

A NON-SPLIT PERFECTLY MATCHED LAYER ABSORBING BOUNDARY CONDITION FOR THE SECOND-ORDER WAVE EQUATION MODELING

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ABSTRACT

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The perfectly matched layer (PML) absorbing boundary conditions (ABC) have been well studied for seismic wavefield modeling. However, existing approaches are either based on a wavefield variable-split or are only applicable to first-order wave equations. In this paper, we present a non-split PML ABC for the second order wave equations in displacement. The principle of the proposed method lies in introducing a series of auxiliary variables to represent the partial derivatives associated with the stretching axis. We derive the non-split PML formula by using basic tensor algebra. The derived equations are in a compact form which makes the ABC condition easier for implementation in practice. Furthermore, as no extra splitting wavefield variables are introduced, the computer memory usage of wave equation modeling can be reduced accordingly. Numerical results for both acoustic and elastic examples show the quality of the performance of the proposed new method.

KEY WORDS: perfectly matched layer, absorbing boundary condition, second-order, wave equation, seismic modeling, finite difference.

INTRODUCTION

Because of the rapid development of computer performance, wave equation based seismic imaging and inversion methods like Reverse Time Migration (RTM) (Baysal et al., 1983; McMechan, 1983; Whitmore, 1983) and Full Waveform Inversion (FWI) (Tarantola, 1984) have become popular for seismic exploration. A highly accurate numerical modeling of seismic wave propagation is an essential stage for successful implementations of these methods. Many different approaches have been examined to solve the seismic

wave equations. Finite difference (FD) methods (Kelly et al., 1976; Virieux, 1984; Dablain, 1986) are most simple and efficient tools for modeling of wave equations. Now they are routinely used for the RTM and FWI. For wave equation modeling by finite difference methods, in order to approximate an unbounded area, ABC are normally introduced to damp the energy at the artificial boundaries of the finite model domain. Over the past decades, numerous methods have been proposed regarding ABC such as damping layers or "sponge zones" (Cerjan et al., 1985), one-way or paraxial conditions (Clayton and Engquist, 1977), Mur's condition (Mur, 1981), PML (Berenger, 1994), and hybrid method (Liu and Sen, 2010). Discussions about the strengths and weaknesses of those methods can be found in (Festa and Vilotte, 2005) and (Komatitsch and Martin, 2007). Berenger (1994) introduced the PML technique that has the desired property of absorbing the incidence waves over a wide range with only ten or less grid points. The PML has been successfully applied to both acoustic (e.g., Liu and Tao, 1997; Qi and Geers, 1998; Hagstrom and Hariharan, 1998) and elastic wave equation modeling problems (e.g. Chew and Liu 1996; Hastings et al., 1996; Collino and Monk, 1998; Collino and Tsogka, 2001; Basu and Chopra, 2003; Liu et al., 2009). All of these papers focused on the PML implementation in first-order systems in velocity and stress. Komatitsch and Tromp (2003) applied the PML to a second-order elastic wave equation in displacement. Their method introduced an intermediate variable to overcome the third-order partial derivative with respect to time. However, as a standard implementation of the PML, their method is still variable-split, which is nonphysical and mathematically weakly well-posed (Abarbanel and Gottlieb, 1997). Also, it is a little bit complex for code programming in practice. On the other hand, non-split based PML ABC has been well studied for the first-order wave equation (e.g., Sacks et al., 1995; Gedney, 1996; Chew and Weedon, 1994; Teixeira and Chew, 2000; Wang and Tang, 2003; Ramadan, 2003; Zeng and Liu, 2004; Komatitsch and Martin, 2007).

In the context of electromagnetic simulation, Ramadan (2003) proposed a non-split implementation of the PML by using auxiliary differential equations (ADEs). Wang and Liang (2006) extended this method to complex-frequency-shift (CFS) PML with a 2D alternating-direction-implicit (ADI) finite-difference time-domain (FDTD) method. Zhang and Shen (2010) implemented the auxiliary differential equations based CFS-PML in the non staggered-grid finite difference method using a fourth-order Runge-Kutta time-marching scheme. However, all previous non-split approaches are used for first-order equations. In this paper, we propose an approach based on ADE and focus on the non-split algorithm for second-order systems. The principle of the method lies in introducing a series of auxiliary variables to replace the partial derivatives associated with the stretching coordinate in frequency domain. The PML wave equation is transformed into a normal second order wave equation and several first order auxiliary equations. As shown in Fig. 1, the auxiliary variables are only calculated in the PML domain. As no extra splitting variables are introduced,

computational memory burden is significantly reduced for implementation. In the following, we will describe our method and present the main formula. We will then verify our method with numerical examples through comparison with one-way conditions (Clayton and Engquist, 1977, eqs. (8) and (9)). In the Appendix, we will show related mathematical derivations in detail.

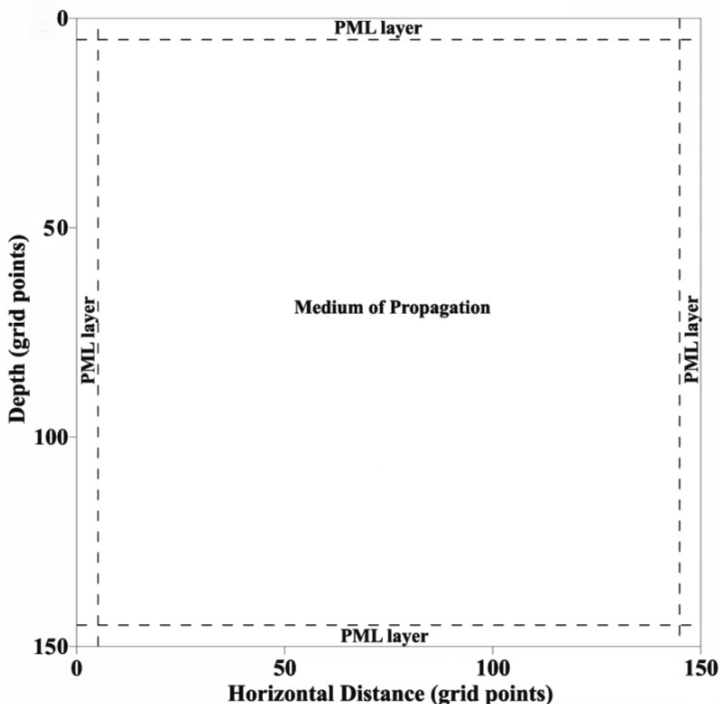


Fig. 1. Schematic diagram of the PML settings.

THEORY

Consider a three dimensional Cartesian coordinate system, in an isotropic homogeneous elastic space. The source free particle displacement elastic wave equations can be expressed as,

$$(\lambda + \mu)\nabla(\nabla \cdot \mathbf{u}) + \mu(\nabla \cdot \nabla)\mathbf{u} = \rho \partial_t^2 \mathbf{u} \quad , \quad (1)$$

where the $\mathbf{u} = (u_1, u_2, u_3)$ is the particle displacement vector of the wavefield, λ and μ are the Lamé coefficients and ρ is the density of the media (Aki and Richards, 1980). The second order partial derivative with respect to time is given by ∂_t^2 . It is assumed that readers are familiar with the basics of tensor algebra, like the subscript ", " for derivatives and Einstein summation convention so that eq. (1) may be written as

$$(\lambda + \mu)u_{j,ji} + \mu u_{i,jj} = \rho \ddot{u}_i \quad (i, j = 1, 2, 3) \quad , \quad (2)$$

where u_i^2 is equivalent to $\delta_i^2 u_i$. Eq. (2) is defined in a Cartesian coordinate system where the coordinates are denoted as x_i , $i = 1, 2, 3$. In the PML implementation, one introduces an analytic continuation of spatial variables d crossing the PML zone, where $d > 0$ controls the decay rates in the PML. In this paper we use a cubic function define as $d(l) = \sigma^{\max}[(h - l + 1)/h]^3$, where h is the number of grid points for the PML, l is the current grid number. The effect of PML may be understood as a complex coordinate stretching system transforming propagating waves into decaying waves, defined as

$$x'_i = x_i - [\sqrt{(-1)/\omega}] \int_0^{x_i} d(s) ds \quad , \quad (3)$$

from which it follows that

$$\partial x'_i / \partial x_i = \alpha_{ii'} = \begin{cases} 1 - [\sqrt{(-1)/\omega}] d(x_i), & \text{for } i' = i \\ 0 & , \text{ otherwise} \end{cases} \quad (4)$$

and

$$\partial x_i / \partial x'_i = \alpha_{i'i} = \begin{cases} \sqrt{(-1)\omega} / [\sqrt{(-1)\omega} + d(x_i)], & \text{for } i' = i \\ 0 & , \text{ otherwise} \end{cases}$$

where the i' denotes the index of the new coordinates. It will be convenient to introduce the quantity $\beta_{i'i}$, defined as

$$\beta_{i'i} = \alpha_{i'i} - \delta_{i'i} = \begin{cases} d(x_i) / [i\omega + d(x_i)], & \text{for } i' = i \\ 0 & , \text{ otherwise} \end{cases} \quad (5)$$

where $\delta_{i'i}$ is the Kronecker delta function.

With eq. (4), the gradient operator in the new coordinate system is

$$\nabla' = \alpha_{i'i} - \partial_i \mathbf{e}_{i'} \quad , \quad i' = 1, 2, 3 \quad (6)$$

with $\mathbf{e}' = (\mathbf{e}_1', \mathbf{e}_2', \mathbf{e}_3')$ being the basis vectors in the new coordinate system.

By transforming eq. (1) into the frequency domain and then replacing the gradient operator using eq. (6), we obtain the following equation for the PML.

$$(\lambda + \mu) \nabla' (\nabla' \cdot \hat{\mathbf{u}}) + \mu (\nabla' \cdot \nabla') \hat{\mathbf{u}} = -\rho \omega^2 \hat{\mathbf{u}} \quad , \quad (7)$$

where $\hat{\mathbf{u}}$ denotes the displacement vector after the application of a Fourier time transform.

We introduce two auxiliary variables $\hat{p}_{i'}$ and $\hat{q}_{i'j}$ (see the Appendix) which play key roles in our non-split PML algorithm:

$$\hat{p}_{i'} = \beta_{i'j} \hat{u}_{i,j} \quad , \quad (8.1)$$

$$\hat{q}_{i'j} = \beta_{i'k} \delta_k (\hat{u}_{i,j} + \hat{p}_{ij}) \quad . \quad (8.2)$$

Eqs. (8.1) and (8.2) are defined in the frequency domain. Applying an inverse Fourier time transform to these two equations and incorporating eq. (5), we have

$$-d(x_i)u_{j,i} = -d(x_i)p_{ji} = \dot{p}_{ji} \quad , \quad (9.1)$$

$$-d(x_i)(u_{k,ji} + p_{kj,i}) - d(x_i)q_{kij} = \dot{q}_{kij} \quad . \quad (9.2)$$

Substituting eqs. (6), (8.1) and (8.2) into eq. (7), yields

$$(\lambda + \mu)(\hat{u}_{j,ji} + \hat{p}_{jj,i} + \hat{q}_{jj}) + \mu(\hat{u}_{i,jj} + \hat{p}_{ij,j} + \hat{q}_{ijj}) = -\rho\omega^2\hat{u}_i \quad . \quad (10)$$

Detailed derivations of the above are given in the Appendix. After applying the inverse Fourier time transform to eq. (10), we have the final equation for the non-split PML in the time domain:

$$(\lambda + \mu)(u_{j,ji} + p_{jj,i} + q_{jj}) + \mu(u_{i,jj} + p_{ij,j} + q_{ijj}) = \rho\ddot{u}_i \quad . \quad (11)$$

Combining with eqs. (9) and (11), we get the non-split PML formula for second-order elastic wave equations. Solving eq. (11) also requires the determination of the auxiliary variables p_{ij} and q_{ijk} in eqs. (9.1) and (9.2). It should be noted that eqs. (9.1) and (9.2) reduce to the original elastic wave, eq. (2), if both p_{ij} and q_{ijk} are set to zero.

For the acoustic wave equation, we can set $(\lambda + \mu) = 0$ and $\mu/\rho = V_p^2$ in eq. (11) to obtain the non-split PML formulae:

$$-V_p^2(u_{i,jj} + p_{ij,j} + q_{ijj}) = \rho u_i \quad . \quad (12)$$

For the acoustic case, the vector \mathbf{u} only has one component as acoustic pressure. We only evaluate $i = 1$ in eq. (12). The equation for the auxiliary variable is the same as eqs. (9). However, we will only consider the reduced system within eqs. (9.1) and (9.2). As shown in eq. (12), we only need to evaluate $p_{ij,j} = p_{11,1} + p_{12,2} + p_{13,3}$. Other terms shown in eq. (9.1) do not need to be calculated for the acoustic case. It is the same for evaluation the auxiliary variable q_{ijj} in eq. (12), i.e., $q_{ijj} = q_{111} + q_{122} + q_{133}$.

For numerical implementation of the non-split PML, we use a forward difference scheme to update the auxiliary variables p_{ij} and q_{ijk} in eqs. (9.1) and (9.2). Then a central difference scheme is used to update the wavefield u_i in eq. (11). As non-splitting wavefield variables are introduced and the auxiliary variables are only computed in the PML domain, the computer memory burden for practical implementation of the PML can be much reduced.

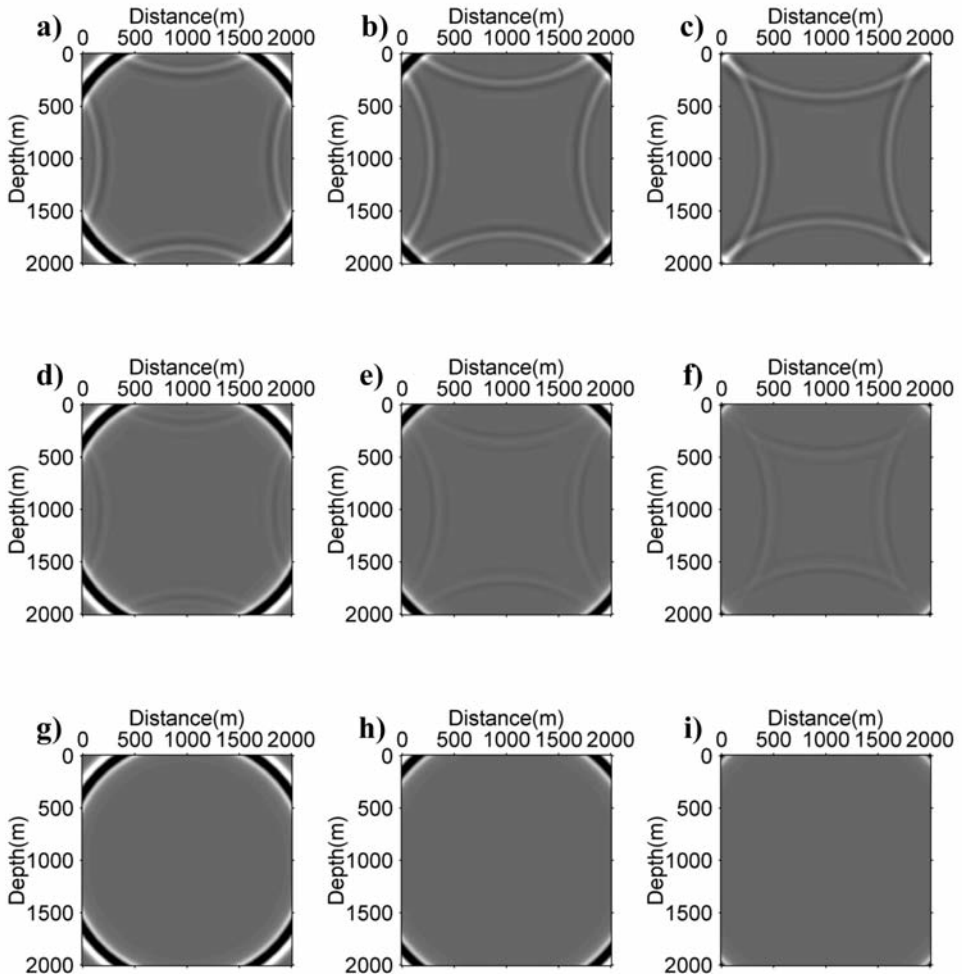


Fig. 2. Snapshots of the 2D homogeneous medium acoustic modeling wavefield by using different ABC at 550 ms, 600 ms and 650 ms, respectively. (a)-(c) are using Clayton A1 ABC; (d)-(f) are using Clayton A2 ABC; (g)-(i) are using the proposed non-split PML ABC.

NUMERICAL EXAMPLES

The first example is a 2D acoustic model with a constant velocity of 2500m/s. The size of the model is 201 grid points in depth, and 201 grid points in the horizontal direction. The vertical and horizontal grid steps are both 10 m. The 15 Hz Ricker wavelet point source is placed at ($z = 1000$ m, $x = 1000$ m). The receiver depth is 1000 m. The time step is 1 ms for computation. We have ABC at each of the four boundaries and evaluate the performance of the proposed non-split PML method by comparing it with the Clayton-A1 ABC and Clayton-A2 ABC proposed by Clayton and Engquist [1977, eqs. (8) and (9)]. The number of grid points for ABC is set the same at 10. Fig. 2 shows the snapshots of the wavefield, at times $t = 350$ ms, 500 ms and 650 ms. Fig. 2 (a-c) is for the Clayton-A1, (d-f) is for Clayton-A2, and (g-i) is for the proposed

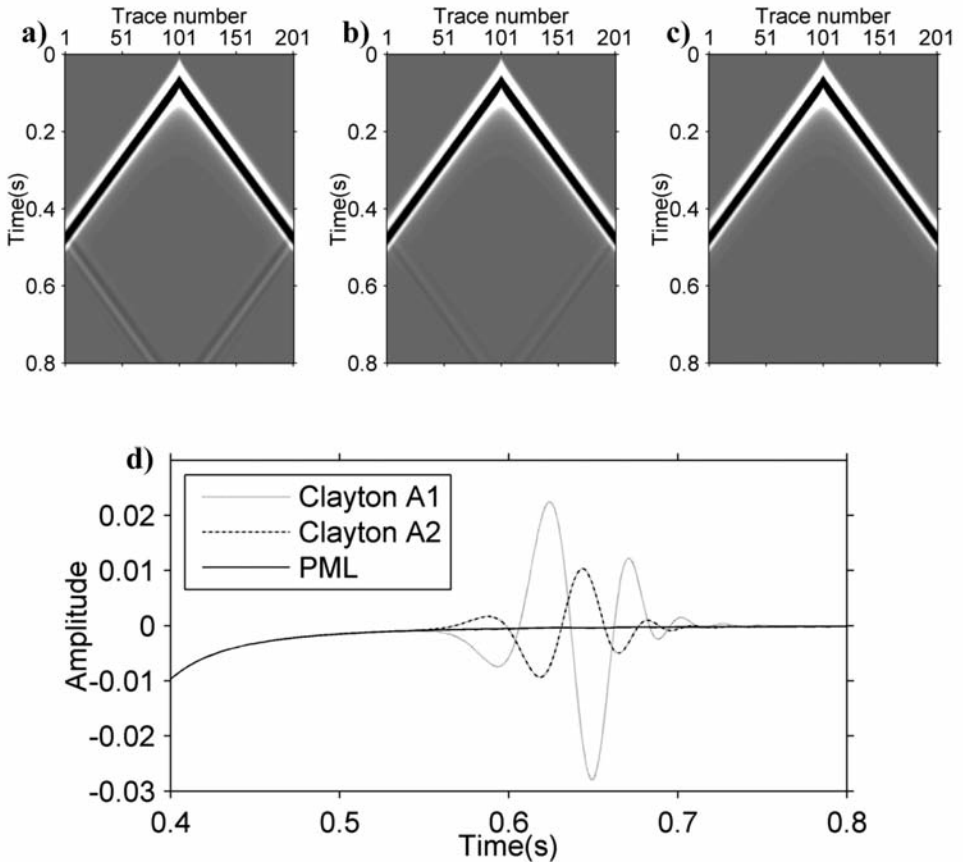


Fig. 3. Shot records of the 2D homogeneous medium acoustic modeling by using different ABC. (a) Clayton-A1. (b) Clayton-A2. (c) proposed non-split PML. (d) Zoomed plot of the 41-th trace extracted from (a), (b) and (c) with time from $t = 0.4$ to $t = 0.8$ s, respectively.

non-split PML ABC. It can be seen from the figures that the PML achieves the best results where no visible reflections occur near the boundary. Fig. 3 (a) shows the shot records for each ABC and Fig. 3 (b) shows the zoomed 41-th trace extracted from Fig. 3 (a-c) in the time range from $t = 0.4$ to $t = 0.8$ s, respectively.

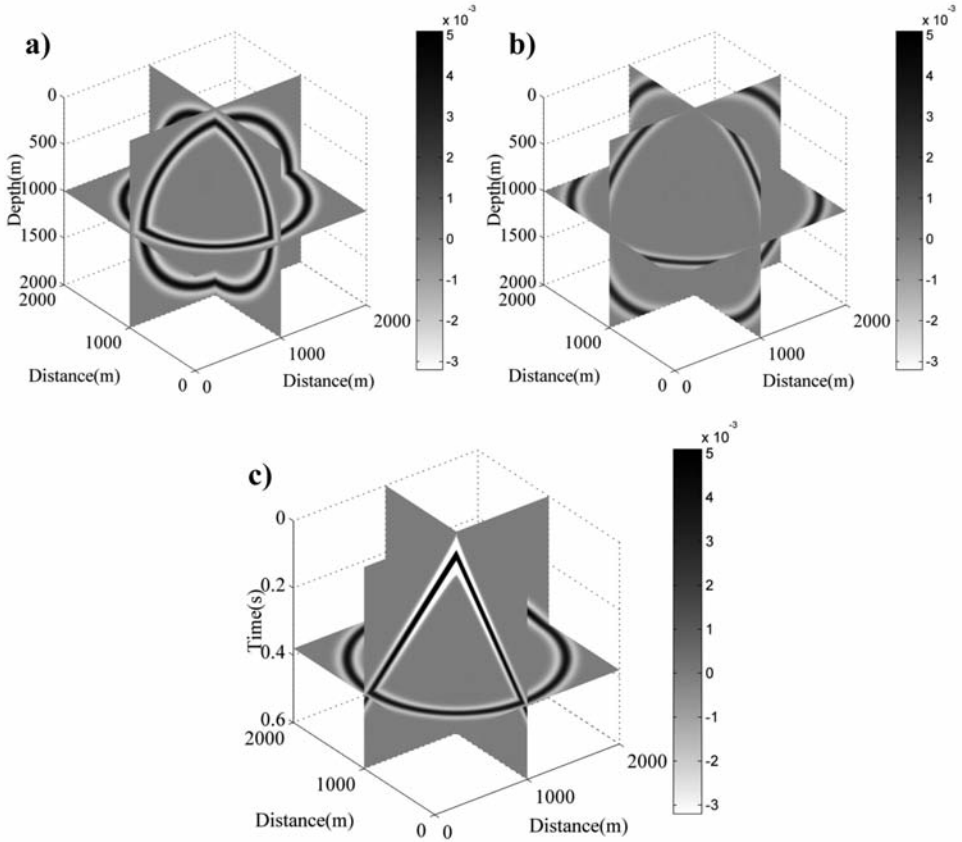


Fig. 4. Snapshots and shot records of 3D homogeneous medium forward modeling. The proposed non-split PML has been used in all boundaries. (a) and (b) show snapshots slices at time $t = 350$ ms and $t = 450$ ms; c) shows the shot records slices.

The second example is for a 3D acoustic media with constant velocity of 3000 m/s. The grid points of all three directions are 201, with a step of 10 m. The calculation time is up to 0.6 s with a time step of 1 ms. The 15 Hz Ricker wavelet is placed at grid ($z = 1000$ m, $x = 1000$ m, $y = 1000$ m). The depth of the receivers is 1000 m. We apply the proposed non-split PML at all boundaries. The number of grid points for the PML is 10. Fig. 4 (a-b) shows snapshots slice at times $t = 350$ ms and $t = 450$ ms. Fig. 4 (c) shows slices of shot records.

We apply the non-split PML ABC to the elastic model in the third example. The model is a constant velocity model with $V_p = 4000$ m/s and $V_s = 3000$ m/s. The vertical and horizontal grid numbers are 201 and 401, respectively, and the grid spacing is 10 m. We have a 15 Hz point source Ricker wavelet placed at ($z = 1000$ m, $x = 2000$ m). The time step is 1 ms and the number of grid points for the ABC is set to be 20. Figs. 5(a) and 5(b) show the snapshots of the vertical component of the displacement vector at 300 ms and 500 ms, respectively. The PML also appears to behave very well for the elastic case.

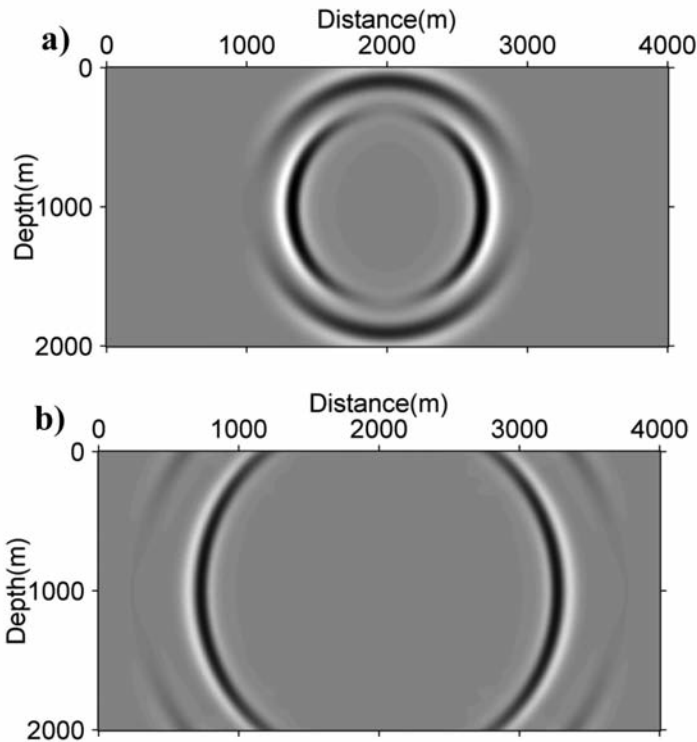


Fig. 5. Snapshots of the vertical component in elastic model at different time: (a) 300 ms; (b) 500 ms.

CONCLUSIONS

In this paper, we proposed a non-split PML formula for the second-order wave equation modeling. The main idea is based on augmented variable substitution. We evaluated the proposed methods with both acoustic and elastic wave equation modeling. The results verified the performance of the proposed PML method in comparison with the conventional Clayton ABC methods. In addition, the proposed method avoids wavefield splitting, which simplifies the practical applications and also saves memory storage space.

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APPENDIX

NON-SPLIT PML FORMULATION DERIVATION

In this Appendix, we provide an alternate form of eq. (1) by substituting eqs. (8.1) and (8.2) into eq. (7). Using eq. (5) the gradient operator, eq. (6), in the new coordinate system can be written as

$$\nabla' = \alpha_{i'i} \partial_i \mathbf{e}_{i'} = (\delta_{i'i} + \beta_{i'i}) \partial_i \mathbf{e}_{i'} \quad . \quad (\text{A-1})$$

The above definition is then introduced into the left hand side of eq. (7) to obtain

$$\begin{aligned} & (\lambda + \mu) \nabla' (\nabla' \cdot \hat{\mathbf{u}}) + \mu (\nabla' \cdot \nabla') \hat{\mathbf{u}} = L_1 + L_2 \\ & = (\lambda + \mu) (\delta_{i'i} + \beta_{i'i}) \partial_i \mathbf{e}_{i'} [(\delta_{j'j} + \beta_{j'j}) \partial_j \mathbf{e}_{j'} \cdot (\mathbf{u}_{k'} \mathbf{e}_{k'})] \\ & + \mu \mathbf{e}_{i'} \cdot (\delta_{i'i} + \beta_{i'i}) \partial_i [\mathbf{e}_{i'} (\delta_{j'j} + \beta_{j'j}) \partial_j (\mathbf{u}_{k'} \mathbf{e}_{k'})] \quad . \end{aligned} \quad (\text{A-2})$$

where

$$\begin{aligned} L_1 & = (\lambda + \mu) (\delta_{i'i} + \beta_{i'i}) \partial_i \mathbf{e}_{i'} [(\delta_{k'j} + \beta_{k'j}) \hat{u}_{k,j}] \\ & = (\lambda + \mu) (\delta_{i'i} + \beta_{i'i}) \mathbf{e}_{i'} \partial_i (\hat{u}_{j,j} + \beta_{k'j} \hat{u}_{k,j}) \\ & = (\lambda + \mu) (\delta_{i'i} + \beta_{i'i}) \mathbf{e}_{i'} \partial_i (\hat{u}_{j,j} + \hat{p}_{k'k'}) \\ & = (\lambda + \mu) \mathbf{e}_{i'} \partial_i (\hat{u}_{j,j} + \hat{p}_{k'k'}) + (\lambda + \mu) \mathbf{e}_{i'} \beta_{i'i} \partial_i (\hat{u}_{j,j} + \hat{p}_{jj}) \\ & = (\lambda + \mu) \mathbf{e}_{i'} (\hat{u}_{j,ji} + \hat{p}_{jj,i}) + (\lambda + \mu) \mathbf{e}_{i'} \hat{q}_{jij} \\ & = [(\lambda + \mu) (\hat{u}_{j,ji} + \hat{p}_{jj,i} + \hat{q}_{jij})] \mathbf{e}_{i'} \quad . \end{aligned} \quad (\text{A-3})$$

In the third and fifth lines of eq. (A-3), we have introduced eqs. (8.1) and (8.2), respectively.

Proceeding in a manner similar to the above equation, we have

$$\begin{aligned} L_2 & = \mu (\delta_{i'i} + \beta_{i'i}) \partial_i [(\delta_{i'j} + \beta_{i'j}) (\hat{u}_{k',j} \mathbf{e}_{k'})] \\ & = \mu (\delta_{i'i} + \beta_{i'i}) \partial_i (\hat{u}_{k',i'} \mathbf{e}_{k'} + \beta_{i'j} \hat{u}_{k'j} \mathbf{e}_{k'}) \\ & = \mu (\delta_{i'i} + \beta_{i'i}) \partial_i (\hat{u}_{k',i'} + \hat{p}_{k'i'}) \mathbf{e}_{k'} \end{aligned}$$

$$\begin{aligned}
&= \mu \partial_{i'} (\hat{u}_{k',i'} + \hat{p}_{k',i'}) \mathbf{e}_{k'} + \mu \beta_{i'i} \partial_i (\hat{u}_{k',i'} + \hat{p}_{k',i'}) \mathbf{e}_{k'} \\
&= \mu (\hat{u}_{i,jj} + \hat{p}_{ij,j} + \hat{q}_{jij}) \mathbf{e}_i .
\end{aligned} \tag{A-4}$$

Combining the last lines of the formulae in eqs. (A-3) and (A-4) results in

$$\begin{aligned}
&(\lambda + \mu) \nabla' (\nabla' \cdot \hat{\mathbf{u}}) + \mu (\nabla' \cdot \nabla') \hat{\mathbf{u}} \\
&= [(\lambda + \mu) (\hat{u}_{j,ji} + \hat{p}_{jj,i} + \hat{q}_{jij}) + \mu (\hat{u}_{i,jj} + \hat{p}_{ij,j} + \hat{q}_{jij})] \mathbf{e}_i .
\end{aligned} \tag{A-5}$$

This is just the left hand side of eq. (10) in vector form.