Ultrasonics, 50 (3). pp. 431-438. ISSN 0041-624X ,
http://dx.doi.org/10.1016/j.ultras.2009.10.009
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Stability analysis of second- and fourth-order finite-difference modelling of wave propagation in orthotropic media

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Abstract

The stability of the finite-difference approximation of elastic wave propagation in orthotropic homogeneous media in the three-dimensional case is discussed. The model applies second- and fourth-order finite-difference approaches with staggered grid and stress-free boundary conditions in the space domain and second-order finite-difference approach in the time domain. The numerical integration of the wave equation by central differences is conditionally stable and the corresponding stability criterion for the time domain discretisation has been deduced as a function of the material properties and the geometrical discretization. The problem is discussed by applying the method of VonNeumann. Solutions and the calculation of the critical time steps is presented for orthotropic material in both the second- and fourth-order case. The criterion is verified for the special case of isotropy and results in the well-known formula from the literature. In the case of orthotropy the method was verified by long time simulations and by calculating the total energy of the system.

Key words: finite differences, numerical simulation, stability analysis

1. Introduction

Numerical and semi-analytical description of wave propagation problems are widely discussed in the literature. The solution requires spatial and temporal discretization, whereby the most common techniques are the methods of the finite elements and finite differences. The spatial discretization is usually carried out with the finite elements [1] or the finite differences technique [2]; for temporal discretization the central difference technique is often applied.

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The finite-difference time domain method [2] is adapted in several form to simulate and analyze wave propagation in arbitrary structures with isotropic or anisotropic material properties. By this method the equations of motion and the generalized Hooke’s law are approximated in the space and time domain by finite-differences and the stress and displacement (or velocity) components are calculated in discrete points.

This method is used in several form and many references are available. A second-order approximation in the two-dimensional isotropic case is presented by Virieux [3, 4] and Madariaga [5]. The three-dimensional case in cylindrical coordinates is discussed in [6, 7, 8, 9] and a special formulation in cartesian coordinates is presented by Schubert and Fellinger et al. [10, 11].

In the case of strongly anisotropic materials, such as wood, an approximation with higher accuracy may be necessary. The fourth-order approach is solved by Levander [12] and a quasi fourth-order approach (fourth-order in the axial and tangential, second-order approach in the radial direction) is shown by Leutenegger [13, 14].

Temporal discretization of the equation of motion with the central difference technique - independently of the spatial discretization - is only conditionally stable [1]; the stability criterion must be fulfilled. The basic concepts of the stability analysis are presented by VonNeumann et al. [15] and by O’Brien et al. [16] however, only for the one-dimensional case. For the two-dimensional isotropic case stability analysis was presented several times [5]. Fellinger et al. presented [10] a special formulation of the finite-difference time domain method in 3D with detailed stability analysis, but only for isotropic material. The application of this method in cylindrical coordinates - only for isotropic material - was shown by Gsell et al. [17]. The same technique could also be applied for finite element discretization. Bathe [1] applied a generalized study for the analysis of the numerical integration techniques with finite element spatial discretization and presents critical time steps for different element types.

In the following sections wave propagation problems are considered in finite orthotropic media. Second- and fourth-order finite-difference approximations are presented to simulate the wave propagation phenomenon in orthotropic media. The numerical model is applied to simulate the wave propagation in an orthotropic (wooden) rectangular bar.

Stability analysis of the numerical model is presented via the concepts of VonNeumann [1, 15, 16] which results in a generalized solution for the critical time step. The method is applicable in simulation with orthotropic material for the second-, fourth- and mixed-order approximation of the wave equation. It is shown that the solution results in the well-known analytical solutions in the special case of isotropy. The calculated stability criterion is verified by the calculation of the eigenvalues of the approximation matrix and by numerical simulations, whereby the stability was controlled by the calculated energy of the model [17].
2. Governing equations

The governing equations of wave propagation within a three-dimensional homogeneous, orthotropic, linear elastic material is described by the equations of motion, the generalized Hooke’s law and the kinematic relations. Using the summation convention they are given as

\[ \rho u_{p,t,t} = \sigma_{pq,q}, \]
\[ \sigma_{pq} = C_{pqrs} \epsilon_{rs}, \]
\[ \epsilon_{rs} = \frac{1}{2} (u_{r,s} + u_{s,r}), \]

where \( u_p \) are the displacement, \( \sigma_{pq} \) the stress, \( \epsilon_{rs} \) the strain components and \( C_{pqrs} \) is the stiffness tensor for orthotropic materials. In the generalized Hooke’s law, Eq.(1) the strain can be replaced by the kinematic relations given in Eq.(1), resulting in two sets of equations

\[ \rho u_{p,t,t} = \sigma_{pq,q}, \]
\[ \sigma_{pq} = C_{pqrs} \frac{1}{2} (u_{r,s} + u_{s,r}). \]

2.1. Second-order approximation

The two sets of equations in Eqs.(2) are solved numerically in the space and time domain by the finite-difference technique [3, 13] with a staggered grid (Fig.1). The applied grid is staggered only in the space domain but not in the time domain. According to the grid positions the normal stresses are calculated on the boundaries of the body. Due to this choice some values of the shear stresses and displacements are outside of the material boundaries. These fictitious points are used to satisfy the stress-free boundary conditions. The second-order finite difference approximation of the first derivative, with the staggered grid in the space domain, results in [3, 17]

\[ \frac{\partial f}{\partial x} \bigg|_{x_i} \approx \frac{1}{\Delta x} \left[ -f(x_i - \frac{\Delta x}{2}) + f(x_i + \frac{\Delta x}{2}) \right]. \]

The second-order approximation of the second derivative without a staggered grid in the time domain is given by [2]

\[ \frac{\partial^2 f}{\partial t^2} \bigg|_{t_n} \approx \frac{1}{\Delta t^2} \left[ f(t_n - \Delta t) - f(t_n) + f(t_n + \Delta t) \right]. \]

In accordance with Eqs.(2) first derivatives appear only in the space domain (with staggered grid), and second derivatives only in the time domain.

The governing equations in Eqs.(2) were discretized by these second-order approximation and the equations obtained are presented in Appendix A.
2.2. Fourth-order approximation

The applied staggered grids must be extended at the boundaries [13, 12] incurring additional fictions layers and points. Moreover, the fourth-order approximation is only applied in the space domain, which is given as [13]

\[
\frac{\partial f}{\partial x} \Big|_{x_i} \approx \frac{1}{24\Delta x} \left[ f(x_i - \frac{3\Delta x}{2}) - 27f(x_i - \frac{\Delta x}{2}) + 27f(x_i + \frac{\Delta x}{2}) - f(x_i + \frac{3\Delta x}{2}) \right].
\]

(5)

In the time domain the second-order approximation given in Eq.(4) will be kept. The fourth-order approximations of Eqs.(2) are presented in Appendix B.

3. Stability analysis

For a specific direct integration method for the equation of motion the following relationship can be established [1] to calculate the required solution for the time \( t + \Delta t \)

\[
\mathbf{u}^{t+\Delta t} = \mathbf{G}\mathbf{u}^t + \mathbf{L}\mathbf{r}^{t+\Delta t},
\]

(6)

where the vectors \( \mathbf{u}^t \), \( \mathbf{u}^{t+\Delta t} \) and \( \mathbf{r}^{t+\Delta t} \) are the solutions in the time \( t \) and \( t + \Delta t \) and the load in the time \( t + \Delta t \), respectively. The matrices \( \mathbf{G} \) and \( \mathbf{L} \) are the integration approximations and load operator.
The stability of an integration method means that any arbitrary initial condition at time $t$ given by errors in the displacements, velocities and accelerations does not grow as a result of the integrations. Therefore, we can consider the equations for the unloaded case for the time $t + \Delta t$

$$u^{t+\Delta t} = G u^t,$$

and the solution in the time $t + n\Delta t$ can be obtained by

$$u^{t+n\Delta t} = G^n u^t.$$  \hfill (7)

For symmetric, quadratic matrices the spectral decomposition \cite{19} of the matrix $G$ results in

$$G = V D V^T, \quad \text{and} \quad G^n = V D^n V^T,$$ \hfill (9)

and for nonsymmetric, quadratic matrices the decomposition results in

$$G = V_L D V_L^{-1}, \quad \text{and} \quad G^n = V_L D^n V_L^{-1}.$$ \hfill (10)

In the diagonal matrix $D$ are the eigenvalues, and in the matrix $V$ the eigenvectors of the symmetric matrix $G$ and the left eigenvectors of the nonsymmetric matrix $G$, respectively.

The stability criterion is fulfilled if the absolute values of all eigenvalues of $G$ are smaller or equal to 1 ($|\lambda_i| \leq 1$), since $D^n$ then is bounded for $n \to \infty$. Therefore, the stability of an integration method depends only on the eigenvalues of the approximation matrix \cite{1}.

For conditionally stable integration methods, such as the central differences method, a stability criterion could be used to fulfill the above condition. This criterion relates the time domain discretization to the material properties and the geometrical discretization, and results in a critical time step.

3.1. Stability of the FDM approach

In the following section the stability criterion for second- and fourth-order finite-difference approximations with orthotropic material properties is deduced. In order to obtain a stable finite-difference simulation the time step $dt$ must satisfy the stability criterion \cite{10, 17}: $dt \leq dt_{cr}$. The critical time step $dt_{cr}$ can be deduced as a function of the cell dimensions and the material properties for a general point on the grid, neglecting the boundaries. However, as the relationships in Eqs.(7-8) are related to the whole system of equations and to the whole structure, a general point could be considered within the grid without loss of generality \cite{2, 10}. To obtain the approximation matrix for the staggered grid the following harmonic ansatz will be taken in the space domain

$$u = u_0 e^{I(k_x i dx + k_y j dy + k_z k dz)},$$

$$\sigma = \sigma_0 e^{I(k_x i dx + k_y j dy + k_z k dz)},$$ \hfill (11)
where \( i, j, k \) denote the node number in the \( x, y, z \) directions, respectively, \( dx, dy, dz \) are the dimensions of one cell, \( \rho \) is the density, \( I = \sqrt{-1} \) and \( k_x, k_y, k_z \) are the wavenumbers in the \( x, y, z \) directions respectively. The vectors \( \mathbf{u}_0, \mathbf{\sigma}_0 \) are

\[
\mathbf{u}_0 = [u_{x0}, u_{y0}, u_{z0}]^T, \\
\mathbf{\sigma}_0 = \left[ \sigma_{x0}, \sigma_{y0}, \sigma_{z0}, \sigma_{xy}, \sigma_{xz}, \sigma_{yz} \right]^T.
\]

Inserting Eqs.(11) into Eqs.(51)-(68) with regard to the relative locations of the components in Fig. 2 and to the identity

\[
e^{I\alpha} - e^{-I\alpha} = 2I \sin \alpha,
\]

the following matrix equations will be taken

\[
\frac{\rho}{dt^2} \left[ \mathbf{u}_{n+1}^0 - 2\mathbf{u}_n^0 + \mathbf{u}_{n-1}^0 \right] \mathbf{u}_0 = \mathbf{A}\mathbf{\sigma}_0, \\
\mathbf{\sigma}_0 = \mathbf{C}\mathbf{A}^T \mathbf{u}_0^n,
\]

where \( \mathbf{C} \) is the matrix representation of the stiffness tensor and the matrix \( \mathbf{A} \) is

\[
\mathbf{A} = 2I \begin{bmatrix}
\frac{s_x}{dx} & 0 & 0 & \frac{s_y}{dy} & \frac{s_z}{dz} & 0 \\
0 & \frac{s_y}{dy} & 0 & \frac{s_z}{dz} & 0 & \frac{s_x}{dx} \\
0 & 0 & \frac{s_z}{dz} & 0 & \frac{s_x}{dx} & \frac{s_y}{dy}
\end{bmatrix}.
\]

Eqs.(14) hold for both second- and fourth-order approximations, however, the definitions for the coefficients \( s_x, s_y, s_z \) are different. For the second order
approximation they are given as

\[ s_x = \sin \left( k_x \frac{dx}{T} \right), \]
\[ s_y = \sin \left( k_y \frac{dy}{T} \right), \]
\[ s_z = \sin \left( k_z \frac{dz}{T} \right), \]  

and for the fourth-order approximation they are defined as

\[ s_x = \frac{1}{24} \left( 27 \sin(k_x \frac{dx}{T}) - \sin(3k_x \frac{dx}{T}) \right), \]
\[ s_y = \frac{1}{24} \left( 27 \sin(k_y \frac{dy}{T}) - \sin(3k_y \frac{dy}{T}) \right), \]
\[ s_z = \frac{1}{24} \left( 27 \sin(k_z \frac{dz}{T}) - \sin(3k_z \frac{dz}{T}) \right). \]  

Inserting the second equation in Eq.(14) into the first one the form of Eq.(6) can be obtained

\[ \frac{\rho}{dt^2} \left[ u_{n+1}^0 - 2u_n^0 + u_{n-1}^0 \right] = \mathbf{A}\mathbf{C}^T u_n^0, \]  

and regrouping yields

\[ \begin{pmatrix} u_{n+1}^0 \\ u_n^0 \end{pmatrix} = \begin{pmatrix} \frac{\rho}{dt^2} \mathbf{A}\mathbf{C}^T + 2\mathbf{E} \\ \mathbf{E} \end{pmatrix} \begin{pmatrix} u_n^0 \\ u_{n-1}^0 \end{pmatrix}, \]  

or

\[ w_{n+1} = \mathbf{G} w_n, \]  

where \( \mathbf{E} \) is the identity matrix. The eigenvalues of \( \mathbf{G} \) must fulfill the condition of stability and therefore their absolute value must be smaller than or equal to 1. To resolve the equation and receive the eigenvalues and the corresponding stability criterion a second harmonic wave ansatz \( u_0^0 = u_0 e^{-i\omega ndt} \) in the time domain in Eq.(18) must be applied. It yields

\[ \frac{\rho}{dt^2} \left[ \Psi + \frac{1}{\Psi} - 2 \right] u_0 = \mathbf{A}\mathbf{C}^T u_0, \]  

with \( \Psi = e^{i\omega dt} \). Inserting the following expression

\[ \nu = \frac{\rho}{dt^2} \left( \Psi + \frac{1}{\Psi} - 2 \right), \]  

into Eq.(21) the final matrix equation is obtained

\[ \nu u_0 = \mathbf{A}\mathbf{C}^T u_0, \]  

which is an eigenvalue problem:

\[ (\mathbf{A}\mathbf{C}^T - \nu \mathbf{E}) u_0 = 0. \]  

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Solving Eq.(22) it yields for $\Psi$

$$\Psi_{1,2} = F \pm \sqrt{F^2 - 1}, \quad \text{with:} \quad F = 1 + \nu \frac{dt^2}{2\rho}.$$  \hspace{1cm} (25)

Furthermore it will be shown, that $\Psi$ is the eigenvalue of $G$ in Eq.(19) and therefore it is required for stability that $|\Psi| \leq 1$. This requirement is satisfied if $-1 \leq F \leq 1$, which yields the conditions for the eigenvalues

$$\nu \leq 0 \quad \text{and} \quad -4 \frac{\rho}{dt^2} \leq \nu.$$  \hspace{1cm} (26)

Since the expression $ACA^T$ is determined by the material properties $C$ and by the cell dimensions $dx, dy, dz$ the second condition can be used to deduce the stability condition for a given spatial discretization. According to the first condition ($\nu \leq 0$) the eigenvalues must be negative, therefore applying the replacement $\tilde{\nu} = -\nu$ and by regrouping the second expression the critical time step can be obtained as

$$dt \leq dt_{cr} = \sqrt{\frac{4\rho}{\tilde{\nu}}}.$$  \hspace{1cm} (27)

Next it should be shown that $\Psi$ is the eigenvalue of $G$. Regrouping Eq.(21) one obtains

$$\Psi^2 E u_0 - \Psi \left( \frac{dt^2}{\rho} ACA^T + 2E \right) u_0 + Eu_0 = 0,$$  \hspace{1cm} (28)

which is a quadratic eigenvalue problem for $\Psi$ [20]. With the definition of $\Psi = e^{I_w dt}$ it can be easily seen that the corresponding linear eigenvalue problem

$$\begin{bmatrix} 0 & E \\ E & \frac{dt^2}{\rho} ACA^T + 2E \end{bmatrix} - \Psi \begin{bmatrix} E & 0 \\ 0 & E \end{bmatrix} \left\{ \begin{array}{c} u_0 \\ \Psi u_0 \end{array} \right\} = 0,$$  \hspace{1cm} (29)

is identical with Eq.(19) and therefore $\Psi$ must also be the eigenvalue of $G$.

3.2. Analysis of the results

The eigenvalue problem given as

$$(ACA^T - \nu E) u_0 = 0.$$  \hspace{1cm} (30)

and the conditions

$$\nu \leq 0 \quad \text{and} \quad -4 \frac{\rho}{dt^2} \leq \nu.$$  \hspace{1cm} (31)
determine a generalized stability condition. The presented relationship is valid for orthotropic materials and can be used for second- or fourth-order approximations using the different definitions of \( s_x, s_y, s_z \).

Eq. (30)-(31) relates physical properties (spatial discretisation \( dx, dy, dz \), material properties \( C, \rho \)) to the temporal discretisation \( dt \). Using the eigenvalues of Eq. (30), in analytical or numerical form, the critical time step could be exactly evaluated with the conditions. Eq. (30) has three eigenvalues which results in three time steps with Eq. (31); the smallest one corresponds to the critical time step.

In some special cases the eigenvalue problem Eq. (30) could be solved analytically and inserting the eigenvalues into the conditions Eq. (31) the critical time step is obtained in closed form. In other cases the numerical eigenvalues must be inserted into the conditions to receive the critical time step.

3.3. Solution in the isotropic case

The relationship in Eq. (23) and Eqs. (31) correspond to an orthotropic material law. However, isotropy is a special case of orthotropy, therefore inserting the isotropic material law into Eq. (23) the corresponding critical time step can be obtained and compared to the existing solutions [10].

The isotropic material law can be obtained by the following substitutions:

\[
\begin{align*}
C_{11} &= C_{22} = C_{33} = \lambda + 2\mu, \\
C_{44} &= C_{55} = C_{66} = \mu, \\
C_{12} &= C_{13} = C_{23} = \lambda,
\end{align*}
\]

where \( \lambda \) and \( \mu \) are the Lamé constants.

The eigenvalues of the simplified problem in Eq. (23) were evaluated by Mathematica

\[
\begin{align*}
\nu_{1,2} &= -4\mu \left[ \frac{s_x^2}{dx^2} + \frac{s_y^2}{dy^2} + \frac{s_z^2}{dz^2} \right] , \\
\nu_3 &= -4(\lambda + 2\mu) \left[ \frac{s_x^2}{dx^2} + \frac{s_y^2}{dy^2} + \frac{s_z^2}{dz^2} \right].
\end{align*}
\]

The first condition in Eq. (31) is satisfied since \( \nu_{1,2,3} < 0 \). The second condition results in

\[
\begin{align*}
dt^2 &\leq \frac{1}{c_s^2} \frac{s_x^2}{dx^2} + \frac{1}{c_p^2} \frac{s_y^2}{dy^2} + \frac{s_z^2}{dz^2} , \\
dt^2 &\leq \frac{1}{c_s^2} \frac{s_x^2}{dx^2} + \frac{1}{c_p^2} \frac{s_y^2}{dy^2} + \frac{s_z^2}{dz^2} ,
\end{align*}
\]

where \( c_s = \sqrt{\frac{\mu}{\rho}} \) and \( c_p = \sqrt{\frac{\lambda + 2\mu}{\rho}} \) are the shear and the bulk wave velocities, respectively.
The expressions \( s_x, s_y, s_z \) are periodic functions (Eqs.(16)-(17)). To minimize the right side of the expressions in Eqs.(34), \( s_x^2, s_y^2, s_z^2 \) must be maximal and \( dx^2, dy^2, dz^2 \) must be minimal. For the second-order case it can be achieved by \( s_x = s_y = s_z = 1 \), since \( \sin(k \frac{\Delta}{2}) \leq 1 \). For a non-uniform grid the minimal spatial discretisation \((dx_{\min}, dy_{\min}, dz_{\min})\) must be used.

The second condition in Eq.(34) is more restrictive because \( c_p > c_s \) and results in the well-known inequality \([10]\)

\[
\frac{dt}{2 \omega} \leq \frac{1}{c_p} \sqrt{\frac{1}{dx^2} + \frac{1}{dy^2} + \frac{1}{dz^2}}.
\]

(35)

For the fourth-order case Eqs.(34) still hold, however according to Eq.(17) the definitions of \( s_x, s_y, s_z \) are different: \( s_x = s_y = s_z = \frac{7}{6} \), since \( \frac{1}{24} (27 \sin (k \frac{\Delta}{2}) - \sin (3k \frac{\Delta}{2})) \leq \frac{7}{6} \). It results in

\[
\frac{dt}{4 \omega} \leq \frac{6}{7} \frac{1}{c_p} \sqrt{\frac{1}{dx^2} + \frac{1}{dy^2} + \frac{1}{dz^2}}.
\]

(36)

which is identical to previously derived solutions\([12, 2]\).

3.4. Solution in the orthotropic case

In the isotropic case the stability criterium can be used in the following form:

\[
\frac{dt}{\omega} \leq \frac{p}{c_{\max}} \frac{1}{\sqrt{\frac{1}{dx^2} + \frac{1}{dy^2} + \frac{1}{dz^2}}},
\]

(37)

where \( c_{\max} \) denotes the largest wave velocity in the medium, \( p = 1 \) for the second-order case and \( p = \frac{6}{7} \) for the fourth-order case. In an orthotropic or anisotropic material, however, the wave velocity depends on the propagation direction. Using only one wave velocity - the highest one in the medium - gives a false critical time step, but it is always smaller than the correct one, and therefore robust, because it assumes that the highest wave velocity is valid for every direction. In materials with strong orthotropy or anisotropy, however, the difference between correct time step and the approach by Eq.(37) is large and valuable computer time could be spared.

In the orthotropic case the eigenvalue problem in Eq.(23) should be solved with orthotropic material properties

\[
(ACA^T - \nu E) u_0 = 0.
\]

(38)

and the corresponding critical time step should be obtained by Eq.(27) as

\[
\frac{dt}{\omega} \leq \frac{dt_{cr}}{\omega} = \sqrt{\frac{4p}{\nu}}.
\]

(39)

An expression in closed form such as Eq.(35-36) for \( dt_{cr} \) cannot be found in the orthotropic case. First Eq.(38) must be solved for the eigenvalues with
given material properties \((C, \rho)\), cell dimensions \((dx, dy, dz)\) and setting \(s_x = s_y = s_z = 1\) (second order approximation), or \(s_x = s_y = s_z = \frac{7}{6}\) (fourth-order approximation). Using the calculated eigenvalues the critical time step is than given by Eq.(39).

### 3.5. Solution for the mixed-order approximation

In some cases it could be useful to use approximations with different order in different directions. Modelling of long structures like beams or pipelines, for example, requires a very large amount of cells. Using a higher-order approach in the axial direction, the necessary number of cells could be reduced [13] avoiding the additional complexity of the fourth-order approximation at the boundaries in two directions at the same time. For the isotropic case the eigenvalue problem in Eq.(38) can be solved analytically to get the critical time step by setting different values for the coefficients \(s_x, s_y, s_z\) in Eq.(34). For the orthotropic case the eigenvalue problem in Eq.(38) should be solved numerically. For a beam with a fourth-order approximation in the axial \((z)\) direction and second-order approximation in both other directions the following values must be used: \(s_x = s_y = 1, s_z = \frac{7}{6}\).

### 4. Numerical examples

In all numerical examples an orthotropic material (wood) will be used to verify the stability criterion and the finite-difference numerical model.

#### 4.1. Material properties

A wooden bar will be considered with the following dimensions: 20mm x 25mm x 2200mm. The density is \(\rho = 520 \text{ kg/m}^3\). The material properties of the bar were determined by wave propagation experiments described in [18]. The stiffness matrix \((GPa)\) is given as

\[
\mathbf{C} = \begin{bmatrix}
1.26 & 0.59 & 0.54 & 0 & 0 & 0 \\
0.59 & 2.42 & 0.84 & 0 & 0 & 0 \\
0.54 & 0.84 & 15.65 & 0 & 0 & 0 \\
0 & 0 & 0 & 0.18 & 0 & 0 \\
0 & 0 & 0 & 0 & 1.02 & 0 \\
0 & 0 & 0 & 0 & 0 & 0.76
\end{bmatrix}.
\]  

(40)

#### 4.2. Determination of the critical time step

The bar will be modelled by a uniform discrete grid with 10x10x1000 cells. One single cell has therefore the dimensions \(dx = 2\) mm, \(dy = 2.5\) mm, \(dz = 2.2\) mm. To obtain the critical time step by Eq.(38) the matrix \(\mathbf{ACA}^T\) and its eigenvalues will be calculated by Eq.(15) and Eq.(40) setting \(s_x = s_y = s_z = 1\)

\[
\mathbf{ACA}^T = \begin{bmatrix}
-0.221 & -0.062 & -0.141 \\
-0.062 & -0.235 & -0.116 \\
-0.141 & -0.116 & -1.444
\end{bmatrix} \times 10^{16},
\]  

(41)
\[ \nu_1 = -1.472 \times 10^{16}, \]
\[ \nu_2 = -0.263 \times 10^{16}, \]
\[ \nu_3 = -0.165 \times 10^{16}. \] (42)

The critical time step is given by the minimum of the second condition in Eq. (31)

\[ dt \leq \min \sqrt{\frac{\nu_q}{\rho}}, \quad q = 1, 2, 3 \] (43)
\[ dt_{2o}^{cr} = 3.760 \times 10^{-7} s. \] (44)

For the fourth-order case in Eq. (15) \( s_x = s_y = s_z = \frac{7}{6} \) will be replaced and the critical time step is given as

\[ dt_{4o}^{cr} = 3.222 \times 10^{-7} s. \] (45)

The results can be compared to the solution in Eq. (37), using only the highest wave velocity to calculate the critical time step. The maximum wave velocity in the bar is \( c_{max} = \sqrt{\frac{C_{33}}{\rho}} = 5486.7 \text{ m/s}. \) The critical time steps by Eq. (37) are:

\[ \tilde{dt}_{2o}^{cr} = 2.321 \times 10^{-7} s, \]
\[ \tilde{dt}_{4o}^{cr} = 1.9895 \times 10^{-7} s. \] (46)

The ratios of the values given in Eqs. (44)-(45) and Eq. (46) are:

\[ \frac{dt_{4o}^{cr}}{dt_{2o}^{cr}} = \frac{dt_{4o}^{cr}}{\tilde{dt}_{2o}^{cr}} = 1.62. \] (47)

For this strongly orthotropic material the correct critical time step is 62% higher than the approximation calculated by Eq. (37) reducing the computational time by 38%.

4.3. Eigenvalues of the approximation matrix

The stability of the simulation depends only on the eigenvalues of the approximation matrix \( G \) in Eq. (19). If the absolute value of the largest eigenvalue is larger than 1, the simulation becomes instable. Using the parameters calculated in section 4.1-4.2 the approximation matrix and its maximal eigenvalue could be determined by Eq. (19) for different values of \( dt \). The results are plotted on Fig. 3 for the second- and fourth-order approximation.

The absolute value of the largest eigenvalue remains 1 until the time step reaches the critical values \( dt_{2o}^{cr} = 3.760 \times 10^{-7} s \) and \( dt_{4o}^{cr} = 3.222 \times 10^{-7} s. \) However, as the time step exceeds the critical point the absolute value of the largest eigenvalue exceeds 1 and shows a tendency to monotonic growth. Above the critical time step the approximation matrix \( G^n \) is therefore not bounded for \( n \to \infty \) resulting in a monotonically increasing - and instable - tendency in \( G^n \) and in the simulation.
Eigenvalues of the approximation matrix

Figure 3: Eigenvalues of the approximation matrix with varying time steps; second- (circles) and fourth-order (crosses) approximation. The absolute value of the largest eigenvalue remains 1 until the time step reaches the critical values. However, above the critical time step the absolute value of the largest eigenvalue exceeds 1 and shows a monotonic growth.

5. Verification by calculating the energy of the system

The discrete FDM model represents a conservative system, therefore, energy can only be introduced externally and it cannot vanish from the model. In other words, after the excitation period the total energy must remain constant. This property can be used to verify stability, because in an unstable simulation the displacements and stresses, and accordingly the energy, increase with the $n$th power ($G^n$) [2, 17].

The kinetic ($T$) and strain energy ($U$) for one cell at the $n$th time step are calculated as [17]

$$i,j,k dT^n = \frac{\rho}{2} \left[ (i,j,k v_x^n)^2 + (i,j,k v_y^n)^2 + (i,j,k v_z^n)^2 \right] dV,$$

$$i,j,k dU^n = \frac{1}{2} i,j,k \sigma_{pq}^n S_{pqrs} i,j,k \sigma_{rs}^n dV,$$

where $S_{pqrs}$ is the compliance tensor, $v_x^n$, $v_y^n$, $v_z^n$ are the velocities in the $n$th
time step and $dV = dx \, dy \, dz$. The total energy of the discrete system at the $n$th time step is therefore

$$E^n = \sum_i \sum_j \sum_k \left[ i,j,k \, dT^n + i,j,k \, dU^n \right], \quad (49)$$

In Eq.(48) the strain energy for the discrete grid is calculated using the stresses determined by the equations in Appendix A - B. The velocities of the discrete grid cells for Eq.(48) are calculated from the displacements by a finite difference approach as

$$v^n = \frac{-u^{n-1} + u^n}{2 \, dt}. \quad (50)$$

The numerical stability with the critical time step given in Eqs.(44-45) were verified by numerical simulations (excitation frequency: 20 kHz, pulsform: sinusoidal with 5 cycles multiplied by a hanning window). The simulation was calculated for a high number of time step (50000 time steps) using $0.99 \times dt^{cr}$ as the time step, and the stability of the calculation was verified by the energy of the system. The total energy of the system after 50000 time steps (18.78 respectively 16.11 ms), was still constant.
To compare the stable and unstable behaviors simulations were carried out with higher time steps than the critical one. The energy of the system was calculated in every time step and the results are plotted on Fig. 4. It can be seen that for every time step beyond the critical one, even with a small increment \((1.0015 \times dt_{cr}^2)\), instabilities occur within a few hundred steps, in this case within the excitation time (the monotone increase of the energy within the first 550 steps is occurred by the excitations, over this time the energy remains constant). The explanation for this behavior might be the non-linear dependence of the approximation matrix upon on the time step in Eq.(23).

6. Conclusion

Second- and fourth-order finite-difference approximations of wave propagation in orthotropic medium were discussed in this work. The numerical stability of the simulation was considered and the stability criterion was deduced in a generalized form as an eigenvalue problem. The presented relationship is valid for orthotropic materials and can be used for second- or fourth-order approximations. In the special case of isotropy the eigenvalue problem was directly solved and it was shown that the criterion results in a well-known formula. In the case of orthotropy the method was verified by the calculation of the total energy of the system and by the calculation of the eigenvalues of the corresponding eigenvalue problem.

It was shown that in the orthotropic case a higher critical time step can be applied than the one calculated by classical approximations. This result can be explained by the fact that the classical approximation uses only the highest wave velocity instead of considering its correct values in different directions, analogous to the spatial discretisation \(dx, dy, dz\) in Eq.(37). This result leads to a decrease in the computational time, and in material with strong orthotropy the difference can be high (according to the numerical example the computational time can be reduced by 38%).

The relationship deduced in Eq.(23) and Eqs.(31) corresponds to an orthotropic material law. Further research should be undertaken to develop a stability relationship for more generalized materials. The deduced relationship in the form of an eigenvalue problem is the most general criterion and it could be generalized to develop stability criteria for anisotropic materials or for higher order approaches.
A. Second order approximation

The sets of Eqs.(2) are discretized by the finite differences given in Eqs.(3)-(4) and solved for the displacement in the \((n + 1)\)th time step:

\[
i_{j,k}u_{x}^{n+1} = 2i_{j,k}u_{x}^{n} - i_{j,k}u_{x}^{n-1} + \frac{dt^2}{\rho} \times \
\left\{ \begin{array}{l}
\frac{1}{dx} \left( -i_{j,k}\sigma_{xx}^{n} + i_{j,k}\sigma_{xx}^{n} \right) \\
+ \frac{1}{dy} \left( -i_{j,k}\sigma_{xy}^{n} + i_{j,k}\sigma_{xy}^{n} \right) \\
+ \frac{1}{dz} \left( -i_{j,k}\sigma_{xz}^{n} + i_{j,k}\sigma_{xz}^{n} \right) \end{array} \right\},
\]

\[(51)\]

\[
i_{j,k}u_{y}^{n+1} = 2i_{j,k}u_{y}^{n} - i_{j,k}u_{y}^{n-1} + \frac{dt^2}{\rho} \times \
\left\{ \begin{array}{l}
\frac{1}{dx} \left( -i_{j,k}\sigma_{xy}^{n} + i_{j,k}\sigma_{xy}^{n} \right) \\
+ \frac{1}{dy} \left( -i_{j,k}\sigma_{yy}^{n} + i_{j,k}\sigma_{yy}^{n} \right) \\
+ \frac{1}{dz} \left( -i_{j,k}\sigma_{yz}^{n} + i_{j,k}\sigma_{yz}^{n} \right) \end{array} \right\},
\]

\[(52)\]

\[
i_{j,k}u_{z}^{n+1} = 2i_{j,k}u_{z}^{n} - i_{j,k}u_{z}^{n-1} + \frac{dt^2}{\rho} \times \
\left\{ \begin{array}{l}
\frac{1}{dx} \left( -i_{j,k}\sigma_{xz}^{n} + i_{j,k}\sigma_{xz}^{n} \right) \\
+ \frac{1}{dy} \left( -i_{j,k}\sigma_{yz}^{n} + i_{j,k}\sigma_{yz}^{n} \right) \\
+ \frac{1}{dz} \left( -i_{j,k}\sigma_{zz}^{n} + i_{j,k}\sigma_{zz}^{n} \right) \end{array} \right\},
\]

\[(53)\]

The stresses by Eqs.(2) are:

\[
i_{j,k}\sigma_{xx}^{n} = \frac{C_{11}}{dx} \left( -i_{j,k}u_{x}^{n} + i+1,j,ku_{x}^{n} \right) \\
+ \frac{C_{12}}{dy} \left( -i_{j,k}u_{y}^{n} + i,j+1,ku_{y}^{n} \right) \\
+ \frac{C_{13}}{dz} \left( -i_{j,k}u_{z}^{n} + i,j,k+1u_{z}^{n} \right),
\]

\[(54)\]
\[ i,j,k \sigma_{yy}^n = \frac{C_{12}}{dx} \left( -i,j,k u_{x}^n + i+1,j,k u_{x}^n \right) + \frac{C_{22}}{dy} \left( -i,j,k u_{y}^n + i,j+1,k u_{y}^n \right) + \frac{C_{23}}{dz} \left( -i,j,k u_{z}^n + i,j,k+1 u_{z}^n \right), \] 

(55)

\[ i,j,k \sigma_{zz}^n = \frac{C_{13}}{dx} \left( -i,j,k u_{x}^n + i+1,j,k u_{x}^n \right) + \frac{C_{23}}{dy} \left( -i,j,k u_{y}^n + i,j+1,k u_{y}^n \right) + \frac{C_{33}}{dz} \left( -i,j,k u_{z}^n + i,j,k+1 u_{z}^n \right), \] 

(56)

\[ i,j,k \sigma_{xy}^n = C_{44} \left[ \frac{1}{dy} \left( -i,j-1,k u_{x}^n + i,j,k u_{x}^n \right) + \frac{1}{dx} \left( -i-1,j,k u_{y}^n + i,j,k u_{y}^n \right) \right], \] 

(57)

\[ i,j,k \sigma_{xz}^n = C_{55} \left[ \frac{1}{dz} \left( -i,j,k-1 u_{x}^n + i,j,k u_{x}^n \right) + \frac{1}{dx} \left( -i-1,j,k u_{z}^n + i,j,k u_{z}^n \right) \right], \] 

(58)

\[ i,j,k \sigma_{yz}^n = C_{66} \left[ \frac{1}{dz} \left( -i,j,k-1 u_{y}^n + i,j,k u_{y}^n \right) + \frac{1}{dy} \left( -i,j-1,k u_{z}^n + i,j,k u_{z}^n \right) \right], \] 

(59)

where \( C_{pq} \) are the elements of the stiffness matrix.

B. Fourth-order approximation

The discrete equations by fourth-order approximation are:

\[ i,j,k u_{x}^{n+1} = 2i,j,k u_{x}^n - i,j,k u_{x}^{n-1} + \frac{dt^2}{24 \rho} \]

\[ \left[ \frac{1}{dx} \left( i-2,j,k \sigma_{xx}^n - 2T_{i-1,j,k} \sigma_{xx}^n + 2T_{i,j,k} \sigma_{xx}^n - i+1,j,k \sigma_{xx}^n \right) \right] + \frac{1}{dy} \left( i,j,k \sigma_{xy}^n - 2T_{i,j,k} \sigma_{xy}^n + 2T_{i,j+1,k} \sigma_{xy}^n - i,j,k+1 \sigma_{xy}^n \right) + \frac{1}{dz} \left( i,j,k \sigma_{xz}^n - 2T_{i,j,k} \sigma_{xz}^n + 2T_{i,j,k+1} \sigma_{xz}^n - i,j,k+2 \sigma_{xz}^n \right) \] 

(60)
\begin{align}
  i,j,k u^n_{y}^{+1} &= 2i,j,k u^n_{y} - i,j,k u^{n-1}_{y} + \frac{dt^2}{24\rho} \times \\
  &\left[ \frac{1}{dx} \left( i-1,j,k \sigma^n_{xy} - 27i,j,k \sigma^n_{xy} + 27i+1,j,k \sigma^n_{xy} - i+2,j,k \sigma^n_{xy} \right) \\
  &+ \frac{1}{dy} \left( i,j-1,k \sigma^n_{yy} - 27i,j,-1,k \sigma^n_{yy} + 27i,j+1,k \sigma^n_{yy} - i,j+2,k \sigma^n_{yy} \right) \\
  &+ \frac{1}{dz} \left( i,j,k-1 \sigma^n_{yz} - 27i,j,k \sigma^n_{yz} + 27i,j,k+1 \sigma^n_{yz} - i,j,k+2 \sigma^n_{yz} \right) \right] \\
  \end{align}

(61)

\begin{align}
  i,j,k u^n_{z}^{+1} &= 2i,j,k u^n_{z} - i,j,k u^{n-1}_{z} + \frac{dt^2}{24\rho} \times \\
  &\left[ \frac{1}{dx} \left( i-1,j,k \sigma^n_{xz} - 27i,j,k \sigma^n_{xz} + 27i+1,j,k \sigma^n_{xz} - i+2,j,k \sigma^n_{xz} \right) \\
  &+ \frac{1}{dy} \left( i,j-1,k \sigma^n_{yz} - 27i,j,-1,k \sigma^n_{yz} + 27i,j+1,k \sigma^n_{yz} - i,j+2,k \sigma^n_{yz} \right) \\
  &+ \frac{1}{dz} \left( i,j,k-2 \sigma^n_{zz} - 27i,j,k \sigma^n_{zz} + 27i,j,k+1 \sigma^n_{zz} - i,j,k+2 \sigma^n_{zz} \right) \right] \\
  \end{align}

(62)

and the stresses are:

\begin{align}
  i,j,k \sigma^n_{xx} &= \frac{1}{24} \times \\
  &\left[ C_{11} \left( i-1,j,k u^n_{x} - 27i,j,k u^n_{x} + 27i+1,j,k u^n_{x} - i+2,j,k u^n_{x} \right) \\
  &+ C_{12} \left( i,j-1,k u^n_{y} - 27i,j,-1,k u^n_{y} + 27i,j+1,k u^n_{y} - i,j+2,k u^n_{y} \right) \\
  &+ C_{13} \left( i,j,k-1 u^n_{z} - 27i,j,k u^n_{z} + 27i,j,k+1 u^n_{z} - i,j,k+2 u^n_{z} \right) \right] \\
  \end{align}

(63)

\begin{align}
  i,j,k \sigma^n_{yy} &= \frac{1}{24} \times \\
  &\left[ C_{12} \left( i-1,j,k u^n_{x} - 27i,j,k u^n_{x} + 27i+1,j,k u^n_{x} - i+2,j,k u^n_{x} \right) \\
  &+ C_{22} \left( i,j-1,k u^n_{y} - 27i,j,-1,k u^n_{y} + 27i,j+1,k u^n_{y} - i,j+2,k u^n_{y} \right) \\
  &+ C_{23} \left( i,j,k-1 u^n_{z} - 27i,j,k u^n_{z} + 27i,j,k+1 u^n_{z} - i,j,k+2 u^n_{z} \right) \right] \\
  \end{align}

(64)
\[ i,j,k \sigma_{zz}^n = \frac{1}{24} \times \]
\[ \left[ \frac{C_{13}}{dx} (i-1,j,k u_x^m - 27i,j,k u_x^n + 27i+1,j,k u_x^n - i+2,j,k u_x^n) \right. \]
\[ + \frac{C_{33}}{dy} (i,j-1,k u_y^m - 27i,j,k u_y^n + 27i,j+1,k u_y^n - i,j+2,k u_y^n) \]
\[ + \frac{C_{53}}{dz} (i,j,k-1 u_z^m - 27i,j,k u_z^n + 27i,j,k+1 u_z^n - i,j,k+2 u_z^n) \left. \right] \]

\[ i,j,k \sigma_{xy}^n = \frac{C_{44}}{24} \times \]
\[ \left[ \frac{1}{dy} (i,j-2,k u_y^m - 27i,j-1,k u_y^n + 27i,j,k u_y^n - i,j+1,k u_y^n) \right. \]
\[ + \frac{1}{dx} (i-2,j,k u_x^m - 27i-1,j,k u_x^n + 27i,j,k u_x^n - i+1,j,k u_y^n) \left. \right] \]

\[ i,j,k \sigma_{xz}^n = \frac{C_{55}}{24} \times \]
\[ \left[ \frac{1}{dz} (i,j,k-2 u_z^m - 27i,j,k-1 u_z^n + 27i,j,k u_z^n - i,j,k+1 u_z^n) \right. \]
\[ + \frac{1}{dx} (i-2,j,k u_x^m - 27i-1,j,k u_x^n + 27i,j,k u_x^n - i+1,j,k u_z^n) \left. \right] \]

\[ i,j,k \sigma_{yz}^n = \frac{C_{66}}{24} \times \]
\[ \left[ \frac{1}{dz} (i,j,k-2 u_y^m - 27i,j,k-1 u_y^n + 27i,j,k u_y^n - i,j,k+1 u_y^n) \right. \]
\[ + \frac{1}{dy} (i-2,j,k u_y^m - 27i-1,j,k u_y^n + 27i,j,k u_y^n - i+1,j,k u_z^n) \left. \right] \]

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