A Fractional Step Method for the Solution of the Compressible Navier-Stokes Equations

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A Fractional Step Method for the Solution of the Compressible Navier–Stokes Equations

R. Codina¹, M. Vázquez¹ and O.C. Zienkiewicz²

Abstract. In this paper we present a summary of the splitting technique for both compressible and incompressible flows previously proposed in [22, 23, 7]. Also, we extend it to the case of a fully implicit treatment of the viscous and convective terms of the momentum equations. For incompressible flows this scheme reduces to classical fractional step methods, except for a non-standard treatment of the boundary conditions. For compressible flows the continuity equation involves two variables which must be related through the equation of state. Convective terms of the conservation equations to be solved are stabilized by means of a Characteristic - Galerkin scheme. Also, in the presence of shocks some additional dissipation is needed. Both numerical techniques are explained here taking the transport of a scalar quantity as a model problem.

1 INTRODUCTION

The algorithm here described is designed to deal equally well with a broad spectrum of problems, all of them physically modeled by the Navier - Stokes equations of fluids (either viscous or inviscid, compressible or incompressible, laminar or turbulent and so on). A *fractional step* or *splitting*, a technique first thought for incompressible flows and proposed by Chorin [3] and Temam [20], allows the use of equal interpolation spaces for pressure and velocity fields. Further, the split of the linear momentum equation produces a stabilizing effect on the pressure, which eliminates the need for special interpolation when the incompressible limit is reached. Therefore not only separate incompressible or compressible problems can be solved using the same algorithm, but compressible problems with regions of very low Mach number can be properly solved too.

In [7] we discuss the semi-implicit version of the algorithm, in which only the pressure gradient term is treated implicitly. Here we extend the scheme to the case in which both the viscous and the convective

terms of the momentum equation may be treated implicitly. In principle, this introduces a *splitting error* in the scheme that will be discussed below. However, we propose a method for eliminating the splitting error due to the implicit treatment of the convective term, and therefore only that due to the viscous term will remain. This is applicable to all types of flow and in particular to incompressible cases, when the algorithm described here reduces to the classical fractional step or projection methods, except for the treatment of the boundary conditions.

The reformulation of the equations in a characteristics co-moving frame provides a consistent artificial diffusion when space discretization is done. This diffusion, which is similar to that of some other classical methods, like SUPG, can handle the purely numerical oscillations that usually appear when the Galerkin method is applied to equations with dominant convective terms. But if shock waves are present in the solution (very likely to appear in compressible flows), the artificial diffusion supplied by the method itself is not enough to eliminate spurious localized oscillations produced around the shock in the numerical solution. Additional “shock capturing” diffusion is needed there. We use in these cases a numerical diffusion proportional to the element residual of each of the scalar transport equations to be solved.

We have organized this paper as follows. In the following section we state the problem and introduce some notation. Next we describe briefly the explicit version of the characteristic Galerkin method and the shock capturing technique used here for each of the scalar equations of the Navier–Stokes equations. In section 4 we describe the splitting method applied to the continuous equations, and then we obtain their weak form incorporating boundary conditions. The discrete problem is analyzed in section 5, where the choice of the variables in the case of compressible flows is discussed. Finally, we present some simple numerical examples and draw some conclusions.

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2 NAVIER-STOKES EQUATIONS

Let us picture a fluid contained in a given domain Ω . Its velocity $\mathbf{u} = \mathbf{u}(\mathbf{x}, t)$ can be described by means of a vectorial function of position $\mathbf{x}$, within Ω , and time t , within $[0, \infty)$. To complete the dynamic description, two of the following three variables are needed: $\rho = \rho(\mathbf{x}, t)$, $p = p(\mathbf{x}, t)$ and $T = T(\mathbf{x}, t)$ which describe its thermodynamic state variables density, pressure and temperature respectively. The linear momentum

$$U_i := \rho u_i,$$

and the total energy

$$E := \rho e,$$

where the total energy per unit mass

$$e := e_o + \frac{1}{2} u_i u_i,$$

can be defined as above. Here, the first term e_o is the internal energy, and the second, the kinetic energy.

Different types of fluids (or flows) are described by their equation of state. In particular, we shall consider the cases of incompressible flows, barotropic flows and the flow of ideal gases. In this last case, the state variables are related according to the following state law:

$$p = \rho R T, \quad (1)$$

where R is the universal gas constant. If, besides, the gas is polytropic, the internal energy is dependent only on T linearly

$$e_o = C_v T,$$

with the constant of proportionality C_v , the specific heat at constant volume.

The equations that model the behaviour of a fluid are known as the Navier-Stokes equations, a problem that is widely described in many books, for instance, [1, 16, 9]. This set of differential equations is derived from general conservation principles of mass, energy and momentum. In its pure conservative form, they can be written

$$\frac{\partial V}{\partial t} + \frac{\partial C_i}{\partial x_i} + \frac{\partial D_i}{\partial x_i} + S = 0, \quad (2)$$

where the conservative variables

$$V^T = (\rho, \rho u_1, \rho u_2, \rho u_3, \rho e)$$

are transported by means of convection, through the convective fluxes:

$$C_i^T = (\rho u_i, \rho u_i u_1 + \delta_{i1} p, \rho u_i u_2 + \delta_{i2} p, \rho u_i u_3 + \delta_{i3} p, u_i (\rho e + p))$$

and of diffusion, through the diffusive fluxes:

$$D_i^T = (0, -\tau_{i1}, -\tau_{i2}, -\tau_{i3}, q_i - \rho u_{ij} u_j).$$

The source is

$$S^T = (0, \rho g_1, \rho g_2, \rho g_3, \rho(g_i u_i + r)),$$

where g_i is the acceleration due to gravity, which points vertically downwards, and r is the heat source per unit mass.

The thermal flux is assumed proportional to temperature gradients, i.e. it is assumed the Fourier law:

$$q_i = -k(\mathbf{x}) \frac{\partial T}{\partial x_i},$$

where $k(\mathbf{x})$ is the thermal conductivity.

The deviatoric (i.e. excluding pressure isotropic term) stress tensor τ_{ij} is related linearly to velocity gradients as is usual in newtonian fluids:

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

where $\mu = \rho \nu$ is the viscosity, and ν is the kinematic viscosity. For some types of flow, kinematic viscosity is found to be temperature dependent through the Sutherland law:

$$\mu = AT^\alpha / (T + B),$$

where A, B, α are given constants.

3 A MODEL PROBLEM: CONVECTION-DIFFUSION-REACTION EQUATION

In this section we describe the numerical formulation employed to stabilize the convective terms of the transport equations to be solved. If this is done, some local overshoots and undershoots may appear in the vicinity of sharp gradients of the unknowns, in particular near shocks. A further numerical dissipation needs to be introduced in these cases. We describe both numerical techniques using the convection-diffusion-reaction equation as model problem.

3.1 Characteristic based schemes

In order to unveil one possible solution to the problem arising by the convective fluxes, consider a general convection-diffusion equation. In it, these fluxes can be written as $C_i = u_i V$. For that reason

$$\frac{\partial V}{\partial t} + \frac{\partial(u_i V)}{\partial x_i} + \frac{\partial D_i(V)}{\partial x_i} + S = 0$$

can be rewritten as

$$\frac{\partial V}{\partial t} + u_i \frac{\partial V}{\partial x_i} + V \frac{\partial u_i}{\partial x_i} + \frac{\partial D_i(V)}{\partial x_i} + S = 0. \quad (4)$$

As we shall see, the fractional momentum introduced in section 4 is solution of a time-discrete problem of this form.

Now consider each component of (4) separately and suppose that the diffusive terms are uncoupled. The first two terms of (4) compose the material derivative of V (now a scalar):

$$\frac{dV}{dt} := \frac{\partial V}{\partial t} + u_i \frac{\partial V}{\partial x_i}.$$

A material derivative of variable V means the rate of change of V , as it is observed from a reference system in which the fluid is locally and instantaneously at rest: the *co-moving reference frame*. In it, the convective terms disappear. As was said early, equations containing convective terms are often satisfied by non-smooth solutions. In this case, the usual Galerkin finite element method loses accuracy and can produce a numerical solution with spurious effects, very far away from the physical one (cf. [14]). But if we want to solve the transport equation for the variable V taking profit of the fact that the convective term vanishes in a different coordinate frame, the equation must be wholly reformulated in the co-moving system. If we note

$$L(V) := \frac{\partial D_i(V)}{\partial x_i} + V \frac{\partial u_k}{\partial x_k},$$

then (4) is simplified to

$$\frac{dV}{dt} + L(V) - S = 0. \quad (5)$$

Until the end of the section we consider the source S as zero to simplify the algebra. Let us label a particle and follow it as it wanders within the fluid. Then, its motion can be described by the *characteristics equation*

$$\frac{d\tilde{x}(t)}{dt} = u(\tilde{x}(t)), \quad (6)$$

where the tilde means “the trajectory of a particle of fluid that was at a reference point x_{ref} at a reference time t_{ref} ”. This statement is in fact the initial condition for the equation (6):

$$\tilde{x}(t_{\text{ref}}) = x_{\text{ref}}.$$

Time integration of this ordinary differential equation with this initial condition would solve the problem of tracking particles of fluid, the “carriers” of co-moving frames. In this form, equation (5) can be restated in that frame. Let S be the fixed reference spatial system, with origin pinned at x_{ref} . Let S' be the co-moving frame. If the origin of S' coincides at the t_{ref} with that of S , i.e., x_{ref} , then

$$\left. \frac{dV}{dt}(\tilde{x}(t), t) \right|_{x_{\text{ref}}, t_{\text{ref}}} = \left[\frac{\partial V}{\partial t} + u_i \frac{\partial V}{\partial x_i} \right]_{x_{\text{ref}}, t_{\text{ref}}},$$

so that

$$\frac{dV}{dt}(\tilde{x}(t), t) + L(V(\tilde{x}(t), t)) = 0.$$

This equation can be time - discretized using the trapezoidal rule:

$$\frac{1}{\Delta t} (V(\tilde{x}^{n+1}, t^{n+1}) - V(\tilde{x}^n, t^n)) + \theta L(V(\tilde{x}^{n+1}, t^{n+1})) + (1 - \theta) L(V(\tilde{x}^n, t^n)) = 0, \quad (7)$$

where $\Delta t = t^{n+1} - t^n$ (assumed constant, for simplicity of notation) and $\tilde{x}^k$ is an approximation to $\tilde{x}(t^k)$, $k = n$ and $k = n + 1$.

Once the time - discretization is done, it is necessary to choose the pair $x_{\text{ref}}, t_{\text{ref}}$ according to it. If S' coincides with $\tilde{x}^n$, the trajectory of our particle of fluid is integrated forwards in time using the values at $\tilde{x}^n$. And backwards if $x_{\text{ref}} := \tilde{x}^{n+1}$, expanding from the values at $\tilde{x}^{n+1}$. A point between them can be used too. We choose $x_{\text{ref}} := \tilde{x}^{n+1}$ (fig. 1). As was said above, Galerkin method is going to be used to discretize the space because in the co-moving frame the convective terms disappear. For that reason, the space convergence for Galerkin method is optimal, but in frame S' (i.e. $(\Delta x')^2$). If $\theta = 1/2$ is chosen (*Crank-Nicholson*) in (8), the trapezoidal rule gives the highest possible order in time: $O(\Delta t^2)$. Then, as $(\Delta x')^2 = (\Delta x)^2 + (u \Delta t)^2$, second order in space, but in S (i.e. $O(\Delta x^2)$) is reached in the streamline direction.

Through four successive steps, a second order time-discretized transport equation can be obtained in the co-moving frame, but with values obtained at the same point in the same, fixed, reference frame:

1. Integrate trajectory backwards, with $O(\Delta t^2)$:

$$\begin{aligned} \tilde{x}^n &\approx \tilde{x}^{n+1} - \Delta t u(\tilde{x}^{n+1}, t^n) \\ &\approx x - \Delta t u^n. \end{aligned}$$

2. Approximate velocity of this particle at $(\tilde{x}^n, t^n)$:

$$\begin{aligned} u(\tilde{x}^n, t^n) &\approx u(x - \Delta t u^n, t^n) \\ &\approx u^n - \Delta t u_i^n \frac{\partial u^n}{\partial x_i}. \end{aligned}$$

3. Integrate trajectory backwards, now with $O(\Delta t^3)$:

$$\begin{aligned} \tilde{x}^n &\approx \tilde{x}^{n+1} - \frac{\Delta t}{2} [u(\tilde{x}^{n+1}, t^{n+1}) + u(\tilde{x}^n, t^n)] \\ &\approx x - \frac{\Delta t}{2} u^{n+1} - \frac{\Delta t}{2} u^n + \frac{\Delta t^2}{2} u_i^n \frac{\partial u^n}{\partial x_i} \\ &\approx x - \Delta t u^{n+1/2} + \frac{\Delta t^2}{2} u_i^n \frac{\partial u^n}{\partial x_i}, \end{aligned}$$

where $u^{n+1/2} = (u^{n+1} + u^n) / 2$.

4. Calculate the variable V at $(\tilde{x}^n, t^n)$:

$$\begin{aligned} V(\tilde{x}^n, t^n) &= V(x - \Delta t u^{n+1/2} \\ &\quad + \frac{\Delta t^2}{2} u_i^n \frac{\partial u^n}{\partial x_i} + O(\Delta t^3), t^n) \\ &= V^n - \Delta t u_j^{n+1/2} \frac{\partial V^n}{\partial x_j} \\ &\quad + \frac{\Delta t^2}{2} \left[u_i^n \frac{\partial u_j^n}{\partial x_i} \frac{\partial V^n}{\partial x_j} \right. \\ &\quad \left. + u_i^{n+1/2} u_j^{n+1/2} \frac{\partial^2 V^n}{\partial x_i \partial x_j} \right] + O(\Delta t^3). \end{aligned}$$

As $u^{n+1/2} = u^n + O(\Delta t)$ and

$$\begin{aligned} u_i^n u_j^n \frac{\partial^2 V^n}{\partial x_i \partial x_j} &= \\ u_i^n \frac{\partial}{\partial x_i} \left(u_j^n \frac{\partial V^n}{\partial x_j} \right) - u_i^n \frac{\partial u_j^n}{\partial x_i} \frac{\partial V^n}{\partial x_j}, \end{aligned}$$

Figure 1. The co-moving reference frame.

we have for the variable V :

$$V(\tilde{x}^n, t^n) = V^n - \Delta t u_j^{n+1/2} \frac{\partial V^n}{\partial x_j} + \frac{\Delta t^2}{2} u_i^n \frac{\partial}{\partial x_i} \left(u_j^n \frac{\partial V^n}{\partial x_j} \right) + O(\Delta t^3). \quad (8)$$

To find an approximation for $L(V(\tilde{x}^n, t^n))$, it is done

$$\begin{aligned} L(V(\tilde{x}^n, t^n)) &= L \left(V^n - \Delta t u_j^{n+1/2} \frac{\partial V^n}{\partial x_j} + O(\Delta t^2) \right) \\ &= L(V^n) - \Delta t u_j^n \frac{\partial L(V^n)}{\partial x_j} + O(\Delta t^2). \end{aligned} \quad (9)$$

Finally, using (8) and (9) in (8)

$$\begin{aligned} V^{n+1} - V^n &= -\Delta t \left[u_j^{n+1/2} \frac{\partial V^n}{\partial x_j} + L(V^{n+1/2}) \right] \\ &\quad + \frac{\Delta t^2}{2} \left[u_i \frac{\partial}{\partial x_i} \left(u_j \frac{\partial V}{\partial x_j} + L(V) \right) \right]^n, \end{aligned}$$

which can be now approximated evaluating all the right hand side explicitly or implicitly.

In brief, if we note

$$R(V) := -u_i \frac{\partial V}{\partial x_i} - L(V)$$

the continuum equation

$$\frac{\partial V}{\partial t} = R(V) \quad (10)$$

is discretized in time, according to the methodology hitherto exposed, as:

$$\Delta V = \Delta t R(V)^{n+\theta} - \frac{\Delta t^2}{2} u_i^n \frac{\partial R(V)^n}{\partial x_i} \quad (11)$$

with $\theta \in [0, 1]$, that is: time-discretization of transport equation (10) using this method has led us to conclude

that the temporal variation of V is controlled by both the residual of the equation (at first order) and the convective derivative of it (at second order).

Consider now the operator $L(V)$ purely as diffusive, only to fix the main ideas, and also take $\theta = 0$. Thus

$$R(V) := u_i \frac{\partial V}{\partial x_i} - k \frac{\partial^2 V}{\partial x_i \partial x_i},$$

with $k > 0$. Assuming that $R(V)$ vanishes on the boundary Γ we have that

$$\begin{aligned} \int_{\Omega} W u_i \frac{\partial R(V)}{\partial x_i} d\Omega &= \underbrace{\int_{\Omega} n_i W u_i R(V) d\Gamma}_0 - \int_{\Omega} \frac{\partial}{\partial x_i} (W u_i) R(V) d\Omega \\ &= - \int_{\Omega} \left(u_i \frac{\partial W}{\partial x_i} \right) R(V) d\Omega - \int_{\Omega} \left(W \frac{\partial u_i}{\partial x_i} \right) R(V) d\Omega \end{aligned}$$

for all test functions W . Using this fact, the weak form of the time-discrete equation to be solved is

$$\begin{aligned} \int_{\Omega} W V^{n+1} d\Omega &= \int_{\Omega} W V^n d\Omega \\ &\quad - \Delta t \left[\int_{\Omega} W u_j \frac{\partial V}{\partial x_j} d\Omega + \int_{\Omega} k \frac{\partial W}{\partial x_j} \frac{\partial V}{\partial x_j} d\Omega \right]^n \\ &\quad - \frac{\Delta t^2}{2} \left[\int_{\Omega} \left(u_i \frac{\partial W}{\partial x_i} \right) R(V) d\Omega \right. \\ &\quad \left. + \int_{\Omega} \left(W \frac{\partial u_i}{\partial x_i} \right) R(V) d\Omega \right]^n + \Delta t \int_{\Gamma_N} W g d\Gamma \end{aligned} \quad (12)$$

for all test functions W vanishing on Γ_D , where Γ_D and Γ_N means respectively contours with a Dirichlet's condition and with a Neumann's condition (normal derivative = g).

The main features of this last equation are two. First, the terms linear in Δt are integrals evaluated over all the domain and boundary terms coming from boundary conditions. And second, the terms quadratic in Δt are a SUPG-like term (see [2, 12, 13]), different only in that the *intrinsic time* (τ) of SUPG is here replaced by a linear function of time, plus a term which depends on velocity divergence, and for that reason, mainly active in the case of compressible flows. Although the final outcome of SUPG is very similar, its starting point is quite different: in its simpler formulation, the test functions are slightly modified by adding to them a term linear in its convective derivative. See [6] for a further discussion about different stabilization techniques for transport equations.

3.2 A DISCONTINUITY CAPTURING TECHNIQUE

Although the method proposed adds artificial diffusion needed when the physical diffusion vanishes in the differential equations of the type here considered, localized overshoots and undershoots can appear around

the strong discontinuities that could be present at the solution. For that reason, some techniques have been developed in order to deal consistently with them.

One of these techniques (proposed in [4, 5]) consists of adding an anisotropic diffusion tensor in that particular places where it is not enough the streamline diffusion of the Characteristic-Galerkin method. It is based on two concepts. First, to preserve consistency, this diffusion tensor must be proportional to the residual of the equation evaluated within each of the elements. Second, it must be small where the convection is small.

If a convection-diffusion-reaction (CDR) equation

$$\frac{\partial V}{\partial t} + u_i \frac{\partial V}{\partial x_i} - k \frac{\partial^2 V}{\partial x_k \partial x_k} + sV = Q, \quad (13)$$

is considered, to the artificial elementary diffusion due to the Characteristic-Galerkin (CG) method, given by

$$k_{cg} = \frac{1}{2} \frac{\Delta t}{\Delta x} u^2,$$

where $u^2 = u_i u_i$, we propose to add a numerical, discontinuity capturing elementary diffusion

$$k_{dc} = \frac{1}{2} \frac{\alpha_{dc} h}{|\nabla V^h|} |R(V^h)|,$$

where $R(V^h)$ is the residual (only spatial terms considered) of (13) and

$$\alpha_{dc} = \max \left(0, C - \frac{2k |\nabla V^h|}{h R(V^h)} \right)$$

C is a constant depending on the interpolation order (0.7 if linear and 0.35 if quadratic). Superscript “h” means that it belongs to the discretized usual FEM space.

But while the former only acts along the streamlines, the latter do it in all directions, taking into account both of the previous concepts. Like the streamline CG diffusion, the final discontinuity capturing tensor diffusion is not diagonal: in the streamline direction it is compared to the CG diffusion. So, the terms added to the right hand side of equation (12), once space discretization in N_{el} elements is done, are:

$$\sum_{e=1}^{N_{el}} \int_{\Omega^e} \left[k_{dc} \frac{\partial W^h}{\partial x_i} \delta_{ij} \frac{\partial V^h}{\partial x_j} + (k_{sl} - k_{dc}) \frac{\partial W^h}{\partial x_i} \left(\frac{u_j u_i}{u^2} \right) \frac{\partial V^h}{\partial x_j} \right] d\Omega, \quad (14)$$

where $k_{sl} = \max(0, k_{dc} - k_{cg})$.

As in the preceding section, in order to apply these concepts to Navier-Stokes equations, they must be rewritten in a CDR form. Then, those same identifications can be done.

4 FRACTIONAL STEP METHOD FOR THE COMPRESSIBLE NAVIER-STOKES EQUATIONS

In this section the basic algorithm is presented. We start with the formulation of the splitting technique for the continuous equations and then we obtain the weak form of each of the equations to be solved incorporating boundary conditions. This weak form is the starting point for the finite element discretization.

4.1 Splitting

Let us write the conservation equations for the momentum $U_i := \rho u_i$ and the density ρ (continuity equation) as

$$\frac{\partial U_i}{\partial t} = M_i - \frac{\partial p}{\partial x_i} =: R_i, \quad (15)$$

$$\frac{\partial \rho}{\partial t} = - \frac{\partial U_i}{\partial x_i}. \quad (16)$$

where R_i is the i -th component of the steady-state residual and we have used the abbreviation

$$M_i := - \frac{\partial}{\partial x_j} (\rho u_i u_j - \tau_{ij}) - \rho g_i. \quad (17)$$

The convective contribution $u_j \partial(\rho u_i)/\partial x_j$ appearing in M_i could lead to numerical instabilities if the standard Galerkin formulation is used to discretize the space. In order to stabilize this effect, we first discretize (15) in time along the characteristics of the total derivative $\partial/\partial t + u_j \partial/\partial x_j$ as explained in section 2. This leads to the following equations:

$$\frac{\Delta U_i^n}{\Delta t} = M_i^{n+\theta_3} - \frac{\partial p^{n+\theta_2}}{\partial x_i} - \frac{\Delta t}{2} u_k^n \frac{\partial R_i^n}{\partial x_k}, \quad (18)$$

$$\frac{\Delta \rho^n}{\Delta t} = - \frac{\partial U_i^{n+\theta_1}}{\partial x_i}, \quad (19)$$

where Δt is the time step size (assumed to be constant for simplicity), the superscripts denote time step level, $\theta_1, \theta_2, \theta_3 \in [0, 1]$ and we use the notation $f^{n+\theta} = \theta f^{n+1} + (1-\theta)f^n$, $\Delta f^n = f^{n+1} - f^n$ for any function f and $\theta \in [0, 1]$.

Observe that in (18) the term coming from the discretization along the characteristics has been treated explicitly, but the rest are allowed to be treated implicitly. In [7] we described the same algorithm as here but with $\theta_3 = 0$, that is, treating explicitly the contribution from the viscous and convective terms. The case $\theta_3 > 0$ will introduce an important difference, as will be shown below.

A deeper insight of the implicit treatment of M_i can be achieved by separating its convective and viscous parts. We define them respectively as

$$M_{c,i} := - \frac{\partial}{\partial x_j} (u_j U_i), \quad (20)$$

$$M_{v,i} := \frac{\partial}{\partial x_j} \tau_{ij}, \quad (21)$$

so that

$$M_i = M_{c,i} + M_{v,i} - \rho g_i.$$

In order to avoid the need for solving a nonlinear problem within each time step, we take

$$M_{c,i}^{n+\theta_3} = -\frac{\partial}{\partial x_j} (u_j^n U_i^{n+\theta_3}), \quad (22)$$

that is, the convective velocity is evaluated at the previous time step. This approach is used for example in [19] for incompressible flows.

Let

$$\Delta \tilde{U}_i^n := \Delta U_i^n + \Delta t \frac{\partial p^{n+\theta_2}}{\partial x_i}. \quad (23)$$

Having introduced this new variable, (23) and (19) can be written as

$$\frac{\Delta \tilde{U}_i^n}{\Delta t} = M_{c,i}^{n+\theta_3} - \frac{\Delta t}{2} u_k^n \frac{\partial R_i^n}{\partial x_k}, \quad (24)$$

$$\frac{\Delta \rho^n}{\Delta t} = -\frac{\partial}{\partial x_i} \left(U_i^n + \theta_1 \Delta \tilde{U}_i^n - \theta_1 \Delta t \frac{\partial p^{n+\theta_2}}{\partial x_i} \right), \quad (25)$$

$$\frac{\Delta U_i^n}{\Delta t} = \frac{\Delta \tilde{U}_i^n}{\Delta t} - \frac{\partial p^{n+\theta_2}}{\partial x_i}. \quad (26)$$

Hereafter, we shall refer to $\tilde{U}_i^{n+1} := U_i^n + \Delta \tilde{U}_i^n$ as the *fractional momentum*.

In principle, the term $M_{c,i}^{n+\theta_3}$ in (24) must be computed using U_j^{n+1} . If this is done, (24), (25) and (26) are exactly equivalent to (18) and (19) for the continuous in space problem that we consider for the moment. However, the use of U_j^{n+1} in (24) prevents from the possibility of computing directly the fractional momentum from this equation. This can be avoided by replacing $M_{c,i}^{n+\theta_3}$ by $\tilde{M}_{c,i}^{n+\theta_3}$, which is obtained by computing M_i with $\tilde{U}_j^{n+1}$ instead of U_j^{n+1} . This introduces of course a splitting error.

There is the possibility of eliminating the error coming from the fact that the convective contribution to M_i is computed with the fractional momentum and not with the momentum itself. Using (22) and (23) it is found that, up to second order accuracy for the pressure term,

$$\begin{aligned} M_{c,i}^{n+\theta_3} &= -\frac{\partial}{\partial x_j} (u_j^n U_i^n) \\ &\quad - \theta_3 \frac{\partial}{\partial x_j} (u_j^n \Delta \tilde{U}_i^n) + \theta_3 \Delta t \frac{\partial}{\partial x_j} \left(u_j^n \frac{\partial p^n}{\partial x_i} \right) \\ &= \tilde{M}_{c,i}^{n+\theta_3} + \theta_3 \Delta t \frac{\partial}{\partial x_j} \left(u_j^n \frac{\partial p^n}{\partial x_i} \right). \end{aligned} \quad (27)$$

The last term corrects the splitting error in the convective fluxes and only that corresponding to the viscous fluxes will remain.

If in (24) $M_{c,i}^{n+\theta_3}$ is replaced by $\tilde{M}_{c,i}^{n+\theta_3}$, using the correction given by (27) or not, we obtain an equation for the fractional momentum alone, which can be solved. Once this is done, (25) may be used to compute either

ρ^{n+1} if $\theta_2 = 0$ or p^{n+1} if $\theta_2 > 0$. In this last case, the equation of state is needed to express ρ^{n+1} in terms of p^{n+1} . This point is treated in the following section.

Finally, (26) can be used to compute the momentum U_i^{n+1} . The important point is the substitution of ΔU_i^n in (25) using (23), all this at the continuous level. This will lead to a stabilizing pressure dissipation term in the discrete finite element scheme that allows to use this scheme for incompressible flows with the same velocity-pressure finite element interpolation if the semi-implicit version of the algorithm is employed.

4.2 Fractional momentum equation

Let us obtain now the weak form of (24), (25) and (26). Considering first (24), let $\tilde{W}_i$ be the i -th component of the test function for the fractional momentum. We shall compute it in the problem domain Ω and also on its boundary $\Gamma = \partial\Omega$, and therefore $\tilde{W}_i$ is subject to no conditions. Multiplying (24) by $\tilde{W}_i$, integrating over Ω and integrating the viscous term and the term coming for the discretization along the characteristics by parts we get

$$\begin{aligned} \int_{\Omega} \tilde{W}_i \frac{\Delta \tilde{U}_i^n}{\Delta t} d\Omega &= \int_{\Omega} \tilde{W}_i \tilde{M}_{c,i}^{n+\theta_3} d\Omega \\ &\quad - \theta_3 \Delta t \int_{\Omega} \frac{\partial \tilde{W}_i}{\partial x_j} u_j^n \frac{\partial p^n}{\partial x_i} d\Omega + \theta_3 \Delta t \int_{\Gamma} n_j u_j^n \tilde{W}_i \frac{\partial p^n}{\partial x_i} d\Gamma \\ &\quad + \int_{\Omega} \tilde{W}_i \rho g_i - \int_{\Omega} \frac{\partial \tilde{W}_i}{\partial x_j} \tilde{\tau}_{ij}^{n+\theta_3} d\Omega + \int_{\Gamma} \tilde{W}_i n_j \tilde{\tau}_{ij}^{n+\theta_3} d\Gamma \\ &\quad + \frac{\Delta t}{2} \int_{\Omega} \frac{\partial}{\partial x_k} (u_k^n \tilde{W}_i) R_i^n d\Omega, \end{aligned} \quad (28)$$

where $\mathbf{n}$ is the unit outward normal to Γ and we have assumed that $R_i^n = 0$ on Γ . Observe that the two terms in the second row correspond to the modification introduced in (27).

If in (28) the viscous stresses defined in (3) are all computed at $n + \theta_3$, this equation couples all the components of the fractional momentum, that is to say, it is a system of d coupled scalar equations and d unknowns, $d = 2$ or 3 being the number of space dimensions. In order to avoid this coupling, we evaluate the part of the viscous stresses that couples the d equations explicitly. Also, in order to avoid the need for using the density at $n + \theta_3$ (which is unknown at the moment of solving (28)) we also evaluate it explicitly. After doing this, the viscous stresses are approximated by

$$\begin{aligned} \tilde{\tau}_{ij}^{n+\theta_3} &\approx \frac{\mu}{\rho^n} \frac{\partial \tilde{U}_i^{n+\theta_3}}{\partial x_j} - \frac{\mu}{(\rho^n)^2} \tilde{U}_i^{n+\theta_3} \frac{\partial \rho^n}{\partial x_j} \\ &\quad + \mu \left(\frac{\partial u_j^n}{\partial x_i} - \frac{2}{3} \frac{\partial u_k^n}{\partial x_k} \delta_{ij} \right). \end{aligned} \quad (29)$$

Boundary conditions expressed in terms of traction can be (weakly) prescribed in (28). Apart from the prescription of the momentum itself (directly or by imposition of the velocity), we consider the following possibilities of boundary conditions:

- a) The whole traction prescribed on Γ_T : $-pn_i + n_j \tau_{ij} = t_i$ (given).
- b) Only the pressure component of the traction prescribed on Γ_P : $-pn_i = t_i^p$ (given).
- c) Free part of the boundary Γ_F .

Conditions a) and b) are standard, especially a). However, condition c) is not as clear as the others. The idea is to leave Γ_F free, without any prescription neither on the velocity nor on the traction or part of it. This approach has been commonly used in compressible flow problems at supersonic outflows, but can be used as an outflow boundary condition for other types of flow (see [17]).

The prescription of boundary conditions a) in (28), taking the pressure at time step n , leads to replace

by

$$\int_{\Gamma} \tilde{W}_i n_j \tilde{\tau}_{ij}^{n+\theta_3} d\Gamma + \int_{\Gamma-\Gamma_T} \tilde{W}_i n_j \tilde{\tau}_{ij}^{n+\theta_3} d\Gamma + \int_{\Gamma_P} \tilde{W}_i (t_i + p^n n_i) d\Gamma. \quad (30)$$

It is observed that boundary integrals have to be evaluated if the fractional momentum is to be computed also on the boundary.

4.3 Continuity equation

Let us consider now (25) and weight it by a test function W_p . We have that

$$\begin{aligned} \int_{\Omega} W_p \frac{\Delta \rho^n}{\Delta t} d\Omega = & - \int_{\Omega} W_i \frac{\partial U_i^n}{\partial x_i} d\Omega \\ & + \theta_1 \int_{\Omega} \frac{\partial W_p}{\partial x_i} \left(\Delta \tilde{U}_i^n - \Delta t \frac{\partial p^{n+\theta_2}}{\partial x_i} \right) d\Omega \\ & - \theta_1 \int_{\Gamma} W_p n_i \left(\Delta \tilde{U}_i^n - \Delta t \frac{\partial p^{n+\theta_2}}{\partial x_i} \right) d\Gamma. \end{aligned} \quad (31)$$

As a boundary condition, we impose that the normal component of (26) be also verified on Γ , a condition equivalent to impose that the normal component of the momentum equation (18) be verified on Γ . This leads to

$$n_i \left(\Delta \tilde{U}_i^n - \Delta t \frac{\partial p^{n+\theta_2}}{\partial x_i} \right) = n_i \Delta U_i^n. \quad (32)$$

on the part of the boundary Γ_C where the test function for the continuity equation W_p doesn't vanish. Observe that if $\theta_2 > 0$ both the pressure and the density appear in (31). Either of these can be chosen as the variable for the continuity equation, as will be discussed in the following section. Thus, Γ_C is the part of Γ where either p or ρ are free, depending on which variable is used. Suppose for example that the choice is p . According to the type of boundary conditions above, we have that

- a) On Γ_T : $p = n_i \tau_{ij} n_j - n_i t_i$.

- b) On Γ_P : $p = n_i t_i^p$.

In both cases, we have a Dirichlet type of boundary condition for the pressure, so that $W_p = 0$ on that part of Γ and $\Gamma_C = \Gamma - \Gamma_T - \Gamma_P$. On the other hand, ΔU_i^n is also known on the part of the boundary where the momentum is given. The problem arises on Γ_F , that is, for condition c) stated above. In this case, neither $W_p = 0$ nor ΔU_i^n is known. If (32) is used in the boundary integral of (31), we obtain an equation that involves U_i^{n+1} , which is not yet known. Therefore, this equation becomes coupled with the weak form of (26) discussed next. In order to avoid this coupling, we take $n_i \Delta U_i^n$ as 0. For transient calculations, if the normal component of the momentum varies on Γ_F this will be an approximation of order Δt . In any case, the steady-state solution (if reached) will be correct. Recall that this approximation is needed only when Γ_F is not empty, that is, when the non-standard boundary condition c) is used.

Let Γ_D be the part of Γ where the momentum is known. Using (32) and the approximation just described, (31) can be written as

$$\begin{aligned} \int_{\Omega} W_p \frac{\Delta \rho^n}{\Delta t} d\Omega = & - \int_{\Omega} W_p \frac{\partial U_i^n}{\partial x_i} d\Omega \\ & + \theta_1 \int_{\Omega} \frac{\partial W_p}{\partial x_i} \left(\Delta \tilde{U}_i^n - \Delta t \frac{\partial p^{n+\theta_2}}{\partial x_i} \right) d\Omega \\ & - \theta_1 \int_{\Gamma_D} W_p n_i \Delta U_i^n d\Gamma. \end{aligned} \quad (33)$$

This is the weak form of the continuity equation that we use, either if the unknown is the pressure or the density. In the second case, the pressure may be considered known where the density is given by using the equation of state and a guess for the temperature, if required.

4.4 Momentum equation

Finally, for (26) we have that

$$\begin{aligned} \int_{\Omega} W_i \frac{\Delta U_i^n}{\Delta t} d\Omega = & \int_{\Omega} W_i \frac{\Delta \tilde{U}_i^n}{\Delta t} d\Omega \\ & - \int_{\Omega} W_i \frac{\partial p^{n+\theta_2}}{\partial x_i} d\Omega, \end{aligned} \quad (34)$$

where W_i is the i -th component of the test function. In this equation all the components of the momentum can be prescribed. This is possible due to the fact that the fractional momentum has been computed precisely by imposing that (26) be also satisfied on the boundary.

In summary, the equations that we have now are (28), (31) and (34), and the boundary conditions that have been introduced are the traction conditions and (32), that can be considered as the normal component of the momentum equations. Moreover, since the fractional momentum is also computed on the boundary, all the components of the momentum itself can be prescribed on it. However, the momentum is usually not

directly fixed for compressible flows, but instead the velocity is given as boundary condition. We use the common approach of taking the momentum as prescribed using the given velocity values and the density computed in the current time step. This prescription is performed at the end of this step.

4.5 Energy equation

Once (28), (31) and (34) are solved, we have the momentum and either the pressure or the density at the current time step. It remains to compute the total energy. For that, one can solve explicitly or implicitly the last scalar equation in the vector equation (2). To simplify the exposition, we use here the former option with a discretization along the characteristics, which leads to

$$\frac{\Delta E^n}{\Delta t} = R_E^n - \frac{\Delta t}{2} u_k^n \frac{\partial R_E^n}{\partial x_k} \quad (35)$$

where R_E is defined as

$$R_E := -\frac{\partial}{\partial x_i} \left[u_i (E + p) - k \frac{\partial T}{\partial x_i} - \tau_{ij} u_j \right].$$

Weighting this equation by a test function W_E , integrating the diffusion and heat production terms by parts, setting $R_E = 0$ on the boundary and prescribing the total heat flux (from production and from conduction) to H on a part of the boundary Γ_H we get

$$\begin{aligned} \int_{\Omega} W_E \frac{\Delta E^n}{\Delta t} d\Omega &= \\ &- \int_{\Omega} W_E \frac{\partial}{\partial x_i} [u_i (E + p)]^n d\Omega \\ &- \int_{\Omega} \frac{\partial W_E}{\partial x_i} \left(k \frac{\partial T}{\partial x_i} + \tau_{ij} u_j \right)^n d\Omega \\ &+ \frac{\Delta t}{2} \int_{\Omega} \frac{\partial}{\partial x_k} (u_k^n W_E) R_E^n d\Omega \\ &+ \int_{\Gamma_H} W_E H d\Gamma. \end{aligned} \quad (36)$$

On $\Gamma - \Gamma_H$ we assume that $W_E = 0$ (that is, the energy is known there. As for the momentum, the total energy is not normally prescribed, but instead of this the temperature is given. In this case we prescribe the total energy using the values already known of velocity and density and the prescribed temperatures.

If the solution of the flow equation has no shocks, instead of the energy equation written in conservation form one can solve the heat equation

$$\begin{aligned} \frac{\partial T}{\partial t} = R_T := &-u_i \frac{\partial T}{\partial x_i} + \frac{1}{C_v \rho} \frac{\partial}{\partial x_i} \left(k \frac{\partial T}{\partial x_i} \right) \\ &+ \frac{1}{C_v \rho} \sigma_{ij} \frac{\partial u_i}{\partial x_j}. \end{aligned} \quad (37)$$

Usually, this equation is written with the heat capacity $C_v \rho$ multiplying the temporal derivative of the temperature. However, this would prevent the possibility of

using a constant diagonal approximation to the mass matrix (via nodal numerical quadrature, for example) in the case of variable densities.

If an explicit time approximation along the characteristics is used for (37) we get

$$\frac{\Delta T^n}{\Delta t} = R_T^n - \frac{\Delta t}{2} u_k^n \frac{\partial R_T^n}{\partial x_k}. \quad (38)$$

Let us weight now this equation by a test function W_T , integrate the diffusion term by parts, set $R_T = 0$ on the boundary and prescribe the conduction heat flux to H on a part of the boundary Γ_H . The result is

$$\begin{aligned} \int_{\Omega} W_T \frac{\Delta T^n}{\Delta t} d\Omega &= \\ &\int_{\Omega} W_T \left[\left(-u_i + \frac{k}{C_v \rho^2} \frac{\partial \rho}{\partial x_i} \right) \frac{\partial T}{\partial x_i} \right]^n d\Omega \\ &+ \int_{\Omega} W_T \left[\frac{1}{C_v \rho} \sigma_{ij} \frac{\partial u_i}{\partial x_j} \right]^n d\Omega \\ &- \int_{\Omega} \frac{\partial W_T}{\partial x_i} \left(\frac{k}{C_v \rho} \frac{\partial T}{\partial x_i} \right)^n d\Omega \\ &+ \frac{\Delta t}{2} \int_{\Omega} \frac{\partial}{\partial x_k} (u_k^n W_T) R_T^n d\Omega \\ &+ \int_{\Gamma_H} \frac{1}{C_v \rho^n} W_T H d\Gamma. \end{aligned} \quad (39)$$

The temperature is assumed to be known on $\Gamma - \Gamma_H$.

4.6 Time increment calculation

Based on stability criteria, the time increment can be calculated for Convection-diffusion-reaction (CDR) equations [4, 10]. Then, to be used here, Navier-Stokes terms must be identified with the analogue terms in a CDR equation. In this case, for the whole set of equations we use the same time increment. This is evaluated for each node using the following:

$$\Delta t = \frac{F^{TI}}{\left(\frac{1}{\Delta t_c} + \frac{1}{\Delta t_u} \right)} \quad (40)$$

where Δt_c is the ‘‘crosswind’’ time increment, calculated using the diffusive limit for the 1-D CDR equation and Δt_u is the ‘‘upwind’’ one, calculated using the general form of for the 1-D CDR equation, which depends on a ratio between diffusion and convection (through Péclet or Reynolds number). F^{TI} is a factor that for explicit advance can be considered as a safety factor, always lower than 1.0. For implicit treatment this factor can be larger than 1.0. In the numerical diffusion which comes from Characteristic - Galerkin method the Δt which appears divided by two is evaluated using $F^{TI} = 1.0$ in all cases.

5 DISCRETE PROBLEM AND SOLUTION STRATEGIES

With the weak form of the differential equations already established, we can proceed to discretize the space. We do this using the standard Galerkin method, since the term coming from the discretization in time along the characteristics will stabilize the convective terms. This means that we take all the test functions $\tilde{W}_i$, W_p , W_i , W_E and W_T equal to the shape functions. Also, some additional shock-capturing viscosity will be needed in the presence of discontinuities or sharp gradients of the solution, as explained in Section 3.2.

Let us consider first the equations for the fractional momentum (28) and for the end-of-step momentum (34). For the sake of simplicity, we take $\theta_3 = 0$ in what follows. Once the spatial discretization has been performed, the discrete version of these equations can be written in matrix form, the structure of which is

$$\mathbf{M} \frac{\Delta \tilde{\mathbf{U}}^n}{\Delta t} = \mathbf{F}_1 - \mathbf{K} \tilde{\mathbf{U}}^n, \quad (41)$$

$$\mathbf{M}_0 \frac{\Delta \tilde{\mathbf{U}}_0^n}{\Delta t} = \mathbf{M}_0 \frac{\Delta \tilde{\mathbf{U}}_0^n}{\Delta t} - \mathbf{G}_0 \tilde{\mathbf{p}}^{n+\theta_2} + \mathbf{F}_2. \quad (42)$$

Vectors of nodal unknowns have been indicated by a boldface character and an overbar. Matrices $\mathbf{M}$, $\mathbf{K}$ and $\mathbf{G}$ are the standard mass matrix for vector fields, the matrix coming from the viscous and convective terms in the equation for the fractional momentum and the matrix coming from the gradient operator, respectively. Subscript naught in the previous equations refers to not prescribed degrees of freedom for the momentum (in the sense indicated above), and $\mathbf{F}_2$ contains precisely the contribution from $\Delta \tilde{\mathbf{U}}^n$ and $\Delta \tilde{\mathbf{U}}^n$ corresponding to the prescribed degrees of freedom for the latter. Here and below we use $\mathbf{F}$ with subscripts to denote a vector which is known at the moment of solving a particular equation.

The discrete version of the energy equation written in conservation form (36) or the heat equation (39) can be solved at the beginning or at the end of the time step. These equations have the structure

$$\mathbf{M}_{s,0} \frac{\Delta \tilde{\mathbf{T}}^n}{\Delta t} = \mathbf{F}_T \quad \text{and} \quad \mathbf{M}_{s,0} \frac{\Delta \tilde{\mathbf{E}}^n}{\Delta t} = \mathbf{F}_E, \quad (43)$$

where $\mathbf{M}_s$ is the mass matrix for scalar unknowns and $\mathbf{M}_{s,0}$ its modification to account for Dirichlet boundary conditions.

It remains to write the discrete version of the continuity equation (33). We consider different cases according to the type of flow being analyzed. We will see that it is useful to introduce the matrices $\mathbf{M}_\alpha$ and $\mathbf{L}_\beta$, of components

$$\begin{aligned} M_{\alpha,ij} &= \int_{\Omega} \alpha N_i N_j \, d\Omega, \\ L_{\beta,ij} &= \int_{\Omega} \beta \frac{\partial N_i}{\partial x_k} \frac{\partial N_j}{\partial x_k} \, d\Omega, \end{aligned}$$

where N_i is the shape function associated to the i -th node of the finite element mesh with which we assume

that all the variables are interpolated and α and β are functions that depend on the type of flow.

5.1 Incompressible and slightly compressible flows

These two types of flows can be defined by the relation

$$\Delta \rho^n = \alpha \Delta p^n, \quad (44)$$

with $\alpha = 0$ for fully incompressible flows and $\alpha = 1/c^2$ (a positive constant) for slightly compressible flows. In this case, (33) can be written as

$$\begin{aligned} \int_{\Omega} \alpha W_p \frac{\Delta p^n}{\Delta t} \, d\Omega + \theta_1 \Delta t \int_{\Omega} \frac{\partial W_p}{\partial x_i} \frac{\partial p^{n+\theta_2}}{\partial x_i} \, d\Omega = \\ - \int_{\Omega} W_p \frac{\partial U_i^n}{\partial x_i} \, d\Omega + \theta_1 \int_{\Omega} \frac{\partial W_p}{\partial x_i} \Delta \tilde{U}_i^n \, d\Omega \\ - \theta_1 \int_{\Gamma_D} W_p n_i \Delta U_i^n \, d\Gamma. \end{aligned} \quad (45)$$

Once the finite element discretization of this equation has been done, the matrix form of the discrete problem is

$$\mathbf{M}_\alpha \frac{\Delta \tilde{\mathbf{p}}^n}{\Delta t} + \theta_1 \Delta t \mathbf{L}_\beta \tilde{\mathbf{p}}^{n+\theta_2} = \mathbf{F}_C, \quad (46)$$

with α the parameter appearing in (44) and $\beta = 1$ in this case. In (46) we have introduced

$$\mathbf{F}_C := -\mathbf{D} \tilde{\mathbf{U}}^n + \theta_1 \mathbf{G}^t \Delta \tilde{\mathbf{U}}^n + \mathbf{F}_D,$$

where $\mathbf{F}_D$ is the vector coming from the last term in (45) that is, from the boundary values of the momentum, and $\mathbf{D}$ is the matrix coming from the divergence operator. Dirichlet boundary conditions for the pressure are assumed to be included in (46).

Of special interest is the case of fully incompressible flows, that is, $\alpha = 0$. It is well known that in this case the velocity and pressure finite element interpolations must satisfy the Babuška-Brezzi conditions when the classical $\mathbf{U}$ - p approach is used. This is not the case using the type of fractional step methods that we are considering. We justify this in the following. To simplify the discussion, we assume that $\mathbf{U}$ is prescribed to zero on the whole boundary Γ .

Omitting the subscript β for a moment (it is 1), the matrix form of (41), (42) and (46) can be written as

$$\mathbf{M}_0 \frac{\Delta \tilde{\mathbf{U}}_0^n}{\Delta t} = \mathbf{F}_1^* - \mathbf{K}_0 \tilde{\mathbf{U}}_0^n, \quad (47)$$

$$\theta_1 \Delta t \mathbf{L} \tilde{\mathbf{p}}^{n+\theta_2} = -\mathbf{D}_0 \tilde{\mathbf{U}}_0^n + \theta_1 \mathbf{G}_0^t \Delta \tilde{\mathbf{U}}_0^n + \mathbf{F}^*, \quad (48)$$

$$\mathbf{M}_0 \frac{\Delta \tilde{\mathbf{U}}_0^n}{\Delta t} = \mathbf{M}_0 \frac{\Delta \tilde{\mathbf{U}}_0^n}{\Delta t} - \mathbf{G}_0 \tilde{\mathbf{p}}^{n+\theta_2} + \mathbf{F}_2. \quad (49)$$

Now subscript naught refers to degrees of freedom of interior nodes. Matrices $\mathbf{D}_0$ and $\mathbf{G}_0^t$ are the submatrices of $\mathbf{D}$ and $\mathbf{G}^t$ corresponding to these nodes. They are related by $\mathbf{D}_0 = -\mathbf{G}_0^t$. Vectors $\mathbf{F}_1^*$ and $\mathbf{F}^*$ have been

introduced to take into account the boundary values of the fractional momentum.

From (49) we get that

$$\Delta \bar{\bar{U}}_0^n = \Delta \bar{U}_0^n + \Delta t M_0^{-1} G_0 \bar{p}^{n+\theta_2} - \Delta t M_0^{-1} F_2,$$

and using this in (47) and (48) we obtain

$$\begin{aligned} M_0 \frac{\Delta \bar{U}_0^n}{\Delta t} + K_0 \bar{U}_0^n + G_0 \bar{p}^{n+\theta_2} &= F_1^* + F_2, \\ D_0 \bar{U}_0^{n+\theta_1} + \theta_1 \Delta t (L - G_0^t M_0^{-1} G_0) \bar{p}^{n+\theta_2} &= F_C^*, \end{aligned} \quad (50)$$

with

$$F_C^* := F^* - \theta_1 \Delta t G_0^t M_0^{-1} F_2.$$

Clearly, we must have $\theta_1 > 0$ and $\theta_2 > 0$ in order to have a solvable problem.

The important point in (50) is the presence of the matrix $B := L - G_0^t M_0^{-1} G_0$, that can be understood as the difference between two discrete Laplacian operators. This matrix provides additional stability and, in particular, allows to use equal velocity pressure finite element interpolations in the incompressible case, as it had been noticed for example in [18] and [15]. This is so because this matrix is *positive semidefinite*. The proof of this fact can be found in [7].

5.2 Barotropic flows

Let us consider now the flow of compressible barotropic fluids, that is to say, fluids for which there is an equation of state that involves only the density and the pressure, and not the temperature. In general, we write this equation as $p = p(\rho)$, but we will particularize it to the case

$$p = A \rho^\gamma, \quad (51)$$

where A and γ , the *adiabatic exponent*, are physical constants. This situation is found for example in the case of isentropic flow of perfect gases.

In the case of incompressible or slightly compressible flows we have formulated the continuity equation in terms of the pressure only. However, now we have the possibility of choosing either the density or the pressure as unknown of the problem. Let us start with the former option:

Density as variable If we choose to write the continuity equation (33) using the density we have to express the pressure gradient in terms of the density. For this we use the approximation

$$\frac{\partial p^{n+\theta_2}}{\partial x_i} = \left(\frac{dp}{d\rho} \right)^n \frac{\partial \rho^{n+\theta_2}}{\partial x_i} = \frac{\gamma p^n}{\rho^n} \frac{\partial \rho^{n+\theta_2}}{\partial x_i}. \quad (52)$$

The approximation relies on the fact that we evaluate the derivative of p with respect to ρ (the square of the speed of sound) at n instead of at $n + \theta_2$. This may be thought of as a linearization of the problem.

Using (52) in (33), it is found that the discrete continuity equation can be written in this case as:

$$M_\alpha \frac{\Delta \bar{p}^n}{\Delta t} + \theta_1 \Delta t L_\beta \bar{p}^{n+\theta_2} = F_C, \quad (53)$$

now with $\alpha = 1$ and $\beta = \gamma p^n / \rho^n$. Observe that this equation has the same structure as (46) but with the density being the unknown instead of the pressure.

Pressure as variable If instead of using the density we use the pressure, the approximation that we employ is

$$\Delta \rho^n = \left(\frac{d\rho}{dp} \right)^n \Delta p^n$$

which is of order $O((\Delta p^n)^2)$. This approximation leads to

$$\frac{\Delta \rho^n}{\Delta t} = \left(\frac{d\rho}{dp} \right)^n \frac{\Delta p^n}{\Delta t} = \frac{\rho^n}{\gamma p^n} \frac{\Delta p^n}{\Delta t},$$

and the discrete continuity equation can now be written again as

$$M_\alpha \frac{\Delta \bar{p}^n}{\Delta t} + \theta_1 \Delta t L_\beta \bar{p}^{n+\theta_2} = F_C, \quad (54)$$

that is, exactly as (46), but now with $\alpha = \rho^n / (\gamma p^n)$ and $\beta = 1$.

For this type of flows, unlike the incompressible case, the continuity equation (53) or (54) can be solved explicitly ($\theta_2 = 0$) also. The fully explicit form of the algorithm allows very fast calculations at each time step, for matrix inversions are avoided. On the other hand, smaller time increments are to be used which leads to a poorer convergence rate to stationary states.

5.3 Perfect gases

In this case the equation of state involves not only the pressure and the density, but also the temperature. This equation is (1). The appearance of the temperature in it complicates a little the treatment of the continuity equation. As before, we may use either the density or the pressure as variables.

Density as variable Again, if $\theta_2 > 0$ we need to relate the pressure gradient to the density. We have that

$$\frac{\partial p^{n+\theta_2}}{\partial x_i} = \frac{\partial \rho^{n+\theta_2}}{\partial x_i} R T^{n+\theta_2} + \rho^{n+\theta_2} R \frac{\partial T^{n+\theta_2}}{\partial x_i}. \quad (55)$$

Clearly, if $\theta_2 = 0$ the pressure gradient term is on the right hand side of the continuity equation, and it is entirely evaluated in the previous time step explicitly. But for $\theta_2 > 0$, if we use directly this expression in (33) the continuity equation will be coupled to the energy (or heat) conservation equation. In order to avoid this, for the implicit solution of this equation we use an iterative strategy based on assuming that $T^{n+\theta_2}$ is known and then correcting it. There is also another aspect that is computationally inconvenient. If we take

$\rho^{n+\theta_2}$ as unknown in the second term of the RHS of (55) this will lead to a non-symmetric matrix (see (33)). This can be circumvented if we also assume that $\rho^{n+\theta_2}$ is known and then we correct it.

Let then T_g be a guess for $T^{n+\theta_2}$ within the time step under consideration and ρ_g a guess for $\rho^{n+\theta_2}$. Equation (55) may be replaced by

$$\frac{\partial p^{n+\theta_2}}{\partial x_i} = \frac{\partial \rho^{n+\theta_2}}{\partial x_i} R T_g + \rho_g R \frac{\partial T_g}{\partial x_i}$$

The second term in this equation contributes to the RHS of the discrete continuity equation. If we denote by F_ρ this contribution, this discrete equation is

$$M_\alpha \frac{\Delta \bar{p}^n}{\Delta t} + \theta_1 \Delta t L_\beta \bar{p}^{n+\theta_2} = F_C + F_\rho. \quad (56)$$

with $\alpha = 1$ and $\beta = R T_g$. This equation is similar to (53). Apart from the coefficients α and β , the only difference is the term F_ρ , which comes from the spatial derivative of the temperature.

Pressure as variable As for the case of barotropic flows, we may also use the pressure as the unknown of the continuity equation. For that we only need to use the equation of state (1), from which we have

$$\rho^{n+1} = \frac{p^{n+1}}{R T^{n+1}}. \quad (57)$$

As in the previous case, we need to guess the value of T^{n+1} by T_g in order to uncouple the resulting continuity equation and the energy equation. We may then write

$$\Delta \rho^n = \frac{\Delta p^n}{R T_g} + \left[\frac{p^n}{R T_g} - \frac{p^n}{R T^n} \right].$$

The bracketed term contributes to the RHS of the discrete continuity equation with a vector F_p . This equation can be written as

$$M_\alpha \frac{\Delta \bar{p}^n}{\Delta t} + \theta_1 \Delta t L_\beta \bar{p}^{n+\theta_2} = F_C + F_p, \quad (58)$$

with $\alpha = 1/(R T_g)$ and $\beta = 1$. Again, this equation has the same structure as (54) with a modification of the RHS due to the variation (now in time) of the temperature.

From numerical experiments we have found that this approach doesn't work well in the presence of strong shocks, in the sense that we haven't been able to obtain a converged steady state solution in these cases. We attribute this to the appearance of the temperature as a denominator in the function α . This makes the coefficients of M_α difficult to evaluate numerically and with possibly high variations from one time step to the other in the vicinity of shocks.

For the case $\theta_2 = 0$, in general compressible cases, the algorithm scheme is:

1. Solve for the fractional momentum (41).
2. Advance the rest of the variables, all at a time.

Step 2 is different for barotropic flow because no energy or heat equation is needed. Besides, the fully explicit algorithm is not correct for incompressible flow.

On the other hand $\theta_2 > 0$ leads to a more complex although more general scheme. If we use either the pressure or the density as unknown, within each time step we need an iterative scheme to correct the temperature that has been guessed. This iterative scheme is:

1. Solve the energy equation or the heat equation (43).
2. Solve for the fractional momentum (41).
3. Guess a temperature T_g .
4. Solve the continuity equation (58) for p^{n+1} (or (56) for ρ^{n+1}).
5. Obtain ρ^{n+1} from the equation of state (57) (or p^{n+1} , if ρ^{n+1} has been used in 4).
6. Solve for the end-of-step momentum (42).
7. Correct T_g using T^{n+1} and ρ_g using ρ^{n+1} , if needed.
8. Check convergence. If not, go to 4.

In the case of barotropic or incompressible flow at constant temperature, only steps 2, 4 and 5 are to be done in this order. Let us make some remarks about this algorithm. The first concerns the use of the heat equation in step 1. If this is done, we already have T^{n+1} and therefore there is *no need to iterate* at all. However, we have found that this approach may yield wrong results in the presence of shocks, with a wrong location for them and/or without satisfying the jump conditions. It is well known that in these situations it is necessary to use the energy equation written in conservation form. By doing this, after step 1 we have E^{n+1} . A natural way to compute T_g is to use this and the density and velocity of the previous time step.

There is the possibility of not checking convergence, that is to say, take T_g computed as indicated before as T^{n+1} in the continuity equation and also ρ_g as ρ^{n+1} in the vector F_ρ if the density is used as unknown. This is an approximation of order $O(\Delta t)$ that works well if only the steady-state is of interest.

The steady-state is reached slightly faster and time steps slightly larger can be used if a couple of iterations of the previous scheme are performed. We have found almost no difference neither in the numerical results nor in the convergence behavior if more than two iterations are done.

Again, if $\theta_2 = 0$ and the explicit scheme is used, smaller time steps are allowed and convergence rates to steady states can be worsened. However, due to the smaller amount of arithmetic operations per time step this is the best option for compressible flow, unless more terms are implicitly treated in the equations (viz. convective or diffusive terms, using $\theta_3 > 0$).

5.4 General expression of the continuity equation

For all the type of flows considered we have written the continuity equation in a very similar way. Using

the pressure as variable the general form is

$$M_\alpha \frac{\Delta \bar{p}^n}{\Delta t} + \theta_1 \Delta t L_\beta \bar{p}^{n+\theta_2} = F'_C,$$

with $\beta = 1$ and

$$\alpha = \begin{cases} 0 & \text{for incompressible flows} \\ \frac{1}{c^2} & \text{for slightly compressible flows} \\ \frac{\rho^n}{\gamma p^n} & \text{for barotropic flows} \\ \frac{1}{RT_g} & \text{for perfect gases} \end{cases}$$

and $F'_C = F_C$, except in the case of perfect gases, for which $F'_C = F_C + F_p$.

The density can be used as variable only for barotropic fluids and perfect gases. In this case the discrete continuity equation is

$$M_\alpha \frac{\Delta \bar{\rho}^n}{\Delta t} + \theta_1 \Delta t L_\beta \bar{\rho}^{n+\theta_2} = F'_C,$$

now with $\alpha = 1$ and

$$\beta = \begin{cases} \frac{\gamma p^n}{\rho^n} & \text{for barotropic flows} \\ \frac{1}{RT_g} & \text{for perfect gases} \end{cases}$$

and $F'_C = F_C$ for barotropic fluids and $F'_C = F_C + F_p$ for perfect gases.

In all the cases, the matrix of the algebraic system of equations to be solved is symmetric and positive-definite (for incompressible confined flows a pressure needs to be specified). We use the conjugate gradient method to solve it. In general, very few iterations are needed to converge, since the unknown at the previous time step is a good initial guess for its value at the current one.

6 NUMERICAL EXAMPLES

In this section some numerical results are shown. These few examples are presented in order to show the correct behavior of the algorithm under different regimes of flow. More examples can be seen in [21, 22, 23, 7]. Even though some of these examples are very simple, we have considered convenient to include them, since the algorithm presented herein has several original features.

6.1 Incompressible flows

In these two examples no volume forces are considered and the problems are solved keeping the temperature constant in all the domain. Parameters θ_1 and θ_2 are fixed to one in both cases, whereas θ_3 varies according to the case analyzed.

6.1.1 Inviscid flow passing a wing profile

In this example inviscid flow passing a NACA 0012 airfoil, placed at an attack angle of 5° is modeled. It is well known (see, for instance, [11]) that although no condition is imposed in the circulation around the airfoil (the so called *Kutta condition*) the final stationary solution

Figure 2. NACA 0012 profile. Detail of the mesh around stagnation point.

reached is that corresponding to the viscous problem, viz. with the downstream stagnation point at the very trailing edge. This fact seems to violate Kelvin's theorem, because if the initial condition is circulation free then if no diffusion is present, the final stationary state must be also circulation free. However, this is not the case, and a circulation which is different from zero appears around the airfoil. The mechanism that triggers this process is the artificial diffusion added by the numerical method, which in turn is supposed to be small. Therefore, the convergence rate to the final state could be very poor unless the equations are treated implicitly. For that reason, this is a good problem for testing the behaviour and possible advantages of the implicit form of the scheme. As no energy equation must be solved, time factors F^{TI} (see (40)) much larger than 1.0 can be used improving the convergence to the steady state.

The 2-D domain is discretized using a mesh made of 15075 P1 elements (7838 nodal points) slightly refined from the exterior, far from the wing, to the profile itself (fig. 2). The velocity is fixed to 1.0 at the inflow and the pressure to 0.0 at the outflow. Normal component of the velocity is prescribed to 0.0 at the airfoil and at the upper and lower boundaries.

Parameters θ_2 and θ_3 are in this case 1.0 (both fractional momentum and pressure equations are solved implicitly). If this is done, the time factor F^{TI} can be between two and three orders of magnitude greater than in the case $\theta_2 = 1.0$ and $\theta_3 = 0.0$. Although an additional linear system of equations needs to be solved per time step, the time step size may be taken much larger, making the total CPU time needed much smaller. This fact strongly favours the use of an implicit method for solving this equation in most of the types of flow. The stationary state reached is shown in fig. 3.

As time increments are here so large, our suggestion for correcting the splitting error (see (27) and (28))

Figure 3. NACA 0012 profile. Pressure contours around airfoil.

Figure 5. NACA 0012 profile. Pressure contours around stagnation point. Splitting error of stationary state produces an overdiffusive result.

is also tested: fig. 4 and fig. 5 show the difference in pressure level contours around the stagnation point either if it is taken into account or not. The analytical value for the pressure at the stagnation point is 0.5. If the correction is done, the value is 0.515. If not, the pressure value reached there is 0.309 being much more diffusive due to the splitting error. This becomes more apparent when larger F^{TI} are used, due to the fact that this error is $O(\Delta t)$.

Figure 4. NACA 0012 profile. Pressure contours around stagnation point. Splitting error of stationary state corrected.

6.1.2 Flow passing a cylinder at $Re=100$

In this case the mesh is made of 2000 Q1 elements (2100 nodal points). An inlet horizontal velocity of norm 1 is prescribed, whereas the outlet is left free. There, pressure is fixed to $n_j \tau_{ij} n_i$. The no slip condition is prescribed on the cylinder. At this Reynolds number, the stationary state is oscillatory: a trail of vortices is left behind the cylinder. The onset of the oscillatory behaviour was produced by a small initial perturbation on the velocity. Fully developed flow is shown in fig. 6.

In this problem we have used $\theta_3 = 0$, i.e. the semi-implicit form of the algorithm, which has no splitting error.

The period obtained is around 5.7, which is very close to that obtained in [19]. The period can be evaluated in many ways: through the evolution of a variable at a point behind the cylinder or the net force over it, or through the evolution of the error norm, etc. In the example shown here, one period of time is covered in approximately 270 time steps.

6.2 Compressible inviscid flow passing a cylinder

In this example, flow at Mach 3 reaches a cylinder and a steady shock is formed upstream of it. At the inflow, velocity, density and temperature are prescribed, for it is a supersonic inlet. The normal velocity on the cylinder is fixed to zero. The domain is discretized using a uniform mesh of 5351 P1 elements (2772 nodal points).

Pressure coefficient

$$P_c = \frac{-2(p - p_{\text{ref}})}{\rho v_{\text{ref}}^2},$$

where reference values are those of the inflow, and Mach number level contours are shown in fig. 7. Also

Figure 6. Flow passing a cylinder, $Re=100$. Streamlines and pressure contours.

their profile along a horizontal cut through the mid point of the domain is shown in fig. 8. It can be seen in this last graph that at the stagnation point (which correspond to x coordinate 3.0) the Mach number is slightly larger than zero, being the reason for that both a non-symmetric mesh and the interpolating procedure of the variables along the cut.

6.3 Compressible viscous flow over a flat plate

The supersonic flow over a plate (*Carter's Flat Plate Problem*) develops many different features that can appear when solving the complete Navier-Stokes equations, like boundary layers and shocks, and the interaction between them.

The Mach number at the inflow is $M_\infty = 3.0$. The viscosity μ depends on the temperature according to Sutherland's law:

$$\mu = \frac{0.0906T^{1.5}}{T + 0.0001406}.$$

Prandtl number ($Pr = \mu C_p / k$) is in this case 0.72, where $C_p = \gamma C_v$ is the specific heat at constant pres-

Figure 7. Supersonic flow passing a cylinder, Mach 3. Left: pressure coefficient. Right: Mach number.

sure, $C_v = 715$ and $\gamma = 1.4$. The state law is that of an ideal gas.

The domain is divided using a uniform mesh of 112×64 (7168) Q1 elements, corresponding to 7345 nodal points. If the coordinates origin is at the left bottom corner, the domain goes from 0.0 to 0.8 vertically and from 0.0 to 1.4 horizontally. Density, temperature and velocity are prescribed at the inflow, because this inlet is supersonic. The values prescribed at the inflow are 1.0 and 2.8×10^{-4} for the first two and (1.0; 0.0) for the horizontal and vertical components of the velocity. The non-slip condition is imposed at the floor of the plate, which starts at $x = 0.25$.

The stagnation temperature is calculated according to:

$$T_{\text{stag}} = T_\infty \left(1 + \frac{\gamma - 1}{2} M_\infty^2 \right),$$

which is the prescription of this variable along the plate. No prescriptions are made at the outflow. This point must be remarked, because most of the outlet is subsonic, eventually requiring a prescription on the density. Nevertheless, the only prescribed node of the outflow is that of the right bottom corner which is considered belonging to the plate, with its boundary conditions on temperature and velocity.

In fig. 9, fig. 10, fig. 11 and fig. 12 the results obtained for this example are shown. Note the sharpness of the shock and the gradual change of the variables along the boundary layer. In fig. 11 and fig. 12 a comparison with the original results of Carter (as appearing

Figure 8. Supersonic flow passing a cylinder, Mach 3. Top: Mach number. Bottom: pressure coefficient. The cut is done horizontally at half of domain, normal to the shock.

in [8]) is made, showing a good agreement with them. These figures correspond to the profiles of some variables along a cut at $x = 1.25$. Density, pressure and temperature are normalized using their inflow values.

For the velocity, density and temperature, the only and slight difference is in the very maximum value at the shock. Carter's pressure profile is not shown because it presents some oscillations. In this problem, shock capturing diffusion is artificially put according to section 3.2. It is activated for all the equations. The algorithm works equally well for both the strong and low compression regions of the domain, viz. the shock and the boundary layer respectively.

7 CONCLUSIONS

In this paper we have presented an overview of the splitting technique that we have developed for both compressible and incompressible flow problems. We have also extended it to the case in which the fractional momentum equation is treated implicitly and discussed some implementation issues related to the implicit treatment of the viscous and convective terms.

Figure 9. Flow over a flat plate. Contour levels. Top: density. Bottom: pressure.

Besides the split of the momentum equation, the basic ingredients of the numerical formulation are the use of an explicit version of the Characteristic-Galerkin scheme together with the introduction of a nonlinear shock capturing diffusion for each scalar equation depending on the spatial residual.

Numerical examples have shown that these techniques are effective to solve convection dominated flows. Shocks have been reproduced with their correct strength and without local oscillations.

Two important aspects of the model presented are the treatment of boundary conditions and the correction of the splitting error coming from the convective term when it is treated implicitly. Both can be applied to incompressible cases as well, thus improving the original fractional step method.

From the numerical examples presented it can be concluded that the formulation proposed here works well in very different flow regimes, compressible and incompressible, viscous and inviscid.

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Figure 10. Flow over a flat plate. Contour levels. Top: temperature. Bottom: Mach number.

Figure 11. Flow over a flat plate. Profile along $x = 1.25$. Top: density. Bottom: temperature. (Normalized using inflow values)

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Figure 12. Flow over a flat plate. Profile along $x = 1.25$.
Top: vertical component of velocity. Bottom: pressure.
(Normalized using inflow values)

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