EXPLICIT AND IMPLICIT TVD AND ENO HIGH RESOLUTION ALGORITHMS APPLIED TO THE EULER AND NAVIER-STOKES EQUATIONS IN THREE-DIMENSIONS – THEORY

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Abstract. *In the present work, the Harten and Osher TVD/ENO and the Yee TVD symmetric schemes are implemented, on a finite volume context and using a structured spatial discretization, to solve the Euler and the laminar Navier-Stokes equations in the three-dimensional space. The Harten and Osher TVD/ENO schemes are flux difference splitting type, whereas the Yee TVD scheme is a symmetric one, which incorporates TVD properties due to the appropriated definition of a limited dissipation function. All three schemes are second order accurate in space. An implicit formulation is employed to all schemes in the solution of the Euler equations. The flux difference splitting schemes employ approximate factorizations in Linearized Nonconservative Implicit LNI form, whereas the symmetric scheme employs approximate factorization in ADI form. A spatially variable time step procedure is also implemented aiming to accelerate the convergence of the algorithms to the steady solution. The gains in convergence with this procedure were demonstrated in Maciel. The schemes are applied to the solution of the physical problems of the transonic flow along a convergent-divergent nozzle and of the supersonic flow along a compression corner in the inviscid case, whereas the laminar case studies a particular ramp problem. The results have demonstrated that the most accurate results are obtained with the Harten and Osher ENO and Yee TVD VL and Min1 schemes. This paper is the first part of this work, THEORY, considering the descriptions of the TVD/ENO schemes of Harten and Osher and of the TVD symmetic scheme of Yee, as also the employed implicit formulations.*

Keywords*: Harten and Osher TVD/ENO algorithms, Yee TVD symmetric algorithm, Euler and Navier-Stokes equations, Laminar case, Explicit and implicit algorithms.*

1. INTRODUCTION

Yee (1989) gives a very extensive survey of the state of the art of second order high resolution schemes for the Euler/Navier-Stokes equations of gas dynamics in general coordinates for both ideal and equilibrium real gases. Also, excellent reviews on modern upwind conservative shock capturing schemes and upwind shock fitting schemes based on wave propagation property have been given by Roe (1986) and Moretti (1987), respectively.

Recently, a new class of uniformly high order accurate, essentially non-oscillatory (ENO) schemes has been developed by Harten *et al.* (1986) and Harten and Osher (1987). They presented a hierarchy of uniformly high order accurate schemes that generalize Godunov (1958) scheme, and its second order accurate extension of monotonic upstream schemes for conservation laws (MUSCL) (Van Leer, 1979, and Colella and Woodward, 1984) and total variation diminishing (TVD) schemes (Harten, 1983, and Osher and Chakravarthy, 1984) to arbitrary order of accuracy.

In contrast to the earlier second order TVD schemes, which drop to first order accuracy at local extreme and maintain second order accuracy in smooth regions, the new ENO schemes are uniformly high order accurate throughout even at critical points. Theoretical results for the scalar conservation law and for the Euler equations of gas dynamics have been reported with highly accurate results. Preliminary results for two-dimensional problems were reported in Harten (1986).

Roe (1984) has proposed a very enlightening generalized formulation of TVD Lax and Wendroff (1964) schemes. Roe's result, in turn, is a generalization of Davis (1984) work. Yee (1987) incorporated the results of Roe (1984) and of Davis (1984) with minor modification to a one parameter family of explicit and implicit TVD schemes (Harten, 1984, and Yee, Warming and Harten, 1983) so that a wider group of limiters could be represented in a general but rather simple form which is at the same time suitable for steady-state applications. The final scheme could be interpreted as a three-point, spatially central difference explicit or implicit scheme which has a whole variety of more rational numerical dissipation terms than the classical way of handling shock-capturing algorithms.

In the present work, the Harten and Osher (1987) TVD/ENO and the Yee (1987) TVD symmetric schemes are implemented, on a finite volume context and using a structured spatial discretization, to solve the Euler and the laminar Navier-Stokes equations in the three-dimensional space. The Harten and Osher (1987) TVD/ENO schemes are flux difference splitting type, whereas the Yee (1987) TVD scheme is a symmetric one, which incorporates TVD properties due to the appropriated definition of a limited dissipation function. All schemes are second order accurate in space and their numerical implementation is based on the concept of Harten's modified flux function. All three schemes are implemented following an implicit formulation to solve the Euler equations. The flux difference splitting schemes employ approximate factorizations in Linearized Nonconservative Implicit LNI form, whereas the symmetric scheme employs approximate factorization in ADI form. The viscous simulations are treated with the explicit versions of the present algorithms, which employ a time splitting method. 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 (Maciel, 2005 and 2008). The algorithms are applied to the solution of the physical problems of the transonic flow along a convergent-divergent nozzle and of the supersonic flow along a compression corner in the inviscid case, whereas the laminar case studies a particular ramp problem. The results have demonstrated that the most accurate results are obtained with the Harten and Osher (1987) ENO and Yee (1987) TVD VL and Min1 schemes.

The main contribution of the present work to the CFD (Computational Fluid Dynamics) community is the extension of the Harten and Osher (1987) TVD/ENO schemes, as also the Yee (1987) TVD symmetric scheme, to three-dimensions, following a finite volume context, and their implicit implementation to inviscid problems, which characterizes a original contribution in the field of high resolution structured numerical algorithms.

2. NAVIER-STOKES EQUATIONS

As the Euler equations can be obtained from the Navier-Stokes ones by discarding the viscous vectors, only the formulation to the later will be presented. The Navier-Stokes equations in integral conservative form, employing a finite volume formulation and using a structured spatial discretization, to three-dimensions, can be written as:

$$\partial Q/\partial t + 1/V \int_V \vec{\nabla}\cdot\vec{P}\,dV = 0\,, \tag{1}$$

where V is the cell volume, which corresponds to an hexahedron in the three-dimensional space; Q is the vector of conserved variables; and $\vec{P} = (E_e - E_v)\vec{i} + (F_e - F_v)\vec{j} + (G_e - G_v)\vec{k}$ represents the complete flux vector in Cartesian coordinates, with the subscript "e" related to the Euler contributions and "v" is related to the viscous contributions. These components of the complete flux vector, as well the vector of conserved variables, are described below:

$$Q = \begin{Bmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ e \end{Bmatrix},\quad E_e = \begin{Bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ \rho uw \\ (e+p)u \end{Bmatrix},\quad F_e = \begin{Bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ \rho vw \\ (e+p)v \end{Bmatrix},\quad G_e = \begin{Bmatrix} \rho w \\ \rho uw \\ \rho vw \\ \rho w^2 + p \\ (e+p)w \end{Bmatrix}; \tag{2}$$

$$E_v = \frac{1}{\mathrm{Re}}\begin{Bmatrix} 0 \\ \tau_{xx} \\ \tau_{xy} \\ \tau_{xz} \\ \tau_{xx}u + \tau_{xy}v + \tau_{xz}w - q_x \end{Bmatrix},\quad F_v = \frac{1}{\mathrm{Re}}\begin{Bmatrix} 0 \\ \tau_{yx} \\ \tau_{yy} \\ \tau_{yz} \\ \tau_{yx}u + \tau_{yy}v + \tau_{yz}w - q_y \end{Bmatrix}\ \text{and}\ G_v = \frac{1}{\mathrm{Re}}\begin{Bmatrix} 0 \\ \tau_{zx} \\ \tau_{zy} \\ \tau_{zz} \\ \tau_{zx}u + \tau_{zy}v + \tau_{zz}w - q_z \end{Bmatrix}. \tag{3}$$

In these equations, the components of the viscous stress tensor are defined as:

$$\tau_{xx} = 2\mu_M\,\partial u/\partial x - 2/3\mu_M(\partial u/\partial x + \partial v/\partial y + \partial w/\partial z),\ \tau_{xy} = \mu_M(\partial u/\partial y + \partial v/\partial x),\ \tau_{xz} = \mu_M(\partial u/\partial z + \partial w/\partial x); \tag{4}$$

$$\tau_{yy} = 2\mu_M\,\partial v/\partial y - 2/3\mu_M(\partial u/\partial x + \partial v/\partial y + \partial w/\partial z),\ \tau_{yz} = \mu_M(\partial v/\partial z + \partial w/\partial y); \tag{5}$$

$$\tau_{zz} = 2\mu_M\,\partial w/\partial z - 2/3\mu_M(\partial u/\partial x + \partial v/\partial y + \partial w/\partial z). \tag{6}$$

The components of the conductive heat flux vector are defined as follows:

$$q_x = -\gamma(\mu_M/\mathrm{Pr}d)\partial e_i/\partial x\,,\ q_y = -\gamma(\mu_M/\mathrm{Pr}d)\partial e_i/\partial y\ \text{ and }\ q_z = -\gamma(\mu_M/\mathrm{Pr}d)\partial e_i/\partial z\,. \tag{7}$$

The quantities that appear above are described as follows: ρ is the fluid density, u, v and w are the Cartesian components of the flow velocity vector in the x, y and z directions, respectively; e is the total energy per unit volume of the fluid; p is the fluid static pressure; e_i is the fluid internal energy, defined as:

$$e_i = e/\rho - 0.5(u^2 + v^2 + w^2); \tag{8}$$

the τ's represent the components of the viscous stress tensor; Prd is the laminar Prandtl number, which assumed a value of 0.72 in the present simulations; the q's represent the components of the conductive heat flux; μ_M is the fluid molecular viscosity; γ is the ratio of specific heats at constant pressure and volume, respectively, which assumed a value 1.4 to the atmospheric air; and Re is the Reynolds number of the viscous simulation, defined by:

$$\mathrm{Re} = \rho u_{REF} l / \mu_M \ , \tag{9}$$

where u_{REF} is a characteristic flow velocity and l is a configuration characteristic length. The molecular viscosity is estimated by the empiric Sutherland formula:

$$\mu_M = bT^{1/2} / \left(1 + S/T\right), \tag{10}$$

where T is the absolute temperature (K), b = 1.458x10^{-6} Kg/(m.s.K$^{1/2}$) and S = 110.4 K, to the atmospheric air in the standard atmospheric conditions (Fox and McDonald, 1988).

The Navier-Stokes equations were nondimensionalized in relation to the stagnation density, ρ_*, the critical speed of the sound, a_*, and the stagnation viscosity, μ_*, for the nozzle problem, whereas in relation to the freestream density, ρ_∞, the freestream speed of sound, a_∞, and the freestream molecular viscosity, μ_∞, for the compression corner and ramp problems. To allow the solution of the matrix system of five equations to five unknowns described by Eq. (1), it is employed the state equation of perfect gases, in its two versions, presented below:

$$p = (\gamma - 1)\left[e - 0.5\rho(u^2 + v^2 + w^2)\right] \quad \text{or} \quad p = \rho RT \ , \tag{11}$$

with R being the specific gas constant, which to atmospheric air assumes the value 287 J/(Kg.K). Finally, the total enthalpy can be expressed by:

$$H = \left(e + p\right)/\rho \ . \tag{12}$$

Details of the geometrical characteristics of the spatial discretization are obtained in Maciel (2002, 2006).

3. NUMERICAL SCHEME OF HARTEN AND OSHER (1987) – TVD AND ENO METHODS

The Harten and Osher (1987) algorithm, second order accurate in space, is specified by the determination of the numerical flux vector at (i+1/2,j,k) interface. The implementation of the other numerical flux vectors at the other interfaces is straightforward.

Following a finite volume formalism, which is equivalent to a generalized system, the right and left cell volumes, as well the interface volume, necessary to coordinate change, are defined by:

$$V_R = V_{i+1,j,k} \ , \ \ V_L = V_{i,j,k} \quad \text{and} \quad V_{\mathrm{int}} = 0.5\left(V_R + V_L\right). \tag{13}$$

The metric terms to this generalized coordinate system are defined as:

$$h_x = S_{x\_\mathrm{int}} / V_{\mathrm{int}} \ , \ h_y = S_{y\_\mathrm{int}} / V_{\mathrm{int}} \ , \ h_z = S_{z\_\mathrm{int}} / V_{\mathrm{int}} \quad \text{and} \quad h_n = S / V_{\mathrm{int}} \ , \tag{14}$$

where $S_{x\_\mathrm{int}} = n_x S$, $S_{y\_\mathrm{int}} = n_y S$, $S_{z\_\mathrm{int}} = n_z S$ are the Cartesian components of the flux area and S is the flux area, calculated as described in Maciel (2002, 2006).

The properties calculated at the flux interface are obtained either by arithmetical average or by Roe (1981) average. In this work, the Roe (1981) average was used:

$$\rho_{\mathrm{int}} = \sqrt{\rho_L \rho_R} \ , \ u_{\mathrm{int}} = \left(u_L + u_R\sqrt{\rho_R/\rho_L}\right) / \left(1 + \sqrt{\rho_R/\rho_L}\right), \ v_{\mathrm{int}} = \left(v_L + v_R\sqrt{\rho_R/\rho_L}\right) / \left(1 + \sqrt{\rho_R/\rho_L}\right), \ w_{\mathrm{int}} = \left(w_L + w_R\sqrt{\rho_R/\rho_L}\right) / \left(1 + \sqrt{\rho_R/\rho_L}\right); \tag{15}$$

$$H_{\mathrm{int}} = \left(H_L + H_R\sqrt{\rho_R/\rho_L}\right) / \left(1 + \sqrt{\rho_R/\rho_L}\right) \ \text{and} \ a_{\mathrm{int}} = \sqrt{(\gamma - 1)\left[H_{\mathrm{int}} - 0.5\left(u_{\mathrm{int}}^2 + v_{\mathrm{int}}^2 + w_{\mathrm{int}}^2\right)\right]} \ . \tag{16}$$

where a_{int} is the speed of sound at the interface. The eigenvalues of the Euler equations, in the ξ direction, are given by:

$$U_{cont} = u_{\mathrm{int}} h_x + v_{\mathrm{int}} h_y + w_{\mathrm{int}} h_z \ , \ \lambda_1 = U_{cont} - a_{\mathrm{int}} h_n \ , \ \lambda_2 = \lambda_3 = \lambda_4 = U_{cont} \ , \text{ and } \lambda_5 = U_{cont} + a_{\mathrm{int}} h_n \ . \tag{17}$$

The jumps of the conserved variables, necessary to the construction of the Harten and Osher (1987) dissipation function, are given by:

$$\Delta\rho = V_{int}(\rho_R - \rho_L),\ \Delta(\rho u) = V_{int}[(\rho u)_R - (\rho u)_L],\ \Delta(\rho v) = V_{int}[(\rho v)_R - (\rho v)_L],\ \Delta(\rho w) = V_{int}[(\rho w)_R - (\rho w)_L], \text{ and } \Delta e = V_{int}(e_R - e_L). \quad (18)$$

The α vectors at the (i+1/2,j,k) interface are calculated by the following expressions:

$$\{\alpha_{i+1/2,j,k}\} = [R^{-1}]_{i+1/2,j,k}\{\Delta_{i+1/2,j,k}\overline{Q}\}, \quad (19)$$

with:

$$[R^{-1}] = \begin{bmatrix} 0.5[((\gamma-1)/a_{int}^2)0.5q^2 + \phi/a_{int}] & -0.5[((\gamma-1)/a_{int}^2)u_{int} + h_x'/a_{int}] & -0.5[((\gamma-1)/a_{int}^2)v_{int} + h_y'/a_{int}] & -0.5[(\gamma-1)/a_{int}^2 w_{int} + h_z'/a_{int}] & 0.5(\gamma-1)/a_{int}^2 \\ 1-((\gamma-1)/a_{int}^2)0.5q^2 & ((\gamma-1)/a_{int}^2)u_{int} & ((\gamma-1)/a_{int}^2)v_{int} & (\gamma-1)/a_{int}^2 w_{int} & -(\gamma-1)/a_{int}^2 \\ -(h_y'u_{int} + h_z'v_{int} + h_x'w_{int}) & h_y' & h_z' & h_x' & 0 \\ -(h_z'u_{int} + h_x'v_{int} + h_y'w_{int}) & h_z' & h_x' & h_y' & 0 \\ 0.5[((\gamma-1)/a_{int}^2)0.5q^2 - \phi/a_{int}] & 0.5[-((\gamma-1)/a_{int}^2)u_{int} + h_x'/a_{int}] & 0.5[-((\gamma-1)/a_{int}^2)v_{int} + h_y'/a_{int}] & 0.5[-(\gamma-1)/a_{int}^2 w_{int} + h_z'/a_{int}] & 0.5(\gamma-1)/a_{int}^2 \end{bmatrix}; \quad (20)$$

$$\{\Delta_{i+1/2,j,k}\overline{Q}\} = \{\Delta\rho \quad \Delta(\rho u) \quad \Delta(\rho v) \quad \Delta(\rho w) \quad \Delta e\}^T, \text{ defined by Eq. (18);} \quad (21)$$

$$q^2 = u_{int}^2 + v_{int}^2 + w_{int}^2; \quad (22)$$

$$\phi = u_{int}h_x' + v_{int}h_y' + w_{int}h_z'; \quad (23)$$

$$h_x' = h_x/h_n,\ h_y' = h_y/h_n \text{ and } h_z' = h_z/h_n. \quad (24)$$

The Harten and Osher (1987) dissipation function uses the right-eigenvector matrix of the normal to the flux face Jacobian matrix in generalized coordinates:

$$[R] = \begin{bmatrix} 1 & 1 & 0 & 0 & 1 \\ u_{int} - h_x'a_{int} & u_{int} & h_y' & h_z' & u_{int} + h_x'a_{int} \\ v_{int} - h_y'a_{int} & v_{int} & h_z' & h_x' & v_{int} + h_y'a_{int} \\ w_{int} - h_z'a_{int} & w_{int} & h_x' & h_y' & w_{int} + h_z'a_{int} \\ H_{int} - h_x'u_{int}a_{int} - h_y'v_{int}a_{int} - h_z'w_{int}a_{int} & 0.5q^2 & h_x'w_{int} + h_z'v_{int} + h_y'u_{int} & h_y'w_{int} + h_x'v_{int} + h_z'u_{int} & H_{int} + h_x'u_{int}a_{int} + h_y'v_{int}a_{int} + h_z'w_{int}a_{int} \end{bmatrix}. \quad (25)$$

To construct the TVD/ENO schemes of Harten and Osher (1987), it is necessary to define the parameter σ at the interface (i+1/2,j,k) to calculate the numerical speed of propagation of information, which contributes to the second order of the scheme:

$$\sigma(z) = 0.5\left[\Psi(z) - \Delta t_{i,j,k}z^2\right]; \quad (26)$$

$$\Psi(z) = \begin{cases} |z|, & if\ |z| \ge \varepsilon \\ (z^2 + \varepsilon^2)/2\varepsilon, & if\ |z| < \varepsilon \end{cases}, \text{ z and } \varepsilon \text{ scalars.} \quad (27)$$

The nonlinear limited flux function, based on Harten's idea of a modified flux function, is constructed by:

$$\overline{\beta}^l_{i,j,k} = m\left[\alpha^l_{i+1/2,j,k} - \zeta\overline{m}\left(\Delta_+\alpha^l_{i+1/2,j,k},\Delta_-\alpha^l_{i+1/2,j,k}\right),\alpha^l_{i-1/2,j,k} + \zeta\overline{m}\left(\Delta_+\alpha^l_{i-1/2,j,k},\Delta_-\alpha^l_{i-1/2,j,k}\right)\right], \quad (28)$$

where the limiters m and $\overline{m}$ are defined by:

$$m(y,z) = \begin{cases} s\times\min(|y|,|z|), & if \ \operatorname{sgn} y = \operatorname{sgn} z = s \\ 0, & otherwise \end{cases}; \quad (29)$$

$$\overline{m}(y,z) = \begin{cases} y, & if \ |y| \le |z| \\ z, & if \ |y| > |z| \end{cases}; \quad (30)$$

and the forward and backward operators are defined according to:

$$\Delta_+ = (\cdot)_{i+1,j,k} - (\cdot)_{i,j,k} \quad \text{and} \quad \Delta_- = (\cdot)_{i,j,k} - (\cdot)_{i-1,j,k}. \quad (31)$$

The numerical speed of propagation of information is calculated by:

$$\overline{\gamma}^l_{i+1/2,j,k} = \sigma\left(\lambda^l_{i+1/2,j,k}\right)\begin{cases} \left(\overline{\beta}^l_{i+1,j,k} - \overline{\beta}^l_{i,j,k}\right)/\alpha^l_{i+1/2,j,k}, & if \ \alpha^l_{i+1/2,j,k} \ne 0 \\ 0, & otherwise \end{cases}. \quad (32)$$

The dissipation function to the Harten and Osher (1987) TVD/ENO schemes is defined as follows:

$$\left(\phi^l_{i+1/2,j,k}\right)_{HO} = \sigma\left(\lambda^l_{i+1/2,j,k}\right)\left(\overline{\beta}^l_{i,j,k} + \overline{\beta}^l_{i+1,j,k}\right) - \Psi\left(\lambda^l_{i+1/2,j,k} + \overline{\gamma}^l_{i+1/2,j,k}\right)\alpha^l_{i+1/2,j,k}, \quad (33)$$

with: "l" assuming values from 1 to 5 (three-dimensional space), ε assumes value 0.2 recommended by Harten and Osher (1987), Ψ is an entropy function to guarantee only physical relevant solutions, and ζ assumes the value 0.0 to obtain the second order TVD scheme of Harten (1983) and 0.5 to obtain the uniformly second order essentially non-oscillatory scheme of Harten and Osher (1987).

Finally, the Harten and Osher (1987) dissipation operator, to second order of spatial accuracy, in TVD or ENO versions, is constructed by the following matrix-vector product:

$$\{D_{HO}\}_{i+1/2,j,k} = [R]_{i+1/2,j,k}\{\phi_{HO}\}_{i+1/2,j,k}. \quad (34)$$

The convective numerical flux vector to the (i+1/2,j,k) interface is described by:

$$F^{(l)}_{i+1/2,j,k} = \left(E^{(l)}_{\text{int}}h_x + F^{(l)}_{\text{int}}h_y + G^{(l)}_{\text{int}}h_z\right)V_{\text{int}} + 0.5D^{(l)}_{HO}, \quad (35)$$

with:

$$E^{(l)}_{\text{int}} = 0.5\left(E^{(l)}_R + E^{(l)}_L\right),\ F^{(l)}_{\text{int}} = 0.5\left(F^{(l)}_R + F^{(l)}_L\right) \quad \text{and} \quad G^{(l)}_{\text{int}} = 0.5\left(G^{(l)}_R + G^{(l)}_L\right). \quad (36)$$

The right-hand-side of the Harten and Osher (1987) scheme, necessaries to the resolution of the implicit version of this algorithm, is determined by:

$$RHS(HO)^n_{i,j,k} = -\Delta t_{i,j,k}/V_{i,j,k}\left(F^n_{i+1/2,j,k} - F^n_{i-1/2,j,k} + F^n_{i,j+1/2,k} - F^n_{i,j-1/2,k} + F^n_{i,j,k+1/2} - F^n_{i,j,k-1/2}\right). \quad (37)$$

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

$$\Delta Q^*_{i,j,k} = -\Delta t_{i,j,k}/V_{i,j,k}\left(F^n_{i+1/2,j,k} - F^n_{i-1/2,j,k}\right); \quad Q^*_{i,j,k} = Q^n_{i,j,k} + \Delta Q^*_{i,j,k}; \quad (38)$$

in the intermediate step, η direction:

$$\Delta Q^{**}_{i,j,k} = -\Delta t_{i,j,k} / V_{i,j,k} \left(F^{*}_{i,j+1/2,k} - F^{*}_{i,j-1/2,k}\right); \quad Q^{**}_{i,j,k} = Q^{*}_{i,j,k} + \Delta Q^{**}_{i,j,k} ; \tag{39}$$

and in the end step, ζ direction:

$$\Delta Q^{n+1}_{i,j,k} = -\Delta t_{i,j,k} / V_{i,j,k} \left(F^{**}_{i,j,k+1/2} - F^{**}_{i,j,k-1/2}\right); \quad Q^{n+1}_{i,j,k} = Q^{**}_{i,j,k} + \Delta Q^{n+1}_{i,j,k} . \tag{40}$$

The viscous vectors at the flux interface are obtained by arithmetical average between the primitive variables at the left and at the right states of the flux interface, as also arithmetical average of the primitive variable gradients also considering the left and the right states of the flux interface. The gradients of the primitive variables present in the viscous flux vectors are calculated employing the Green Theorem which considers that the gradient of a primitive variable is constant in the volume and that the volume integral which defines this gradient is replaced by a surface integral (Long, Khan and Sharp, 1991); For instance, to $\partial u / \partial x$:

$$\frac{\partial u}{\partial x} = \frac{1}{V}\int_V \frac{\partial u}{\partial x} dV = \frac{1}{V}\int_S u\left(\vec{n} \bullet d\vec{S}\right) = \frac{1}{V}\int_{S_x} u dS_x \cong \frac{1}{V_{i,j,k}}\Big[0.5\left(u_{i,j,k} + u_{i,j-1,k}\right)S_{x_{i,j-1/2,k}} + 0.5\left(u_{i,j,k} + u_{i+1,j,k}\right)S_{x_{i+1/2,j,k}} +$$
$$0.5\left(u_{i,j,k} + u_{i,j+1,k}\right)S_{x_{i,j+1/2,k}} + 0.5\left(u_{i,j,k} + u_{i-1,j,k}\right)S_{x_{i-1/2,j,k}} + 0.5\left(u_{i,j,k} + u_{i,j,k-1}\right)S_{x_{i,j,k-1/2}} + 0.5\left(u_{i,j,k} + u_{i,j,k+1}\right)S_{x_{i,j,k+1/2}}\Big]. \tag{41}$$

3. NUMERICAL SCHEME OF YEE (1987) – SYMMETRIC TVD METHOD

The second order symmetric TVD scheme of Yee (1987) employs Eqs. (13) to (25). The next step consists in determining the different limiters which incorporate the TVD properties to the Yee (1987) symmetric scheme. According to Yee (1987), five different limiters are implemented. The limited dissipation function Q is defined to the five options as:

$$Q\left(r^-, r^+\right) = \min\text{mod}\left(1, r^-\right) + \min\text{mod}\left(1, r^+\right) - 1 ; \tag{42}$$
$$Q\left(r^-, r^+\right) = \min\text{mod}\left(1, r^-, r^+\right); \tag{43}$$
$$Q\left(r^-, r^+\right) = \min\text{mod}\left[2, 2r^-, 2r^+, 0.5\left(r^- + r^+\right)\right]; \tag{44}$$
$$Q\left(r^-, r^+\right) = \max\left[0, \min\left(2r^-, 1\right), \min\left(r^-, 2\right)\right] + \max\left[0, \min\left(2r^+, 1\right), \min\left(r^+, 2\right)\right] - 1 ; \tag{45}$$
$$Q\left(r^-, r^+\right) = \frac{r^- + \left|r^-\right|}{1 + r^-} + \frac{r^+ + \left|r^+\right|}{1 + r^+} - 1 , \tag{46}$$

where:

$$\left(r^-_{i+1/2,j,k}\right)^l = \alpha^l_{i-1/2,j,k} / \alpha^l_{i+1/2,j,k} \quad \text{and} \quad \left(r^+_{i+1/2,j,k}\right)^l = \alpha^l_{i+3/2,j,k} / \alpha^l_{i+1/2,j,k} , \tag{47}$$

with the α vectors defined by Eq. (19). Equations (42) to (44) are referenced by this author as minmod1 (Min1), minmod2 (Min2) and minmod3 (Min3), respectively. Equation (45) is referred in the CFD literature as the "Superbee" (SB) limiter due to Roe (1983) and Eq. (46) is referred as the Van Leer (VL) limiter due to Van Leer (1974).

The dissipation function to the symmetric TVD scheme of Yee (1987) is defined as follows:

$$\left(\phi^l_{i+1/2,j,k}\right)_{Yee} = \Psi\left(\lambda^l_{i+1/2,j,k}\right)\left(1 - Q^l_{i+1/2,j,k}\right)\alpha^l_{i+1/2,j,k} , \tag{48}$$

with Ψ entropy function defined by Eq. (27). The Yee (1987) TVD dissipation operator is finally constructed by the following matrix-vector product:

$$\left\{D_{Yee}\right\}_{i+1/2,j,k} = \left[R\right]_{i+1/2,j,k} \left\{\phi_{Yee}\right\}_{i+1/2,j,k} , \tag{49}$$

The convective numerical flux vector to the (i+1/2,j,k) interface is described by:

$$F^{(l)}_{i+1/2,j,k} = \left(E^{(l)}_{\text{int}} h_x + F^{(l)}_{\text{int}} h_y + G^{(l)}_{\text{int}} h_z\right)V_{\text{int}} - 0.5 D^{(l)}_{Yee} , \tag{50}$$

with: $E_{int}^{(l)}$, $F_{int}^{(l)}$ and $G_{int}^{(l)}$ defined by Eq. (36) and the calculation of the viscous terms according to Eq. (41). The right-hand-side of the Yee (1987) symmetric scheme, necessaries to the resolution of the implicit version of this algorithm, is determined by:

$$RHS(Yee)_{i,j,k}^{n} = -\Delta t_{i,j,k} / V_{i,j,k} \left(F_{i+1/2,j,k}^{n} - F_{i-1/2,j,k}^{n} + F_{i,j+1/2,k}^{n} - F_{i,j-1/2,k}^{n} + F_{i,j,k+1/2}^{n} - F_{i,j,k-1/2}^{n} \right). \tag{51}$$

The explicit version to the viscous simulations is defined by Eqs. (38)-(40).

4. IMPLICIT FORMULATION

All implicit schemes implemented in this work used backward Euler in time and ADI or LNI approximate factorization to solve a three-diagonal system in each direction.

4.1. Implicit formulation to flux difference splitting schemes

In the flux difference splitting cases, a Linearized Nonconservative Implicit (LNI) form is applied that, although the resulting schemes loss the conservative property, preserve their unconditionally TVD property. Moreover, the LNI form is mainly useful to steady state calculations, since the schemes are only conservative after the solution reaches steady state. This LNI form to the solution of the implicit schemes of Harten and Osher (1987) TVD/ENO was proposed by Yee, Warming and Harten (1985). The LNI form presents three stages as described below:

$$\left[I - \Delta t_{i,j,k} J_{i+1/2,j,k}^{-} \Delta_{i+1/2,j,k} + \Delta t_{i,j,k} J_{i-1/2,j,k}^{+} \Delta_{i-1/2,j,k} \right] \Delta Q_{i,j,k}^{*} = \left[RHS_{(HO)} \right]_{i,j,k}^{n}; \tag{52}$$

$$\left[I - \Delta t_{i,j,k} K_{i,j+1/2,k}^{-} \Delta_{i,j+1/2,k} + \Delta t_{i,j,k} K_{i,j-1/2,k}^{+} \Delta_{i,j-1/2,k} \right] \Delta Q_{i,j,k}^{**} = \Delta Q_{i,j,k}^{*}; \tag{53}$$

$$\left[I - \Delta t_{i,j,k} L_{i,j,k+1/2}^{-} \Delta_{i,j,k+1/2} + \Delta t_{i,j,k} L_{i,j,k-1/2}^{+} \Delta_{i,j,k-1/2} \right] \Delta Q_{i,j,k}^{n+1} = \Delta Q_{i,j,k}^{**}, \tag{54}$$

where $RHS_{(HO)}$ is defined by Eq. (37). The difference operators are defined as:

$$\Delta_{i+1/2,j,k}(\cdot) = (\cdot)_{i+1,j,k} - (\cdot)_{i,j,k},\ \Delta_{i-1/2,j,k}(\cdot) = (\cdot)_{i,j,k} - (\cdot)_{i-1,j,k},\ \Delta_{i,j+1/2,k}(\cdot) = (\cdot)_{i,j+1,k} - (\cdot)_{i,j,k}; \tag{55}$$

$$\Delta_{i,j-1/2,k}(\cdot) = (\cdot)_{i,j,k} - (\cdot)_{i,j-1,k},\ \Delta_{i,j,k+1/2}(\cdot) = (\cdot)_{i,j,k+1} - (\cdot)_{i,j,k},\ \Delta_{i,j,k-1/2}(\cdot) = (\cdot)_{i,j,k} - (\cdot)_{i,j,k-1}. \tag{56}$$

and the update of the conserved variable vector is proceeded as follows:

$$Q_{i,j,k}^{n+1} = Q_{i,j,k}^{n} + \Delta Q_{i,j,k}^{n+1}. \tag{57}$$

This system of 5x5 block three-diagonal linear equations is solved using LU decomposition and the Thomas algorithm applied to systems of block matrices.

The splitting matrices J^+, J^-, K^+, K^-, L^+ and L^- are defined as:

$$J^{+} = R_{\xi} diag\left(D_{\xi}^{+}\right) R_{\xi}^{-1},\ J^{-} = R_{\xi} diag\left(D_{\xi}^{-}\right) R_{\xi}^{-1},\ K^{+} = R_{\eta} diag\left(D_{\eta}^{+}\right) R_{\eta}^{-1}; \tag{58}$$

$$K^{-} = R_{\eta} diag\left(D_{\eta}^{-}\right) R_{\eta}^{-1},\ L^{+} = R_{\zeta} diag\left(D_{\zeta}^{+}\right) R_{\zeta}^{-1} \quad \text{and} \quad L^{-} = R_{\zeta} diag\left(D_{\zeta}^{-}\right) R_{\zeta}^{-1}, \tag{59}$$

where R_{ξ}, R_{η}, R_{ζ}, R_{ξ}^{-1}, R_{η}^{-1} and R_{ζ}^{-1} are defined by Eqs. (20) and (25), applied to each coordinate direction; $diag(\cdot)$ represents a diagonal matrix such as:

$$D_{\xi}^{+} = \begin{bmatrix} D_1^{\xi,+} & & & & \\ & D_2^{\xi,+} & & & \\ & & D_3^{\xi,+} & & \\ & & & D_4^{\xi,+} & \\ & & & & D_5^{\xi,+} \end{bmatrix} \text{ and } D_{\xi}^{-} = \begin{bmatrix} D_1^{\xi,-} & & & & \\ & D_2^{\xi,-} & & & \\ & & D_3^{\xi,-} & & \\ & & & D_4^{\xi,-} & \\ & & & & D_5^{\xi,-} \end{bmatrix}. \tag{60}$$

and the terms D are defined as:

$$D_\xi^\pm = 0.5\left[Q\left(\lambda_\xi^l + \gamma_\xi^l\right) \pm \left(\lambda_\xi^l + \gamma_\xi^l\right)\right],\ D_\eta^\pm = 0.5\left[Q\left(\lambda_\eta^l + \gamma_\eta^l\right) \pm \left(\lambda_\eta^l + \gamma_\eta^l\right)\right],\text{ and } D_\zeta^\pm = 0.5\left[Q\left(\lambda_\zeta^l + \gamma_\zeta^l\right) \pm \left(\lambda_\zeta^l + \gamma_\zeta^l\right)\right], \quad (61)$$

with:

$$Q(x_l) = \begin{cases} |x_l|, & if\ |x_l| \geq \varepsilon \\ 0.5\left(x_l^2 + \varepsilon^2\right)/\varepsilon, & if\ |x_l| < \varepsilon \end{cases},\ \varepsilon \text{ defined by Eq. (27);} \quad (62)$$

λ_ξ^l, λ_η^l and λ_ζ^l are the eigenvalues of the Euler equations, defined by Eq. (17), in each coordinate direction;

$$\left(\gamma_\xi^l\right)_{i+1/2,j,k} = \begin{cases} \left[\left(g_\xi^{'}\right)_{i+1,j,k}^l - \left(g_\xi^{'}\right)_{i,j,k}^l\right] \Big/ \left(\alpha_\xi^l\right)_{i+1/2,j,k}, & if\ \left(\alpha_\xi^l\right)_{i+1/2,j,k} \neq 0.0 \\ 0.0, & if\ \left(\alpha_\xi^l\right)_{i+1/2,j,k} = 0.0 \end{cases}; \quad (63)$$

$$\left(\gamma_\eta^l\right)_{i,j+1/2,k} = \begin{cases} \left[\left(g_\eta^{'}\right)_{i,j+1,k}^l - \left(g_\eta^{'}\right)_{i,j,k}^l\right] \Big/ \left(\alpha_\eta^l\right)_{i,j+1/2,k}, & if\ \left(\alpha_\eta^l\right)_{i,j+1/2,k} \neq 0.0 \\ 0.0, & if\ \left(\alpha_\eta^l\right)_{i,j+1/2,k} = 0.0 \end{cases}; \quad (64)$$

$$\left(\gamma_\zeta^l\right)_{i,j,k+1/2} = \begin{cases} \left[\left(g_\zeta^{'}\right)_{i,j,k+1}^l - \left(g_\zeta^{'}\right)_{i,j,k}^l\right] \Big/ \left(\alpha_\zeta^l\right)_{i,j,k+1/2}, & if\ \left(\alpha_\zeta^l\right)_{i,j,k+1/2} \neq 0.0 \\ 0.0, & if\ \left(\alpha_\zeta^l\right)_{i,j,k+1/2} = 0.0 \end{cases}; \quad (65)$$

$$\left(g_\xi^{'}\right)_{i,j,k}^l = signal_\xi^l MAX\left[0.0, MIN\left(\sigma_{i+1/2,j,k}^l \left|\left(\alpha_\xi^l\right)_{i+1/2,j,k}\right|, signal_\xi^l \sigma_{i-1/2,j,k}^l \left(\alpha_\xi^l\right)_{i-1/2,j,k}\right)\right]; \quad (66)$$

$$\left(g_\eta^{'}\right)_{i,j,k}^l = signal_\eta^l MAX\left[0.0, MIN\left(\sigma_{i,j+1/2,k}^l \left|\left(\alpha_\eta^l\right)_{i,j+1/2,k}\right|, signal_\eta^l \sigma_{i,j-1/2,k}^l \left(\alpha_\eta^l\right)_{i,j-1/2,k}\right)\right]; \quad (67)$$

$$\left(g_\zeta^{'}\right)_{i,j,k}^l = signal_\zeta^l MAX\left[0.0, MIN\left(\sigma_{i,j,k+1/2}^l \left|\left(\alpha_\zeta^l\right)_{i,j,k+1/2}\right|, signal_\zeta^l \sigma_{i,j,k-1/2}^l \left(\alpha_\zeta^l\right)_{i,j,k-1/2}\right)\right]; \quad (68)$$

$$\sigma^l = 0.5Q^l\left(\lambda^l\right) \text{ to steady state simulations.} \quad (69)$$

Finally, $signal_\xi^l$ = 1.0 if $\left(\alpha_\xi^l\right)_{i+1/2,j,k} \geq 0.0$ and -1.0 otherwise; $signal_\eta^l$ = 1.0 if $\left(\alpha_\eta^l\right)_{i,j+1/2,k} \geq 0.0$ and -1.0 otherwise and $signal_\zeta^l$ = 1.0 if $\left(\alpha_\zeta^l\right)_{i,j,k+1/2} \geq 0.0$ and -1.0 otherwise.

This implicit formulation to the LHS of the Harten and Osher (1987) scheme is second order accurate in time and space due to the presence of the numerical characteristic speed γ associated to the numerical flux function g'. In this case, the solution accuracy in space is definitively of second order because both LHS and RHS are also of second order.

It is important to emphasize that as the right-hand-side of the implicit flux difference splitting schemes tested in this work presents steady state solutions which depends of the time step, the use of large time steps with the implicit schemes can affect the steady solutions, as mentioned in Yee, Warming and Harten (1982). This is an initial study with implicit schemes and improvements of the implementation of these schemes with steady state solutions independent of the time step is a goal to be aimed in future works by this author.

4.2. Implicit formulation to symmetric scheme

The ADI form of the implicit symmetric TVD scheme of Yee (1987) is represented by:

$$E_1 \Delta Q_{i-1,j,k}^* + E_2 \Delta Q_{i,j,k}^* + E_3 \Delta Q_{i+1,j,k}^* = \left[RHS_{(Yee)}\right]_{i,j,k}^n \text{, to the } \xi \text{ direction;} \quad (70)$$

$$F_1 \Delta Q_{i,j-1,k}^{**} + F_2 \Delta Q_{i,j,k}^{**} + F_3 \Delta Q_{i,j+1,k}^{**} = \Delta Q_{i,j,k}^* \text{, to the } \eta \text{ direction;} \quad (71)$$

$$G_1 \Delta Q_{i,j,k-1}^{n+1} + G_2 \Delta Q_{i,j,k}^{n+1} + G_3 \Delta Q_{i,j,k+1}^{n+1} = \Delta Q_{i,j,k}^{**} \text{, to the } \zeta \text{ direction;} \quad (72)$$

$$Q_{i,j,k}^{n+1} = Q_{i,j,k}^n + \Delta Q_{i,j,k}^{n+1}, \quad (73)$$

where:

$$E_1 = \frac{\Delta t_{i,j,k}\theta}{2}\left(-A_{i-1/2,j,k} - K_{i-1/2,j,k}\right)^n;\ E_2 = I + \frac{\Delta t_{i,j,k}\theta}{2}\left(K_{i-1/2,j,k} + K_{i+1/2,j,k}\right)^n; \quad (74)$$

$$E_3 = \frac{\Delta t_{i,j,k}\theta}{2}\left(A_{i+1/2,j,k} - K_{i+1/2,j,k}\right)^n ;\ F_1 = \frac{\Delta t_{i,j,k}\theta}{2}\left(-B_{i,j-1/2,k} - J_{i,j-1/2,k}\right)^n ; \quad (75)$$

$$F_2 = I + \frac{\Delta t_{i,j,k}\theta}{2}\left(J_{i,j-1/2,k} + J_{i,j+1/2,k}\right)^n ;\ F_3 = \frac{\Delta t_{i,j,k}\theta}{2}\left(B_{i,j+1/2,k} - J_{i,j+1/2,k}\right)^n ; \quad (76)$$

$$G_1 = \frac{\Delta t_{i,j,k}\theta}{2}\left(-C_{i,j,k-1/2} - L_{i,j,k-1/2}\right)^n ;\ G_2 = I + \frac{\Delta t_{i,j,k}\theta}{2}\left(L_{i,j,k-1/2} + L_{i,j,k+1/2}\right)^n ; \quad (77)$$

$$G_3 = \frac{\Delta t_{i,j,k}\theta}{2}\left(C_{i,j,k+1/2} - L_{i,j,k+1/2}\right)^n ;\ A^n_{i\pm1/2,j,k} = [R]^n_{i\pm1/2,j,k}\, diag\left(\lambda^l_\xi\right)^n_{i\pm1/2,j,k}\left[R^{-1}\right]^n_{i\pm1/2,j,k} ; \quad (78)$$

$$B^n_{i,j\pm1/2,k} = [R]^n_{i,j\pm1/2,k}\, diag\left(\lambda^l_\eta\right)^n_{i,j\pm1/2,k}\left[R^{-1}\right]^n_{i,j\pm1/2,k} ;\ C^n_{i,j,k\pm1/2} = [R]^n_{i,j,k\pm1/2}\, diag\left(\lambda^l_\zeta\right)^n_{i,j,k\pm1/2}\left[R^{-1}\right]^n_{i,j,k\pm1/2} ; \quad (79)$$

$$K^n_{i\pm1/2,j,k} = [R]^n_{i\pm1/2,j,k}\,\Omega^n_{i\pm1/2,j,k}\left[R^{-1}\right]^n_{i\pm1/2,j,k} ;\ J^n_{i,j\pm1/2,k} = [R]^n_{i,j\pm1/2,k}\,\Phi^n_{i,j\pm1/2,k}\left[R^{-1}\right]^n_{i,j\pm1/2,k} ; \quad (80)$$

$$L^n_{i,j,k\pm1/2} = [R]^n_{i,j,k\pm1/2}\,\Theta^n_{i,j,k\pm1/2}\left[R^{-1}\right]^n_{i,j,k\pm1/2} ;\ \Omega^n_{i\pm1/2,j,k} = diag\left[\Psi\left(\lambda^l_\xi\right)\right]^n_{i\pm1/2,j,k} ; \quad (81)$$

$$\Phi^n_{i,j\pm1/2,k} = diag\left[\Psi\left(\lambda^l_\eta\right)\right]^n_{i,j\pm1/2,k} ;\ \Theta^n_{i,j,k\pm1/2} = diag\left[\Psi\left(\lambda^l_\zeta\right)\right]^n_{i,j,k\pm1/2} . \quad (82)$$

In Equations (78) to (81), the R and R^{-1} matrixes are defined by Eqs. (20) and (25); in Eqs. (78), (79), (81) and (82), "l" assumes values from 1 to 5; the Ψ entropy function is defined by Eq. (27); and I is the identity matrix. The $RHS_{(Yee)}$ operator required in Eq. (70) is defined by Eq. (51).

This implementation is first order accurate in time due to the definition of Ω, of Φ and of Θ, as reported in Yee (1987). The θ parameter defines the particular implicit time integration method studied in this work. A value of 0.0 to this parameter results in an explicit method; the value 0.5 implies the trapezoidal method; and, the value 1.0 results in the backward Euler method. In the present experiments, the backward Euler method was used.

5. SPATIAL VARIABLE TIME STEP, INITIAL AND BOUNDARY CONDITIONS

The description of the spatially variable time step procedure, as also the initial and boundary conditions to the three-dimensional space are described in Maciel (2002, 2006).

6. CONCLUSIONS

In the present work, the description of the Harten and Osher (1987) TVD/ENO schemes and of Yee (1987) symmetric TVD scheme is presented, including the implicit formulation. This scheme is implemented, on a finite volume context and using a structured spatial discretization, to solve the Euler and the laminar Navier-Stokes equations in the three-dimensional space. The Harten and Osher (1987) TVD/ENO schemes are flux difference splitting type, whereas the Yee (1987) TVD scheme is a symmetric one, which incorporates TVD properties due to the appropriated definition of a limited dissipation function. Both schemes are second order accurate in space and their numerical implementation is based on the concept of Harten's modified flux function. All schemes are implemented following an implicit formulation to solve the Euler equations. The flux difference splitting schemes employ approximate factorizations in Linearized Nonconservative Implicit LNI form, whereas the symmetric scheme employs approximate factorization in ADI form. The viscous simulations are treated with the explicit versions of the present algorithms, which employ the time splitting method. 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 (Maciel, 2005 and 2008). The algorithms are applied to the solution of the physical problems of the transonic flow along a convergent-divergent nozzle and of the supersonic flow along a compression corner in the inviscid case, whereas the laminar case studies a particular ramp problem.

The results have demonstrated that the most accurate results are obtained with the Harten and Osher (1987) ENO and Yee (1987) TVD VL and Min1 schemes. This paper is the first part of this work, THEORY, focusing in the description of the TVD/ENO Harten and Osher (1987) schemes and of the TVD symmetric Yee (1987) scheme, as also the implicit formulation to the inviscid cases.

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