

A locally-adaptive truly-explicit time-marching formulation for acoustic analyses

Lucas Ruffo Pinto¹, Delfim Soares Jr.², Webe João Mansur¹

¹*COPPE/Federal University of Rio de Janeiro*

CEP 21941-611, Rio de Janeiro, Brazil

lucas.ruffo@engenharia.uff.br, webe@coc.uffj.br

²*Structural Engineering Department, Federal University of Juiz de Fora*

CEP 36036-330, Juiz de Fora, MG, Brazil

delfim.soares@uff.edu.br

Abstract. This study discusses a novel explicit time-marching procedure for solving acoustic problems in the time domain. The procedure is designed to adapt to the characteristics of the spatially discretized model, providing a fully automated and highly effective solution. The approach is second-order accurate, explicitly formulated, and self-starting, offering the advantages of adaptive algorithmic dissipation and extended stability limits. Furthermore, the paper discusses automated subdomain/sub-cycling splitting procedures that enhance the performance of the proposed formulation. By partitioning the model domain into multiple subdomains based on the discretization properties, different time-step values can be utilized to ensure stability and enable more precise and efficient analyses. The method incorporates adaptive values for the time integration parameters, which are determined based on the characteristics of the spatial discretization. This locally-defined self-adjustable formulation establishes a link between the spatial and temporal solution procedures, better compensating for their errors. The paper presents and discusses expressions for the adaptive time integration parameters and the limiting time-step values of the discretized domain elements. Finally, numerical results are presented at the end of the paper, comparing them to those obtained using standard techniques, thereby illustrating the performance of the discussed approach.

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

1 Introduction

Wave propagation models involve governing equations that require both spatial and temporal discretization techniques for their numerical solutions. Typically, in this case, space and time domains are separately analyzed, and spatial discretization methods are initially applied. This process generates a semi-discrete time-domain system of equations, which is then solved using a time-marching procedure. Finite element formulations based on local approximations have been extensively used in engineering to solve problems based on partial differential equations. While local approaches are commonly employed for spatial discretization, they are not as commonly used for time integration. In such cases, local approximations have been mostly considered just by defining the time-step value, often utilizing adaptive time stepping techniques and/or multi-time-steps/sub-cycling splitting procedures [1-7].

A new explicit time-integration procedure, incorporating self-adjusting time-integrators, is here discussed to advance the development of locally defined time-marching formulations. This procedure is combined with adaptive time-steps/sub-cycling splitting techniques, resulting in a highly effective approach for solving problems in the time domain [7]. The time-steps and time-integration parameters of this method are locally computed, taking into account the adopted spatial discretization and model properties. This automated formulation eliminates the need for user decisions, effort, and/or expertise. As a result, this methodology is highly recommended for regular use in commercial codes. In the current methodology, the time-integration parameters are designed to attenuate spurious high-frequency modes while preserving the influence of significant low-frequency modes, resulting in a very accurate dissipative time-marching technique. The efficacy of the solution procedure can be further enhanced by implementing appropriate multiple time-step values throughout the model, as demonstrated by sub-cycling splitting techniques [4-7]. In this case, since the time-integration parameters of the method also depend on the considered time-step size, by considering appropriate multiple time-step values and employing sub-cycling

splitting techniques, these parameters may be better evaluated, further enhancing the effectiveness of the solution procedure.

The present formulation stands as a second-order accurate, truly explicit, truly self-starting approach, and it offers extended stability limits, as well as advanced controllable algorithm dissipation. In this manuscript, acoustic analyses and geophysical applications are mainly focused, although the discussed technique can be applied to analyze innumerable wave propagation models. Geophysics often involves the analysis of heterogeneous domains comprising multiple layers of different materials. In such cases, automatic sub-cycling techniques have proved to be valuable as they enable efficient analysis of these distinct layers or media by dividing them into appropriate subdomains [5-7].

2 Governing equations and time integration strategy

The governing equation describing a semi-discrete wave propagation model may be written as:

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

where \mathbf{M} , \mathbf{C} , and \mathbf{K} stand for the mass, damping, and stiffness matrix, respectively. The acceleration, velocity, and displacement vectors of the system are represented by $\ddot{\mathbf{U}}(t)$, $\dot{\mathbf{U}}(t)$ and $\mathbf{U}(t)$, respectively, while the external force acting on the system is represented by vector $\mathbf{F}(t)$. The initial conditions are defined as $\mathbf{U}^0 = \mathbf{U}(0)$ and $\dot{\mathbf{U}}^0 = \dot{\mathbf{U}}(0)$, representing the initial displacement and velocity vectors, respectively. As this manuscript focuses on explicit analyses, lumped mass matrices are used to define the discretized model described above, as usual. This approach avoids the need to solve systems of algebraic equations when using truly-explicit time-marching formulations, leading to significantly more efficient analyses. Additionally, classical Rayleigh damping is considered in this paper, where the viscous damping matrix \mathbf{C} is assumed to be proportional to the mass and stiffness matrices of the model; i.e., $\mathbf{C} = \alpha_m \mathbf{M} + \alpha_k \mathbf{K}$, where α_m and α_k are constants of proportionality, providing a straightforward representation of damping effects in the system.

The time-integration procedure discussed in this paper is an extension of a previous methodology presented by Soares [8], which proposed three truly explicit time-marching procedures utilizing appropriate coefficients and chained compositions of stiffness and damping matrix multiplications to achieve second-, third-, and fourth-order accuracy in time-domain solutions. The current time-integration procedure can be described by the following recurrence relationships:

$$\mathbf{M}\mathbf{V}_1 = \int_{t^n}^{t^{n+1}} \mathbf{F}(t) dt - \Delta t[\mathbf{C}\dot{\mathbf{U}}^n + \mathbf{K}(\mathbf{U}^n + \frac{1}{2}\Delta t\dot{\mathbf{U}}^n)], \quad (2a)$$

$$\mathbf{M}\mathbf{V}_2 = \Delta t\mathbf{C}\mathbf{V}_1, \quad (2b)$$

$$\dot{\mathbf{U}}^{n+1} = \dot{\mathbf{U}}^n + \mathbf{V}_1 - \frac{1}{2}\mathbf{V}_2, \quad (2c)$$

$$\mathbf{M}\mathbf{V}_3 = \Delta t\mathbf{K}(\mu_1\Delta t\dot{\mathbf{U}}^{n+1} + \mu_2\Delta t\dot{\mathbf{U}}^n), \quad (2d)$$

$$\mathbf{U}^{n+1} = \mathbf{U}^n + \frac{1}{2}\Delta t(\dot{\mathbf{U}}^n + \dot{\mathbf{U}}^{n+1} - \mathbf{V}_3) \quad (2e)$$

where Δt represents the time-step of the analysis, and the auxiliary vectors \mathbf{V}_1 , \mathbf{V}_2 and \mathbf{V}_3 are defined based on equations (2a), (2b), and (2d), respectively. The auxiliary vector \mathbf{V}_3 is computed at the element level, taking into account the local properties of the spatially discretized model, which are considered when locally calculating the time-integration parameters μ_1 and μ_2 . In this sense, a local vector \mathbf{V}_e is computed as $\mathbf{V}_e = \mathbf{K}_e(\bar{\mu}_1^e \dot{\mathbf{U}}_e^{n+1} + \bar{\mu}_2^e \dot{\mathbf{U}}_e^n)$, where the subscripts and superscripts "e" indicate variables defined at the element level (with $\bar{\mu}_i^e = \mu_i^e \Delta t$), and a global vector \mathbf{V} is assembled by combining \mathbf{V}_e . \mathbf{V}_3 is calculated as $\mathbf{V}_3 = \Delta t\mathbf{M}^{-1}\mathbf{V}$, as described by equation (2d). This locally defined approach enables the specification of μ_1 and μ_2 for each element of the discretized model, considering its local properties and resulting in a more effective solution procedure. In this case, the following expressions are considered to define μ_1 and μ_2 :

$$\mu_1^e = 4(\xi_e \Omega_e^{\max} - 1)^{-1} \Omega_e^{\max-4} + 4\xi_e \Omega_e^{\max-3} + 2\Omega_e^{\max-2}, \quad (3a)$$

$$\mu_2^e = -2(\xi_e \Omega_e^{\max} - 1)^{-1} \Omega_e^{\max-4} - 4\xi_e \Omega_e^{\max-3}, \quad (3b)$$

where $\Omega_e^{\max} = \omega_e^{\max} \Delta t$ and $\xi_e = \alpha_m (2\omega_e^{\max})^{-1} + \alpha_k \omega_e^{\max} / 2$ are defined as the maximal sampling frequency and damping ratio of element "e", respectively, with ω_e^{\max} representing the highest natural frequency of the element. Expressions (3a-b) are formulated to ensure that the spectral radius of the method is zero at Ω_e^{\max} , thereby providing maximum numerical damping at the element's highest sampling frequency. This optimized design aims to minimize the impact of spurious high-frequency modes, leading to improved analyses. The introduction of numerical damping is intended to eliminate non-physical spurious oscillations caused by unresolved modes. However, striking a balance between introducing high-frequency dissipation while preserving low-frequency modes is challenging. The new methodology adapts by enforcing low spectral radius values at the highest frequencies and relatively high spectral radius values at the important low frequencies.

As it is well-known, when non-zero values of α_k are utilized, physical damping is already incorporated at the highest frequencies of the model. Consequently, there is no need to introduce numerical damping into the analysis, allowing for the adoption of $\mu_1^e = \mu_2^e = 0$. By eliminating the evaluation of equation (2d), the solution algorithm's efficiency is further enhanced. Therefore, in this study, if $\xi_e > 0.222$ (refer to [7] for more details regarding this threshold), numerical damping is not applied in the analysis and the time integration parameters are set to zero (i.e., $\mu_1^e = \mu_2^e = 0$).

The solution algorithm described by equations (2a-e) is straightforward to implement and does not require any user input as all parameters are automatically evaluated based on the properties of the model, as described by equations (3a-b). This algorithm describes a self-starting and truly explicit technique that does not involve solving any system of equations, only requiring the inversion of the diagonally adopted \mathbf{M} matrix. By following equations (3a-b), the proposed time-marching formulation establishes a connection between the adopted spatial and temporal discretization procedures, resulting in improved error balances and in more accurate responses. This technique also offers enhanced stability conditions, with a stability limit over 1.7 times greater than that of the Central Difference (CD) method. Indeed, the maximum time-step value for each element of the discretized model can be determined based on two possible configurations, depending on whether $\mu_1^e = \mu_2^e = 0$ or not, as indicated below:

$$\text{if } \xi_e \leq 0.222, \quad \Delta t_e = (2 + 2^{1/2})(\omega_e^{\max})^{-1}, \quad (4a)$$

$$\text{if } \xi_e > 0.222, \quad \Delta t_e = (\xi_e \omega_e^{\max})^{-1}, \quad (4b)$$

Thus, the discussed technique, as shown in equations (4a-b), enables a straightforward estimation of the limiting time-step value, which is not typically found in standard truly explicit approaches. This estimation is crucial for automated subdomain divisions and adaptive computations of local time-step values, as discussed in the next subsection. Additionally, a minimum value of Ω_e^{\max} is suggested in equations (3a-b) to prevent excessive numerical damping when subdomain/sub-cycling splitting procedures are not considered, with a recommended value of $2^{1/2}$.

3 Sub-cycling

Sub-cycling is a technique proposed by Belytschko et al. [4] that involves dividing a domain into subdomains and performing computations at multiple "sub-steps". This approach allows for an explicit time-marching solution without restricting the entire domain to its shortest critical time-step value. It enables the consideration of larger time-step values for different subdomains, reducing computational efforts. Sub-cycling is necessary when a mesh contains both stiff and soft subdomains, which would otherwise require using an excessively small time-step value for the entire model. To achieve an efficient computational approach, these regions need to be solved separately, employing different time-step values for different subdomains, and then connecting the computed responses. However, excessive subdivisions can lead to a compromise in both accuracy and efficiency, emphasizing the significance of appropriate sub-cycling considerations.

This study reports an automated algorithm for subdividing the model domain, aiming to improve efficiency

while maintaining accuracy. The algorithm calculates and assigns a time-step (Δt) to each node of the model through a controlled subdivision procedure. Elements with similar stability limits are grouped together, creating subdomains with different time-step values, enabling an efficient and accurate solution. The following sequence of commands is used to define this subdomain division automatically: (i) calculate the limiting time-steps of all elements (Δt_e) using equations (4a-b) and find the smallest Δt_e of the model (Δt_e^{\min} , where $\Delta t_e^{\min} = \min(\Delta t_e)$), which serves as the basic time-step for subdivision; (ii) calculate subsequent time-step values as multiples of 2 of Δt_e^{\min} (Δt_i , where $\Delta t_i = 2^{(i-1)}\Delta t_e^{\min}$); (iii) associate each element with a computed time-step value (Δt_i , where $\Delta t_i \leq \Delta t_e \leq \Delta t_{i+1}$, and i denotes the subdomain of that element); (iv) associate a time-step value (subdomain) to each degree of freedom of the model based on the lowest time-step value of the surrounding elements.

After implementing the subdomain division and sub-cycling algorithm, it is sometimes necessary to interpolate the displacement and velocity values near the boundaries of the time-step subdomains. This study utilizes the following expressions for these interpolations:

$$\mathbf{U}(t) = \frac{1}{2}(\dot{\mathbf{U}}^{n+1} - \dot{\mathbf{U}}^n)t^2/\Delta t + \dot{\mathbf{U}}^n t + \mathbf{U}^n, \quad (5a)$$

$$\dot{\mathbf{U}}(t) = (\dot{\mathbf{U}}^{n+1} - \dot{\mathbf{U}}^n)t/\Delta t + \dot{\mathbf{U}}^n, \quad (5b)$$

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. A similar expression to equation (5b) is used to interpolate \mathbf{V}_1 , if required, based on equation (2b).

4 Numerical applications

This study evaluates the performance of the proposed solution procedure by analyzing two acoustic models. The first model represents a homogeneous infinite medium, and its analytical solution is given by the Green's function of this acoustic problem. The availability of this analytical solution allows for a precise assessment of the errors in the numerically computed responses. The second model simulates a synthetic scenario with complexity similar to real-world geological applications, serving as a demonstration of the effectiveness of the proposed methodology in analyzing large-scale geophysical problems, such as those encountered in the OIL & GAS industry. In particular, this study considers a benchmark case provided by the PETROBRAS research laboratory, focusing on the Búzios region, where ten well-defined stratified layers are present [9].

The results obtained from the discussed adaptive formulation, both with (New/sub) and without (New) considering multi-time-steps/sub-cycling splitting procedures, are compared to those obtained using standard explicit approaches. These approaches included the widely used Central Difference (CD) method, the explicit generalized α (EG- α) method developed by Hulbert and Chung [10] (where $\rho_b = 0.3665$ is chosen, as recommended by the authors to minimize errors in period elongation), and the composite Noh-Bathe (NB) method [11] (where $p = 0.54$ is selected, as recommended by the authors). For each technique, the maximum allowable time-step value for stability, evaluated at element level, is utilized to enable more efficient analyses for each approach.

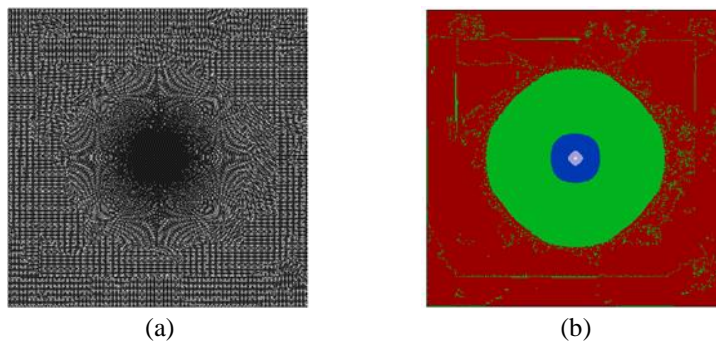


Fig.1 – (a) adopted FEM mesh and (b) computed time-step subdomains.

4.1 Application 1

In this first example, a numerical analysis is conducted on an infinite acoustic model with an impulsive source. The model is discretized using a square mesh measuring 5m x 5m, consisting of 310,253 linear quadrilateral elements. To simulate the infinite medium, perfectly matched layers (PMLs) [12] are incorporated at the boundaries of the model. This setup prevents wave reflection, allowing for longer analyses. The exact solution for this application can be found in Mansur [13]. Figure 1a illustrates the mesh used in the analysis, whereas, in Fig. 1b, the sub-cycling subdomain decompositions of the analyzed model are presented. This figure demonstrates that by employing subdomain decomposition, it becomes possible to use time-step values up to 8 times larger compared to standard analyses.

Table 1 provides the corresponding CPU times and relative errors (computed at a distance of 15 meters from the application point of the load) for each approach. The New/sub method utilizes different time-step values, with its largest time-step value indicated in the table. As may be observed, the new procedure enables more accurate responses to be computed within shorter CPU times, resulting in a significant reduction in computational effort compared to standard techniques. In this particular case, the computational effort of the proposed New/sub formulation amounts to only 55% of that required by the standard techniques.

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

Method	Δt (10^{-2} s)	Error u (10^{-1})	CPU Time (s)
CD	0.81175 (1.11)	6.66 (3.84)	88.80 (1.79)
EG- α	0.73160 (1.00)	6.38 (3.67)	114.9 (2.32)
NB	1.52001 (2.08)	6.59 (3.79)	126.7 (2.56)
New	0.81175 (1.11)	4.18 (2.40)	89.04 (1.80)
New/sub	12.9880 (17.8)	1.74 (1.00)	49.49 (1.00)

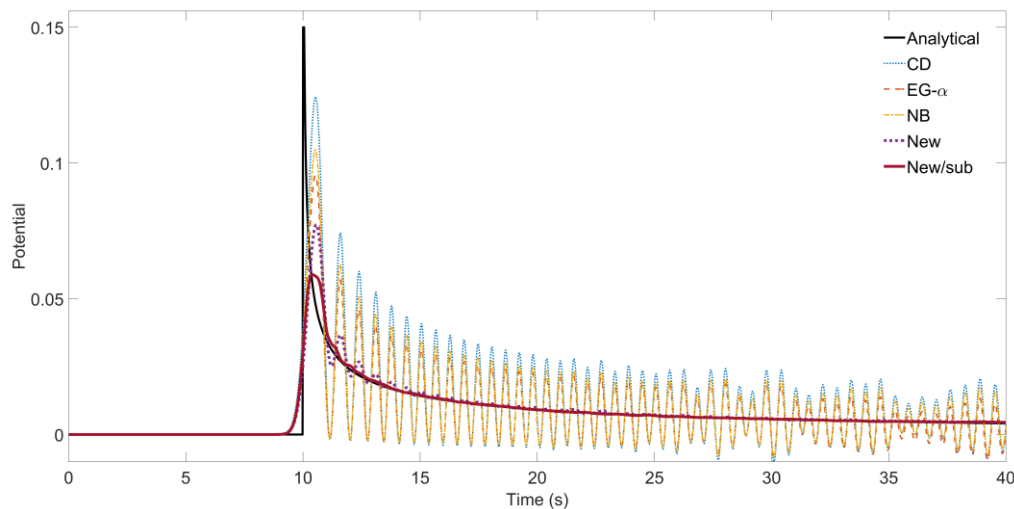


Fig.2 – Time history results for U , at a point located 15m horizontally away from the applied load.

In Figure 2, time-history results are presented at a location 15 meters away from the applied source, highlighting the improved accuracy achieved with the discussed adaptive approach. As depicted in this figure, the adaptive formulation effectively dissipates spurious numerical oscillations, leading to significantly improved responses compared to standard techniques. In Figure 3, snapshots of the computed results at $t = 20$ s are shown, comparing the outcomes obtained using different time-marching techniques. From this figure, it becomes evident that the Central Difference method, Noh-Bathe method, and EG- α method fail to produce accurate results, as their computed responses are dominated by spurious oscillations. In contrast, the New and New/sub techniques exhibit much more satisfactory results. This demonstrates the capability of the discussed adaptive approach to accurately capture the dynamic behavior of the system and mitigate undesirable numerical oscillations.

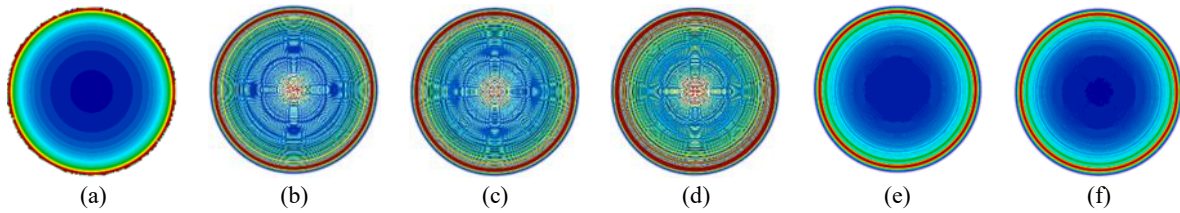


Fig.3 – Computed fields at 20s: (a) analytical, (b) CDM, (c) EG- α , (d) Noh-Bathe, (e) New and (f) New/sub.

4.2 Application 2

In this second example, a geophysical model of the Búzios region in Brazil is considered. The model represents a realistic depiction of a 7.9km x 16km area [9]. The properties of the model are based on fundamental rock properties, with subtle variations at the boundaries of the macro-layer, resulting in synthetic data that closely resembles real-world scenarios. Figure 4a illustrates the representation of these synthetic data. To analyze the model, the original synthetic data obtained from finite difference discretization is converted into a finite element mesh comprising 4,864,312 linear triangular elements. The conversion process ensures that the elements of the finite element mesh are structured and have uniform sizes, so the variability in the time-step value (Δt_e) is determined by the wave propagation speed of each material within the model. As a result, the model is divided into three time-step subdomains, as depicted in Figure 4b. In order to simulate the infinite medium accurately, perfectly matched layers (PMLs) with a thickness of 800m are implemented at the left, right, and bottom borders of the model. By incorporating PMLs, the model can be analyzed in a manner that is consistent with an infinite medium, enabling more accurate and reliable simulations.

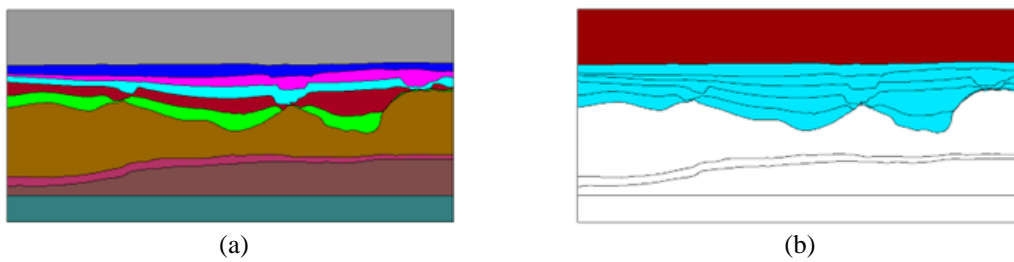


Fig.4 – (a) Geological model and (b) computed time-step subdomains.

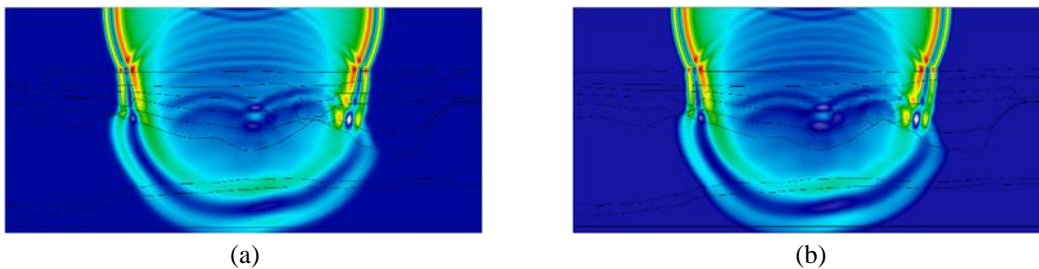


Fig.5 – Computed fields at $t = 4s$: (a) EG- α ; (b) New/sub.

Method	$\Delta t (10^{-3}s)$	CPU Time (s)
CD	0.64051 (1.11)	5233.7 (1.68)
EG- α	0.57727 (1.00)	5462.8 (1.75)
NB	1.19936 (2.08)	5683.6 (1.83)
New	0.64051 (1.11)	5261.2 (1.69)
New/sub	2.56204 (4.44)	3112.9 (1.00)

Table 2 presents a comprehensive overview of the performance of the analyzed methods, reaffirming the good efficiency of the proposed formulation. The computational effort of the proposed approach is significantly reduced compared to standard procedures, with a decrease of up to 40%. Remarkably, this enhanced efficiency does not compromise the quality of the obtained results, as demonstrated in Figure 5, where the responses obtained using the proposed formulation are shown to be equivalent to those obtained using standard procedures.

5 Conclusions

This study discusses an explicit time-marching technique that incorporates subdomain/sub-cycling splitting procedures for solving acoustic models. The time-steps and time-integration parameters of the method are determined locally and automatically based on the characteristics of the spatially discretized model. The key features of this formulation can be summarized as follows: (i) it is a truly explicit approach that does not involve solving any system of equations by utilizing lumped mass matrices; (ii) it is self-starting and relies on simple single-step displacement-velocity relations; (iii) it allows for advanced controllable algorithmic dissipation through optimized, adaptive, locally computed parameters; (iv) it establishes a connection between the temporal and spatial discretization methods, allowing their errors to be better counterbalanced; (v) it provides extended stability limits (that may not be reduced by the presence of physical damping, as typically occur in truly explicit analyses); (vi) it is fully automated and easy to implement, requiring no user expertise or effort; (vii) it offers high accuracy and efficiency, particularly when combined with subdomain/sub-cycling splitting procedures.

The paper demonstrates that the discussed technique is highly versatile and consistently outperforms traditional time-marching methods. It showcases the technique's robustness in adapting to different model properties and its ability to handle complex and refined large-scale problems, significantly reducing the computational burden of their analyses. As illustrated in this manuscript, the discussed methodology stands as an effective and attractive option for modeling complex wave propagation problems.

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