PML Implementation for 2D Wave Equation

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The standard wave equation describes wave propagation in space and time. However, when we solve it numerically on a finite computational domain, waves reflect off the boundaries, creating artificial reflections that contaminate our simulation. Perfectly Matched Layers (PML) are absorbing boundary conditions designed to eliminate these reflections by attenuating waves as they approach the domain boundaries.

Part 1 – Using First Order Equations via an Auxiliary Differential Equation

Step 1: Coordinate Transformation and Derivative Scaling

The Core Concept

The foundation of PML is a coordinate stretching technique that introduces damping into the wave equation. We start by transforming our spatial derivatives to incorporate an absorbing function.

Note: A PML is not a physical absorber but a mathematical transformation of the wave equation within a special layer surrounding the main computational domain. The key idea is to perform a complex coordinate stretching.

The Coordinate Transform

Spatial Coordinate Transformation: The fundamental step is to transform the spatial coordinate x into a complex plane:

$$x \to x + j\frac{f(x)}{\omega} \tag{1}$$

- j is the imaginary unit
- ω is the angular frequency
- $f(x)$ is a function we design (zero in main domain, gradually increases in PML)

Effect of the Transformation

This complex shift makes the wave solution inside the PML become exponentially decaying:

$$u(x,t) \to e^{-c^{-1}f(x)}u(x,t) \tag{2}$$

This achieves the desired attenuation while preserving the wave's phase properties.

So, in a regular domain, we have spatial derivatives $\frac{\partial}{\partial x}$. PML modifies this by introducing a complex-valued coordinate transformation. The first step is to see how the coordinate transformation affects derivatives. Using the chain rule for the transformation $\tilde{x} = x + j\frac{f(x)}{\omega}$:

$$\partial x \to \left(1 + j\frac{1}{\omega}\frac{\partial f}{\partial x}\right)\partial x \tag{3}$$

where j is the imaginary unit and ω is the angular frequency.

Simplification Through Redefinition

For computational simplicity, we redefine the normalized absorbed derivative gradient:

$$\frac{1}{\omega}\frac{\partial f}{\partial x} = \frac{\sigma_x}{\omega} \tag{4}$$

where σ_x is the absorption coefficient in the x-direction. σ_x is our control parameter. This coefficient is:

- Zero in the interior of the computational domain
- Non-zero (positive) in the PML region near boundaries
- Smoothly transitions from interior to boundary

Derivative Transformation

With this redefinition, all spatial derivatives transform as:

$$\boxed{\frac{\partial}{\partial x} \to \frac{1}{1 + j\frac{\sigma_x}{\omega}}\frac{\partial}{\partial x}} \tag{5}$$

This transformation ensures that:

- Waves propagating in the x-direction experience exponential decay in the PML region
- The attenuation is proportional to σ_x
- Frequency-dependent behavior provides broadband absorption

Step 2: Wave Equation Splitting

The standard second-order wave equation in 2D is:

$$\frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} = \nabla^2 u + \phi \tag{6}$$

where:

- $u(x, y, t)$ is the scalar wave field (pressure, displacement, amplitude, etc.)
- c is the wave velocity (constant in homogeneous media)
- $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$ is the 2D Laplacian operator
- $\phi(x, y, t)$ represents source terms (point sources, distributed sources, etc.)
- In free space, $\phi = 0$ for homogeneous propagation

Introduce an Auxiliary Vector Field

The key is to reduce the order of the time derivative. We introduce a new vector field $\mathbf{v}(\mathbf{x}, t)$, defined such that its relationship to u mimics the structure of common physical systems (like acoustics or electromagnetics):

$$\frac{\partial \mathbf{v}}{\partial t} = \nabla u \tag{7}$$

This definition is chosen because the gradient of a scalar field (∇u) naturally gives a vector field. The time derivative of $\mathbf{v}$ is equal to this gradient. Auxiliary vector field, $\mathbf{v} = (v_x, v_y)$

Construct a Second First-Order Equation

We now need an equation for $\frac{\partial u}{\partial t}$. Let's manipulate the original wave equation. First, take the divergence of both sides of Equation (7):

$$\nabla \cdot \left(\frac{\partial \mathbf{v}}{\partial t} \right) = \nabla \cdot (\nabla u)$$

The divergence and time derivative operators commute (assuming sufficient smoothness of $\mathbf{v}$), so:

$$\frac{\partial}{\partial t}(\nabla \cdot \mathbf{v}) = \nabla^2 u \tag{8}$$

From 6, we can solve this for $\nabla^2 u$:

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

Substitute this expression for $\nabla^2 u$ into Equation (8):

$$\frac{\partial}{\partial t}(\nabla \cdot \mathbf{v}) = \frac{1}{c^2} \frac{\partial^2 u}{\partial t^2} - \phi \tag{9}$$

Integrate with Respect to Time

To eliminate the second time derivative on the right-hand side, we integrate the entire equation 9 with respect to time, from 0 to t:

$$\int_0^t \frac{\partial}{\partial t}(\nabla \cdot \mathbf{v}) dt = \int_0^t \left(\frac{1}{c^2} \frac{\partial^2 u}{\partial t^2} - \phi \right) dt$$

Evaluating the integrals:

- The left-hand side becomes: $\nabla \cdot \mathbf{v}(t) - \nabla \cdot \mathbf{v}(0)$
- The right-hand side becomes:

$$\frac{1}{c^2} \left[\frac{\partial u}{\partial t} \right]_0^t - \int_0^t \phi dt = \frac{1}{c^2} \frac{\partial u}{\partial t} - \frac{1}{c^2} \frac{\partial u}{\partial t}(0) - \int_0^t \phi dt$$

Apply Initial Conditions

We now make the standard assumption of **quiescent initial conditions**. This means that at $t = 0$, the fields and their time derivatives are zero:

- $u(\mathbf{x}, 0) = 0$

- $\frac{\partial u}{\partial t}(\mathbf{x}, 0) = 0$
- $\mathbf{v}(\mathbf{x}, 0) = \mathbf{0}$

With these initial conditions:

- $\nabla \cdot \mathbf{v}(0) = 0$
- $\frac{\partial u}{\partial t}(0) = 0$

Substituting these into the integrated equation gives the final, clean first-order equation:

$$\nabla \cdot \mathbf{v} = \frac{1}{c^2}\frac{\partial u}{\partial t} - \int_0^t \phi dt$$

Rewriting this in the more standard form:

$$\frac{1}{c^2}\frac{\partial u}{\partial t} = \nabla \cdot \mathbf{v} + \int_0^t \phi dt \tag{10}$$

Final First-Order System

The original second-order wave equation (6) has been replaced by a system of two first-order equations:

$$\boxed{\begin{aligned} &(1) \quad \frac{1}{c^2}\frac{\partial u}{\partial t} = \nabla \cdot \mathbf{v} + \int_0^t \phi \, dt \\ &(2) \quad \frac{\partial \mathbf{v}}{\partial t} = \nabla u \end{aligned}} \tag{11}$$

Why Split the Wave Equation?

1. **PML Implementation:** It allows for a more straightforward incorporation of the complex coordinate stretching, as seen in the original derivation, by applying the transformation rules directly to the two first order equations 11. The coordinate stretching technique works naturally with first-order systems but becomes complicated with second-order time derivatives.

2. **Numerical Stability:** Explicit time-stepping schemes work more reliably with first-order systems. A split system allows us to use simpler, more stable numerical methods like Forward Euler with staggered grids.

Verification: Recovering the Original Equation

We can recover the original second-order equation (6) from this first-order system.

1. Take the time derivative $\frac{\partial}{\partial t}$ of (1) of equation 11:

$$\frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial t}(\nabla \cdot \mathbf{v}) + \phi$$

   (The time derivative of the integral $\int_0^t \phi dt$ is simply ϕ, by the Fundamental Theorem of Calculus).

2. On the right-hand side, the divergence and time derivative commute:

$$\frac{\partial}{\partial t}(\nabla \cdot \mathbf{v}) = \nabla \cdot \left(\frac{\partial \mathbf{v}}{\partial t}\right)$$

3. Now substitute (2) of equation 11, $\frac{\partial \mathbf{v}}{\partial t} = \nabla u$, into this expression:

$$\nabla \cdot \left(\frac{\partial \mathbf{v}}{\partial t}\right) = \nabla \cdot (\nabla u) = \nabla^2 u$$

4. Putting it all together:

$$\boxed{\frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} = \nabla^2 u + \phi}$$

   This is indeed the original second-order wave equation. The transformation is exact and reversible.

Step 3: Frequency Domain Analysis and Substitution

Fourier Transform to Frequency Domain

To understand how PML affects wave propagation, we apply the Fourier Transform over time. This converts temporal derivatives to frequency multipliers:

$$\frac{\partial}{\partial t} \to -j\omega \tag{12}$$

and spatial derivatives remain as partial derivatives: $\frac{\partial}{\partial x}$, $\frac{\partial}{\partial y}$

Transformed Equations

Applying the Fourier Transform to our split equations and incorporating the coordinate stretching transformation:

$$\frac{\partial}{\partial x} \to \frac{1}{1+j\frac{\sigma_x}{\omega}}\frac{\partial}{\partial x}$$

$$\frac{\partial \mathbf{v}}{\partial t} = \nabla u$$

Focusing on the $x-$ component:

$$\frac{\partial v_x}{\partial t} = \frac{\partial u}{\partial x}$$

$$\frac{\partial v_x}{\partial t} = \frac{1}{1+j\frac{\sigma_x}{\omega}}\frac{\partial u}{\partial x}$$

In Fourier Domain:

$$\boxed{-j\omega v_x = \frac{1}{1+j\frac{\sigma_x}{\omega}}\frac{\partial u}{\partial x}} \tag{13}$$

Multiply both sides by the complex denominator to eliminate the fraction:

$$-j\omega v_x\left(1+j\frac{\sigma_x}{\omega}\right) = \frac{\partial u}{\partial x} \tag{14}$$

Expanding:

$$-j\omega v_x + v_x\sigma_x = \frac{\partial u}{\partial x} \tag{15}$$

$$\boxed{-j\omega v_x = \frac{\partial u}{\partial x} - v_x\sigma_x} \tag{16}$$

Transform back to time domain ($-j\omega \to \frac{\partial}{\partial t}$):

$$\boxed{\frac{\partial \mathbf{v}}{\partial t} = \nabla u - \mathbf{v}\odot\sigma} \tag{A}$$

where $\odot$ denotes an hadamard or element-wise product. This is our first final equation. The term $-\mathbf{v}\odot\sigma$ acts as damping term or damping contribution, active only within the PML.

- In regions where $\sigma_x = 0$ (interior), we get pure wave propagation

- In PML regions where $\sigma_x > 0$, this additional term causes exponential attenuation
- The attenuation coefficient directly scales with σ_x

Step 4: Complete 2D System with Absorbing Coefficients

Expanding the Full System

For 2D wave propagation, we apply the coordinate stretching in both x and y directions. The divergence of the vector field, $\mathbf{v}$, requires both components:
Remember:

$$\frac{1}{c^2}\frac{\partial u}{\partial t} = \nabla \cdot \mathbf{v} + \int_0^t \phi \; dt$$

$$\frac{1}{c^2}\frac{\partial u}{\partial t} = \frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial x} + \int_0^t \phi \; dt$$

In the frequency domain, the equation becomes:

$$\int_0^t \phi \; dt = \frac{j}{\omega}\phi$$

$$-\frac{1}{c^2}j\omega u = \frac{1}{1+j\frac{\sigma_x}{\omega}}\frac{\partial v_x}{\partial x} + \frac{1}{1+j\frac{\sigma_y}{\omega}}\frac{\partial v_y}{\partial y} + \frac{j}{\omega}\phi \tag{17}$$

Multiplying through by both complex denominators:

$$\begin{aligned} -\frac{1}{c^2}j\omega\left(1+j\frac{\sigma_x}{\omega}\right)\left(1+j\frac{\sigma_y}{\omega}\right)u \\ = \frac{\partial v_x}{\partial x}\left(1+j\frac{\sigma_y}{\omega}\right) + \frac{\partial v_y}{\partial y}\left(1+j\frac{\sigma_x}{\omega}\right) \\ + \frac{j}{\omega}\phi\left(1+j\frac{\sigma_x}{\omega}\right)\left(1+j\frac{\sigma_y}{\omega}\right) \end{aligned} \tag{18}$$

Left-hand side:

$$(1+j\frac{\sigma_x}{\omega})(1+j\frac{\sigma_y}{\omega}) = 1 + j\frac{\sigma_x+\sigma_y}{\omega} + j^2\frac{\sigma_x\sigma_y}{\omega^2} = 1 + j\frac{\sigma_x+\sigma_y}{\omega} - \frac{\sigma_x\sigma_y}{\omega^2}.$$

$$-\frac{1}{c^2}j\omega\Big(1+j\frac{\sigma_x}{\omega}\Big)\Big(1+j\frac{\sigma_y}{\omega}\Big)u = -\frac{1}{c^2}j\omega\left[1 + j\frac{\sigma_x+\sigma_y}{\omega} - \frac{\sigma_x\sigma_y}{\omega^2}\right]u.$$

Multiply $j\omega$ through the bracket:

$$j\omega\,[1] = j\omega, \qquad j\omega\left[j\frac{\sigma_x+\sigma_y}{\omega}\right] = j^2(\sigma_x+\sigma_y) = -(\sigma_x+\sigma_y),$$

$$j\omega\left[-\frac{\sigma_x\sigma_y}{\omega^2}\right] = -j\frac{\sigma_x\sigma_y}{\omega}.$$

So the LHS becomes

$$-\frac{1}{c^2}\Big[j\omega-(\sigma_x+\sigma_y)-j\frac{\sigma_x\sigma_y}{\omega}\Big]u = \frac{1}{c^2}\Big[-j\omega+(\sigma_x+\sigma_y)+j\frac{\sigma_x\sigma_y}{\omega}\Big]u.$$

Right-hand side:
Expand each factor:

$$\frac{\partial v_x}{\partial x}\Big(1+j\frac{\sigma_y}{\omega}\Big) = \frac{\partial v_x}{\partial x}+j\frac{\sigma_y}{\omega}\frac{\partial v_x}{\partial x},$$
$$\frac{\partial v_y}{\partial y}\Big(1+j\frac{\sigma_x}{\omega}\Big) = \frac{\partial v_y}{\partial y}+j\frac{\sigma_x}{\omega}\frac{\partial v_y}{\partial y}.$$

For the source term,

$$\frac{j}{\omega}\phi\Big(1+j\frac{\sigma_x}{\omega}\Big)\Big(1+j\frac{\sigma_y}{\omega}\Big) = \phi\frac{j}{\omega}\Big[1+j\frac{\sigma_x+\sigma_y}{\omega}-\frac{\sigma_x\sigma_y}{\omega^2}\Big].$$

Multiply $\dfrac{j}{\omega}$ through:

$$\phi\Big[\frac{j}{\omega}-\frac{\sigma_x+\sigma_y}{\omega^2}-j\frac{\sigma_x\sigma_y}{\omega^3}\Big].$$

Now collect the three RHS parts:

$$\frac{\partial v_x}{\partial x}+j\frac{\sigma_y}{\omega}\frac{\partial v_x}{\partial x}+\frac{\partial v_y}{\partial y}+j\frac{\sigma_x}{\omega}\frac{\partial v_y}{\partial y}+\phi\Big[\frac{j}{\omega}-\frac{\sigma_x+\sigma_y}{\omega^2}-j\frac{\sigma_x\sigma_y}{\omega^3}\Big].$$

Full expanded equation:

$$\boxed{\frac{1}{c^2}\Big[-j\omega+(\sigma_x+\sigma_y)+j\frac{\sigma_x\sigma_y}{\omega}\Big]u = \frac{\partial v_x}{\partial x}+\frac{\partial v_y}{\partial y}+j\frac{\sigma_y}{\omega}\frac{\partial v_x}{\partial x}+j\frac{\sigma_x}{\omega}\frac{\partial v_y}{\partial y}+\phi\Big(\frac{j}{\omega}-\frac{\sigma_x+\sigma_y}{\omega^2}-j\frac{\sigma_x\sigma_y}{\omega^3}\Big)}$$

Simplification with Non-Overlapping Assumption

We may assume that will be no overlap between the source location and the region where our wave attenuates. This mean our source ϕ stay far away from the PML. So, we can assume any product of damping term and source is zero. ($\sigma_x\phi = 0$, $\sigma_y\phi = 0$).

After expanding and grouping:

$$\frac{1}{c^2}\Big[-j\omega+(\sigma_x+\sigma_y)+j\frac{\sigma_x\sigma_y}{\omega}\Big]u=\frac{\partial v_x}{\partial x}+\frac{\partial v_y}{\partial y}+j\frac{\sigma_y}{\omega}\frac{\partial v_x}{\partial x}+j\frac{\sigma_x}{\omega}\frac{\partial v_y}{\partial y}+\phi\Big(\frac{j}{\omega}-\frac{\sigma_x+\sigma_y}{\omega^2}-j\frac{\sigma_x\sigma_y}{\omega^3}\Big)$$

$$\frac{1}{c^2}\Big[-j\omega+(\sigma_x+\sigma_y)+j\frac{\sigma_x\sigma_y}{\omega}\Big]u=\frac{\partial v_x}{\partial x}+\frac{\partial v_y}{\partial y}+j\frac{\sigma_y}{\omega}\frac{\partial v_x}{\partial x}+j\frac{\sigma_x}{\omega}\frac{\partial v_y}{\partial y}+\phi\Big(\frac{j}{\omega}\Big)-\phi\frac{\sigma_x+\sigma_y}{\omega^2}-j\frac{\sigma_x\sigma_y}{\omega^3}\phi$$

$$\frac{1}{c^2}\Big[-j\omega+(\sigma_x+\sigma_y)+j\frac{\sigma_x\sigma_y}{\omega}\Big]u=\frac{\partial v_x}{\partial x}+\frac{\partial v_y}{\partial y}+j\frac{\sigma_y}{\omega}\frac{\partial v_x}{\partial x}+j\frac{\sigma_x}{\omega}\frac{\partial v_y}{\partial y}+\phi\Big(\frac{j}{\omega}\Big)$$

$$\boxed{-\frac{1}{c^2}j\omega u+\frac{1}{c^2}(\sigma_x+\sigma_y)u=\nabla\cdot\mathbf{v}+\frac{j}{\omega}\left(\sigma_x\frac{\partial v_y}{\partial y}+\sigma_y\frac{\partial v_x}{\partial x}-\frac{\sigma_x\sigma_y}{c^2}u+\phi\right)} \tag{19}$$

Step 5: Introduction of Auxiliary Field ψ

The term multiplied by $\frac{j}{\omega}$ in equation 19 is problematic because it represents an integral in the time domain $\left(\frac{j}{\omega}\to\int_0^t dt\right)$. To avoid storing the history of the solution, a standard trick is to define an **auxiliary variable** ψ that encapsulates this term:

$$\psi=\frac{j}{\omega}\left(\sigma_y\frac{\partial v_x}{\partial x}+\sigma_x\frac{\partial v_y}{\partial y}-\frac{1}{c^2}\sigma_x\sigma_y u+\phi\right) \tag{20}$$

Reduction to First-Order System

Multiplying both sides by ω/j:

$$-j\omega\psi=\sigma_y\frac{\partial v_x}{\partial x}+\sigma_x\frac{\partial v_y}{\partial y}-\frac{1}{c^2}\sigma_x\sigma_y u+\phi \tag{21}$$

Transforming back to the time domain (where $-j\omega\leftrightarrow\frac{\partial}{\partial t}$):

$$\boxed{\frac{\partial\psi}{\partial t}=\sigma_y\frac{\partial v_x}{\partial x}+\sigma_x\frac{\partial v_y}{\partial y}-\frac{1}{c^2}\sigma_x\sigma_y u+\phi} \tag{B}$$

This decouples the problem into manageable first-order equations.

Now, tranform equation 19 to time domain:

$$-\frac{1}{c^2}j\omega u + \frac{1}{c^2}(\sigma_x + \sigma_y)u = \nabla \cdot \mathbf{v} + \frac{j}{\omega}\left(\sigma_x \frac{\partial v_y}{\partial y} + \sigma_y \frac{\partial v_x}{\partial x} - \frac{\sigma_x \sigma_y}{c^2}u + \phi\right)$$

$$-\frac{1}{c^2}j\omega u + \frac{1}{c^2}(\sigma_x + \sigma_y)u = \nabla \cdot \mathbf{v} + \psi$$

$$-\frac{1}{c^2}j\omega u = \nabla \cdot \mathbf{v} - \frac{1}{c^2}(\sigma_x + \sigma_y)u + \psi$$

$$\boxed{\frac{1}{c^2}\frac{\partial u}{\partial t} = \nabla \cdot \mathbf{v} - \frac{1}{c^2}(\sigma_x + \sigma_y)u + \psi} \tag{C}$$

Step 6: Time-Domain Implementation Algorithm

Now, to simulate a wave in a domain with a PML, we no longer need to solve the original wave equation (6). Instead, we solve a system of three coupled equations simultaneously inside the PML region (in the main domain, $\sigma_x = \sigma_y = 0$, and the system reduces to the original first-order system).

Auxillairy Vector Field equation:

$$\boxed{\frac{\partial \mathbf{v}}{\partial t} = \nabla u - \mathbf{v} \odot \sigma} \tag{22}$$

Auxiliary field equation:

$$\boxed{\frac{\partial \psi}{\partial t} = \sigma_y \frac{\partial v_x}{\partial x} + \sigma_x \frac{\partial v_y}{\partial y} - \frac{1}{c^2}\sigma_x \sigma_y u + \phi} \tag{23}$$

Wave field equation:

$$\boxed{\frac{1}{c^2}\frac{\partial u}{\partial t} = \nabla \cdot \mathbf{v} - \frac{1}{c^2}(\sigma_x + \sigma_y)u + \psi} \tag{24}$$

Numerical Solution: Forward Euler Method

At each time step n, we compute the solution at step $n+1$ using forward differences:

Step 1 – Compute the $\dot{\mathbf{v}}$:

Calculate ∇u and then solve for $\mathbf{v}$ using the vector field equation with an explicit method (Forward Euler):

$$\frac{\partial \mathbf{v}}{\partial t} = \nabla u - \mathbf{v} \odot \sigma \tag{25}$$

Forward differences in time (easiest):

$$\mathbf{v}^{n+1} = \mathbf{v}^n + \Delta t \left(\nabla u^n - \mathbf{v}^n \odot \sigma \right) \tag{26}$$

Step 2 – Update auxiliary field:

Update ψ using current derivatives and field values:

$$\frac{\partial \psi}{\partial t} = \sigma_y \frac{\partial v_x}{\partial x} + \sigma_x \frac{\partial v_y}{\partial y} - \frac{1}{c^2} \sigma_x \sigma_y u + \phi \tag{27}$$

$$\psi^{n+1} = \psi^n + \Delta t \left(\sigma_y \frac{\partial v_x^{n+1}}{\partial x} + \sigma_x \frac{\partial v_y^{n+1}}{\partial y} - \frac{1}{c^2} \sigma_x \sigma_y u^n + \phi^n \right)$$

Use the newly updated $\mathbf{v}^{n+1}$ and the current u^n.

Step 3 – Update wave field:

Using the updated velocity components v_x^{n+1} and v_y^{n+1}, compute the divergence $\nabla \cdot \mathbf{v}$ and find the x-derivative of v_x needed for the next step. Then explicitly step forward using:

$$\frac{1}{c^2} \frac{\partial u}{\partial t} = \nabla \cdot \mathbf{v} - \frac{1}{c^2} (\sigma_x + \sigma_y) u + \psi$$

$$\frac{\partial u}{\partial t} = c^2 (\nabla \cdot \mathbf{v}) - (\sigma_x + \sigma_y) u + c^2 \psi \tag{28}$$

$$u^{n+1} = u^n + \Delta t \left(c^2 \nabla \cdot \mathbf{v}^{n+1} - (\sigma_x + \sigma_y) u^n + c^2 \psi^{n+1} \right)$$

Use the newly updated $\mathbf{v}^{n+1}$ and ψ^{n+1}

<u>Initial Conditions</u>

To launch the simulation correctly:

- Set all fields (u, $\mathbf{v}$, ψ) to zero at $t = 0$
- Inject energy through the source term ϕ

- The absorbing layer parameters σ_x and σ_y are defined spatially and remain constant in time

This algorithm "marches" the fields forward in time, and the damping terms ($-\mathbf{v} \odot \sigma$, $-(\sigma_x + \sigma_y)u$, etc.) ensure that any wave entering the PML region is effectively absorbed.

1 Full Discretization

We discretize the system using the Forward Euler method on a 2D spatial grid with temporal discretization.

Grid Definition

- **Spatial Grid:** Indices i and j for x and y directions
- Spatial steps: Δx, Δy
- Grid points: $(x_i, y_j) = (i\Delta x, j\Delta y)$
- **Temporal Grid:** Index n for time
- Time step: Δt
- Time points: $t_n = n\Delta t$
- **Discrete Fields:**

$$\begin{aligned} u(i,j,n) &\approx u^n[i,j] \\ v_x(i,j,n) &\approx v_x^n[i,j] \\ v_y(i,j,n) &\approx v_y^n[i,j] \\ \psi(i,j,n) &\approx \psi^n[i,j] \end{aligned}$$

Discretize the Auxiliary Vector Field Equation

Continuous Equation:

$$\frac{\partial \mathbf{v}}{\partial t} = \nabla u - \mathbf{v} \odot \sigma$$

This is a vector equation. Let's write it component-wise, assuming $\sigma = (\sigma_x, \sigma_y)$ and the $\odot$ operator denotes element-wise multiplication.

$$\frac{\partial v_x}{\partial t} = \frac{\partial u}{\partial x} - \sigma_x v_x$$

$$\frac{\partial v_y}{\partial t} = \frac{\partial u}{\partial y} - \sigma_y v_y$$

Forward Euler Discretization:
The Forward Euler scheme is:

$$\frac{\partial f}{\partial t} \approx \frac{f^{n+1} - f^n}{\Delta t}$$

Applying this to the v_x equation:

$$\frac{v_x^{n+1}[i,j] - v_x^n[i,j]}{\Delta t} = \left.\frac{\partial u}{\partial x}\right|_{i,j}^{n} - \sigma_x[i,j] \cdot v_x^n[i,j]$$

We now need to discretize the spatial derivative $\frac{\partial u}{\partial x}$. A central difference scheme is common for accuracy:

$$\left.\frac{\partial u}{\partial x}\right|_{i,j}^{n} \approx \frac{u^n[i+1,j] - u^n[i-1,j]}{2\Delta x}$$

Putting it all together and solving for v_x^{n+1}:

$$\boxed{v_x^{n+1}[i,j] = v_x^n[i,j] + \Delta t \left(\frac{u^n[i+1,j] - u^n[i-1,j]}{2\Delta x} - \sigma_x[i,j] \cdot v_x^n[i,j] \right)}$$

Similarly, for the v_y equation, using a central difference for $\frac{\partial u}{\partial y}$:

$$\left.\frac{\partial u}{\partial y}\right|_{i,j}^{n} \approx \frac{u^n[i,j+1] - u^n[i,j-1]}{2\Delta y}$$

$$\boxed{v_y^{n+1}[i,j] = v_y^n[i,j] + \Delta t \left(\frac{u^n[i,j+1] - u^n[i,j-1]}{2\Delta y} - \sigma_y[i,j] \cdot v_y^n[i,j] \right)}$$

Forward Euler discretization with central spatial differences

$$v_x^{n+1}[i,j] = v_x^n[i,j] + \Delta t \left(\frac{u^n[i+1,j] - u^n[i-1,j]}{2\Delta x} - \sigma_x[i,j] \cdot v_x^n[i,j] \right) \tag{29}$$

$$v_y^{n+1}[i,j] = v_y^n[i,j] + \Delta t \left(\frac{u^n[i,j+1] - u^n[i,j-1]}{2\Delta y} - \sigma_y[i,j] \cdot v_y^n[i,j] \right) \tag{30}$$

Discretize the Auxiliary Field Equation

The continuous equation:

$$\frac{\partial \psi}{\partial t} = \sigma_y \frac{\partial v_x}{\partial x} + \sigma_x \frac{\partial v_y}{\partial y} - \frac{1}{c^2} \sigma_x \sigma_y u + \phi$$

Forward Euler Discretization:

$$\frac{\psi^{n+1}[i,j] - \psi^n[i,j]}{\Delta t} = \sigma_y[i,j] \cdot \left.\frac{\partial v_x}{\partial x}\right|_{i,j}^n + \sigma_x[i,j] \cdot \left.\frac{\partial v_y}{\partial y}\right|_{i,j}^n - \frac{1}{c^2} \sigma_x[i,j] \sigma_y[i,j] \cdot u^n[i,j] + \phi^n[i,j]$$

Discretize the spatial derivatives with central differences:

$$\left.\frac{\partial v_x}{\partial x}\right|_{i,j}^n \approx \frac{v_x^n[i+1,j] - v_x^n[i-1,j]}{2\Delta x}$$

$$\left.\frac{\partial v_y}{\partial y}\right|_{i,j}^n \approx \frac{v_y^n[i,j+1] - v_y^n[i,j-1]}{2\Delta y}$$

Putting it all together and solving for ψ^{n+1}:

$$\begin{aligned} \psi^{n+1}[i,j] = \psi^n[i,j] + \Delta t \Bigg(& \sigma_y[i,j] \cdot \frac{v_x^n[i+1,j] - v_x^n[i-1,j]}{2\Delta x} \\ & + \sigma_x[i,j] \cdot \frac{v_y^n[i,j+1] - v_y^n[i,j-1]}{2\Delta y} \\ & - \frac{\sigma_x[i,j] \sigma_y[i,j]}{c^2} \cdot u^n[i,j] + \phi^n[i,j] \Bigg) \end{aligned} \tag{31}$$

Discretize the Wave Field Equation

The continuous Equation:

$$\frac{1}{c^2}\frac{\partial u}{\partial t} = \nabla \cdot \mathbf{v} - \frac{1}{c^2}(\sigma_x + \sigma_y)u + \psi$$

Forward Euler Discretization:

$$\frac{1}{c^2} \cdot \frac{u^{n+1}[i,j] - u^n[i,j]}{\Delta t} = \nabla \cdot \mathbf{v} \,\Big|_{i,j}^{n} - \frac{1}{c^2}(\sigma_x[i,j] + \sigma_y[i,j])u^n[i,j] + \psi^n[i,j]$$

Discretize the divergence $\nabla \cdot v$ with central differences:

$$\nabla \cdot \mathbf{v} \,\Big|_{i,j}^{n} = \frac{\partial v_x}{\partial x}\Big|_{i,j}^{n} + \frac{\partial v_y}{\partial y}\Big|_{i,j}^{n} \approx \frac{v_x^n[i+1,j] - v_x^n[i-1,j]}{2\Delta x} + \frac{v_y^n[i,j+1] - v_y^n[i,j-1]}{2\Delta y}$$

Putting it all together and solving for u^{n+1}:

$$\begin{aligned} u^{n+1}[i,j] - u^n[i,j] = c^2 \Delta t \left(\frac{v_x^n[i+1,j] - v_x^n[i-1,j]}{2\Delta x} + \frac{v_y^n[i,j+1] - v_y^n[i,j-1]}{2\Delta y} \right) \\ - \Delta t\big(\sigma_x[i,j] + \sigma_y[i,j]\big)u^n[i,j] + c^2 \Delta t\, \psi^n[i,j] \end{aligned} \tag{32}$$

$$\begin{aligned} u^{n+1}[i,j] = u^n[i,j] + c^2 \Delta t \left(\frac{v_x^n[i+1,j] - v_x^n[i-1,j]}{2\Delta x} + \frac{v_y^n[i,j+1] - v_y^n[i,j-1]}{2\Delta y} \right) \\ - \Delta t\big(\sigma_x[i,j] + \sigma_y[i,j]\big)u^n[i,j] + c^2 \Delta t\, \psi^n[i,j] \end{aligned} \tag{33}$$

2 Implementation Algorithm

The update procedure at each time step is:

1. Update velocities v_x and v_y using equations (29) and (30)
2. Update auxiliary field ψ using equation (31)
3. Update wave field u using equation (33)

3 Stability Considerations

The Forward Euler method requires satisfying the Courant-Friedrichs-Lewy (CFL) condition:

$$\Delta t \leq \frac{1}{c\sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}}}$$

The damping terms σ_x, σ_y may impose additional restrictions on the time step.

Step 7: Summary

Why PML Works

Derivation of Exponential Decay in a PML

1. **Coordinate Stretch:**
$$\tilde{x} = x + j\frac{f(x)}{\omega}$$
where $f(x)$ is zero in the main domain and positive in the PML.

2. **General Wave Solution:** The general, steady-state solution for a wave propagating in free space can be described in the frequency domain as a superposition of plane waves. A single Fourier component (a single (a single k and ω) has the form:

   A plane wave component is:
$$u(x,t) = U(k,\omega)e^{j(kx-\omega t)}$$
This is a standard plane wave solution to the wave equation, where $U(k,\omega)$ is the amplitude.

Applying the Transformation

The core idea is to analytically continue the solution into the complex coordinate $\tilde{x}$.

Step 1: Substitute $x \to \tilde{x}$ into the solution:

$$u(x,t) \to u(\tilde{x},t) = U(k,\omega)e^{j(k\tilde{x}-\omega t)}$$

Step 2: Expand the exponent using the definition of $\tilde{x}$:

$$u(\tilde{x},t) = U(k,\omega)e^{j\left[k\left(x+j\frac{f(x)}{\omega}\right)-\omega t\right]}$$

Step 3: Simplify the exponent:

$$u(\tilde{x},t) = U(k,\omega)e^{j\left(kx+jk\frac{f(x)}{\omega}-\omega t\right)} = U(k,\omega)e^{j(kx-\omega t)+j^2\frac{kf(x)}{\omega}}$$

Since $j^2 = -1$:

$$u(\tilde{x}, t) = U(k, \omega)e^{j(kx-\omega t)} \cdot e^{-\frac{kf(x)}{\omega}}$$

Step 4: Use the phase velocity $c = \omega/k \Rightarrow k = \omega/c$:

$$e^{-\frac{kf(x)}{\omega}} = e^{-\frac{(\omega/c)f(x)}{\omega}} = e^{-\frac{f(x)}{c}}$$

The ω cancels out, making the attenuation frequency-independent.
Step 5: The final transformed solution:

$$u(\tilde{x}, t) = \left[e^{-\frac{f(x)}{c}}\right] U(k, \omega)e^{j(kx-\omega t)}$$

The term $U(k, \omega)e^{j(kx-\omega t)}$ is the original wave $u(x, t)$. Therefore:

$$\boxed{u(x, t) \to e^{-c^{-1}f(x)}u(x, t)} \tag{34}$$

This is the derivation of equation 2 above.

- The transformation $x \to x + jf(x)/\omega$ is mathematically equivalent to multiplying the original wave solution by a real, spatially dependent exponential decay factor $e^{-f(x)/c}$.
- **Role of $f(x)$**: The function $f(x)$ controls the attenuation. Inside the main domain where $f(x) = 0$, the exponential factor is 1, and the wave is unchanged. Inside the PML layer where $f(x) > 0$, the wave is exponentially damped.
- **Why it's "Perfectly Matched"**: Because this transformation is an analytic continuation of the original wave equation, the wave impedance at the interface between the main domain and the PML remains unchanged. This is the "perfect match" that prevents reflections at the interface. Reflections only occur due to discretization in the numerical implementation, not from the theoretical formulation.

This derivation shows the elegant theoretical foundation of the PML technique: a complex coordinate stretch in the frequency domain directly translates to an exponential attenuation of the wave in the time domain.

Design Choices

Derivation of PML Sigma Profile

The goal is to ensure that a wave entering the PML is attenuated to a very small amplitude, R, by the time it reaches the outer boundary of the computational domain. This prevents the wave from reflecting back into the main simulation region.

So, we start with the fundamental result from the complex coordinate stretching (see equation 29 above), which shows that the wave inside the PML is multiplied by an exponential decay factor:

$$u(x,t) \to e^{-c^{-1}f(x)}u(x,t)$$

We want this decay factor to equal our desired reflection coefficient R at the outer boundary of the PML ($x = x_{\max}$):
Set the decay factor equal to R at $x = x_{\max}$:

$$e^{-c^{-1}f(x_{\max})} = R \tag{35}$$

Relating the Attenuation to the PML parameter σ

From the PML definition:

$$\frac{\partial f}{\partial x} = \sigma_x(x) \qquad (2)$$

Integrate from the PML start x_0 to its end $x_{\max}$:

$$\int_{x_0}^{x_{\max}} \frac{\partial f}{\partial x} dx = \int_{x_0}^{x_{\max}} \sigma_x(x) dx$$

$$f(x_{\max}) - f(x_0) = \int_{x_0}^{x_{\max}} \sigma_x(x) dx$$

$$f(x_{\max}) = \int_{x_0}^{x_{\max}} \sigma_x(x) dx \qquad (3)$$

Take the natural log of equation 1:

$$\ln\left(e^{-c^{-1}f(x_{\max})}\right) = \ln(R) \Rightarrow f(x_{\max}) = -c\ln(R) \qquad (4)$$

Substitute (4) into (3):

$$\boxed{\int_{x_0}^{x_{\max}} \sigma_x(x) dx = -c\ln(R)} \qquad (5)$$

This is the key design equation. It states that the integral of σ_x across the PML must equal $-c\ln(R)$ to achieve the desired attenuation R.

Choosing a Polynomial Profile

To minimize numerical reflections at the interface x_0, the PML should "turn on" gradually. A common and effective choice is a polynomial profile:

$$\sigma_x(x) = \sigma_{\max} (x - x_0)^m \qquad (6)$$

Where:

1. $\sigma_{\max}$ is the maximum value of σ_x at the outer boundary.
2. m is the order of the polynomial (a positive integer, e.g., $m = 2, 3, 4$). A higher m makes the transition smoother.

Solving for $\sigma_{\max}$

Substitute (6) into (5):

$$\int_{x_0}^{x_{\max}} \sigma_{\max} (x - x_0)^m \, dx = -c \ln(R)$$

Let $u = x - x_0$, $du = dx$. When $x = x_0$, $u = 0$; when $x = x_{\max}$, $u = L = x_{\max} - x_0$:

$$\sigma_{\max} \int_0^L u^m du = -c \ln(R)$$

$$\sigma_{\max} \int_0^L u^m du = -c \ln(R)$$

$$\sigma_{\max} \left[\frac{u^{m+1}}{m+1} \right]_0^L = -c \ln(R)$$

$$\sigma_{\max} \cdot \frac{L^{m+1}}{m+1} = -c \ln(R)$$

$$\boxed{\sigma_{\max} = -\frac{c \ln(R)(m+1)}{L^{m+1}} = -\frac{c \ln(R)(m+1)}{(x_{\max} - x_0)^{m+1}}}$$

Discretization

In simulation, space is discretized into cells of width Δx. The PML width is therefore an integer number of these cells:

$$L = n \Delta x$$

Where n is the number of cells in the PML. The final formula for implementation becomes:

$$\sigma_{\max} = -\frac{c \ln(R)(m+1)}{(n\Delta x)^{m+1}}$$

<u>NOTE</u>:

Sigma Profile: The absorption coefficient σ typically increases from zero (at the PML-interior interface) to a maximum value (at the boundary).
Thickness: PML thickness should be roughly $\lambda/10$ to $\lambda/4$, where λ is the smallest wavelength in the simulation.