A Well-posed PML Absorbing Boundary Condition For 2D Acoustic Wave Equation

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ABSTRACT

An perfectly matched layers absorbing boundary condition (PML) with an un-split field is derived for the acoustic wave equation by introducing the auxiliary variables and their associated partial differential equations. Unlike the conventional split-variable PML which is only weakly well-posed, the unsplit PML is proven to be strongly well-posed. Both the split-field PML (SPML) and the well-posed PML (WPML) are tested on a homogeneous velocity model by applying the 2-4 staggered-grid finite-difference scheme. Test results are compared with those by Cerjan’s sponge zone absorbing boundary condition. The comparison indicates that WPML and SPML have almost the same performance and are significantly more effective and efficient in absorbing spurious reflections. The advantage of WPML over SPML is that it is theoretically more robust.

INTRODUCTION

In numerical simulations with an open domain, robust absorbing boundary conditions are highly desirable in eliminating spurious reflections from the artificial boundaries of the bounded computational domain. The perfectly matched layer (PML) proposed by Berenger (1994) in 2D time-domain EM simulations has become very popular because it is highly effective and enjoys excellent CPU efficiency. The PML has been successfully extended to the field of elasticity, poroelasticity and anisotropic media for acoustic/elastodynamic wave propagation simulations (Chew and Liu, 1996; Zeng et al., 2001; Collino and Tsogka, 2001; Becache et al., 2001). In the continuum limit, PML is proven to be mostly reflection free regardless of the incidence angle and frequency (Chew and Liu, 1996; Zeng et al., 2001; Festa and Nielsen, 2003). Although there are weak reflections associated with the discretization, PML provides excellent results with less computational cost than the sponge absorber method and does not have the instability problem (Mahrer, 1986; Stacey, 1988) associated with the Clay-
ton and Engquist absorbing boundary condition (Clayton and Engquist, 1977) when the \( \frac{V_s}{V_p} \) ratio is less than 0.5.

Conventionally, PML is implemented by splitting variables in the PML domain (referred to as SPML hereafter), i.e., the velocity, and pressure fields are split into two independent parts based on the spatial derivative terms in the original equations. However, it has been shown (Abarbanel et al., 1998) to be only weakly well-posed, i.e., it may become ill-posed under certain perturbations. Considerable efforts have been made to develop well-posed PML (WPML) formulations (Turkel and Yefet, 1998; Abarbanel et al., 1999; Hu, 2001; Zeng and Liu, 2002). These WPML formulations are mostly unsplit-field PML formulations where the auxiliary variables and augment equations are introduced instead of splitting the physical variables.

In this paper, an unsplit-field PML formulation for the 2D acoustic wave equation is developed and proven to be strongly well-posed. WPML and SPML are tested on a homogeneous velocity model and with a 2-4 (second-order accurate in time and fourth-order accurate in space) staggered grid finite-difference method. Results are compared with those from the sponge method, a combination of Clayton absorbing boundary conditions (Clayton and Engquist, 1977) and Cerjan’s sponge absorber boundary conditions (Cerjan et al, 1985).

**WELL-POSED PML FORMULATIONS**

The PML absorbing layer is a non-physical region located outside the artificial numerical boundary as shown in Figure 1. Hereafter, the PML absorbing layer is referred to the PML region, and the internal model space is referred to as the interior model region or inner region. In Cartesian coordinates, the 2D acoustic wave-equation can be expressed as a system of first-order differential equations in terms of the particle velocities and stresses:

\[
\begin{align*}
\frac{\partial u_x}{\partial t} &= \frac{1}{\rho} \frac{\partial p}{\partial x}, \\
\frac{\partial u_z}{\partial t} &= \frac{1}{\rho} \frac{\partial p}{\partial z}, \\
\frac{\partial p}{\partial t} &= c^2 \rho \left( \frac{\partial u_x}{\partial x} + \frac{\partial u_z}{\partial z} \right),
\end{align*}
\]

where \( \mathbf{u}(\mathbf{x}, t) \) is the particle velocity in term of position \( \mathbf{x} \) and time \( t \), \( \rho(\mathbf{x}, t) \) is the stress tensor, \( c(\mathbf{x}, t) \) is the acoustic velocity of the medium, and \( \rho(\mathbf{x}) \) is density.

The PML formulations can be derived by a complex coordinate stretching approach (Chew and Liu, 1996; Chew and Weedon, 1997; Liu, 1997; Zeng et al., 2001) expressed as
\[ \partial x \Rightarrow \left[ 1 + \frac{id(x)}{\omega} \right] \partial x \quad \partial x \Rightarrow \left[ 1 + \frac{id(z)}{\omega} \right] \partial z, \]  

where \( \omega \) is the temporal frequency, \( d(x) \) and \( d(z) \) represent the exponential damping coefficients in the PML region along \( x \) and \( z \) directions, respectively. By using this complex coordinate approach, PML formulations can also be extended to cylindrical, spherical and general orthogonal curvilinear coordinates (Teixeira et al., 2001).

The split-field formulation of PML for the 2D acoustic wave equation requires a splitting only with the pressure field (Liu and Tao, 1997) \( p = p_x + p_z \) with \( p_x \) and \( p_z \) associated with spatial derivatives in the \( x \) and \( z \) directions, respectively. Equations 1 are first split according to the spatial derivatives

\[
\begin{align*}
\frac{\partial u_x}{\partial t} &= \frac{1}{\rho} \frac{\partial p}{\partial x}, \\
\frac{\partial u_z}{\partial t} &= \frac{1}{\rho} \frac{\partial p}{\partial z}, \\
\frac{\partial p_x}{\partial t} &= c^2 \rho \frac{\partial u_x}{\partial x}, \\
\frac{\partial p_z}{\partial t} &= c^2 \rho \frac{\partial u_z}{\partial z}, \\
p &= p_x + p_z.
\end{align*}
\]

The SPML formulation is then obtained by applying coordinate stretching to equations 3

\[
\begin{align*}
\frac{\partial p_x}{\partial t} + d(x)p_x &= c^2 \rho \frac{\partial u_x}{\partial x}, \\
\frac{\partial p_z}{\partial t} + d(z)p_z &= c^2 \rho \frac{\partial u_z}{\partial z}, \\
p &= p_x + p_z, \\
\frac{\partial u_x}{\partial t} + d(x)u_x &= \frac{1}{\rho} \frac{\partial p}{\partial x}, \\
\frac{\partial u_z}{\partial t} + d(z)u_z &= \frac{1}{\rho} \frac{\partial p}{\partial z}.
\end{align*}
\]

SPML expressed in equations 4 can be easily extended to 3D and its implementation with a finite-difference scheme is also straightforward. An effective use of PML requires the thickness of the PML region to be, typically, 5 to 10 grid points wide. The computational costs for the extra variables and equations are not significant because the damping terms \( d(x) \) and \( d(z) \) only have supports within the PML region in the \( x \) and \( z \) directions, respectively. So the SPML is also highly efficient. However,
the variable and equation splitting destroys the well-posedness of the original acoustic wave equations so that SPML is only weakly well-posed which means it may be ill-posed under certain perturbations (Abarbanel et al., 1998). An alternative is to derive well-posed PML equations which do not split the variables and equations.

The unspilt-field formulation of PML can be derived by applying the complex coordinate stretching expressed in equations 2 to the original wave equation (equations 1) in the frequency domain

\[-i\omega(1 + \frac{d(x)}{-i\omega})\tilde{u}_x = \frac{1}{\rho} \frac{\partial \tilde{p}}{\partial x},\]
\[-i\omega(1 + \frac{d(z)}{-i\omega})\tilde{u}_z = \frac{1}{\rho} \frac{\partial \tilde{p}}{\partial z},\]
\[-i\omega(1 + \frac{d(x)}{-i\omega})(1 + \frac{d(z)}{-i\omega})\tilde{p} = c^2 \rho [(1 + \frac{d(x)}{-i\omega}) \frac{\partial \tilde{u}_x}{\partial x} + (1 + \frac{d(z)}{-i\omega}) \frac{\partial \tilde{u}_z}{\partial z}],\]

where \(\tilde{u}_x, \tilde{u}_z,\) and \(\tilde{p}\) are the temporal Fourier transforms of \(u_x, u_z,\) and \(p,\) respectively. Equations 5 are transformed back to time domain to get the unsplit-field PML formulations

\[\frac{\partial u_x}{\partial t} = \frac{1}{\rho} \frac{\partial p}{\partial x} - d(x)u_x,\]
\[\frac{\partial u_z}{\partial t} = \frac{1}{\rho} \frac{\partial p}{\partial z} - d(z)u_z,\]
\[\frac{\partial p}{\partial t} = c^2 \rho \left[ (1 + \frac{d(x)}{-i\omega}) \frac{\partial u_x}{\partial x} + (1 + \frac{d(z)}{-i\omega}) \frac{\partial u_z}{\partial z} \right] - (d(x) + d(z))p - d(x)d(z)p^{(1)},\]

where the auxiliary variables \(u_x^{(1)}, u_z^{(1)},\) and \(p^{(1)}\) are the time-integrated components for velocity and pressure fields. They are defined as

\[u_x^{(1)}(x, t) = \int_{-\infty}^{t} u_x(x, t') dt',\]
\[u_z^{(1)}(x, t) = \int_{-\infty}^{t} u_z(x, t') dt',\]
\[p^{(1)}(x, t) = \int_{-\infty}^{t} p(x, t') dt'.\]

Define the new variables for the PML region as Turkel and Yefet (1998)

\[U_x = u_x + d(z)u_x^{(1)}, \quad U_z = u_z + d(x)u_z^{(1)},\]

the unsplit PML can be expressed as
\[
\frac{\partial U_x}{\partial t} = \frac{1}{\rho} \frac{\partial p}{\partial x} + (d(z) - d(x))(U_x - d(z)u_x^{(1)}),
\]
\[
\frac{\partial U_z}{\partial t} = \frac{1}{\rho} \frac{\partial p}{\partial z} + (d(x) - d(z))(U_z - d(x)u_z^{(1)}),
\]
\[
\frac{\partial p}{\partial t} = c^2 \rho \left( \frac{\partial U_x}{\partial x} + \frac{\partial U_z}{\partial z} \right) - (d(x) + d(z))p - d(x)d(z)p^{(1)},
\]

with the auxiliary variables and equations to represent the time integrals of the wave fields

\[
\frac{\partial u_x^{(1)}}{\partial t} = u_x = U_x - d(z)u_x^{(1)},
\]
\[
\frac{\partial u_z^{(1)}}{\partial t} = u_z = U_z - d(x)u_z^{(1)},
\]
\[
\frac{\partial p^{(1)}}{\partial t} = p.
\]

The unsplit PML equations for the 2D acoustic wave equation in equations 8 and 9 form a strongly well-posed linear hyperbolic system. To prove this, equations 8 and 9 are expressed in vector form as

\[
\frac{\partial}{\partial t} \begin{pmatrix} u \\ q \end{pmatrix} = A \frac{\partial}{\partial x} \begin{pmatrix} u \\ q \end{pmatrix} + B \frac{\partial}{\partial z} \begin{pmatrix} u \\ q \end{pmatrix} + C \begin{pmatrix} u \\ q \end{pmatrix},
\]

where vectors \( u = (\rho c U_x, \rho c U_z, p)^T \), \( q = (\rho c u_x^{(1)}, \rho c u_z^{(1)}, p^{(1)})^T \), and \( A, B, \) and \( C \) are matrices with

\[
A = \begin{pmatrix}
0 & 0 & c & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
c & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix},
B = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & c & 0 & 0 & 0 \\
c & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}.
\]

Since matrices \( A \) and \( B \) are both real symmetric matrices, they have real eigenvalues and can be diagonalized which ensures that the linear hyperbolic system in equation 10 is strongly well-posed (Gustafsson, et al., 1995).

Although the WPML equations 8 and 9 seem more complicated than the SPML equations 4, they are more computationally efficient because the auxiliary variables \( \tilde{u}_x, \tilde{u}_z, \) and \( \tilde{p} \) are only needed at \( d(z) > 0, d(x) > 0, \) and the corners where both \( d(x) \) and \( d(z) \) are nonzero, respectively, while the split variables \( p_x \) and \( p_z \) are needed for all PML region. In the 2D case, the memory requirement of the sponge and PML approaches can be estimated by defining
\[ m_{\text{sponge}} = m_o [1 + 2n_b \left( \frac{1}{n_x} + \frac{1}{an_z} \right)], \]
\[ m_{\text{WPML}} = m_o [1 + 2.4n_b \left( \frac{1}{n_x} + \frac{1}{an_z} \right)], \]
\[ m_{\text{SPML}} = m_o [1 + 2.8n_b \left( \frac{1}{n_x} + \frac{1}{an_z} \right)], \]
\[ m_o = 5n_xn_z, \tag{12} \]

where \( m_{\text{sponge}}, m_{\text{SPML}}, m_{\text{WPML}} \) and \( m_o \) represents the memory requirement for the sponge method, split-field PML, unsplit-field/well-posed PML and the one without a boundary condition applied, respectively; \( n_x \) and \( n_z \) define the number of nodes along the \( x \) and \( z \) directions of the model; \( n_b \) denotes the number of nodes used for the sponge and PML regions; and \( a \) is a constant (\( a = 2 \) when there is a free surface on the top and \( a = 1 \) when the absorbing boundary conditions are applied to all boundaries). In \( m_o \), particle velocity variables \( u_x \) and \( u_z \), pressure \( p \), acoustic velocity \( c \), and the density \( \rho \) are considered.

The unsplit-field PML formulations are prone to be well-posed because they preserve the well-posedness of the original equations. It is proved that the unsplit-field PML formulations for the acoustic wave equations in a lossy medium are also strongly well-posed (Fan and Liu, 2001). However, the unsplit-field PML formulations are not always well-posed. For example, the unsplit-field PML formulations for the acoustic wave equations with convective mean flow are only weakly well-posed (Hu, 2001).

**FD IMPLEMENTATION OF PML**

The reasons why PML has become so popular are not only because of its excellent numerical efficiency and high performance in eliminating the artificial boundary reflections, but also because of the ease of implementation with finite-difference, finite-element and other numerical schemes. For the inner region, the PML equations are the same as the original wave equations, only in the PML region, the auxiliary variables and equations should be taken care of. So the FD implementation is straightforward. Festa and Nielsen (2003) proved that the stability condition of the 2-2 FD scheme for PML is the same as the classical FD scheme.

A 2-4 FD scheme is used in this report and the stability condition is

\[ \frac{\Delta x}{\Delta t} \geq \frac{7\sqrt{n}}{6} c_{\text{max}}, \tag{13} \]

where \( \Delta t \) and \( \Delta x \) are the temporal and spatial sampling interval for FD scheme, respectively; \( n = 2 \) for 2D and \( n = 3 \) for 3D; \( c_{\text{max}} \) represents the maximum acoustic velocity in the model. To suppress the numerical dispersion, a condition of \( \Delta x \leq \)
\( \frac{c_{\text{min}}}{10 f_{\text{max}}} \) is used which ensures a minimum 10 grid points per wavelength. Here, \( c_{\text{min}} \) and \( f_{\text{max}} \) represent the minimum acoustic velocity and the maximum frequency of the signal.

The careful selection of the damping parameters \( d(x) \) and \( d(z) \) is essential to the performance of PML because the PML error is proportional to the product of the spatial discretization and the damping contrast (Chew and Liu, 1996). Zeng and Liu (2001) and Zeng et al. (2001) related the damping parameters to the dominant source frequency and PML thickness. Collino and Tsogka (2001) presented a relation based on a theoretical reflection coefficient, where the PML thickness and the \( p \)-wave velocity

\[
d(x) = d_0 \frac{x^2}{\delta},
\]

\[
d_0 = \log\left(\frac{1}{R}\right) \frac{3V_p}{2\delta},
\]

and \( \delta = n_b \Delta h \) is the PML thickness, \( n_b \) is the PML thickness in term of nodes, \( \Delta h \) is the node interval, and \( d_0 \) is the maximum damping parameter which is a function of the theoretical reflection coefficient \( R \) (Collino and Tsogka, 2001).

I have found that equations 14 and 15 serve as a satisfactory guide for estimating the damping parameter. The theoretical reflection coefficients are related with the PML thickness \( n_b \) as follows (Collino and Tsogka, 2001): \( PML(n_b = 5)R = 0.01 \), \( PML(n_b = 10)R = 0.001 \), and \( PML(n_b = 20)R = 0.0001 \).

**NUMERICAL RESULTS**

I tested the PML absorbing boundary conditions on the constant model with the shot/receiver geometries in Figure 2. The velocity model is discretized into 101 by 101 nodes with an interval of 10 meters. A line source is located at a depth of 500 m and a horizontal position of 0 m, and the receiver line is located on top of the model. The source time history is a Ricker wavelet with a dominant frequency of 20 Hz and is added to the pressure field. The receivers record the pressure field with a sampling interval of 1 ms and a total record length of 1.0 s. The results are compared with those by the sponge absorber method.

Figure 3 shows the synthetic seismograms by the PML and the sponge absorber approaches. Figures 3a and 3b demonstrate the SPML and WPML results for an absorbing region of 10 nodes in thickness, namely SPML(10) and WPML(10), respectively. Figure 3c shows the seismograms obtained by applying sponge absorbing boundary condition with a sponge zone of 10 nodes in thickness and a damping parameter of 0.95 (called sponge(10) hereafter). There are no visible artificial reflections observed in the seismograms by SPML(10) and WPML(10). It indicates that both PMLs are very effective in absorbing the artificial reflections. Figures 4a-c show the snapshots by SPML(10), WPML(10) and sponge(50) at \( t = 0.1 \) s and \( t = 0.5 \) s,
Figure 1: The PML system. The interior model propagation region is surrounded by the PML absorbing regions which are separated into different parts: in the corners, both damping parameters $d(x)$ and $d(z)$ are positive, and either $d(z) = 0$ or $d(x) = 0$ inside the PML region in the x and z directions. For WPML, the auxiliary integral variables $u_z^{(1)}$ and $u_x^{(1)}$ are needed when $d(x) > 0$ and $d(z) > 0$, respectively, $p^{(1)}$ is needed in the corners where $d(x)$ and $d(z)$ are both positive.
respectively. Snapshots at $t = 0.5$ s are amplified by a factor of 500. Large artificial reflections can be observed in the snapshot at $t = 0.5$ s by sponge(50), while it is quite clean in the PML snapshots.

Figures 5 and 6 show the artificial reflections by SPML(10), WPML(10), sponge(10), and sponge(50), respectively. The artificial reflections are evaluated by the relative errors with respect to the reflection-free traces obtained by the sponge method with a sponge zone of 200 nodes in thickness, and then normalized with respect to the reflection-free traces. According to Figures 5 and 6, the amplitudes of the artificial reflections by the PMLs are about 0.5% of the amplitudes of the incidence waves, while those by sponge(10) and sponge(50) are about 25%−30% and 2% of the amplitudes of the incidence events, respectively. SPML(10) and WPML(10) perform 4 times better in suppressing artificial reflections than sponge(50) for the current model size (101 by 101 nodes). To evaluate the efficiency of PML, the PML CPU time to sponge CPU time ratios are given in Table 1. WPML(10) is almost as fast as sponge(10) while the artificial reflections are about 50−60 times weaker. In addition, WPML(10) is about 20% faster than SPML(10) and 80% faster than sponge(20). These results indicate that the WPML approach is both effective and efficient in suppressing artificial reflections.

Table 1. CPU time for PML and sponge approaches.

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<th>PML (nodes)</th>
<th>Sponge (nodes)</th>
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<tr>
<td></td>
<td>SPML(10)</td>
<td>WPML(10)</td>
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<td>CPU time (s)</td>
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<td>CPU time ratio</td>
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**DISCUSSION**

The WPML formulations for the 2D acoustic wave-equation are derived and tested on a homogeneous model. The results are compared with those from the SPML which is only weakly well-posed and sponge methods with different damping thicknesses. The amplitudes of the artificial reflections by PML(10) are about 0.5% of the amplitudes of the incidence events; WPML(10) is almost as fast as sponge(10) while the artificial reflections are about 50−60 times weaker; WPML(10) is more than 6 times faster than sponge(50) while the artificial reflections are about 4 times weaker for current model with size of 101 by 101 points; WPML(10) is about 20% faster than SPML(10) and 80% faster than sponge(20) due to less memory requirements and computational costs. These results indicate that the WPML approach is both effective and efficient in suppressing artificial reflections.

Following the same procedure as in 2D case, the unsplit PML formulations for the 3D acoustic wave equation are a straight forward derivation and they are also strongly well-posed. The only complexity in the 3D case is that the second-order
Figure 2: Velocity models and shot/receiver geometry used in the tests. A 1000 m by 1000 m constant velocity model of 5000 m/s with a density of 2600 kg/m$^3$. The shot is located in a depth of 500 m and a horizontal position of 0 m, and the receiver line is located in a depth of 0 m with an interval of 10 meters.
Figure 3: Synthetic seismograms of the pressure field for a constant velocity model by PML and sponge methods. The velocity model with no free surface and shot/receiver geometry are shown in Figure 2a. a) SPML(10); b) WPML(10); c) sponge(10) with a damping parameter of 0.95. There are no visible artificial reflections in both PML seismograms.
Figure 4: Snapshots of the pressure fields at $t = 0.1\ s$ and $t = 0.5\ s$ by PML and sponge methods. a) SPML(10); b) WPML(10); c) sponge(50) with a damping parameter of 0.95. Snapshots at $t = 0.5\ s$ are amplified by a factor of 500. Note the large artificial reflections in the snapshot at $t = 0.5\ s$ by the sponge method.
Figure 5: Artificial reflections (errors) of three traces by (a) SPML(10), and (b) WPML. The traces are located at $x = -0.5\ km$ (top), $x = -0.0\ km$ (middle), and $x = 0.5\ km$ (bottom), respectively. The artificial reflections are the normalized relative errors with respect to the corresponding reflection-free reference traces obtained by sponge(200). The energy of the artificial reflections by SPML(10) and WPML(10) is about 0.5% of the incident one in the reference traces.
Figure 6: The artificial reflections (errors) of three traces by (a) sponge(10), and (b) sponge(50). The traces are located at $x = -0.5 \text{ km}$ (top), $x = 0.0 \text{ km}$ (middle), and $x = 0.5 \text{ km}$ (bottom), respectively. The artificial reflections are the normalized relative errors with respect to the the corresponding reflection-free reference traces obtained by sponge(200). The energy of the artificial reflections by sponge(10) and sponge(50) is about $25\% - 30\%$ and $2\%$ of the incident one in the reference traces, respectively.
time integrals of the wave fields are needed, and this can be solved by introduce more auxiliary variables and equations.

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REFERENCES


