PML absorbing boundary condition for structure-preserving seismic wave modeling

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Abstract. Some efficient structure preserving algorithms have been proposed for high precision seismic exploration and detection in recent years. However, feasible artificial boundary conditions to truncate unbounded medium are never discussed in structure preserving seismic modeling. We pay our emphasis on application of perfectly matched layer absorbing boundary condition (PML ABC) to fit the structure preserving algorithms. In the domain of interest, a typical structure preserving algorithm is presented to discretize the conservative dynamic system, while in the PML region, traditional central difference is applied to solve the dissipative system. In the adjacent region of the interior and exterior domains, the temporary values of wave field between two time steps are approximated by interpolation using the present and the updated value of the wave fields in the PML region. A numerical experiment is adopted to demonstrate compatibility of the algorithms and no visible reflections of outgoing waves occur on the edge of interior domain.

1. Introduction
High-precision and long-term seismic wave modeling becomes increasingly important for seismic exploration and seismological research. Sometimes, one needs to investigate seismic waveform after millions of time steps for large scale seismic migration and detection. Structure-preserving algorithms [1,2], which can preserve some properties of dynamic system, have significant capacity for these special requirements. These structure-preserving methods (e.g. symplectic methods) have been discussed widely in some articles. So far valid artificial boundary conditions, especially perfectly matched layer absorbing boundary condition (PML ABC) has never been discussed for those structure preserving methods [3,4].

Here we contribute our effort to implement PML absorbing boundary to absorb the outgoing waves in modeling by symplectic schemes. The 2nd-order form of PML ABC is formulated. To calculate the derivatives of the conservative ordinary differential equations near the interfaces of interior region, we use linear interpolation methods to approximate the values of displacement field on non-integer time nodes by virtue of the present and updated wave fields in the PML region.

A numerical experiment was presented to demonstrate the efficiency of the PML ABC. Results show that the energy of seismic wave preserves well when wave propagates in the domain of interest and no obvious artificial reflections occur.
2. Theory

First-order PML ABC has been fully discussed in past literatures, while the corresponding 2nd-order PML ABC has had little attention. Here, the 2nd-order PML ABC formulated in displacement is discussed, and a new method to split PML ABC equations into fewer terms than the method presented by Komatitsch [4] is proposed.

In heterogeneous medium, the formulation of wave equation in Cartesian coordinates has the following form in frequency domain:

\[-\rho \omega^2 \ddot{\textbf{u}} = \frac{1}{2} \nabla \cdot \left[ \nabla \ddot{\textbf{u}} + \left( \nabla \ddot{\textbf{u}} \right)^T \right] \tag{1}\]

Where \(\rho\) is the density, \(\omega\) is the frequency, \(\ddot{\textbf{u}}\) is the displacement solution, \(\mathbf{C}\) is the 4th-order elastic coefficients tensor.

In exterior domain, considering the gradient operator can be expressed into two parts: the vertical component \(\nabla^v\) and the parallel component \(\nabla^p\), equation (1) in the exterior can be written as

\[-\rho \omega^2 \ddot{\textbf{u}} = \frac{1}{2} \left( \nabla^v \cdot \mathbf{C} \left[ \nabla^v \ddot{\textbf{u}} + \left( \nabla^v \ddot{\textbf{u}} \right)^T \right] + \nabla^v \cdot \mathbf{C} \left[ \nabla^p \ddot{\textbf{u}} + \left( \nabla^p \ddot{\textbf{u}} \right)^T \right] \right) + \nabla^p \cdot \mathbf{C} \left[ \nabla^v \ddot{\textbf{u}} + \left( \nabla^v \ddot{\textbf{u}} \right)^T \right] + \nabla^p \cdot \mathbf{C} \left[ \nabla^p \ddot{\textbf{u}} + \left( \nabla^p \ddot{\textbf{u}} \right)^T \right] \] \tag{2}

The PML is introduced by an analytic continuation of spatial variables to the complex-variable domain such that

\[\frac{\partial}{\partial \beta_p} = \frac{i \omega}{\omega + d(\rho)} \frac{\partial}{\partial \rho},\] \tag{3}

For \(\rho = x, y, z\) where

\[\beta_p = \rho - \frac{i}{\omega} \int_0^\rho d(s)ds,\] \tag{4}

In which \(d(s)\) is a frequency-independent loss coefficient. Substituting equations (3) and (4) into equation (2), it becomes:

\[-\rho \omega^2 \ddot{\textbf{u}} = \frac{1}{2} \left( \nabla^v \cdot \mathbf{C} \left[ \nabla^v \ddot{\textbf{u}} + \left( \nabla^v \ddot{\textbf{u}} \right)^T \right] \right) \left( \frac{\partial \rho}{\partial \beta_p} \right)^2 + \frac{1}{2} \left( \nabla^v \cdot \mathbf{C} \left[ \nabla^v \ddot{\textbf{u}} + \left( \nabla^v \ddot{\textbf{u}} \right)^T \right] \right) \left( \frac{\partial \rho}{\partial \beta_p} \right) \left( \frac{\partial \rho}{\partial \beta_p} \right)^2 + \frac{1}{2} \left( \nabla^p \cdot \mathbf{C} \left[ \nabla^v \ddot{\textbf{u}} + \left( \nabla^v \ddot{\textbf{u}} \right)^T \right] \right) \left( \frac{\partial \rho}{\partial \beta_p} \right) + \frac{1}{2} \left( \nabla^p \cdot \mathbf{C} \left[ \nabla^p \ddot{\textbf{u}} + \left( \nabla^p \ddot{\textbf{u}} \right)^T \right] \right) \left( \frac{\partial \rho}{\partial \beta_p} \right) + \frac{1}{2} \left( \nabla^p \cdot \mathbf{C} \left[ \nabla^p \ddot{\textbf{u}} + \left( \nabla^p \ddot{\textbf{u}} \right)^T \right] \right) \] \tag{5}

The components of displacement are split into three parts by introducing intermediate variable, and converting back to the time domain, the following equation is obtained:

\[\rho \left( \partial_{\tau} + d \right)^2 \textbf{u}_i = \frac{1}{2} \left( \nabla^v \cdot \mathbf{C} \left[ \nabla^v \textbf{u} + \left( \nabla^v \textbf{u} \right)^T \right] \right) + \textbf{P},\]

\[\left( \partial_{\tau} + d \right) \textbf{P} = \frac{d}{2} \nabla^v \cdot \mathbf{C} \left[ \nabla^v \textbf{u} + \left( \nabla^v \textbf{u} \right)^T \right],\] \tag{6}

\[\partial_{\tau} \left( \partial_{\tau} + d \right) \textbf{u}_i = \frac{1}{2} \left( \nabla^p \cdot \mathbf{C} \left[ \nabla^p \textbf{u} + \left( \nabla^p \textbf{u} \right)^T \right] \right) + \nabla^p \cdot \mathbf{C} \left[ \nabla^v \textbf{u} + \left( \nabla^v \textbf{u} \right)^T \right],\]

\[\partial_{\tau}^2 \textbf{u}_i = \frac{1}{2} \nabla^p \cdot \mathbf{C} \left[ \nabla^p \textbf{u} + \left( \nabla^p \textbf{u} \right)^T \right].\]
As is well-known, seismic wave propagating in the PML domain decays exponentially. By coordinate transformation, suppose the interface is perpendicular to x-axis, and the solution in PML domain can be written as

$$ u = u_0 \exp(\omega t - ik_x x - ik_y y - ik_z z) \exp(-\frac{k_x}{\omega} \int_0^t d(s) ds), $$

Where $L$ is the thickness of the PML region.

Various methods are available for spatial discretization for equations (1) and (6), the optimal convolution differentiator operator developed by Liu et al(2013) for spatial discretization is used here. The discretized equations (1) and (6) can be written as in a general form

$$ (\partial_t + d)^2 \rho U = DU - P, $$

$$ (\partial_t + d) P = D'U, $$

Where $D$ and $D'$ are operators for spatial discretization. In the interior region, there are $d = 0$, $P = 0$ and $D' = 0$ (conservative system); while in the PML region, there are $d \neq 0$, $P \neq 0$ and $D' \neq 0$ (dissipative system). After discussing the temporal discretization schemes for equation (8), one can use the PML ABC for this scheme.

Symplectic algorithm does not exist for dissipative system, so we have to use non-symplectic schemes such as the central difference method for the discretization of equation (7) in PML domain, which achieves 2nd-order accuracy, and we get

$$ \frac{U^{n+1} - 2U^n + U^{n-1}}{\Delta t^2} + d \frac{U^{n+1} - U^{n-1}}{\Delta t} + d^2 U^n = \frac{1}{\rho} (DU^n - P^n), $$

$$ \frac{P^{n+1} - P^{n-1}}{2\Delta t} + dP^n = D'U^n. $$

We find an approach that we update the displacement in the PML domain earlier than in the interior domain, then approximate the intermediate displacements by interpolation method. The intermediate displacements in the PML domain can be written as

$$ u_1^n = u^n + c_1 \Delta t (u^{n+1} - u^n), $$

$$ u_2^n = u^n + c_2 \Delta t (u^{n+1} - u^n), $$

$$ u_3^n = u^n + c_3 \Delta t (u^{n+1} - u^n). $$

3. Examples

In this section, an example is designed to demonstrate that the PML ABC is suitable for absorbing the outgoing waves. The profile of the homogeneous model is as shown in Figure 1. The model size is 4000 m × 4000 m, the spatial step is 10 m in both directions, and time step is 0.5 ms. An explosive source, which is a Ricker wavelet with dominant frequency of 30 Hz, is located at the center of the model. Two receivers are placed at the points (3800 m, 2000 m) and (3800 m, 200 m), respectively. In the numerical calculation, the model parameters are $V_p = 3000$ m/s, $V_s = 1732$ m/s and $\rho = 2000$ kg/m$^3$. Two numerical methods, RKN method and Newmark method [5] are used to demonstrate the validity of our algorithm. The PML region has 20 cells.

Figure 2 shows that the waveforms generated by these two methods are all most the same, and no obvious reflected waveforms from the edge can be found in this figure. The Newmark method we used is an algorithm for conservation of total energy. It is obviously that these two methods are comparable in short-term seismic modeling, but the performances of RKN are far superior to Newmark method in long-term calculation [1]. However, we only demonstrate the validity of PML ABC works in structure-preserving seismic modeling here. Figure 3 illustrates that if boundary condition is not dealt correctly (e. g., stiff boundary condition is implemented), the reflected waves are quite strong.
Figure 1. 2-D homogeneous medium model: configuration and parameters. The source is located at the centre of model; two receivers are placed very close to the right edge of the model.

Figure 2. The seismic waveform records of R1 (a) and R2 (b). The solid lines are generated by RKN method; the dotted lines are generated by Newmark method.

Figure 3. Snapshots of wavefield of horizontal component at t=0.4s modelled by symplectic RKN method; (a) PML ABC is implemented; (b) stiff boundary condition is implemented.
4. Conclusion
A new method to implement the PML ABC to absorb the outgoing waves modeled by structure-preserving method is presented by introducing displacement field interpolation method, and the 2nd-order PML ABC formulas is reformulated for dynamic equation in terms of displacement. The validity of PML ABC is also demonstrated by an experiment. The results hold the promise that this kind of PML ABC works well not only for homogeneous model but also for heterogeneous case. The PML ABC is also suitable for structure-preserving SEM or FEM in seismic wave simulations.

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