Mathematical Properties of PML in time domain

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Overview

- Some properties of hyperbolic systems of first order PDE
- Well-posedness of the PML model
- Stability of the PML-method

Cauchy problem in $\mathbb{R}^2$

Lets have a look at a Cauchy problem in $\mathbb{R}^2$

$$\begin{cases} \frac{\partial V}{\partial t} + A_x \frac{\partial V}{\partial x} + A_y \frac{\partial V}{\partial y} + BV = 0, (x, y) \in \mathbb{R}^2, t < 0 \\ V(x, y, 0) = V_0(x, y), (x, y) \in \mathbb{R}^2 \\ V \in \mathbb{R}^d, (A_x, A_y, B) \in \mathcal{L}(\mathbb{R}^d)^3 \end{cases}$$

Observe that the PML-System in two dimensions:

$$\frac{\partial U^x}{\partial t} + \sigma U^x + \mathbf{A}_x \frac{\partial}{\partial x}(U^x + U^y) = 0$$

$$\frac{\partial U^y}{\partial t} + \mathbf{A}_y \frac{\partial}{\partial y}(U^x + U^y) = 0$$

is a problem of this type if we set:

$$V = \begin{pmatrix} U^x \\ U^y \end{pmatrix}, A_x = \begin{pmatrix} \mathbf{A}_x & \mathbf{A}_x \\ 0 & 0 \end{pmatrix}, A_y = \begin{pmatrix} 0 & 0 \\ \mathbf{A}_y & \mathbf{A}_y \end{pmatrix}, B = \begin{pmatrix} \sigma I & 0 \\ 0 & 0 \end{pmatrix}$$

Definition 1. *We say that the Cauchy problem is well-posed if for every V_0 in H^s, there exists a unique solution $V \in C^0(\mathbb{R}^+, L^2)$ that satisfies a estimation on the type:*

$$\forall t > 0, \|V(t)\|_{L^2} \leqslant C(t) \|V_0\|_{H^s}$$

It is called strongly well-posed if $s = 0$, otherwise it is called weakly well-posed.

When is the above Cauchy problem a well-posed problem?

Applying the Fourier transform in space: $V(x, y, t) \longrightarrow \hat{V}(k_x, k_y, t)$

$$\frac{\partial \hat{V}}{\partial t} + (\, i\underbrace{(k_x A_x + k_y A_y)}_{A(k)} + B \,) \hat{V} = 0$$
$$\hat{V}(k_x, k_y, 0) = \hat{V}_0(k_x, k_y)$$

The solution to this problem is:

$$\hat{V}(k_x, k_y, t) = e^{i(A(k)-iB)t}\hat{V}_0$$

If we want an estimation like in the definition, we have to estimate the exponential term.

In practice, this is the same as finding particular solution in forms of plane waves:

$$V(x, y, t) = V(k)e^{i(k_x x + k_y y)}e^{i\omega(k)t},\ k = (k_x, k_y) \in \mathbb{R}^2,\ \omega(k) \in \mathbb{C}$$

This leads us to the dispersion relation: $\det(A(k) - iB - \omega I) = 0$

We denote by $\{\omega(k)\}$ the set of all branch of solutions.

For the problem to be well-posed it is necessary that:

$$Im\,\omega(k) \text{ is bounded below, } \forall k \in \mathbb{R}^2$$

This is because of: $e^{i\omega(k)t} = e^{iRe(\omega(k))t}e^{-Im(\omega(k))t}$

Geometrically this can be interpreted as:

All the complex curves $|k| \to \omega(|k| \cdot K), K = \frac{k}{|k|}$ stay above a half plane.

Because the functions $\omega(k)$ are continuous, we only have to look at what happens if $|k|$ goes to ∞.

The original problem can be interpreted as a perturbation of a homogenous system, where $B = 0$. So we first have a look at that.

The unperturbed system

Definition 2. *The unperturbed system is called hyperbolic if*

$$\forall k \in \mathbb{R}^2, \text{ the eigenvalues of } A(k) \text{ are real.}$$

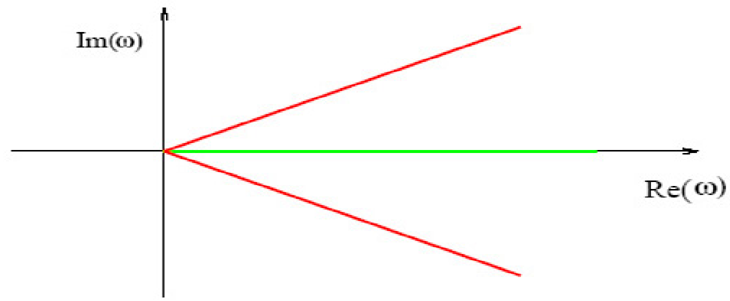
It is called strongly hyperbolic (otherwise weakly hyperbolic) if

$$\forall k \in \mathbb{R}^2, A(k) \text{ can be diagonalised.}$$

The dispersion relation $\det(A(k) - \omega I) = 0$ becomes the characteristic equation of the Matrix $A(k)$: ω has to be an eigenvalue of $A(k)$.

The solutions $\omega(k)$ are homogenous functions of order 1 in k, so in this case the curves are straight lines.

$A(k)$ is real and therefore the eigenvalues are paired by complex conjugation. So the curves are also paired by symmetry to the reel axis.



We have a well-posed problem, if all curves are on the real axes, which means that the system is hyperbolic. In fact there is a more precise result:

Theorem 1. *(Kreiss) In the case $B = 0$, the problem is well-posed if and only if the system is hyperbolic, and:*

- *strongly hyperbolic $\Rightarrow$ strongly well-posed*
  and $\forall t > 0, \|V(t)\|_{L^2} \leq C \|V_0\|_{L^2}$

- *weakly hyperbolic $\Rightarrow$ weakly well-posed*
  and $\forall t > 0, \|V(t)\|_{L^2} \leq C(1+t)^s \|V_0\|_{H^s}, \ s \geq 1$

The perturbed system $(B \neq 0)$

Theorem 2. *If the unperturbed system is strongly hyperbolic, then the problem is strongly well-posed and it exists a constant* $K > 0$ *such that:*

$$\forall t > 0, \|V(t)\|_{L^2} \leq Ce^{Kt} \|V_0\|_{L^2}$$

If the unperturbed system is only weakly hyperbolic, then for certain matrices B the problem is ill-posed.

The notation of well-posedness guarantees a unique solution, but it does not exclude exponential growth in time.

Therefore this isn't sufficient for a PML, witch should be absorbing.

Definition 3. *We suppose that the Cauchy problem is well-posed. Then the system is called strongly stable if the solution holds:*

$$\forall t > 0, \quad \|V(t)\|_{L^2} \leq C \|V_0\|_{L^2}$$

or weakly stable if it holds:

$$\forall t > 0, \quad \|V(t)\|_{L^2} \leq C(1+t)^s \|V_0\|_{H^s}, \; s \geq 1$$

The Cauchy problem is stable if and only if

$$\forall k \in \mathbb{R}^2 \text{ the solutions } \omega(k) \text{ satisfy } Im\omega(k) \geq 0.$$

The existence of solutions ω with negative imaginary parts would correspond to plane wave solutions with exponential growth in time.
A stable system does not admit such solutions.

Example in one dimension

$$\frac{\partial}{\partial t}\begin{pmatrix} u \\ v \\ w \end{pmatrix} + A\frac{\partial}{\partial x}\begin{pmatrix} u \\ v \\ w \end{pmatrix} + B\begin{pmatrix} u \\ v \\ w \end{pmatrix} = 0$$

where the matrix A is given by: $A = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 2 & 1 \\ 0 & -1 & 0 \end{pmatrix}$

The eigenvalues of A are 0 (simple) and 1 (double), and it is not diagonalisable.
Consider successively $(a \in \mathbb{R})$:

$$B = B_1 = \begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & a \\ 0 & 0 & 0 \end{pmatrix}, B = B_2 = \begin{pmatrix} 0 & -1 & 0 \\ a & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

With $B = B_1$ we obtain the following equation for u if we eliminate v and w

$$\frac{\partial}{\partial t}\Big(\frac{\partial^2 u}{\partial t^2} + 2\frac{\partial^2 u}{\partial x \partial t} + \frac{\partial^2 u}{\partial x^2} + a\frac{\partial u}{\partial x}\Big) = 0$$

The dispersion relation is $i\omega(-\omega^2 - 2k\omega - k^2 - iak) = 0$, and the solutions are:

$$\omega = 0, \omega = -k \pm |ak|^{\frac{1}{2}} \tfrac{1+i}{\sqrt{2}}$$

One of them has a imaginary part that goes to $-\infty$ when $|k|$ goes to $+\infty$. So in this case the problem is ill-posed.

With $B = B_2$ we obtain a slightly different equation for u

$$\frac{\partial}{\partial t}\Big(\frac{\partial^2 u}{\partial t^2} + 2\frac{\partial^2 u}{\partial x \partial t} + \frac{\partial^2 u}{\partial x^2} + au\Big) = 0$$

Now the dispersion relation is $i\omega(-\omega^2 - 2k\omega - k^2 + a) = 0$, and the solutions are:

$$\omega = 0, \omega = -k \pm \sqrt{a}$$

There imaginary parts are uniformly bounded and therefore the problem is well-posed.

But we see also, that the system is stable if $a \geq 0$ and instable if $a < 0$.

Well-posedness of the PML model

First, have a look at the PML system for acoustic waves:

$$\begin{cases} \rho(\frac{\partial u^x}{\partial t} + \sigma u^x) - \frac{\partial v_x}{\partial x} = 0 \\ \mu^{-1}(\frac{\partial v_x}{\partial t} + \sigma v_x) - \frac{\partial}{\partial x}(u^x + u^y) = 0 \\ \rho\frac{\partial u^y}{\partial t} - \frac{\partial v_y}{\partial y} = 0 \\ \mu^{-1}\frac{\partial v_y}{\partial t} - \frac{\partial}{\partial y}(u^x + u^y) = 0 \end{cases}$$

If we set $\rho = \mu = 1$ and $\sigma = const.$, we can simplify:

$$\left(\frac{\partial}{\partial t} + \sigma\right)^2 (\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial y^2}) - \frac{\partial^4 u}{\partial x^2 \partial t^2} = 0$$

From this we get the dispersion relation:

$$\det(A(k) - iB - \omega I) = (i\omega + \sigma)^2(\omega^2 - k_y^2) + \omega^2 k_x^2 = 0$$

And the one for the unperturbed system: $\omega^2(\omega^2 - k_y^2 - k_x^2) = 0$

$\omega = 0$ is a double eigenvalue of $A(k)$ and it is not diagonalisable.

$\Rightarrow$ not strongly hyperbolic

To show that the system stays well-posed anyway, we have to look at the development of the four solutions $\omega(k)$ for great values of $|k|$:

$$\begin{cases} \omega(k) = \pm |k| + i\sigma k_x^2 / |k|^2 + O(|k|^{-1}), \\ \omega(k) = \sigma \frac{\pm k_x k_y + i k_y^2}{|k|^2} + O(|k|^{-1}), \end{cases}$$

The imaginary parts are bounded regardless of the sign of σ.
One can show that: $\sigma > 0 \Rightarrow 0 \leq Im\, \omega(k) \leq \sigma, \forall k \in \mathbb{R}^2$

Theorem 3. *The Cauchy problem associated to the PML system for acoustic waves with constant coefficients is weakly well-posed. More precisely, for every initial data* $V_0 = (u_0^x, u_0^y, v_{x,0}, v_{y,0})$ *in* $L^2(\mathbb{R}^2)$ *there exists a unique solution:*

$$(u = u^x + u^y, v_x, v_y) \in C^0(\mathbb{R}^+, L^2(\mathbb{R}^2)), e = u^x - u^y \in C^0(\mathbb{R}^+, H^{-1}(\mathbb{R}^2)),$$

and if $\sigma > 0$*, we have the estimations:*

$$\begin{cases} \|u(.,t)\|_{L^2} + \|v_x(.,t)\|_{L^2} + \|v_y(.,t)\|_{L^2} \leq C \|V_0\|_{L^2} \\ \|e(.,t)\|_{H^{-1}} \leq C(1+t) \|V_0\|_{L^2} \end{cases}$$

If $\sigma < 0$ there are similar estimations with $Ce^{|\sigma|t}$ in place of C.
The loss of regularity concerns only the "not physical" value e.

Energy estimation

For the unperturbed system:

$$\begin{cases} \rho \frac{\partial u}{\partial t} - \frac{\partial v_x}{\partial x} - \frac{\partial v_y}{\partial y} = 0 \\ \mu^{-1} \frac{\partial v_x}{\partial t} - \frac{\partial u}{\partial t} = 0 \\ \mu^{-1} \frac{\partial v_y}{\partial t} - \frac{\partial u}{\partial t} = 0 \end{cases}$$

we have conservation of the energy:

$$\frac{d}{dt} \left\{ \frac{1}{2} \int \rho \left| u \right|^2 + \mu^{-1} \left| v \right|^2 dx \right\} = 0$$

Is there also a energy estimation for the PML system?

The formulation of Zhao-Cangellaris

We have to make a change of the unknown functions:

$$(u^x, u^y, v_x, v_y) \longrightarrow (u, v_x, v_y, v_y^*)$$

where the new functions are given by: $u = u^x + u^y, \quad \frac{\partial v_y^*}{\partial t} = \frac{\partial v_y}{\partial t} + \sigma v_y$

From the first and the third equations we get:

$$\frac{\partial}{\partial t}\left[\rho\left(\frac{\partial u^x}{\partial t} + \sigma u^x\right) - \frac{\partial v_x}{\partial x}\right] = 0$$

$$\left(\frac{\partial}{\partial t} + \sigma\right)\left[\rho\frac{\partial u^y}{\partial t} - \frac{\partial v_y}{\partial y}\right] = 0$$

After summation, it becomes

$$\frac{\partial}{\partial t}\left(\rho\left(\frac{\partial}{\partial t} + \sigma\right)u - \frac{\partial v_x}{\partial x}\right) - \frac{\partial}{\partial y}\left(\frac{\partial}{\partial t} + \sigma\right)v_y = 0$$

Finally we get:

$$\rho \left(\frac{\partial}{\partial t} + \sigma \right) u - \frac{\partial v_x}{\partial x} - \frac{\partial v_y^*}{\partial y} = 0$$

together with the second and fourth equation and the one for v_y^*, we have the new system:

$$\begin{cases} \rho \left(\frac{\partial u}{\partial t} + \sigma u \right) - \frac{\partial v_x}{\partial x} - \frac{\partial v_y^*}{\partial y} = 0 \\ \mu^{-1} (\frac{\partial v_x}{\partial t} + \sigma v_x) - \frac{\partial u}{\partial x} = 0 \\ \mu^{-1} \frac{\partial v_y}{\partial t} - \frac{\partial u}{\partial y} = 0 \\ \frac{\partial v_y^*}{\partial t} = \frac{\partial v_y}{\partial t} + \sigma v_y \end{cases}$$

Theorem 4. *The solution of the Cauchy problem associated to the system above satisfies:*

$$\frac{1}{2}\frac{d}{dt}\left\{\int \rho \left|\frac{\partial u}{\partial t} + \sigma u\right|^2 dx + \int \mu^{-1} \left|\frac{\partial v_x}{\partial t}\right|^2 + \left|\frac{\partial v_y^*}{\partial t}\right|^2 dx\right\}$$

$$+\frac{1}{2}\frac{d}{dt}\left\{\int \sigma^2 \mu^{-1} \left|v_x\right|^2 dx\right\} + 2\int \sigma \mu^{-1} \left|\frac{\partial v_x}{\partial t}\right|^2 dx = 0$$

This shows the dissipative character of the PML system if $\sigma > 0$

Attention: This is only true, if σ is constant.

The general case

Let's come back to the general PML system in 2 dimensions:

$$\begin{cases} \frac{\partial U^x}{\partial t} + \sigma U^x + \mathbf{A}_x \frac{\partial}{\partial x}(U^x + U^y) = 0 \\ \frac{\partial U^y}{\partial t} + \mathbf{A}_y \frac{\partial}{\partial y}(U^x + U^y) = 0 \end{cases}$$

which can be rewritten as: $V = \begin{pmatrix} U^x \\ U^y \end{pmatrix}$

$$\frac{\partial V}{\partial t} + \begin{pmatrix} \mathbf{A}_x & \mathbf{A}_x \\ 0 & 0 \end{pmatrix} \frac{\partial V}{\partial x} + \begin{pmatrix} 0 & 0 \\ \mathbf{A}_y & \mathbf{A}_y \end{pmatrix} \frac{\partial V}{\partial y} + \begin{pmatrix} \sigma I & 0 \\ 0 & 0 \end{pmatrix} V = 0$$

the Matrix $A(k)$ becomes:

$$A(k) = k_x \begin{pmatrix} \mathbf{A}_x & \mathbf{A}_x \\ 0 & 0 \end{pmatrix} + k_y \begin{pmatrix} 0 & 0 \\ \mathbf{A}_y & \mathbf{A}_y \end{pmatrix} = \begin{pmatrix} k_x \mathbf{A}_x & k_x \mathbf{A}_x \\ k_y \mathbf{A}_y & k_y \mathbf{A}_y \end{pmatrix}$$

and the eigenvalues are given by the equation:

$$\begin{aligned}
\det(A(k) - \omega I_{2d}) &= \det \begin{pmatrix} k_x \mathbf{A}_x - \omega I_d & k_x \mathbf{A}_x \\ k_y \mathbf{A}_y & k_y \mathbf{A}_y - \omega I_d \end{pmatrix} \\
&= \det \begin{pmatrix} -\omega I_d & k_x \mathbf{A}_x \\ 0 & k_x \mathbf{A}_x + k_y \mathbf{A}_y - \omega I_d \end{pmatrix} \\
&= \det(-\omega I_d) \det(k_x \mathbf{A}_x + k_y \mathbf{A}_y - \omega I_d) \\
&= (-\omega)^d \det(k_x \mathbf{A}_x + k_y \mathbf{A}_y - \omega I_d) = 0
\end{aligned}$$

$\omega = 0$ is d-times eigenvalue and moreover $A(k)$ is not diagonalisable.

$\Rightarrow$ not strongly hyperbolic

One can show that the character of weakly well-posedness stays preserved.
But there is no general result about the stability.

Stability of the PML-method

Let's start with an example:
Elastic waves in an anisotropic medium in 2D

$$\rho\frac{\partial^2 u}{\partial t^2} - P(i\frac{\partial}{\partial x}, i\frac{\partial}{\partial y})u = 0$$

where $u = (u_i)$ denotes the displacement field, $\rho > 0$ the density and the matrix P is given by:

$$P(K_x, K_y) = \begin{pmatrix} c_{11}K_x^2 + c_{33}K_y^2 & (c_{12} + c_{33})K_xK_y \\ (c_{12} + c_{33})K_xK_y & c_{33}K_x^2 + c_{22}K_y^2 \end{pmatrix}$$

If we want solutions in the form of plane waves:

$$u(x, y, t) = De^{i(\omega t - (k_x x + k_y y))}$$

we have to solve the dispersion relation:

$$F(\omega, k) = \det(P(k_x, k_y) - \rho\omega^2 I) = 0$$

The function $F(\omega, k)$ is homogeneous of order 4

For every k, we get 4 solutions $\omega(k) = |k|\,\omega(K)$,

and the equation can be rewritten as

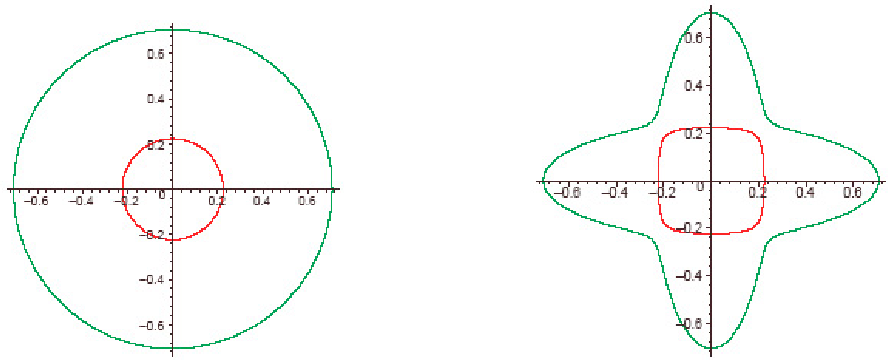
$$F(1, \frac{k}{\omega}) = F(1, \vec{S}) = 0$$

$k = (k_x, k_y)$
$K = k/\,|k|$: unit propagation direction
$S = k/\omega$: slowness vector

Slowness diagram

the slowness diagram: set of all points in the plane of slowness vectors $S = k/\omega$ that satisfy $F(1, \vec{S}) = 0$

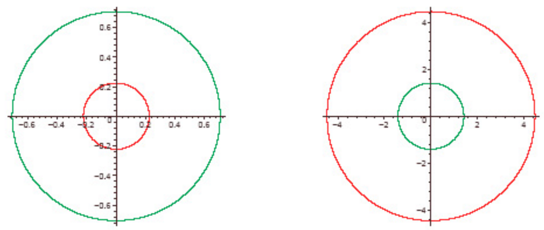
On each straight line with direction K we get 4 points $K/\omega(|K|)$ that belong to the diagram. Altogether we have 2 closed curves, the slowness curves:



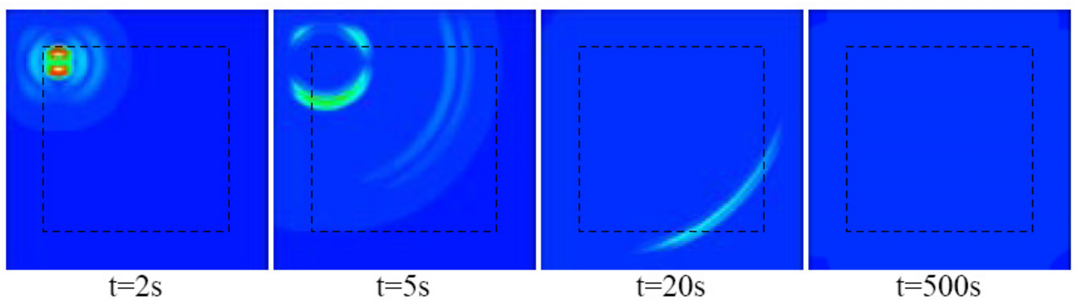
Slowness diagrams. Left: isotropic medium. Right: orthotropic medium.

Some numerical simulations

Numerical calculations with PML of a wave emitted by a point source.
Case I: Isotropic Medium

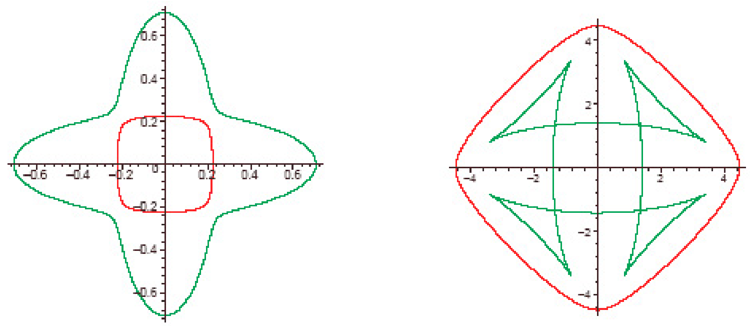


Slowness curves and Wave fronts for the isotropic media.

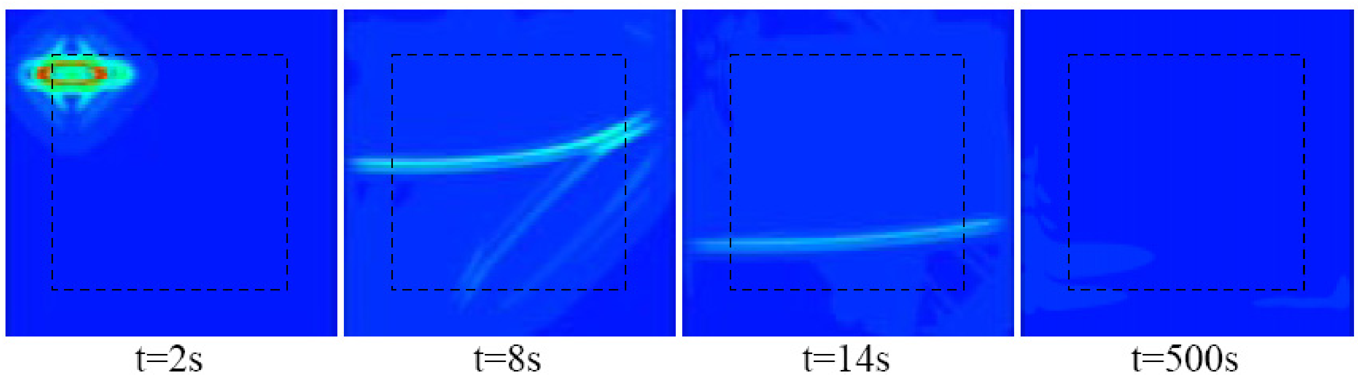


Some snapshots at different times for the isotropic media.

Case II: anisotropic medium with $c_{11} = c_{22} = 20, c_{33} = 2, c_{12} = 3.8$

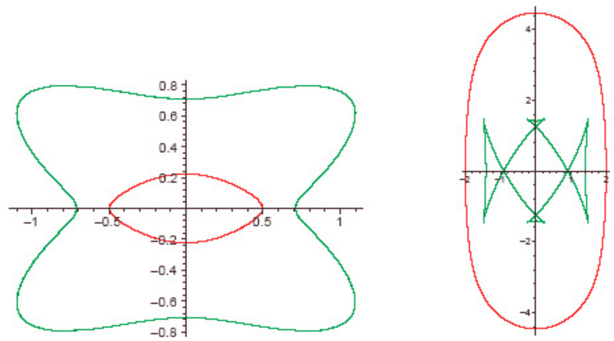


Slowness curves and Wave front for the orthotropic medium (II).



Some snapshots at different times for the orthotropic medium (II).

Case III: anisotropic medium with $c_{11} = 4, c_{22} = 20, c_{33} = 2, c_{12} = 7.5$



Slowness curves and Wave front for the orthotropic media (III).

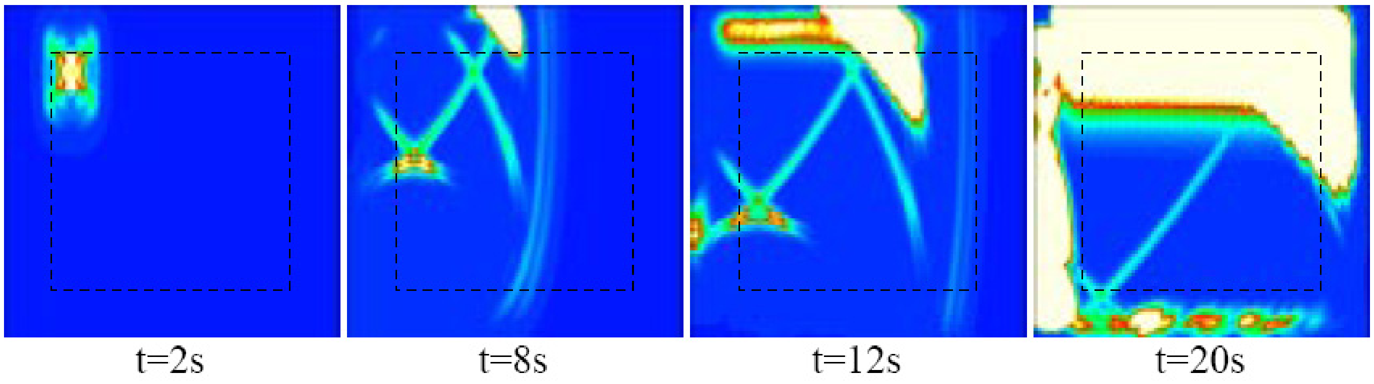


Figure 13: Some snapshots at different times for the orthotropic media (III).

A necessary stability condition

Let's come back to a general model of propagation described by the hyperbolic system:

$$\frac{\partial U}{\partial t} + \mathbf{A}_x \frac{\partial U}{\partial x} + \mathbf{A}_y \frac{\partial U}{\partial y} = 0$$

The dispersion relation has also the form of a homogenous function

$$F(\omega, k) = 0.$$

So the notation of the slowness curves can be generalised to this system.

We define: group velocity associated to the mode $\omega(k)$

$$V_g(k) := \nabla_k \omega(k) \quad (= (V_x(k), V_y(k))\ )$$

By differentiation of $F(\omega, k) = 0$ we get:

$$\frac{\partial F}{\partial \omega}(\omega, k)\ \nabla_k \omega(k) + \nabla_k F(\omega, k) = 0$$

witch gives us: $\nabla_k \omega(k) = \left(-\frac{\partial F}{\partial \omega}(\omega, k)\right)^{-1} \nabla_k F(\omega, k)$

So the group velocities are orthogonal to the slowness curves. The direction of $V_g(k)$ is given by the normal to the slowness curves at the point $k/\omega(k)$.

Theorem 5. *For the PML model in x-direction to be stable it is necessary that for all mode $\omega(k)$, it holds:*

$$\forall K = (K_x, K_y) \quad K_x \cdot V_x(K) \geq 0$$

For the PML model in y-direction: simply replace x by y

Geometric interpretation

The geometrical interpretation of this necessary property is the following:

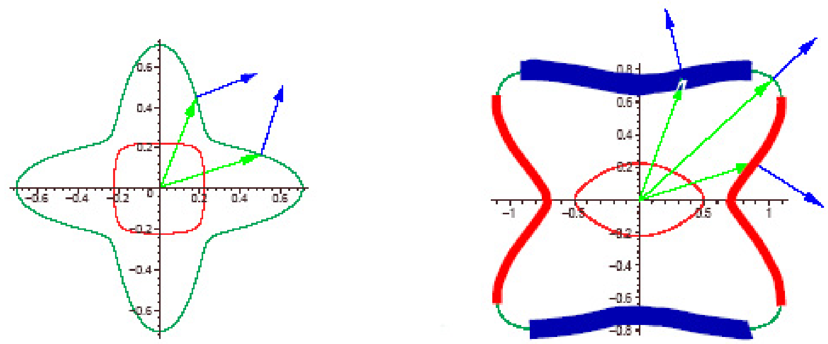
Stable Not stable

The vectors K (and therefore S) and $V_g(k)$ must have the same orientations with respect to the vertical line parallel to the y-axes.

If the condition is not fulfilled, we speak about backward propagative mode.

Interpretation of the numerical simulations

For the two anisotropic mediums we had this two slowness diagrams:



Slowness diagrams. Left: material (II) - Right: material (III).

There we can see, why the third case is not stable. The coloured sections are the backward propagative modes for the x-direction (blue) resp. y-direction (red).

Summary

- homogeneous and anisotropic wave equation:
  - weakly well-posedness
  - stability of the PML methode if $\sigma > 0$
  - dissipation result

- general media
  - leads also to a weakly well-posed problem
  - necessary but not sufficient stability condition