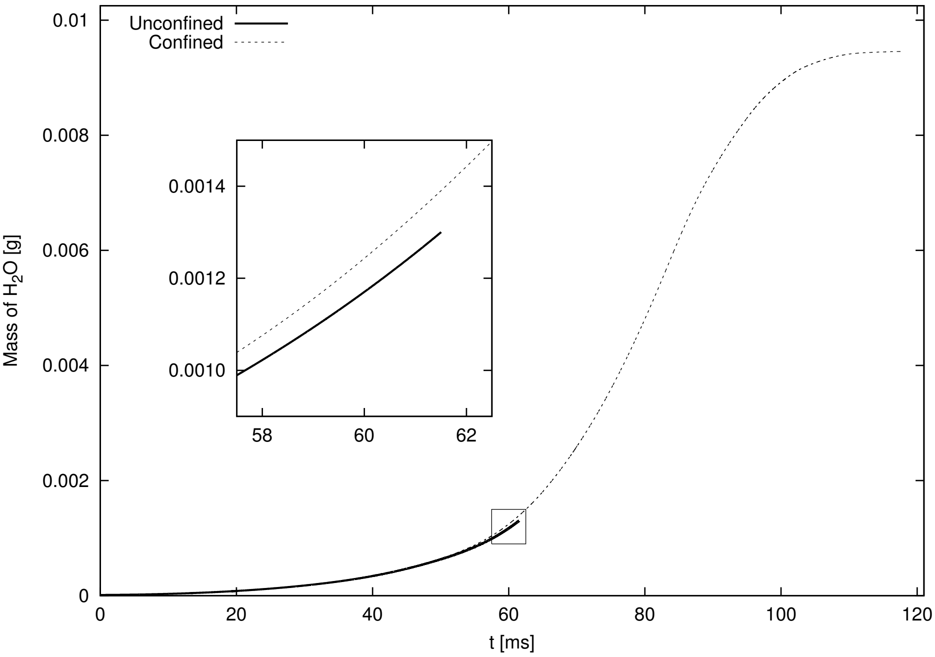

Figure 8. Mass of product as a function of time for the confined and unconfined cases.

correcting p_0. In future work, we also plan to extend this algorithm to more general equations of state, which will allow improved fidelity simulations at high pressure.

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