# Perfectly matched layers (PML) for full-waveform modeling of seismic and electromagnetic wave propagation in unbounded domains

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**ABSTRACT**

In this work, I present the theory of perfectly matched layer for numerical modeling of seismic and electromagnetic waves in unbounded domains.

## INTRODUCTION

Full-waveform modeling of seismic and electromagnetic wave propagation is a very important tool for geophysical exploration, especially for imaging techniques based on two-way wave equations such as reverse-time migration and full-waveform inversion. Many numerical methods have been proposed to solve the wave equations including the finite-difference method, the finite-element method, spectral and pseudo-spectral methods, boundary-element method, and wavelet-based method. Typically, the computational domain is bounded and represents only a region of interest of the physical medium. When wavefields propagate to the boundary of the computational domain, we would like the wavefields to leave the domain, i.e., there is no reflection from the boundary. Many absorbing boundary conditions and layers have been proposed in the past decades including the absorbing boundary conditions proposed by Clayton and Engquist (1980) and Keys (1985), the sponge boundary layer proposed by (Cerjan et al., 1985), and the perfectly matched layer (PML) proposed by Berenger (1994). Among the three, PML is the most efficient and effective one. Many efforts have been spent to improve the efficiency and effectiveness of PML until it is now the most widely used absorbing boundary layers for numerical modeling of wave propagation.

In this paper, I present PML formulas for numerical modeling of seismic and electromagnetic wave propagation in the time domain.

## FINITE DIFFERENCE METHOD

Finite-difference methods (FDMs) are a numerical method based on the Taylor's expansion for solving partial differential equations (PDEs). Continuous problems solved by FDM will be discretized, e.g., on to a regular grid (see Figure 1). For simplicity, only a uniform grid ($\Delta x = \Delta z$ everywhere in the domain) will be used here. A one-dimensional forward Taylor's expansion for a uniform grid is given as

$$\begin{aligned} f(x_{i+1}) &= f(x_i) + \Delta x f'(x_i) + \frac{\Delta x^2}{2!} f''(x_i) + \\ &\quad \frac{\Delta x^3}{3!} f'''(x_i) + \frac{\Delta x^4}{4!} f^{(4)}(x_i) + ... \end{aligned} \tag{1}$$

where $x_i = i\Delta x$ for $i = 0, 1, 2, ..., n$. As an example, we can rearrange and truncate terms in equation 1 to obtain a first-order approximation of the first-order derivative of function $f$, namely

$$f'(x_i) \approx \frac{f(x_{i+1}) - f(x_i)}{\Delta x} + O(\Delta x). \tag{2}$$

Let's have another example before we apply FDM to solve the acoustic wave equation. To improve the order of accuracy of the forward FDM scheme in equation 2, we can use the backward Taylor's expansion of the function $f$ at $x_(i-1)$

$$\begin{aligned} f(x_{i-1}) &= f(x_i) - \Delta x f'(x_i) + \frac{\Delta x^2}{2!} f''(x_i) - \\ &\quad \frac{\Delta x^3}{3!} f'''(x_i) + \frac{\Delta x^4}{4!} f^{(4)}(x_i) - ... \end{aligned} \tag{3}$$

Subtracting equation 3 from equation 1 yields

$$f(x_{i+1}) - f(x_{i-1}) = 2\Delta x f'(x_i) + \frac{\Delta x^3}{3!} f'''(x_i) + O(\Delta x^5). \tag{4}$$

Rearranging equation 4 gives us

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2\Delta x} + O(\Delta x^2), \quad (5)$$

which is a central FDM scheme with a second order of accuracy.

To demonstrate how FDM can be used to solve a PDE, let's solve the first-order coupled acoustic wave equations

$$p_{,t}(\mathbf{r}, t) = c^2(\mathbf{r})\rho(\mathbf{r})\nabla \cdot \mathbf{u}, \quad (6)$$

$$u_{,t}(\mathbf{r}, t) = \frac{1}{\rho(\mathbf{r})}\nabla p(\mathbf{r}, t), \quad (7)$$

where $p$ is the pressure field, $u$ is the particle velocity field, $c$ is velocity, $\kappa$ is bulk density, $\mathbf{r}$ is position vector, and $t$ is time. A derivative of variable $f$ with respect to variable $x$ is denoted as $f_{,x}$. This notation was used in equations 6 and 7, and will be used later on.

### *Staggered-Grid Finite-Difference Method*

The standard FDM method for solving the first-order coupled acoustic wave equations is the staggered-grid FDM. More details on this method are described in Levander (1988) for an elastic case.

To solve the acoustic wave equations using FDM on the staggered grid, let's first rewrite equations 6 and 7 for two dimensions as

$$p_{,t}(x, z, t) = c^2(x, z)\rho(x, z)\left(u_{,x}(x, z, t) + w_{,z}(x, z, t)\right), \quad (8)$$

$$u_{,t}(x, z, t) = \frac{1}{\rho(x, z)} p_{,x}(x, z, t), \quad (9)$$

$$w_{,t}(x, z, t) = \frac{1}{\rho(x, z)} p_{,z}(x, z, t), \quad (10)$$

where $u$ and $w$ is the $x$- and $z$-components of the particle velocity $\mathbf{u}$. Then approximate the temporal and spatial derivatives in equations 8-10 using finite differences, i.e.,

$$p_{,t}(x, z, t) = p_{,t}(x_i, z_j, t_k) \approx \frac{p_{ij}^{k+1/2} - p_{ij}^{k-1/2}}{2\frac{\Delta t}{2}} + O(\Delta t^2), \quad (11)$$

$$u_{,x}(x, z, t) = u_{,x}(x_i, z_j, t_k) \approx \frac{u_{i+1/2,j}^{k} - u_{i-1/2,j}^{k}}{2\frac{\Delta x}{2}} + O(\Delta x^2), \quad (12)$$

where

$$x = x_i = i\Delta x \quad for \quad i = 0, 1, 2, ..., n_x \quad (13)$$

$$z = z_j = j\Delta z \quad for \quad j = 0, 1, 2, ..., n_z \quad (14)$$

$$t = t_k = k\Delta t \quad for \quad k = 0, 1, 2, ..., n_t \quad (15)$$

$$p_{ij}^{k+\frac{1}{2}} = p(x_i, z_j, t_k + \frac{\Delta t}{2}), \quad (16)$$

$$u_{i+\frac{1}{2},j}^{k} = u(x_i + \frac{\Delta x}{2}, z_j, t_k). \quad (17)$$

We will use a second-order FDM to approximate both time and spatial derivatives. By replacing the derivatives in equations 8-10 with finite differences and rearranging the resulting difference equations we obtain

$$p_{ij}^{k+\frac{1}{2}} = p_{ij}^{k-\frac{1}{2}} + \frac{c_{ij}^2\rho_{ij}\Delta t}{\Delta x}\left(u_{i+\frac{1}{2},j}^{k} - u_{i-\frac{1}{2},j}^{k} + w_{i,j+\frac{1}{2}}^{k} - w_{i,j-\frac{1}{2}}^{k}\right), \quad (18)$$

$$u_{i+\frac{1}{2},j}^{k+1} = u_{i+\frac{1}{2},j}^{k} + \frac{\Delta t}{\rho_{ij}\Delta x}\left(p_{i+1,j}^{k+\frac{1}{2}} + p_{ij}^{k+\frac{1}{2}}\right), \quad (19)$$

$$w_{i,j+\frac{1}{2}}^{k+1} = w_{i,j+\frac{1}{2}}^{k} + \frac{\Delta t}{\rho_{ij}\Delta x}\left(p_{i,j+1}^{k+\frac{1}{2}} + p_{ij}^{k+\frac{1}{2}}\right). \quad (20)$$

Equations 18-20 represent an explicit staggered-grid FD scheme with second-order accuracy in space and time. In the class, we will derive a FD scheme with fourth-order accuracy in space.

## PERFECTLY MATCHED LAYER

In many applications, we want to model wavefield propagation in a bounded domain. When the wavefield propagates to a boundary, there will be some reflection from the boundary. This boundary reflection is not desirable and we want to eliminate it from our numerical simulation. Absorbing boundary conditions (ABCs) are normally used for this purpose. There are various kinds of ABCs in the literature but one of the standard and most widely used ABCs is perfectly matched layer (PML) boundary conditions (Berenger, 1994).

Before we go into more details on PML, let's first introduce the simplest ABC which is based on a one-way propagation operator (Clayton and Engquist, 1980). Recalling the second-order acoustic wave equation in 1D, namely,

$$\frac{1}{c^2}p_{,tt} - p_{,xx} = \left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2}\right)p = 0. \quad (21)$$

The two-way propagation operator in the parentheses can be decomposed into two one-way propagation operators, and equation 21 becomes

$$\left(\frac{1}{c}\frac{\partial}{\partial t} - \frac{\partial}{\partial x}\right)\left(\frac{1}{c}\frac{\partial}{\partial t} + \frac{\partial}{\partial x}\right)p = 0. \quad (22)$$

Either of the one-way propagation operators in equations 22 can be used as an absorbing boundary condition at the boundary of the computation domain to reduce boundary reflections by approximating the derivatives by finite differences. The main drawback of this ABC is that it perfectly absorbs only normal-incident wavefields. So oblique-incident wavefields will still produce spurious reflections from the boundary. Nonetheless, this one-way-propagator ABC works nicely in 1D case since the wavefields always propagate perpendicular to the boundary.

Boundary reflections can be significantly reduced by using PML. The key idea of PML is to turn propagating waves into decaying waves in the region of PML. To demonstrate this idea, let's assume a 1D homogeneous medium so the wavefield can be represented by a plane wave

$$p(x,t) = e^{i(kx-\omega t)}. \quad (23)$$

Since the wavefield is an analytic function, we can use analytic continuation by replacing the real coordinate x with a complex coordinate (Johnson, 2010)

$$\tilde{x} = x + \frac{i\sigma(x)}{\omega}, \quad (24)$$

where $\sigma(x)$ vanishes when $x < 0$. Substituting equation 24 into equation 23 and rearranging yields

$$p(x,t) = e^{i(kx-\omega t)}e^{-k\sigma/\omega} \quad (25)$$

which shows that the wavefield is exponentially decaying wherever $\sigma(x)$ is nonzero.

To make use of the complex coordinate, we just simply replace a spatial derivative operator with a modified form

$$\frac{\partial}{\partial x} \rightarrow \frac{\partial}{\partial \tilde{x}} = \frac{1}{1+\frac{i\sigma}{\omega}}\frac{\partial}{\partial x} = \frac{-i\omega}{\sigma - i\omega}\frac{\partial}{\partial x}. \quad (26)$$

Let's apply PML to 1D first-order wave equations

$$p_{,t}(x,t) = c^2(x)\rho(x)u_{,x}(x,t), \quad (27)$$

$$u_{,t}(x,t) = \frac{1}{\rho(x)}p_{,x}(x,t). \quad (28)$$

Applying Fourier transform in time to equations 27 and 28 yields

$$-i\omega\tilde{p}(x,\omega) = c^2(x)\rho(x)\frac{\partial u(x,\omega)}{\partial x}, \quad (29)$$

$$-i\omega\tilde{u}(x,\omega) = \frac{1}{\rho(x)}\frac{\partial \tilde{p}(x,\omega)}{\partial x}, \quad (30)$$

where $\tilde{p}$ and $\tilde{u}$ are the Fourier transforms in time of $p$ and $u$. The regular coordinate $x$ in equations 26 and 27 is then replaced by the complex coordinate in equation 24, and we obtain

$$-i\omega\tilde{p} = c^2\rho\frac{\partial\tilde{u}}{\partial\tilde{x}}, \quad (31)$$

$$-i\omega\tilde{u} = \frac{1}{\rho}\frac{\partial\tilde{p}}{\partial\tilde{x}}. \quad (32)$$

Using equation 26, equations 28 and 29 become

$$-i\omega\tilde{p} = c^2\rho\left(\frac{1}{1+\frac{i\sigma}{\omega}}\right)\frac{\partial\tilde{u}}{\partial x}, \quad (33)$$

$$-i\omega\tilde{u} = \frac{1}{\rho}\left(\frac{1}{1+\frac{i\sigma}{\omega}}\right)\frac{\partial\tilde{p}}{\partial x}. \quad (34)$$

Rearranging equations 31 and 32, we obtain

$$-i\omega\tilde{p} + \sigma\tilde{p} = c^2\rho\frac{\partial\tilde{u}}{\partial x}, \quad (35)$$

$$-i\omega\tilde{u} + \sigma\tilde{u} = \frac{1}{\rho}\frac{\partial\tilde{p}}{\partial x}. \quad (36)$$

Taking the inverse Fourier transforms to equations 33 and 34 yields the PML formulation of the first-order wave equations

$$\frac{\partial p}{\partial t} + \sigma p = c^2\rho\frac{\partial u}{\partial x}, \quad (37)$$

$$\frac{\partial u}{\partial t} + \sigma u = \frac{1}{\rho}\frac{\partial p}{\partial x}, \quad (38)$$

Using the steps above, we can derive PML formulations in other cases as shown in Appendix A.

## SUMMARY

Formulations of the perfectly matched layers for numerical modeling of seismic and electromagnetic wave propagation have been presented.

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## APPENDIX A: PML FORMULATIONS

## PML Formulations for Second-Order Wave Equations

*1D Case*

The governing equation for the 1D case is given by

$$p_{,tt} - c^2 p_{,xx} = 0. \quad (39)$$

Applying temporal Fourier transform to equation 39 yields

$$-\omega^2\tilde{p} - c^2\tilde{p} = 0, \quad (40)$$

where $\tilde{p}$ is the pressure field in the frequency domain. Applying the PML transformation 26 to equation 40 yields

$$-\omega^2\tilde{p} - c^2\left[\frac{-i\omega}{\sigma - i\omega}\frac{\partial}{\partial x}\left(\frac{-i\omega}{\sigma - i\omega}\frac{\partial\tilde{p}}{\partial x}\right)\right] = 0, \quad (41)$$

$$\tilde{p} - c^2\left[\frac{1}{\sigma - i\omega}\frac{\partial}{\partial x}\left(\frac{1}{\sigma - i\omega}\frac{\partial\tilde{p}}{\partial x}\right)\right] = 0. \quad (42)$$

Let

$$\psi = \frac{1}{\sigma - i\omega}\frac{\partial \tilde{p}}{\partial x}. \tag{43}$$

Then equation 42 becomes

$$\tilde{p} - \frac{c^2}{\sigma - i\omega}\frac{\partial \tilde{\psi}}{\partial x} = 0, \tag{44}$$

$$(\sigma - i\omega)\tilde{p} - c^2\frac{\partial \tilde{\psi}}{\partial x} = 0. \tag{45}$$

Taking inverse temporal Fourier transform to equations 43 and 45 yields

$$\frac{\partial p}{\partial t} + \sigma p - c^2\frac{\partial \psi}{\partial x} = 0 \tag{46}$$

and

$$\frac{\partial \psi}{\partial t} + \sigma\psi - \frac{\partial p}{\partial x} = 0, \tag{47}$$

which are the PML formulations for the first-order coupled wave equation; the auxiliary field $\psi$ has the physical meaning of the particle velocity $u$.

To obtain the second-order PML formulation, differentiate equation 46 with respect to time and use equation 47:

$$\left(p_{,tt} - c^2 p_{,xx}\right) + \left(\sigma p_{,t} - c^2(\sigma\psi)_{,x}\right) = 0, \tag{48}$$

$$\psi_{,t} + \sigma\psi - p_{,x} = 0. \tag{49}$$

Comparing the first- and second-order PML formulations, it is obvious that the first-order formulation is simpler and thus easier to implement. The staggered-grid finite-difference method is required to implement both formulations. Nonetheless, for the 1D case the absorbing boundary condition of Clayton and Engquist is the method of choice since it can perfectly absorp normally incident wavefield.

*2D Case*

The governing equation for the 2D case is given by

$$p_{,tt} - c^2(p_{,xx} + p_{,zz}) = 0. \tag{50}$$

Applying temporal Fourier transform to equation 50 yields

$$-\omega^2\tilde{p} - c^2(\tilde{p}_{,xx} + \tilde{p}_{,zz}) = 0. \tag{51}$$

Applying the PML transformation 26 to equation 51 yields

$$-\omega^2\tilde{p} - c^2\left[\frac{-i\omega}{\sigma_x - i\omega}\frac{\partial}{\partial x}\left(\frac{-i\omega}{\sigma_x - i\omega}\frac{\partial \tilde{p}}{\partial x}\right) + \frac{-i\omega}{\sigma_z - i\omega}\frac{\partial}{\partial z}\left(\frac{-i\omega}{\sigma_z - i\omega}\frac{\partial \tilde{p}}{\partial z}\right)\right] = 0, \tag{52}$$

$$\tilde{p} - c^2\left[\frac{1}{\sigma_x - i\omega}\frac{\partial}{\partial x}\left(\frac{1}{\sigma_x - i\omega}\frac{\partial \tilde{p}}{\partial x}\right) + \frac{1}{\sigma_z - i\omega}\frac{\partial}{\partial z}\left(\frac{1}{\sigma_z - i\omega}\frac{\partial \tilde{p}}{\partial z}\right)\right] = 0, \tag{53}$$

Let

$$\tilde{\psi}_x = \frac{1}{\sigma_x - i\omega}\frac{\partial \tilde{p}}{\partial x}, \tag{54}$$

and

$$\tilde{\psi}_z = \frac{1}{\sigma_z - i\omega}\frac{\partial \tilde{p}}{\partial z}. \tag{55}$$

Using equations 54 and 55, equation 53 becomes

$$\tilde{p} - c^2\left(\frac{1}{\sigma_x - i\omega}\frac{\partial \tilde{\psi}_x}{\partial x} + \frac{1}{\sigma_z - i\omega}\frac{\partial \tilde{\psi}_z}{\partial z}\right) = 0, \tag{56}$$

$$(\sigma_x - i\omega)(\sigma_z - i\omega)\tilde{p} - c^2\left[(\sigma_z - i\omega)\frac{\partial \tilde{\psi}_x}{\partial x} + (\sigma_x - i\omega)\frac{\partial \tilde{\psi}_z}{\partial z}\right] = 0, \tag{57}$$

Multiplying equation 57 by $1/(-i\omega)$ yields

$$\left[(-i\omega) + (\sigma_x + \sigma_z) + \frac{\sigma_x\sigma_z}{-i\omega}\right]\tilde{p} - c^2\left[\left(\frac{\sigma_z}{-i\omega} + 1\right)\frac{\partial \tilde{\psi}_x}{\partial x} + \left(\frac{\sigma_x}{-i\omega} + 1\right)\frac{\partial \tilde{\psi}_z}{\partial z}\right] = 0. \tag{58}$$

Let

$$\tilde{\phi} = \frac{\tilde{p}}{-i\omega}, \tag{59}$$

$$\tilde{\phi}_x = \frac{\tilde{\psi}_x}{-i\omega}, \tag{60}$$

and

$$\tilde{\phi}_z = \frac{\tilde{\psi}_z}{-i\omega}. \tag{61}$$

Using equations 59-61, equation 58 becomes

$$-i\omega\tilde{p} + (\sigma_x + \sigma_z)\tilde{p} + \sigma_x\sigma_z\tilde{\phi} - c^2\left(\sigma_z\frac{\partial \tilde{\phi}_x}{\partial x} + \frac{\partial \tilde{\psi}_x}{\partial x} + \sigma_x\frac{\partial \tilde{\phi}_z}{\partial z} + \frac{\partial \tilde{\psi}_z}{\partial z}\right) = 0. \tag{62}$$

Taking inverse temporal Fourier transform to equation 62 yields

$$\frac{\partial p}{\partial t} + (\sigma_x + \sigma_z)p + \sigma_x\sigma_z\phi - c^2\left(\sigma_z\frac{\partial \phi_x}{\partial x} + \frac{\partial \psi_x}{\partial x} + \sigma_x\frac{\partial \phi_z}{\partial z} + \frac{\partial \psi_z}{\partial z}\right) = 0. \tag{63}$$

To obtain the second-order PML formulation, differentiate equation 63 with respect to time:

$$\frac{\partial^2 p}{\partial t^2} + (\sigma_x + \sigma_z)\frac{\partial p}{\partial t} + \sigma_x\sigma_z\frac{\partial \phi}{\partial t} - c^2\left(\sigma_z\frac{\partial^2 \phi_x}{\partial x\partial t} + \frac{\partial^2 \psi_x}{\partial x\partial t} + \sigma_x\frac{\partial^2 \phi_z}{\partial z\partial t} + \frac{\partial^2 \psi_z}{\partial z\partial t}\right) = 0. \tag{64}$$

Taking inverse temporal Fourier transform to equations 54-55 and 59-61 we obtain

$$\phi_t = p, \tag{65}$$

$$\phi_{x,t} = \psi_x, \tag{66}$$

$$\phi_{z,t} = \psi_z, \tag{67}$$

$$\psi_{x,t} = -\sigma_x \psi_x + p_{,x}, \tag{68}$$

and

$$\psi_{z,t} = -\sigma_z \psi_z + p_{,z}. \tag{69}$$

Substituting equations 65-69 into equation 64 yields

$$\begin{aligned} &\left[p_{,tt} - c^2(p_{,xx} + p_{,zz})\right] + \left[(\sigma_x + \sigma_z)p_{,t} + \sigma_x\sigma_z p \right. \\ &\left. -c^2 \left\{\sigma_z \psi_{x,x} - (\sigma_x \psi_x)_{,x} + \sigma_x \psi_{z,z} - (\sigma_z \psi_z)_{,z}\right\}\right] = 0. \end{aligned} \tag{70}$$

## PML Formulations for First-Order Wave Equations

Similar to the second-order PML formulation, we obtain the following first-order PML formulations.

*1D Case*

$$p_{,t} + \sigma_x p - \rho c^2 u_{,x} = 0, \tag{71}$$

$$u_{,t} + \sigma_x u - \frac{1}{\rho} p_{,x} = 0. \tag{72}$$

*2D Case*

$$p_{,t} + (\sigma_x + \sigma_z)p + \sigma_x\sigma_z\phi - \rho c^2(\sigma_z \phi_{x,x} + u_{,x} + \sigma_x \phi_{z,z} + w_{,z}) = 0, \tag{73}$$

$$u_{,t} + \sigma_x u - \frac{1}{\rho} p_{,x} = 0, \tag{74}$$

$$w_{,t} + \sigma_z w - \frac{1}{\rho} p_{,z} = 0, \tag{75}$$

$$\phi_{,t} = p, \tag{76}$$

$$\phi_{x,t} = u, \tag{77}$$

and

$$\phi_{z,t} = w, \tag{78}$$

It turns out that the auxiliary field $\phi$ is not necessary in the first-order formulation.