EXTENSION OF THE ROE AND VAN LEER ALGORITHMS TO SECOND ORDER ACCURACY AND IMPLICIT FORMULATIONS APPLIED TO THE EULER EQUATIONS IN TWO-DIMENSIONS - THEORY

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Abstract. *In this work, the first part of this study, the Roe and the Van Leer schemes are implemented following a MUSCL ("Monotone Upstream-centered Schemes for Conservation Laws") approach, aiming to guarantee second order accuracy and to achieve TVD ("Total Variation Diminishing") properties, and employing an implicit formulation to solve the Euler equations in the two-dimensional space. These schemes are implemented according to a finite volume formulation and using a structured spatial discretization. The former scheme is a flux difference splitting one, whereas the latter is a flux vector splitting scheme. The MUSCL approach employs five different types of nonlinear limiters, which assure TVD properties, namely: Van Leer limiter, Van Albada limiter, minmod limiter, Super Bee limiter and β-limiter. All variants of the MUSCL approach are second order accurate in space. The implicit schemes employ an ADI ("Alternating Direction Implicit") approximate factorization to solve implicitly the Euler equations. Explicit and implicit results are compared trying to emphasize the advantages and disadvantages of each formulation. The schemes are accelerated to the steady state solution using a spatially variable time step, which has demonstrated effective gains in terms of convergence rate according to Maciel. The algorithms are applied to the solution of the physical problem of the moderate supersonic flow along a compression corner. The results have demonstrated that the most accurate solutions are obtained with the Roe TVD scheme using minmod and Super Bee nonlinear limiters, when implemented in its implicit version. The numerical results and the analyses of this study are the subjects of the part II of this work (RESULTS).*

Keywords*: Roe algorithm, Van Leer algorithm, MUSCL procedure, Implicit formulations, Euler equations.*

1. INTRODUCTION

Conventional non-upwind algorithms have been used extensively to solve a wide variety of problems (Kutler, 1975). Conventional algorithms are somewhat unreliable in the sense that for every different problem (and sometimes, every different case in the same class of problems) artificial dissipation terms must be specially tuned and judicially chosen for convergence. Also, complex problems with shocks and steep compression and expansion gradients may defy solution altogether.

Upwind schemes are in general more robust but are also more involved in their derivation and application. Some first order upwind schemes that have been applied to the Euler equations are:

Roe (1981) method, whose author presented a work that emphasized that several numerical schemes to the solution of the hyperbolic conservation equations were based on exploring the information obtained in the solution of a sequence of Riemann problems. It was verified that in the existent schemes the major part of these information was degraded and that only certain solution aspects were solved. It was demonstrated that the information could be preserved by the construction of a matrix with a certain "U property". After the construction of this matrix, its eigenvalues could be considered as wave velocities of the Riemann problem and the U_L-U_R projections over the matrix's eigenvectors would be the jumps which occur between intermediate stages.

Van Leer (1982) method, whose author suggested an upwind scheme based on the flux vector splitting concept. This scheme considered the fact that the convective flux vector components could be written as flow Mach number polynomial functions, as main characteristic. Such polynomials presented the particularity of having the minor possible degree and the scheme had to satisfy seven basic properties to form such polynomials.

Second order spatial accuracy can be achieved by introducing more upwind points or cells in the schemes. It has been noted that the projection stage, whereby the solution is projected in each cell face (i-1/2,j; i+1/2,j) on piecewise constant states, is the cause of the first order space accuracy of the Godunov schemes (Hirsch, 1990). Hence, it is sufficient to modify the first projection stage without modifying the Riemann solver, in order to generate higher spatial approximations. The state variables at the interfaces are thereby obtained from an extrapolation between neighboring cell averages. This method for the generation of second order upwind schemes based on variable extrapolation is often referred to in the literature as the MUSCL ("Monotone Upstream-centered Schemes for Conservation Laws") approach. The use of nonlinear limiters in such procedure, with the intention of restricting the amplitude of the gradients appearing in the solution, avoiding thus the formation of new extrema, allows that first order upwind schemes be transformed in TVD ("Total Variation Diminishing") high resolution schemes with the appropriate definition of such nonlinear limiters, assuring monotone preserving and total variation diminishing methods.

Traditionally, implicit numerical methods have been praised for their improved stability and condemned for their large arithmetic operation counts (Beam and Warming, 1978). On the one hand, the slow convergence rate of explicit

methods become they so unattractive to the solution of steady state problems due to the large number of iterations required to convergence, in spite of the reduced number of operation counts per time step in comparison with their implicit counterparts. Such problem is resulting from the limited stability region which such methods are subjected (the Courant condition). On the other hand, implicit schemes guarantee a larger stability region, which allows the use of CFL numbers above 1.0, and fast convergence to steady state conditions. Undoubtedly, the most significant efficiency achievement for multidimensional implicit methods was the introduction of the Alternating Direction Implicit (ADI) algorithms by Douglas (1955), Peaceman and Rachford (1955), and Douglas and Gunn (1964), and fractional step algorithms by Yanenko (1971). ADI approximate factorization methods consist in approximating the Left Hand Side (LHS) of the numerical scheme by the product of one-dimensional parcels, each one associated with a different spatial coordinate direction, which retract nearly the original implicit operator. These methods have been largely applied in the CFD community and, despite the fact of the error of the approximate factorization, it allows the use of large time steps, which results in significant gains in terms of convergence rate in relation to explicit methods.

In this work, the first part of this study, the Roe (1981) and the Van Leer (1982) schemes are implemented following a MUSCL approach, aiming to guarantee second order accuracy and to achieve TVD properties, and employing an implicit formulation to solve the Euler equations in the two-dimensional space. These schemes are implemented according to a finite volume formulation and using a structured spatial discretization. The former scheme is a flux difference splitting one, whereas the latter is a flux vector splitting scheme. The MUSCL approach employs five different types of nonlinear limiters, which assure TVD properties, namely: Van Leer limiter, Van Albada limiter, minmod limiter, Super Bee limiter and β-limiter. All variants of the MUSCL approach are second order accurate in space. The implicit schemes employ an ADI approximate factorization to solve implicitly the Euler equations. Explicit and implicit results are compared trying to emphasize the advantages and disadvantages of each formulation. The schemes are accelerated to the steady state solution using a spatially variable time step, which has demonstrated effective gains in terms of convergence rate according to Maciel (2005, 2008). The algorithms are applied to the solution of the physical problem of the moderate supersonic flow along a compression corner. The results have demonstrated that the most accurate solutions are obtained with the Roe (1981) TVD scheme using minmod and Super Bee nonlinear limiters, when implemented in its implicit version. The numerical results and the analyses of this study are the subjects of the part II of this work (RESULTS).

2. EULER EQUATIONS

The fluid movement is described by the Euler equations, which express the conservation of mass, of the linear momentum and of the energy to an inviscid mean, heat non-conductor and compressible, in the absence of external forces. These equations can be represented, in the integral and conservative forms, to a finite volume formulation, by:

$$\partial/\partial t \int_V Q dV + \int_S \left[E n_x + F n_y \right] dS = 0 , \tag{1}$$

where Q is written to a Cartesian system, V is the cell volume, n_x and n_y are components of the normal unit vector to the flux face, S is the flux area, and E and F are components of the convective flux vector. The Q, E and F vectors are represented by:

$$Q = \begin{Bmatrix} \rho \\ \rho u \\ \rho v \\ e \end{Bmatrix}, \quad E = \begin{Bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ (e+p)u \end{Bmatrix} \quad \text{and} \quad F = \begin{Bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ (e+p)v \end{Bmatrix}, \tag{2}$$

with ρ being the fluid density; u and v are Cartesian components of the velocity vector in the x and y directions, respectively; e is the total energy per unit volume of the fluid mean; and p is the static pressure of the fluid mean.

The Euler equations were nondimensionalized in relation to the freestream density, ρ_∞, and in relation to the freestream speed of sound, a_∞, to the studied problem in this work. The matrix system of the Euler equations is closed with the state equation of a perfect gas

$$p = (\gamma - 1)\left[e - 0.5\rho (u^2 + v^2) \right], \tag{3}$$

considering the ideal gas hypothesis. γ is the ratio of specific heats. The total enthalpy is determined by $H = (e + p)/\rho$.

3. NUMERICAL ALGORITHMS

3.1 Roe (1981) algorithm

The Roe (1981) algorithm, first order accurate in space, is specified by the determination of the numerical flux vector at *(i+½,j)* interface. The extension of this numerical flux to the *(i,j+½)* interface is straightforward, without any additional complications. The right and the left cell volumes, as well the interface volume, necessary to the coordinate change, following the finite volume formulation, which is equivalent to a generalized coordinate system, are defined as:

$$V_R = V_{i+1,j}\,,\; V_L = V_{i,j} \quad \text{and} \quad V_{int} = 0.5\left(V_R + V_L\right), \tag{4}$$

where "R" and "L" represent right and left states, respectively. The interface area components are defined by:

$$S_{x\_int} = s_x^{'} S \quad \text{and} \quad S_{y\_int} = s_y^{'} S\,, \tag{5}$$

where $s_x^{'}$ and $s_y^{'}$ are defined as: $s_x^{'} = s_x / S$ and $s_y^{'} = s_y / S$, being $S = \left(s_x^2 + s_y^2\right)^{0.5}$. Expressions for s_x and s_y, as well for the cell volume, are defined in Maciel (2006). The metric terms to this generalized coordinate system are defined as:

$$h_x = S_{x\_int} / V_{int}\,,\; h_y = S_{y\_int} / V_{int} \quad \text{and} \quad h_n = S / V_{int}\,. \tag{6}$$

The calculated properties at the flux interface are obtained by arithmetical average or by Roe average. The Roe average was used in this work:

$$\rho_{int} = \sqrt{\rho_L \rho_R}\,,\; u_{int} = \left(u_L + u_R\sqrt{\rho_R/\rho_L}\right)\Big/\left(1+\sqrt{\rho_R/\rho_L}\right),\; v_{int} = \left(v_L + v_R\sqrt{\rho_R/\rho_L}\right)\Big/\left(1+\sqrt{\rho_R/\rho_L}\right); \tag{7}$$

$$H_{int} = \left(H_L + H_R\sqrt{\rho_R/\rho_L}\right)\Big/\left(1+\sqrt{\rho_R/\rho_L}\right) \quad \text{and} \quad a_{int} = \sqrt{(\gamma-1)\left[H_{int} - 0.5\left(u_{int}^2 + v_{int}^2\right)\right]}\,. \tag{8}$$

The eigenvalues of the Euler equations, in the ξ direction, to the convective flux are given by:

$$U_{cont} = u_{int} h_x + v_{int} h_y\,,\; \lambda_1 = U_{cont} - a_{int} h_n\,,\; \lambda_2 = \lambda_3 = U_{cont} \quad \text{and} \quad \lambda_4 = U_{cont} + a_{int} h_n\,. \tag{9}$$

The jumps in the conserved variables, necessary to the construction of the Roe (1981) dissipation function, are given by:

$$\Delta e = V_{int}\left(e_R - e_L\right),\; \Delta\rho = V_{int}\left(\rho_R - \rho_L\right),\; \Delta(\rho u) = V_{int}\left[(\rho u)_R - (\rho u)_L\right] \text{ and } \Delta(\rho v) = V_{int}\left[(\rho v)_R - (\rho v)_L\right]. \tag{10}$$

The components of the α vector to the *(i+½,j)* interface are calculated by the following expressions:

$$\alpha_1 = 0.5\left(aa - bb\right),\;\; \alpha_2 = \Delta\rho - aa\,,\;\; \alpha_3 = cc \quad \text{and} \quad \alpha_4 = 0.5\left(aa + bb\right), \tag{11}$$

with:

$$aa = (\gamma-1)\Big/ a_{int}^2\left[\Delta e + 0.5\left(u_{int}^2 + v_{int}^2\right)\Delta\rho - u_{int}\Delta(\rho u) - v_{int}\Delta(\rho v)\right]; \tag{12}$$

$$bb = 1/a_{int}\left[h_x^{'}\Delta(\rho u) - \left(h_x^{'} u_{int} + h_y^{'} v_{int}\right)\Delta\rho + h_y^{'}\Delta(\rho v)\right]; \tag{13}$$

$$cc = h_x^{'}\Delta(\rho v) + \left(h_y^{'} u_{int} - h_x^{'} v_{int}\right)\Delta\rho - h_y^{'}\Delta(\rho u)\,; \tag{14}$$

$$h_x^{'} = h_x / h_n \quad \text{and} \quad h_y^{'} = h_y / h_n\,. \tag{15}$$

The Roe (1981) dissipation function is constructed using the following matrix:

$$R_{i+1/2,j} = \begin{bmatrix} 1 & 1 & 0 & 1 \\ u_{int} - h_x^{'} a_{int} & u_{int} & -h_y^{'} & u_{int} + h_x^{'} a_{int} \\ v_{int} - h_y^{'} a_{int} & v_{int} & h_x^{'} & v_{int} + h_y^{'} a_{int} \\ H_{int} - h_x^{'} u_{int} a_{int} - h_y^{'} v_{int} a_{int} & 0.5\left(u_{int}^2 + v_{int}^2\right) & h_x^{'} v_{int} - h_y^{'} u_{int} & H_{int} + h_x^{'} u_{int} a_{int} + h_y^{'} v_{int} a_{int} \end{bmatrix}. \tag{16}$$

The entropy condition is implemented of the following way:

$$\psi_l = \begin{cases} |\lambda_l|, & if\ |\lambda_l| \geq \varepsilon_{\xi_l} \\ 0.5\left(\lambda_l^2 + \varepsilon_{\xi_l}^2\right)/\varepsilon_{\xi_l}, & if\ |\lambda_l| < \varepsilon_{\xi_l} \end{cases}, \text{ non-linear fields, and } \psi_l = |\lambda_l|, \text{ linear fields,} \tag{17}$$

with "*l*" assuming values of 1 and 4 to non-linear fields and 2 and 3 to linear fields; and ε_{ξ_l} assuming a value of 0.2, as recommended by Roe (1981). The Roe (1981) dissipation function is finally constructed by the following matrix-vector product:

$$\{D_{Roe}\}_{i+1/2,j} = [R]_{i+1/2,j}\{-\psi\alpha\}_{i+1/2,j}. \tag{18}$$

The convective numerical flux vector to the *(i+½,j)* interface is described by:

$$F_{i+1/2,j}^{(l)} = \left(E_{\boldsymbol{int}}^{(l)} h_x + F_{\boldsymbol{int}}^{(l)} h_y\right) V_{\boldsymbol{int}} + 0.5 D_{Roe}^{(l)},\ E_{\boldsymbol{int}}^{(l)} = 0.5\left(E_R^{(l)} + E_L^{(l)}\right) \quad \text{and} \quad F_{\boldsymbol{int}}^{(l)} = 0.5\left(F_R^{(l)} + F_L^{(l)}\right). \tag{19}$$

The explicit time integration follows the time splitting method, first order accurate, which divides the integration in two steps, each one associated with a specific spatial direction. In the initial step, it is possible to write for the ξ direction:

$$\Delta Q_{i,j}^{*} = -\Delta t_{i,j}/V_{i,j}\left(F_{i+1/2,j}^{n} - F_{i-1/2,j}^{n}\right);\ Q_{i,j}^{*} = Q_{i,j}^{n} + \Delta Q_{i,j}^{*}; \tag{20}$$

and at the end step, η direction:

$$\Delta Q_{i,j}^{n+1} = -\Delta t_{i,j}/V_{i,j}\left(F_{i,j+1/2}^{*} - F_{i,j-1/2}^{*}\right);\ Q_{i,j}^{n+1} = Q_{i,j}^{*} + \Delta Q_{i,j}^{n+1}. \tag{21}$$

3.2 Van Leer (1982) algorithm

The approximation to the integral equation (1) to a rectangular finite volume yields an ordinary differential equation system with respect to time:

$$V_{i,j}\, dQ_{i,j}/dt = -R_{i,j}, \tag{22}$$

with $R_{i,j}$ representing the neat flux (residual) of the conservation of mass, of linear momentum and of energy in the $V_{i,j}$ volume. The residual is calculated as:

$$R_{i,j} = R_{i+1/2,j} - R_{i-1/2,j} + R_{i,j+1/2} - R_{i,j-1/2}, \tag{23}$$

where $R_{i+1/2,j} = R_{i+1/2,j}^{c}$, in which "c" is related to the flow convective contribution. The discrete convective flux calculated by the AUSM scheme ("Advection Upstream Splitting Method") can be interpreted as a sum involving the arithmetical average between the right (*R*) and the left (*L*) states of the *(i+½,j)* cell face, related to cells *(i,j)* and *(i+1,j)*, respectively, multiplied by the interface Mach number, and a scalar dissipative term, as shown in Liou and Steffen Jr. (1993). Hence,

$$R_{i+1/2,j} = |S|_{i+1/2,j}\left\{\frac{1}{2}M_{i+1/2,j}\left[\begin{pmatrix}\rho a\\ \rho a u\\ \rho a v\\ \rho a H\end{pmatrix}_L + \begin{pmatrix}\rho a\\ \rho a u\\ \rho a v\\ \rho a H\end{pmatrix}_R\right] - \frac{1}{2}\phi_{i+1/2,j}\left[\begin{pmatrix}\rho a\\ \rho a u\\ \rho a v\\ \rho a H\end{pmatrix}_R - \begin{pmatrix}\rho a\\ \rho a u\\ \rho a v\\ \rho a H\end{pmatrix}_L\right]\right\} + \begin{pmatrix}0\\ S_x p\\ S_y p\\ 0\end{pmatrix}_{i+1/2,j}, \tag{24}$$

where $S_{i+1/2,j} = \begin{bmatrix} S_x & S_y \end{bmatrix}_{i+1/2,j}^{T}$ defines the normal area vector to the *(i+½,j)* surface. The "*a*" quantity represents the speed of sound. $M_{i+½,j}$ defines the advective Mach number in the *(i+½,j)* face of the cell *(i,j)*, which is calculated according to Liou and Steffen Jr. (1993) as:

$$M_{i+1/2,j} = M_L^+ + M_R^-, \tag{25}$$

where the $M^{+/-}$ separated Mach numbers are defined by Van Leer (1982) as:

$$M^+ = \begin{cases} M, & if\ M \geq 1; \\ 0.25(M+1)^2, & if\ |M| < 1; \\ 0, & if\ M \leq -1; \end{cases} \quad \text{and} \quad M^- = \begin{cases} 0, & if\ M \geq 1; \\ -0.25(M-1)^2, & if\ |M| < 1; \\ M, & if\ M \leq -1. \end{cases} \tag{26}$$

M_L and M_R represent the Mach numbers associated to the left and right states, respectively. The advection Mach number is defined as:

$$M = \left(S_x u + S_y v\right) / \left(a|S|\right). \tag{27}$$

The pressure at the *(i+½,j)* face of the *(i,j)* cell is calculated from a similar way:

$$p_{i+1/2,j} = p_L^+ + p_R^-, \tag{28}$$

with $p^{+/-}$ representing the pressure separation defined according to Van Leer (1982):

$$p^+ = \begin{cases} p, & if\ M \geq 1; \\ 0.25p(M+1)^2(2-M), & if\ |M| < 1; \\ 0, & if\ M \leq -1; \end{cases} \quad \text{and} \quad p^- = \begin{cases} 0, & if\ M \geq 1; \\ 0.25p(M-1)^2(2+M), & if\ |M| < 1; \\ p, & if\ M \leq -1. \end{cases} \tag{29}$$

The definition of the ϕ dissipation term determines the particular formulation to the convective fluxes. The following choice corresponds to the Van Leer (1982) scheme, according to Radespiel e Kroll (1995):

$$\phi_{i+1/2,j} = \phi_{i+1/2,j}^{VL}, \tag{30}$$

where:

$$\phi_{i+1/2,j}^{VL} = \begin{cases} |M_{i+1/2,j}|, & if\ |M_{i+1/2,j}| \geq 1; \\ |M_{i+1/2,j}| + 0.5(M_R - 1)^2, & if\ 0 \leq M_{i+1/2,j} < 1; \\ |M_{i+1/2,j}| + 0.5(M_L + 1)^2, & if\ -1 < M_{i+1/2,j} \leq 0. \end{cases} \tag{31}$$

The explicit time integration follows the method presented in the Roe (1981) scheme [Eqs. (20) and (21)]. This version of the Van Leer (1982) algorithm is first order accurate in space.

4. MUSCL PROCEDURE

Second order spatial accuracy can be achieved by introducing more upwind points or cells in the schemes. It has been noted that the projection stage, whereby the solution is projected in each cell face (i-1/2,j; i+1/2,j) on piecewise constant states, is the cause of the first order space accuracy of the Godunov schemes (Hirsch, 1990). Hence, it is sufficient to modify the first projection stage without modifying the Riemann solver, in order to generate higher spatial approximations. The state variables at the interfaces are thereby obtained from an extrapolation between neighboring cell averages. This method for the generation of second order upwind schemes based on variable extrapolation is often referred to in the literature as the MUSCL ("Monotone Upstream-centered Schemes for Conservation Laws") approach. The use of nonlinear limiters in such procedure, with the intention of restricting the amplitude of the gradients appearing in the solution, avoiding thus the formation of new extrema, allows that first order upwind schemes be transformed in TVD high resolution schemes with the appropriate definition of such nonlinear limiters, assuring monotone preserving and total variation diminishing methods. Details of the present implementation of the MUSCL procedure, as well the incorporation of TVD properties to the schemes, are found in Hirsch (1990). The expressions to calculate de fluxes following a MUSCL procedure and the nonlinear flux limiter definitions employed in this work, which incorporates TVD properties, are defined as follows.

The conserved variables at the interface *(i+½,j)* can be considered as resulting from a combination of backward and forward extrapolations. To a linear one-sided extrapolation at the interface between the averaged values at the two upstream cells (i,j) and (i-1,j), one has:

$$Q^{L}_{i+1/2,j} = Q_{i,j} + \frac{\varepsilon}{2}\left(Q_{i,j} - Q_{i-1,j}\right), \text{ cell (i,j);} \tag{32}$$

$$Q^{R}_{i+1/2,j} = Q_{i+1,j} - \frac{\varepsilon}{2}\left(Q_{i+2,j} - Q_{i+1,j}\right), \text{ cell (i+1,j),} \tag{33}$$

leading to a second order fully one-sided scheme. If the first order scheme is defined by the numerical flux

$$F_{i+1/2,j} = F\left(Q_{i,j}, Q_{i+1,j}\right) \tag{34}$$

the second order space accurate numerical flux is obtained from

$$F^{(2)}_{i+1/2,j} = F\left(Q^{L}_{i+1/2,j}, Q^{R}_{i+1/2,j}\right). \tag{35}$$

Higher order flux vector splitting or flux difference splitting methods, such as those studied in this work, are obtained from:

$$F^{(2)}_{i+1/2,j} = F^{+}\left(Q^{L}_{i+1/2,j}\right) + F^{-}\left(Q^{R}_{i+1/2,j}\right). \tag{36}$$

All second order upwind schemes necessarily involve at least five mesh points or cells. To reach high order solutions without oscillations around discontinuities, nonlinear limiters are employed, replacing the term ε in Eqs. (32) and (33) by these limiters at the left and at the right states of the flux interface. To define such limiters, it is necessary to calculate the ratio of consecutive variations of the conserved variables. These ratios are defined as follows:

$$r^{+}_{i-1/2,j} = \left(Q_{i+1,j} - Q_{i,j}\right)/\left(Q_{i,j} - Q_{i-1,j}\right) \quad \text{and} \quad r^{+}_{i+1/2,j} = \left(Q_{i+2,j} - Q_{i+1j}\right)/\left(Q_{i+1,j} - Q_{i,j}\right), \tag{37}$$

where the nonlinear limiters at the left and at the right states of the flux interface are defined by $\Psi^{L} = \Psi\left(r^{+}_{i-1/2,j}\right)$ and $\Psi^{R} = \Psi\left(1/r^{+}_{i+1/2,j}\right)$. In this work, five options of nonlinear limiters were considered to the numerical experiments. These limiters are defined as follows:

$$\Psi^{VL}_{l}(r_l) = \frac{r_l + |r_l|}{1 + r_l}, \text{ Van Leer (1974) limiter;} \tag{38}$$

$$\Psi^{VA}_{l}(r_l) = \frac{r_l + r_l^2}{1 + r_l^2}, \text{ Van Albada limiter;} \tag{39}$$

$$\Psi^{MIN}_{l}(r_l) = signal_l\, MAX\left(0, MIN\left(|r_l|, signal_l\right)\right), \text{ minmod limiter;} \tag{40}$$

$$\Psi^{SB}_{l}(r_l) = MAX\left(0, MIN\left(2r_l, 1\right), MIN\left(r_l, 2\right)\right), \text{ “Super Bee” limiter, due to Roe (1983);} \tag{41}$$

$$\Psi^{\beta-L}_{l}(r_l) = MAX\left(0, MIN\left(\beta r_l, 1\right), MIN\left(r_l, \beta\right)\right), \text{ β-limiter,} \tag{42}$$

with “*l*” varying from 1 to 4 (two-dimensional space), $signal_l$ being equal to 1.0 if $r_l \geq 0.0$ and -1.0 otherwise, r_l is the ratio of consecutive variations of the *l*th conserved variable and β is a parameter assuming values between 1.0 and 2.0, being 1.5 the value assumed in this work. With the implementation of the numerical flux vectors following this MUSCL procedure, second order spatial accuracy and TVD properties are incorporated in the algorithms.

5. IMPLICIT FORMULATIONS

All implicit schemes studied in this work used an ADI formulation to solve the algebraic nonlinear system of equations. Initially, the nonlinear system of equations is linearized considering the implicit operator evaluated at the time “*n*” and, posteriorly, the pentadiagonal system of linear algebraic equations is factored in two tridiagonal systems of linear algebraic equations, each one associated with a particular spatial direction. Thomas algorithm is employed to solve these two tridiagonal systems. The implicit schemes studied in this work were only applicable to the solution of

the Euler equations, which implies that only the convective contributions were considered in the RHS ("Right Hand Side") operator.

5.1 Roe (1981) TVD implicit scheme

The ADI form of the Roe (1981) TVD scheme is defined by the following two step algorithm:

$$\left\{I + \Delta t_{i,j}\Delta_\xi^- K_{i+1/2,j}^+ + \Delta t_{i,j}\Delta_\xi^+ K_{i+1/2,j}^-\right\}\Delta Q_{i,j}^* = \left[RHS_{(Roe)}\right]_{i,j}^n, \text{ to the } \xi \text{ direction;} \tag{43}$$

$$\left\{I + \Delta t_{i,j}\Delta_\eta^- J_{i,j+1/2}^+ + \Delta t_{i,j}\Delta_\eta^+ J_{i,j+1/2}^-\right\}\Delta Q_{i,j}^{n+1} = \Delta Q_{i,j}^*, \text{ to the } \eta \text{ direction;} \tag{44}$$

$$Q_{i,j}^{n+1} = Q_{i,j}^n + \Delta Q_{i,j}^{n+1}, \tag{45}$$

where:

$$K_{i\pm1/2,j}^\pm = \left[R\right]_{i\pm1/2,j}^n \Omega_{i\pm1/2,j}^\pm \left[R^{-1}\right]_{i\pm1/2,j}^n;\ J_{i,j\pm1/2}^\pm = \left[R\right]_{i,j\pm1/2}^n \Phi_{i,j\pm1/2}^\pm \left[R^{-1}\right]_{i,j\pm1/2}^n; \tag{46}$$

$$\Omega_{i\pm1/2,j}^\pm = diag\left[\left(\lambda_\xi^l\right)^\pm\right]_{i\pm1/2,j}^n;\ \Phi_{i,j\pm1/2}^\pm = diag\left[\left(\lambda_\eta^l\right)^\pm\right]_{i,j\pm1/2}^n; \tag{47}$$

$$\left(\lambda_\xi^l\right)^\pm = 0.5\left(\lambda_\xi^l \pm \left|\lambda_\xi^l\right|\right),\ \left(\lambda_\eta^l\right)^\pm = 0.5\left(\lambda_\eta^l \pm \left|\lambda_\eta^l\right|\right),\ \Delta_\xi^- = (\cdot)_{i,j} - (\cdot)_{i-1,j},\ \Delta_\xi^+ = (\cdot)_{i+1,j} - (\cdot)_{i,j}; \tag{48}$$

$$\Delta_\eta^- = (\cdot)_{i,j} - (\cdot)_{i,j-1},\ \Delta_\eta^+ = (\cdot)_{i,j+1} - (\cdot)_{i,j}. \tag{49}$$

In Equation (47), *diag*[·] is a diagonal matrix; in Eqs. (47) and (48), "*l*" assumes values from 1 to 4 and λ's are the eigenvalues of the Euler equations, described by Eq. (9). The matrix R^{-1} is defined as:

$$R^{-1} = \begin{bmatrix} \frac{1}{2}\left[\frac{\gamma-1}{a_{int}^2}\frac{\left(u_{int}^2+v_{int}^2\right)}{2} + \frac{1}{a_{int}}\left(u_{int}h_x' + v_{int}h_y'\right)\right] & \frac{1}{2}\left(-\frac{\gamma-1}{a_{int}^2}u_{int} - \frac{h_x'}{a_{int}}\right) & \frac{1}{2}\left(-\frac{\gamma-1}{a_{int}^2}v_{int} - \frac{h_y'}{a_{int}}\right) & \frac{\gamma-1}{2a_{int}^2} \\ 1 - \frac{\gamma-1}{a_{int}^2}\frac{\left(u_{int}^2+v_{int}^2\right)}{2} & \frac{\gamma-1}{a_{int}^2}u_{int} & \frac{\gamma-1}{a_{int}^2}v_{int} & -\frac{\gamma-1}{a_{int}^2} \\ -\left(h_x'v_{int} - h_y'u_{int}\right) & -h_y' & h_x' & 0 \\ \frac{1}{2}\left[\frac{\gamma-1}{a_{int}^2}\frac{\left(u_{int}^2+v_{int}^2\right)}{2} - \frac{1}{a_{int}}\left(u_{int}h_x' + v_{int}h_y'\right)\right] & \frac{1}{2}\left(-\frac{\gamma-1}{a_{int}^2}u_{int} + \frac{h_x'}{a_{int}}\right) & \frac{1}{2}\left(-\frac{\gamma-1}{a_{int}^2}v_{int} + \frac{h_y'}{a_{int}}\right) & \frac{\gamma-1}{2a_{int}^2} \end{bmatrix}, \tag{50}$$

The interface properties are defined either by arithmetical average or by Roe (1981) average. In this work, the Roe (1981) average was used. The $RHS_{(Roe)}$ operator required in Eq. (43) is defined as:

$$\left[RHS_{(Roe)}\right]_{i,j}^n = -\Delta t_{i,j}/V_{i,j}\left(F_{i+1/2,j}^{(Roe)} - F_{i-1/2,j}^{(Roe)} + F_{i,j+1/2}^{(Roe)} - F_{i,j-1/2}^{(Roe)}\right)^n, \tag{51}$$

with $F_{i+1/2,j}^{(Roe)}$ calculated according to Eq. (19). This implementation is first order accurate in time due to the definition of Ω and of Φ, as reported in Yee, Warming and Harten (1985), but is second order accurate in space due to the RHS solution at the steady state, when a MUSCL procedure is employed.

5.2 Van Leer (1982) TVD implicit scheme

The ADI form of the Van Leer (1982) TVD scheme is defined by the following two step algorithm:

$$\left\{I + \Delta t_{i,j}\Delta_\xi^- A_{i+1/2,j}^+ + \Delta t_{i,j}\Delta_\xi^+ A_{i+1/2,j}^-\right\}\Delta Q_{i,j}^* = \left[RHS_{(VL)}\right]_{i,j}^n, \text{ to the } \xi \text{ direction;} \tag{52}$$

$$\left\{I + \Delta t_{i,j}\Delta_\eta^- B_{i,j+1/2}^+ + \Delta t_{i,j}\Delta_\eta^+ B_{i,j+1/2}^-\right\}\Delta Q_{i,j}^{n+1} = \Delta Q_{i,j}^*, \text{ to the } \eta \text{ direction;} \tag{53}$$

$$Q_{i,j}^{n+1} = Q_{i,j}^n + \Delta Q_{i,j}^{n+1}, \tag{54}$$

where the matrices $A^\pm$ and $B^\pm$ are defined as:

$$A^{\pm}_{i\pm1/2,j} = \left[T\right]^{n}_{i\pm1/2,j}\Omega^{\pm}_{i\pm1/2,j}\left[T^{-1}\right]^{n}_{i\pm1/2,j};\ B^{\pm}_{i,j\pm1/2} = \left[T\right]^{n}_{i,j\pm1/2}\Phi^{\pm}_{i,j\pm1/2}\left[T^{-1}\right]^{n}_{i,j\pm1/2}; \tag{55}$$

$$\Omega^{\pm}_{i\pm1/2,j} = diag\left[\left(\lambda^{l}_{\xi}\right)^{\pm}\right]^{n}_{i\pm1/2,j};\ \Phi^{\pm}_{i,j\pm1/2} = diag\left[\left(\lambda^{l}_{\eta}\right)^{\pm}\right]^{n}_{i,j\pm1/2}; \tag{56}$$

with the similarity transformation matrices defined by:

$$T = \begin{bmatrix} 1 & 0 & \alpha & \alpha \\ u_{int} & h'_y\rho_{int} & \alpha\left(u_{int}+h'_x a_{int}\right) & \alpha\left(u_{int}-h'_x a_{int}\right) \\ v_{int} & -h'_x\rho_{int} & \alpha\left(v_{int}+h'_y a_{int}\right) & \alpha\left(v_{int}-h'_y a_{int}\right) \\ \dfrac{\phi^2}{\gamma-1} & \rho_{int}\left(h'_y u_{int}-h'_x v_{int}\right) & \alpha\left(\dfrac{\phi^2+a^2_{int}}{\gamma-1}+a_{int}\tilde{\theta}\right) & \alpha\left(\dfrac{\phi^2+a^2_{int}}{\gamma-1}-a_{int}\tilde{\theta}\right) \end{bmatrix}; \tag{57}$$

$$\alpha = \rho_{int}/\left(\sqrt{2}a_{int}\right),\ \beta = 1/\left(\sqrt{2}\rho_{int}a_{int}\right),\ \phi^2 = (\gamma-1)\frac{u^2_{int}+v^2_{int}}{2},\ \tilde{\theta} = h'_x u_{int}+h'_y v_{int}; \tag{58}$$

$$T^{-1} = \begin{bmatrix} 1-\dfrac{\phi^2}{a^2_{int}} & (\gamma-1)\dfrac{u_{int}}{a^2_{int}} & (\gamma-1)\dfrac{v_{int}}{a^2_{int}} & -\dfrac{\gamma-1}{a^2_{int}} \\ -\dfrac{h'_y u_{int}-h'_x v_{int}}{\rho_{int}} & \dfrac{h'_y}{\rho_{int}} & -\dfrac{h'_x}{\rho_{int}} & 0 \\ \beta\left(\phi^2-a_{int}\tilde{\theta}\right) & \beta\left[h'_x a_{int}-(\gamma-1)u_{int}\right] & \beta\left[h'_y a_{int}-(\gamma-1)v_{int}\right] & \beta(\gamma-1) \\ \beta\left(\phi^2+a_{int}\tilde{\theta}\right) & -\beta\left[h'_x a_{int}+(\gamma-1)u_{int}\right] & -\beta\left[h'_y a_{int}+(\gamma-1)v_{int}\right] & \beta(\gamma-1) \end{bmatrix}. \tag{59}$$

The properties defined at interface are calculated by arithmetical average. The $RHS_{(VL)}$ operator required in Eq. (52) is defined as:

$$\left[RHS_{(VL)}\right]^{n}_{i,j} = -\Delta t_{i,j}/V_{i,j}\left(R^{(VL)}_{i+1/2,j}-R^{(VL)}_{i-1/2,j}+R^{(VL)}_{i,j+1/2}-R^{(VL)}_{i,j-1/2}\right)^{n}, \tag{60}$$

with the numerical flux vector $R^{(VL)}_{i+1/2,j}$ calculated according to Eq. (24).

6. SPATIALLY VARIABLE TIME STEP

The basic idea of this procedure consists in keeping constant the CFL number in all calculation domain, allowing, hence, the use of appropriated time steps to each specific mesh region during the convergence process. Hence, according to the definition of the CFL number, it is possible to write:

$$\Delta t_{i,j} = CFL\left(\Delta s\right)_{i,j}/c_{i,j}, \tag{61}$$

where CFL is the "Courant-Friedrichs-Lewy" number to provide numerical stability to the scheme; $c_{i,j} = \left[\left(u^2+v^2\right)^{0.5}+a\right]_{i,j}$ is the maximum characteristic speed of information propagation in the calculation domain; and $\left(\Delta s\right)_{i,j}$ is a characteristic length of information transport. On a finite volume context, $\left(\Delta s\right)_{i,j}$ is chosen as the minor value found between the minor centroid distance, involving the (i,j) cell and a neighbor, and the minor cell side length.

7. INITIAL AND BOUNDARY CONDITIONS

7.1 Initial conditions

Values of freestream flow are adopted for all properties as initial condition, in the whole calculation domain, to the studied problem in this work (Jameson and Mavriplis, 1986, and Maciel, 2002):

$$Q_{\infty} = \left\{1 \quad M_{\infty}\cos\theta \quad M_{\infty}\sin\theta \quad \left[1/\left[\gamma(\gamma-1)\right]+0.5M^2_{\infty}\right]\right\}^{T}, \tag{62}$$

where M_∞ represents the freestream Mach number and θ is the flow attack angle.

7.2 Boundary conditions

The boundary conditions are basically of three types: solid wall, entrance and exit. These conditions are implemented in special cells named ghost cells.

(a) Wall condition: This condition imposes the flow tangency at the solid wall. This condition is satisfied considering the wall tangent velocity component of the ghost volume as equals to the respective velocity component of its real neighbor cell. At the same way, the wall normal velocity component of the ghost cell is equaled in value, but with opposite signal, to the respective velocity component of the real neighbor cell.

The pressure gradient normal to the wall is assumed be equal to zero, following an inviscid formulation. The same hypothesis is applied to the temperature gradient normal to the wall, considering adiabatic wall. The ghost volume density and pressure are extrapolated from the respective values of the real neighbor volume (zero order extrapolation), with these two conditions. The total energy is obtained by the state equation of a perfect gas.

(b) Entrance condition:

(b.1) Subsonic flow: Three properties are specified and one is extrapolated, based on analysis of information propagation along characteristic directions in the calculation domain (Maciel, 2002). In other words, three characteristic directions of information propagation point inward the computational domain and should be specified. Only the characteristic direction associated to the "(q_{normal}-a)" velocity can not be specified and should be determined by interior information of the calculation domain. Pressure was the extrapolated variable to the present problem. Density and velocity components had their values determined by the freestream flow properties. The total energy per unity fluid volume is determined by the state equation of a perfect gas.

(b.2) Supersonic flow: All variables are fixed with their freestream flow values.

(c) Exit condition:

(c.1) Subsonic flow: Three characteristic directions of information propagation point outward the computational domain and should be extrapolated from interior information (Maciel, 2002). The characteristic direction associated to the "(q_{normal}-a)" velocity should be specified because it penetrates the calculation domain. In this case, the ghost volume's pressure is specified by its freestream value. Density and velocity components are extrapolated and the total energy is obtained by the state equation of a perfect gas.

(c.2) Supersonic flow: All variables are extrapolated from the interior domain due to the fact that all four characteristic directions of information propagation of the Euler equations point outward the calculation domain and, with it, nothing can be fixed.

8. CONCLUSIONS

In the present work, first part of this study, the theories involving the extension of the first order versions of the numerical schemes of Roe (1981) and of Van Leer (1982) to second order spatial accuracy, incorporating hence TVD properties through a MUSCL approach, and the implicit numerical implementation of these second order schemes are detailed. The schemes are implemented on a finite volume context, using a structured spatial discretization. First order time integrations like ADI approximate factorization are programmed. The Euler equations in conservation and integral forms, in two-dimensions, are solved. The steady state physical problem of the moderate supersonic flow along a compression corner is studied and compared with theoretical results. A spatially variable time step procedure is also implemented aiming to accelerate the convergence to the steady solution. The gains in convergence with this procedure were demonstrated in Maciel (2005, 2008). The results have demonstrated that the most accurate solutions are obtained with the Roe (1981) TVD scheme using minmod and Super Bee nonlinear limiters, when implemented in its implicit version. The numerical results and the analyses of this study are the subjects of the part II of this work (RESULTS).

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