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Wave propagation analyses considering a truly-explicit time-marching formulation

Lucas Ruffo Pinto[1], Delfim Soares Jr.[2], Webe João Mansur[1]

[1]*COPPE/Federal University of Rio de Janeiro*
CEP 21941-611, Rio de Janeiro, Brazil
lucas.ruffo@engenharia.ufjf.br, webe@coc.ufrj.br
[2]*Structural Engineering Department, Federal University of Juiz de Fora*
CEP 36036-330, Juiz de Fora, MG, Brazil
delfim.soares@ufjf.edu.br

Abstract. This work discusses a truly-explicit time-marching formulation to analyse wave propagation models, which is based on locally-defined adaptive time-integrators and time-step values. The discussed technique considers single-step displacement/velocity recurrence relations, providing an easy to implement, truly self-starting methodology. The stability limit of the discussed approach may become larger than that of the central difference method, and it enables controllable adaptive numerical dissipation to be locally applied, improving the accuracy and versatility of the solution procedure. As an explicit approach, the technique does not require the solution of any system of equations, standing as a very efficient methodology. To solve problems regarding wave propagation in complex media, subdomain decomposition procedures, associated to multiple time-step values and sub-cycling, are also considered, improving the performance and accuracy of the technique. The entire formulation is carried out taking into account automated computations, requiring no effort and/or expertise from the user. At the end of the paper, numerical results are presented and compared to those of standard techniques, illustrating the great effectiveness of the discussed approach.

Keywords: Time-marching, Explicit analysis, Adaptive parameters.

1 Introduction

Time-dependent hyperbolic equations have numerous applications in geophysics and other areas, as they make it possible to describe time-dependent continuous domain physical problems. Nevertheless, they are challenging to be solved and their analytical resolution is often unfeasible. Therefore, in order to solve these equations, numerical methods are commonly used to find approximate solutions. These methods usually employ step-by-step time integration procedures, solving initial value problems considering a temporal discretization. Numerical methods are basically divided into two main groups: explicit methods [1-4], whose main advantage is that there is no need to deal with solver procedures, making them computationally efficient, but with stability restrictions; and implicit methods [4-7], which usually provide unconditional stability, but are considerably more computationally expensive per time step (for a comprehensive review, see [8]).

In this paper, a new truly explicit formulation is studied considering the implementation of sub-cycling techniques to improve the efficiency and accuracy of the discussed time integration algorithm. In this context, the standard Finite Element Method (FEM) is used for the spatial discretization of the models, and an extended version of the adaptive explicit technique proposed by Soares [9] is adopted for the temporal discretization. This adopted adaptive explicit technique is based on time integration procedures with adaptive parameters that focus on providing effective numerically dissipative algorithms, aiming to eliminate the influence of spurious high frequency modes and to reduce amplitude decay errors. Following this approach, a connection between the adopted spatial and temporal discretization is created. Furthermore, these adaptive parameters are associated with adaptive time-steps/subcycling splitting strategies [10], permitting fully adaptive time-domain solution procedures. As a consequence, the time-steps and time-integrators of the time-marching technique become locally computed,

depending on the spatial discretization and properties of the model. Hence, highly effective solution analyses may be achieved.

The technique discussed in this work can be used to solve problems of different nature, however, here, acoustic applications are focused. In geophysics, it is often necessary to directly analyse very heterogeneous domains that feature several layers of different materials. In this sense, automatic sub-cycling techniques become very attractive, since these different layers/media may be efficiently analysed considering proper subdomain divisions.

This paper is divided into five sections, the first being this introduction. In the second section, the equations that govern the time integration strategy are presented. In the third section, a generic automatic methodology for sub-cycling is discussed. In the fourth section, two numerical applications are considered, illustrating the good performance of the proposed technique (in this case, the obtained results are compared to those of the central difference method (CDM), the explicit generalized α method (EG-α) [1] and the Noh-Bathe method [3], as well as with analytical solutions, whenever available). In the fifth and final section, conclusions are presented.

2 Governing equations and solution strategy

The governing system of equations describing a dynamic model is given by:

$$\mathbf{M}\ddot{\mathbf{U}}(\mathrm{t}) + \mathbf{C}\dot{\mathbf{U}}(\mathrm{t}) + \mathbf{K}\mathbf{U}(\mathrm{t}) = \mathbf{F}(\mathrm{t}), \tag{1}$$

where $\mathbf{M}$, $\mathbf{C}$, and $\mathbf{K}$ stand for the mass, damping, and stiffness matrices, respectively; $\ddot{\mathbf{U}}(\mathrm{t})$, $\dot{\mathbf{U}}(\mathrm{t})$ and $\mathbf{U}(\mathrm{t})$ are acceleration, velocity, and displacement vectors, respectively; and $\mathbf{F}(\mathrm{t})$ stands for the force vector. The initial conditions of the model are given by: $\mathbf{U}^0 = \mathbf{U}(0)$ and $\dot{\mathbf{U}}^0 = \dot{\mathbf{U}}(0)$, where $\mathbf{U}^0$ and $\dot{\mathbf{U}}^0$ stand for initial displacement and velocity vectors, respectively.

The standard Finite Element Method (FEM) is here considered for the spatial discretization, so that the domain of the problem is divided into elements, allowing the calculation of local matrices and vectors, which can then be assembled to generate the global matrices $\mathbf{M}$, $\mathbf{C}$, and $\mathbf{K}$, and vector $\mathbf{F}$.

Once the semi-discrete system of equations is established, its solution is here carried out considering the following time-marching algorithm:

$$\mathbf{M}\mathbf{V}_1 = \bar{\mathbf{F}} - \Delta\mathrm{t}\left[\mathbf{C}\dot{\mathbf{U}}^{\mathrm{n}} + \mathbf{K}\left(\mathbf{U}^{\mathrm{n}} + \tfrac{1}{2}\alpha\Delta\mathrm{t}\dot{\mathbf{U}}^{\mathrm{n}}\right)\right], \tag{2a}$$

$$\mathbf{M}\mathbf{V}_2 = \Delta\mathrm{t}\mathbf{C}\mathbf{V}_1, \tag{2b}$$

$$\dot{\mathbf{U}}^{\mathrm{n}+1} = \dot{\mathbf{U}}^{\mathrm{n}} + \mathbf{V}_1 - \tfrac{1}{2}\mathbf{V}_2, \tag{2c}$$

$$\mathbf{U}^{\mathrm{n}+1} = \mathbf{U}^{\mathrm{n}} + \tfrac{1}{2}\Delta\mathrm{t}\left(\dot{\mathbf{U}}^{\mathrm{n}} + \dot{\mathbf{U}}^{\mathrm{n}+1}\right), \tag{2d}$$

where $\Delta\mathrm{t}$ represents the adopted time-step of the analysis, α stands for the time integration parameter of the method, $\mathbf{V}_1$ and $\mathbf{V}_2$ stand as auxiliary vectors (computed as indicated by equations (2a) and (2b), respectively), $\bar{\mathbf{F}} = \int_{\mathrm{t}^{\mathrm{n}}}^{\mathrm{t}^{\mathrm{n}+1}} \mathbf{F}(\mathrm{t})\,\mathrm{dt}$ and $\mathbf{C} = \alpha_m\mathbf{M} + \alpha_k\mathbf{K}$.

As one can observe, this solution algorithm is based only on single-step relations regarding displacement and velocity fields. Hence, the technique is truly self-starting, avoiding cumbersome initial calculations. In addition, it stands as a truly explicit approach, requiring no treatment of any system of equations, demanding only the "inversion" of the $\mathbf{M}$ matrix (which is here diagonally adopted, i.e., lumped matrices are regarded). Another important feature of this algorithm is that its critical time-step value increases for low and moderate physical damping values and it does not drastically decrease regarding highly damped models, enabling explicit analyses (i.e., analyses without considering solver procedures) to be carried out taking into account convenient time-step values.

In this work, adaptive locally-defined α parameters are considered, providing a very effective time-domain solution methodology. In this case, different values for α may occur across the different finite elements, and they may vary for each time step of the analysis, allowing a quite versatile and flexible approach to be provided. The α parameter controls the algorithmic damping of the formulation and the following notation is here adopted: $\alpha_{\mathrm{e}}^{\mathrm{n}}$, indicating that its value is defined for each element "e" of the spatially discretized model and for each time step "n" of the analysis.

The strategy here is to adopt $\alpha_e^n > 1$ wherever and whenever numerical damping may be necessary, and α_e^n=1 otherwise. This strategy can be executed automatically based on an oscillatory criterion defined by a φ_e^n parameter, which is also calculated at each time step and for each element of the model. The calculation of this oscillatory parameter may be expressed as: $\varphi_e^n = \Sigma_{i=1}^{\eta}\left|\left|U_i^n - U_i^{n-2}\right| - \left|U_i^n - U_i^{n-1}\right| - \left|U_i^{n-1} - U_i^{n-2}\right|\right|$, where η stands for the total number of degrees of freedom of the element. Therefore, when $\varphi_e^n \neq 0$, at least one degree of freedom of the focused element is oscillating along time. In this case, the algorithm activates maximal numerical dissipation at the maximal sampling frequency of the element Ω_e^{max} (where $\Omega_e^{max} = \omega_e^{max}\Delta t$, and ω_e^{max} stands for the highest square root of the generalized eigenvalues that are computed based on the local matrices $\mathbf{M}_e$ and $\mathbf{K}_e$), more effectively dissipating the influence of the highest modes of the problem. So, when $\varphi_e^n \neq 0$, α_e^n assumes the following value:

$$\alpha_e^{act} = \left[-4\zeta_e + (4\zeta_e^2 - 1)\Omega_e^{max} + \zeta_e\Omega_e^{max^2} + 4(1 - \zeta_e\Omega_e^{max})^{1/2}\right]\left[(1 - \zeta_e\Omega_e^{max})\Omega_e^{max}\right]^{-1}, \tag{3}$$

where the superscript "act" (abbreviation for active) highlights that this amount is applied only when numerical damping is to be introduced into the analysis. When $\varphi_e^n = 0$, $\alpha_e^n = 1$. In equation (3), ζ_e is given by:

$$\zeta_e = \alpha_m(2\omega_e^{max})^{-1} + 0.5\alpha_k\omega_e^{max}, \tag{4}$$

and this value characterizes the so-called physical damping ratio of the element.

For truly explicit formulations, the critical time-step of the analysis also becomes function of the physical damping of the model. In this case, the following expression for the element critical time-step, as function of ζ_e, can be established, for the discussed formulation:

$$\text{if } \zeta_e \leq 0.225, \qquad \Delta t_e = 2(\omega_e^{max})^{-1}, \tag{5a}$$

$$\text{if } \zeta_e > 0.225, \qquad \Delta t_e = (\zeta_e\omega_e^{max})^{-1}, \tag{5b}$$

where equation (5a) stands for a simple conservative expression, assuming $\Omega_c = 2$ for $\zeta_e \leq 0.225$, which is the minimal Ω_c value in that range, equaling the critical sampling frequency of the CDM, and equation (5b) considers $\Omega_c = 1/\zeta_e$ for $\zeta_e > 0.225$. As one can observe regarding equations (5a-b), the critical time-step value of the discussed technique can be very easily estimated, which is rarely the case considering standard truly explicit approaches. This estimative is highly important to the automated subdomain divisions and adaptive computations of local time-step values that are carried out in this work, as it is discussed in the next subsection.

3 Sub-cycling

Subcycling is a subdomain decomposition associated with multiple time-steps. This technique allows a domain to be discretized considering different refinement levels without limiting its explicit time-marching solution to be restricted to its shortest critical time-step. This allows greater time-step values for different subdomains, enabling lower computational costs. However, sub-cycling must be properly considered, once excessive subdivisions may provide deterioration in both accuracy and efficiency. Here, an automatic algorithm is developed to improve efficiency without compromising accuracy. In this algorithm, the following steps are followed to define the subdomain decomposition: (i) calculate the critical time-steps of all elements (following equations (5a-b)), finding the smallest Δt_e of the model (i.e., Δt_b, where $\Delta t_b = \min(\Delta t_e)$), which is the basic time-step for the controlled subdivision of the domain; (ii) with Δt_b defined, calculate subsequent time-step values as multiple of the power of 2 of this minimal time-step value (i.e., calculate Δt_i, where $\Delta t_i = 2^{(i-1)}\Delta t_b$); (iii) associate each element to a computed time-step value (i.e., to Δt_i, where $\Delta t_i \leq \Delta t_e \leq \Delta t_{i+1}$ and i indicates the subdomain of that element); (iv) associate a time-step value (i.e., associate a subdomain) to each degree of freedom of the model considering the lowest time-step value of its surrounding elements. In addition, the algorithm allows the control of the percentage of elements that have inexpressive numerical damping, that is, $\alpha_e^{act} \approx 1$, due to $\Delta t_i \approx \Delta t_c$ (in this case, the dissipative capability of the element is greatly reduced), assigning a Δt to the subdomain slightly lower than its critical value (i.e., $\Delta t = \gamma\Delta t_c$, where γ stands for this reduction factor, which guarantees $\alpha_e^{act} > 1$). In this work, the following criterion is adopted, in this case: if more than 25% of the computed α_e^{act} values are lower than 1.05, $\gamma = 0.95$; otherwise, $\gamma = 1$.

Once the subdomains of the model are stablished, displacement and velocity values along the boundaries of

these subdomains may need to be interpolated. In this work, the following expressions are adopted for these interpolations:

$$\boldsymbol{U(t) = ½\Delta t\left(\dot{U}^{n+1} - \dot{U}^{n}\right)t^2 + \dot{U}^{n}t + U^{n}}, \tag{6a}$$

$$\boldsymbol{\dot{U}(t) = 1/\Delta t\left(\dot{U}^{n+1} - \dot{U}^{n}\right)t + \dot{U}^{n}}, \tag{6b}$$

where t is the current increment of time ($0 \leq t \leq \Delta t$) for the focused subdomain and Δt is the time-step value of the degree of freedom being interpolated, which is related to another subdomain.

4 Numerical applications

In this section, two numerical applications are considered to illustrate the performance and potentialities of the discussed adaptive explicit time-marching technique with sub-cycling. First, a square homogeneous membrane is studied, and, subsequently, the propagation of acoustic waves in the "Marmousi2" model by Martin et al. [11] is analysed. The computed results are compared to those of the CDM, EG-α and Noh-Bathe method. In the following analyses, lumped mass matrices are always considered. For physically dampened models, appropriate time-step values are established for the EG-α and Noh-Bathe method, once reduced stability limits are provided by these techniques in this case. In addition, since the CDM does not stand as a truly explicit approach, this technique is not here employed for solution once non-null α_k values are regarded.

4.1 Application 1

In this application, the transversal motion of a membrane is analysed. A constant unit displacement value is prescribed along the left boundary of the body and null displacements are prescribed along the remaining boundaries. The model is defined by a unit side length and mass density, as well as a wave propagation velocity of $10m\ /\ s$. Initially, null values are considered for α_m and α_k, defining a physically undamped configuration, and, in the sequence, $\alpha_m = 10$ and $\alpha_k = 0.0001$ are applied, describing a damped model. The symmetry of the problem is regarded and only its upper half is spatially discretized by the FEM. The adopted mesh is composed of 125000 elements and refinement towards the upper-left border of the model is considered. The exact solution for this application (undamped model) can be found in Soares [4].

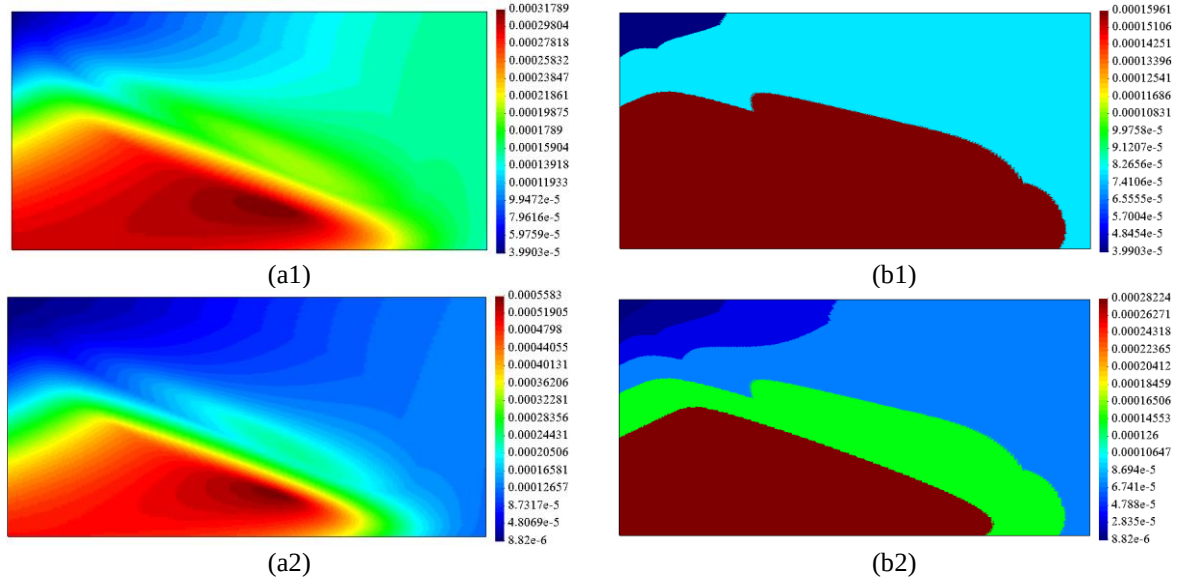


Figure 1. Subdomain decomposition for the (1) undamped and (2) damped model (first application): (a) Δt_e and (b) Δt_i.

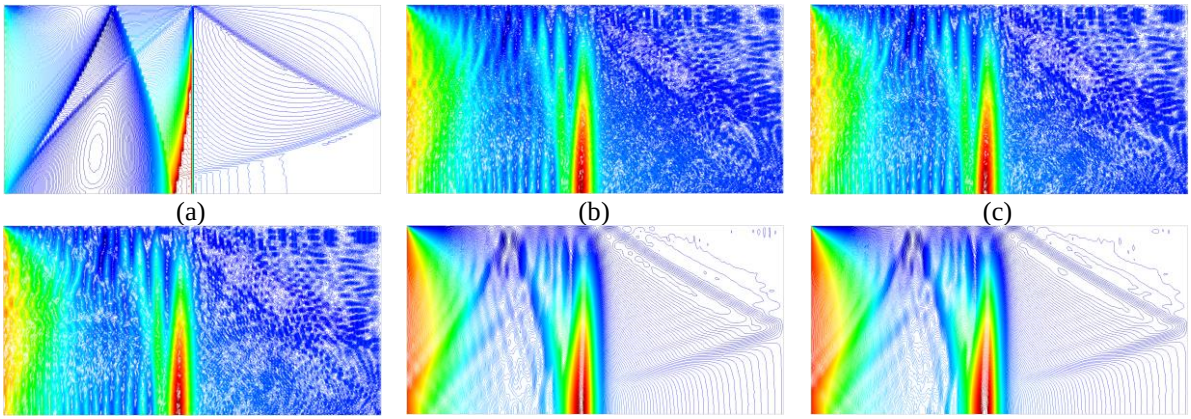
In Fig.1, the sub-cycling subdomain decompositions of the reported undamped and damped models are depicted. In Fig.1a, the time-steps calculated for each element of the adopted mesh are presented, whereas, in Fig.1b, the computed time-step value for each established subdomain is provided. As this figure indicates, the use of subdomains decomposition allows considering time-steps up to 32 times greater than those of standard analyses,

in this case (see Fig.1b2).

Table 1. Computed errors and CPU times for the first application

Method	Undamped Model			Damped Model	
	Δt (10^{-4})	Error (10^{-1})	CPU time	Δt (10^{-4})	CPU time
CDM	0.3990 (0.249)	1.6369 (1.414)	82.23 (2.792)	-	-
Noh-Bathe	0.7471 (0.468)	1.6158 (1.395)	86.01 (2.920)	0.0786 (0.027)	1142.75 (9.996)
EG-α	0.3596 (0.225)	1.6195 (1.399)	84.56 (2.871)	0.0567 (0.020)	856.63 (7.493)
New	0.3990 (0.249)	1.2314 (1.063)	81.82 (2.778)	0.0882 (0.031)	631.24 (5.521)
New/sub	1.5961 (1.000)	1.1576 (1.000)	29.45 (1.000)	2.8224 (1.000)	114.32 (1.000)

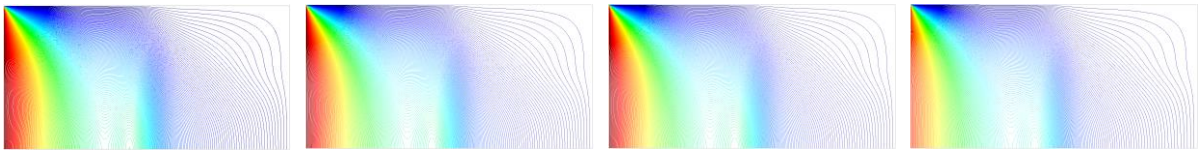
Table 1 shows the obtained CPU times and relative errors (computed at the middle of the model) for each approach. The New/sub method, which describes the new approach applied with subdomain divisions and sub-cycling, runs with different time-steps and its largest time-step value is indicated in the table. As one can observe, the new procedure allows computing more accurate responses at lower CPU times, and the computational effort of the proposed New/sub formulation may then become just 10% of that of standard techniques, in this case.



(a) (b) (c)

(d) (e) (f)

Figure 2. Computed fields for the undamped model at 0.25s: (a) analytical, (b) CDM, (c) Noh-Bathe, (d) EG-α, (e) New and (f) New/sub



(a) (b) (c) (d)

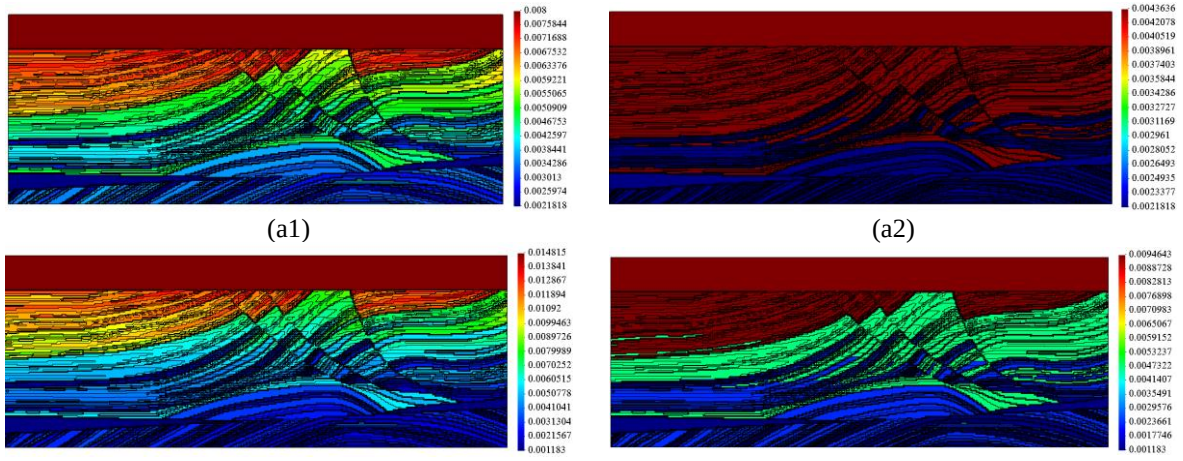
Figure 3. Computed fields for the damped model at 0.25s: (a) Noh-Bathe, (b) EG-α, (c) New and (d) New/sub

In Fig. 2, snapshots of the results computed at time t = 0.25s are depicted, taking into account the referred time-marching techniques. As can be observed in this figure, the CDM, Noah-Bathe and EG-α do not provide appropriate results and spurious oscillations dominate their computed responses. On the other hand, much more adequate results are provided by New and New/sub, demonstrating their good performance. For non-null α_k values, higher modes may be physically damped and, in this case, spurious oscillations do not occur, no matter the adopted time integration procedure, as illustrated in Fig.3.

4.2 Application 2

In this second application, an extension of the original Marmousi model created by Martin et al. [11] is analysed. The model has a lateral extent of 17 km and a depth of 3.5 km and includes a total of 199 geological layers, as well as an upper water layer that is 450 m deep. Here, the original finite difference synthetic data is transformed into an FEM mesh with 224,731 nodes and 223,672 linear square elements. As this FEM mesh is

created from a finite difference discretization, its elements are structured and all have the same size. Thus, just the wave propagation speed of each material controls the variability of Δt_e. As in the previous example, undamped and damped models are also considered in this application. Initially, null values are considered for α_m and α_k, defining a physically undamped configuration, and, in the sequence, $\alpha_m = 10$ and $\alpha_k = 0.002$ are applied, describing a damped model.



(a1) (a2)

(b1) (b2)

Figure 4. Subdomain decomposition for the (1) undamped and (2) damped model (second application): (a) Δt_e and (b) Δt_i.

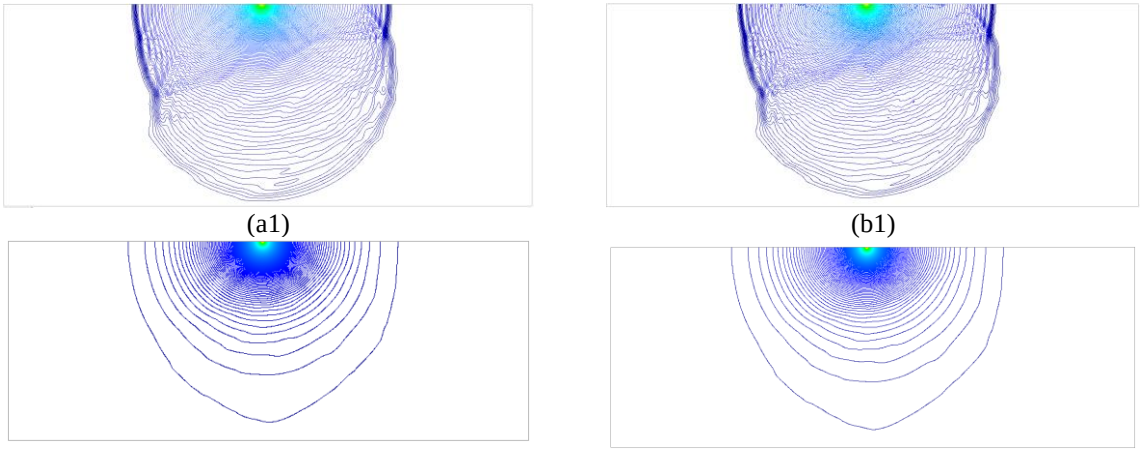
Table 2 describes the performance of the discussed analyses, indicating once again the excellent efficiency of the proposed formulation. In this case, the computational effort of the proposed approach may become less than 9% of that of standard procedures, still providing equivalent responses, as indicated in Figure 5.

Table 2. Computed CPU times for the second application

Method	Undamped		Damped	
	Δt (10^{-3})	CPU time	Δt (10^{-3})	CPU time
CDM	2.1818 (0.500)	66.73 (1.792)	-	-
Noh-Bathe	4.0854 (0.936)	69.95 (1.878)	0.4085 (0.043)	502.18 (12.221)
EG-α	1.9664 (0.450)	67.69 (1.818)	0.2949 (0.031)	361.72 (8.803)
New	2.1818 (0.500)	66.54 (1.787)	1.1830 (0.125)	106.06 (2.581)
New/sub	4.3636 (1.000)	37.23 (1.000)	9.464 (1.000)	41.90 (1.000)

5 Conclusions

This paper describes a new truly explicit formulation for hyperbolic models. In this approach, both the time-step and time integration parameter values adapt to the properties of the discretized model, yielding a more efficient and accurate solution methodology. Additionally, when considering damped models, the methodology may provide greater stability limits, allowing computing larger time-step values, further improving the efficiency of the discussed technique. Two examples are discussed in this work, illustrating the good performance of the proposed formulation. As these examples describe, the referred technique regularly provides better results than standard solution procedures, considering lower computational efforts. In the second example, a complex heterogeneous model is studied, demonstrating the robustness of the proposed automated formulation for multiple time-step analyses.



(a1) (b1)

(a2) (b2)

Figure 5. Computed fields for the (1) undamped and (2) damped models, at 1.5s: (a) EG-α (b) New/Sub.

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