ANALYSIS OF CONVERGENCE ACCELERATION TECHNIQUES USED IN UNSTRUCTURED ALGORITHMS IN THE SOLUTION OF AEROSPACE PROBLEMS – PART II

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Abstract. This work is the second part of the study that deals with convergence acceleration techniques applied to the solution of steady state problems. Techniques like spatially variable time step, implicit residual smoothing, enthalpy damping and increase of the CFL number during iterative process are studied. The Jameson and Mavriplis explicit algorithm, with symmetrical spatial discretization and the artificial dissipation operator of Mavriplis, is implemented to perform the two-dimensional numerical experiments. This scheme is second order accurate in space. The Euler equations in conservative form, employing a finite volume formulation and an unstructured spatial discretization, are solved. The techniques are studied and compared with themselves in the solution of the physical problem of the supersonic flow around a blunt body, with zero attack angle. The employed time march is the Runge-Kutta method of five stages and second order. The results have shown that the best studied techniques were the spatially variable time step and the implicit residual smoothing, having good convergence gains, moderate computational costs and more regular behavior. These techniques also presented good behavior in the first paper of this series, where the enthalpy damping was the best. An analysis of the computational performances of the techniques is accomplished (cost, maximum CFL number and iterations to convergence).

Keywords: Spatially variable time step, Implicit residual smoothing, Enthalpy damping, Increase of CFL, Unstructured algorithm.

1. INTRODUCTION

A point of great research in CFD, Computational Fluid Dynamics, is the development of convergence acceleration techniques to steady state problems. The great amount of aerodynamics data required for aeronautical and aerospace vehicle projects are obtained from these problems: Kutler (1985) and Long and Radespiel (1991). Convergence acceleration techniques always were great objectives of CFD following the development of fluid mechanics equation solvers. A great amount of techniques were elaborated and several works tried to develop convergence acceleration computational tools which produces more efficient and, at the same time, less expensive codes.

On the context of convergence gains, an efficient technique that raised to numerical calculation was the "multigrid" procedure. Such technique was initially presented to obtain solutions of problems involving elliptic partial differential equations (Brandt, 1981) and, posteriorly, was extended to hyperbolic partial differential equations. Some works that used this procedure were: Jameson and Mavriplis (1986) and Radespiel (1989).

Techniques of convergence acceleration simpler and less expensive to explicit and implicit schemes, when applied to the solution of fluid mechanics equations, also were studied: spatially variable time step, enthalpy damping, residual smoothing and increase of CFL number during the iterative process. The spatially variable time step aims to use the maximum time step allowed by a local stability limit in each computational cell. This technique was initially applied by Jameson, Schmidt and Turkel (1981). Other works that used such technique were: Jameson and Yoon (1986) and Mavriplis (1990).

The enthalpy damping strategy is based on the fact that the Euler equations are inviscid and the total enthalpy keeps constant in all computational domain when the steady state is reached and the mass and the energy equations are satisfied. Forcing terms proportional to the difference between local total enthalpy and the freestream total enthalpy are added to the mass, momentum and energy conservation equations, aiming to accelerate the convergence process to steady state condition. This procedure was suggested by Jameson, Schmidt and Turkel (1981). Others works were: Jameson and Mavriplis (1986) and Baruzzi, Habashi and Hafez (1991).

The maximum time step that can be used is limited by the CFL condition (Courant, Friedrichs and Lewy, 1928), which defines that the dependence domain of the discretized equations need no minimal contains the dependence domain of the original differential equation. To reduce this restriction, an implicit residual smoothing is developed to increase the scheme stability. Such strategy consists in determining an average residual value, weighted by neighbor residual values. This technique was introduced by Jameson and Mavriplis (1986) work. Others works were: Mavriplis (1990) and Luo, Baum and Löhner (1994).

Other convergence acceleration technique simpler than the others is the increase of the CFL number during the convergence process to reach steady state. This technique consists in increasing the CFL number all time that a prescribed number of iterations are reached. The user determines the number of iterations to increase the CFL as the increase value to be considered too.

Maciel (2005), the first paper of this series, studied four convergence acceleration techniques applied to the solution of steady state problems. Techniques like spatially variable time step, implicit residual smoothing, enthalpy damping and increase of the CFL number during iterative process were studied. The Jameson and Mavriplis explicit algorithm, with symmetrical spatial discretization and the artificial dissipation operator of Mavriplis, was implemented to perform the two-dimensional numerical experiments. The scheme is second order accurate in space. The Euler equations in conservative form, employing a finite volume formulation and an unstructured spatial discretization were solved. The techniques were studied and compared with themselves in the solution of the physical problem of the transonic flow around a NACA 0012 airfoil, with zero angle of attack. The employed time marching algorithm was the Runge-Kutta method of five stages and second order. The results have shown that the best technique studied was enthalpy damping, having better convergence gain than the others and have moderate computational cost.

This work is the second part of the study started with Maciel (2005) that presents some convergence acceleration techniques generally applied to CFD community. The objective of this paper, as in the first paper of this series, is to present the best results obtained, in terms of convergence ratio and computational cost, with the studied techniques. The spatially variable time step, the implicit residual smoothing, the enthalpy damping and the increase of the CFL number are again studied. The Jameson and Mavriplis (1986) scheme, on an unstructured context, is again used to generate the numerical results to comparison. Tests with a convergent-divergent nozzle and a double ellipse configuration, involving transonic and "cold gas" hypersonic flows, respectively, are performed. The results have indicated that the spatially variable time step and the implicit residual smoothing are the best choices due to the most regular behavior among the studied techniques and the meaningful computational gains. These techniques also presented good behavior in the first paper of this series, where the enthalpy damping was the best.

2. EULER EQUATIONS

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

$$\partial/\partial t \int_{V} Q dV + \int_{S} \left(E_{e} n_{x} + F_{e} n_{y} \right) dS = 0 , \qquad (1)$$

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

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

where ρ is 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 unity volume; and p is the static pressure.

The nondimensionalization applied to the Euler equations for all problems was accomplished in relation to the freestream density, ρ_{∞} , and the freestream speed of sound, a_{∞} . Hence, the density is nondimensionalized in relation to ρ_{∞} , the velocity components u and v are nondimensionalized in relation to a_{∞} and the pressure and the total energy are nondimensionalized in relation to the product $\rho_{\infty}(a_{\infty})^2$. The matrix system of the Euler equations is closed using the perfect gas state equation $p = (\gamma - 1)[e - 0.5\rho(u^2 + v^2)]$, with γ being the ratio of specific heats. The total enthalpy is determined by $h = [\gamma/(\gamma - 1)](p/\rho) + 0.5(u^2 + v^2)$.

3. JAMESON AND MAVRIPLIS (1986) ALGORITHM

The Euler equations in conservative and integral forms, according to a finite volume formulation, can be written, on a context of unstructured spatial discretization (Jameson, Schmidt and Turkel, 1981, Jameson and Mavriplis, 1986, and Maciel, 2002), as:

$$d(V_iQ_i)/dt + C(Q_i) = 0, (3)$$

where $C(Q_i) = \sum_{k=1}^{3} \left[E_e(Q_{i,k}) \Delta y_{i,k} - F_e(Q_{i,k}) \Delta x_{i,k} \right]$ is the discrete approximation to the flux integral of Eq. (1). The cell

volume is defined in Maciel (2002). In this work, it was adopted that:

$$Q_{i,k} = 0.5(Q_i + Q_k), \quad \Delta y_{i,k} = y_{n2} - y_{n1} \text{ and } \Delta x_{i,k} = x_{n2} - x_{n1},$$
 (4)

with "i" indicating a given mesh volume and "k" being its respective neighbor; and n1 and n2 represent consecutive nodes of volume "i", in counter-clockwise orientation.

The spatial discretization proposed by the authors is equivalent to a centered scheme with second order of accuracy, on a finite difference context. The introduction of a dissipation operator "D" is necessary to guarantee numerical stability in the presence, for example, of even-odd uncoupled solutions and nonlinear instabilities, like shock waves. So, Equation (3) is rewritten as:

$$d(V_iQ_i)/dt + [C(Q_i) - D(Q_i)] = 0.$$
(5)

The time integration is accomplished using a Runge-Kutta explicit method of second order and five stages and can be represented in generalized form as:

$$Q_{i}^{(0)} = Q_{i}^{(n)}$$

$$Q_{i}^{(k)} = Q_{i}^{(0)} - \alpha_{k} \Delta t_{i} / V_{i} \Big[C(Q_{i}^{(k-1)}) - D(Q_{i}^{(m)}) \Big],$$

$$Q_{i}^{(n+1)} = Q_{i}^{(k)}$$
(6)

where k = 1,...,5; m = 0 to 4; $\alpha_1 = 1/4$, $\alpha_2 = 1/6$, $\alpha_3 = 3/8$, $\alpha_4 = 1/2$ e $\alpha_5 = 1$. The artificial dissipation operator should be evaluated only in the first two stages (m = 0, k = 1, e m = 1, k = 2), aiming CPU time economy, according to Jameson and Mavriplis (1986). It is "frozen" for the reminiscent stages, exploring the hyperbolic properties of the Euler equations, aiming to guarantee steady state condition.

3.1. Artificial dissipation operator

The artificial dissipation operator employed in this work is based on Mavriplis (1990) and can be described as:

$$D(Q_i) = d^{(2)}(Q_i) - d^{(4)}(Q_i), \tag{7}$$

where: $d^{(2)}(Q_i) = \sum_{k=1}^{3} 0.5 \varepsilon_{i,k}^{(2)} (A_i + A_k) (Q_k - Q_i)$, named undivided laplacian operator, is responsible to the numerical

stability in the presence of shock waves; and $d^{(4)}(Q_i) = \sum_{k=1}^3 0.5 \varepsilon_{i,k}^{(4)} (A_i + A_k) (\nabla^2 Q_k - \nabla^2 Q_i)$, named bi-harmonic operator, is responsible to the background stability (for example, even-odd uncoupled instabilities). In this last term, $\nabla^2 Q_i = \sum_{k=1}^3 (Q_k - Q_i)$. Every time that "k" represents a special boundary cell, named "ghost" cell, its contribution in terms of $\nabla^2 Q_k$ is extrapolated from its real neighbor volume. The ε terms are defined as:

$$\varepsilon_{i,k}^{(2)} = K^{(2)} MAX \left(\mathbf{v}_i, \mathbf{v}_k \right) \text{ and } \varepsilon_{i,k}^{(4)} = MAX \left[0, \left(K^{(4)} - \varepsilon_{i,k}^{(2)} \right) \right],$$
 (8)

where $v_i = \sum_{k=1}^{3} \left| p_k - p_i \right| / \sum_{k=1}^{3} \left(p_k + p_i \right)$ represents a pressure sensor. It is employed to identify regions of high gradients. $K^{(2)}$ and $K^{(4)}$ are constants and typical values are 1/4 and 3/256, respectively. Every time that "k" represents a ghost cell, $v_g = v_i$. The A_i terms are the sum of the contributions of the maximum normal eigenvalue of the Euler equations integrated along each cell face. They are defined as:

$$A_{i} = \sum_{k=1}^{3} \left[\left| u_{i,k} \Delta y_{i,k} - v_{i,k} \Delta x_{i,k} \right| + a_{i,k} \left(\Delta x_{i,k}^{2} + \Delta y_{i,k}^{2} \right)^{0.5} \right], \tag{9}$$

where $u_{i,k}$, $v_{i,k}$ and $a_{i,k}$ are calculated by arithmetical average between values of properties associated with volume "i" and its respective neighbour "k".

4. CONVERGENCE ACCELERATION TECHNIQUES

4.1. Spatially variable time step

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

$$\Delta t_{cell} = CFL(\Delta s)_{cell} / c_{cell} , \tag{10}$$

where CFL is the "Courant-Friedrichs-Lewy" number to provide numerical stability to the scheme; $c_{cell} = \left[\left(u^2 + v^2 \right)^{0.5} + a \right]_{cell}$ is the maximum characteristic velocity of information propagation in the calculation

domain; and $(\Delta s)_{cell}$ is a characteristic length of information propagation. On a finite volume context, $(\Delta s)_{cell}$ is chosen as the minimum value found between the centroid distance, involving cell "i" and its neighbor "k", and the minimum cell side length.

4.2. Implicit residual smoothing

The implicit residual smoothing technique employed in this work is based on Jameson and Mavriplis (1986) paper. The residual is initially defined as follows:

$$R(Q) = 1/V[C(Q) - D(Q)]. (11)$$

The smoothing is performed replacing the residual associated with a given computational cell by the average residual \overline{R} , obtained by the solution of the equation:

$$\overline{R} - \varepsilon \nabla^2 \overline{R} = R \,, \tag{12}$$

where to a cell centered data base,

$$\nabla^2 \overline{R} = \sum_{k=1}^{tnnc} (\overline{R}_k - \overline{R}), \tag{13}$$

with "k" being the index of the neighbor cell of the respective cell under study and "tnnc" is the total number of neighbor cells. The Equation (12) represents a diagonal dominant system and due to its high cost to solution, Jameson and Mavriplis (1986) suggest that a few iterations with the Jacobi method are sufficient to obtain residual smoothing. The resultant algorithm to the solution of Eq. (12) is written as:

$$(1 + tnnc \times \varepsilon)\overline{R}^{(m)} = R + \varepsilon \sum_{k=1}^{tnnc} \overline{R}_k^{(m-1)}, \qquad (14)$$

where $\overline{R}^{(0)}=R$. Jameson and Mavriplis (1986) suggest that only two iterations are necessary to solve Eq. (14), to steady state problems. These authors also suggest that the implicit residual smoothing should be accomplished in alternate stages of the time integration method with the purpose of computational cost reduction. The parameter ϵ assumes values between 0.0 and 1.0, 0.5 being the value suggested by Jameson and Mavriplis (1986).

4.3. Enthalpy damping

The enthalpy damping technique suggested by Jameson, Schmidt and Turkel (1981) paper is applied to the Euler equations in this work to accelerate the convergence process to steady state. In this technique, forcing terms proportional to the difference between the local total enthalpy and the freestream total enthalpy are added to each conservation equation. In this work, this procedure will be employed.

The conservation equation system is written as:

$$\partial/\partial t \int_{V} Q dV + \int_{S} \left(E_{e} n_{x} + F_{e} n_{y} \right) dS - \int_{V} Z dV = 0,$$

$$\tag{15}$$

where $Z = -(H - H_{\infty})\beta[\rho \quad \rho u \quad \rho v \quad \rho H]^t$ and β is an user specified coefficient. The forcing terms do not alter the steady state solution if the physical problem satisfies the constant total enthalpy condition.

In centered schemes, the artificial dissipation operator often introduces variations in the total enthalpy, which produces a non-conservative effect to this property. Mavriplis (1988) suggests that the artificial dissipation provided by the operator in the energy equation should be imposed to the total enthalpy " ρH " as conserved variable. It guarantees the constant total enthalpy in the field and allows the application of the enthalpy damping technique.

4.4. Increase of the CFL number

This procedure consists in increase the CFL number during the convergence process every time that a determined number of iterations is performed by the solver. The user specifies the number of iterations to increase the CFL number and its increase value too.

5. INITIAL AND BOUNDARY CONDITIONS

5.1. Initial condition

Values of freestream flow are adopted for all properties as initial condition for the blunt body problem, in the whole computational domain (Jameson and Mavriplis, 1986, and Maciel, 2002).

5.2. Boundary conditions

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

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

The normal pressure gradient of the fluid to the wall is assumed be equal to zero according to an inviscid formulation. The same hypothesis is applied to the normal temperature gradient to the wall. From these considerations, the density and pressure of the ghost volume are extrapolated from the respective values of its real neighbor volume (zero order extrapolation). 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 extrapolated, based on information propagation analysis along characteristic directions in the calculation domain (Maciel, 2002). In other words, to subsonic flow, three characteristic directions of propagation information point inward to the computational domain and should be fixed. Just the characteristic direction associated to the " $(q_n$ -a)" velocity can not be specified and should be determined by interior information from the calculation domain. The pressure was the extrapolated variable from the real neighbor volumes, for the studied problems. Density and velocity components adopted values of freestream flow. The total energy is determined by the state equation of a perfect gas.
- (b.2) Supersonic flow: All variables are fixed with values of freestream flow.
- (c) Exit condition:
- (c.1) Subsonic flow: Three characteristic directions of propagation information point outward to the computational domain. Hence, the associated variables should be extrapolated from interior information. The characteristic direction associated to the " $(q_n$ -a)" velocity should be specified because it point inward to the computational domain (Maciel, 2002). In this case, the ghost volume pressure is specified from its initial value. Density and velocity components are extrapolated and total energy is obtained from the state equation of a perfect gas.
- (c.2) Supersonic flow: All variables are extrapolated from interior domain due to all four characteristic directions of information propagation of the Euler equations point outward to the computational domain and nothing can be fixed.

6. RESULTS

Tests were performed in a CELERON-1.2GHz and 128 Mbytes of RAM memory microcomputer. Converged results occurred to 4 orders of reduction of the maximum residual value. The parameter γ assumed a value of 1.4. A zero attack angle was adopted for the blunt body problem.

The unstructured mesh was created transforming each rectangular cell of the given structured mesh into two triangular cells. All necessary tables were generated and a volume-based data structure was implemented. Although this procedure of mesh generation does not produce meshes with the best spatial discretization, meshes with reasonable quality have been obtained for the present problem.

An algebraic mesh of 103x100 points or composed of 20,196 triangular volumes and 10,300 nodes around the blunt body configuration was used. The far field boundary (entrance and exit boundaries) was located at 20.0 chords in relation to the configuration nose ratio.

The freestream Mach number adopted for the numerical simulation was 5.0, characterizing a supersonic flow regime. A CFL number of 2.0 was used by the Jameson and Mavriplis (1986) scheme, using a constant time step. The convergence was obtained in 826 iterations, with a computational cost of 0.0000186s/per volume/per iteration.

Figures 1 and 2 show the pressure and Mach number contours, while Fig. 3 and Fig. 4 show the -Cp distribution around the blunt body and the convergence history, respectively.

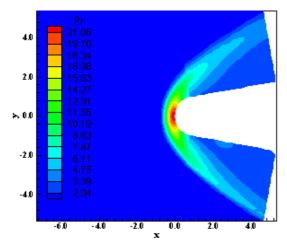


Figure 1. Pressure contours.

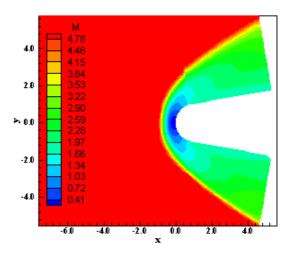


Figure 2. Mach number contours.

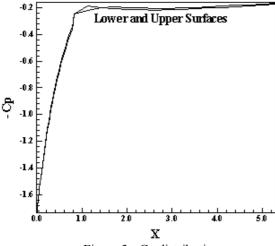


Figure 3. -Cp distribution.

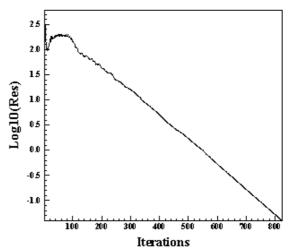


Figure 4. Convergence history.

6.1. Spatially variable time step

The spatially variable time step accelerated the convergence process of the Jameson and Mavriplis (1986) scheme. A CFL number of 1.5, less than that used to the constant time step case, was used and the convergence occurred in 503 iterations, with a computational cost of 0.0000558s/per volume/per iteration. This cost is about 200% more expensive than that obtained with the constant time step case. The CFL number equals to 1.5 was the maximum value allowed using the spatially variable time step technique. The gain in terms of iterations to convergence is of 39.1%. So, the computational cost is more expensive but there is a meaningful convergence gain.

6.2. Implicit residual smoothing

The time step was kept constant to use this technique and the residual smoothing was accomplished in odd stages of the time integration method.

The CFL number used was 2.0, kept constant during the numerical experiments. Table 1 shows the values of ϵ used and the number of convergence iterations. The best result occurred to $\epsilon = 0.14$, presenting convergence in 554 iterations. The computational cost of this technique is 0,0000581s/per volume/per iteration, which corresponds to about 212.4% more expensive than that used with a constant time step.

Table 1. Values of ε and the respective iterations to convergence.

Value of ε:	Iterations:	Value of ε:	Iterations:
0.10	610	0.12	581
0.13	567	0.14	554

The computational gain, taking into account the best performance, was 32.9 %, which is worse than that obtained with the spatially variable time step.

6.3. Enthalpy damping

The time step was kept constant during the simulations and a CFL number of 2.0 was used. Table 2 shows values of β with the respective number of iterations to reach the steady state condition. Values of β were adopted between 0.1 and 1.0. The maximum value of 1.0 to this parameter was determined aiming do not meaningfully alter the pressure and the Mach number fields. Although greater values of β can be used, meaningful modifications occur in the pressure and Mach number contours that alter the solution. However, only values of β varying from 0.0 to 0.6 are presented because no improvement in convergence gain was verified with values above 0.6.

Table 2. Values of β and the respective iterations to convergence.

Value of β:	Iterations:	Value of β:	Iterations:
0.10	966	0.40	1,323
0.20	1,092	0.50	1,431
0.30	1,210	0.60	1,537

As can be seen, no improvement in terms of convergence gain was verified, which limits this technique to just some problems were the enthalpy damping causes this gain. The reason for this unexpected result behavior can be that the total enthalpy is not totally conserved for this more severe problem. This situation can cause the convergence ratio degradation. The computational cost of this technique is 0.0000431s/per volume/per iteration, which is about 131.7% more expensive than that of the constant time step.

6.4. Increase of CFL

The increase of the CFL number procedure was employed to accelerate the convergence of the Jameson and Mavriplis (1986) scheme. The CFL number was again kept constant and the procedure was employed varying the number of iterations to increase the CFL number as well the step adopted to increase the CFL number (Δ CFL). The main characteristics of this study are indicated in Tab. 3.

Table 3. Main characteristics of the increase of CFL procedure.

Interactions to increase the CFL:	Value of the increase of CFL, ΔCFL:	Final CFL:	Iterations to convergence:
300	0.1	2.2	Divergence
350	0.1	2.2	738
350	0.2	2.2	Divergence
400	0.1	2.1	749
400	0.2	2.2	Divergence

As can be seen from Table 3, some improvement in terms of convergence gain is perceptible to the second and fourth cases. Other cases above 400 iterations to increase the CFL number converged to no more meaningful results.

The convergence gain to this procedure, taking into account the best case, was 10.7%, worse than the spatially variable time step and the implicit residual smoothing. The computational cost of this technique depends of the number of times that the CFL number is increased. To the best convergence gain obtained above, its computational cost is 0.0000422s/per volume/per iteration, which is 126.9% more expensive than the constant time step procedure.

7. CONCLUSIONS

In this work, the continuation of Maciel (2005), was presented four techniques of convergence acceleration implemented in the Jameson and Mavriplis (1986) scheme, on the context of unstructured discretization of the Euler equations. A constant time step solution, without any acceleration technique, was initially presented. Posteriorly, the techniques of spatially variable time step, implicit residual smoothing, enthalpy damping and increase of CFL were applied. The implicit residual smoothing, enthalpy damping and increase of CFL techniques were always applied considering a constant time step aiming to compare with initial results. The physical problem of the supersonic flow around a blunt body configuration was studied.

The numerical experiments have shown that the spatially variable time step and the implicit residual smoothing have presented good convergence properties and are the best choices in terms of convergence gain to supersonic steady state problems and of best regular properties (they both were more regular than the others because they always produced converged results and meaningful convergence gains).

Hence, the spatially variable time step, with a computational gain of 39.1%, and the implicit residual smoothing, with a computational gain of 32.9%, are the best choices in terms of acceleration techniques applied to supersonic flows, on an unstructured context. In relation to the first paper of this series, Maciel (2005), the spatially variable time step, 20.6% computational gain, and the implicit residual smoothing, 24.4% computational gain, also presented good convergence acceleration properties to transonic flows. As conclusion, in general terms, the spatially variable time step and the implicit residual smoothing are the recommended techniques to be applied to any flow problem.

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