Introduction to PML in time domain

Alexander Thomann

Overview

Introduction

PML in one dimension

- Classical absorbing layers
- One-dimensional PML's
- Approach with complex change of variables

PML in two dimensions

- PML for a general linear system
- Accoustic waves
- Discretization and numerical problems

Task

- Solution of wave scattering problem.
- Interesting region is bounded.
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- Construct artificial boundary.
- Transparent for the solution.
- Totally absorbs incoming waves, no reflections.

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- Solution of wave scattering problem.
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Solution

- Absorbing Boundary Conditions: Differential equations at the boundary.
- "Classical" absorbing layers.
- Perfectly Matched Layers.

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Absorbing Layers in 1D

Consider the 1D wave equation with velocity 1:

$$\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} = 0, \quad x \in \mathbb{R}, \quad t > 0.$$

- As a first illustrative example we restrict the computational domain to x < 0.
- We therefore have to impose an Absorbing Boundary Condition at x = 0.
- In fact we dispose of a very simple and even local condition:

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0, \quad x = 0, \quad t > 0.$$

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$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0, \quad x = 0, \quad t > 0.$$

\implies No exact local analogue in higher dimensions!

Let us therefore find a transparent condition through an absorbing layer, infinite first and then in the interval [0, L].

Classical Absorbing Layers

In order to damp waves through a physical mechanism, we can add two terms to the wave equation,

- fluid friction: $\nu \frac{\partial u}{\partial t}, \ \nu \geq 0$,
- viscous friction: $-\frac{\partial}{\partial x}(\nu^*\frac{\partial^2 u}{\partial x\partial t}), \ \nu^* \ge 0.$

We then obtain the equation

$$\frac{\partial^2 u}{\partial t^2} + \nu \frac{\partial u}{\partial t} - \frac{\partial}{\partial x} \left(\frac{\partial u}{\partial x} + \nu^* \frac{\partial^2 u}{\partial x \partial t} \right) = 0.$$

The solution is

$$u(x,t) = Ae^{i(\omega t - k(\omega)x)} + Be^{i(\omega t + k(\omega)x)}, \quad k(\omega)^2 = \frac{\omega^2 - i\omega\nu}{1 + i\omega\nu^*}, \quad \Im k(\omega) \le 0.$$

A natural choice thus would be

$$\nu(x) = 0, \ \nu^*(x) = 0, \ x < 0,
\nu(x) > 0, \ \nu^*(x) > 0, \ x > 0.$$

$$\frac{\partial^2 u}{\partial t^2} - \frac{\partial}{\partial x} \left(\frac{\partial u}{\partial x} \right) = 0, \qquad \frac{\partial^2 u}{\partial t^2} + \nu \frac{\partial u}{\partial t} - \frac{\partial}{\partial x} \left(\frac{\partial u}{\partial x} + \nu^* \frac{\partial^2 u}{\partial x \partial t} \right) = 0.$$

The larger ν and ν^* , the smaller can we later on choose the length L of the absorbing layer.

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The larger ν and ν^* , the smaller can we later on choose the length *L* of the absorbing layer.

But consider

$$u(x,t) = \begin{cases} e^{i\omega(t-x)} + R(\omega)e^{i\omega(t+x)}, & x < 0, & \frac{1}{1} \\ T(\omega)e^{i(\omega t - k(\omega)x)}, & x > 0. & \frac{R(\omega)}{1} \\ \end{array}$$

We impose the right boundary conditions,

$$u(0^{-}) = u(0^{+}),$$

$$\frac{\partial u}{\partial x}(0^{-}) = \left(\frac{\partial u}{\partial x} + \nu^{*}\frac{\partial^{2} u}{\partial x \partial t}\right)(0^{+}).$$

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This leads to

$$R(\omega) = \frac{\omega - k(\omega)(1 + i\omega\nu^*)}{\omega + k(\omega)(1 + i\omega\nu^*)}, \quad \lim_{\nu \to \infty} |R(\omega)| = \lim_{\nu^* \to \infty} |R(\omega)| = 1$$
$$T(\omega) = 1 + R(\omega),$$

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Reflection at a visco-elastic layer. On the right side the absorption and therefore the reflection is stronger (Joly).

Perfectly Matched Layers in 1D

This was not satisfactory. In order to suppress reflections we want perfect adaption.

For that reason, we return to the wave-equation with variable coefficients. With $\rho, \mu > 0$ we have

$$o(x)\frac{\partial^2 u}{\partial t^2} - \frac{\partial}{\partial x}\left(\mu(x)\frac{\partial u}{\partial x}\right) = 0,$$

and define

- the velocity of propagation $c(x) = \sqrt{\mu(x)/\rho(x)}$,
- the impedance $z(x) = \sqrt{\mu(x)\rho(x)}$.

We impose

$$u(x) = e^{i(\omega t - kx)} + R(\omega)e^{i(\omega t + kx)}, \quad k = \frac{\omega}{c(x)}, \ c(x) = c, \ z(x) = z, \quad x < 0,$$

$$u(x) = T(\omega)e^{i(\omega t - k(\omega)x)},$$
 $k = \frac{\omega}{c(x)}, c(x) = c_*, \ z(x) = z_*, \ x > 0.$

With the right boundary conditions,

$$u(0^{-}) = u(0^{+}),$$

$$\mu(0^{-})\frac{\partial u}{\partial x}(0^{-}) = \mu(0^{+})\frac{\partial u}{\partial x}(0^{+}),$$

we find

$$R = \frac{z - z_*}{z + z_*}, \qquad T = \frac{2z}{z + z_*}.$$

- It is obvious that R = 0 if $z = z_*$.
- We thus need **impedance-matching**.
- But how can we make the layer absorbing at the same time?
- For that reason we change to frequency-space. Then we arrive at the Helmholtz-equation

$$-\widehat{\rho}(x,\omega)\omega^2 u - \frac{\partial}{\partial x}\left(\widehat{\mu}(x,\omega)\frac{\partial u}{\partial x}\right) = 0, \quad \widehat{\rho}, \widehat{\mu} > 0$$

The Idea

The idea is simple but effective: We choose $d(\omega) \in \mathbb{C}$ and

$$\widehat{\rho}(x,\omega) \equiv \rho, \quad \widehat{\mu}(x,\omega) \equiv \mu, \qquad x < 0,$$
$$\widehat{\rho}(x,\omega) = \frac{\rho}{d(\omega)}, \quad \widehat{\mu}(x,\omega) = \mu \cdot d(\omega), \qquad x > 0.$$

This then actually leads to

$$\widehat{z}(x < 0) = \widehat{z}(x > 0) = \sqrt{\rho\mu} \implies \text{we have impedance-matching,}$$

$$\widehat{c}(x < 0) = \sqrt{\mu/\rho} = c, \quad \widehat{c}(x > 0) = c \cdot d(\omega) \in \mathbb{C} \implies \text{we can make the layer absorbing.}$$

- It must be possible to return to time domain.
- Then the equation needs to be constructed out of differential operators.
- ⇒ A crucial condition is thus that $d(\omega)$ is a rational function in the variable $i\omega$ with real coefficients.

Analysis of the Solution

Writing $d(\omega)^{-1} = a + ib$, we have the solutions

$$u(x) = e^{i\omega(t \pm \frac{ax}{c}) \mp \omega \frac{bx}{c}}, \quad \omega b < 0,$$

with

- phase velocity c/a,
- that decay with penetration depth $l(\omega) = \frac{c}{|\omega b|}$ in the direction of propagation.

Possible choice: $a = 1, b = -\frac{\sigma}{\omega}$, where σ is called the coefficient of absorption.

Then we have the simple case where

- $l = \frac{c}{\sigma}$: absorption does not depend on the frequency,
- the phase velocity remains *c*,

•
$$d(\omega) = \frac{i\omega}{i\omega + \sigma}$$
.

In frequency domain the wave-equation becomes

$$\rho(\sigma + i\omega)u - \frac{\partial}{\partial x} \underbrace{\left(\mu(\sigma + i\omega)^{-1} \frac{\partial u}{\partial x}\right)}_{v} = 0,$$

which corresponds in time domain to the differential equation

$$\frac{\partial^2 u}{\partial t^2} + 2\sigma \frac{\partial u}{\partial t} + \sigma^2 u - c^2 \frac{\partial^2 u}{\partial x^2} = 0,$$

or as a first order system, describing a PML,

$$\rho\left(\frac{\partial u}{\partial t} + \sigma u\right) - \frac{\partial v}{\partial x} = 0,$$
$$\mu^{-1}\left(\frac{\partial v}{\partial t} + \sigma v\right) - \frac{\partial u}{\partial x} = 0.$$

In 1D we have the energy identity

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

As one can see,

- we do not only have dissipation in space but
- we additionally have proof for temporal dissipation!

All solutions to the 1D-equation are decaying!

There will be NO such proof in higher dimensions!

Alternative Method

- The solutions of the Helmholtz-equation can be analytically continued on the complex plane.
- Think of a complex path, were the physical world is the real trace.
- Parametrize it through the physical coordinate (X = X(x)).
- For x < 0 it shall be the real axis.
- For x > 0 the solution shall be exponentially decaying ($\Rightarrow \Im X < 0$).
- After returning to the time domain, the equation must be written in terms of partial differential equations.
- \Rightarrow The change of variables has to be rationally dependent of $i\omega$.

The following change of variables satisfies the conditions:

$$X(x) = x + \frac{1}{i\omega} \int_{o}^{x} \sigma(\xi) d\xi,$$

where $\sigma(x)$ typically is chosen to be $\sigma(x) = 0$ for x < 0 and $\sigma(x) > 0$ for x > 0.

If $\widetilde{u}(x) = u(X(x))$, and u(x) is a solution of the Helmholtz-equation, then

$$-\frac{i\omega}{i\omega+\sigma}\frac{\partial}{\partial x}\left(\frac{i\omega}{i\omega+\sigma}\mu\frac{\partial\widetilde{u}}{\partial x}\right)-\rho\omega^{2}\widetilde{u}=0.$$

- This is the equation we already found for the absorbing layer!
- We can thus always find a Perfectly Matched Layer.
- Even with a spatially dependent absorption profile $\sigma(x)$.

Returning to $\rho = \mu = 1$, one can even show that if u(x, t), v(x, t) are the solutions for given initial data to

$$\frac{\partial u}{\partial t} - \frac{\partial v}{\partial x} = 0, \quad \frac{\partial v}{\partial t} - \frac{\partial u}{\partial x} = 0,$$

then the associated solutions for the (infinite) PML are

 $u^*(x,t) = u(x,t)e^{-\int_0^x \sigma(\xi)d\xi}, \qquad v^*(x,t) = v(x,t)e^{-\int_0^x \sigma(\xi)d\xi}.$

Infinite Layer



The propagation of a wave in with an infinite PML, with constant absorption profile σ on the left and variable profile $\sigma(x)$ on the right (Joly).

But the goal is a finite layer,

 \implies homogeneus Neumann-condition at x = L:

$$\frac{\partial u}{\partial x}(L,t) = 0.$$

Finite Layer

Boundary condition at $x = L \implies$ reflected wave, with total solution

$$\overline{u}(x,t) = u^*(x,t) + u^*(2L - x,t), \overline{v}(x,t) = v^*(x,t) - v^*(2L - x,t).$$



The propagation of a wave entering a finite PML, with constant profile σ on the left and variable profile $\sigma(x)$ on the right (Joly).

PML in Two Dimensions

Consider $(x, y) \in \mathbb{R}^2$ and the general linear hyperbolic system

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

where $U(x, y, t) \in \mathbb{R}^m, m \ge 1$ and $\mathbf{A}_x, \mathbf{A}_y \in \mathbb{R}^{m \times m}$.

Let's

- limit the computational domain to x < 0 (or x < L),
- and thus add a perfectly matched and absorbing layer to the normal region x < 0.
- We first split $U = U^x + U^y$, where (U^x, U^y) is the solution to the system

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

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

- We have isolated the derivative in the x- and y-direction.
- We now add an absorption-term σU^x with $\sigma \ge 0$ to the equation containing the derivative in the *x*-direction and obtain

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

It is clear that we can describe the one-dimensional PML-equation with this system:

$$U^{x} = \begin{bmatrix} u \\ v \end{bmatrix}, \quad U^{y} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \quad A = \begin{bmatrix} 0 & \rho^{-1} \\ \mu & 0 \end{bmatrix}$$

- Of course one will choose $\sigma = 0$ for x < 0 and $\sigma > 0$ for x > 0.
- One will not split the equations in the physical region but only in the PML and couple the two solutions by $U(0^-) = U^x(0^+) + U^y(0^+)$ at x = 0.

Complex Change of Variables

Changing to frequency space with a temporal fourier transform we arrive at the "generalized Helmholtz-equation",

$$i\omega\widehat{U} + \mathbf{A}_x \frac{\partial\widehat{U}}{\partial x} + \mathbf{A}_y \frac{\partial\widehat{U}}{\partial y} = 0.$$

Supposing that we can extend the solution \widehat{U} onto the complex plane, we can look at the function

$$\widetilde{U}(x) = \widehat{U}\left(x + \frac{1}{i\omega}\int_0^x \sigma(\xi)d\xi\right).$$

 $\widetilde{U}(x)=\widehat{U}(x)$ for x<0 and

$$i\omega \widetilde{U} + \mathbf{A}_x \frac{\partial \widetilde{U}}{\partial x} \left(\frac{i\omega}{i\omega + \sigma} \right) + \mathbf{A}_y \frac{\partial \widetilde{U}}{\partial y} = 0,$$

$$\implies \widetilde{U} = \underbrace{\left(-\frac{1}{i\omega + \sigma} \mathbf{A}_x \frac{\partial \widetilde{U}}{\partial x} \right)}_{\widetilde{U}_x} + \underbrace{\left(-\frac{1}{i\omega} \mathbf{A}_y \frac{\partial \widetilde{U}}{\partial y} \right)}_{\widetilde{U}_y}.$$

Going back to time domain, we finally have

$$\left(\frac{\partial}{\partial t} + \sigma\right)\widetilde{U}_x + \mathbf{A}_x\frac{\partial\widetilde{U}}{\partial x} = 0, \qquad \frac{\partial}{\partial t}\widetilde{U}_y + \mathbf{A}_y\frac{\partial\widetilde{U}}{\partial y} = 0,$$

which is the previously found system.

But we have not yet proven the absorbing character of the constructed layer:

Special solutions of the not-absorbing equation in a (special) homogeneous region are plane waves:

$$U(x, y, t) = U_0 e^{i(\omega t - k_x x - k_y y)}, \quad k_x, k_y, \omega \in \mathbb{R},$$

- k and ω are related through the dispersion relation.
- The solutions propagate with phase-velocity $c = \omega/|k|$.

In the PML, we have the change of variables

$$x \to x + {1 \over i\omega} \int_0^x \sigma(\xi) d\xi,$$

and the plane wave becomes

$$U(x, y, t) = U_0 e^{i(\omega t - k_x x - k_y y) - \frac{k_x}{\omega} \int_0^x \sigma(\xi) d\xi}$$

- As the wave propagates, the wave is evanescent.
- In this manner we can speak of an absorbing layer.
- But our argument on the absorbance of the wave is dependent on its propagation. To be correct, we would have to argument using the group velocity.
- We do not have proof of temporal dissipation through the energy identity as in one dimension.

Acoustic Wave Equation

We start from the 2-dimensional acoustic wave equation,

$$p \frac{\partial^2 u}{\partial t^2} - \operatorname{div}(\mu \nabla u) = 0,$$

and rewrite it as a system of order 1,

$$p \frac{\partial u}{\partial t} - \frac{\partial v_x}{\partial x} - \frac{\partial v_y}{\partial y} = 0,$$
$$\mu^{-1} \frac{\partial v_x}{\partial t} - \frac{\partial u}{\partial x} = 0,$$
$$\mu^{-1} \frac{\partial v_y}{\partial t} - \frac{\partial u}{\partial y} = 0.$$

- In order to rewrite the system as PML, we would have to split the vector $U = (u, v_x, v_y)$.
- But we can avoid splitting v_x and v_y .

Writing the PML System

Splitting u and introducing the absorption coefficient σ we find the system

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

$$\mu^{-1} \left(\frac{\partial v_x}{\partial t} + \sigma v_x \right) - \frac{\partial}{\partial x} (u^x + u^y) = 0,$$

$$\rho \frac{\partial u^y}{\partial t} - \frac{\partial v_y}{\partial y} = 0,$$

$$\mu^{-1} \frac{\partial v_y}{\partial t} - \frac{\partial}{\partial y} (u^x + u^y) = 0.$$

If ρ, μ and σ are constant, we can eliminate v_x and v_y and find the 4th order equation

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

Absorption and Reflection of Plane Waves

In a homogeneous acoustic region we have $c = \sqrt{\mu/\rho}$ and the dispersion-relation

$$k_x^2 + k_y^2 = \frac{\omega^2}{c^2}.$$

If θ is the angle of incidence, the solution is

$$u(x,t) = \underbrace{e^{i\frac{\omega}{c}(ct-x\cos\theta-y\sin\theta)}}_{\forall x} \underbrace{e^{-\frac{\cos\theta}{c}\int_0^x \sigma(\xi)d\xi}}_{x>0}.$$

- We end the PML at x = L with a homogeneous Neumann-condition.
- In the PML we get through simple reflection a particular solution of the form

$$u(x,t) = e^{i\frac{\omega}{c}(ct-x\cos\theta-y\sin\theta)}e^{-\frac{\cos\theta}{c}\int_0^x\sigma(\xi)d\xi} + e^{i\frac{\omega}{c}(ct-(2L-x)\cos\theta-y\sin\theta)}e^{-\frac{\cos\theta}{c}\int_0^{2L-x}\sigma(\xi)d\xi}.$$

In the region x < 0 the solution becomes

$$u(x,t) = e^{i\frac{\omega}{c}(ct - x\cos\theta - y\sin\theta)} + R_{\sigma}(\theta)e^{i\frac{\omega}{c}(ct + x\cos\theta - y\sin\theta)},$$

where we have set the coefficient of reflection to



The total reflection is exponentially decreasing with

- the absorption σ ,
- the length of the layer L,
- the angle of incidence $\cos(\theta)$.

So far so good, but we have only analyzed exact solutions to the problem. What happens if we treat the system numerically?

Numerical Problems

Our goal A very thin layer *L* in order to accelerate the simulation.

Solution Let $\sigma > 0$ and constant arbitrarily big to let *L* become arbitrarily small.

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Therefore, the incident wave will give rise to two reflected waves:

- A wave reflected at x = L, the PML-wave.
- A wave reflected at x = 0, the numerical or discretization-wave.



• The PML-wave is of the same nature as in the exact case. The amplitude is $(\Delta x \text{ is the step of discretization in space})$

$$R_{\rm PML} = e^{-2\frac{\sigma L}{c}\cos\theta} (1 + O(\Delta x^2)).$$

• The amplitude of the numerical wave is found to be

$$R_{\rm disc} \sim const. \cdot \sigma^2 \Delta x^2, \quad (\Delta x \to 0).$$

- The amplitude of the numerical wave vanishes with Δx .
- But it also grows quadratically with σ and the layer is less perfectly matched.

In order to fasten calculation,

we should increase both Δx and σ ,

but in order to minimize the errors

we should take them to be small.

Variable Profiles

We actually choose a compromise:

- We impose many thin layers with increasing absorption coefficients σ_i .
- $(\sigma_{i+1} \sigma_i)$ shall be small.
- ⇒ Additionally to the normal PML-reflection we will have a superposition of small numerical reflections proportional to $(\sigma_{i+1} \sigma_i)^2$.
- ⇒ Their amplitudes will be exponentially damped by a factor of $\rho_i = e^{-\frac{2}{c} \int_0^{x_i} \sigma(\xi) d\xi}$.

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Examples (1)



- 1 Propagation of an accoustic wave with $\sigma = const.$ at the left and right boundary.
- 2 $\sigma = const$ but a finer grid: The reflections are smaller.
- 3 Quadratic absorption profile $\sigma(x)$: The reflected waves have disappeared.

(Joly)

Examples (2)



The solution at a single point and its evolution in time (Joly).

- Blue: Constant profile with coarse grid.
- Red: Constant profile with fine grid.
- Green: Quadratic profile.

Rectangular Domain

In most problems all boundaries need to be absorbing.

For a rectangular domain and a layer of length *L*, we impose the following equations on the domain $[-a - L, a + L] \times [-b - L, b + L]$:

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

$$\mu^{-1} \left(\frac{\partial v_x}{\partial t} + \sigma_x(x)v_x \right) - \frac{\partial}{\partial x}(u^x + u^y) = 0,$$

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

$$\mu^{-1} \left(\frac{\partial v_y}{\partial t} + \sigma_y(y)v_y \right) - \frac{\partial}{\partial y}(u^x + u^y) = 0,$$

where σ_x (σ_y) depends only on x (y) and its support is $\{0 < |x| - a < L\}$ ($\{0 < |y| - b < L\}$).in With this procedure, the corners of the rectangle are automatically treated quite simple.

Below, we see an illustration of this:

The calculation of an 2D-acoustic wave emitted by a single point-source (Joly).



Summary

We have seen

- the reflections that occur at "physical" absorbing layers.
- that (exact) PML do suppress the reflections (impedance matching) and lead to complex velocity.
- that we can describe this via a complex change of variables.
- the easy generalization of this method to higher dimension.
- that a convex (quadratic) absorption-profile $\sigma(x)$ minimizes the numerical reflections.

Conclusion

The PML-method seems to have outranked the other available boundary conditions. Especially since

- the PML are particularly simple to implement, at least with respect Absorbing Boundary Conditions.
- they offer remarkable performance in many cases.
- they adapt without complications to a large number of problems/equations.

Although,

- even if essential progress has been made recently, the mathematical analysis of these methods has not yet been completed.
- the competition between the PML and the Absorbing Boundary Conditions has not come to an end yet.