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The normal flux method at the boundary for multidimensional finite volume approximations in CFD

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Abstract

This paper presents a general method for imposing boundary conditions in the context of hyperbolic systems of conservation laws. This method is particularly well suited for approximations in the framework of Finite Volume Methods in the sense that *it computes directly the normal flux at the boundary*. We generalize our approach to nonconservative hyperbolic systems and discuss both the characteristic and the noncharacteristic cases. We present several applications to models occurring in Computational Fluid Mechanics like the Euler equations for compressible inviscid fluids with real equation of state, shallow water equations, magnetohydrodynamics equations and two fluid models.

Keywords: Boundary conditions; Finite volumes; Hyperbolic Systems; Euler equations; Two fluid models

1. Introduction

A lot of physical models occurring in continuous mechanics appear to be systems of conservation laws. These equations express in general fundamental laws of physics, namely the conservation of mass, charge, momentum, total energy, etc. When dealing with multidimensional models, essentially the only way of obtaining quantitative results is to use numerical simulation. That is working with a discrete approximation of the system. If one insists on the fact that conservation laws must be rigorously fulfilled (and according to physical considerations this is often a minimal requirement) one is naturally led to use the so-called finite volume approach.

The purpose of this paper is to propose a numerical method for handling the boundary condition value problem in a multidimensional finite volume approximation of hyperbolic systems. We want to achieve the following goals. The numerical method should be (i) general, (ii) easy to implement and efficient in terms of computational cost, (iii) physically relevant, (iv) mathematically founded. A few comments are in order. By general, we understand that no a priori hypothesis should be required on the finite volume method used, in particular we want to be able to consider all kind of control volumes and meshes. By general, we also mean that we do not want to rely on putative particular features of the system under consideration, like e.g. existence of Riemann invariants or Riemann solvers. Concerning the computational aspects, we look for simplicity in the implementation because we have in mind important cases where the computational platform is not only used to produce good predictions on a single well established model but also to serve as a tool for comparison between different models. This is in particular the case in the context of two phase flow modelling that was one of the motivation of this work. As it is well

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known, physical relevance is essential even for "numerical boundary conditions" since failure in this direction might produce spurious, albeit converged, solutions. Last but not least, mathematical relevance is also seminal, first to a priori ensure that the implemented numerical algorithm produces a solution (existence of solution) but also that the problem is well-posed i.e. that there is continuous dependence of the solution with respect to the data.

The modern theory of partial differential equations relies on Distribution theory and boundary conditions problems have been first studied in this context. A reference in this direction is the famous treatise written in the late sixties by Lions and Magenes [1,2]. The objective of their program was to study in a systematic way the boundary values problems associated with *linear* partial differential equations. Let us deal more particularly with hyperbolic type equations. For these, wave propagation phenomena are determinant and we refer to Whitham [3] in which a deep exposition is provided.

Concerning the discrete problem associated with these equations, roughly speaking there are two situations. In the first one, one deals with linear and quite general (wave) equations while in the second one, one deals with nonlinear particular ones. For linear (wave) equations like e.g. the wave equation, Maxwell's equations or elasticity equations, a lot of works rely on the theoretic and explicit solution to the continuous equations and this leads in general to nonlocal boundary conditions. Then usually, an approximation procedure, e.g. an asymptotic expansion with respect to a small parameter, is applied in order to derive local boundary conditions. Next these conditions are discretized by classical difference techniques. This has led to a very wide body of knowledge and we refer to the review article by S. Tsynkov [4] for numerous results and references. On the opposite, concerning nonlinear equations, most of the works are devoted to particular equations and since no explicit solutions are available, authors use in general *ad hoc* procedures that rely usually on physical considerations. On the one hand, there are a few recent reference books dealing with the numerical approximation of hyperbolic systems of conservation laws e.g. Godlewski and Raviart [5], LeVeque [6]. However they mostly concentrate on the discretization inside the computational domain. On the other hand, the most achieved treatise on the subject is according to us Hirsch [7] but it is solely devoted to the Euler equations of gas dynamics.

In this paper, we provide a *general theory* for the boundary condition treatment at the discrete level in the finite volume framework. Our work transfers in a certain sense knowledge in the linear case to the nonlinear one and gives a systematic approach that can be used in either cases (linear and nonlinear). Moreover, and in contrast with most of the works on the subject, we do not rely on either specific or computationally expansive functions like e.g. Riemann invariants. *Actually we just use the hyperbolic nature of the system and nothing else.* Last but not least, we address directly the key problem, which consists in determining directly the *normal flux* on the boundary, while other methods rely on the finding of a state on this boundary, a problem that can be ill-posed.

As a result of our method, we are able to take into account any physically reasonable boundary condition. In the non-characteristic case i.e. in the case where no waves are crawling on the boundary, Theorem 1 gives a sufficient condition under which the problem of finding the normal flux is well-posed. Moreover this condition is natural and straightforward to check in each example. For the characteristic case, although no general result is obtained in the nonlinear case (at the continuous level, this is a well known open problem), we are able to treat the case of characteristic boundaries in the context of a wall in fluid mechanics. In contrast with methods that require the determination of a state on the boundary, we do not impose artificial conditions since in this case the problem is under determined. Indeed dealing directly with the normal flux leads us to a system with the same number of equations and unknowns.

This general theory was initially motivated by the finite volume approximation of the so called averaged models for two phase fluid dynamics, see Boure and Delhaye [8], Drew and Lahey [9], Ishii [10], Ransom [11]. These models, which can predict kinematic and thermal non-equilibrated flows, are derived by the application of an average process (with respect to time or space or even a statistical averaging) to the classical compressible Navier–Stokes equations in each fluid or phase, separated by interfaces. This leads to a simplified system of six balance equations (simplified in the sense that we have omitted in its right-hand side the contributions related to dissipative phenomena) that reads as follows ($k = 1$ or 2):

$$\frac{\partial(\alpha_k\rho_k)}{\partial t} + \nabla\cdot(\alpha_k\rho_k u_k) = \Gamma_k, \tag{1}$$

$$\frac{\partial(\alpha_k\rho_k u_k)}{\partial t} + \nabla\cdot\big(\alpha_k(\rho_k u_k\otimes u_k + p\,\mathtt{Id})\big) - p\nabla\alpha_k = \alpha_k\rho_k g + M_k + u_{k,i}\Gamma_k, \tag{2}$$

$$\frac{\partial(\alpha_k\rho_k E_k)}{\partial t} + \nabla\cdot(\alpha_k\rho_k H_k u_k) + p\frac{\partial\alpha_k}{\partial t} = (\alpha_k\rho_k g + M_k)\cdot u_k + H_k\Gamma_k + Q_k, \tag{3}$$

where α_k, ρ_k, u_k are respectively the volume fraction, the density, the velocity of the fluid k and where p is the thermodynamic pressure. We have denoted by $a\otimes b$ the matrix defined by $(a\otimes b)_{ij} = a_i b_j$ and by $\mathtt{Id}$ the identity matrix. Denoting by e_k the specific internal energy of the phase k, we have set $E_k = e_k + \frac{1}{2}|u|^2$ and $H_k = E_k + p/\rho_k$, respectively the total specific energy and the total specific enthalpy of the fluid k. The Γ_k's denote mass transfers term with $\Gamma_1 + \Gamma_2 = 0$, the M_k's momentum transfers, Q_k's heat transfers and finally the $u_{k,i}$ are interfacial velocities. Gravity is denoted by g. We have the

relation $\alpha_1 + \alpha_2 = 1$ and in order to close the system (1)–(3), we have to write two equations of state, one for each fluid: $\mathcal{F}_k(p, \rho_k, e_k) = 0$ for $k = 1, 2$.

Such systems that arise in two phase fluid mechanics are nonconservative and fall into the following formalism

$$\frac{\partial v}{\partial t} + \nabla \cdot F(v) + \sum_{j=1}^{nd} \tilde{C}_j(v) \frac{\partial v}{\partial x_j} + D(v) \frac{\partial v}{\partial t} = \tilde{S}(v), \tag{4}$$

with $v = (v_1, \ldots, v_m) \in \mathbb{R}^m$ and where $\tilde{C}_j(v)$ and $D(v)$ are $m \times m$ matrices, $F(v)$ the conservative fluxes and $\tilde{S}(v)$ the source term. Here $\nabla \cdot F(v) = \sum_{j=1}^{nd} \partial F^j(v)/\partial x_j$ and F^j maps G into $\mathbb{R}^m$ where G is an open subset of $\mathbb{R}^m$ corresponding to the physically admissible states.

The paper is organized as follows. In the next section we describe our method in the case of an hyperbolic system of conservation equations. Also several systems of practical interest are given. Section 3 is devoted to the extension of this method to the nonconservative case while the last section addresses all the practical issues one is faced to when applications to actual equations are intended. Conclusions end the paper.

2. The conservative case

Let us first consider the conservative form of system (4) where the matrices $\tilde{C}_j(v)$ and $D(v)$ are taken to be zero and for simplicity in the exposition, we take $\tilde{S}(v) = 0$. The system of m conservation equations defined on a nd-dimensional domain Ω (with $nd = 1, 2$ or 3 in practice) then reads as

$$\frac{\partial v}{\partial t} + \nabla \cdot F(v) = 0 \quad \text{in } \Omega \times \mathbb{R}^+, \quad v = (v_1, \ldots, v_m) \in \mathbb{R}^m. \tag{5}$$

Before describing the finite volume approach and the discrete boundary conditions treatment, let us give some applications.

2.1. Applications

Application 1. The first application concerns a model of ideal magnetohydrodynamics. The system satisfied by *magnetics fluids* reads in conservative form as

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0, \tag{6}$$

$$\frac{\partial (\rho u)}{\partial t} + \nabla \cdot (\rho u \otimes u + P) = 0, \tag{7}$$

$$\frac{\partial (\rho E)}{\partial t} + \nabla \cdot (\rho E u + P u) = 0, \tag{8}$$

$$\frac{\partial B}{\partial t} + \nabla \cdot (u \otimes B - B \otimes u) = 0, \tag{9}$$

where the scalar ρ is the density, the vector u in $\mathbb{R}^{nd}$ represents the velocity, the divergence free vector field B (i.e. $\nabla \cdot B = 0$) is the magnetic field, the scalar $E = e + \frac{1}{2}|u|^2 + \frac{1}{2\rho}|B|^2$ is the total energy and the matrix P satisfies $P = (p + \frac{1}{2}|B|^2)\mathtt{Id} - B \otimes B$. In order to close this system, one should provide an equation of state (EOS) linking the pressure p, the internal energy e and the density ρ. Let us emphasize that this system is of the form (5) with $v \in \mathbb{R}^{2nd+2}$, $v = (\rho, \rho u_1, \ldots, \rho u_{nd}, \rho E, B_1, \ldots, B_{nd})$, $m = 2nd + 2$ and for all ω in $\mathbb{R}^{nd}$

$$\sum_{i=1}^{nd} \omega_i F^i(v) \equiv F(v) \cdot \omega = u \cdot \omega(\rho, \rho u, \rho E, -B) + \left(p + \frac{1}{2}|B|^2\right)(0, \omega, u \cdot \omega, 0) - B \cdot \omega(0, B, B \cdot u, -u). \tag{10}$$

Application 2. The *compressible Euler system of equations* reduces to the 3 first equations (6)–(8) where this times $E = e + \frac{1}{2}|u|^2$ and the matrix P is spherical: $P = p\mathtt{Id}$, with p denoting the thermodynamical pressure. Again in order to close this system, one should provide an equation of state (EOS) linking the pressure p, the internal energy e and the density ρ. This system is of the form (5) with $v \in \mathbb{R}^{nd+2}$, $v = (\rho, \rho u_1, \ldots, \rho u_{nd}, \rho E)$, $m = nd + 2$ and

$$F(v) \cdot \omega = u \cdot \omega(\rho, \rho u, \rho E) + p(0, \omega, u \cdot \omega), \quad \forall \omega \in \mathbb{R}^{nd}. \tag{11}$$

Introducing the specific entropy function s and the temperature T that satisfy $T\,\mathrm{d}s = \mathrm{d}e - \frac{p}{\rho^2}\,\mathrm{d}\rho$, it is classical to derive for continuous solutions of (6)–(8) the fact that the specific entropy is convected by the flow: $\frac{\partial s}{\partial t} + u \cdot \nabla s = 0$.

Application 3. Since $s =$ constant is an obvious solution to this equation, in certain physical cases, it might be relevant to address the reduced system, known as the *isentropic compressible Euler system of equations*, which consists in the two conservation laws (6) and (7). This time the EOS is a relation between the pressure and the density: $p = p(\rho)$. This system is of the form (5) with $v \in \mathbb{R}^{nd+1}$, $v = (\rho, \rho u_1, \ldots, \rho u_{nd})$, $m = nd + 1$ and

$$F(v) \cdot \omega = u \cdot \omega(\rho, \rho u) + p(0, \omega), \quad \forall \omega \in \mathbb{R}^{nd}. \tag{12}$$

The function $p = p(\rho)$ is arbitrary and depends on the considered fluid. The only constraint is that the derivative of p with respect to ρ is nonnegative, which corresponds to the physical property that pressure perturbations propagate at finite speed: the speed of sound, $c = \sqrt{\mathrm{d}p/\mathrm{d}\rho}$. There are two asymptotic cases, which are sometimes considered and yield the last two applications.

Application 4. In the first one, known as *isothermal flows*, the relation between pressure and temperature is linear, which physically corresponds to the limit case where the two heat capacities C_v and C_p are equal. In such a case a change in the temperature requires an infinite amount of energy, that is an impossible fact. Hence the temperature cannot vary. Since now the speed of sound is constant, the system (6), (7) with the normal flux (12) is closed by the EOS: $p = c_0^2 \rho$.

Application 5. In the second one, known as *the shallow water equations*, a very thin layer of fluid is considered. This fluid is in general a liquid and is therefore slightly compressible. In the limit where the fluid is incompressible, the density is constant but the height, h, of the fluid might depend on space and time. In this situation one arrives again (see e.g. Whitham [3]) to the model (6), (7) with the normal flux (12) but this time $p = \frac{1}{2}\bar{\rho} g h^2$ and $\rho = \bar{\rho} h$ where $\bar{\rho}$ is the constant density of the fluid and g denotes the gravity.

2.2. On the continuous system of equations

Given an arbitrary point $\underline{v} \in G$, if we linearize the system (5) around the trivial constant solution $\underline{v}$, we obtain

$$\frac{\partial w}{\partial t} + \sum_{j=1}^{nd} \underline{A}^j \frac{\partial w}{\partial x_j} = 0 \quad \text{with } \underline{A}^j = A^j(\underline{v}) \equiv \frac{\partial F^j(\underline{v})}{\partial v}. \tag{13}$$

Now this equation can be explicitly solved thanks to the Fourier transform, which leads to the eigenvalue problem for the $m \times m$ matrix $A_\omega(\underline{v})$ where

$$A_\omega(v) = \sum_{j=1}^{nd} \omega_j \frac{\partial F^j(v)}{\partial v} \equiv \frac{\partial F(v) \cdot \omega}{\partial v}. \tag{14}$$

It is now natural to introduce the classical definition of hyperbolicity (see the Appendix for a study of the hyperbolic character for the previously described applications):

Definition 1. The multidimensional system of conservation laws (5) is said to be hyperbolic if for every $\omega \in \mathbb{R}^{nd}$ and every $v \in G$ the $m \times m$ matrix $A_\omega(v)$ has m linearly independent real eigenvectors. In such case, an eigensystem of $A_\omega(v)$ is composed of

- the set of the real eigenvalues: $\lambda_1(v, \omega) \leqslant \cdots \leqslant \lambda_m(v, \omega)$,
- a set $(l_1(v, \omega), \ldots, l_m(v, \omega))$ of left eigenvectors satisfying:

$$^t A_\omega(v)\, l_k(v, \omega) = \lambda_k(v, \omega) l_k(v, \omega), \quad \text{for } k = 1, \ldots, m,$$

- a set $(r_1(v, \omega), \ldots, r_m(v, \omega))$ of right eigenvectors satisfying:

$$A_\omega(v)\, r_k(v, \omega) = \lambda_k(v, \omega) r_k(v, \omega), \quad \text{for } k = 1, \ldots, m$$

and the following normalization: $l_k(v, \omega) \cdot r_p(v, \omega) = \delta_{k,p}$ for $k, p = 1, \ldots, m$.

Now for the hyperbolic linearized system (13), it is then straightforward to show that the initial value problem in the whole space is well posed in various functional spaces. Then by fixed point techniques, one can extend these results to the nonlinear system (5). We refer e.g. to the books by Serre [12] and Dafermos [13] for that purpose. However when one is interested in the mixed initial and boundary value problem, the situation is much more involved. In the linear case, a lot can be done while in the nonlinear one very little is known. Let us briefly give a flavor of the problem by considering the very simple example of the linear transport equation. Given $c \in \mathbb{R}^*$, the one-dimensional linear transport equation (called the advection equation) reads

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0. \tag{15}$$

Here hyperbolicity is automatic and if this equation is posed on a bounded interval, say $]a, b[$, one can prescribe only one of the two boundary values $u(a, t)$ or $u(b, t)$ depending on the sign of c. More precisely, one can only give the information that enters into the domain $]a, b[$: if $c > 0$ one can give for instance $u(a, t)$, while if $c < 0$ one can give for instance $u(b, t)$. In the nonlinear case, the situation is more complex, even in the one-dimensional case, since the "speed" c (and therefore its sign) will depend on the solution. We refer to the paper of Oliger and Sundström [14] for a study on how formulate boundary conditions to yield well-posed problems for the Eulerian equations for gas dynamics.

2.3. The discrete system of equations

The computational domain Ω is taken to be a polygonal domain and is decomposed in small volumes K (the so-called control volumes) such that $\Omega = \bigcup_{K\in\mathcal{T}} K$. We assume that the control volumes K are polyhedra such that the interior boundary is the union of hypersurfaces $K \cap L$ where L belongs to the set $\mathcal{N}(K) = \{L \in \mathcal{T} \mid L \neq K$ and $K \cap L$ has positive $(nd-1)$-measure$\}$.

2.3.1. The finite volume approach

In order to approximate $v_K(t)$ the average of the solution on the control volume K, system (5) is integrated on K and leads to a system where the time evolution of $v_K(t)$ is governed by the normal flux on the boundary of K:

$$F_{\partial K}(t) = \int_{\partial K} F\big(v(\sigma, t)\big) \cdot \nu(\sigma)\, \mathrm{d}\sigma, \tag{16}$$

where ∂K is the boundary of K, $\nu(\sigma)$ the unit external normal on ∂K and $d\sigma$ denotes the $(nd-1)$-volume element on this hypersurface. The heart of the matter in finite volume methods consists in providing a formula for the normal fluxes $F_{\partial K}$ in terms of the $\{v_L\}_{L\in\mathcal{T}}$ and the given data. There are two kind of control volumes. Those whose intersection with the boundary of Ω has zero $(nd-1)$-dimensional measure and those with positive measure intersection with the boundary of Ω. Concerning the first ones, we decompose the normal flux (16) into a sum:

$$F_{\partial K} = \sum_{L\in\mathcal{N}(K)} F_{K,L} \quad \text{with } F_{K,L} = \int_{K\cap L} F\big(v(\sigma, t)\big) \cdot \nu_{K,L}\, \mathrm{d}\sigma, \tag{17}$$

where the unit normal on $K \cap L$ denoted by $\nu_{K,L}$ points into L. To get an ordinary differential equation for the $v_K(t)$'s, the normal flux (17) has to be expressed in terms of the $\{v_M\}_{M\in\mathcal{T}}$. In general, system (5), when it is hyperbolic, is strongly dominated by *finite* speed nonlinear wave propagation phenomena and therefore we are led to consider a formula, which uses a finite stencil. For practical reasons, including CPU and storage costs, it turns out that using the two neighboring values v_K and v_L is enough at least for first order approximations. This means that we are looking for a formula that reads as

$$F_{K,L} \approx \mathrm{area}(K \cap L)\, \Phi(v_K, v_L, K, L), \tag{18}$$

where Φ is the numerical flux to be constructed and $\mathrm{area}(K \cap L)$ stands for the $(nd-1)$-dimensional volume of the hypersurface $K \cap L$. At this level of generality, let us note that the numerical flux has to satisfy two properties. The first one is consistency that is $\Phi(w, w, K, L) = F(w) \cdot \nu_{K,L}$. The second one concerns conservation: $\Phi(v, w, K, L) = -\Phi(w, v, L, K)$.

Concerning now the control volumes that have positive measure intersection with the boundary of Ω, we have also to find the numerical flux $\Phi(v_K, K, \partial\Omega)$ that approximates the integral

$$F_{K,\partial\Omega} = \int_{K\cap\partial\Omega} F\big(v(\sigma, t)\big) \cdot \nu_K\, \mathrm{d}\sigma. \tag{19}$$

Here ν_K denotes (instead of $\nu_{K,\partial\Omega}$) the unit normal to the face $K \cap \partial\Omega$ that points outside Ω. It is the goal of this paper to provide a formula for $\Phi(v_K, K, \partial\Omega)$, which is done in Section 2.4.

Hence the finite volume semi discretization of (5) is a system of o.d.e.'s that reads ($\mathrm{vol}(K)$ denotes the *nd*-dimensional volume of K)

$$\mathrm{vol}(K)\frac{\mathrm{d}v_K}{\mathrm{d}t} + \sum_{L\in\mathcal{N}(K)} \mathrm{area}(K\cap L)\,\Phi(v_K, v_L, K, L) + \sum_{\mathrm{area}(K\cap\partial\Omega)\neq 0} \mathrm{area}(K\cap\partial\Omega)\,\Phi(v_K, K, \partial\Omega) = 0. \tag{20}$$

2.3.2. The numerical fluxes

Let us recall in this section how to provide a formula for the numerical flux $\Phi(v_K, v_L, K, L)$ at the interface between two control volumes K and L. Since this vector is an approximation to the normal flux (17), a natural choice would be e.g.

$$\Phi(v_K, v_L, K, L) = \frac{F(v_K) + F(v_L)}{2}\cdot \nu_{K,L}, \tag{21}$$

but as it is well known and understood, this leads to unstable schemes. Actually this flux has to take into account the direction of propagation of information between the two volumes during the time step. This is the basis for the upwind schemes and we can cite among them the Godunov scheme, the Roe scheme (see Godlewski and Raviart [5] and reference therein) and the VFFC scheme from Ghidaglia et al. [15,16]. The last two schemes belong to the family of flux schemes according to the following definition.

Definition 2 (*Ghidaglia* [17]). The numerical flux $\Phi(v, w, K, L)$ corresponds to a flux scheme when there exists a matrix $U(v, w, K, L)$ such that

$$\Phi(v, w, K, L) = \frac{F(v) + F(w)}{2}\cdot \nu_{K,L} - U(v, w, K, L)\frac{F(w) - F(v)}{2}\cdot \nu_{K,L}. \tag{22}$$

The VFFC scheme corresponds to the following choice of matrix U.

Definition 3. The numerical flux of the VFFC method is obtained by formula (22) when we take

$$U(v, w, K, L) = \mathrm{sgn}\big(A_{\nu_{K,L}}(\mu)\big), \tag{23}$$

where $\mu = \mu(v, w, K, L)$ is a mean between v and w that only depends on the geometry of K and L, e.g. $\mu = (\mathrm{vol}(K)v + \mathrm{vol}(L)w)/(\mathrm{vol}(K) + \mathrm{vol}(L))$ and where $sgn(M)$ is the matrix that has the same eigenvectors as M but whose eigenvalues are the sign ($\in\{-1, 0, +1\}$) of those of M.

2.4. Discretization of the boundary conditions

Let K be a control volume that meets the boundary $\partial\Omega$ and ν_K the unit normal to the face $K\cap\partial\Omega$ that points outside Ω. Our goal is to provide a formula for $\Phi(v_K, K, \partial\Omega)$ that approximates the flux at the boundary i.e. the integral (19). In practice, this flux is not given by the physical boundary conditions and moreover, in general, (5) is an ill-posed problem if we try to impose either v or $F(v)\cdot\nu_K$ on $\partial\Omega$. This can simply be understood by analyzing the characteristics. Let us consider the linearization of the system around a state $\underline{v}$ and its projection on the normal direction to the face

$$\frac{\partial v}{\partial t} + \underline{A}_{\nu_K}\frac{\partial v}{\partial v} = 0, \tag{24}$$

where $\frac{\partial v}{\partial v} = \nabla v\cdot\nu_K$ and where $\underline{A}_{\nu_K}$ is the advection matrix $A_{\nu_K}(\underline{v})$. Since (5) is assumed to be hyperbolic, by a change of coordinates, the system (24) has the form of an uncoupled set of m advection equations: ($\eta_k \equiv l_k(\underline{v}, \nu_K)\cdot v$)

$$\frac{\partial \eta_k}{\partial t} + \lambda_k(\underline{v}, \nu_K)\frac{\partial \eta_k}{\partial v} = 0, \quad k = 1, \ldots, m. \tag{25}$$

Let us assume that $\lambda_k(\underline{v}, \nu_K) \neq 0$. According to the sign of these numbers, waves are going either into the domain Ω ($\lambda_k(\underline{v}, \nu_K) < 0$) or out of the domain Ω ($\lambda_k(\underline{v}, \nu_K) > 0$). Hence we expect that it is only possible to impose χ conditions on $K\cap\partial\Omega$ where

$$\chi \equiv \sharp\{k\in\{1, \ldots, m\} \text{ such that } \lambda_k(\underline{v}, \nu_K) < 0\}.$$

At this point there are two different situations. The first one, which is termed as the noncharacteristic case in the literature, refers to the case where the matrix $\underline{A}_{\nu_K}$ is invertible, while the second one refers to the complementary case.

2.4.1. The noncharacteristic case

We label the eigenvalues $\lambda_k(\underline{v}, \nu_K)$ of $\underline{A}_{\nu_K}$ by increasing order

$$\lambda_1(\underline{v}, \nu_K) \leqslant \lambda_2(\underline{v}, \nu_K) \leqslant \cdots \leqslant \lambda_\chi(\underline{v}, \nu_K) < 0 < \lambda_{\chi+1}(\underline{v}, \nu_K) \cdots \leqslant \lambda_m(\underline{v}, \nu_K).$$

The case $\chi = 0$. In this case, all the information comes from inside Ω and therefore, like in the Computational Fluid Dynamics literature where it is known as the "supersonic outflow" case, we take

$$\Phi(v_K, K, \partial\Omega) = F(v_K) \cdot \nu_K. \tag{26}$$

The case $\chi = m$. In this case, all the information comes from outside Ω and therefore, like in the Computational Fluid Dynamics literature where it is known as the "supersonic inflow" case, we take

$$\Phi(v_K, K, \partial\Omega) = \Phi_{\text{given}}, \tag{27}$$

where Φ_{given} is the flux computed from the given physical boundary conditions.

The case $1 \leqslant \chi \leqslant m-1$. As already discussed in the introduction of this Section, we need χ scalar information coming from outside of Ω. Hence we assume that we have on physical ground χ relations on the boundary:

$$g_k(v) = 0, \quad k = 1, \ldots, \chi. \tag{28}$$

Remark 1. The notation $g_k(v) = 0$ means that we have a relation between the components of v. However, in general, the function g_k is not given explicitly in terms of v. In Application 2, for Euler equations, $g_k(v)$ could be the pressure, which is not one of the components of v.

Since we have to determine the m components of $\Phi(v_K, K, \partial\Omega)$, we need $m - \chi$ supplementary scalar information. Let us write them as

$$h_k(v) = 0, \quad k = \chi + 1, \ldots, m. \tag{29}$$

In general conditions (28) are named as "physical boundary conditions" while conditions (29) are named as "numerical boundary conditions". Then we take

$$\Phi(v_K, K, \partial\Omega) = F(v) \cdot \nu_K, \tag{30}$$

where v is solution to (28), (29) (see however Section 4.1 for a practical point of view).

Remark 2. The system (28), (29) for the m unknowns $v \in G$ is a $m \times m$ nonlinear system of equations. We are going to study its solvability in Theorem 1.

Let us now first discuss the numerical boundary conditions (29). The $m - \chi$ supplementary information we need, come from inside of Ω. A natural idea is then to use the advection equation (25) that is, of course, a first order approximation of the nonlinear equation (5). Since for $k \geqslant \chi + 1$ we have $\lambda_k(\underline{v}, \nu_K) > 0$, we know that $l_k(\underline{v}, \nu_K) \cdot v(x, t)$ on the boundary (i.e. for $x \in \partial\Omega$) at time t depends on the values of $l_k(\underline{v}, \nu_K) \cdot v$ inside Ω. This suggests that the so-called characteristic boundary conditions

$$l_k(\underline{v}, \nu_K) \cdot v = l_k(\underline{v}, \nu_K) \cdot v_K, \quad k = \chi + 1, \ldots, m, \tag{31}$$

are good candidates for (29). Actually we prefer a slightly different boundary condition that reads for $k = \chi + 1, \ldots, m$

$$h_k(v) \equiv l_k(\underline{v}, \nu_K) \cdot \big(F(v) \cdot \nu_K\big) - l_k(\underline{v}, \nu_K) \cdot \big(F(v_K) \cdot \nu_K\big) = 0. \tag{32}$$

In fact (31) was derived with $\underline{v} = v_K$ in the context of finite differences (we refer to the book of Hirsch [7], Chapter 19). We think, and this is also confirmed by our numerical experience, that (32) is more adapted to the finite volume approach since the unknown is the normal flux $F(v) \cdot \nu_K$ on the boundary $K \cap \partial\Omega$. In Ghidaglia and Pascal [18], we prove the following result on the solvability of (28)–(32).

Theorem 1. *In the case where* $1 \leqslant \chi \leqslant m-1$ (*let us recall that we are in the noncharacteristic case*: $\lambda_k(\underline{v}, \nu_K) \neq 0$, $k = 1, \ldots, m$) *and if*

$$\det_{1 \leqslant k,l \leqslant \chi} \left(\sum_{i=1}^{m} r_l^i(\underline{v}, \nu_K) \frac{\partial g_k}{\partial v_i}(\underline{v}) \right) \neq 0 \tag{33}$$

then the nonlinear system (28)–(32) *has one and only one solution* v, *for* $v - \underline{v}$, $g_k(\underline{v})$ *and* $h_k(\underline{v})$ *sufficiently small.*

Remark 3. It follows immediately from (33) that the functions g_k are functionally independent.

2.4.2. The characteristic case

If $n_0 \geqslant 1$ denotes the dimension of the kernel of the matrix $\underline{A}_{v_K}$, we label its eigenvalues as follows:

$$\lambda_1(\underline{v}, v_K) \leqslant \cdots \leqslant \lambda_\chi(\underline{v}, v_K) < 0 < \lambda_{\chi+n_0+1}(\underline{v}, v_K) \leqslant \cdots \leqslant \lambda_m(\underline{v}, v_K),$$
$$\lambda_{\chi+1}(\underline{v}, v_K) = \cdots = \lambda_{\chi+n_0}(\underline{v}, v_K) = 0.$$

The case $\chi = 0$. In this case, we simply follow the noncharacteristic case where we consider that all the information comes from inside and we take again

$$\Phi(v_K, K, \partial\Omega) = F(v_K) \cdot v_K. \tag{34}$$

The case $\chi + n_0 = m$. Again we simply follow the noncharacteristic case where we consider that all the information comes from outside and we take

$$\Phi(v_K, K, \partial\Omega) = \Phi_{\text{given}}. \tag{35}$$

The case $1 \leqslant \chi \leqslant m - 1 - n_0$. We have χ scalar information coming from outside of Ω. Hence we assume that we have, on the physical ground, χ relations on the boundary:

$$g_k(v) = 0, \quad k = 1, \ldots, \chi. \tag{36}$$

Since we have to determine the m components of $\Phi(v_K, K, \partial\Omega)$, we need $m - \chi$ supplementary scalar information. Let us first write $m - \chi - n_0$ conditions according to what we have done in the noncharacteristic case:

$$l_k(\underline{v}, v_K) \cdot \big(F(v) \cdot v_K\big) = l_k(\underline{v}, v_K) \cdot \big(F(v_K) \cdot v_K\big), \quad k = \chi + n_0 + 1, \ldots, m. \tag{37}$$

At first sight, we need n_0 supplementary information to determine the m components of the normal flux $F(v) \cdot v_K$. But since the mapping $v \to F(v) \cdot v_K$ has a noninvertible Jacobian for $v = \underline{v}$, it happens that it may be not true. For instance in the case of the Euler equations, for the wall boundary condition, since the relation (36) simply reads $u \cdot v_K = 0$, the normal flux $F(v) \cdot v_K = (0, pv_K, 0)$ depends on only one variable, the pressure p that may indeed be determined with relation (37). In the general nonlinear case, the question is open but in the linear case, the situation is more simple: $F(v) \cdot v_K = \underline{A}_{v_K} v$ has exactly $m - n_0$ independent components and although v satisfying (36), (37) is no longer unique, there is only one numerical flux $F(v) \cdot v_K$ satisfying (36), (37) provided again condition (33) holds true.

3. Extension to the nonconservative case

Let us now address the case of nonconservative systems like the system (1)–(3).

3.1. On the continuous system of equations

We assume that the matrix $\mathtt{Id} + D(v)$ is invertible (i.e. that (4) is an evolution partial differential equation) and we rewrite Eq. (4) as

$$\frac{\partial v}{\partial t} + \nabla \cdot F(v) + \sum_{j=1}^{nd} C_j(v) \frac{\partial v}{\partial x_j} = S(v), \tag{38}$$

with

$$S(v) = \big(\mathtt{Id} + D(v)\big)^{-1} \tilde{S}(v),$$
$$C_j(v) = \big(\mathtt{Id} + D(v)\big)^{-1} \left(\tilde{C}_j(v) + \frac{\partial F^j(v)}{\partial v}\right) - \frac{\partial F^j(v)}{\partial v} \quad \text{for } j = 1, \ldots, nd,$$

in order to keep the flux $F(v)$ unchanged between (4) and (38). The reason for this is given in Ghidaglia et al. [16].

3.2. The discrete system of equations

Here the integration of (38) on K leads to

$$\mathrm{vol}(K)\frac{\mathrm{d}v_K}{\mathrm{d}t} + F_{\partial K} + \int_K \sum_{j=1}^{nd} C_j(v)\frac{\partial v}{\partial x_j}\,\mathrm{d}x = \int_K S(v)\,\mathrm{d}x. \tag{39}$$

Hence the time evolution of $v_K(t)$ is governed by three terms. Their discrete treatment, which was introduced in Ghidaglia et al. [16], is discussed in details in Ghidaglia and Pascal [18]. Let us summarize terms by terms their approximation. The source term i.e. $\int_K S(v)\,\mathrm{d}x$ contains no derivative and a natural discretization reads as

$$\int_K S(v)\,\mathrm{d}x \approx \mathrm{vol}(K)S(v_K). \tag{40}$$

The term $F_{\partial K}(t)$ is the normal flux on the boundary of K and the integral $F_{K,L} = \int_{K\cap L} F(v(\sigma,t))\cdot \nu_{K,L}\,\mathrm{d}\sigma$ is again approximated by the numerical flux $\Phi(v_K, v_L, K, L)$ that is obtained from the VFFC method by formula (22) where we take

$$U(v, w, K, L) = \mathrm{sgn}\big(\tilde{A}_{\nu_{K,L}}(\mu)\big). \tag{41}$$

Here $\mu = \mu(v, w, K, L)$ is still an average between v and w depending on the geometry but since a formal argument leads to the following approximate convection equation for the flux $F_{K,L}$

$$\frac{\partial F_{K,L}}{\partial t} + \tilde{A}_{\nu_{K,L}}(\mu)\frac{\partial F_{K,L}}{\partial \nu} = \mathrm{area}(K\cap L)J_{\nu_{K,L}}(\mu)S(\mu), \tag{42}$$

the advection matrix $\tilde{A}_\nu(v)$ is now given by

$$\tilde{A}_\nu(v) = J_\nu(v) + J_\nu(v)C_\nu(v)J_\nu(v)^{-1}, \tag{43}$$

where $J_\nu(v) = \partial F(v)\cdot\nu/\partial v$ is the normal Jacobian matrix and $C_\nu(v) = C(v)\cdot\nu \equiv \sum_{j=1}^{nd} C_j(v)\nu^j$ is the normal non-conservative matrix.

The starting point of the discretization of the nonconservative product in (39) is a constant approximation of $C_j(v)$ by $C_j(v_K)$ on each control volume. A formal Taylor expansion on $K\cap L$ gives

$$J_{\nu_{K,L}}(v_K)\big(v(\sigma,t) - v_K\big) \approx F\big(v(\sigma,t)\big)\cdot\nu_{K,L} - F(v_K)\cdot\nu_{K,L} \tag{44}$$

and leads, for approximating $\int_K \sum_{j=1}^{nd} C_j(v)\frac{\partial v}{\partial x_j}\,\mathrm{d}x$, to the formula

$$\sum_{L\in\mathcal{N}(K)} \mathrm{area}(K\cap L)E_{K,L}\big(\Phi(v_K, v_L, K, L) - F(v_K)\cdot\nu_{K,L}\big) \tag{45}$$

with $E_{K,L} = C_{\nu_{K,L}}(v_K)J_{\nu_{K,L}}(v_K)^{-1}$.

Finally from the introduction of $\Phi(v_K, K, \partial\Omega)$, an approximation of the conservative flux on the boundary that is discussed in the next section, and from an easy extension of the previous discussion for a control volume that meets the boundary, the finite volume discretization of (38) yields to the following o.d.e.'s:

$$\begin{aligned}\mathrm{vol}(K)\frac{\mathrm{d}v_K}{\mathrm{d}t} &+ \sum_{L\in\mathcal{N}(K)} \mathrm{area}(K\cap L)(\mathtt{Id} + E_{K,L})\big(\Phi(v_K, v_L, K, L) - F(v_K)\cdot\nu_{K,L}\big)\\ &+ \sum_{\mathrm{area}(K\cap\partial\Omega)\neq 0} \mathrm{area}(K\cap\partial\Omega)\,(\mathtt{Id} + E_{K,\partial\Omega})\big(\Phi(v_K, K, \partial\Omega) - F(v_K)\cdot\nu_K\big) = \mathrm{vol}(K)S(v_K)\end{aligned} \tag{46}$$

with $E_{K,\partial\Omega} = C_{\nu_K}(v_K)J_{\nu_K}(v_K)^{-1}$ and ν_K the unit normal to $K\cap\partial\Omega$ that points outside Ω.

3.3. Discretization of the boundary conditions

Let us study the extension of our method in the nonconservative case. Exactly as for the conservative case, we have to find the numerical flux $\Phi(v_K, K, \partial\Omega)$ that approximates $\int_{K\cap\partial\Omega} F(v(\sigma,t))\cdot\nu_K\,\mathrm{d}\sigma$. Here the linearization around the state $\underline{v}$ still reads (24) but this time the advection matrix $\underline{A}_{\nu_K}$ is

$$\underline{A}_{\nu_K} = J_{\nu_K}(\underline{v}) + C_{\nu_K}(\underline{v}), \tag{47}$$

which is equivalent to the matrix $\tilde{A}_{\nu_K}(\underline{v})$. As in the conservative case, there are two different situations. The first one (the non-characteristic case) refers to the case where the matrix $\underline{A}_{\nu_K}$ is invertible, while the second one refers to the complementary case.

3.3.1. The noncharacteristic case

Let us assume that the eigenvalues $\lambda_k(\underline{v}, v_K)$ of $\underline{A}_{v_K}$, which are also the eigenvalues of $\tilde{A}_{v_K}(\underline{v})$, are

$$\lambda_1(\underline{v}, v_K) \leqslant \lambda_2(\underline{v}, v_K) \leqslant \cdots \leqslant \lambda_\chi(\underline{v}, v_K) < 0 < \lambda_{\chi+1}(\underline{v}, v_K) \cdots \leqslant \lambda_m(\underline{v}, v_K).$$

Then like in the conservative case, we have to discuss according to the value of χ. There is no change for the cases $\chi = 0$ and $\chi = m$. In the case $1 \leqslant \chi \leqslant m-1$, the discussion is exactly that of Section 2.4.1. There is only one difference, we take for $h_k(v)$, $k = \chi+1, \ldots, m$,

$$h_k(v) \equiv \tilde{l}_k(\underline{v}, v_K) \cdot \big(F(v) \cdot \nu_K\big) - \tilde{l}_k(\underline{v}, v_K) \cdot \big(F(v_K) \cdot \nu_K\big), \tag{48}$$

but this time $\tilde{l}_k(\underline{v}, v)$ denotes a left eigenvector of $\tilde{A}_{v_K}(\underline{v})$ defined by (43), this choice being justified by the approximate convection equation (42) for the normal flux.

3.3.2. The characteristic case

Here we label the eigenvalues of the matrix $\underline{A}_{v_K}$ as follows:

$$\lambda_1(\underline{v}, v_K) \leqslant \cdots \leqslant \lambda_\chi(\underline{v}, v_K) < 0 < \lambda_{\chi+n_0+1}(\underline{v}, v_K) \cdots \leqslant \lambda_m(\underline{v}, v_K),$$
$$\lambda_{\chi+1}(\underline{v}, v_K) = \cdots = \lambda_{\chi+n_0}(\underline{v}, v_K) = 0.$$

Again $n_0 \geqslant 1$ denotes the dimension of the kernel of $\underline{A}_{v_K}$. There is no change for the case $\chi = 0$. In the case $1 \leqslant \chi \leqslant m-1$, the discussion is exactly that of Section 2.4.2. There is again only one difference, we take again for the $h_k(v)$'s the functions given by (48).

4. Applications and implementation in CFD

4.1. On the effective normal flux at the boundary and on the choice of $\underline{v}$

In the two previous sections, we have exposed a general principle for obtaining the normal flux at the boundary. In this section, our goal is to provide the complementary steps that allows one to turn this principle into lines of code. We first propose a practical point of view for the implementation of our boundary condition treatment: we investigate the numerical resolution to the central nonlinear system of equation and we discuss the choice of $\underline{v}$. We limit ourselves to the conservative case since there are no major differences to this respect with the nonconservative case.

Let us summarize the proposed method. If K is a control volume that meets the boundary $\partial\Omega$, we take at the boundary the following normal flux

$$\Phi(v_K, K, \partial\Omega) = \Phi, \tag{49}$$

where Φ satisfies the following nonlinear system of equations (here we assume that $\underline{v}$ is given)

$$\begin{cases} g_k(v) = 0, \quad k = 1, \ldots, \chi, \\ l_k(\underline{v}, v_K) \cdot \Phi = l_k(\underline{v}, v_K) \cdot \big(F(v_K) \cdot \nu_K\big), \quad k = \chi+1, \ldots, m, \\ \Phi = F(v) \cdot \nu_K. \end{cases} \tag{50}$$

In practice, the flux $F(v) \cdot \nu_K$ can be seen (at least in general) as a "small" perturbation of $F(v_K) \cdot \nu_K$ and system (50) can be written in a parametric way:

$$\begin{cases} \Phi = F(v_K) \cdot \nu_K + \displaystyle\sum_{k=1}^{\chi} \epsilon_k r_k(\underline{v}, v_K), \\ (\epsilon_1, \ldots, \epsilon_\chi) \in \mathbb{R}^\chi \text{ such that } g_k(v) = 0 \text{ for } k = 1, \ldots, \chi. \end{cases} \tag{51}$$

This system is a nonlinear system of $m + \chi$ equations with $m + \chi$ unknowns (for instance the components of Φ and the ϵ_k) and it is solved by a few iteration of the Newton–Raphson method. Theorem 1 guarantees that the Jacobian matrix is invertible.

Let us now investigate the choice of $\underline{v}$. From Theorem 1, $g_k(\underline{v})$ for $k = 1, \ldots, \chi$ and $h_k(\underline{v})$ for $k = \chi+1, \ldots, m$ have to be "sufficiently small". Therefore the best choice should be the state v, solution to the system (28)–(32) for which g_k and h_k are zero. But since v is a priori unknown and since the computation of the eigenelements of the matrix $\underline{A}_{v_K}$ is complex, in practice an "easily computed" approximation of v is used. So $\underline{v}$ is taken equal to the interior state: $\underline{v} = v_K$. However, from a practical point of view, it may be more interesting to use other approximations as we are going to illustrate it now.

4.1.1. Boundary conditions at infinity

Let us discuss the case where the physical domain is unbounded, for example the case of an external flow. For practical reasons, the computational domain must be bounded and this leads to introduce a boundary, which is called the boundary at infinity. On this boundary denoted Γ_∞, we consider that the physical data correspond to a given state v_∞ also called the free-stream state. Let us remark that if the boundary is not sufficiently far then a numerical boundary has to be determined and this issue is discussed in Section 4.1.2. For a control volume that meets the boundary Γ_∞, we have to find the normal flux $\Phi(v_K, K, \Gamma_\infty)$ that approximates $\int_{K\cap\Gamma_\infty} F(v(\sigma,t))\cdot \nu_K \,\mathrm{d}\sigma$. We propose to chose $\underline{v}$ equal to v_∞, then to compute the eigenvalues $\lambda_k(v_\infty, \nu_K)$ of $A_{\nu_K}(v_\infty)$ and to take in the conservative case

$$\Phi(v_K, K, \Gamma_\infty) = \sum_{k/\lambda_k(v_\infty,\nu_K)<0} l_k(v_\infty,\nu_K)\cdot\big(F(v_\infty)\cdot\nu_K\big)r_k(v_\infty,\nu_K) + \sum_{k/\lambda_k(v_\infty,\nu_K)\geqslant 0} l_k(v_\infty,\nu_K)\cdot\big(F(v_K)\cdot\nu_K\big)r_k(v_\infty,\nu_K). \tag{52}$$

This approach is different from taking

$$\Phi(v_K, K, \Gamma_\infty) = F(v_\infty)\cdot\nu_K. \tag{53}$$

In the case where the code is run in order to find a steady state (i.e. a solution of $\nabla\cdot F(v)=0$), it is clear that close to convergence, formulation (52) and (53) for the normal flux at infinity will give almost the same results. However during transients, formulation (52) is better.

4.1.2. Numerical boundary conditions

In Section 4.1.1, it was assumed that the boundary Γ_∞ was sufficiently far, in order to take v_∞ on this boundary as if it was at infinity. If the truncation of the domain affects the value on the boundary Γ_∞ (by taking a smaller computational domain), therefore one has to modify the previous boundary condition (52) in order to get more accurate boundary condition at infinity. A possible method consists in correcting the state v_∞ into an other state say $\tilde{v}_\infty$. This has to be done via an *ad hoc* procedure depending on the system. For instance in the case of an internal flow, one obtains $\tilde{v}_\infty$ by linearizing the Euler system (Application 2) and by using the so called far field correction (see e.g. Chapter 19.3 of Hirsch [7]). Once the state $\tilde{v}_\infty$ has been chosen, we replace (52) by

$$\Phi(v_K, K, \Gamma_\infty) = \sum_{k/\lambda_k(\tilde{v}_\infty,\nu_K)\leqslant 0} l_k(\tilde{v}_\infty,\nu_K)\cdot\big(F(\tilde{v}_\infty)\cdot\nu_K\big)r_k(\tilde{v}_\infty,\nu_K) + \sum_{k/\lambda_k(\tilde{v}_\infty,\nu_K)>0} l_k(\tilde{v}_\infty,\nu_K)\cdot\big(F(v_K)\cdot\nu_K\big)r_k(\tilde{v}_\infty,\nu_K). \tag{54}$$

Remark 4. Let us remark that the following numerical boundary condition

$$\Phi(v_K, K, \partial\Omega) = F(v_K)\cdot\nu_K, \tag{55}$$

can be implemented in at least two cases where numerical boundary reduces the computational domain: the case where the solution is symmetric with respect to an hyperplane and the case where the system does not depend on one of the space variables (e.g. one-dimensional computation with a two-dimensional code).

4.2. Applications to single fluid models

In this section, we discuss the issue with the multidimensional Euler system for inviscid fluids, which is described in Application 2.

4.2.1. The case of subsonic inlet boundary condition

Let us first address to the case where on a part of the boundary the fluid goes inside the domain at a subsonic speed, that is $-c < u\cdot\nu_K < 0$. We need one information that comes from inside of Ω and we have to prescribe $\chi = nd+1$ boundary conditions. In general one prescribes the direction of the flow on the boundary i.e. $u=\mu\alpha$ where α is a unit vector which makes an obtuse angle with ν_K with $\alpha\cdot\nu_K<0$ and where μ is a positive number such that $-\alpha\cdot\nu_K\,\mu < c$. Giving α amounts to give $nd-1$ conditions and therefore it remains to prescribe two supplementary boundary conditions.

$$g_1(v)=0, \qquad g_2(v)=0. \tag{56}$$

Table 1
Inlet boundary condition: values of Δ, determinant in Theorem 1

Variable	$g_1(v)$	$g_2(v)$	Δ
Thermodynamic	$\rho - \rho_{\text{in}}$	$e - e_{\text{in}}$	$-\frac{1}{2\underline{\rho}\underline{c}}$
Thermodynamic & velocity	$p - p_{\text{in}}$	$u - u_{\text{in}}$	0
	$\rho - \rho_{\text{in}}$	$u - u_{\text{in}}$	$\frac{\underline{p}}{\underline{\rho}} - \frac{\underline{c}^2}{\underline{k}}$
	$h - h_{\text{in}}$	$u - u_{\text{in}}$	$\underline{c}^2$
Thermodynamic & mass flow	$p - p_{\text{in}}$	$\rho u - (\rho u)_{\text{in}}$	$\underline{uc}$
	$e - e_{\text{in}}$	$\rho u - (\rho u)_{\text{in}}$	$\underline{uc} - \underline{c}^2 + \frac{\underline{kp}}{\underline{\rho}}$
Entropy & enthalpy	$s - s_{\text{in}}$	$H - H_{\text{in}}$	$\underline{c} - \underline{u}$

Table 2
Outlet boundary condition: values of Δ, the determinant in Theorem 1

Variable	$g_1(v)$	Δ
Pressure	$p - p_{\text{out}}$	$\underline{c}^2$
Velocity	$u - u_{\text{out}}$	$-\frac{\underline{c}}{\underline{\rho}}$
Mass flux	$\rho u - (\rho u)_{\text{out}}$	$\underline{u} - \underline{c}$
Temperature (perfect gas)	$T - T_{\text{out}}$	$\frac{2\underline{c}^2 + 3\gamma \underline{u}^2}{6\gamma C_v \underline{\rho}}$
Total enthalpy	$H - H_{\text{out}}$	$\frac{\underline{c}(\underline{c} - \underline{u})}{\underline{\rho}}$
Entropy	$s - s_{\text{out}}$	0

In the case where the flow is normal to the boundary, according to Theorem 1, the local solvability of (28)–(32) is reduced to the condition

$$\det_{1 \leqslant k,l \leqslant 2} \left(\sum_{i=1}^{m} r_k^i(\underline{v}, \nu_K) \frac{\partial g_l}{\partial v_i}(\underline{v}) \right) \neq 0. \tag{57}$$

Denoting by Δ this determinant, its values are gathered in Table 1 depending on whether thermodynamic variables, velocity or enthalpy are imposed. All combinations of conservative and primitive variables can be selected as physical boundary condition with the exception of the well known pair composed of the velocity and the pressure. Let us observe that the often used pair of stagnation temperature and pressure is equivalent to the entropy and total enthalpy pair, which is displayed in the last line of the table.

4.2.2. The case of subsonic outlet boundary condition

Usually at a subsonic outlet where $0 < u \cdot \nu_K < c$ and where we have $nd + 1$ information that come from inside of Ω and $\chi = 1$, it is standard to impose the pressure, that is to take $g_1(v) = p - p_{\text{out}}$ where p_{out} is a given pressure. Theorem 1 yields that $\underline{c}^2$ is different from 0, an obvious fact. One can also wish to impose another quantity like velocity, mass flux, temperature, etc and we obtain the following results gathered in Table 2. These results show that indeed it is appropriate to impose either the pressure or the velocity, which are the most often imposed condition respectively for internal flow and for external flow. The entropy cannot be prescribed but it is also possible to fix the temperature, the mass flux or the total enthalpy. However in these two last cases, an instability may occur if the flow becomes critical (sonic point) at the outlet.

4.2.3. The case of wall boundary condition

On a wall, the normal velocity of the fluid $u \cdot \nu_K$ is equal to zero. Hence the normal flux $F(v) \cdot \nu_K$ is equal to

$$F(v) \cdot \nu_K = (0, p\nu_K, 0). \tag{58}$$

Therefore, to determine the flux $\Phi(v_K, K, \partial\Omega)$, we only have to find the unknown p. Let us notice that it is much simpler and much more physically relevant to try to find the normal flux on the boundary rather than the variable $v = (\rho, \rho u, \rho E)$.

According to the value of the eigenvalues, only one, namely $\lambda_{nd+2}(v, \nu_K) = c$, is positive. Then only one information comes from inside Ω and if we follow our strategy, we have to impose (37) which reads

$$l_{nd+2}(\underline{v}, \nu_K) \cdot (0, p\nu_K, 0) = l_{nd+2}(\underline{v}, \nu_K) \cdot \big(F(v_K) \cdot \nu_K\big). \tag{59}$$

If $\underline{v}$ consists in the interior state v_K, then pressure p is automatically given by the explicit formula

$$p = \frac{l_{nd+2}(v_K, \nu_K) \cdot (F(v_K) \cdot \nu_K)}{l_{nd+2}(v_K, \nu_K) \cdot (0, \nu_K, 0)}, \tag{60}$$

that is (where the indexed quantities correspond to v_K)

$$p = p_K + \frac{\rho_K c_K^2 u_K \cdot \nu_K}{c_K - k_K u_K \cdot \nu_K}. \tag{61}$$

Remark 5. For a polytropic gas, for which the EOS is $p = (\gamma - 1)\rho e$ where $\gamma > 1$ is a given constant, we have $k = \gamma - 1$ and $c^2 = \frac{\gamma p}{\rho}$. Then formula (61) reads as

$$p = p_K \left(1 + \frac{\gamma u_K \cdot \nu_K}{c_K - (\gamma - 1) u_K \cdot \nu_K}\right). \tag{62}$$

4.2.4. Comparison between the Riemann invariant technique and our method

As it is well known, the Riemann problem for one-dimensional hyperbolic equations has played a very important role for the numerical computations of its solutions. Although, up to now, this strategy has not been generalized to higher space dimensions (even on Cartesian meshes and for linear equations, the solution to the Riemann problem is not simple to obtain and no closed formulas are available), multidimensional problems benefit from one-dimensional ones by considering at each interface the normal equation. Nevertheless at a boundary, it is not possible to solve the classical Riemann problem since the exterior state is not known. Then (see the monograph by Godlewski and Raviart [5] and references therein) some strategies are proposed to overcome these difficulties. For instance, the technique developed by Dubois [19] consists in solving an "incomplete" Riemann problem. For a case where $1 \leqslant \chi \leqslant m - 1$ i.e. where χ information are entering into the domain, this strategy aims at solving the projection of (5) on the normal direction:

$$\frac{\partial v}{\partial t} + \frac{\partial F(v) \cdot \nu_K}{\partial x} = 0, \tag{63}$$

with the initial data

$$v(x, 0) = \underline{v} \quad \text{for } x < 0 \quad \text{and} \quad v(x, 0) \text{ satisfies (28) for } x > 0 \tag{64}$$

and where we assume that $\underline{v} = v_K$. The "incomplete" Riemann problem method consists then in finding $\chi - 1$ intermediate states $\mu_1, \ldots, \mu_{\chi-1}$ such that $\underline{v}$ is connected to μ_1 through a 1-simple wave, μ_1 is connected to μ_2 through a 2-simple wave, $\ldots$, $\mu_{\chi-1}$ is connected to v through a χ-simple wave. We can rewrite these conditions, with $\mu_0 \equiv \underline{v}$ and $\mu_\chi \equiv v$, as

$$W_k^\ell(\mu_{\ell-1}) = W_k^\ell(\mu_\ell), \quad k = 1, \ldots, m-1, \ell = 1, \ldots, \chi, \tag{65}$$

where $\{W_k^\ell\}_{k=1,\ldots,m-1}$ is a family of $m - 1$ independent ℓ-pseudo Riemann invariants (in the vicinity of $\underline{v}$). The system (28)-(65) is made of $m \times \chi$ scalar equations for $m \times \chi$ scalar unknowns: the coordinates of $\mu_1, \ldots, \mu_\chi$ (provided the pseudo Riemann invariants have been computed). Let us emphasize that the method we propose in this paper replaces the system (65) by the system (32) of $m - \chi$ equations. Hence our method appears to be much simpler than the one that uses an incomplete Riemann problem. In a certain sense, (32) provides an approximation for the solution of (65).

Let us study now the relationship between these two systems for a typical example. We consider the case where $\chi = m - 1$ that is the case where $m - 1$ information are entering into the domain and which occurs e.g. in the context of fluid dynamics for a subsonic inlet. We are able to prove (Ghidaglia and Pascal [18]) the following theorem that confirms numerical experiments with subsonic inlet and oulet where we observed a tiny difference between the results obtained by the two methods.

Theorem 2. *Given $\epsilon > 0$, the set of solutions $v \in G$ satisfying $\|v - \underline{v}\| \leqslant \epsilon$ and* (32) *i.e. corresponding to our method and the set of solutions $v \in G$ satisfying $\|v - \underline{v}\| \leqslant \epsilon$ and* (65) *with $\|\mu_i - \underline{v}\| \leqslant \epsilon$ i.e. that corresponds to the incomplete Riemann solution are tangent at $\underline{v}$ to the hyperspace orthogonal to $l_m(\underline{v}, \nu_K)$.*

4.3. An application to a two fluid model

4.3.1. An isentropic model

An isentropic version of the system (1)–(3) can be obtained as follows. Introducing the specific entropy of the fluid k, s_k, defined by

$$T_k \, \mathrm{d}s_k = \mathrm{d}e_k - \frac{p}{\rho_k^2} \mathrm{d}\rho_k, \tag{66}$$

and *assuming that there is no production of entropy into the shocks*, Eq. (3) leads to

$$\frac{\partial(\alpha_k\rho_k s_k)}{\partial t} + \nabla\cdot(\alpha_k\rho_k s_k u_k) = \frac{Q_k}{T_k} + \left(\frac{u_k - u_{k,i}}{T_k}u_k + s_k\right)\Gamma_k. \tag{67}$$

In the case of absence of mass transfers between the two fluids ($\Gamma_k \equiv 0$) and of heat transfers ($Q_k \equiv 0$), these equations read as

$$\frac{\partial(\alpha_k\rho_k s_k)}{\partial t} + \nabla\cdot(\alpha_k\rho_k s_k u_k) = 0. \tag{68}$$

In view of (1) and (68), we can have solutions with constant entropies i.e. with s_1 and s_2 constant. The system then reduces to Eqs. (1), (2) and the equations of states are replaced by isentropic ones: $\mathcal{G}_k(p,\rho_k) = 0$ for $k = 1, 2$.

For the sake of simplicity in the exposition, let us concentrate on the following simplified system:

$$\frac{\partial(\alpha_k\rho_k)}{\partial t} + \nabla\cdot(\alpha_k\rho_k u_k) = 0, \tag{69}$$

$$\frac{\partial(\alpha_k\rho_k u_k)}{\partial t} + \nabla\cdot\big(\alpha_k(\rho_k u_k\otimes u_k + p\mathtt{Id})\big) - p\nabla\alpha_k = \alpha_k\rho_k g + M_k, \tag{70}$$

with the two equations of states and where we only take into account interfacial pressure in the momentum transfer. Hence the forces M_k which satisfy $M_1 + M_2 = 0$ reads $M_k = -(p - p_{\text{interface}})\nabla\alpha_k$ for $k = 1, 2$ where as Bestion [20], we take

$$(p - p_{\text{interface}}) \equiv \delta\frac{\alpha_1\alpha_2\rho_1\rho_2}{\alpha_1\rho_2 + \alpha_2\rho_1}(u_1 - u_2)^2. \tag{71}$$

The order of magnitude of the parameter δ is about 1 and its role is to allow the system (69), (70) to be hyperbolic.

This system has already the nonconservative form (4) provided we take $nd = 3$, $m = 8$, $u_k \in \mathbb{R}^3$, $v = (\alpha_1\rho_1, \alpha_1\rho_1 u_1, \alpha_2\rho_2, \alpha_2\rho_2 u_2)$ and

$$F(v)\cdot\omega = \big(\alpha_1\rho_1(u_1\cdot\omega), \alpha_1\rho_1(u_1\cdot\omega)u_1 + \alpha_1(p-\pi)\omega, \alpha_2\rho_2(u_2\cdot\omega), \alpha_2\rho_2(u_2\cdot\omega)u_2 + \alpha_2(p-\pi)\omega\big),$$
$$\forall\omega\in\mathbb{R}^3, \tag{72}$$

$$\sum_{j=1}^{3} C_j(v)\frac{\partial v}{\partial x_j} = (0, -\Gamma\nabla\alpha_1, 0, -\Gamma\nabla\alpha_2), \tag{73}$$

$$S(v) = (0, \alpha_1\rho_1 g, 0, \alpha_2\rho_2 g), \tag{74}$$

where g denotes the gravity, $\pi = \pi(t)$ is a time-dependent function chosen as in [16] in order that the Jacobian matrix $J_v(v)$ is invertible and finally we have denoted

$$\Gamma \equiv p - \pi - \delta\frac{\alpha_1\alpha_2\rho_1\rho_2}{\alpha_1\rho_2 + \alpha_2\rho_1}(u_1 - u_2)^2. \tag{75}$$

Remark 6. The relation (73) does not give explicitly the matrices $C_j(v)$. In order to obtain these quantities, we have to compute the derivatives $\partial\alpha_k/\partial v_j$. This is done by using the (EOS) as follows. The system allowing to compute the α_k and p from the components of v is

$$\alpha_1 + \alpha_2 = 1, \qquad \mathcal{G}_1\left(p, \frac{v_1}{\alpha_1}\right) = 0, \qquad \mathcal{G}_2\left(p, \frac{v_5}{\alpha_2}\right) = 0. \tag{76}$$

The differentiation of this system with respect to the v_k's will then produce a linear system for the $\partial\alpha_k/\partial v_j$.

4.3.2. On the determination of the normal flux at the boundary

In order to apply the characteristic boundary conditions (3.3.1), we have to construct the Jacobian matrix $J_\nu = A_\nu(v) - C_\nu(v)$. Let us denote by $q^{(\ell)} \equiv \partial q/\partial v_\ell$ then we have $A_\nu(v) =$

$$\begin{pmatrix} 0 & \nu & 0 & 0 \\ \alpha_1 p^{(1)}\nu - u_1\cdot\nu u_1 & u_1\otimes\nu + u_1\cdot\nu\mathtt{Id} & \alpha_1 p^{(5)}\nu & 0 \\ 0 & 0 & 0 & \nu \\ \alpha_2 p^{(1)}\nu & 0 & \alpha_2 p^{(5)}\nu - u_2\cdot\nu u_2 & u_2\otimes\nu + u_2\cdot\nu\mathtt{Id} \end{pmatrix}$$

and

$$C_\nu(v) = -\Gamma\begin{pmatrix} 0 & 0 & 0 & 0 \\ \alpha_1^{(1)}\nu & 0 & \alpha_1^{(5)}\nu & 0 \\ 0 & 0 & 0 & 0 \\ \alpha_2^{(1)}\nu & 0 & \alpha_2^{(5)}\nu & 0 \end{pmatrix}. \tag{77}$$

According to the method of this article, we have to find the eigensystem of the matrix $\tilde{A}_\nu(v)$, see (43). In fact the analytical expressions for the eigenelements of this 8 by 8 matrix is available but it is not numerically efficient to make use of these formulas. Let us explain why and describe what is done in practice. Due to the physical origin of this system, $u_1 \cdot \nu$ and $u_2 \cdot \nu$ are eigenvalues with multiplicity equal to 2 each. Hence the degree 8 characteristic polynomial $P(\lambda) \equiv \det(A_\nu(v) - \lambda \mathtt{Id})$ can be factorized as $P(\lambda) = (u_1 \cdot \nu - \lambda)^2 (u_2 \cdot \nu - \lambda)^2 R(\lambda)$ where R is a degree 4 polynomial. The 4 remaining eigenvalues can be found by analytical expression (using e.g. Maple). Once these eigenvalues are determined, the eigensystem follows by simple algebraic computations. Although leading to exact values, this method is not numerically efficient and the reason for this is two fold. First these analytical expressions involve a very large number of operations (divisions and algebraic roots in the complex plane). Second, and more important, they are very sensitive to round off errors. The strategy we recommend (and use ourselves) in practice consists in making use of Newton's algorithm for finding the two "large" roots of R. Indeed from the physical background of the problem, we expect that R has two real eigenvalues $u \cdot \nu - c$ and $u \cdot \nu + c$ with $c \gg |u|$. These eigenvalues are well isolated from the others and therefore Newton's algorithm is fast and robust. Moreover it involves only the 4 basic operations. Once these two eigenvalues are determined, the two remaining eigenvalues are the solutions to a known degree 2 equation in λ and this time the analytic expression for its roots are used. Once the eigensystem of $\tilde{A}_\nu(v)$ is obtained, the determination of the normal flux at the boundary follows Section 3.3.

5. Conclusions

In this paper we have presented a general method for imposing boundary conditions in the context of hyperbolic systems of conservation laws. This method is particularly well suited for approximations in the framework of Finite Volume Methods in the sense that *it computes directly the normal flux at the boundary*. This method is *general* since it only relies on the hyperbolic character of the system and neither on its conservative form nor on sophisticated and sometimes numerically expansive tools like Riemann's solvers or Riemann's invariant. However when such objects are available, our method is faster at the same precision. Our method is mathematically founded (Theorem 1) and easy to implement. Moreover it considers physical boundary conditions as natural inputs. We have given some material that indeed allows to achieve to the actual coding of our method in the main applications in Fluid Mechanics. Concerning numerical results, we refer the reader to the report Ghidaglia and Pascal [18].

Appendix

A.1. Eigenvalues for Application 1

For the ideal magnetohydrodynamics equations, the matrix $A_\omega(v)$ is

$$\begin{pmatrix} 0 & \omega & 0 & 0 \\ K\omega - u\cdot\omega u & u\otimes\omega - k\omega\otimes u + u\cdot\omega\,\mathtt{Id} & k\omega & (1-k)\omega\otimes B - B\cdot\omega\,\mathtt{Id} \\ -\frac{2u\cdot\omega|B|^2}{\rho} + (K-H)u\cdot\omega & (H+\frac{|B|^2}{\rho})\omega - k(u\cdot\omega)u & (1+k)u\cdot\omega & (1-k)u\cdot\omega B - B\cdot\omega u \\ \frac{B\cdot\omega u - B\cdot u\omega}{\rho} & \frac{B\otimes\omega - B\cdot\omega\,\mathtt{Id}}{\rho} & 0 & u\cdot\omega\,\mathtt{Id} \end{pmatrix}$$

and the eight real eigenvalues are as follows:

$$\begin{aligned} \lambda_1(v,\omega) = u\cdot\omega - |\omega|c_+ \leqslant \lambda_2(v,\omega) = u\cdot\omega - |\omega|c_- \leqslant \lambda_3(v,\omega) = u\cdot\omega - \frac{B\cdot\omega}{\sqrt{\rho}} \\ \leqslant \lambda_4(v,\omega) = \lambda_5(v,\omega) = u\cdot\omega \leqslant \lambda_6(v,\omega) = u\cdot\omega + \frac{B\cdot\omega}{\sqrt{\rho}} \\ \leqslant \lambda_7(v,\omega) = u\cdot\omega + |\omega|c_- \leqslant \lambda_8(v,\omega) = u\cdot\omega + |\omega|c_+, \end{aligned}$$

where

$$c_\pm = \frac{1}{\sqrt{2}}\sqrt{c^2 + \frac{|B|^2}{\rho} \pm \sqrt{\left(c^2 + \frac{|B|^2}{\rho}\right)^2 - \frac{4c^2(B\cdot\omega)^2}{\rho}}}.$$

The analytical expression of the corresponding eigenvectors can be found in Ghidaglia and Pascal [18].

A.2. Eigensystem of Application 2

For the multidimensional Euler system, the matrix $A_\omega(v)$ is found to be equal to

$$A_\omega(v) = \begin{pmatrix} 0 & \omega & 0 \\ K\omega - (u\cdot\omega)u & u\otimes\omega - k\omega\otimes u + u\cdot\omega\,\mathtt{Id} & k\omega \\ (K-H)u\cdot\omega & H\omega - k(u\cdot\omega)u & (1+k)u\cdot\omega \end{pmatrix},$$

where

$$k = \frac{1}{\rho T}\left(\frac{\partial p}{\partial s}\right)_\rho, \quad c = \sqrt{\left(\frac{\partial p}{\partial \rho}\right)_s}, \quad H = e + \frac{p}{\rho} + \frac{|u|^2}{2}, \quad K = c^2 + k\big(|u|^2 - H\big).$$

Note that according to the second principle of thermodynamics, we have $(\partial p/\partial\rho)_s > 0$. Then the eigenvalues of $A_\omega(v)$ are as follows:

$$\lambda_1(v,\omega) \equiv u\cdot\omega - |\omega|c \leqslant \lambda_2(v,\omega) = \cdots = \lambda_{nd+1}(v,\omega) \equiv u\cdot\omega \leqslant \lambda_{nd+2}(v,\omega) \equiv u\cdot\omega + |\omega|c.$$

Now if $\Omega_1,\ldots,\Omega_{nd-1}$ denotes an orthonormal basis of the hyperplane orthogonal to ω, the right eigenvectors can be taken equal to

$$\begin{cases} r_1(v,\omega) = \big(1, u - c\frac{\omega}{|\omega|}, H - u\cdot\frac{\omega}{|\omega|}c\big), \\ r_{nd+2}(v,\omega) = \big(1, u + c\frac{\omega}{|\omega|}, H + u\cdot\frac{\omega}{|\omega|}c\big), \\ r_2(v,\omega) = \big(1, u, H - \frac{c^2}{k}\big), \\ r_3(v,\omega) = (0,\Omega_1, u\cdot\Omega_1),\ldots, r_{nd+1}(v,\omega) = (0,\Omega_{nd-1}, u\cdot\Omega_{nd-1}). \end{cases}$$

The dual basis of the $(r_k(v,\omega))_{k=1,\ldots,nd+2}$ is then

$$\begin{cases} l_1(v,\omega) = \frac{1}{2c^2}\big(K + \frac{u\cdot\omega}{|\omega|}c, -ku - \frac{\omega c}{|\omega|}, k\big), \\ l_{nd+2}(v,\omega) = \frac{1}{2c^2}\big(K - \frac{u\cdot\omega}{|\omega|}c, -ku + \frac{\omega c}{|\omega|}, k\big), \\ l_2(v,\omega) = \frac{k}{c^2}\big(H - |u|^2, u, -1\big), \\ l_3(v,\omega) = (-u\cdot\Omega_1,\Omega_1,0),\ldots, l_{nd+1}(v,\omega) = (-u\cdot\Omega_{nd-1},\Omega_{nd-1},0). \end{cases}$$

A.3. Eigensystems of Applications 3, 4 and 5

For the isentropic multidimensional Euler equations (Application 3) the matrix $A_\omega(v)$ is

$$A_\omega(v) = \begin{pmatrix} 0 & \omega \\ c^2\omega - u\cdot\omega u & u\otimes\omega + u\cdot\omega\,\mathtt{Id} \end{pmatrix}.$$

The eigenvalues are as follows,

$$\lambda_1(v,\omega) \equiv u\cdot\omega - |\omega|c \leqslant \lambda_2(v,\omega) = \cdots = \lambda_{nd}(v,\omega) \equiv u\cdot\omega \leqslant \lambda_{nd+1}(v,\omega) \equiv u\cdot\omega + |\omega|c.$$

If $\Omega_1,\ldots,\Omega_{nd-1}$ is an orthonormal basis of the hyperplane orthogonal to ω, the right eigenvectors associated to these eigenvalues can be taken equal to

$$\begin{cases} r_1(v,\omega) = \big(1, u - c\frac{\omega}{|\omega|}\big), r_{nd+1}(v,\omega) = \big(1, u + c\frac{\omega}{|\omega|}\big), \\ r_2(v,\omega) = (0,\Omega_1),\ldots, r_{nd}(v,\omega) = (0,\Omega_{nd-1}). \end{cases}$$

The dual basis of the $(r_k(v,\omega))_{k=1,\ldots,nd+2}$ is then

$$\begin{cases} l_1(v,\omega) = \frac{1}{2c}\big(c + \frac{\omega.u}{|\omega|}, -\frac{\omega}{|\omega|}\big), \quad l_{nd+1}(v,\omega) = \frac{1}{2c}\big(c - \frac{\omega.u}{|\omega|}c, \frac{\omega}{|\omega|}\big), \\ l_2(v,\omega) = (-u\cdot\Omega_1,\Omega_1),\ldots, l_{nd}(v,\omega) = (-u\cdot\Omega_{nd-1},\Omega_{nd-1}). \end{cases}$$

Concerning Application 4 one has simply to take into the previous formulas $c \equiv c_0$ while for Application 5 one takes $c \equiv \sqrt{gh}$.

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