A Ghost-fluid method for large-eddy simulations of premixed combustion in complex geometries

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1. Motivation and objectives

Large-eddy simulation of premixed combustion is a computational challenge, because complex diffusion and reaction processes often occur in very thin layers. The interaction of these processes with turbulence determines the main properties of the flame brush, such as its burning velocity or its thickness. In turbulent flows, the large vortices wrinkle the flame brush and increase its surface, while the small scales may penetrate into the flame brush and increase its thickness. In both cases, the turbulence leads to an increase in the burning velocity. This feature has to be captured by the combustion model. Even if the turbulent scales increase the flame thickness, the flame brush remains difficult to resolve on LES meshes. Numerically, the premixed flame brush is very close to an interface, but its non-zero thickness must be taken into account to represent the proper flame-turbulence interactions.

In state-of-the-art combustion models, the issue of thin flames is overcome in very different ways. The Thickened-Flame model (TFLES) (Colin et al. 2000) artificially thickens the flame brush and the source terms in the species, and energy equations are corrected to recover the right burning velocity. The thickening factor that is needed to resolve the flame on a usual unstructured mesh is of the order of 20. This factor can be decreased slightly if naturally thicker quantities are used to represent the flame. This is the case in flame surface density approaches (Boger et al. 1998), but the thickening factor remains large. Instead of transporting reacting scalars, the flame can also be described using a flamelet hypothesis. That is, the reaction zone in the flame is considered to retain a laminar structure. The problem is then reduced to finding the position of the thin reaction layer. This is the principle of the G-equation model (Williams 1985; Peters 2000) in which a level set technique is used to track accurately the flame front. The displacement velocity of the level set is usually given by a model based on asymptotic analysis or experimental correlations (Peters 2000; Pitsch 2002). Then the level set has to be coupled to the Navier-Stokes solver by imposing the temperature profile in the flame brush. Often, Navier-Stokes solvers are not able to deal with large density and momentum gradients, and the imposed temperature profile has to be resolved on more than one, typically on the order of five cells.

In all the described models, the flame brush is more or less thickened, and the interactions with the smallest resolved scales are modified. The proposed method overcomes this artificial thickening using a numerical method that better couples the level set technique and the Navier-Stokes solver. This method is based on the Ghost-Fluid Method (GFM) (Fedkiw et al. 1998), which tracks discontinuities without introducing any smearing or numerical instabilities. While the original GFM has been developed to track infinitely

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thin discontinuities, the present method extends the GFM formalism to deal with interfaces of finite thickness.

2. A Ghost-Fluid Method for thin flame brushes

2.1. The classical variable-density method for low-Mach number flows

In reacting flows, the density is not constant, and incompressible methods cannot be used. Taking the low-Mach limit without the constant-density assumption, the filtered Navier-Stokes equations reduce to the continuity and momentum equations:

\[
\frac{\partial \bar{\rho}}{\partial t} + \nabla \cdot (\bar{\rho} \bar{u}) = 0 \tag{2.1}
\]

\[
\frac{\partial \bar{\rho} \bar{\bar{u}}}{\partial t} + \nabla \cdot (\bar{\rho} \bar{\bar{u}}) = -\nabla \bar{P} + \nabla \cdot \mathbf{t}, \tag{2.2}
\]

where the density is usually given from the combustion model. The pressure in (2.2) is not the thermodynamic pressure but rather a Lagrange multiplier called dynamic pressure. Similar to incompressible flows, these equations can be solved using a fractional-step method. A time-staggered discretization of (2.1) is given as:

\[
\frac{\bar{\rho}^{n+3/2} - \bar{\rho}^{n+1/2}}{\Delta t} + \nabla \cdot (\bar{\rho} \bar{\bar{u}}^{n+1}) = 0. \tag{2.3}
\]

If the density is known at \( t^{n+1/2} \) and \( t^{n+3/2} \), this equation provides a constraint on the velocity divergence. The first step of the fractional-step method is to advance the momentum equation to

\[
\frac{\bar{\rho} \bar{\bar{u}}^{n+1} - \bar{\rho} \bar{\bar{u}}^{n}}{\Delta t} + \nabla \cdot (\bar{\rho} \bar{\bar{u}}^{n+1/2} \bar{\bar{u}}^{n+1/2}) = \nabla \cdot \mathbf{t}. \tag{2.4}
\]

In the second step, the momentum is corrected with the dynamic pressure gradient:

\[
\frac{\bar{\rho} \bar{\bar{u}}^{n+1} - \bar{\rho} \bar{\bar{u}}^{n}}{\Delta t} = -\nabla \bar{P}^{n+1/2}. \tag{2.5}
\]

The dynamic pressure \( \bar{P} \) is found solving the variable-density Poisson equation:

\[
\nabla \cdot \nabla \bar{P}^{n+1/2} = \frac{\bar{\rho}^{n+3/2} - \bar{\rho}^{n+1/2}}{\Delta t^2} + \frac{1}{\Delta t} \nabla \cdot (\bar{\rho} \bar{\bar{u}}^{n+1}). \tag{2.6}
\]

Solving (2.4) to (2.6) for a propagating premixed flame may present several challenges. First, since the flame essentially occurs on the sub-filter scale, the filtered velocity and momentum flux may have steep gradients, which are difficult to integrate in the momentum equation. This may lead to spurious numerical instabilities. Second, the density variations in the flame may also be large. These density variations have to be integrated in the RHS of the Poisson equation, which may lead to the generation of non-physical velocity waves that are immediately propagated throughout the whole computational domain.

2.2. The Ghost-Fluid Method principle

The Ghost-Fluid Method (Fedkiw et al. 1998), when applied to premixed combustion, removes the steep gradients in the spatial derivatives by solving two continuous problems in the unburned and burned gases and by satisfying jump conditions at the interface, as
The Ghost-Fluid Method decomposition. $\phi_u$ and $\phi_b$ are the pre- and post-interface states, the unburned and burned gases in the case of premixed combustion, and $[\phi]$ is the jump.

shown in Fig. 1. To impose the jump conditions, the two continuous problems have to be solved in an overlapping region around the flame brush. The level set formalism is well adapted to track the flame position and to define the regions in which each problem has to be solved.

The main idea of the present method is to advance the momentum in the unburned and burned gases independently and then to use a modified Poisson equation to impose the jump conditions and the continuity constraint.

2.3. Decomposition of the conservative variables in a premixed flame brush

If the filtered density and momentum jumps due to the flame brush are discretized on a couple of points, they can be represented with a single function $\tilde{\alpha}$ that equals one in the burned gases and equals zero in the unburned gases:

$$\bar{\rho} = \tilde{\alpha}\bar{\rho}_b + (1 - \tilde{\alpha})\bar{\rho}_u \quad (2.7)$$
$$\bar{\rho}\bar{u} = \tilde{\alpha}\bar{\rho}_b\bar{u}_b + (1 - \tilde{\alpha})\bar{\rho}_u\bar{u}_u \quad (2.8)$$

The Favre average in (2.8) is defined with respect to the density in the burned and unburned gases:

$$\bar{\rho}_b\bar{u}_b = \bar{\rho}_u\bar{u}_u \quad (2.9)$$

This decomposition of (2.7) and (2.8) can be derived rigorously, assuming that the instantaneous flame is infinitely thin. Then, the function $\tilde{\alpha}$ is simply the filtered probability of finding burned gases. However, this decomposition remains a good approximation for thicker flames resolved on few points if the fluctuations of density and momentum due to turbulence are small compared to the jumps caused by the flame.

2.4. The continuity constraint

The continuity constraint (2.1) can be reformulated using (2.7) and (2.8). Further assumption that the continuity is satisfied in the burned and unburned gases leads to

$$\frac{\partial\tilde{\alpha}}{\partial t} + \frac{[\bar{\rho}\bar{u}]}{\bar{\rho}} \cdot \nabla\tilde{\alpha} = 0 \quad (2.10)$$

where $[\bar{\rho}]$ and $[\bar{\rho}\bar{u}]$ denote the density and momentum jumps. The continuity constraint therefore leads to a propagation equation for the flame profile. If $\tilde{\alpha}$ is only a function of
the level set field $G$, then (2.10) is also a constraint on $G$:

$$\frac{\partial G}{\partial t} + \left[ \frac{\hat{\rho} \hat{u}}{\hat{\rho}} \right] \cdot \nabla G = 0. \quad (2.11)$$

### 2.5. The coupled Poisson equation

The fractional-step algorithm presented in Section 2.1 is supposed to be satisfied for the burned, unburned, and global quantities through the flame brush. Then, if the pressure gradient is decomposed similar to the conservative variables

$$\nabla \hat{P} = \hat{\alpha} \nabla \hat{P}_b + (1 - \hat{\alpha}) \nabla \hat{P}_u, \quad (2.12)$$

the pressure Laplacian of (2.6) becomes

$$\nabla \cdot \nabla \hat{P} = \hat{\alpha} \nabla \cdot \nabla \hat{P}_b + (1 - \hat{\alpha}) \nabla \cdot \nabla \hat{P}_u + [\nabla \hat{P}] \cdot \nabla \hat{\alpha}. \quad (2.13)$$

The two first terms on the RHS of (2.13) are the pressure Laplacians in the burned and unburned gases multiplied by the profile function. The third term is the pressure gradient jump. It corrects the momentum jump, and it is computed after the momentum advancement. The two Laplacians can be expressed as functions of the density variations and of the predicted velocity divergence on both sides of the flame. This leads to the coupled Poisson equation:

$$\nabla \cdot \nabla \hat{P} = [\nabla \hat{P}] \cdot \nabla \hat{\alpha} + \frac{1}{\Delta t} \left( \hat{\alpha} \frac{\partial \hat{\rho}_b}{\partial t} + (1 - \hat{\alpha}) \frac{\partial \hat{\rho}_u}{\partial t} + \hat{\alpha} \nabla \cdot \hat{\rho}_b \hat{u}_b^* + (1 - \hat{\alpha}) \nabla \cdot \hat{\rho}_u \hat{u}_u^* \right). \quad (2.14)$$

It should be noted that (2.14) has been obtained using (2.12), i.e. by assuming that the pressure gradient can be decomposed similarly to the conservative variables. This is possible if and only if the RHS of (2.12) is irrotational, and this condition is satisfied if and only if

$$\nabla \times (\hat{\alpha} \nabla \hat{P}_b + (1 - \hat{\alpha}) \nabla \hat{P}_u) = \nabla \hat{\alpha} \wedge [\nabla \hat{P}] = 0. \quad (2.15)$$

This implies that in the flame brush, the pressure gradient obtained by solving (2.13) mainly consists of the pressure correction due to the pressure gradient jump along the flame normal. The tangential component of the pressure gradient jump is recovered when computing the pressure corrections in the unburned and burned gases:

$$\nabla \hat{P}_u = \nabla \hat{P} - \hat{\alpha} [\nabla \hat{P}], \quad \nabla \hat{P}_b = \nabla \hat{P} + (1 - \hat{\alpha}) [\nabla \hat{P}]. \quad (2.16)$$

These pressure corrections ensure that the momentum jump at the end of the time-step is well imposed.

### 2.6. Jump conditions

The density jump $[\hat{\rho}]$ is given by the thermo-chemistry in the flame, and it is an input of the computation. The momentum jump is obtained from the continuity equation expressed in a Galilean frame that is moving at a speed $U_S$ in the reference frame. The flame is then steady in this frame, and the continuity equation becomes:

$$\nabla \cdot (\hat{\rho} (\hat{u} - U_S)) = 0. \quad (2.17)$$

Integrating this equation in the flame brush leads to

$$[\hat{\rho} \hat{u}] = [\hat{\rho}] U_S. \quad (2.18)$$
The frame speed $U_S$ can be expressed as the sum of a flow speed and an intrinsic flame speed. Taking these values in the unburned gases gives

$$\left[ \rho \hat{u} \right] = \left[ \rho \right] (\hat{u} - S_{T,u} \mathbf{N}),$$

where $\mathbf{N}$ is the flame brush normal:

$$\mathbf{N} = -\frac{\nabla G}{\| \nabla G \|}.$$

The level set propagation equation given by (2.11) can therefore be rewritten in the usual form:

$$\frac{\partial G}{\partial t} + (\hat{u}_u + S_{T,u} \mathbf{N}) \cdot \nabla G = 0.$$  

(2.21)

Finally, the jump of the gradient of the dynamic pressure $[\nabla \hat{P}]$ is obtained by taking the difference of the pressure correction steps in the burned and unburned gases:

$$[\nabla \hat{P}] = \frac{1}{\Delta t} \left( [\rho \hat{u}^n] - [\rho \hat{u}^{n+1}] \right).$$

(2.22)

2.7. The combustion model

To determine the burning velocity in the unburned gases $S_{T,u}$, the LES model developed by Pitsch (2002) is used. This model is an extension of the $G$-equation model originally derived for the Reynolds-Averaged Navier-Stokes (RANS) formalism (Williams 1985; Peters 2000). The burning velocity $S_{T,u}$ is given by the relation:

$$\frac{S_{T,u} - S_{L,u}}{S_{L,u}} = -\frac{b_2^3 C_s}{2 b_1 \text{Sc}_{t,G}} \frac{\Delta}{t_F} + \sqrt{\left( \frac{b_2^3 C_s}{2 b_1 \text{Sc}_{t,G}} \frac{\Delta}{t_F} \right)^2 + \frac{b_3^2 D_{t,G}}{S_{L,u} t_F}},$$

(2.23)

where $S_{L,u}$ is the laminar burning velocity, $\Delta$ is the filter width, $t_F$ is the laminar flame thickness, $C_s$ is the Smagorinsky constant, $\text{Sc}_{t,G} = 0.5$ is a turbulent Schmidt number, and $b_1 = 2.0$ and $b_2 = 1.0$ are two model constants. The turbulent diffusivity $D_{t,G}$ is computed using a Smagorinsky-type model:

$$D_{t,G} = \frac{C_s \Delta u'_\Delta}{\text{Sc}_{t,G}}.$$  

(2.24)

where $u'_\Delta$ is the intensity of the sub-filter velocity fluctuations.

2.8. The full algorithm

The full algorithm consists of the following steps:

**Step 1: Advance the level set equation from $G^{n+1/2}$ to $G^{n+3/2}$**

The propagation equation given by (2.21) is advanced with estimates of $\hat{u}_u^{n+1}$ and $S_{T,u}^{n+1}$. The time integration is done using a 3-step Back and Forth Error Correction (BFEC) method (Dupont & Liu 2003), and the spatial discretization is done using a first-order upwind scheme. It can be proven that the combination of these two integration techniques leads to a low-dispersive scheme that is second-order in space and time. Then, to keep the level set field $G$ equal to a distance function, a fast-marching reinitialization method (Sethian 1996) is used.
Step 2: Compute the flame brush profile $\tilde{\alpha}^{n+3/2}$ and the density field $\tilde{\rho}^{n+3/2}$

These two quantities are computed using a user-defined profile for $\tilde{\alpha}^{n+3/2}$, which is a function of the distance to the flame front. The density is then computed according to (2.7), where the density in the burned and the unburned gases is taken constant. The thickness of the flame is therefore given by the user-defined function.

Step 3: Advance the momentum in the unburned and burned gases $\tilde{\rho}_u \tilde{u}_u^*$ and $\tilde{\rho}_b \tilde{u}_b^*$

The momentum in the unburned and in the burned gases is advanced independently following (2.4) and using an implicit Gauss-Seidel method with relaxation. The spatial scheme is a second-order central scheme that conserves the kinetic energy (Mahesh et al. 2004).

Step 4: Compute the pressure gradient jump $[\nabla P]$.

This jump is computed according to (2.22), in which the momentum jump at $t^{n+1}$ is evaluated using (2.19).

Step 5: Solve the Poisson equation.

This constant-coefficient Poisson equation (2.14) is solved using an algebraic multi-grid solver.

Step 6: Correct the unburned and burned momentum.

The pressure gradients in the unburned and burned gases are computed using (2.16) and are then used to correct the momentum in the unburned and burned gases.

3. Results

In this section, the proposed method is verified by computing 2D flame-vortex interactions. Then, the method is applied to the LES computation of a turbulent flame anchored by a triangular-flame holder. Finally, LES computations of a reacting industrial lean-premixed swirl-burner are presented and discussed.

3.1. Flame-vortex interactions

The proposed method is verified by computing 2D flame-vortex interactions. This unsteady laminar test case has been studied experimentally (Mueller et al. 1998), and it has been used extensively to build DNS databases and combustion regime diagrams (Poinset et al. 1991) and to validate combustion models (Colin et al. 2000). Recently, Lessani & Papalexandris (2005) have used this test to verify a low-Mach fractional-step method.

The flame-vortex computations performed in this study consist of a steady laminar premixed flame interacting with a vortex dipole convected at the laminar burning speed. The parameters used in this study are the same as in Lessani & Papalexandris (2005) ($Le = 1, r/\delta = 5.5, u'/S_L = 10.6$), and these parameters are close to one case of the database of Poinset et al. (1991) ($Le = 1.2, r/\delta = 5, u'/S_L = 12$). The flame profile $\tilde{\alpha}$ has been extracted from the 1D computations of Lessani & Papalexandris (2005). The initial conditions are given in Fig. 2(a). The distances are non-dimensionalized by the flame thickness. The inlet is located at $Y = 0$, and the inlet velocity is set equal to the burning velocity $S_L$. Before the interaction with the vortex dipole, the flame is steady and located at $Y = 100$. When the vortices arrive in the vicinity of the flame, their vorticity decreases rapidly as they wrinkle the flame front. Between the vortices, the flow speed increases,
whereas on the sides of the dipole the flow speed decreases. This decrease leads to the formation of an unburned gas pocket as shown in Fig. 2(b). The form of the flame on this figure is very close to the results of Poinsot et al. (1991).

For a verification of the proposed method, a mesh refinement study is performed. Three Cartesian meshes of dimensions $64 \times 256$, $128 \times 256$ and $256 \times 512$ are used. Snapshots of the $G_0$-level set are presented on Fig. 3. The results obtained with the three different resolutions are in very good agreement, and they show the same behavior as those obtained by Poinsot et al. (1991). However, the results are quite different from those of Lessani & Papalexandris (2005), in which no pocket of unburned gas is formed. These differences can be explained by the fact that the formation of this pocket is very sensitive to the numerical dissipation and to the actual burning velocity of the flame. These two key aspects are the main impetus for using a level set formalism coupled to non-dissipative numerical schemes in the present method.

3.2. Triangular flame-holder

3.2.1. Description

This configuration consists of a turbulent premixed flame anchored to a triangular flame-holder. It has been studied experimentally (Nottin et al. 2000; Knikker et al. 2002) with the objective of providing data for the validation of RANS and LES combustion models. This burner is operated at atmospheric conditions with a stoichiometric propane/air mixture. The inlet speed $u_{in}$ and the main flame characteristics are given in Table 1. A 3D computation of this configuration has been performed with an unstructured mesh of approximately 2 million hexahedral cells. The flame profile $\tilde{\alpha}$ has been chosen to have a thermal thickness approximately equal to twice the filter width near the flame-holder. A snapshot of the computed flame and of the coherent structures of
the flow is presented in Fig. 4. The Q criterion (Dubief & Delcayre 2000), which is the second invariant of the deformation tensor, is used to visualize the coherent structures. It compares the magnitude of the rotation and shear rates. Most of the vortices are created in the shear zone between the flame-holder recirculation and the burned gases accelerated by the thermal expansion. These vortices, which are originally transverse, are elongated by the burned gases and become streamwise in the tail of the recirculation zone.
3.2.2. Progress-variable statistics

The values of the mean progress-variable \( \bar{c} \) given by the 3D LES computation and extracted from OH-LIF images are compared in Fig. 5. The contours are in very good agreement, demonstrating that the dynamics of the flame are captured accurately by the LES computation. The four dashed lines on Fig. 5 represent the locations chosen to compare the mean and RMS progress-variable profiles. The results of these are given in Fig. 6. The RMS profiles are reconstructed from the mean progress variable assuming that the flame is infinitely thin (Poinsot & Veynante 2001):

\[
c_{\text{rms}} = \sqrt{\bar{c}(1 - \bar{c})} \quad (3.1)
\]

The mean and RMS progress-variable profiles, shown in Fig. 6, are in very good agreement with experimental data. The discrepancy between RMS profiles far from the flame-holder can be due to the fact that the flame thickness is taken to be constant in the entire domain.
3.3. Industrial lean-premixed swirl-burner

3.3.1. Description

In this section, the proposed method is applied to the complex swirl-burner shown in Fig. 7. It features a plenum, a swirl-injector, and a combustion chamber. A lean premixed mixture of methane and air is injected at atmospheric pressure in the plenum, and the turbulent flame is anchored at the outlet of the swirler. The swirl plays an important role in the stabilization of the lean premixed flame. The main parameters of the burner are given in Table 2. Velocity LDV measurements (Roux et al. 2005) are available for several locations in the combustion chamber. This burner has been computed by Roux et al. (2005) using the Thickened-Flame model (TFLES) (Colin et al. 2000), and their results are in good agreement with experimental data.

Two different unstructured meshes have been used to perform the LES computations. The first is based mostly on tetrahedral elements and is the same as in Roux et al. (2005). The second is based mostly on hexahedral elements. Both meshes count 3 million control volumes. Given these meshes, the computed turbulent flames can be located in the LES combustion diagram (Fig. 8) proposed by Pitsch (2005). These flames are at the interface between the thin reaction zones regime and the broken reaction zones regime. The combustion model described in Section 2.7 is actually only valid for the corrugated and the thin reaction zones regime. The flame profile $\bar{c}$ has been defined to give a thermal thickness approximately equal to twice the filter width.

The vortices are formed in two main regions. The first region is the sudden enlargement on the exterior of the swirler, and the second region is the head of the injector, where the separation of the flow occurs. Although the exterior vortices are of small intensity, the vortices in the core region strongly affect the flame brush. These interior vortices have the same nature as the Precessing Vortex Core (PVC) described by Roux et al. (2005) for the non-reactive flow.
Table 2. Swirl-burner. Parameters.

<table>
<thead>
<tr>
<th>Re</th>
<th>$u_{in}$</th>
<th>$\phi$</th>
<th>$S_L$</th>
<th>$\delta$</th>
<th>$\rho_u$</th>
<th>$\rho_b$</th>
<th>$\rho_u/\rho_b$</th>
</tr>
</thead>
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<td>45000</td>
<td>24 m/s</td>
<td>0.75</td>
<td>0.23 m/s</td>
<td>0.6 mm</td>
<td>1.14 kg/m$^3$</td>
<td>0.18 kg/m$^3$</td>
<td>6.3</td>
</tr>
</tbody>
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Figure 7. Swirl-burner. Instantaneous flame and azimuthally-projected stream-lines.

Figure 8. Swirl-burner. Location of the computations in the LES regime diagram.

3.3.2. Velocity statistics

The mean and RMS velocities from the LES computations are compared to the experimental data in Figs. 10 and 11. The comparisons are performed for five 1D profiles at different distances from the chamber head. Only the axial profiles are presented because the radial and azimuthal profiles show a similar agreement. Both mean and RMS profiles are in a very good agreement, especially in the near field of the injector. The 1.5 mm RMS profiles in Fig. 11 clearly show the velocity fluctuations due to the exterior and interior vortices. The exterior vortices are well captured on both meshes by the present method,
whereas they do not seem to be captured with the Thickened-Flame model (TFLES) results of Roux et al. (2005).

4. Conclusions

A new Ghost-Fluid Method for premixed flames of finite thickness has been developed. This method provides a robust and accurate coupling of the G-equation model with a low-Mach Navier-Stokes solver while allowing the use of kinetic-energy conserving schemes. The combination of these state-of-the-art algorithms results in a very accurate description of the flame transport and ensures very low numerical dissipation. The proposed method has first been verified using the basic test case of laminar flame-vortex interactions. The results demonstrate the high accuracy of the method even on coarse
meshes. Furthermore, the method has been applied in the LES computation of a turbulent flame anchored by a triangular flame-holder. Computed mean and RMS progress-variable profiles are compared to the experimental data, showing good agreement. Finally, the method has been used to compute the combustion process in a complex swirl-burner. The dynamic behavior of the device is discussed, and mean and RMS velocity profiles have been compared with experimental measurements. The remarkable agreement obtained for this complex geometry attests to the high fidelity of the method.

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