An adaptive implicit-explicit time-marching technique for elastodynamic analysis

Isabelle de Souza Sales[1], Delfim Soares Jr.[2], Webe João Mansur[1], Lucas Ruffo Pinto[1]

[1]*COPPE/Federal University of Rio de Janeiro*
CEP 21941-611, Rio de Janeiro, Brazil
Isabelle.sales@coc.ufrj.br, lucas.ruffo@coc.ufrj.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. In this work, we discuss an implicit-explicit time-marching procedure with adaptive time integration parameters for the analysis of hyperbolic models. This methodology utilizes two locally evaluated time integration parameters, allowing for their different spatial and temporal distributions. The first parameter defines implicit/explicit subdomains within the model, ensuring stability and reducing errors related to period elongation. The second parameter controls the dissipative properties of the methodology, effectively eliminating the influence of spurious high-frequency modes and reducing amplitude decay errors. Moreover, this implicit-explicit approach reduces computational effort by obtaining reduced systems of equations and serves as an efficient non-iterative single-step procedure. The key features of this novel methodology can be summarized as follows: it is simple, locally defined, guarantees stability, provides enhanced accuracy, enables advanced controllable algorithmic dissipation in higher modes, establishes a connection between temporal and spatial discretizations, operates as a single-solve framework based on reduced systems of equations, is self-starting, and fully automated. The paper concludes with the presentation and comparison of numerical results with those obtained using standard techniques, illustrating the remarkable effectiveness of the discussed approach.

Keywords: Time-Marching, Implicit-Explicit Analysis, Adaptive Parameters.

1 Introduction

Time-dependent hyperbolic equations are widely used in science and engineering, but finding analytical solutions for these equations is often impractical. As a result, numerical methods, especially step-by-step time integration algorithms, are commonly employed to obtain approximate solutions. The literature presents numerous classical explicit and implicit algorithms for time-marching analysis [1-4], each with its own advantages and disadvantages. Explicit algorithms are generally preferred due to their lower computational costs, but their use is limited by stability conditions. On the other hand, implicit algorithms can be defined as unconditionally stable but require higher computational costs. Various techniques can be employed to enhance the accuracy and stability of time-integration algorithms, such as subcycling, mass scaling, high-order schemes, and automatic time step control. Ongoing research in this field has led to the development of several time-marching techniques available today for transient analyses [5-11].

This work discusses an implicit-explicit time-marching algorithm that combines the strengths of both explicit and implicit methods. It employs implicit integrators for "stiffer" subdomains and explicit integrators for "flexible" subdomains, making it easier to meet stability requirements and enabling the use of larger time steps. This approach also leads to reduced systems of equations, resulting in more efficient analyses. Previous studies on implicit-explicit time-marching techniques focused on merging different integration procedures, whereas this work presents a unified time-marching framework and a model/solution-adaptive implicit-explicit time integration procedure. The algorithm dynamically selects time integration parameters at a local level, allowing different values to be used for each element of the model and each time step. It is adaptive and computes integration parameters automatically based on the properties of the discrete model and the evolution of the computed fields. Consequently, this approach offers a high degree of flexibility and effectiveness.

The methodology utilized in this work involves two time integration parameters, γ and α, which are employed to determine the explicit/implicit and dissipative/non-dissipative aspects of the model, respectively [5]. The

calculation of γ ensures stability and improved accuracy, while α is evaluated to eliminate the influence of spurious modes. The approach is non-iterative, directly computing the values of the time integration parameters based on local properties of the spatial discretization, the chosen time step, and the results from previous time steps. It is also self-starting, eliminating the need for complex initial procedures.

In the field of geophysics, the analysis of heterogeneous domains with multiple layers consisting of different materials is common. Therefore, the methodology discussed in this work automatically handles the more "flexible" layers of the geological model explicitly, while treating the other layers implicitly. This approach enables the consideration of larger time steps, leading to improved efficiency. Additionally, the methodology evaluates an optimal time-step value that ensures the most efficient distribution of explicit and implicit elements throughout the model. This guarantees that the implicit-explicit approach described in this work is always more efficient compared to conducting the analysis entirely using either explicit or implicit methods.

2 Governing equations and time integration strategy

The governing equation describing a semi-discrete hyperbolic system may be written as:

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

where $\mathbf{M}$, $\mathbf{C}$, and $\mathbf{K}$ represent its mass, damping, and stiffness matrices, respectively. The system's acceleration, velocity, and displacement vectors are denoted as $\ddot{\mathbf{U}}(\mathrm{t})$, $\dot{\mathbf{U}}(\mathrm{t})$ and $\mathbf{U}(\mathrm{t})$, respectively, and the external force acting on the system is represented by vector $\mathbf{F}(\mathrm{t})$. Furthermore, the initial conditions are defined as $\mathbf{U}^0 = \mathbf{U}(0)$ and $\dot{\mathbf{U}}^0 = \dot{\mathbf{U}}(0)$, representing its initial displacement and velocity vectors, respectively.

The adopted time-domain solution methodology utilizes locally and adaptively computed time integration parameters, which take into account the properties of the discretized model and its computed responses. This approach enhances the accuracy of the discussed solution procedure, which is here carried out considering the following recurrence equations:

$$\left(\mathbf{M} + \frac{1}{2}\Delta\mathrm{t}\mathbf{C} + \frac{1}{2}\gamma^{\mathrm{n}}\Delta\mathrm{t}^2\mathbf{K}\right)\dot{\mathbf{U}}^{\mathrm{n+1}} = \int_{\mathrm{t^n}}^{\mathrm{t^{n+1}}} \mathbf{F}(\mathrm{t})\,\mathrm{dt} + \mathbf{M}\dot{\mathbf{U}}^{\mathrm{n}} - \frac{1}{2}\Delta\mathrm{t}\mathbf{C}\dot{\mathbf{U}}^{\mathrm{n}} - \Delta\mathrm{t}\mathbf{K}\left(\mathbf{U}^{\mathrm{n}} + \frac{1}{2}\alpha^{\mathrm{n}}\Delta\mathrm{t}\dot{\mathbf{U}}^{\mathrm{n}}\right) \tag{2a}$$

$$\mathbf{U}^{\mathrm{n+1}} = \mathbf{U}^{\mathrm{n}} + \frac{1}{2}\Delta\mathrm{t}\dot{\mathbf{U}}^{\mathrm{n}} + \frac{1}{2}\Delta\mathrm{t}\dot{\mathbf{U}}^{\mathrm{n+1}} \tag{2b}$$

where $\Delta\mathrm{t}$ represents the time-step used in the analysis. An important feature of this method is that it solely relies on the first temporal derivative of $\mathbf{U}$ and does not necessitate the calculation of its second temporal derivative. This characteristic renders it a truly self-starting method, eliminating the need for complex initial procedures such as computing initial second temporal derivatives or using multistep initial values. Another important characteristic is that, in the discussed adaptive approach, the time integration parameters are computed spatially and temporally to more effectively explore specific features. This is achieved by defining α_e^n and γ_e^n, where "e" represents the element of the spatial discretization used in the analysis.

In this approach, the parameter $\gamma_{\mathrm{e}}^{\mathrm{n}}$ plays a crucial role in defining explicit and implicit subdomains. When $\gamma_{\mathrm{e}}^{\mathrm{n}} = 0$, explicit elements are generated, resulting in a local system of equations that has a diagonal effective matrix when lumped mass and damping matrices are employed. On the other hand, implicit elements are obtained when $\gamma_{\mathrm{e}}^{\mathrm{n}} \neq 0$. For improved accuracy in the implicit elements, it is recommended to use $0 < \gamma_{\mathrm{e}}^{\mathrm{n}} < 1/2$. Notably, when $\alpha_{\mathrm{e}}^{\mathrm{n}} = 1$ and $\gamma_{\mathrm{e}}^{\mathrm{n}} = 0$, the proposed technique reproduces the characteristics of the central difference (CD) method, while $\alpha_{\mathrm{e}}^{\mathrm{n}} = 1/2$ and $\gamma_{\mathrm{e}}^{\mathrm{n}} = 1/2$ replicate the trapezoidal rule (TR). Therefore, by selecting $0 < \gamma_{\mathrm{e}}^{\mathrm{n}} < 1/2$ and $\alpha_{\mathrm{e}}^{\mathrm{n}} = 1 - \gamma_{\mathrm{e}}^{\mathrm{n}}$ (representing a non-dissipative formulation), an intermediate methodology between the CD and the TR is achieved. This intermediate methodology reduces period elongation errors compared to the CD and the TR, as the CD provides negative period elongation and the TR provides positive period elongation. The value of $\gamma_{\mathrm{e}}^{\mathrm{n}}$ is determined using equations (3a) and (3b), which depend on the maximum sampling frequency of the element: $\Omega_{\mathrm{e}}^{\max} = \omega_{\mathrm{e}}^{\max}\Delta\mathrm{t}$, where $\omega_{\mathrm{e}}^{\max}$ represents the highest natural frequency of the element.

$$If\ \Omega_e^{max} \leq 2, \gamma_e^n = 0 \tag{3a}$$

$$\mathrm{If}\ \Omega_{\mathrm{e}}^{\max} > 2, \gamma_{\mathrm{e}}^{\mathrm{n}} = \frac{1}{2}\tanh\left(\frac{1}{4}\Omega_{\mathrm{e}}^{\max}\right) \tag{3b}$$

The proposed implicit solution is always stable, while the explicit analysis is conditionally stable with a critical value of $\Omega_{\mathrm{c}} = 2$, the same as that of the central difference method. By using this criterion to compute $\gamma_{\mathrm{e}}^{\mathrm{n}}$,

the implicit-explicit algorithm is ensured to maintain stability. When the element properties remain constant throughout the analysis, such as in standard linear analyses, the values of γ_e^n remain unchanged over time. Consequently, if the model matrices remain unchanged, the time integration parameter γ_e^n also remains constant, resulting in a constant effective matrix (see the left-hand-side of equation (2a)) throughout the analysis. In this scenario, the effective matrix can be calculated and treated only once, leading to increased efficiency.

Additionally, the inclusion of explicit elements into the analysis results in a portion of the effective matrix consisting solely of diagonal entries. These entries can be easily eliminated from the global system of equations, reducing the system dimension and the computational effort required for its solution. Thus, the proposed hybrid implicit-explicit analysis offers a stable algorithm with a smaller system of equations, making it more efficient compared to traditional implicit methods. It is important to emphasize that this automatic reduction of the global system dimension is achieved solely by considering the diagonal terms of the effective matrix, without any predetermined subdomain specifications or user input, which may not be practical for complex models.

The α_e^n parameter governs the dissipative characteristics and can be adjusted based on the solution evolution. It allows for the introduction of numerical dissipation when and where it is needed to mitigate spurious non-physical oscillations. By locally computing α_e^n, the technique aims to optimize the incorporation of numerical damping into the analysis, minimizing its adverse effects. Thus, when $\alpha_e^n = 1 - \gamma_e^n$, no numerical dissipation is introduced into the analysis. However, when α_e^n is greater than $1 - \gamma_e^n$, numerical damping is present. This capability allows for the selective activation of dissipation at specific locations or instants where oscillations occur, while deactivating it when unnecessary. This approach avoids the imposition of a permanent algorithmic dissipative pattern and helps prevent excessive numerical damping errors. The activation of dissipation can be based on an oscillatory criterion, where the α_e^n parameters of neighboring elements to an oscillating degree of freedom are adjusted to introduce numerical dissipation. If no oscillatory behavior is detected, $\alpha_e^n = 1 - \gamma_e^n$ is used. This process involves computing an oscillatory parameter φ_e^n for each element and time step of the analysis. If $\varphi_e^n = 0$ (indicating no oscillation), $\alpha_e^n = 1 - \gamma_e^n$; otherwise, $\alpha_e^n > 1 - \gamma_e^n$, as shown:

$$\varphi_e^n = \sum_{i=1}^{\eta_e} \left| \left| u_i^n - u_i^{n-2} \right| - \left| u_i^n - u_i^{n-1} \right| - \left| u_i^{n-1} - u_i^{n-2} \right| \right| / \left| u_i^n - u_i^{n-2} \right| \tag{4a}$$

$$\text{If } \varphi_e^n = 0,\ \alpha_e^n = 1 - \gamma_e^n \tag{4b}$$

$$\text{If } \varphi_e^n \neq 0,\ \alpha_e^n = 2\left[2\gamma_e^n + \left(1 + \frac{\xi_e \Delta t}{2\rho_e}\right)\left(\frac{2}{\Omega_e^{max}}\right)^2\right]^{1/2} - 1 - \gamma_e^n - \frac{\xi_e \Delta t}{2\rho_e}\left(\frac{2}{\Omega_e^{max}}\right)^2 \tag{4c}$$

where $\xi_e = \varsigma_e/(2\rho_e\omega_e^{max})$ and ρ_e and ς_e represent the physical properties of the medium that define matrices $\mathbf{M}$ and $\mathbf{C}$, respectively. Equation (4c) is formulated so that maximum numerical dissipation is applied to the higher frequency of the element [5], making this procedure highly effective in dissipating the influences of spurious high-frequency modes.

In the discussed implicit-explicit analysis, increasing the chosen time-step value reduces the number of required time steps for the solution within a fixed period of analysis, which is beneficial for efficiency. However, simultaneously, enlarging Δt results in a higher number of implicit elements throughout the discretized model, increasing the computational effort required for the solver procedure. Consequently, an optimization algorithm can be employed to determine an optimal Δt value with respect to computational efficiency. In this study, the Particle Swarm Optimization (PSO) algorithm [12] is utilized to compute the optimal Δt by minimizing the expected total number of operations involved in the solution process.

3 Numerical applications

In this section, we present two numerical examples to showcase the effectiveness of the discussed hybrid technique. The first example involves a heterogeneous rod consisting of two materials, for which analytical solutions are available. This allows us to assess the accuracy of the proposed technique. The second example involves a synthetic model that closely resembles real geological applications, demonstrating the efficacy of the methodology for analyzing large-scale geophysical problems encountered in the OIL & GAS industry. Specifically, the study focuses on the elastic 2DEW model, which encompasses multiple layers with varying properties and significant salt regions, representing complex configurations of elastodynamic wave propagation.

The performance of the discussed implicit-explicit adaptive formulation, referred to as the "New" method,

is compared to that of standard explicit methods. The explicit methods used for comparison include the classic Central Difference (CD) method, the explicit generalized α (EG-α) method developed by Hulbert and Chung [2], and the Noh-Bathe (NB) method [4]. The EG-α method adopts a value of ρ_b = 0.3665 to minimize period elongation errors, as recommended by the authors, while the NB method uses a value of p = 0.54, also recommended by the authors. Each explicit method applies the maximum allowable time-step value for stability, evaluated at element level, to ensure more efficient analyses for each approach. In contrast, the implicit-explicit approach evaluates an optimal time-step value for each analysis, as discussed at the end of the previous section.

3.1 Application 1

In this first example, we examine a rectangular heterogeneous rod composed of different combinations of two materials. Two model configurations were analyzed, with each material occupying 50% of the rod proportion. For both analyses, material 1 has the physical properties E = 100 KPa and $\rho = 1 Kg/m^3$, with material 2 having the same density. The modulus of elasticity of material 2 is chosen to generate different wave propagation speeds (c_2/c_1) between the two materials, with the first analysis having a ratio of 4 and the second analysis having a ratio of 6. The model is spatially discretized using a structured finite element mesh consisting of 32,000 linear square elements. The analytical solution for the horizontal displacements of the rod is known in the literature and can be found in [13], allowing for proper evaluation of the accuracy of the referred solution techniques.

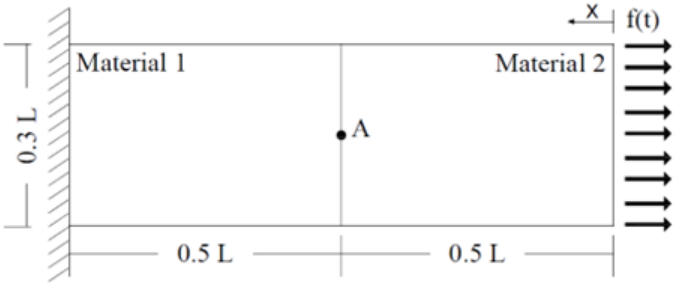


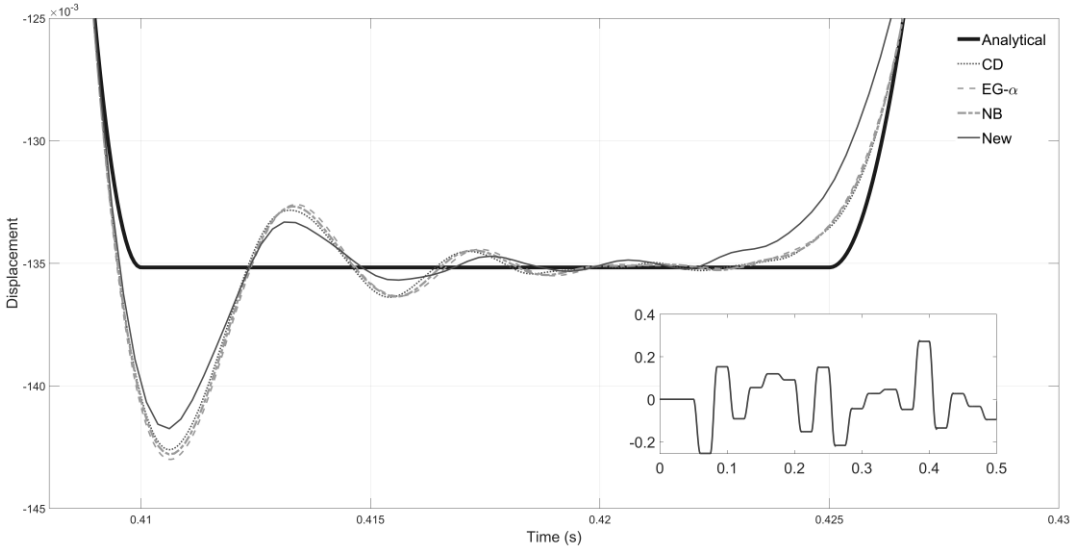
Fig.1 – Sketch of the heterogeneous rod.

Table 1 presents the CPU times and relative errors (computed at point A, located at the center of the model, as shown in Figure 1) for each approach. The "New" method employs the same time step for both implicit and explicit subdomains, with the more rigid region treated implicitly and the less rigid region treated explicitly. This allows for the use of a larger time step for the overall analysis. As observed, the new procedure achieves similar or greater accuracy compared to the standard methods but with shorter CPU times, resulting in a significant reduction in computational effort. In these specific cases, the computational effort of the discussed "New" formulation amounts to only 89% ($c_2/c_1 = 4$) and 55% ($c_2/c_1 = 6$) of that required by the standard techniques.

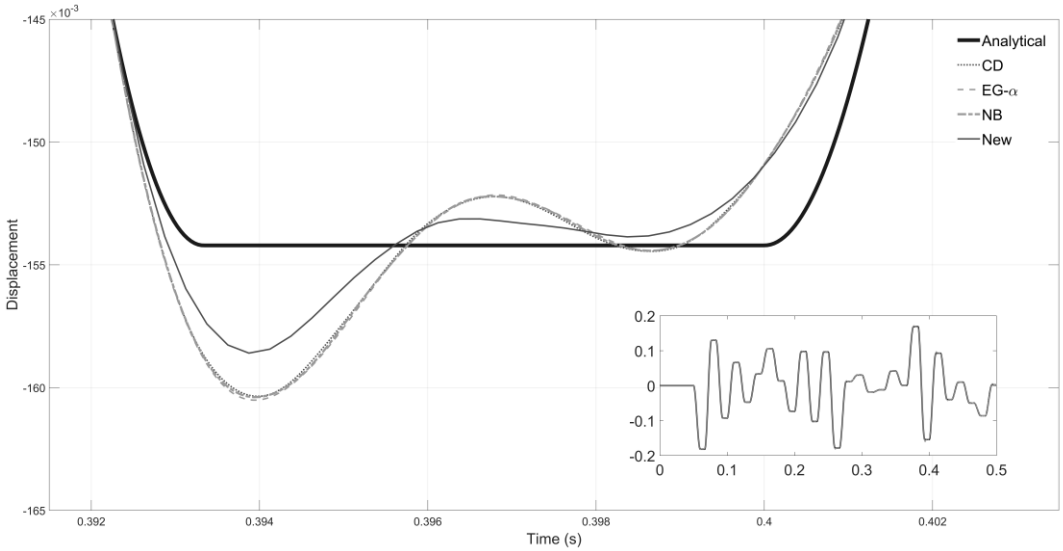
Table 1 - Performance of the methods for the first example

c_2/c_1	Method	Δt (10^{-4}s)	Error u (10^{-2})	CPU Time (s)
4	CD	0.61874 (1.11)	1.02 (1.00)	86.1 (1.12)
	EG-α	0.55765 (1.00)	1.10 (1.08)	90.7 (1.18)
	NB	1.15861 (2.08)	1.08 (1.06)	103.2 (1.35)
	New	2.49920 (4.48)	1.15 (1.12)	76.7 (1.00)
6	CD	0.41249 (1.11)	1.50 (1.00)	139.8 (1.81)
	EG-α	0.37177 (1.00)	1.55 (1.03)	147.4 (2.18)
	NB	0.77241 (2.08)	1.55 (1.03)	167.7 (2.18)
	New	2.49920 (6.72)	1.51 (1.00)	77.0 (1.00)

In Figure 2, time-history results are presented at the same point A for both analyses, highlighting the improved accuracy achieved with the proposed adaptive approach. It is evident that the "New" method obtains results similar to the other techniques, even when using time steps 6 times larger.

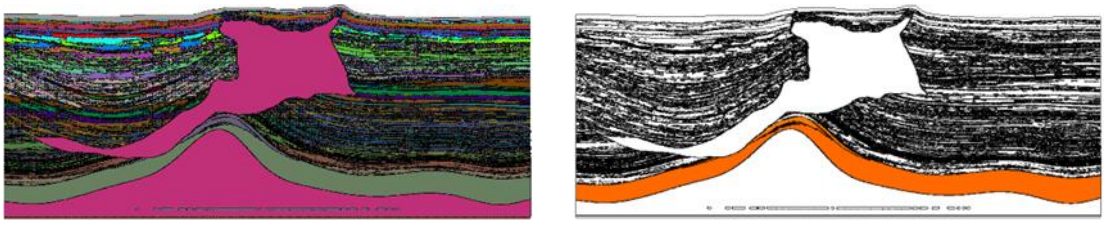


(a)



(b)

Fig.2 – Time history results for u_x, at the middle of the rod, considering: (a) $c_2/c_1 = 4$; and (b) $c_2/c_1 = 6$.



(a) (b)

Fig.3 – (a) Geological model and (b) division of implicit (orange) and explicit (white) subdomains.

3.2 Application 2

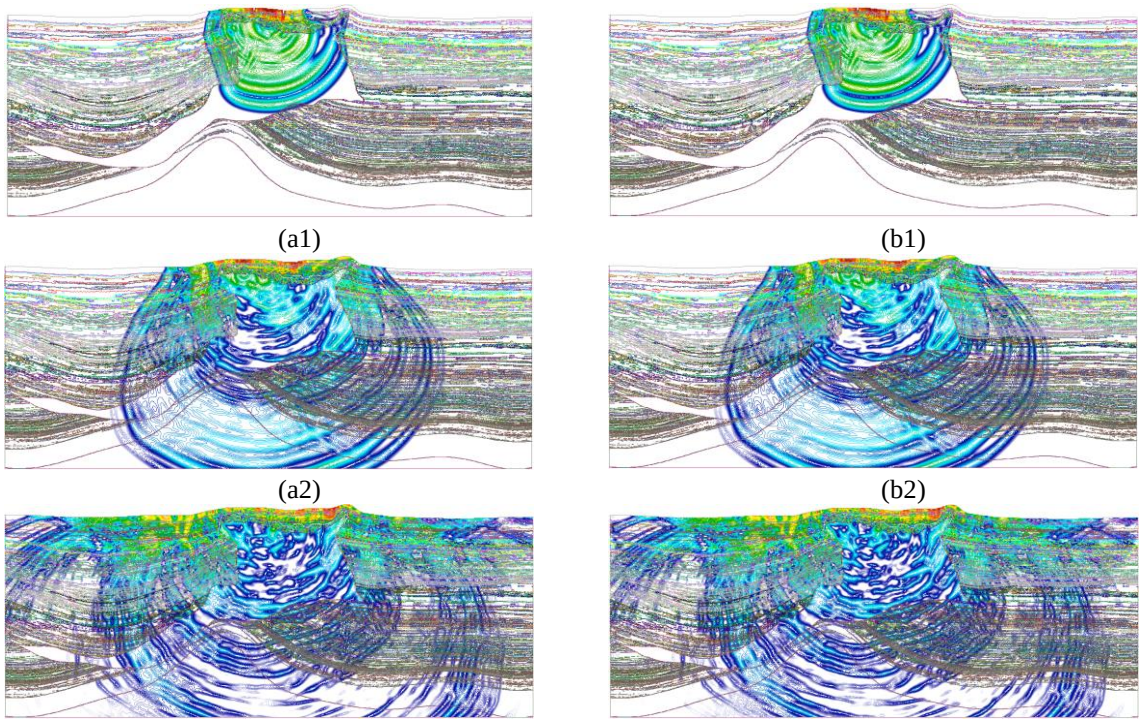
In the second example, a geophysical model generated in SEAM (SEG Advanced Modeling) is considered. This model simulates a realistic soil environment in a salt region in the Gulf of Mexico, incorporating stratigraphy and including oil and gas reservoirs. All properties of the model are derived from fundamental rock properties, which exhibit subtle contrasts at the boundaries of the macro-layer. This generates realistic synthetic data for analysis. The model distribution used is the Elastic Earth Model, specifically the Elastic 2DEW Classic model [14], is represented in Figure 3a. The distribution consists of three binary files containing data for density, P-wave

velocity (dilation), and S-wave velocity (shear). In this case, for the discussed implicit-explicit approach, an optimal time-step of 0.42489s is computed, resulting in 16.78% implicit elements and 83.22% explicit elements along the referred mesh, as illustrated in Figure 3b.

Table 2 - Performance of the methods for the geological model

Method	Δt (10^{-3}s)	CPU Time (s)
CD	0.32415 (1.11)	11322.8 (2.15)
EG-α	0.29215 (1.00)	12283.3 (2.34)
NB	0.60698 (2.08)	14773.1 (2.81)
New	0.42489 (1.45)	5259.40 (1.00)

Similar to Table 1, Table 2 showcases the performance of the selected techniques for the second example, further emphasizing the superior efficiency of the discussed hybrid approach. Figures 4(a) and 4(b) present snapshots of the displacements computed using the studied implicit-explicit formulation and explicit generalized α method, respectively. These figures demonstrate that both techniques yield very similar results, with the discussed hybrid approach offering more efficient evaluations, as indicated in Table 2.



(a1) (b1)

(a2) (b2)

(a3) (b3)

Fig.4 – Computed results along the discretized domain at different time instants:
(a) New, (b) EG-α; (1) 2s, (2) 4s, and (3) 8s.

4 Conclusions

This work presents an adaptive implicit-explicit time-marching technique for analyzing elastodynamic problems. The discussed formulation exhibits several noteworthy characteristics, such as: (i) it is a straightforward hybrid approach, directly combining explicit and implicit formulations; (ii) it is locally and adaptively defined, allowing for better accuracy; (iii) it ensures stability; (iv) it is an efficient non-iterative single-step procedure; (v) it incorporates controllable algorithmic dissipation; (vi) it establishes a connection between the temporal and spatial discretization approaches; (vii) it provides reduced solver efforts; (viii) it is self-starting, eliminating the need for complex initialization procedures; (ix) it is fully automated and user-friendly, requiring minimal input and expertise; (x) it surpasses standard explicit or implicit formulations in efficiency by employing optimized time-step values. As one may observe, the discussed technique stands as a very effective time-marching formulation.

Acknowledgements. The financial support by CNPq (Conselho Nacional de Desenvolvimento Cientifico e Tecnológico), PRH-ANP (Programa de Recursos Humanos da Agência Nacional do Petróleo, Gás Natural e Biocombustíveis) and PETROBRAS (CENPES – 21066) is greatly acknowledged.

Authorship statement. The authors hereby confirm that they are the sole liable persons responsible for the authorship of this work, and that all material that has been herein included as part of the present paper is either the property (and authorship) of the authors, or has the permission of the owners to be included here.

References

[1] Chung, J., & Hulbert, G. A time integration algorithm for structural dynamics with improved numerical dissipation: the generalized-α method, 1993.
[2] Hulbert, G. M., & Chung, J. Explicit time integration algorithms for structural dynamics with optimal numerical dissipation. *Computer Methods in Applied Mechanics and Engineering*, 137(2), 175-188, 1996.
[3] Bathe, K. J., & Baig, M. M. I. On a composite implicit time integration procedure for nonlinear dynamics. *Computers & Structures*, 83(31-32), 2513-2524, 2005.
[4] Noh, G., & Bathe, K. J. An explicit time integration scheme for the analysis of wave propagations. *Computers & structures*, 129, 178-193, 2013.
[5] Soares, D. A model/solution-adaptive explicit-implicit time-marching technique for wave propagation analysis. *International Journal for Numerical Methods in Engineering*, 119(7), 590-617, 2019.
[6] Pinto, L. R., Soares, D., & Mansur, W. J. Elastodynamic wave propagation modelling in geological structures considering fully-adaptive explicit time-marching procedures. *Soil Dynamics and Earthquake Engineering*, 150, 106962, 2021.
[7] Mansur, W. J., Loureiro, F. S., Soares, D., & Dors, C. Explicit time-domain approaches based on numerical Green's functions computed by finite differences–the ExGA family. *Journal of Computational Physics*, 227(1), 851-870, 2007.
[8] Soares, D. An enhanced explicit–implicit time-marching formulation based on fully-adaptive time-integration parameters. *Computer Methods in Applied Mechanics and Engineering*, 403, 115711, 2023.
[9] Soares Jr, D. An improved adaptive formulation for explicit analyses of wave propagation models considering locally-defined self-adjustable time-integration parameters. *Computer Methods in Applied Mechanics and Engineering*, 399, 115324, 2022.
[10] Soares, D. A simple and effective new family of time marching procedures for dynamics. *Computer Methods in Applied Mechanics and Engineering*, 283, 1138-1166, 2015.
[11] Soares, D. A novel single-step explicit time-marching procedure with improved dissipative, dispersive and stability properties. Computer Methods in Applied Mechanics and Engineering, 386, 114077, 2021.
[12] Kennedy, J., & Eberhart, R. Particle swarm optimization. *In Proceedings of ICNN'95- international conference on neural networks* (Vol. 4, pp. 1942-1948). IEEE, 1995.
[13] Soares, D., Pinto, L. R., Mansur, W. J. A truly explicit time-marching formulation for elastodynamic analyses considering locally-adaptive time-integration parameters and time-step values. *International Journal of Solids and Structures*, 112260, 2023.
[14] Fehler, M. Seam update: Seam phase i rpsea update: Status of simulations. *The Leading Edge*, 31(12), 1424-1426, 2012.