

An Adaptive Implicit-Explicit Time-Marching Technique for Wave Propagation Analysis

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Abstract

This work discusses an effective explicit-implicit timemarching procedure with adaptive time integration parameters to analyze wave propagation models. This approach has two parameters that are locally evaluated, providing different spatial and temporal distributions. The first parameter ensures stability and reduces dispersion errors, defining the explicit/implicit subdomains of the model. The second parameter controls the dissipative properties of the methodology, allowing spurious highfrequency modes to be properly eliminated, as well as reducing amplitude decay errors. The discussed approach diminishes the computational effort of the analysis by obtaining reduced systems of equations, making it an efficient adaptive single-step procedure. Additionally, the methodology offers enhanced accuracy and enables advanced controllable algorithmic dissipation in higher modes, linking temporal and spatial discretization. It is also a self-starting, entirely automated process that has been tested through benchmark analyses, demonstrating its effectiveness for real-world applications in the OIL & GAS industry.

Introduction

Time-dependent hyperbolic equations have a wide range of applications in science and engineering, but obtaining analytical solutions for these equations is often impractical. Therefore, numerical methods, particularly step-by-step time integration algorithms, are commonly used to obtain approximate solutions. The literature describes many classical explicit and implicit algorithms for time-marching analysis [1-4], each with their own advantages and drawbacks. Explicit algorithms are generally preferred due to their lower computational costs, but stability conditions can limit their use. On the other hand, implicit algorithms may be defined unconditionally stable, but they come with higher computational costs. Various procedures can be applied to improve the accuracy and stability of timeintegration algorithms, including subcycling, mass scaling, high-order schemes, and automatic time step control. Ongoing research in this field has resulted in several timemarching techniques available today for transient analyses [5-11].

This work presents an explicit-implicit time-marching algorithm that combines the advantages of both explicit

and implicit methods. By treating "stiffer" subdomains with implicit integrators and "flexible" subdomains with explicit integrators, stability requirements are easier to fulfill, allowing larger time steps to be employed. This approach also results in reduced systems of equations, allowing for more efficient analyses. Previous works on explicit-implicit time-marching techniques focused on merging different integration procedures, but this work considers a single time-marching framework and a model/solution-adaptive explicit-implicit time integration procedure. This timemarching algorithm selects time integration parameters at a local level, which allows for different values to be used for each element of the model and each time step. The procedure is adaptive and computes the integration parameters automatically, taking into account the properties of the discrete model and the evolution of the computed fields. As a result, the approach is highly flexible and effective.

The methodology employs two time integration parameters, γ and α , which are used to define the explicit/ implicit and dissipative/non-dissipative elements of the model, respectively [5]. The computation of γ ensures stability and enhanced accuracy, while the evaluation of α aims 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 adopted time step, and previous time-step results. It is also self-starting, eliminating the need for cumbersome initial procedures.

In geophysics, there is often a need to analyze heterogeneous domains with multiple layers of various materials. Thus, the discussed methodology automatically treats the more 'flexible' layers of the geological model explicitly and the others implicitly, allowing larger time-step values to be considered, increasing the efficiency of the analyses. The evaluation of an optimal time-step value, which allows the most efficient distribution of explicit and implicit elements along the model, is also considered here, guaranteeing that the discussed explicit-implicit approach is always more efficient than an entirely explicit or implicit analysis.

Governing equations and time integration strategy

The semi-discrete system of equations governing a wave propagation model may be written as:

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

where M, C, and K stand for the so-called mass, damping, and stiffness matrices of the model, respectively, which are here computed considering the finite element method [12], P(t) stands for the unknown pressure field (with overdots indicating its time derivatives), and vector F(t) represents external applied sources. The initial conditions are defined as $\mathbf{P}^0 = \mathbf{P}(0)$ and $\dot{\mathbf{P}}^0 = \dot{\mathbf{P}}(0)$.

The time integration parameters of the methodology_are locally and adaptively computed based on the properties of the discretized model and the computed responses, allowing for more accurate solution procedures. In this time-marching procedure, the following recurrence equations are considered:

$$\begin{pmatrix} \mathbf{M} + \frac{1}{2}\Delta t\mathbf{C} + \frac{1}{2}\gamma^{n}\Delta t^{2}\mathbf{K} \end{pmatrix} \dot{\mathbf{P}}^{n+1} = \int_{t^{n}}^{t^{n+1}} \mathbf{F}(t) dt + \\ \mathbf{M}\dot{\mathbf{P}}^{n} - \frac{1}{2}\Delta t\mathbf{C}\dot{\mathbf{P}}^{n} - \mathbf{K}(\mathbf{P}^{n} + \frac{1}{2}\alpha^{n}\Delta t^{2}\dot{\mathbf{P}}^{n})$$

$$\mathbf{P}^{n+1} = \mathbf{P}^{n} + \frac{1}{2}\Delta t\dot{\mathbf{P}}^{n} + \frac{1}{2}\Delta t\dot{\mathbf{P}}^{n+1}$$

$$(2b)$$

where Δt represents the time-step of the analysis. It is worth noting that this single-step method depends only on the first temporal derivative of **P**, and does not require the calculation of its second temporal derivative. This property makes it a truly self-starting method, eliminating the need for cumbersome initial procedures like computing initial second temporal derivatives or multistep initial values.

In the discussed adaptive approach, the time integration parameters of the method are spatially and temporally computed to locally better explore specific features (i.e., α_e^n and γ_e^n are defined, where "e" stands for the element of the adopted spatial discretization).

In this case, the γ_e^n parameter controls the definition of explicit and implicit subdomains, with explicit elements being generated when $\gamma_e^n=0$ and implicit elements being engendered when $\gamma_e^n \neq 0.$ If $\gamma_e^n = 0$ is adopted and lumped mass and damping matrices are considered, the local system of equations becomes explicit with a diagonal effective matrix. For implicit elements, better accuracy is achieved when $0 < \gamma_e^n < 1/2$ is considered. In fact, for $\alpha_e^n =$ 1 and $\gamma_e^n = 0$, the proposed technique reproduces the main features of the central difference method (CD), and for $\alpha_e^n = 1/2$ and $\gamma_e^n = 1/2$, it reproduces the trapezoidal rule (TR). Thus, for $0 < \gamma_e^n < 1/2$ and $\alpha_e^n = 1 - \gamma_e^n$ (which represents a non-dissipative formulation), an intermediate methodology between the CD and the TR is enabled. As the CD provides negative period elongation and the TR provides positive period elongation, reduced period elongation errors occur for $0 < \gamma_e^n < 1/2$, enabling a more accurate technique. Here, γ_e^n is determined as indicated in equation (3), which is based on the maximum sampling frequency of element $\Omega_e^{max} = \omega_e^{max} \Delta t$, where ω_e^{max} stands for the highest natural frequency of the element.

If
$$\Omega_{\rm e}^{\rm max} \le 2, \gamma_{\rm e}^{\rm n} = 0$$
 (3a)

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

The proposed implicit solution is always stable, and the proposed explicit analysis is conditionally stable, with $\Omega_c = 2$ (i.e., the same critical value as that of the CD). Thus, by using this criterion to compute γ_e^n , the explicit-implicit algorithm is guaranteed to be stable. If the element's properties remain constant throughout the analysis (as is the case in standard linear analyses), the values of γ_e^n will remain the same over time. Consequently, if the matrices

of the model do not change, the time integration parameter γ_e^n will also remain unchanged, and the effective matrix of the model will remain constant throughout the analysis. In this situation, the effective matrix can be calculated/treated only once, resulting in a more efficient approach. Moreover, incorporating explicit elements in the analysis leads to a portion of the effective matrix consisting only of diagonal entries. These entries can be easily eliminated from the global system of equations, resulting in a reduced dimension and computational effort required for its solution. Hence, the proposed hybrid explicit-implicit analysis offers a stable algorithm that is associated with a smaller system of equations, making it more efficient than conventional implicit methods. It is crucial to emphasize that this automatic reduction of the global system's dimension is achieved by considering only the diagonal terms of the effective matrix without any predetermined subdomains or input information from the user, which may not be practical for intricate geophysical models.

The α_e^n parameter controls the dissipative properties of the technique and can be adapted according to the evolution of the solution, introducing numerical dissipation when/where necessary to reduce spurious non-physical oscillations. The local computation of α_e^n aims to optimize the introduction of numerical damping into the analysis, minimizing its negative effects.

For $\alpha_e^n = 1 - \gamma_e^n$, numerical dissipation is not introduced into the analysis; for $\alpha_e^n > 1 - \gamma_e^n$, however, numerical damping occurs. This feature may be then explored, allowing dissipation to be locally activated when/where necessary (i.e., when oscillations occur) and deactivated when/where not needed. In this sense, a permanent algorithmic dissipative pattern can be avoided, and excessive numerical damping errors prevented. This local activation may be carried out based on an oscillatory criterion, where the α_e^n parameters of the elements surrounding an oscillating degree of freedom are modified to introduce numerical dissipation. If no oscillatory behavior is observed, $\alpha_e^n = 1 - \gamma_e^n$ is used. This process involves computing an oscillatory parameter ϕ_e^n for each element and time step of the analysis, and, if $\phi_e^n = 0$ (i.e., no oscillation is perceived), $\alpha_e^n = 1 - \gamma_e^n$, otherwise, $\alpha_e^n > 1 - \gamma_e^n$ γ_{e}^{n} , as indicated in equation (4):

$$\varphi_{e}^{n} = \sum_{i=1}^{\eta_{e}} \left| \left| u_{i}^{n} - u_{i}^{n-2} \right| - \left| u_{i}^{n} - u_{i}^{n-1} \right| - \left| u_{i}^{n-1} - u_{i}^{n-2} \right| \right| / \left| u_{i}^{n} - u_{i}^{n-2} \right|$$
(4a)

If
$$\varphi_e^n = 0$$
, $\alpha_e^n = 1 - \gamma_e^n$ (4b)

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

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

In the discussed explicit-implicit analysis, by increasing the adopted time-step value, less time steps are necessary for solution (given a fixed period of analysis), which is positive regarding efficiency aspects; however, simultaneously, by enlarging Δt , more implicit elements take place along the discretized model, increasing the computational effort related to the solver procedure. Thus, an optimization algorithm can then be applied in order to compute an optimal Δt value, regarding computational efficiency. In this work, the Particle Swarm Optimization (PSO) [13] algorithm is used, establishing an optimal Δt value by minimizing the expected total number of operations involved in the solution process.

Numerical applications

In this section, we examine two numerical examples that briefly demonstrate the good performance of the discussed hybrid technique. The first example investigates the resulting pressure field that is due to an impulsive load on an infinite domain, while the second application analyzes a geophysical model. For this first example, an analytical solution is available [14], allowing a better comparison of the obtained results through different time-domain solution procedures. The second example is a benchmark case, created by the PETROBRAS research laboratory, of the Búzios region, where ten well-defined stratified layers are present [15].

The performance of the discussed explicit-implicit adaptive formulation (which is here referred as "new") is compared to that of standard explicit methods. The explicit approaches used in this comparison are the classic Central Difference (CD) method, the explicit generalized α (EG- α) method developed by Hulbert and Chung [2] (with a value of $\rho_b = 0.3665$ adopted to minimize period elongation errors, as recommended by the authors), and the Noh-Bathe (NB) method [4] (with a value of p = 0.54, as recommended by the authors). The maximum possible time-step value for stability is applied for these explicit methods (taking into account an element level evaluation), to ensure more efficient analyses for each approach. For the reported explicit-implicit approach, an optimal timestep value is evaluated for each analysis, as discussed at the end of the previous section.

Application 1

In this first example, an infinite acoustic model is subjected to an impulsive source. The model is discretized considering a 5m x 5m square mesh of 310,253 linear quadrilateral elements. Perfectly matched layers (PMLs) are considered at the borders of the model to simulate the infinite medium.

Tab.1 outlines the performances of the techniques that are employed in this study. As one can observe, the discussed hybrid approach yields the most accurate results, also providing the most efficient computations (which are performed on an Intel Core i7 -7700 3.60GHz processor with OpenMP parallelization utilizing 8 threads). For the referred explicit-implicit analysis, an optimal time-step of 5.3831s is obtained, which is almost 3 times larger than the computed maximal possible time-step for the CD. For this optimal Δt value, the adopted mesh becomes composed of 94.974% explicit elements and 5.026% implicit elements.

Table 1 – Performance of the methods for Application 1

Method	<i>∆t</i> (10 ⁻² s)	Error (10 ⁻¹)	CPU Time (s)
CD	1.8563	5.687	30.56
EG-α	1.6730	4.914	31.27
NB	3.4760	4.134	43.21
New	5.3831	1.443	22.39

In Figure 1, time-history results at a location 1 meter away from the applied source are depicted, further illustrating the better accuracy of the discussed adaptive explicit-implicit approach. As one can observe in this figure, the referred adaptive formulation is able to very properly dissipate spurious numerical oscillations, resulting in much better responses than those provided by standard techniques.



Application 2

This second example considers a geophysical model, which describes a realistic representation of a 7.9km x 16km region in Buzios, Brazil [15]. The properties of the model are based on fundamental rock properties that exhibit subtle contrasts at the boundaries of the macro-layer, resulting in realistic synthetic data that is represented in Figure 2a. The model is discretized considering a finite element mesh with 4,864,312 linear triangular elements, and PMLs of 800m are defined at its left, right and bottom borders. In this case, for the discussed explicit-implicit approach, an optimal time-step of 8.6751×10^{-4} s is computed, resulting in 71.46% explicit elements and 28.54% implicit elements along the referred mesh, as illustrated in Figure 2b.

Table 2 - Performance of the methods for Application 2

Method	Δt (10 ⁻³ s)	CPU Time (s)
CD	6.4051	10277
EG-α	5.5394	10562
NB	11.4665	10781
New	8.6751	8342

As in Tab.1, the performance of the selected techniques for this second example are presented in Tab.2, once again illustrating the better efficiency of the discussed hybrid approach. In Figures 3 and 4, snapshots of the computed pressure fields are depicted, considering the explicit generalized α method and the studied explicitimplicit formulation, respectively, illustrating that very similar results are obtained by these techniques, although the discussed hybrid approach is able to provide more efficient evaluations, as described in Tab.2. Finally, in Figure 5, the computed α_e^n values of the explicit-implicit formulation are described, illustrating its adaptive behaviour.





(b)

Fig.2 – Geological model: (a) layers illustrating the different physical properties of the model; (b) implicit (red) and explicit (white) subdomains of the model, for the hybrid analysis.





Fig.3 – Computed results for the EG-α, at different time instants: (a) 3s; (b) 4s.



(b)
 Fig.4 – Computed results for the adaptive explicit-implicit technique, at different time instants: (a) 3s; (b) 4s.





Fig.5 – α_e^n values in the adaptive explicit-implicit analysis: (a) 3s; (b) 4s.

Conclusions

This paper discusses an adaptive explicit-implicit timemarching technique to analyze wave propagation problems. The main characteristics of the discussed formulation may be summarized as follows: (i) it stands as a very straightforward hybrid approach; (ii) it is locally and adaptively defined; (iii) it has guaranteed stability; (iv) it stands as an efficient non-iterative single-step procedure; (v) it provides enhanced accuracy; (vi) it enables advanced controllable algorithmic dissipation; (vii) it considers a link between the adopted temporal and spatial discretization procedures; (viii) it is based on a single-solve framework that enables reduced systems of equations; (ix) it is truly self-starting; (x) it is entirely automated, requiring no input or expertise from the user; (xi) by considering optimized time-step values, it always becomes more efficient than standard purely explicit or implicit formulations. As can be seen, the proposed technique is very attractive, providing several positive attributes that may be required from a highly effective time-marching formulation.

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