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Application of the Method of Manufactured Solutions to the verification of a pressure-based finite-volume numerical scheme

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Abstract

The present work provides the description and verification of a pressure-based finite volume approach for variable density flows representative of those encountered in combustion applications. The algorithm under consideration is based on a classical predictor-corrector time integration scheme that employs a projection method for the momentum equations. Spatial discretization is based on a staggered framework with velocity and scalar quantities evaluated in different grids to avoid the rise of checkerboard pressure patterns. The present study then reports a numerical procedure based on a series of tests that make use of the method of manufactured solutions (MMS) and allows to evaluate the effective numerical performance with respect to the theoretical order of accuracy. It is successfully applied to both fully incompressible and variable density flows, confirming again the interest of the method to conduct a preliminary check of the performance of any numerical algorithm.

Key words: Variable density flows, Combustion, Low Mach number approximation, Pressure based solver, Code verification, Methods of manufactured solutions

1. Introduction

Low Mach number variable density flows arise in several natural as well as technological processes, including meteorological flows or combustion in energy conversion devices (engine, turbojets, etc.). Regarding the prediction and understanding of such a category of flows, the extensive use of mathematical and numerical techniques is unavoidable. Hence, as the mathematical and numerical methods becomes more complex, the procedures of validation and verification of computer codes must evolve as well. The present work aims at demonstrating systematically the procedure of verification of a CFD code designed to perform the numerical simulation of low Mach number flows. **Although** such a procedure appears as a necessary preliminary step before tackling the computational modeling of turbulent combustion problems of interest to the authors [1, 2, 3, 4], **the literature lacks on information over the subject, especially concerning the**

verification of variable density low Mach number flows. In order to clarify the differences between the words verification and validation, we used the following definitions. Verification aims at providing information on whether the mathematical model has been well implemented according to initial design or not, whereas validation refers to how closely the correctly implemented mathematical model mimics a given set of experimental data. The solutions of the balance equations (mass, momentum, energy, species mass fractions, etc.) are deemed sufficient to represent any flows irrespective of their characteristic velocity, provided that the continuum hypothesis holds, and once suitable constitutive equations for the fluids of interest are provided. However, when dealing with discrete approaches for solving such a system of balance equations, the numerical techniques do involve, invariably, errors. These errors have different sources, spanning from unavoidable roundoff errors to mere programming mistakes (bugs), hence emphasizing the crucial need for well defined procedures to evaluate the numerical accuracy [5]. Moreover, it is of fundamental importance to be able to characterize the capabilities of a numerical approach, i.e., it is imperative to determine whether (or not) the retained mathematical / numerical scheme is suitable to cope with the problem of interest. Here, we first briefly review the existing strategies that are usually retained to develop compressible and incompressible solvers for low Mach number calculations. Further, we show the mathematical and numerical modeling adopted herein, and then focus on the procedure retained for the verification of low Mach number codes.

1.1. Compressible vs low Mach number approximations

An important non-dimensional parameter that characterizes a flow field is the Mach number $Ma=U/c$, where U is a characteristic velocity of the flow field, and c is the speed of sound. The incompressible limit is usually defined as the situation associated to Mach number values smaller than 0.3. Above this value the compressibility effects cannot be neglected any longer, and variations of density and pressure are coupled through an equation of state. For incompressible flows a decoupling between the equations of momentum and the energy equation is possible, and in such flows the pressure variations remain typically very small. The possible density variations are no longer related to pressure variations, but to temperature and variations only. The pressure is often said to be thermodynamically constant, and its influence is only felt through the spatial derivatives that appear in the momentum equation.

In fact, there exists a fundamental difference between the behavior of the set of conservation equations in an incompressible flow, with respect to compressible flows. In compressible flows featuring high Mach number values, the fluid velocity reach the same order of magnitude as the velocity of sound waves, i.e., $O(U) \approx O(c)$, and the mathematical system of governing equations follows an hyperbolic behavior [6], whereas in the low Mach number incompressible case, the velocity of sound waves are much higher than the fluid velocity, i.e., $O(U) \ll O(c)$. Such a disparity of magnitudes between the velocity of the flow and the speed of sound waves leads to a great stiffness in the system of balance equations. This severely hampers the accuracy and convergence of the numerical methods that rely on the consideration of density variations, i.e., density-based solvers [7], which remain the most commonly used to perform the numerical simulations of compressible flows. In the case of incompressible flows such a disparity between the wave and flow velocities is also one of the major sources of numerical instability [8, 9, 10].

In the present work, we are interested in low velocity flows, i.e., in the incompressible regime, but featuring non negligible density variations, the so-called low Mach number flows. There are

basically two broad classes of numerical methodologies to deal with this kind of flows: those relying on density-based solvers, i.e., based on methods usually retained for compressible flows, and those relying on pressure-based solvers, such as those retained to perform the numerical simulation of incompressible flows. The application of each one of these two methodologies to low Mach number flows requires the introduction of several modifications and improvements, that are briefly summarized below.

1.2. Density-based methods

The density-based methods represent a wide class of numerical schemes originally developed to study compressible flows [11]. Turkel *et al.* [12] determined that the set of discretized equations retained for the numerical simulation of a compressible flows fails to provide an accurate solution for an incompressible flow. The simulations of incompressible flows based on the fully compressible method, with no modifications to reduce the disparity existing between the flow velocity and the speed of sound, are found impracticable due to the associated computational costs. In this case, temporal integration schemes, whatever they are explicit or implicit, are penalized. In the former case, the Courant-Friedrichs-Lewy (CFL) condition, that must be satisfied at each time step to enforce the numerical stability of the numerical integration scheme, leads to prohibitively small time step values due to the prevailing influence of acoustic waves propagation. In the case of implicit methods such a disparity induces large differences in the characteristic eigenvalues of the algebraic system to be solved, which becomes ill-conditioned, leading therefore to extremely high-cost iterative solutions [13].

Two distinct sets of techniques have been proposed to achieve better convergence properties of density-based solvers, in the limit of low Mach number flows: preconditioning and perturbation methods. Both techniques strive to minimize the stiffness of the algebraic system that results from the discretization of the balance equations.

The first technique pre-multiplies the temporal derivatives by a preconditioning matrix, whose choice is determined according to the problem to be analyzed [7], thus leading to a new set of equations. As a consequence, the initial (stiff) system is altered. The technique essentially aims at re-scaling the characteristic eigenvalues with respect to the original system, so that eigenvalues of similar orders of magnitude can be obtained, leading to a better conditioned system [12, 14]. The major drawback associated with preconditioning methods is that the governing equations are modified in terms of their mathematical nature due to the incorporated transient term. The modified system of equations has only the steady-state solution in common with the original system and becomes therefore devoid of any physical transients. A second limitation is the failure of this methodology, in terms both of efficiency and robustness, in the vicinity of stagnation points, where the characteristic eigenvectors become almost parallel [15]. Furthermore, the design of general purpose pre-conditioners adequate for a large variety of physical problems remains far from being straightforward.

The second set of techniques is the perturbation methods, or asymptotic analysis. In this case, a perturbed form of the equations is used to reduce the stiffness of the algebraic system of equations. A Taylor expansion is performed in terms of the Mach number decoupling the acoustic waves from the equations, and replacing them with a set of pseudo-acoustic forms, where the wave velocities become the same order of magnitude as the fluid velocity. Such a procedure alters the velocity of the acoustic waves in order to allow the numerical integration to be performed

with larger time steps [7, 13].

Other methodologies have been also developed for the purpose of considering density variations, such as the artificial compressibility methods, and the PGS (Pressure Gradient Scaling). The first, described, for instance in [16], has been successfully applied to the numerical simulation of reactive flows and, in particular, to describe the propagation of a planar turbulent premixed flame [17]. The PGS method [18, 19, 20, 21] displays certain similarities to the perturbation methods, and it also acts on the pressure term that appears in the momentum equation. In this method the pressure gradient is multiplied by a factor $1/\alpha^2$, where α is a constant that amplifies the pressure variations. As a consequence, since the velocity of acoustic waves is decreased by a factor α , the pressure variations are amplified by a factor α^2 , thus, improving the robustness of the numerical method as the Mach number tends towards zero [19]. Finally, it is worth adding that one reason for the use of the last two methods rely in the fact that they can be easily implemented within an existing compressible solver.

1.3. Pressure-based methods

In contrast to the methodologies discussed above, that are based on density variations, pressure-based methods have been initially proposed to solve fully incompressible flows, retaining the pressure as one of the primary variables. Such numerical schemes that are often referred to as pressure-corrections methods, or projection methods, evaluate the pressure and velocity fields in a segregated manner [22, 23]. In pressure-based methods, the pressure does not play a thermodynamic role, but ensures the incompressibility condition, which leads to a discretization scheme based on a separation of operators (splitting method). In a first step, momentum equations are solved to obtain an estimated velocity field, based on a previous evaluation of pressure. The velocity field should be solenoidal, and this property is enforced by a subsequent projection step within the subspace of divergence-free vectorial fields. Such projection, which defines the corrector step, relies on the Hodge decomposition theorem [24]. The pioneering works in this field [22, 25] have provided the basis for the development of several projection schemes that are still currently used. More specifically, the work of Patankar and co-workers [25], has led to a family of methodologies refereed to as the SIMPLE (Semi-Implicit Pressure Linked Equations) approach, which undoubtedly remains the most widely used to obtain the solution of incompressible flows.

As previously mentioned, in the low Mach number regime, the compressibility effects have a negligible influence on the momentum transport and the pressure is only a weak function of density. To prevent significant inaccuracies when performing the evaluation of pressure, it is usually divided into two distinct components:

$$P(\mathbf{x}, t) = P_o(t) + P'(\mathbf{x}, t), \quad (1)$$

where P_o is a reference pressure level¹, with $P_o(t)/P_o = O(1)$, and $P(\mathbf{x}, t)/P_o = O(Ma^2)$. It is worth noting that $P_o(t)$ is often referred to as the thermodynamic pressure, whereas $P'(\mathbf{x}, t)$ is called the dynamic pressure since it is directly related to modifications of the velocity field.

¹Since we are interested in gaseous flow fields, the effects of gravity are not considered, hence $P_o(t)$ is a function of the time only.

Using such a decomposition, the thermodynamic pressure appears in the equations of state and energy conservation only, vanishing in the momentum equation. Since its gradient is zero everywhere, only the gradient of the dynamic pressure component remains. It is worth noting that this procedure significantly accelerates the convergence only if the pressure fluctuations remain sufficiently small.

Since one of the objectives of the present work is to provide guidelines for verification and cross-checks of a recently developed incompressible code, the most natural choice for an extension to variable density flows is a formulation based on pressure variations, i.e., to extend a mathematical and numerical model proposed for fully incompressible flows to handle density variations.

A wide class of numerical methods that remains used to perform such simulations of low Mach number flows, is based on predictor-corrector methods. Several works, [8, 9, 10, 26, 27, 28, 29, 30] share such pressure-velocity coupling. Rider *et al.* [31] report an extensive discussion about robust projection methods applied to variable density low Mach number flows. The numerical strategy retained for the purpose of the present study is described below.

2. Mathematical modeling

Since we intend to simulate variable density flows, we consider a mathematical model suitable for a compressible flow, in which the primary transported variables are the density $\rho(\mathbf{x}, t)$, the three velocity components $u_i(\mathbf{x}, t)$ ($i = 1, 2, 3$), and the temperature. The non-dimensional balance equations for the cited variables in space, $(x_i, i = 1, 2, 3)$, and time, t , are summarized below along with an equation of state that relates the thermodynamic component of the pressure to density and temperature. It is worth noting that dimensional quantities are now referred to with the superscript ‘ $\wedge$ ’.

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = S_\rho, \quad (2)$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{1}{Re} \frac{\partial}{\partial x_j} \tau_{ij} + S_{u_i}, \quad (3)$$

$$\tau_{ij} = -\frac{2}{3} \mu \frac{\partial u_k}{\partial x_k} \delta_{ij} + \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right), \quad (4)$$

$$P = P_o(t) + P'(\mathbf{x}, t) ; \quad P_o = \rho \phi. \quad (5)$$

The above set of equations is obtained in a non-dimensional form using:

$$x_i = \hat{x}_i / L_{ref}, \quad t = \hat{t} u_{ref} / L_{ref}, \quad u_i = \hat{u}_i / u_{ref}, \quad (6)$$

$$P = \frac{\hat{P}}{(\rho_{ref} u_{ref}^2)}, \quad \rho = \hat{\rho} / \rho_{ref}, \quad (7)$$

In Eq. (5), $P_o(t)$ is the thermodynamic pressure, a function of time only, $P'(\mathbf{x}, t)$ is the dynamic pressure, henceforth denoted only by p . In the same equation, the variable ϕ stands for a reduced temperature, defined by

$$\phi = (T - T_u) / (T_b - T_u), \quad (8)$$

where T_b (resp. T_u) denotes the maximal (resp. minimal) value of the temperature, in such a manner that $\phi \in [0; 1]$. For instance, if we consider a premixed flame propagating towards unburned reactants, T_u and T_b stand for the temperature in the fresh mixture and fully burned products of combustion respectively. The transport equation for the reduced temperature writes:

$$\rho C_p \frac{\partial \phi}{\partial t} + \rho C_p u_i \frac{\partial \phi}{\partial x_i} = \frac{1}{Re Pr} \frac{\partial}{\partial x_j} \left(\kappa \frac{\partial \phi}{\partial x_j} \right) + \left(\frac{\gamma - 1}{\gamma} \right) \frac{dP_o}{dt} + S_\phi, \quad (9)$$

where $Pr = \mu_{ref} C_{p_{ref}} / \kappa_{ref}$, and $Re = \rho_{ref} u_{ref} L_{ref} / \mu_{ref}$, denote the Prandtl and Reynolds numbers.

It is noteworthy that, in the previous set of conservation equations Eqs. (2), (3), and (9), temperature dependent variables, such as the transport properties: viscosity μ , and thermal conductivity κ , and the heat capacity C_p , have been made non dimensional with respect to their values at temperature T_u . The corresponding values are denoted μ_{ref} , κ_{ref} , and $C_{p_{ref}}$.

Finally, the source terms S_{u_i} , S_ρ , and S_ϕ have been included in Eqs. (2), (3), and (9), just for the sake of generality and will be discussed later.

In transient flows the balance equations must be integrated in time as well, which requires the choice of a suitable time marching scheme. Temporal integration schemes are essentially controlled by the Courant criterion $Co = (u_i \delta t) / \delta x_i$, $i = 1, 2, 3$. Explicit schemes exhibit numerical stability issues when using Courant number values larger than unity. However, such a numerical limitation does not apply to implicit or semi-implicit discretizations. Ferziger and Peric [16] provide an introduction to several types of classical temporal integration methods. Examples of semi-implicit approaches can be found in [36], and a detailed evaluation of various semi-implicit schemes has been reported in [37]. The temporal integration schemes retained in the present work are fully implicit, in such a manner that it is possible to reach statistically steady regimes faster than by resorting to explicit time integration techniques.

Arscher *et al.* [37] proposed a semi-discretized arrangement in such a way that any differential equation could be temporally integrated using second order semi-implicit schemes:

$$\begin{aligned} \frac{1}{\Delta t} \left[\left(\gamma + \frac{1}{2} \right) u^{n+1} - 2\gamma u^n + \left(\gamma - \frac{1}{2} \right) u^{n-1} \right] &= (\gamma + 1) \zeta(u^n) - \gamma \zeta(u^{n-1}) + \\ &\left[\left(\gamma + \frac{c}{2} \right) \epsilon(u^{n+1}) + (1 - \gamma - c) \epsilon(u^n) + \frac{c}{2} \epsilon(u^{n-1}) \right], \end{aligned} \quad (10)$$

where $\zeta(u)$ and $\epsilon(u)$ stand for, respectively, diffusive and advective contributions to the differential equation, and n represents the time level. Depending on the values retained for constants γ and c , different time integration schemes can be obtained [37]:

- Crank-Nicolson Adams-Bashfort (CNAB): $(\gamma, c) = (0.5, 0.0)$;
- Modified Crank-Nicolson Adams-Bashfort (MCNAB): $(\gamma, c) = (0.5, 0.125)$;
- Crank-Nicolson Leap Frog (CNLF): $(\gamma, c) = (0.0, 1.0)$;
- Semi-Backward Difference Formula (SBDF): $(\gamma, c) = (1.0, 0.0)$.

In the present work, instead of a semi-implicit, a fully implicit scheme is adopted. However, the organization allowed by Eq. (10) remains very attractive, since it includes the possibility

of (i) describing several methods of temporal discretization and, hence, (ii) choosing the more adequate for a given problem. Retaining the same values of the constants γ and c , Eq. (10) can be adapted within a fully implicit framework as follows:

$$\begin{aligned} \frac{1}{\Delta t} \left[\left(\gamma + \frac{1}{2} \right) u^{n+1} - 2\gamma u^n + \left(\gamma - \frac{1}{2} \right) u^{n-1} \right] &= \left(\gamma + \frac{c}{2} \right) (\zeta(u^{n+1}) + \epsilon(u^{n+1})) \\ &+ (1 - \gamma - c) (\zeta(u^n) + \epsilon(u^n)) + \frac{c}{2} (\zeta(u^{n-1}) + \epsilon(u^{n-1})), \end{aligned} \quad (11)$$

Applying Eq. (3) in Eq. (11), and re-arranging the different terms, the momentum equation, once discretized in time takes the following form:

$$\begin{aligned} \frac{(\gamma + 0.5)\rho^{n+1}u_i^{n+1} - (2\gamma)\rho^n u_i^n + (\gamma - 0.5)\rho^{n-1}u_i^{n-1}}{\Delta t} &= -\frac{\partial p^{n+1}}{\partial x_i} \\ &+ (\gamma + 0.5c)m_2 + (1 - \gamma - c)m_1 + (0.5c)m_0 + S_{ui}^{n+1}, \end{aligned} \quad (12)$$

where we defined:

$$m_{k+1} = \left(\frac{\partial \tau_{ij}^{n+k}}{\partial x_j} - \frac{\partial \rho^{n+k} u_i^{n+k} u_j^{n+k}}{\partial x_j} \right), k = -1, 0, 1 \quad (13)$$

As mentioned previously, the choice of the constant values γ and c , allows to recover the Crank-Nicolson method $(\gamma, c) = (0.5, 0.0)$, the Modified Crank-Nicolson $(\gamma, c) = (0.5, 0.125)$, the Leap Frog method $(\gamma, c) = (0.0, 1.0)$ and, the Backward Difference Formula - BDF, $(\gamma, c) = (1.0, 0.0)$. Finally, it is worth recalling that, through Eq. (12), the fully implicit framework retained here requires the numerical resolution of a large algebraic system.

2.1. Projection method

Since a fully implicit fractional step method is used in the present work, a Poisson type equation must be solved to apply a pressure correction to both velocity and pressure fields. To provide such an equation, we write Eq. (12), with the pressure derivative evaluated at time level n :

$$\begin{aligned} \frac{(\gamma + 0.5)\rho^{n+1}\tilde{u}_i^{n+1} - (2\gamma)\rho^n u_i^n + (\gamma - 0.5)\rho^{n-1}u_i^{n-1}}{\Delta t} &= -\frac{\partial p^n}{\partial x_i} \\ &+ (\gamma + 0.5c)m_2 + (1 - \gamma - c)m_1 + (0.5c)m_0 + S_{ui}^{n+1}, \end{aligned} \quad (14)$$

where $\tilde{u}_i^{n+1}$ stands for the estimated velocity field. Subtracting Eq. (14) from Eq. (12), defining $Q = p^{n+1} - p^n$, and rearranging the different terms, one obtains:

$$\frac{\rho^{n+1}(\gamma + 0.5)}{\Delta t} (\tilde{u}_i^{n+1} - u_i^{n+1}) = \frac{\partial Q}{\partial x_i}, \quad (15)$$

we then proceed classically by taking the divergence of Eq. (15):

$$\frac{(\gamma + 0.5)}{\Delta t} \left(\frac{\partial \tilde{u}_i^{n+1}}{\partial x_i} - \frac{\partial u_i^{n+1}}{\partial x_i} \right) = \frac{\partial}{\partial x_i} \left(\frac{1}{\rho^{n+1}} \frac{\partial Q}{\partial x_i} \right). \quad (16)$$

In situations where the density can be considered to be constant, at least along a streamline, the second derivative at the LHS of Eq. (16) is zero due the incompressibility condition. However,

when density variations arise from temperature (and potential composition) variations as encountered for instance in reactive flows, such term can no longer be discarded.

In the low Mach number flows under consideration, the density is solely determined by the temperature and thermodynamic pressure fields. The energy equation plays the role of an additional constraint on the velocity field, which is enforced by the dynamic pressure. This constraint acts onto the flow field divergence, and it is related to the total derivative of the density field, which involves - through the equation of state Eq. (5) - the total derivatives of both pressure and temperature. The latter can be expressed thanks to the energy conservation equation, i.e. Eq. (9), thus leading to:

$$\frac{\partial u_i}{\partial x_i} + S_c = \frac{1}{C_p P_o} \left\{ \frac{1}{RePr} \frac{\partial}{\partial x_i} \left(\kappa \frac{\partial \phi}{\partial x_i} \right) + \left(\frac{\gamma - 1}{\gamma} - C_p \right) \frac{dP_o}{dt} + S_\phi + C_p T S_\rho \right\}, \quad (17)$$

where S_c is a mathematical source term associated with the constraint itself. This source term, which is added to the constraint, will be used in the subsequent application of the method of manufactured solutions devoted to the low Mach number scheme verification. Its determination will be discussed in the corresponding section. The equation for pressure correction, for low Mach number flows simulations may therefore be written as:

$$\begin{aligned} \frac{\partial}{\partial x_i} \left(\frac{1}{\rho^{n+1}} \frac{\partial Q}{\partial x_i} \right) &= \frac{(\gamma + 0.5)}{\Delta t} \left\{ \frac{\partial \tilde{u}_i^{n+1}}{\partial x_i} - \frac{1}{C_p P_o} \left[\frac{1}{RePr} \frac{\partial}{\partial x_i} \left(\kappa \frac{\partial \phi}{\partial x_i} \right) \right] \right\} \\ &+ \frac{(\gamma + 0.5)}{\Delta t} \left[\left(\frac{\gamma - 1}{\gamma} - C_p \right) \frac{dP_o}{dt} + S_\phi + C_p T S_\rho - S_c \right] \end{aligned} \quad (18)$$

Once the pressure correction is evaluated, the velocity field can be updated:

$$u_i^{n+1} = \tilde{u}_i^{n+1} - \left(\frac{\Delta t}{(\gamma + 0.5) \rho^{n+1}} \right) \frac{\partial Q}{\partial x_i}. \quad (19)$$

The constraint given by Eq.(17) in variable density flows has been previously discussed, among others, in [28] and [39]. Moreover, an inner iterative process can be used to enhance both stability and convergence of the solution process. Further comments about such a procedure and its effects on the numerical convergence are deferred to the section devoted to the validation of low Mach number manufactured solutions. Finally, it is worth recalling that, for incompressible flows simulations, the constraint presented above is no longer necessary.

3. Numerical modeling

Important factors that directly impact the performances of a numerical method that seeks to solve variable density incompressible flows are: (i) the choice of the variables arrangement in the computational grid, (ii) the type and order of accuracy of the numerical scheme retained to perform the discretization in space of both viscous and advective terms, and (iii) the type and order of accuracy of the method chosen to perform the temporal integration.

If the discretization relies on a finite-volume (FV) approach, it is necessary to evaluate vectorial fields coupled to scalar fields, as it is the case when the Navier-Stokes equations are considered. The issue associated to the positioning of the primary variables in the computational grid

must be carefully accounted. Several options exist, but they may be classified into two principal groups: staggered or co-located grids. In the former case, the vectorial and scalar variables are positioned in different locations. In the latter, all physical variables are evaluated at the same location. This is the simplest choice for implementation, in particular when distributed computing strategies are to be applied. However, in incompressible flows, if the velocity and pressure are positioned in the same location, decoupling instabilities, often referred to as checkerboard patterns can arise [6, 16, 27].

The discretization procedure retained for the momentum equation is basically identical for both the staggered and the co-located arrangements. Nevertheless, with the latter, the velocity components, positioned at the center of the control volumes must be interpolated to their faces. The most common procedure is to use the Rhie-Chow interpolation [32]. Shen *et al.*, [33] underline that the Rhie-Chow interpolation produces excellent results when steady-state solutions are sought for, and large time steps used, but pressure field oscillations may arise for small time steps and during transient simulations. Versteeg and Malalasekera [34], and Ferziger and Peric [16], argue that there is no intrinsic physical requirement that all variables share the same location. For cartesian grids, the concept of staggered grid was introduced in reference [35]. If second order of accuracy schemes are retained for spatial discretization, such an arrangement does not require additional interpolations, which otherwise would be necessary for a co-located grid. Finally, the major advantages of the staggered variable arrangement is that the pressure terms are naturally discretized by second order accuracy central differences scheme, without any resort to interpolation rules, and the evaluation of mass fluxes at the faces of control volumes is straightforward, which leads to a strong coupling between pressure and velocity, thus avoiding spurious instabilities in the calculated pressure field.

The numerical method chosen for solving the variable density momentum, reduced temperature and Poisson equations is based on a three-dimensional, conservative, staggered, finite-volume discretization. The central difference scheme (CDS) is applied to express both diffusive and advective contributions of the present finite-volume scheme. **Depending on the class of flows simulated, some iterative solvers can fail to converge when applied to the algebraic equation systems derived from central difference approximations of convective fluxes. The reason why it can happen is because grid-to-grid oscillations are not solved by central finite-difference schemes, and hence, should be removed because they can lead to numerical instabilities [40]. Practically, the elimination of these spurious short waves is obtained by introducing artificial dissipation through additional damping terms in the equations [41] or, more efficiently, through filtering [40] without affecting the physical long waves. It is possible yet to apply a deferred correction approach on the advective terms of the balance equations. Such approach designed to improve stability is explained in [16].**

A fully implicit approach is adopted, and the resulting linear systems are solved using the MSIP - Modified Strongly Implicit Procedure [42]. The numerical code developed is capable of performing massively parallel distributed computations also. The corresponding parallelization strategy relies on a three-dimensional cartesian topology of domain decomposition, its detailed description is outside the scope of the present study.

The structure adopted for the computational grid, can be non-uniform in such a manner that it is necessary to perform interpolations to discretize any spatial derivatives. Such interpolations are obtained by using classical distance-weighted rules [16] e.g., to determine the value of a scalar property, θ , on a face e , the following expression is used: $\theta_e = \theta_E \Lambda_e + \theta_P (1 - \Lambda_e)$, where:

$$\Lambda_e = \frac{(\delta x)_e^-}{(\delta x)_e} \quad (20)$$

Figure 1: Non-uniform finite-volume grid and distances associated to the face e .

321 The indexes P , E and e , are, respectively, the center of the current control volume, the center
 322 of the left control volume, and the position of the face of the control volume centered in P , that
 323 lies between P and E , as can be seen in Fig. (1).
 324 The iterative procedure, for each time step, is summarized in Table (1):

Table 1:

Algorithm 1- Projection method with inner iteration procedure

-
- [1] The scalar equation for reduced temperature [Eq. (9)] is advanced in time using the Crank Nicolson integration scheme, [Eqs.(12,13)] with $(\gamma, c) = (0.5, 0.0)$
 - [2] The equation of state [Eq. (5)] is evaluated, yielding the density in the actual time step
 - [3] The momentum equations [Eq. (14)] are advanced in time, yielding the estimated velocity field $\tilde{u}_i^{n+1}$
 - [4] The variable-coefficient Poisson equation [Eq. (18)] is solved yielding the pressure correction Q , the pressure and velocity fields are updated [Eq.(19)]
 - [5] The continuity equation [Eq.(2)] is evaluated to check the mass conservation
 - [6] Returns to item [1], until the cycling process is finished
 - [7] Time is advanced: $t^{n+1} = t^n + \delta t^n$
 - [8] Process is repeated from step [1] until $t^{n+1} = t_{end}$
-

325 It is important to underline that the algorithm described above ensures mass conservation
 326 within each single iteration step, however, increasing the number of inner iterations improves
 327 both its precision and numerical stability, as will be shown in the following section.

328 4. Code verification using the Method of Manufactured Solutions - MMS

329 The resort to the method of manufactured solutions is progressively becoming a classical,
 330 and well accepted methodology retained in the framework of numerical code verification [43].
 331 There is an undeniable interest in the use of such a method to quantify accurately numerical ca-
 332 pabilities before using computational programs to perform the simulation of more complicated
 333 physical systems.

The MMS consists in developing *a priori* known analytical solutions of the system of governing equations. These manufactured solutions modify the original equations by adding a ‘source term’, such as those presented in Eqs. (2), (3) and (9). To construct the manufactured solution a set of almost arbitrary functions are selected and substituted into the considered system PDEs, thus allowing to solve its derivatives analytically. The result of such a substitution is the ‘source term’. The source term is then considered as an input to the numerical code, so it becomes able to reproduce the manufactured solution. The pioneering works that make use of manufactured solutions with the objective of verifying the order of accuracy of a given numerical code can be assigned to Steinberg and Roache [43], Roache *et. al.* [44] and Roache [45].

In order to obtain the order of accuracy of the developed numerical implementation, a quantitative metric of the error is chosen, and successive grid refinements are performed. As the error metric decays with the grid refinement, it is evaluated as a function of the characteristic mesh size h .

The arbitrary nature of the analytical functions must satisfy, at least, the following conditions:

- They must be continuous smooth function of independent variables (problems involving discontinuities are generally dealt with using lower order algorithms due to stability issues);
- The solution must be continuously differentiable up to the order required by the corresponding terms in the governing equations;
- To avoid numerical difficulties, manufactured solutions should avoid negative values for quantities that are physically defined as positive semi-definite (e.g. density, molecular viscosity);
- If periodic boundary conditions are chosen, the solution must be periodic as well to avoid the development of discontinuities.

Salari and Knupp [46] provide a well documented guideline for creating manufactured solutions as well as the procedure for obtaining the corresponding source terms and further analysis of the results.

For a given level of resolution, we define $\Phi_{(i,j,k)}^h$ as the discrete value of any variable Φ of interest, e.g. the density, velocity components, pressure or reduced temperature, at any point (i, j, k) , and $\Phi_{(i,j,k)}^e$ the corresponding value of the manufactured solution. The first step of the verification procedure now requires to define a metric of the numerical error, denoted Ψ_h in the following, in order to quantify subsequently the error decay rate obtained for decreasing values of the characteristic grid mesh size h .

Retaining the L_2 -norm as a relevant metric of the numerical error, we introduce:

$$\Psi_h = L_2(\Phi_{(i,j,k)}^h) = \sqrt{\frac{1}{N} \sum_{i,j,k} (\Phi_{(i,j,k)}^h - \Phi_{(i,j,k)}^e)^2}, \quad (21)$$

where N denotes the total number of grid points.

The ratio of error decay is defined according to:

$$r_e = \log\left(\frac{\Psi_{2h}}{\Psi_h}\right), \quad (22)$$

372 with Ψ_{2h} the numerical value of the metric error obtained on a grid with a characteristic mesh
 373 size $2h$.
 374 Following the nomenclature retained in [46], we define also the order of accuracy q as:

$$q \approx \frac{r_e}{\log(2)}. \quad (23)$$

375 Using Eq. (23), it is possible to verify that the characteristic error decay ratio, using grids with
 376 characteristics mesh sizes $2h$ and h , for methods of order of accuracy $q = 1, 2$ and 3 , must be,
 377 approximately, $2, 4$ and 8 , respectively. It is worth noting that, although possible, the value of r_e
 378 does not always converge monotonically as the mesh is progressively refined, and it may exhibit
 379 some oscillations.

380
 381 The process of verification presented herein is divided into two distinct parts. First, the nu-
 382 merical code is tested using a manufactured solution that aims at verifying the order of accuracy
 383 for an incompressible solution (zero Mach number limit). This is performed using solutions
 384 based on sine and cosine functions, built in such a manner that the velocity divergence is zero. A
 385 second set of tests aims at mimicking the propagation of a corrugated flame front that separates
 386 heavy from light gases. The application of the method of manufactured solutions still remains
 387 more scarce for such low Mach number situations. If we except the expression of the equation
 388 of state, the solution retained to perform this analysis is the same as the one previously consid-
 389 ered in the recent studies conducted by Shunn and Ham [47], and Shunn and Knupp [48]. This
 390 second set of tests clearly aims at evaluating the numerical capabilities of the developed code to
 391 deal with variable density flows as those encountered in combustion problems of interest to the
 392 authors.

393 4.1. Verification of an incompressible solution

394 Following the recent work conducted by [49] and [50], the set of functions reported below is
 395 retained as a possible solution for velocity, pressure and scalar fields in the limit of a zero Mach
 396 number scheme:

$$u_e = \sin^2(2\pi x + 2\pi y + 2\pi z + t), \quad (24)$$

$$v_e = \cos^2(2\pi x + 2\pi y + 2\pi z + t), \quad (25)$$

$$w_e = 1, \quad (26)$$

$$p_e = \cos(2\pi x + 2\pi y + 2\pi z + t), \quad (27)$$

$$\phi_e = K_{\phi_1} + \frac{1}{K_{\phi_2}} + \cos(2\pi x + 2\pi y + 2\pi z + t). \quad (28)$$

401 In the previous equations K_{ϕ_1} and K_{ϕ_2} are constant parameters, t is the time. The subscript e
 402 stands for the manufactured solutions of the primary variables, i.e. the three velocity components,
 403 pressure and reduced temperature

404 The computational domain retained for the present numerical simulations is a cube of dimensions
 405 $[0, 1] \times [0, 1] \times [0, 1]$, in x, y and z directions respectively. The time step is set constant and equal
 406 to 10^{-4} . The parameters K_{ϕ_1} and K_{ϕ_2} are fixed respectively to 1 and 0.5 . The constant values of
 407 density and viscosity are set to unity. The variable coefficient Poisson solver is used, however,
 408 no constraint is enforced for such incompressible solution. Table (2) reports the grid refinement,
 409 the decay of L_2 norm and the resulting order of accuracy q .

Table 2:
Order of accuracy for Dirichlet boundary conditions and constant physical properties.

Domain	16^3	q	32^3	q	64^3	q	128^3	q
$L_2 u$	1.60E-02	-	3.80E-03	2.07	9.30E-04	2.03	2.33E-04	2.00
$L_2 v$	1.60E-02	-	3.80E-03	2.07	9.30E-04	2.03	2.33E-04	2.00
$L_2 w$	3.42E-03	-	7.98E-04	2.10	1.94E-04	2.04	4.86E-05	2.00
$L_2 p$	1.82E-01	-	5.44E-02	1.74	1.52E-02	1.84	4.10E-03	1.89
$L_2 \phi$	1.54E-02	-	4.10E-03	2.08	8.88E-04	2.03	2.29E-04	1.96

410 The results gathered in Table (2) are illustrated in Figure (2). For the incompressible solution,
 411 the numerical code is shown to yield at least second order of accuracy for velocity. For the
 412 scalar variable ϕ , second order of accuracy is achieved as well, although minor oscillations arise.
 413 Finally, concerning the pressure, it is possible to note a continuous increase of the order of
 414 accuracy as the computational mesh is refined, however, its value does not exceed 1.89.

Figure 2: L_2 norm of the Zero Mach Number manufactured solution. $\blacksquare$: u , $\blacktriangle$: v , $\blacklozenge$: w , $\blacktriangledown$: ϕ , $\bullet$: p . The solid line stands for the second order decay, and the dashed line stands for first order decay

415 Such an analysis of the incompressible solution under consideration clearly demonstrates
 416 that, in terms of numerical accuracy, the numerical code we developed is a good candidate to
 417 perform Large Eddy Simulations of constant density turbulent flows that requires at least second
 418 order accuracy.
 419 The preliminary key step associated with the verification of the numerical code being performed
 420 for an incompressible regime, we will now turn to variable density flows.

4.2. Verification of the Low-Mach number solution

421 The set of manufactured solutions retained in the present section are similar to those intro-
 422 duced in the previous studies by Shunn and Knupp [48] and Shunn and Ham [47]. However, it
 423 is used here with a different equation of state, which involves a different pressure-velocity cou-
 424 pling. It is also worth mentioning that we are interested in density ratio variations representative
 425

of those encountered in flames, which are significantly smaller than those reported in [47].

The manufactured solutions are not necessarily related to an expected physical solution, however, a solution that attempts to represent some relevant features of a given problem becomes not only a tool to assess the order of accuracy, but also provides a pertaining preview of the behavior of the numerical code, when applied to situations of interest. In this sense, the set of analytical functions reported below gathers some interesting features of a propagative combustion front.

$$\phi_e = \frac{1 + \tanh[b\hat{x}\exp(-\omega t)]}{\left(1 + \frac{\rho_0}{\rho_1}\right) + \left(1 - \frac{\rho_0}{\rho_1}\right)\tanh[b\hat{x}\exp(-\omega t)]}, \quad (29)$$

$$\rho_e = \frac{P_o}{\phi_e}, \quad (30)$$

$$u_e = \frac{\rho_1 - \rho_0}{\rho_e} \left\{ -\omega\hat{x} + \frac{\omega\hat{x} - u_f}{\exp[2b\hat{x}\exp(-\omega t)] + 1} + \frac{\omega \log[\exp(2b\hat{x}\exp(-\omega t)) + 1]}{2b \exp(-\omega t)} \right\}, \quad (31)$$

$$v_e = v_f, \quad (32)$$

$$w_e = 0, \quad (33)$$

$$p_e = 0, \quad (34)$$

where, $\hat{x} = u_f t - x + a \cos[k_2(v_f t - y)]$ and $a, b, k_2, \omega, u_f, v_f$ and P_o are constant parameters.

It is important to point out that the manufactured solution must be compatible with the full set of equations that governs the evolution of the system under consideration, and this also includes the equation of state and the resulting constraint that applies to the velocity field through Eq. (17). The above manufactured solution does not fulfill such a requirement, and the source term S_c , previously introduced in Eqs. (17) and (18), must be now considered. Its expression, which is a rather cumbersome combination of exponential and hyperbolic functions, is not reported here. It is evaluated in the same manner as S_{u_i} and S_ϕ , i.e. the exact functions (Eqs. (29-34)) are substituted in Eq. (17), and, after solving the derivatives analytically, one obtains the expression of S_c . Equations (29 - 34) satisfy the mass balance equation with $S_\rho = 0$, however, non-zero source terms also appear in momentum, (S_{u_i}), and reduced temperature transport equation (S_ϕ).

Table 3:
Values of the constant parameters
for the variable density numerical simulation.

parameter	value	parameter	value
ρ_o	5	a	1/5
ρ_1	1	b	20
u_f	0.25	k_2	4π
v_f	0	ω	1
w_f	0	$\kappa = \mu$	10^{-4}
P_o	5	C_p	1

Figure (3) displays the temporal evolution of the density field. It is possible to note that, as the time passes, the front is simultaneously advected and diffused. The computational domain is

453 a box of $[-1, 2] \times [-0.5, 0.5] \times [-h/2, h/2]$. Five different grids are used, from: $150 \times 50 \times 1$, up
 454 to, $2400 \times 800 \times 1$. These grids are henceforth denoted, respectively, by: $4h$, $2h$, h , $h/2$ and $h/4$.
 455 For velocity components, reduced temperature and density, Dirichlet boundary conditions are set
 456 at $x = 0$, $y = -1/2$ and $y = 1/2$. A Neumann boundary condition is used in the outlet $x = 2.0$.
 457 For the pressure, Neumann boundary conditions are applied at $x = 0$, $y = -1/2$ and $y = 1/2$. At
 458 the outlet a Dirichlet condition is retained. For all variables, periodicity is assumed in spanwise,
 459 (z), direction. Table 3 presents the values considered in this work for simulation of Eqs. (29-31).

Figure 3: Evolution of the density field. Top to bottom, $t = 0.0$, $t = 0.5$ and $t = 1.0$. From left to right, each isolines stands for an increase of 0.5 in density from $\rho_1 = 1$, until $\rho_0 = 5$.

460 The procedure of cycling some parts of the algorithm is used to enhance convergence and
 461 stability of the numerical scheme. Such procedure is based on the recent work of Shunn and
 462 Ham [47], but with some modifications. First a different equation of state is used, second a
 463 constraint on the divergence of the velocity field is added herein, as a part of the strategy retained
 464 to solve the Poisson problem. Finally, it is worth recalling that we are interested in density ratio
 465 values smaller than those considered in [47].

466 4.2.1. Unsteady error behavior

467 In this section we discuss the effects of the outer iterative procedure i.e. number of times that
 468 the balance, state and the Poisson equations are solved, before the numerical time integration
 469 scheme. The influence of the Courant number value on the evolution of the L_2 norm is also
 470 assessed.

471 In order to quantify only the effects of spatial errors and cycling procedure in the analysis of order
 472 of accuracy of low Mach number MMS problems, a Courant number value is chosen, and then,
 473 the grid refinement procedure is performed and the subsequent analysis of order of accuracy is
 474 conducted.

Figure 4: Evolution in time of the L_2 norm for the density variable with 1 (left) and 10 (right) cycles. $\blacksquare$: $4h$, $\blacktriangle$: $2h$, $\bullet$: h , $\blacklozenge$: $h/2$, $\blacktriangleright$: $h/4$. For the sake of better visualization, the L_2 axis is in log scale

Figure (4) shows the unsteady evolution of the L_2 norm evaluated from the density field. In this case, the Courant number value for the simulations is set to 2. It is noteworthy that, specially for the refined grids, the increase in the number of cycles leads to a slight decrease of the magnitude of the L_2 norm and therefore an improvement in order of accuracy. It is also worth noting that such a behavior is also observed for the variables u , v and ϕ . In figure (5) the evolution of the L_2 norm of pressure is reported. Unlike the other primary variables of the system, as the number of cycles increases, the magnitude of the L_2 norm increases as well. However, it will be shown in the next section devoted to the analysis of order of accuracy for the low Mach number MMS that, even with such a negative sensitivity to the number of cycles, its order of accuracy is not penalized.

Although not shown here for the sake of conciseness, we have also found that the L_2 norm of primary variables errors smoothly decays with time as the front diffuses and the number of control volumes within the front increases. In fact, this is the reason that explains why we stopped the numerical simulations at $t = 1.0$.

Figure 5: Evolution in time of the L_2 norm for p with 1 (left) and 10 (right) cycles. $\blacksquare$: $4h$, $\blacktriangle$: $2h$, $\bullet$: h , $\blacklozenge$: $h/2$, $\blacktriangleright$: $h/4$. For the sake of better visualization, the L_2 axis is displayed in log scale

Figure (6) displays L_2 norm for different number of cycles for the h grid. The results clearly show that with higher values of Courant number, the use of more than 5 iterations in the cycling procedure does not provide any further gain in the reduction of error magnitude. However, for Courant number values up to unity, an increase in the number of cycles still gives rise to an improvement of the results.

Figure 6: Decay of the L_2 norm according to the number of cycles $CFL = 0.5$ (left) and $CFL = 2.0$ (right) for density. $\blacksquare$: Single cycle, $\blacktriangle$: 5 cycles, $\bullet$: 10 cycles. For the sake of better visualization, the L_2 axis is plotted in log scale

4.2.2. Order of accuracy analysis

In this section we present and discuss the results of an order of accuracy analysis performed for the low Mach number MMS case. All the simulations presented below have been carried out with a constant value of the Courant number. Although the errors quantified herein by means of

the L_2 norm is a rather complicated combination of both spatial and temporal approximations, performing the grid refinement with such a constant Courant number value allows to focus on the influence of the spatial discretization only, and this despite the presence of a residual temporal error since it will remain the same, provided that the Courant number value is kept constant.

Table 4:
Order of accuracy for low Mach number solution, Single cycle, Co=2.

Domain	$4h$	q	$2h$	q	h	q	$h/2$	q	$h/4$	q
L_2u	8.82E-03	-	4.52E-03	0.96	1.65E-03	1.45	2.29E-04	2.85	1.91E-05	3.58
L_2v	3.06E-03	-	1.28E-03	1.25	3.27E-04	1.97	3.47E-05	3.24	3.44E-06	3.33
L_2p	9.82E-04	-	5.69E-04	0.79	2.44E-04	1.22	5.89E-05	2.05	1.59E-05	1.89
$L_2\phi$	1.03E-01	-	6.73E-02	0.61	2.39E-02	1.50	7.70E-02	1.01	1.40E-03	2.07
$L_2\rho$	2.18E-01	-	1.55E-01	0.49	7.70E-02	1.01	2.69E-02	1.52	7.31E-03	1.88

Tables (4), (5) and (6) display the order of accuracy, and the value of the L_2 norm obtained for velocity, density and reduced temperature for different numbers of cycles and a Courant number value Co=2. These values of error and order of accuracy are measured at $t = 1.0$ [47].

Table 5:
Order of accuracy for low Mach number solution, 5 cycles, Co=2.

Domain	$4h$	q	$2h$	q	h	q	$h/2$	q	$h/4$	q
L_2u	8.19E-03	-	2.50E-03	1.71	5.01E-04	2.32	7.55E-05	2.73	1.00E-05	2.92
L_2v	3.52E-03	-	1.17E-03	1.60	2.29E-04	2.35	2.82E-05	3.02	5.85E-06	2.27
L_2p	2.68E-03	-	1.24E-03	1.11	4.49E-04	1.47	1.36E-04	1.72	6.07E-05	1.17
$L_2\phi$	5.05E-02	-	1.16E-02	2.12	1.96E-03	2.57	2.98E-04	2.72	4.87E-05	2.61
$L_2\rho$	1.15E-01	-	3.83E-02	1.59	8.97E-03	2.09	1.32E-03	2.76	1.76E-04	2.91

Unlike the order of accuracy analysis conducted for the incompressible solution, where the values of the L_2 norm decrease with a constant order of accuracy, the present results show that, as the grid is refined, not only the magnitude of the L_2 norm decreases, but also the order of accuracy increases. Such a trend is even more pronounced for velocity, density and reduced temperature when increasing the number of cycles. On the contrary, as far as the pressure field is concerned, the magnitude of the L_2 norm also increases for an increasing number of cycles.

Table 6:
Order of accuracy for low Mach number solution, 10 cycles, Co=2.

Domain	$4h$	q	$2h$	q	h	q	$h/2$	q	$h/4$	q
L_2u	8.50E-03	-	2.58E-03	1.72	4.52E-04	2.51	6.59E-05	2.78	9.73E-06	2.82
L_2v	3.14E-03	-	1.02E-03	1.63	2.05E-04	2.31	2.12E-05	3.27	4.24E-06	2.32
L_2p	3.90E-03	-	1.81E-03	1.11	6.44E-04	1.49	1.76E-04	1.87	6.49E-05	1.44
$L_2\phi$	4.19E-02	-	8.34E-03	2.33	1.26E-03	2.73	1.32E-04	3.25	1.29E-05	3.35
$L_2\rho$	1.21E-01	-	3.97E-02	1.61	5.55E-03	2.84	1.17E-03	2.24	1.19E-04	3.31

Figure (7) displays the order of accuracy achieved for both the pressure and the u -component of the velocity. The simulations are carried out using a constant value of the Courant number value Co=2. From a careful examination of Tables (4), (5) and (6), and Figure (7), one can notice that the error decay is larger in single cycle simulations. A similar analysis (not reported)

516 demonstrates that such a conclusion also holds for different Courant number values, and for all
 517 the primary variables.

Figure 7: Evolution of the order of accuracy q . Pressure (left), u (right). ■: Single cycle, ▲: 5 cycles, ●: 10 cycles. For the sake of better visualization, the N axis is plotted in log scale

518 The decays of the L_2 norm obtained for the primary variables, corresponding to the results
 519 gathered in Tables (4) - (6), are illustrated in Figure (7). In this figure, one can note a higher value
 520 of the order of accuracy as the number of cycles is increased. Even for the pressure, that is less
 521 sensitive to the number of cycles than the others variables, an increase in the order of accuracy is
 522 observed.

523 With regard to the effects of the number of cycles with respect to the order of accuracy, it is
 524 worth noticing that, as the grid mesh size is halved from h to $h/2$, and with a Courant number
 525 value $Co=2$, the order of accuracy for the density is found to increase from 1.52 (Tab. 4, column
 526 8, line 5) to 2.24 (Tab. 6, column 8, line 5), provided that the number of cycles is increased from
 527 1 to 10.

Figure 8: Evolution in time of the L_2 norm. Single cycle (left), 10 cycles (right). ■: u , ▲: v , ◆: p , ●: ϕ , ►: ρ . The solid line stands for the second order decay, and the dashed line stands for first order decay.

5. Qualitative results of a high speed mixing layer

In order to test the stability of the numerical model here implemented, a high speed mixing layer is simulated. The flow in question based on the work of [51] and [52] is a turbulent high speed mixing layer in a combustion chamber, where a premixed air-methane flow is ignited and stabilized by a parallel flow of hot gases. Profiles of mean velocities, turbulence rate and velocity fluctuations are given for both reactive and non-reactive flows. The combustion chamber is a channel with dimensions $800 \times 100 \times 100$ mm discretized in a finite volume mesh of $100 \times 50 \times 50$ control volumes in the directions x , y and z respectively. Its inlet is divided in two ducts by a splitter plate; a main duct where the fresh gases are injected and an auxiliary duct for the hot gases. No-slip boundary conditions are imposed in the limits of y and z directions. A convective boundary condition is used at the outlet. The turbulence model adopted is the classical Smagorinsky model [53] and its constant is set to 0.18; The Van-Driest damping function is used [16]. The mean velocity profile used in the inlet is represented by an hyperbolic function:

$$\bar{u}(z) = \frac{\bar{u}_q - \bar{u}_p}{2} + \frac{\bar{u}_q + \bar{u}_p}{2} \tanh\left(\frac{2h(z)}{\delta_m} - \frac{2h_p}{\delta_m}\right), \quad (35)$$

where, $\bar{u}_q$ and $\bar{u}_p$ are respectively the mean velocities of the auxiliary burner and of the main duct; h_p is the height of auxiliary duct. δ_m is the width of the mixing layer. The main duct incoming flow is characterized by a maximum longitudinal velocity of 65 m/s. The auxiliary duct incoming flow presents a maximum longitudinal velocity of 130 m/s. The Reynolds number, based on the main duct incoming flow, on its height ($h_q = 80$ mm) and on the value of the kinematic viscosity of air at 600 K is 94540.

Figure 9: Iso surfaces of $Q = 2^6$, at $t = 0.46s$ (46000 iterations). The Reynolds number is 94540

It is well known that a subject of great importance in the simulation of problems of fluid

dynamics is the correct and realistic impositions of boundary conditions, especially inflow and outflow conditions. For the example here described we retain a methodology for generation realistic inlet boundary conditions based of digital filters. Such an approach involves to create a entire set of random number data which can then be processed using digital filters in such a way that the data presents desired statistical properties such as spatial and temporal correlations. An interesting feature of this approach is the ability of generating anisotropic turbulence, which is fundamental in Large Eddy Simulations [54].

A instantaneous snapshot of the three dimensional simulation of the flow just cited is shown in Figure (9). The snapshot was taken at $t = 0.46s$, equivalent to 46000 iterations. An interesting way to evidencing rotational structures is through the property Q [55]. In Figure (9) it is possible to see the isosurface of the property $Q = 2^6$. The high value of such property in this case is due the fact that the flow is a high velocity, high Reynolds number, confined flow. The Kelvin-Helmholtz structures, characteristic of mixing layers are notable near the inlet of the domain. The strong three-dimensionality of the flow is also present, in a major part due the turbulence inlet generator.

The fact that we firstly had a totally verified numerical code was fundamental in the simulation of the above mixing layer. It shows that even tough the MMS are normally applied with smooth well known problems, it does serves (and should be used) as a primary test before coping with problems physically more demanding.

6. Conclusion

We have described a procedure for code verification (*i*) to determine whether, or not, a numerical code solves its governing equations correctly, and (*ii*) to preview how such a numerical scheme behaves when dealing with real problems. The numerical procedure relies on the manufacture of a general solution of the system of governing equations. Generality of the solution is essential because it guarantees that few, if any, code capabilities will remain unverified.

Two MMS problems are considered. First, a fully incompressible manufactured solution is proposed, achieving the expected order of accuracy. Second, an analytical propagating front separating heavy from light gases is considered. A variable coefficient Poisson solver is used to simulate the corresponding low Mach number flow. A physically consistent constraint is used to ensure that the velocity field is solved correctly. Such a combination of the velocity constraint and the variable-coefficient Poisson solver is found of fundamental importance to ensure both the numerical stability and the expected order of accuracy. An inner iteration procedure is implemented, and despite its high numerical cost, the improvements in terms of both the order of accuracy and error magnitude are undeniable. In this respect, further investigations may be carried out since although possible, the order of accuracy q does not always converge monotonically.

The present results also suggest that determining the optimal operating conditions in terms of grid size, Courant number value, number of outer iterations, etc. is a nontrivial and problem-dependent task that deserves more attention than currently afforded.

Finally, although not fully physically consistent - since the MMS is more a mathematical exercise rather than a real attempt of reproducing a real life experiment or physical problem - the procedure of verification allows to gain more insights into the capabilities and limitations of the numerical code we presented to deal with variable density flow fields representative of those encountered in situations relevant of combustion.

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