COMPARISON AMONG PREDICTOR-CORRECTOR, SIMMETRICAL AND TVD UPWIND SCHEMES IN THE SOLUTION OF THE EULER EQUATIONS IN TWO-DIMENSIONS - THEORY

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Abstract. *The present work compares the MacCormack, the Harten, the Yee and Kutler and the Jameson and Mavriplis numerical methods, using a finite volume formulation and a structured spatial discretization, applied to the solution of the Euler equations in the two-dimensional space. All schemes are second order accurate in space. The MacCormack and the Jameson and Mavriplis schemes are also second order accurate in time and both use artificial dissipation operators to guarantee the convergence to the steady state solution. The steady state physical problems of the transonic flows along a convergent-divergent nozzle and around a NACA 0012 airfoil, the supersonic flow along a ramp and the "cold gas" hypersonic flow around a double ellipse configuration are studied. A spatially variable time step is implemented aiming to accelerate the convergence process. The results have demonstrated that the MacCormack scheme predicts the most critical solutions, although unphysical results were obtained in high Mach numbers. Shock pressure ratio, nozzle, and stagnation pressure, double ellipse, were best estimated by this scheme. This paper is concerned with the theories related to the numerical implementation of the schemes. The part II (RESULTS) presents the solutions and comparisons between numerical and experimental or theoretical results.*

Keywords*: MacCormack algorithm, Harten algorithm, Yee and Kutler algorithm, Jameson and Mavriplis algorithm, Euler equations.*

1. INTRODUCTION

The development of aeronautical and aerospace projects require hours of wind tunnel essays. It is necessary to minimize such wind tunnel procedures due to the growing cost of electrical energy. In Brazil, there is the problem of this country has not yet wind tunnels of great capacity, able to generate supersonic flows or even high subsonic flows. So, Computational Fluid Dynamics, CFD, techniques have now great highlight in the aeronautical industry scenario. Analogous to wind tunnel essays, the numerical methods determine physical properties in discrete points of the spatial domain. Hence, the aerodynamic coefficients of lift, drag and momentum can be calculated.

Initially, non-upwind schemes were developed to simulate flow over simple and complex geometries due to their simplicity in numerical implementation. Predictor-corrector and symmetrical schemes were the most employed algorithms during the 60's to 80's years. Some of them are reported below:

MacCormack (1969) developed a numerical method second order accurate in space and time to solve the Navier-Stokes equations in two-dimensions. The scheme was initially developed to a finite difference technique. The method was divided in two steps: a predictor step and a corrector step. In the predictor step, the derivatives of the flux terms were calculated with forward spatial discretization operators and in the corrector step, these derivatives were calculated with backward spatial discretization operators.

Jameson, Schmidt and Turkel (1981) proportioned a great impulse in the solution of the Euler equations in two-dimensions, using a finite volume numerical scheme, a Runge-Kutta time march method and a structured formulation to spatial discretization, although its extension to an unstructured treatment was straightforward. The scheme was symmetrical and used artificial dissipation terms of first and third orders to reduce instabilities originated from pressure gradients and resulting from discretization process errors, respectively. The method was used to calculate the steady state transonic flow around an airfoil using an "O" topology mesh.

Jameson and Mavriplis (1986) emphasized the substantial cost reduction in the calculations of the Euler equation solutions. The method proposed by Jameson, Schmidt and Turkel (1981) had proved robustness, good accuracy and sufficient sophistication to more complete applications. The objective was apply such scheme to geometries like wing-fuselage, involving engines, missiles and other typical components, to represent a whole airplane. The work emphasized the use of triangular cells which allow a bigger flexibility in the description of complex geometries and become the mesh generation process less expensive. The fluid movement equations were spatially discretized on an unstructured context. The scheme used a finite volume formulation with properties determined at the cell centroids. Artificial dissipation operators were constructed to guarantee second order spatial accuracy to the scheme, except in the proximities of shock waves in which the accuracy was reduced to the first order (Jameson, Schmidt and Turkel, 1981). The time integration used a Runge-Kutta method of five stages.

The necessity to construct more elaborated and more robust schemes, which permitted the capture of strong and sharp shocks, become an important goal to be achieved by first order and high resolution upwind schemes. Since 1959, first order and high resolution upwind schemes, which combined the characteristics of robustness, good shock capture properties and good shock quality, have been developed aiming to provide efficient tools to predict accurately the main

features of flow field. The first order and high resolution upwind schemes can be of flux vector splitting type or flux difference splitting type. In the former case, more robust algorithms are yielded, while in the later case, more accuracy is obtained. Several studies were reported involving first order and high resolution algorithms in the international literature, as for example:

Roe (1981) 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 this 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.

Harten (1983) developed a class of new finite difference schemes, explicit and second order accurate in space, to calculation of weak solutions of the hyperbolic conservation laws. These schemes highly non-linear were obtained by the application of a first order non-oscillatory scheme to an appropriated modified flux function. The so derived second order schemes reached high resolution, while preserved the robustness property of the original non-oscillatory first order scheme.

Yee and Kutler (1985) presented a work which extended the Harten (1983) scheme to a generalized coordinate system, in two-dimensions. The method called "TVD scheme" by the authors was tested to the physical problem of a moving shock impinging a cylinder. The numerical results were compared with the MacCormack (1969) scheme, presenting good results.

With this scenario, an important and interesting study can be performed by comparing predictor-corrector, symmetrical and high resolution upwind schemes.

The present work compares the MacCormack (1969), the Harten (1983), the Yee and Kutler (1985) and the Jameson and Mavriplis (1986) numerical methods, using a finite volume formulation and a structured spatial discretization, applied to the solution of the Euler equations in the two-dimensional space. All schemes are second order accurate in space. The MacCormack (1969) and the Jameson and Mavriplis (1986) schemes are also second order accurate in time and both use artificial dissipation operators to guarantee the convergence to the steady state solution. The Harten (1983) and the Yee and Kutler (1985) schemes are first order accurate in time. The steady state physical problems of the transonic flows along a convergent-divergent nozzle and around a NACA 0012 airfoil, the supersonic flow along a ramp and the "cold gas" hypersonic flow around a double ellipse configuration are studied. A spatially variable time step is implemented aiming to accelerate the convergence process. This technique has proved excellent gains in terms of convergence ratio as reported in Maciel (2005).

The results have demonstrated that the MacCormack scheme predicts the most critical solutions, although unphysical results were obtained in high Mach numbers. The pressure ratio at the shock, nozzle problem, and the stagnation pressure, double ellipse problem, were best estimated by the MacCormack (1969) scheme.

This paper is concerned with the theories related to the numerical implementation of the schemes, consisting in part I (THEORY) of this study. The part II (RESULTS) presents the solutions of the numerical simulations, comparisons between numerical and experimental or theoretical results and computational data.

It is important to emphasize that all algorithms presented in this work were implemented by the author, without requiring the use of external packages. Only the Tecplot 8.0 software was used to generate the figures.

2. EULER EQUATIONS

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

$$\partial/\partial t \int_V Q dV + \int_S \left(E_e n_x + F_e n_y\right) dS = 0 \,, \tag{1}$$

where Q is written to a Cartesian system, V is the cell volume, n_x and n_y are the components of the normal unity vector to the flux face, S is the area flux and E_e and F_e represent the components of the convective flux vector. Q, E_e and F_e are represented by:

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

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

The Euler equations were nondimensionalized in relation to the stagnation density, ρ^*, and in relation to the critical speed of sound, a^*, to the nozzle problem, and in relation to the freestream density, ρ_∞, and in relation to the freestream speed of sound, a_∞, to the others problems. The matrix system of the Euler equations is closed with the state equation of a perfect gas:

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

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

3. MACCORMACK (1969) ALGORITHM

Using finite volumes and applying the Green theorem to Equation (1), it is possible to write that:

$$\partial Q_{i,j} / \partial t = -1/V_{i,j} \int_S \left(\vec{F} \bullet \vec{n}\right)_{i,j} dS_{i,j}. \tag{4}$$

In the discretization of the surface integral, the Eq. (4) can be rewritten as:

$$dQ_{i,j} / dt = -1/V_{i,j} \left[\left(\vec{F} \bullet \vec{S}\right)_{i,j-1/2} + \left(\vec{F} \bullet \vec{S}\right)_{i+1/2,j} + \left(\vec{F} \bullet \vec{S}\right)_{i,j+1/2} + \left(\vec{F} \bullet \vec{S}\right)_{i-1/2,j}\right]. \tag{5}$$

Discretizing Equation (5) in time using the Euler explicit method, results in:

$$Q_{i,j}^{n+1} = Q_{i,j}^{n} - \Delta t_{i,j} / V_{i,j} \left[(F \cdot S)_{i,j-1/2} + (F \cdot S)_{i+1/2,j} + (F \cdot S)_{i,j+1/2} + (F \cdot S)_{i-1/2,j}\right]^n. \tag{6}$$

The time integration is now divided in two steps: one predictor and the other corrector. In the predictor step, the flux terms are calculated using the properties of the forward cell in relation to the flux interface. In the corrector step, the properties of the backward cell in relation to the flux interface are used. With this procedure, the scheme is second order accurate in space and time. Hence, the MacCormack (1969) algorithm, based on a finite volume formulation, is described as follows:

Predictor step:

$$\begin{aligned}\Delta Q_{i,j}^{n} = -\Delta t_{i,j} / V_{i,j} \left[\left(\left(E_e\right)_{i,j} S_{x\,i,j-1/2} + \left(F_e\right)_{i,j} S_{y\,i,j-1/2}\right) + \left(\left(E_e\right)_{i+1,j} S_{x\,i+1/2,j} + \left(F_e\right)_{i+1,j} S_{y\,i+1/2,j}\right) + \right. \\ \left. \left(\left(E_e\right)_{i,j+1} S_{x\,i,j+1/2} + \left(F_e\right)_{i,j+1} S_{y\,i,j+1/2}\right) + \left(\left(E_e\right)_{i,j} S_{x\,i-1/2,j} + \left(F_e\right)_{i,j} S_{y\,i-1/2,j}\right)\right];\end{aligned} \tag{7}$$

$$Q_{p\,i,j}^{n+1} = Q_{i,j}^{n} + \Delta Q_{i,j}^{n}; \tag{8}$$

Corrector step:

$$\begin{aligned}\Delta Q_{c\,i,j}^{n+1} = -\Delta t_{i,j} / V_{i,j} \left[\left(\left(E_e\right)_{p_{i,j-1}} S_{x\,i,j-1/2} + \left(F_e\right)_{p_{i,j-1}} S_{y\,i,j-1/2}\right) + \left(\left(E_e\right)_{p_{i,j}} S_{x\,i+1/2,j} + \left(F_e\right)_{p_{i,j}} S_{y\,i+1/2,j}\right) + \right. \\ \left. \left(\left(E_e\right)_{p_{i,j}} S_{x\,i,j+1/2} + \left(F_e\right)_{p_{i,j}} S_{y\,i,j+1/2}\right) + \left(\left(E_e\right)_{p_{i-1,j}} S_{x\,i-1/2,j} + \left(F_e\right)_{p_{i-1,j}} S_{y\,i-1/2,j}\right)\right];\end{aligned} \tag{9}$$

$$Q_{i,j}^{n+1} = 0.5\left(Q_{i,j}^{n} + Q_{p\,i,j}^{n+1} + \Delta Q_{c\,i,j}^{n+1}\right). \tag{10}$$

To guarantee numerical stability to the MacCormack (1969) scheme, an artificial dissipation operator of second differences (Maciel, 2006a) is subtracted from the RHS flux terms in the corrector step aiming to eliminate instabilities originated from shock waves. The operator is of $D = d_{i,j}^{(2)}$ type, defined in section **6.1**, where $A_{i,j} = V_{i,j} / \Delta t_{i,j}$ is assumed, which defines the artificial dissipation operator of Azevedo (1992). The value used to K_2 was 0.06.

4. HARTEN (1983) ALGORITHM

The Harten (1983) algorithm, second order accurate in space, is specified by the determination of the numerical flux vector at *(i+½,j)* interface.

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

$$V_R = V_{i+1,j}\,,\;\; V_L = V_{i,j} \;\;\text{and}\;\; V_{\text{int}} = 0.5\left(V_R + V_L\right), \tag{11}$$

in which "*R*" and "*L*" represent right and left, respectively. The metric terms to this generalized coordinate system are defined as:

$$h_x = S_{x\_\text{int}}/V_{\text{int}}\,,\;\; h_y = S_{y\_\text{int}}/V_{\text{int}} \;\;\text{and}\;\; h_n = S/V_{\text{int}}\,. \tag{12}$$

The cell volume and the interface area components, S_{x_int} and S_{y_int}, are defined in Maciel (2006b).

The properties calculated at the flux interface are obtained either by arithmetical average or by Roe (1981) average. In this work, the arithmetical average was used. The speed of sound at the interface is determined by $a_{\text{int}} = \sqrt{(\gamma-1)\left[H_{\text{int}} - 0.5\left(u_{\text{int}}^2 + v_{\text{int}}^2\right)\right]}$, where H_{int}, u_{int} and v_{int} are the flux interface properties. The eigenvalues of the Euler equations, in the ξ direction, are given by:

$$U_{cont} = u_{\text{int}} h_x + v_{\text{int}} h_y\,,\;\; \lambda_1 = U_{cont} - a_{\text{int}} h_n\,,\;\; \lambda_2 = \lambda_3 = U_{cont} \;\;\text{and}\;\; \lambda_4 = U_{cont} + a_{\text{int}} h_n\,. \tag{13}$$

The jumps of the conserved variables, necessary to the construction of the Harten (1983) dissipation function, are given by:

$$\Delta e = V_{\text{int}}\left(e_R - e_L\right),\; \Delta\rho = V_{\text{int}}\left(\rho_R - \rho_L\right),\; \Delta(\rho u) = V_{\text{int}}\left[(\rho u)_R - (\rho u)_L\right] \;\text{and}\; \Delta(\rho v) = V_{\text{int}}\left[(\rho v)_R - (\rho v)_L\right]; \tag{14}$$

The α vectors at the *(i+½,j)* interface are calculated by the following expressions:

$$\alpha^1 = 0.5(aa - bb),\; \alpha^2 = \Delta\rho - aa\,,\; \alpha^3 = cc \;\;\text{and}\;\; \alpha^4 = 0.5(aa + bb), \tag{15}$$

with:

$$aa = \frac{(\gamma-1)}{a_{\text{int}}^2}\left[\Delta e + 0.5\left(u_{\text{int}}^2 + v_{\text{int}}^2\right)\Delta\rho - u_{\text{int}}\Delta(\rho u) - v_{\text{int}}\Delta(\rho v)\right]; \tag{16}$$

$$bb = \frac{1}{a_{\text{int}}}\left[h_x'\Delta(\rho u) - \left(h_x' u_{\text{int}} + h_y' v_{\text{int}}\right)\Delta\rho + h_y'\Delta(\rho v)\right]; \tag{17}$$

$$cc = h_x'\Delta(\rho v) + \left(h_y' u_{\text{int}} - h_x' v_{\text{int}}\right)\Delta\rho - h_y'\Delta(\rho u); \tag{18}$$

$$h_x' = h_x/h_n \;\;\text{and}\;\; h_y' = h_y/h_n\,. \tag{19}$$

The Harten (1983) dissipation function uses the right-eigenvector matrix associated with the Euler Jacobian matrix in the normal flux direction:

$$R_{i+1/2,j} = \begin{bmatrix} 1 & 1 & 0 & 1 \\ u_{\text{int}} - h_x' a_{\text{int}} & u_{\text{int}} & -h_y' & u_{\text{int}} + h_x' a_{\text{int}} \\ v_{\text{int}} - h_y' a_{\text{int}} & v_{\text{int}} & h_x' & v_{\text{int}} + h_y' a_{\text{int}} \\ H_{\text{int}} - h_x' u_{\text{int}} a_{\text{int}} - h_y' v_{\text{int}} a_{\text{int}} & 0.5\left(u_{\text{int}}^2 + v_{\text{int}}^2\right) & h_x' v_{\text{int}} - h_y' u_{\text{int}} & H_{\text{int}} + h_x' u_{\text{int}} a_{\text{int}} + h_y' v_{\text{int}} a_{\text{int}} \end{bmatrix}, \tag{20}$$

The entropy condition is implemented defining the ψ_l entropy function as:

$$\nu_l = \Delta t\lambda_l = Z_l \;\;\text{and}\;\; \psi_l = \begin{cases} |Z_l|, & \text{if } |Z_l| \geq \delta_f \\ 0.5\left(Z_l^2 + \delta_f^2\right)/\delta_f\,, & \text{if } |Z_l| < \delta_f \end{cases}; \tag{21}$$

where "*l*" varies from 1 to 4 (two-dimensional space) and δ_f assuming values between 0.1 and 0.5, being 0.2 the value recommended by Harten (1983).

The $\tilde{g}$ function at the *(i+½,j)* interface is defined by:

$$\tilde{g}^l = 0.5\left(\psi_l - Z_l^2\right)\alpha^l . \tag{22}$$

The *g* numerical flux function, which is a limited function to avoid the formation of new extremes in the solution and is responsible to the second order of accuracy of the scheme, is given by:

$$g_{i,j}^l = signal_l \times MAX\left(0.0; MIN\left(\left|\tilde{g}_{i+1/2,j}^l\right|, \tilde{g}_{i-1/2,j}^l \times signal_l\right)\right), \tag{23}$$

where $signal_l$ is equal to 1.0 if $\tilde{g}_{i+1/2,j}^l \geq 0.0$ and -1.0 otherwise. The numerical characteristic speed φ_l at the *(i+½,j)* interface, responsible to propagate the numerical information associated with the g numerical flux function, is defined by:

$$\varphi_l = \begin{cases} \left(g_{i+1,j}^l - g_{i,j}^l\right)/\alpha^l, & if\ \alpha^l \neq 0.0 \\ 0.0, & if\ \alpha^l = 0.0 \end{cases}. \tag{24}$$

The entropy function, responsible to guarantee that only relevant physical solutions are to be considered, is redefined considering φ_l: $Z_l = \nu_l + \varphi_l$, and ψ_l is recalculated according to Eq. (21). Finally, the Harten (1983) dissipation function, to second order spatial accuracy, is constructed by the following matrix-vector product:

$$\left\{D_{Harten}\right\}_{i+1/2,j} = \left[R\right]_{i+1/2,j}\left\{\left(g_{i,j} + g_{i+1,j} - \psi\alpha\right)/\Delta t_{i,j}\right\}_{i+1/2,j} . \tag{25}$$

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

$$F_{i+1/2,j}^{(l)} = \left(E_{\text{int}}^{(l)} h_x + F_{\text{int}}^{(l)} h_y\right) V_{\text{int}} + 0.5 D_{Harten}^{(l)}, \text{ with: } E_{\text{int}}^{(l)} = 0.5\left(E_R^{(l)} + E_L^{(l)}\right) \text{ and } F_{\text{int}}^{(l)} = 0.5\left(F_R^{(l)} + F_L^{(l)}\right). \tag{26}$$

The 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:

$$\Delta Q_{i,j}^* = -\Delta t_{i,j}/V_{i,j}\left(F_{i+1/2,j}^n - F_{i-1/2,j}^n\right) \text{ and } Q_{i,j}^* = Q_{i,j}^n + \Delta Q_{i,j}^* ; \tag{27}$$

and in the final step:

$$\Delta Q_{i,j}^{n+1} = -\Delta t_{i,j}/V_{i,j}\left(F_{i,j+1/2}^* - F_{i,j-1/2}^*\right) \text{ and } Q_{i,j}^{n+1} = Q_{i,j}^* + \Delta Q_{i,j}^{n+1} . \tag{28}$$

5. YEE AND KUTLER (1985) ALGORITHM

The Yee and Kutler (1985) algorithm, second order accurate in space, follows Eqs. (11) to (20). The next step consists in determining the θ function, which corresponds to the artificial compression term and is responsible to enhance the resolution of the scheme at discontinuities.

$$\theta_{i,j}^l = \begin{cases} \dfrac{\left|\alpha_{i+1/2,j}^l - \alpha_{i-1/2,j}^l\right|}{\alpha_{i+1/2,j}^l + \alpha_{i-1/2,j}^l}, & if\ \left(\alpha_{i+1/2,j}^l + \alpha_{i-1/2,j}^l\right) \neq 0.0 \\ 0.0, & if\ \left(\alpha_{i+1/2,j}^l + \alpha_{i-1/2,j}^l\right) = 0.0 \end{cases}. \tag{29}$$

The κ function at the *(i+½,j)* interface is defined as follows:

$$\kappa_l = 1/8\left(1 + \omega_l MAX\left(\theta_{i,j}^l, \theta_{i+1,j}^l\right)\right), \tag{30}$$

in which ω_l assumes the following values: $\omega_1 = \omega_4 = 0.25$ (non-linear field), $\omega_2 = \omega_3 = 1.0$ (linear field).

The *g* numerical flux function is determined by:

$$g_{i,j}^{l} = signal_l \times MAX\left(0.0; MIN\left(\left|\alpha_{i+1/2,j}^{l}\right|, \alpha_{i-1/2,j}^{l} \times signal_l\right)\right), \tag{31}$$

where $signal_l$ assumes value 1.0 if $\alpha_{i+1/2,j}^{l} \geq 0.0$ and -1.0 otherwise. The φ_l function at the *(i+½,j)* interface is calculated by the following expression:

$$\varphi_l = \begin{cases} \kappa_l \left(g_{i+1,j}^{l} - g_{i,j}^{l}\right) / \alpha^l, & if\ \alpha^l \neq 0.0 \\ 0.0, & if\ \alpha^l = 0.0 \end{cases}. \tag{32}$$

The ψ_l entropy function at the *(i+½,j)* interface is defined by:

$$\psi_l = \left(\nu_l + \varphi_l\right)^2 + 0.25\,, \tag{33}$$

with ν_l defined according to Eq. (21). Finally, the Yee and Kutler (1985) dissipation function, to second order spatial accuracy, is constructed by the following matrix-vector product:

$$\left\{D_{Yee/Kutler}\right\}_{i+1/2,j} = \left[R\right]_{i+1/2,j} \left\{\left(\kappa\left(g_{i,j} + g_{i+1,j}\right) - \varphi\alpha\right) / \Delta t_{i,j}\right\}_{i+1/2,j}. \tag{34}$$

Equation (26) is used to conclude the numerical flux vector of Yee and Kutler (1985) scheme and the time integration is performed by the time splitting method defined by Eqs (27) and (28).

6. JAMESON AND MAVRIPLIS (1986) ALGORITHM

Equation (5) can be rewritten following a structured discretization context (Jameson, Schmidt and Turkel, 1981, and Jameson and Mavriplis, 1986) as:

$$d\left(V_{i,j} Q_{i,j}\right) / dt + C(Q_{i,j}) = 0\,, \tag{35}$$

where:

$$\begin{aligned} C(Q_{i,j}) = {} & \left[E_e(Q_{i,j-1/2}) S_{x_{i,j-1/2}} + F_e(Q_{i,j-1/2}) S_{y_{i,j-1/2}}\right] + \left[E_e(Q_{i+1/2,j}) S_{x_{i+1/2,j}} + F_e(Q_{i+1/2,j}) S_{y_{i+1/2,j}}\right] + \\ & \left[E_e(Q_{i,j+1/2}) S_{x_{i,j+1/2}} + F_e(Q_{i,j+1/2}) S_{y_{i,j+1/2}}\right] + \left[E_e(Q_{i-1/2,j}) S_{x_{i-1/2,j}} + F_e(Q_{i-1/2,j}) S_{y_{i-1/2,j}}\right] \end{aligned} \tag{36}$$

is the discrete approximation of the flux integral of Eq. (5). In this work, it was adopted that, for example, the values of primitive variables at the *(i,j-1/2)* flux interface are obtained from the arithmetical average between the values of the primitive variables in the *(i,j)* volume and in the *(i,j-1)* volume.

The spatial discretization proposed by the authors is equivalent to a symmetrical scheme with second order accuracy, on a finite difference context. The introduction of an artificial dissipation operator "D" is necessary to guarantee the numerical stability of the scheme in the presence of, for example, odd-even uncoupled solutions and nonlinear instabilities, like shock waves. So, Equation (35) is rewritten as:

$$d\left(V_{i,j} Q_{i,j}\right) / dt + \left[C(Q_{i,j}) - D(Q_{i,j})\right] = 0\,. \tag{37}$$

The time integration is performed using a hybrid explicit Runge-Kutta method of five stages, with second order accuracy, and can be represented in general form as:

$$\begin{aligned} & Q_{i,j}^{(0)} = Q_{i,j}^{(n)} \\ & Q_{i,j}^{(k)} = Q_{i,j}^{(0)} - \alpha_k\, \Delta t_{i,j} / V_{i,j} \left[C\left(Q_{i,j}^{(k-1)}\right) - D\left(Q_{i,j}^{(m)}\right)\right], \\ & Q_{i,j}^{(n+1)} = Q_{i,j}^{(k)} \end{aligned} \tag{38}$$

where $k = 1,...,5$; $m = 0$ until 4; $\alpha_1 = 1/4$, $\alpha_2 = 1/6$, $\alpha_3 = 3/8$, $\alpha_4 = 1/2$ and $\alpha_5 = 1$. Jameson and Mavriplis (1986) suggests that the artificial dissipation operator should only be evaluated in the first two stages when the Euler equations were solved ($m = 0$, $k = 1$ and $m = 1$, $k = 2$). This procedure aims CPU time economy and also better smoothing of the numerical instabilities of the discretization based on the hyperbolic characteristics of the Euler equations.

6.1. Artificial dissipation operator

The artificial dissipation operator implemented in the Jameson and Mavriplis (1986) scheme is based on Mavriplis (1990) model and has the following structure:

$$D\left(Q_{i,j}\right) = d^{(2)}\left(Q_{i,j}\right) - d^{(4)}\left(Q_{i,j}\right) , \tag{39}$$

where:

$$\begin{aligned} d^{(2)}\left(Q_{i,j}\right) = {} & 0.5\varepsilon^{(2)}_{i,j-1/2}\left(A_{i,j} + A_{i,j-1}\right)\left(Q_{i,j-1} - Q_{i,j}\right) + 0.5\varepsilon^{(2)}_{i+1/2,j}\left(A_{i,j} + A_{i+1,j}\right)\left(Q_{i+1,j} - Q_{i,j}\right) + \\ & 0.5\varepsilon^{(2)}_{i,j+1/2}\left(A_{i,j} + A_{i,j+1}\right)\left(Q_{i,j+1} - Q_{i,j}\right) + 0.5\varepsilon^{(2)}_{i-1/2,j}\left(A_{i,j} + A_{i-1,j}\right)\left(Q_{i-1,j} - Q_{i,j}\right), \end{aligned} \tag{40}$$

named undivided Laplacian operator, is responsible to the numerical stability in the presence of shock waves; and

$$\begin{aligned} d^{(4)}\left(Q_{i,j}\right) = {} & 0.5\varepsilon^{(4)}_{i,j-1/2}\left(A_{i,j} + A_{i,j-1}\right)\left(\nabla^2 Q_{i,j-1} - \nabla^2 Q_{i,j}\right) + 0.5\varepsilon^{(4)}_{i+1/2,j}\left(A_{i,j} + A_{i+1,j}\right)\left(\nabla^2 Q_{i+1,j} - \nabla^2 Q_{i,j}\right) + \\ & 0.5\varepsilon^{(4)}_{i,j+1/2}\left(A_{i,j} + A_{i,j+1}\right)\left(\nabla^2 Q_{i,j+1} - \nabla^2 Q_{i,j}\right) + 0.5\varepsilon^{(4)}_{i-1/2,j}\left(A_{i,j} + A_{i-1,j}\right)\left(\nabla^2 Q_{i-1,j} - \nabla^2 Q_{i,j}\right), \end{aligned} \tag{41}$$

named bi-harmonic operator, is responsible by the background stability (for example, instabilities originated from odd-even uncoupled solutions). In this last term,

$$\nabla^2 Q_{i,j} = \left(Q_{i,j-1} - Q_{i,j}\right) + \left(Q_{i+1,j} - Q_{i,j}\right) + \left(Q_{i,j+1} - Q_{i,j}\right) + \left(Q_{i-1,j} - Q_{i,j}\right). \tag{42}$$

In the operator $d^{(4)}$, $\nabla^2 Q_{i,j}$ is extrapolated from its real neighbor every time that it represents a special boundary cell, recognized in the literature as "ghost" cell. The ε terms are defined, for example, as:

$$\varepsilon^{(2)}_{i,j-1/2} = K^{(2)} MAX\left(\nu_{i,j}, \nu_{i,j-1}\right) \quad \text{and} \quad \varepsilon^{(4)}_{i,j-1/2} = MAX\left[0, \left(K^{(4)} - \varepsilon^{(2)}_{i,j-1/2}\right)\right], \tag{43}$$

with:

$$\nu_{i,j} = \left(\left|p_{i,j-1} - p_{i,j}\right| + \left|p_{i+1,j} - p_{i,j}\right| + \left|p_{i,j+1} - p_{i,j}\right| + \left|p_{i-1,j} - p_{i,j}\right|\right) \Big/ \sum_{k=1}^{4}\left(p_{i,j-1} + p_{i+1,j} + p_{i,j+1} + p_{i-1,j} + 4p_{i,j}\right) \tag{44}$$

representing a pressure sensor employed to identify regions of high gradients. The constants $K^{(2)}$ and $K^{(4)}$ has typical values of 1/4 and 3/256, respectively. Every time that a neighbor represents a ghost cell, it is assumed that, for example, $\nu_{ghost} = \nu_{i,j}$. The $A_{i,j}$ terms are contributions of the maximum normal eigenvalue of the Euler equations integrated along each cell face. Based on Mavriplis (1990) work, these terms are defined as:

$$\begin{aligned} A_{i,j} = {} & \left[\left|0.5\left(u_{i,j} + u_{i,j-1}\right)S_{x_{i,j-1/2}} + 0.5\left(v_{i,j} + v_{i,j-1}\right)S_{y_{i,j-1/2}}\right| + 0.5\left(a_{i,j} + a_{i,j-1}\right)\left(S^2_{x_{i,j-1/2}} + S^2_{y_{i,j-1/2}}\right)^{0.5}\right] + \\ & \left[\left|0.5\left(u_{i,j} + u_{i+1,j}\right)S_{x_{i+1/2,j}} + 0.5\left(v_{i,j} + v_{i+1,j}\right)S_{y_{i+1/2,j}}\right| + 0.5\left(a_{i,j} + a_{i+1,j}\right)\left(S^2_{x_{i+1/2,j}} + S^2_{y_{i+1/2,j}}\right)^{0.5}\right] + \\ & \left[\left|0.5\left(u_{i,j} + u_{i,j+1}\right)S_{x_{i,j+1/2}} + 0.5\left(v_{i,j} + v_{i,j+1}\right)S_{y_{i,j+1/2}}\right| + 0.5\left(a_{i,j} + a_{i,j+1}\right)\left(S^2_{x_{i,j+1/2}} + S^2_{y_{i,j+1/2}}\right)^{0.5}\right] + \\ & \left[\left|0.5\left(u_{i,j} + u_{i-1,j}\right)S_{x_{i-1/2,j}} + 0.5\left(v_{i,j} + v_{i-1,j}\right)S_{y_{i-1/2,j}}\right| + 0.5\left(a_{i,j} + a_{i-1,j}\right)\left(S^2_{x_{i-1/2,j}} + S^2_{y_{i-1/2,j}}\right)^{0.5}\right], \end{aligned} \tag{45}$$

where "a" represents the speed of sound.

7. 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:

$$\Delta t_{i,j} = CFL(\Delta s)_{i,j} / c_{i,j} \ , \tag{46}$$

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 $(\Delta s)_{i,j}$ is a characteristic length of information transport. On a finite volume context, $(\Delta s)_{i,j}$ 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.

8. INITIAL AND BOUNDARY CONDITIONS

8.1. Initial conditions

Stagnation values are used as initial condition to the nozzle problem. Only at the exit boundary is imposed a reduction of 1/3 to the density and to the pressure to start the flow along the nozzle. The vector of conserved variables is defined as:

a) Domain except the nozzle exit:

$$Q = \left\{ 1 \quad 0 \quad 0 \quad (\gamma + 1) / [2\gamma(\gamma - 1)] \right\}^t ; \tag{47}$$

b) Nozzle exit:

$$Q = \left\{ 1/3 \quad 0 \quad 0 \quad (\gamma + 1) / [6\gamma(\gamma - 1)] \right\}^t . \tag{48}$$

To the others problems, values of freestream flow are adopted for all properties as initial condition, in the whole calculation domain:

$$Q_\infty = \left\{ 1 \quad M_\infty \cos\theta \quad M_\infty sen\theta \quad \left[1/[\gamma(\gamma - 1)] + 0.5 M_\infty^2 \right] \right\}^t , \tag{49}$$

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

8.2. Boundary conditions

The boundary conditions are basically of four types: solid wall, entrance, exit and continuity. 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 "$(q_n\text{-}a)$" velocity can not be specified and should be determined by interior information of the calculation domain. The u velocity component was the extrapolated variable from the real neighbor volume to the nozzle problem, while the pressure was the extrapolated variable to the others problems. Density and pressure had their values determined by isentropic relations in the nozzle problem, while density and velocity

components had their values determined by the freestream flow properties in the others problems. 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_n-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.
(d) Continuity condition: Just for the airfoil physical problem. It is necessary that the continuity of the flow at the trailing edge should be satisfied (Kutta condition). This condition is assured by imposing that the vector of conserved variables at the lower body surface should be equal to the vector of conserved variables at the upper body surface.

9. CONCLUSIONS

The present work compares the MacCormack (1969), the Harten (1983), the Yee and Kutler (1985) and the Jameson and Mavriplis (1986) numerical methods, using a finite volume formulation and a structured spatial discretization, applied to the solution of the Euler equations in the two-dimensional space. All schemes are second order accurate in space. The MacCormack (1969) and the Jameson and Mavriplis (1986) schemes are also second order accurate in time and both use artificial dissipation operators to guarantee the convergence to the steady state solution. The Harten (1983) and the Yee and Kutler (1985) schemes are first order accurate in time. The steady state physical problems of the transonic flows along a convergent-divergent nozzle and around a NACA 0012 airfoil, the supersonic flow along a ramp and the "cold gas" hypersonic flow around a double ellipse configuration are studied. A spatially variable time step is implemented aiming to accelerate the convergence process. This technique has proved excellent gains in terms of convergence ratio as reported in Maciel (2005).

The results have demonstrated that the MacCormack scheme predicts the most critical solutions, although unphysical results were obtained in high Mach numbers. The pressure ratio at the shock, nozzle problem, and the stagnation pressure, double ellipse problem, were best estimated by the MacCormack (1969) scheme.

This paper is concerned with the theories related to the numerical implementation of the schemes, consisting in part I (THEORY) of this study. The part II (RESULTS) presents the solutions of the numerical simulations, comparisons between numerical and experimental or theoretical results and computational data.

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