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THREE DIMENSIONAL SIMULATION OF HIGH COMPRESSIBLE FLOWS USING A SUBCYCLING ALGORITHM FOR TIME INTEGRATION

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Abstract. *An algorithm to simulate 3-D high compressible flows using the finite element method and a multi-time-step integration technique with subcycles is presented in this work. An explicit two-step Taylor-Galerkin scheme is adopted to integrate in time continuum equations. When explicit schemes are used, the time steps must satisfy some stability conditions. If the smallest critical time-step is adopted uniformely for the whole domain, the integration scheme may consume a large amount of CPU time. Multi-time-step integration techniques are very suitable in these cases because elements and nodes are separated into several groups and a different time-step is assigned to each group. In this way, each group of elements is integrated with a time interval wich is much closer to the critical time steps of the elements in the group. This results in great computational savings, mainly when elements size and properties are very different, leading to significative differences of the local critical time steps values. Multi-time-steps integration techniques are also very useful in transient problems, taking into account that at the end of each subcycle, values of the unknowns at the same time level are obtained. The multi-time-step algorithm is applied to analyze the supersonic flow (Mach=8,5) past a sphere immersed in a non viscous flow, and results and computational performance are compared with those obtained when a uniformly time-step is used over the whole domain.*

Key words: *High compressible flows, Finite element simulation, Multi-time-step integration.*

1. INTRODUCTION

Multi-time-step integration techniques are very suitable aproaches when explicit schemes are involved in the numerical simulation of engineering problems. This is accomplished by separating the elements and nodes into groups and assigning a different time-step to each group. In this way, each group of elements is integrated with a time interval which is much closer to the critical time steps of the elements in the group. This results in great computational savings, mainly when elements size and properties are very different, leading to significative differences of the local critical time steps values.

A mixed time integration technique was first introduced by Belytschko and Mullen (1976) where they presented an "implicit-explicit" method for the second order equations which arise from the semidiscretization of the continuum equation and using a nodal partition. Hughes and Liu (1978) later introduced an "implicit-explicit" method which divided the mesh into groups of elements rather than nodes, using an element partition. An "explicit-explicit" subcycling procedure was then introduced by Belytschko, Yen and Mullen (1979), using nodal partition, where the groups of nodes were integrated explicitly with different time steps for each group.

Mixed time integration procedures for first order semidiscretization have also been proposed by Belytschko *et al.* (1985) and Smolinski *et al.* (1988). In all these previous methods, integer time-steps ratios are required, restricting sometimes the division of the mesh into more then just a few groups. Although Neal and Belytschko (1989) have relaxed the constrain of requiring integer time step ratios, (applying an "explicit-explicit" subcycling technique for structural dynamic systems), this last alternative may be convenient to vectorize and to parallelize the computer program, as indicated by Belytschko and Gilbertsen (1992).

A multi-time-step integration technique, similar to that used by Belytschko and Gilbertsen (1992) for structural dynamics problems, was implemented in this work to analyze 3-D high compressible flows using an explicit Taylor-Galerkin scheme with tetrahedral finite elements. This scheme was applied to analyze the supersonic flow past a sphere immersed in a non viscous fluid.

2. THE EXPLICIT TAYLOR-GALERKIN SCHEME

The equations expressing mass, momentum and energy conservation may be written in a compact form as

$$\frac{\partial \mathbf{V}}{\partial t} + \frac{\partial \mathbf{F}_i}{\partial x_i} = 0 \quad (i=1,2,3) \tag{1}$$

with $\mathbf{F}_i = \mathbf{F}_{iA} + \mathbf{F}_{iD}$ and

$$\mathbf{V} = \begin{Bmatrix} \rho \\ \rho \mathrm{v}_1 \\ \rho \mathrm{v}_2 \\ \rho \mathrm{v}_3 \\ \rho \varepsilon \end{Bmatrix} ; \quad \mathbf{F}_{iA} = \begin{Bmatrix} \rho \mathrm{v}_i \\ \rho \mathrm{v}_1 \mathrm{v}_i + p\,\delta_{i1} \\ \rho \mathrm{v}_2 \mathrm{v}_i + p\,\delta_{i2} \\ \rho \mathrm{v}_3 \mathrm{v}_i + p\,\delta_{i3} \\ \mathrm{v}_i (\rho\varepsilon + p) \end{Bmatrix} ; \quad \mathbf{F}_{iD} = \begin{Bmatrix} 0 \\ -\sigma_{1i} \\ -\sigma_{2i} \\ -\sigma_{3i} \\ -\sigma_{ij}\mathrm{v}_j - k_{ij}\,\partial T / \partial x_j \end{Bmatrix} \quad (i,j=1,2,3) \tag{2}$$

where v_i is the velocity component in the direction of the coordinate x_i, ρ is the specific mass, p is the thermodynamic pressure, σ_{ij} are the components of the deviatoric stress tensor, T is the temperature, ε is the total specific energy and k_{ij} are the components of the conductivity tensor; vector $\mathbf{V}$ contains the conservation or the field variables and $\mathbf{F}_i$ are the components of the flux variables ($\mathbf{F}_{iA}$ contains the advective terms and $\mathbf{F}_{iD}$ the viscous terms). Finally, δ_{ij} is the Kronecker delta. Equation (1) is supplemented by the equation of state for an ideal gas and by the relationship between the temperature and the total and the kinetic energies. Initial and boundary conditions must be added to these equations in order to define uniquely the problem.

In the Taylor-Galerkin scheme, conservation equations are expanded in time by Taylor series, and after, space discretization is accomplised by the classical Bubnov-Galerkin scheme. A two-step method is used, as indicated by Zienkiewicz *et al.* (1988); this aproach can be interpreted as the finite element version of the Lax-Wendroff scheme (Richtmeyer & Morton, 1967) used in finite differences.

In the first step, corresponding to the time interval [t^n, $t^{n+1/2}$], the unknown vector **V** at $t=t^{n+1/2}$ is expanded in Taylor series, and it is obtained the following expression:

$$\mathbf{V}^{n+1/2} = \mathbf{V}^n + \frac{1}{2}\Delta t \frac{\partial \mathbf{V}^n}{\partial t} + O\left(\Delta t^2\right) \cong \mathbf{V}^n - \frac{1}{2}\frac{\partial \mathbf{F}_i^n}{\partial x_i} \quad (i=1,2,3) \tag{3}$$

Using a linear shape function $\mathbf{N}_j$ associated with node j to interpolate $\mathbf{V}^n$, a constant shape function associated with element E to interpolate $\mathbf{V}^{n+1/2}$ and applying the classical Galerkin weighted residual method, it is obtained the following equation:

$$\Omega_E^{n+1/2}\,\mathbf{V}_E^{n+1/2} = \sum_j \left[\int_{\Omega_E^n} \mathbf{N}_j \ \ d\Omega \right] \mathbf{V}_j^n - \frac{1}{2}\Delta t \sum_j \left[\int_{\Omega_E^n} \frac{\partial \mathbf{N}_j}{\partial x_i} \ \ d\Omega \right] \mathbf{F}_{ij}^n \quad (i=1,2,3;\, j=1,2,3,4) \tag{4}$$

where $\Omega_E^{n+1/2}$ is the element volume and $\mathbf{V}_E^{n+1/2}$ is the unknown vector of element E at $t=t^{n+1/2}$.

In the second step, the unknown vector at $t=t^{n+1}$ is expanded in Taylor series, and it is obtained the following expression:

$$\mathbf{V}^{n+1} = \mathbf{V}^n + \Delta t \frac{\partial \mathbf{V}^{n+1/2}}{\partial t} + O\left(\Delta t^2\right) \cong \mathbf{V}^n - \frac{\partial \mathbf{F}_i^{n+1/2}}{\partial x_i} \quad (i=1,2,3) \tag{5}$$

Using again the same shape functions, and applying the Bubnov-Galerkin method, the following equation is obtained for the second step:

$$\sum_j \left[\int_{\Omega_E^{n+1}} \mathbf{N}_k \, \mathbf{N}_j \ \ d\Omega \right] \mathbf{V}_j^{n+1} = \sum_j \left[\int_{\Omega_E^n} \mathbf{N}_k \, \mathbf{N}_j \ \ d\Omega \right] \mathbf{V}_j^n + \Delta t \sum_i \left[\int_{\Omega_E^{n+1/2}} \frac{\partial \mathbf{N}_k}{\partial x_i} \ \ d\Omega \right] \mathbf{F}_{Ei}^{n+1/2}$$

$$+ \Delta t \sum_i \left[\int_{\Gamma_E^{n+1/2}} l_i \, \mathbf{N}_k \ \ d\Gamma \right] \mathbf{F}_{Bi}^{n+1/2} \quad (i=1,2,3),\ (j,k=1,2,3,4) \tag{6}$$

where $\Gamma_E^{n+1/2}$ is the boundary of the element domain $\Omega_E^{n+1/2}$ and l_i is the cosine of the angle formed by the outward normal axis to $\Gamma_E^{n+1/2}$ with the positive direction of the reference axis x_i. Index B is referred to values at the boundary of the element domain.

In compact form, equations (4) and (6) may be written, respectively, as

$$\Omega_E^{n+1/2}\,\mathbf{V}_E^{n+1/2} = \mathbf{Q}_E^n\,\mathbf{V}^n - \frac{1}{2}\Delta t\,\mathbf{H}_{Ei}^n\,\mathbf{F}_i^n \quad (i=1,2,3) \tag{7}$$

$$\mathbf{M}_{E_c}^{n+1}\mathbf{V}^{n+1} = \mathbf{M}_{E_c}^{n}\mathbf{V}^{n} + \mathbf{R}_{Ei}^{n+1/2}\mathbf{F}_{Ei}^{n+1/2} + \mathbf{S}_{Ei}^{n+1/2}\mathbf{F}_{Bi}^{n+1/2} \quad (i=1,2,3) \tag{8}$$

In (8), the consistent mass matrix $\mathbf{M}_{E_c}^{n+1}$ is substituted by the lumped mass matrix $\mathbf{M}_{E_L}^{n+1}$ and then this equation is solved iteratively with an explicit scheme. The proposed scheme is conditionally stable, and the local stability condition for non viscous flows is given by

$$\Delta t_E \leq \frac{\beta\, h_E}{\max_E (\mathrm{v} + c)} \tag{9}$$

where h_E is a characteristic dimension of element E, c is the velocity of sound propagation and β is a safety factor.

In order to stabilize numerically the solution, specially in the presence of strong shocks, it is necessary to add numerical damping to the flow solver. In this work the viscosity model as given by Peraire *et al.* (1988) is adopted. An artificial viscosity is added explicitly to the non-smoothed solution, as follows

$$\mathbf{V}_s^{n+1} = \mathbf{V}^{n+1} + \left(\mathbf{M}_L^{n+1}\right)^{-1} \mathbf{D} \tag{10}$$

where $\mathbf{V}_s^{n+1}$ and $\mathbf{V}^{n+1}$ are the smoothed and non-smoothed solution at $t = t^{n+1}$ respectively. $\mathbf{M}_L^{n+1}$ is the assembled lumped mass matrix at $t = t^{n+1}$. The vector $\mathbf{D}$ is given by

$$\mathbf{D} = \sum_E CFL_E\, C\, \bar{S}_E \left[\mathbf{M}_{E_c}^n - \mathbf{M}_{E_L}^n\right] \mathbf{V}_E^n, \tag{11}$$

where E is an index referred to a specific element, CFL is the local Courant number, C is a constant specified by the user, $\bar{S}_E$ is a coefficient of pressure distribution.

3. THE MULTI-TIME-STEP INTEGRATION PROCEDURE

The multi-time-step integration procedure is implemented by computing the critical time step for each element in the mesh and then dividing the elements into groups according to their time step. Each element group can then be integrated with different time steps, but subject to the following restrictions:

a) the largest group time step must be an integer multiple of all time steps,
b) if any node is shared by elements in two different integration groups, the time step of the groups must be integer multiples of one another.

In this work the first restriction has been satisfied by requiring that all group time steps be integer multiplies of each other. This constrain allows elements to be assigned to groups according to their critical time steps and not to their physical proximity.

Time steps Δt_N and Δt_G are assigned to nodes and elements groups, respectively, at the beginning of the solution. The master time step Δt_{master} is set to the largest element group time step and is used to determine when a cycle has been completed.

In order to assign nodal and element group time steps, the time step of each element is calculated with expression (9). These time steps are then converted to an integer multiple of the smallest element time step. The integer multiples are then adjusted to satisfy the restriction that all time steps must be integer multiples of one another.

The time step for each node is computed considering the smaller time step of all the elements connected to the node. After all Δt_N are computed, each element time step is determined considering the smallest time step of all the nodes of this element. Thus, it is possible to be sure that any node belongs to an element with a larger time step. Then, elements and nodes are separated in groups according to their time steps.

In addition to time steps, a clock is assigned to each nodal and element groups. These clocks, when compared to the current time, indicate when a node group or a element group is ready to be updated. At the beginning of each subcycle, the nodal and element group clocks are advanced for those nodes and elements groups which were updated in the previous subcycle (by design, all nodes and elements groups are updated in the first subcycle).

After the first subcycle, element groups whose clock is behind the current time, i.e. $t_G \leq time$ (where t_G is the element group clock and *time* is the current time) will be updated. After all elements which satisfy expression last condition have been updated, the nodal loop is executed. Each node whose clock is behind the current time, i.e. $t_N \leq time$ (where t_N is the nodal clock) will be updated.

Figure 1 shows the advance in time of each group of elements and nodes along a subcycle when seven groups with its respective time steps (Δt, $2\Delta t$, $4\Delta t$, $8\Delta t$, $16\Delta t$, $32\Delta t$, $64\Delta t$) are adopted. In this case a cycle is finished after $64\Delta t$. It is observed, for example, as when *time*=$25\Delta t$, only the groups 1 to 4 (with Δt, $2\Delta t$, $4\Delta t$ and $8\Delta t$ respectively) are updated.

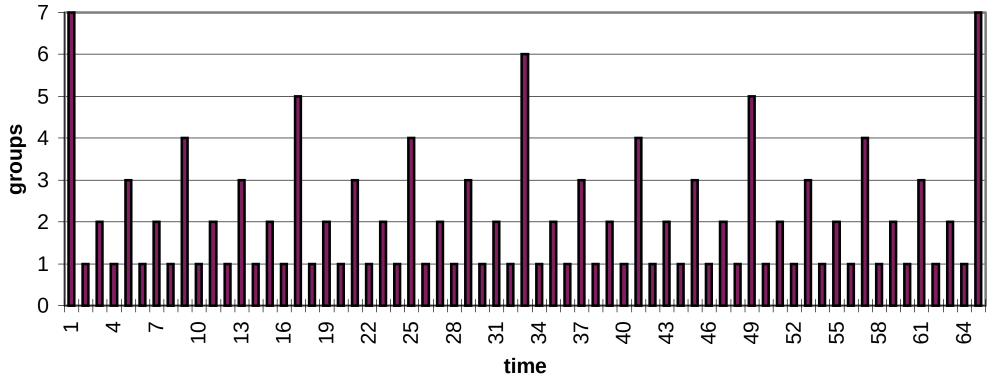

Figure 1 - Updating of nodes and element groups for each subcycle.

When a element is updated, values of the variables at the nodes connected to this element are necessary. But as these nodes may have time step that are different of the element time interval, a linear interpolation is carried out in order to get all the variables values at the same time in the moment where the updating is performed.

The subcycling procedure continues until all nodes and element groups have been updated to the master time. After the final subcycle all nodal variables have been updated to the same point in time. In this instant the cycle is completed and before a new cycle is initiated, element and nodes groups are evaluated again. Only elements and nodes with a critical time step smaller than the current time interval are resorted. An outline of the multi-time-step procedure is given bellow

1. Initial conditions $\mathbf{V}(0)$ and $\mathbf{x}(0)$ are given.
2. Initialize nodal and element group clocks (t_G=0 for all element groups; t_N=0 for all nodes; *time*=0).
3. Compute Δt for each element using expression (9).
4. Separate elements and nodes in groups according with the time step.
5. If the first subcycle will be computed, resort elements (if required) and update all nodal and element group clocks; update *time* (*time*=Δt).
6. For the subcycle n (with n>1), update nodal clocks if t_N<*time* and update element groups clocks if t_G<*time*; update time.
7. Loop on elements to be updated

   (a) Compute $\mathbf{V}_E^{n+1/2}$ with expression (7).

   (b) Compute the terms of the Eq. (8) at element level.
8. For nodes belowing to groups to be updated

(a) Compute the conservation variables $\mathbf{V}^{n+1}$ at $t=t^{n+1}$ using an iterative process, after assembling (8) and prescribing boundary conditions.

(b) Compute the smoothed conservation variables with expression (10).

(c) Compute the dependent variables p^{n+1} and T^{n+1}.

9. Interpolate linearly the variables of the nodes updated in this subcycle.
10. If $time<t_{master}$, select nodal and element groups which will be updated in the next subcycle; for the nodes of these nodal groups reconstruct the values of the interpolated variables and go to step 6.
11. If $t<t_{final}$ then go to step 5, else print results and the process is finished.

Figure 2 illustrates the subcycling procedure for three element groups. Time is represented by the vertical axis. The nodal time is represented by black circles and white circles represent the time where the nodal variables are interpolated. The influences of other nodes in the variables computation of a particular node are indicated with arrows.

In the first subcycle, the current time is *t*, and all nodal and element groups are updated. Nodes 1, 2 and 3 are updated to $t+\Delta t$; nodes 4 and 5 are updated to $t+2\Delta t$ and nodes 6 and 7 to $t+4\Delta t$. In the second subcycle, the current time is $t+\Delta t$; so, only nodal and element groups with step Δt can be updated (nodes 1, 2, 3 and elements 1, 2, 3). It is observed that in this subcycle node 3 receives the influence of the interpolated values of the variables of node 4. In the third subcycle, the current time is $t+2\Delta t$, and nodes 1 to 5 are updated. It can be observed that after this updating the cycle is finished for nodal groups with step $2\Delta t$ and step $4\Delta t$ (this last nodal group needs only the first updating to finish the cycle). In the fourth and last subcycle, only nodal and element groups with step Δt are updated, finishing the cycle.

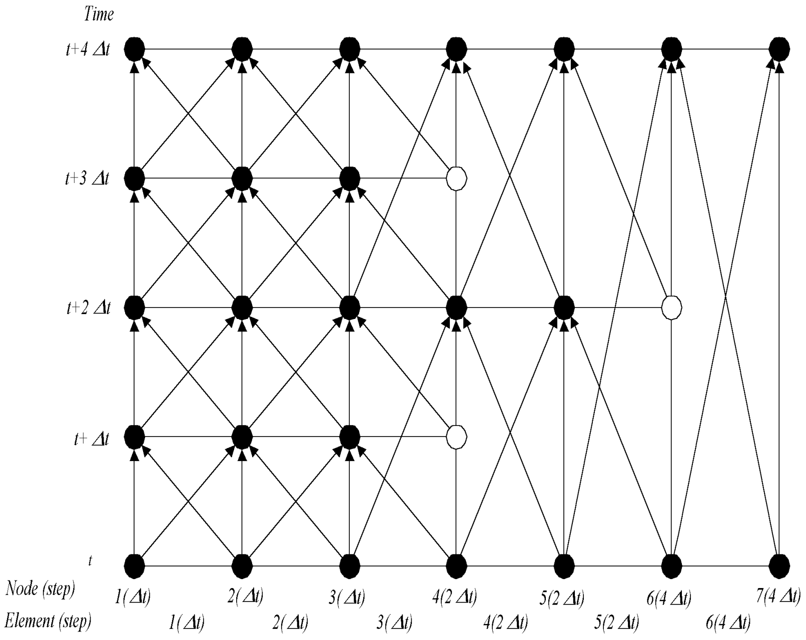

Figure 2 - Multi-time-step scheme for three element groups.

4. EXAMPLE

The supersonic flow (with Mach = 8,15) of a compressible non viscous fluid around a sphere is analyzed. A mixed structured-unstructured mesh with 52732 tetrahedrical elements and 11086 nodes is used. In Figure 3, a general view and details of the frontal region of the sphere are shown. In the planes of symmetry and in the body surface the normal component of the velocity is supressed. Therefore, the velocity vector is tangent to the surface of the sphere. At the far-field, the values for the specific mass, the velocity vector and the total specific energy are: $\rho_\infty = \rho / \rho_{ref} = 1{,}4$; $\vec{\mathbf{v}}_\infty = \vec{\mathbf{v}} / c_{ref} = (8{,}15 \quad 0 \quad 0)$; $\varepsilon_\infty = \varepsilon / c_{ref}^2 = 34{,}997$; where ρ_∞, $\vec{\mathbf{v}}_\infty$, ε_∞ are dimensionless quantities and ρ_{ref}, c_{ref} are references values of the specific mass and the speed of sound propagation, respectively. $\Delta t_{min} c_{ref} / x_{ref} = 6 \text{x} 10^{-5}$ is adopted for the smaller dimensionless time interval (with x_{ref} being a reference length).

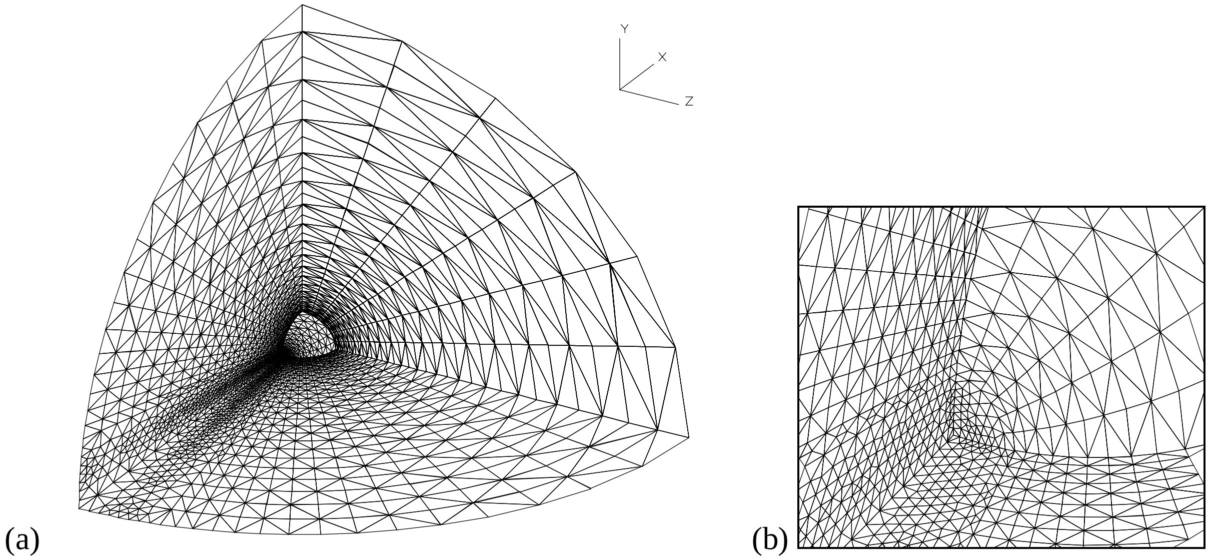

Figure 3 - Finite element mesh. (a) General view; (b) Detail of the frontal region.

The finite element mesh is divided into seven groups with time steps equal to *Δt*, 2*Δt*, 4*Δt*, 8*Δt*, 16*Δt*, 32*Δt* and 64*Δt*. Although it is possible to divide the domain in more than 7 groups, the suggestion given by Belytschko and Gilbertsen (1992), based in numerical experiments obtained in applications to structural dynamics problems, is adopted.

Number of elements and nodes for each group are presented in Table 1.

Table 1 - Number of elements and nodes for each group

GROUP	STEP	NUM. OF ELEM..	NUM. OF NODES
1	*Δt*	194	8
2	*2Δt*	1522	138
3	*4Δt*	4504	726
4	*8Δt*	8644	1768
5	*16Δt*	13068	2645
6	*32Δt*	11086	2519
7	*64Δt*	13714	3282

It is observed that great computational savings may be obtained using the multi-time-step integration scheme in cases such as the example presented in this work, where the variations of the elements size and properties over the finite element domain are very important.

The maximum theoretical value of this computational saving (speed-up) can be computed as follows (Belytschko & Gilbertsen, 1992):

$$speed-up=\frac{t^{ns}}{t^{s}}=\frac{NSUB}{\sum_{i}^{NSUB}PUES_{i}} \qquad (12)$$

where t^{ns} and t^{s} are the processing time required to solve the problem with an uniform time step and with a variable time step in space and time, respectively. *NSUB* is the number of subcycles and $PUES_i$ is the percentage of elements which are updated in the subcycle *i*.

For the example presented in this work, the values of the theoretical computational saving, obtained from expression (12), is 11,62 . However, comparing the CPU time of both cases (with variable time steps and with an uniform time step) the real reduction in processing time is about 9,22 times. The main reasons of this difference are: (a) the operations to control groups of elements and nodes increase the processing time, (b) the performance decreases because some difficulties arise to vectorize the subroutines that define the different groups of elements and nodes, and due to loops executed only for these groups which can be updated at a given instant, introducing indirect adressing (in this case the performance reduction, measured in Mflops, is about 23%).

In Figure 4, results for the specific mass and for the pressure are presented when the smaller time step is taken uniformely for the whole domain, and are very similar to that obtained by Argyris *et al.* (1989).

In Figure 5, results for the specific mass and the pressure are presented when the multi-time-step integration scheme is used. In order to compare results obtained in Figures 4 and 5, the fields with the percentage of differences between the values obtained with both schemes are shown in Figure 6.

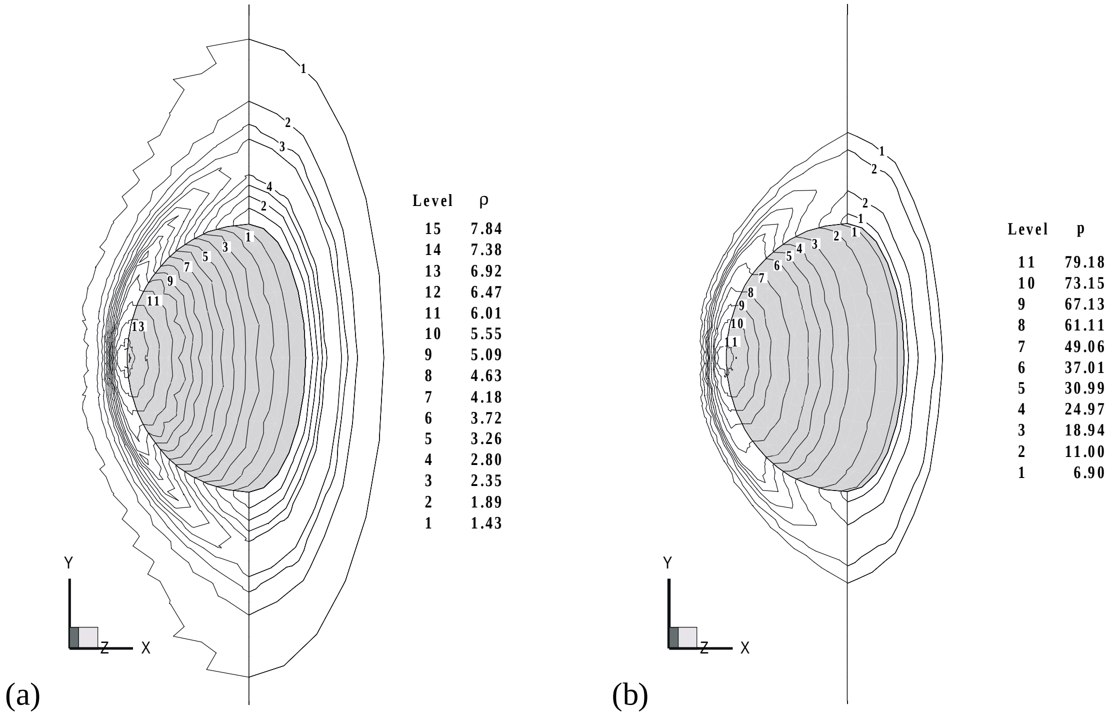

Figure 4 - Distribution of the specific mass (a) and pressure (b) when a constant time step is used.

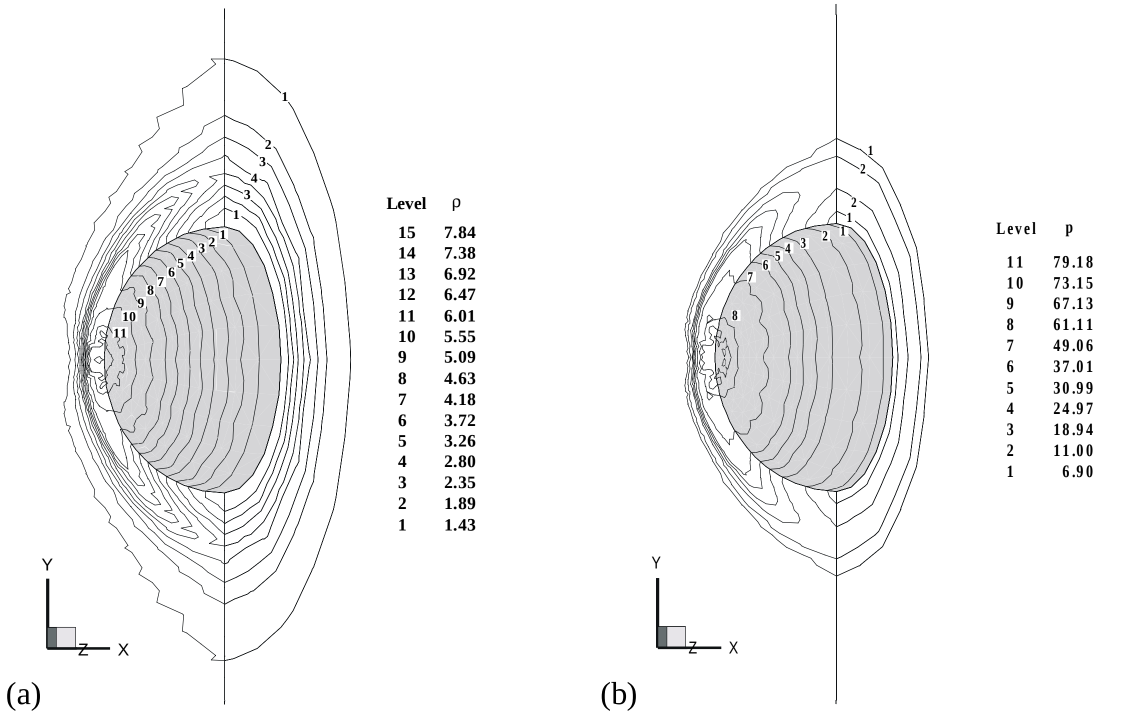

Figure 5 - Distribution of the specific mass (a) and pressure (b) when the multi-time-step scheme is used.

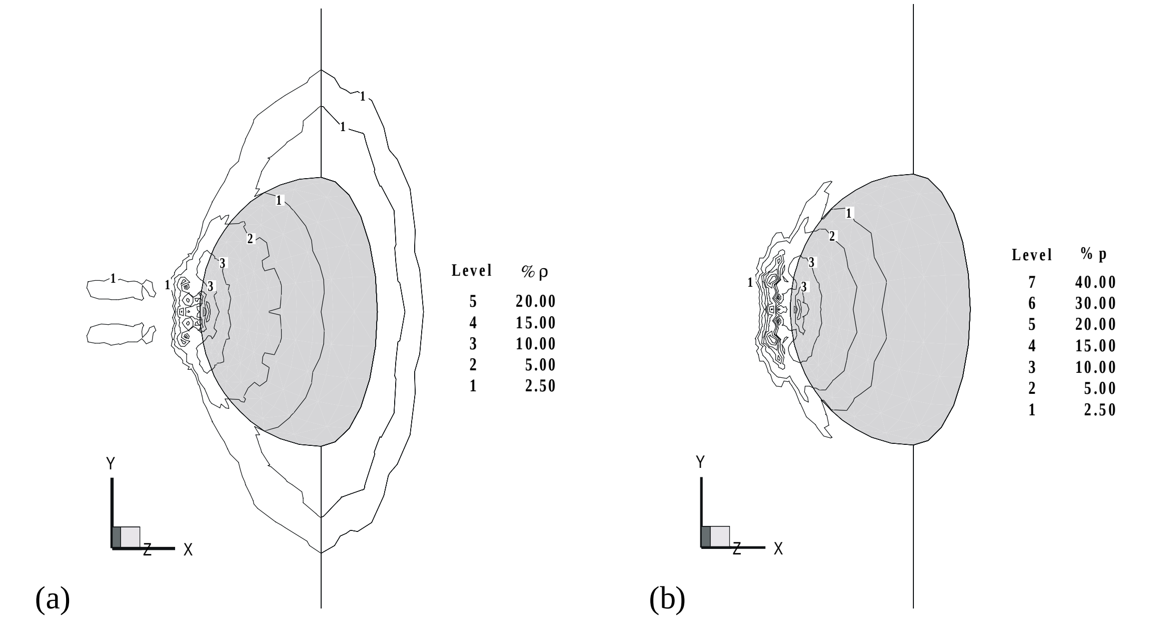

Figure 6 - Fields with the percentage of differences between results obtained in Figure 4 and Figure 5 for specific mass (a) and pressure (b).

Small differences less then 10% are found in pratically the whole finite element domain, although some few isolated nodes, close to the stagnation region, present important differences between the solution with an uniform time step and calculations using subcycles with different time intervals for the several element and node groups.

Results presented in Figure 6 are obtained redefining the groups each 10 complete cycles. These results are improved with respect to those obtained defining the groups only once, at the beggining of the process, without taking into account modifications of some properties. In the first case the algorithm to define the different groups requires 1.76% of the total process time, while in the second case only 0.14% of the total process time is used to define groups of elements and nodes.

5. CONCLUSIONS

It was shown that important computational saving may be obtained if multi-time-step integrations techniques are used, specially for problems where size and properties of the elements vary in space and time.

Although in the example presented in this work the processing time is reduced 9.22 times (with a decrease of 23% in the performance, measured in Mflops) when the multi-time-step technique is used, differences can be observed in zones near the shock line (with some peaks concentrated in small regions). Probably these shortcomings could be overcome if time steps to define element groups would be controlled by indicators in order to detect important physical phenomena, applying techniques very similar to those used in the refinement procedure when adaptive meshes are employed. This aspect will be subject of future works.

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