Stability Issues in Discretization of Wave Equation

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***Abstract*—This paper discusses some of the interesting properties of stability analysis of a discretized wave equation. The solutions of the wave equation are wave functions, hence oscillating, so when testing stability the discretization scheme usually shows marginal stability. Marginal stability is a sufficient condition for a discrete scheme convergence and many authors don't bother with mathematical consistency. However, inadequatly chosen discretization method may lead to the additional unwanted oscillations. This paper illustrates this effect in a different approach. First, the wave equation is introduced together with a Perfectly matched layer (PML). Then the 1D wave equation is discretized by using Finite Differences Method (FDM) and Finite-differences Time-domain method (FDTD). It is shown that the latter method does not produce spurious oscillations in the solution. Eigenvalue analysis is done to explain this effect and discuss stability of the numerical scheme.**

***Index Terms*—wave equation, perfectly matched layer, finite differences method, finite-differences time-domain method, stability**

I. Introduction

The wave equation is the fundamental equation in any wave propagation analysis. Every psyhical phenomena involving the propagation of waves in a continuous medium is based on wave equation or on some of its various generalization. Propagation of water waves, acoustic waves, elastic waves in solids, and electromagnetic waves are all based on this equation. The authors of this paper used wave equation mostly for sound field analysis, but the analysis proposed in this paper could be applied in many other technical areas, and on similar systems of partial differential equations.

Even though a mathematical description of wave propagation problems looks fairly simple, usually described with a linear partial differential equation, finding an analytical solution of the problem is not trivial in case of general initial and boundary conditions. With the ubiquity of computers, solving and analyzing continual analytical problems with some discrete numerical method seems almost natural. Today, there are many discretization methods developed (Finite difference methods (FDM), Finite volume methods, Finite element methods, Domain decomposition methods and many others), from which every one of them has several variations, each with its own advantages and disadvantages [1-2].

Unfortunately, inevitable aproximations arise when numerically solving a continual problem. One of the problems described in this paper is that these approximations can lead to instability of the numerical solution. Usually testing stability and convergence of the discrete numerical scheme is relatively easy using Lax-Richtmayer theorem [2-5]. The main contribution of this paper is the illustration of the stability issues of the discretized wave equation, that are neglected in many research papers (such as [6-7]) because the discretization scheme is inherently not unstable, but marginally stable. This phenomenon is usually hardly visible in "soft" mathematical approach. It will be shown that marginal stability actually doesn't interfere with the numerical results, but yet it may lead to interesting stability consequences.

II. The Wave Equation

The wave equation in its simplest form, known as non-dispersive wave equation with constant wave propagation speed, refers to a scalar function $u = (x_1, x_2, ..., x_n, t) = u(\mathbf{x}, t)$, $\mathbf{x} \in \Omega$, that satisfies:

$$c^2 \nabla^2 u = \frac{\partial^2 u}{\partial t^2} \tag{1}$$

where ∇^2 is the (spatial) Laplacian, c is a fixed constant equal to the propagation speed of the wave, and Ω is the wave equation analysed domain. The wave equation could be described even in a more complex and nonlinear form, depending on the medium and wave type analysed [8]. In this paper the simplest linear wave equation (1) will be analysed.

Wave equation is almost always subject to initial and boundary conditions. Initial conditions are related to the initial perturbation of the wave function, or to variuos wave sources, while boundary conditions are more interesting when analysing wave field with objects that can cause reflection, absorption, refraction or difraction.

There are several types of boundary conditions [1]. The wave equation usually deals with two types of boundary conditions, called Dirichlet and Neumann boundary conditions. Dirichlet boundary condition is important in determining the wave field in the neighborhood of solid boundaries (e.g. closed areas, solid obstacles), while Neumann boundary condition is necessary when modeling open tubes, or elastic boundary conditions.

III. Perfectly matched layer concept

When modeling infinite space in a finite domain, spurious reflections can occurr at the end of the analysed domain, as it was a solid boundary. This problem arises in many technical areas (open sea waves analysis, seizmic processes, electromagnetic radiation etc.). When solving wave function,

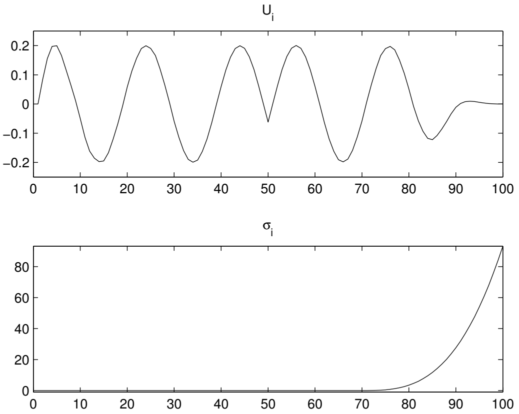


Fig. 1: 1D wave propagation with PML implemented, U_i is the discretized wave function, and σ_i is the absorbing function in time n. On the right side of the x-axis waves are absorbed, while on the left the reflection begins.

some of the conventional methods, such as real coordinate transformations (e.g. $x_T = tanh(x)$), will cause the solutions to oscillate infinitely fast close to the boundary which will again simulate a infinitely hard wall.

While trying to model wave propagation in an infinite open space, it was necessary to exploit the concept of Perfectly Matched Layer (PML). PML is firstly introduced in by Berenger [9-10]. The basic idea of PML is to form a "thin" layer around the analysed domain, which will absorb all the waves entering it. It can be shown (using [10]) that the entire process of deriving the PML layer in one dimension (x) can be described using only a symbolic transformation:

$$\frac{\partial}{\partial x} \longrightarrow \frac{1}{1 + j\frac{\sigma_x(x)}{\omega}} \frac{\partial}{\partial x} \tag{2}$$

where ω is the angular frequency of the wave, j is the imaginary unit, and σ_x is an absorbing real scalar function defined on a domain. Function σ_x determines the absorbing properties of domain. When $\sigma_x > 0$ the oscillating solution has exponential decay, while $\sigma_x = 0$ leads to an ordinary equation (as illustrated on Fig. 1). In practice, usually quadratic or cubic form of σ_x is used in the absorbing layer [11].

In order to implement PML the equation (1) is usually written in the following equivalent form:

$$\nabla \cdot (a \nabla u) = \frac{1}{b} \frac{\partial^2 u}{\partial t^2} \tag{3}$$

where a and b are constants related with wave speed $c = \sqrt{ab}$. The equation (3) is then separated into two first order equations, introducing a vector function: $\mathbf{v}(\mathbf{x}, t)$ and its corresponding auxillary differential equation:

$$\frac{\partial u}{\partial t} = b \nabla \cdot \mathbf{v} \tag{4}$$

$$\frac{\partial v}{\partial t} = a \nabla u \tag{5}$$

After some algebra, which is omitted for brevity, the latter equations for one-dimensional case and implemented PML (2) become:

$$\frac{\partial u}{\partial t} = b \frac{\partial v}{\partial x} - \sigma_x u \tag{6}$$

$$\frac{\partial v}{\partial t} = a \frac{\partial u}{\partial x} - \sigma_x v \tag{7}$$

The equations (6) and (7) will be the starting equations for discretization in the following section.

IV. Discretization of Wave Equation

Two most popular wave equation discretization methods: Finite Differences Method (FDM) and Finite-differences Time-domain method (FDTM) will be used in this paper.

FDM is based on the approximation of m-th order derivation of the function with m-th order forward, backward and central difference [2]. The expression for central differences is given with (8):

$$\delta_h^m[f](x) = \sum_{k=0}^{m} (-1)^k \binom{m}{k} f\left(x + \left(\frac{m}{2} - k\right) h\right) \tag{8}$$

where f represents a function whose finite difference is formed, and h is the grid interval of space (or time) division. Similar relations exist for forward and backward differences. However, the central difference (8) yields a more accurate approximation ($O(h^2)$) than forward and backward differences ($O(h)$) [2]. Also the latter methods lead to an unconditionally unstable dicrete scheme from equations (6) and (7), so (8) is usually preferred in calculation.

In order to use relation (8), space and time domain should be uniformly discretized with discretization intervals Δx and Δt respectively (Fig. 2a). Notation $U_i^n = u(x{=}i\Delta x, t{=}n\Delta t)$ will be adopted in the following text, where i and n are positive integers or zeros.

Using the relation (8) in (6) and (7) gives a discrete difference equation systems for central differences FDM:

$$U_i^{n+\frac{1}{2}} = U_i^{n-\frac{1}{2}} + b\frac{\Delta t}{\Delta x}(V_{i+\frac{1}{2}}^n - V_{i-\frac{1}{2}}^n) - \Delta t \cdot \sigma_i U_i^n \tag{9}$$

$$V_i^{n+\frac{1}{2}} = V_i^{n-\frac{1}{2}} + a\frac{\Delta t}{\Delta x}(U_{i+\frac{1}{2}}^n - U_{i-\frac{1}{2}}^n) - \Delta t \cdot \sigma_i V_i^n \tag{10}$$

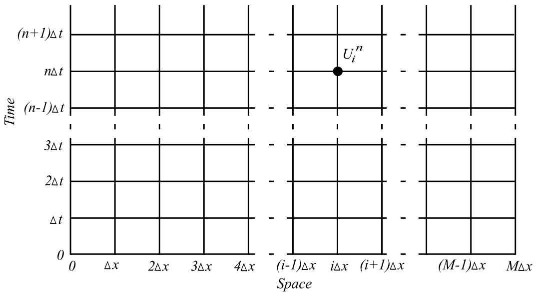
Considering that the values in the centers of the grid cannot be calculated, the equations (9) and (10) are not usable for implementation and the equations after the extension become:

$$U_i^{n+1} = U_i^{n-1} + b\frac{\Delta t}{\Delta x}(V_{i+1}^n - V_{i-1}^n) - 2\Delta t \cdot \sigma_i U_i^n \tag{11}$$

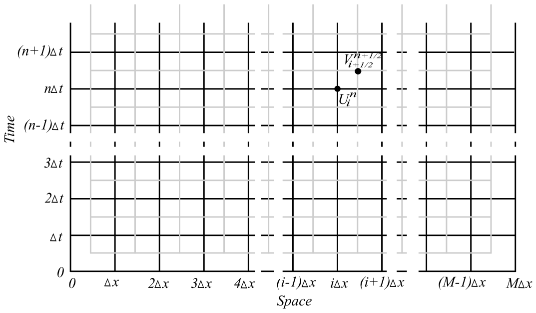
$$V_i^{n+1} = V_i^{n-1} + a\frac{\Delta t}{\Delta x}(U_{i+1}^n - U_{i-1}^n) - 2\Delta t \cdot \sigma_i V_i^n \tag{12}$$

As one can see, the main issue in the latter equations is that the precision of the function derivation which is calculated is reduced, because the derivation is calculated over two grid rectangles.

The Finite-difference Time-domain method (FDTD) is first introduced by Yee [12], and so far it is one of the most popular discretization method for solving many scientific and



(a)



(b)

Fig. 2: Space-Time divisions using: a) FDM, b) FDTD

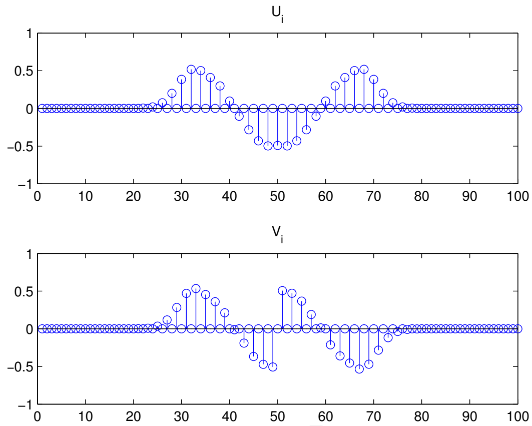


Fig. 3: Unwanted oscillability of the solution using FDM

engineering problems. FDTD is superior over FDM in numerically solving system of differential equations as the one given with (6) and (7). The main idea of the simplest variation of FDTD method is that the functions V_i^n and U_i^n are calculated in different space and time domain divisions using central differences (8), such as in Fig. 2b . This approach has even its own physical interpretation [12]. So the derived equations are (very similar to equations (9) and (10), but programmable after averaging):

$$U_i^{n+\frac{1}{2}} = U_i^{n-\frac{1}{2}} + b\frac{\Delta t}{\Delta x}(V_{i+\frac{1}{2}}^n - V_{i-\frac{1}{2}}^n) - \Delta t \cdot \sigma_i U_i^n \quad (13)$$

$$V_{i+\frac{1}{2}}^{n+1} = V_{i+\frac{1}{2}}^n + a\frac{\Delta t}{\Delta x}(U_{i+1}^{n+\frac{1}{2}} - U_i^{n+\frac{1}{2}}) - \Delta t \cdot \sigma_i V_{i+\frac{1}{2}}^{n+\frac{1}{2}} \quad (14)$$

The FDTD approach has its own drawbacks (increasing memory and computing resource demands), but it is a stable algorithm. Actually, it exploits the advantages and reduces the disadvantages of FDM central difference method.

V. Stability analysis of analysed discretization schemes

It can be easily verified by numerical simulation that the FDTD discrete scheme ((13),(14)) is stable (e.g. Fig. 1), but the FDM scheme ((11),(12)) shows additional unwanted oscillations, as can be seen on Fig. 3). The main idea of this paper is to illustrate and discuss the difference between FDM and FDTM discrete scheme on these unwanted oscillation. Many authors treat these oscillations as instability of the solution, and usually directly use FDTD method without entering into mathematical dicussion. However, both discrete systems are actually marginally stable, which is a sufficient condition for numerical scheme convergence, but the eigenvalues positions on unity circle are different, and that will determine the behaviour of the solution.

The fundamental theorem of numerical mathematics, known as a Lax-Richtmyer theorem shows that an iterational discrete scheme is convergent if and only if it is stable [5]. The finite difference scheme is said to be convergent if U_i^n tends to $u(x,t)$ as Δx and Δt tend to zero. If a numerical scheme is convergent, then a numerical solution actually represent the actual solution. Instead of proving covergence, most authors prove the stability of the scheme. In this paper, stability is discussed using Von Neumann stability analysis as in [6].

On a finite domain, solutions of the difference sheme ((11) and (12)) can be assumed:

$$U_i^n = U_\rho e^{j(-\omega n\Delta t + ki\Delta x)} \quad (15)$$

$$V_i^n = V_\rho e^{j(-\omega n\Delta t + ki\Delta x)} \quad (16)$$

where ω is the angular frequency, and k is the wavenumber. Relations (11) and (12) can be written in the following form:

$$\begin{bmatrix} U_i^{n+1} \\ U_i^n \\ V_i^{n+1} \\ V_i^n \end{bmatrix} = \begin{bmatrix} S & 1 & B & 0 \\ 1 & 0 & 0 & 0 \\ A & 0 & S & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} U_i^n \\ U_i^{n-1} \\ V_i^n \\ V_i^{n-1} \end{bmatrix} = \mathbf{G} \begin{bmatrix} U_i^n \\ U_i^{n-1} \\ V_i^n \\ V_i^{n-1} \end{bmatrix} \quad (17)$$

Where $S = -2\Delta t\sigma_i$, $B = b\frac{\Delta t}{\Delta x}2jsin(k\Delta x)$ and $A = a\frac{\Delta t}{\Delta x}2jsin(k\Delta x)$. Sufficient condition for bounded numerical solution of numerical scheme (17) in Von Neumann sense is that

$$\parallel \mathbf{G} \parallel \leq 1 \quad (18)$$

where $\parallel \ \parallel$ denotes a matrix norm (induced from Euclidean vector norm). This implies that the eigenvalues λ_i of the matrix $\mathbf{G}$ must satisfy:

$$max|\lambda_i| \leq 1 \quad (19)$$

The characteristic polynomial of the system (17) is:

$$P(\lambda) = \lambda^4 - 2S\lambda^3 + (S^2 - 2 - AB)\lambda^2 + 2\lambda S + 1 = 0 \quad (20)$$

If PML is neglected (S=0), using Jury criterion [13-14] on (20) it can be shown that the scheme is stable if the following condition is satisfied:

$$\Delta t \leq \frac{\Delta x}{\sqrt{ab}} \tag{21}$$

Otherwise the scheme is unstable (equation sign implies marginal stability). The inequality (21) is commonly used as the stability criterion in literature [15]. As it can be easily shown from (20), the eigenvalues of the equation must satisfy:

$$\lambda_1 \lambda_2 \lambda_3 \lambda_4 = 1 \tag{22}$$

which means that all eigenvalues of the equation must lie on unity circle (hence causing marginal stability), or the system will be unstable (if all the roots lie inside the unity circle the product in the equation (22) is less then one). This can also be derived directly from Jury criterion.

Using the FDTD method, equations (19) and (14) can be written as:

$$\left[\begin{array}{c} U_i^n \\ V_{i+\frac{1}{2}}^{n+\frac{1}{2}} \end{array} \right] = \left[\begin{array}{cc} S' & B' \\ A'S' & S' + A'B' \end{array} \right] \left[\begin{array}{c} U_i^{n-1} \\ V_{i+\frac{1}{2}}^{n-\frac{1}{2}} \end{array} \right] \tag{23}$$

where $S' = (1 - \frac{\Delta t \sigma_i}{2})/(1 + \frac{\Delta t \sigma_i}{2})$, $A' = \frac{a\Delta t}{\Delta x}(e^{jk\Delta x} - 1)/(1 + \frac{\Delta t \sigma_i}{2})$ and $B' = \frac{b\Delta t}{\Delta x}(1 - e^{-jk\Delta x})/(1 + \frac{\Delta t \sigma_i}{2})$. Now it can be shown that the characteristic polynomial for (23) is:

$$P(\lambda) = \lambda^2 + (-2S' - A'B')\lambda + {S'}^2 = 0 \tag{24}$$

As can be seen, if the PML doesn't exist (S=0, S'=1), the characteristic polynomials (20) and (24) have almost identical form, but the equation (20) has four roots lying on unity circle, while equation (24) has only two. It is easily shown that the discrete stability condition for both equations is the same (given with (21)), but the FDTD method doesn't show additional oscillations.

VI. Discussion

The most important observation to be made is that all discrete schemes describing wave-like equations must be marginally stable, because the solutions are essentially oscillating functions. Stability can be guaranteed only when using a medium whis attennuates the waves (such as PML), but in an ideal lossless medium the sollutions are inherently marginaly stable. FDM method illustrated above, because of its mathematical formulation increases the system order by two, introducing more (fake) poles on unity circle. This introduces two marginally stable sine waves as solutions of the equation (one is the actual solution and one is the consequence of unapropriate discretization).

Let's assume the eigenvalues of equation (24) without PML (S' set to 1) are $\lambda_1 = e^{j\phi}$ and $\lambda_2 = e^{-j\phi}$ which are conjugate-complex pair both lying on unity circle. The numerical solution of the wave equation could be decribed in the form:

$$S(n) = a_1 \lambda_1^n + a_2 \lambda_2^n = a_1 e^{j\phi n} + a_2 e^{-j\phi n} \tag{25}$$

The latter equation represents a solution in the form of a sine function of certain amplitude, frequency and phase. The eigenvalues of equation (20) are actually the square roots of λ_1 and λ_2 respectively, so the eigenvalues are: $\lambda_{11} = e^{j\frac{\phi}{2}}$, $\lambda_{12} = e^{j\frac{\phi+2\pi}{2}}$, $\lambda_{21} = e^{-j\frac{\phi}{2}}$, $\lambda_{22} = e^{-j\frac{\phi+2\pi}{2}}$. Hence, the solution could be described as:

$$S(n) = a_{11}\lambda_{11}^n + a_{12}\lambda_{12}^n + a_{21}\lambda_{21}^n + a_{22}\lambda_{22}^n \tag{26}$$

$$S(n) = a_{11}e^{j\frac{\phi n}{2}} + a_{12}(-1)^n e^{j\frac{\phi n}{2}} + a_{21}e^{-j\frac{\phi n}{2}} + a_{22}(-1)^n e^{-j\frac{\phi n}{2}} \tag{27}$$

Equation (27) clearly illustrates why every odd sample on Fig. 3 is zero, hence introducing this unwanted "oscillability", because it can be shown $a_{11} = a_{12} = \frac{a_1}{2}$ and $a_{21} = a_{22} = \frac{a_2}{2}$ for the same inital conditions. Note that the frequency of the solution is twice reduced. This is a logical consequence because the grid size is two times larger. Also it is clear from the characteristic polynomials and Jury criterion that introducing PML improves stability, because it actually introduces attenuation in the solutions.

VII. Conclusion

This paper illustrates an advantage of using FDTD method instead of FDM in numerical solving wave equations, described by a partial differential equations system. Also, it presents the stability issues in discretization of wave and similar equations, showing that is impossible to prove absolute stability of the convergence scheme whose solutions are oscillating wave functions, which is often oversighted.

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