Convolutional and Non-convolutional PMLs for High-order Schemes Optimized at Grazing Incidence for the Seismic Wave Equation
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Introduction

The Perfectly Matched Layer absorbing boundary condition has proven to be very efficient from a numerical point of view for the elastic wave equation to absorb both body waves with non-grazing incidence and surface waves. However, at grazing incidence the classical discrete Perfectly Matched Layer suffers from large spurious reflections that make it less efficient for instance in the case of very thin mesh slices, in the case of sources located very close to the edge of the mesh, and/or in the case of receivers located at very large offset. Suitable high order time-stepping algorithms are also necessary particularly when high order spatial integration are introduced. In Komatitsch and Martin (2007) we improved the Perfectly Matched Layer at grazing incidence for the seismic wave equation based on an unsplit convolution technique. The results are significantly improved compared with the classical Perfectly Matched Layer technique. But as with the classical model, this technique is intrinsically unstable in the case of some anisotropic materials. In this case, retaining an idea of Meza-Fajardo and Papageorgiou (2008), it can been stabilized by adding correction terms along the other coordinate axes, as implemented by Martin et al. (2008b) for a spectral-element method based on a hybrid first/second order time integration scheme. Unfortunately the Perfectly Matched character of the method is then lost. A Newmark time marching scheme allows us to match perfectly at the base of the absorbing layer a velocity-stress formulation in the PML and a second order displacement formulation in the inner computational domain. Our CPML unsplit formulation has the advantage to reduce the memory storage of CPML by 40% in 2D comparing to the GFPML split formulation of Festa and Vilotte (2005) and by around 70% in viscoelastic cases. We also applied the CPML technique based on a fourth-order staggered finite-difference method to more complex models such as Biot dissipative/non-dissipative poroelastic (Martin et al., 2008a) or viscoelastic (Martin and Komatitsch, 2009) media.

These unsplit CPMLs are usually computed based on a second-order finite-difference time scheme. However, in many situations such as very long time simulations, it is of interest to increase the accuracy of the method by increasing the order of the time marching scheme and of the spatial discretization. The CPML cannot be easily extended to high order because of its convolution formulation. In Martin et al. (2010) we thus study how to design a new unsplit PML (called ADE-PML/Auxiliary Differential Equations PML) that remains optimized at grazing incidence but that can accommodate a high-order time scheme. At second order in time we demonstrate that CPML and ADE-PML are equivalent and that all the advantages of CPML, for instance in terms of memory storage reduction, are preserved. At both second and higher order discretization in time, solutions can be obtained with very good accuracy.

New PML formulations

Let us compare different formulations and discretizations of the elastodynamics equation and show the equivalence between CPML and the non-convolutional ADE-PML for a second-order time discretization. This will also allow us to derive a high-order time-advancement scheme for the ADE-PML.

The elastodynamics equation written as a first-order system in velocity vector and stress tensor is :

$$\begin{aligned} \rho \frac{\partial v_i}{\partial t} &= \frac{\partial \sigma_{ij}}{\partial x_j} + s_i \\ \frac{\partial \sigma_{ij}}{\partial t} &= \lambda \varepsilon_{kk} \delta_{ij} + 2\mu \varepsilon_{ij} \, , \end{aligned} \qquad (1)$$

where $\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial v_j}{\partial x_i} + \frac{\partial v_i}{\partial x_j}\right)$ is the velocity strain tensor, v_i are the components of the velocity vector, σ_{ij} the components of the stress tensor, s_i are the components of the (known) source force vector, ρ is the density and λ and μ are the Lamé parameters. As in the construction of a classical PML or a Convolution PML, the spatial derivatives along the axis perpendicular to the PML layer, say x, are rewritten in a stretched coordinate $\tilde{x}$, based on (see e.g. Komatitsch and Martin (2007)):

$$\partial_{\tilde{x}} = \frac{1}{s_x}\partial_x \tag{2}$$

where

$$s_x = \kappa_x + \frac{d_x}{\alpha_x + i\omega}. \tag{3}$$

Then, following Komatitsch and Martin (2007), we can express:

$$\frac{1}{s_x} = \frac{1}{\kappa_x} - \frac{d_x}{\kappa_x^2}\frac{1}{(d_x/\kappa_x + \alpha_x) + i\omega} \tag{4}$$

where $d_x = d_0\left(\frac{x}{L}\right)^N$ is the damping profile, κ_x is a polynomial acting as a stretching of the mesh and α_x is a polynomial that acts as a shift in the frequency domain or a Butterworth-like filter. The choice of the different parameters involved in these functions allows a good or bad absorption of the waves at the outer boundaries. By sake of simplicity we will study the term $\partial_x\sigma_{xy}$, keeping in mind that similar formulations are derived for the x and y derivatives of v_x, v_y, σ_{xx} and σ_{yy} in 2D when PML layers are present along both axes of the grid. The derivative $\partial_x\sigma_{xy}$ is transformed into

$$\frac{1}{s_x}\partial_x\sigma_{xy} = \frac{1}{\kappa_x}\partial_x\sigma_{xy} - \frac{d_x}{\kappa_x^2}\frac{1}{(d_x/\kappa_x + \alpha_x) + i\omega}\partial_x\sigma_{xy}. \tag{5}$$

Let us denote $Q_x^{\sigma_{xy}}$ the auxiliary memory variable associated with $\partial_x\sigma_{xy}$, i.e.:

$$Q_x^{\sigma_{xy}} = -\frac{d_x}{\kappa_x^2}\frac{1}{(d_x/\kappa_x + \alpha_x) + i\omega}\partial_x\sigma_{xy}\,, \tag{6}$$

which leads to

$$\left(\frac{d_x}{\kappa_x} + \alpha_x + i\omega\right)Q_x^{\sigma_{xy}} = -\frac{d_x}{\kappa_x^2}\partial_x\sigma_{xy}. \tag{7}$$

Written in the time domain this equation becomes

$$\partial_t Q_x^{\sigma_{xy}} + \left(\frac{d_x}{\kappa_x} + \alpha_x\right)Q_x^{\sigma_{xy}} = -\frac{d_x}{\kappa_x^2}\partial_x\sigma_{xy} \tag{8}$$

After discretization at the second order in time it can be shown that the above non-convolution Auxiliary Differential Equation (ADE) formulation of equation (8) is equivalent to the convolution CPML discretization of Komatitsch and Martin (2007). But the advantage of the ADE-PML formulation is that it can be extended to a higher-order time scheme.

Examples

Let us discretize the memory variable equations with high accuracy using a fourth-order time scheme for instance. The Q memory terms are updated at the same time as the velocity and stress components in each inner loop of the time cycle. Simulations are performed using a 8th-order space-discretization. In Figure 1 we show snapshots of wave propagation in a homogeneous thin slice at different times. No spurious modes propagate back into the main domain. Figure 2 shows comparisons between a reference solution and high order semi-implicit and explicit solutions at the third receiver located far from the source. At the three receivers, high order simulations are far more accurate than the second order ADE-PML or CPML solutions which exhibit large discrepancies in terms of amplitude and spurious waves with larger errors at all the receivers, particularly at receiver #3 which is located at large offset far from the source and for which spurious waves have time to develop at grazing incidence. An important

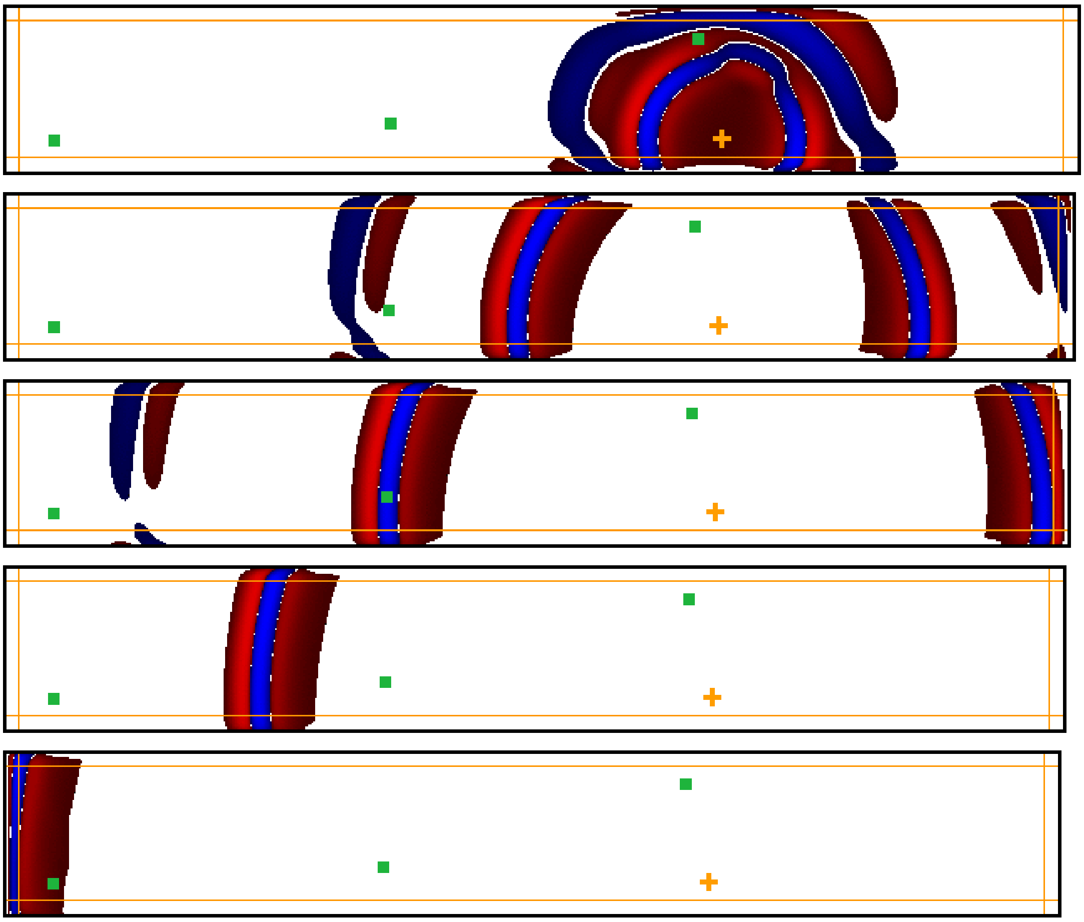

Figure 1 *Snapshots of the horizontal component of the velocity vector in a homogeneous medium for a thin slice with high order PML conditions implemented on its four sides, at time 0.4 s (top), 0.8 s, 1.6 s and 2.4 s (bottom). We represent it in red (positive) or blue (negative) when it has an amplitude higher than a threshold of 1% of the maximum. The orange cross indicates the location of the source and the green squares the position of receivers at which seismograms are recorded. The four vertical or horizontal orange lines represent the edge of each PML layer. No spurious wave of significant amplitude is visible, even at grazing incidence. The snapshots have been rotated by 90° to fit on the page.*

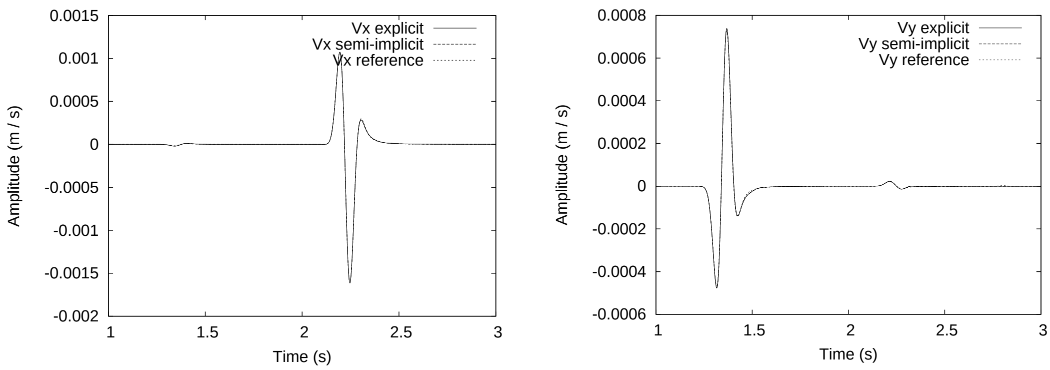

Figure 2 *High-order (fourth-order in time and eighth-order in space) PML solution, using explicit or semi-implicit implementations, for the horizontal (left column) and vertical (right column) component of the velocity vector recorded at the third receiver located at large offset far from the source. At this specific receiver the agreement with a reference solution (dotted line) is good in spite of the grazing incidence and only tiny spurious oscillations are observed, which is difficult to obtain. These solutions are very similar and are more accurate than the second-order solution*

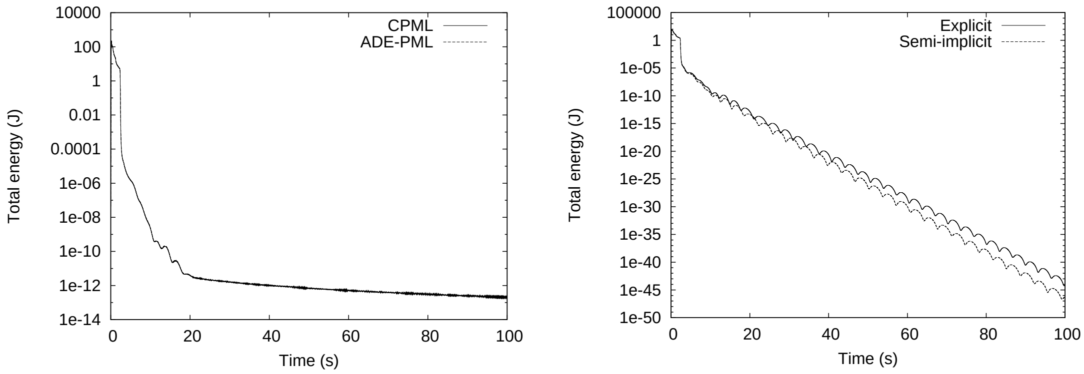

***Figure 3** (Left): Decay with time of total energy in semi-logarithmic scale for the homogeneous elastic medium modeled for long time periods, up to 100 s of simulation for the second-order CPML (dashed line) and second-order ADE-PML (solid line). Both energy curves are superimposed, which illustrates the equivalence of the two formulations. No instabilities appear even at long time periods. (Right): Energy decay for the same period and high order PML. No instabilities are observed in the explicit or semi-implicit solutions, which means that the discrete ADE-PML high order in time and space is stable up to 100,000 time steps. After 100 s total energy is 10^{-44} J in the explicit case and 10^{-46}J in the semi-implicit case, while it is around 10^{-13} J in the second-order case (top). The semi-implicit case seems to lead to faster decay of the energy in all cases by 30 orders of magnitude.*

issue to analyze when designing a perfectly matched layer is the numerical stability of the PML at long time periods. In Figure 3, for a simulation over 10^6 time steps, we observe that in the first 3 s the total energy of the system decays much faster by almost 20 orders of magnitude using high order PMLs than using second-order PML; and a semi-implicit scheme seems to ensure faster energy decay. Then, values around 10^{-44} J are reached, while in the case of the second-order PML total energy reaches values around 10^{-13} J at around 100 s.

Conclusions

We have demonstrated that at the second order the convolutional and non convolutional PMLs are equivalent. We have also shown that a high order non-convolutional PML can be implemented and improve the accuracy of the solution. We have also shown that the high-order technique is numerically stable at long time periods and that total energy is better absorbed by several tens of orders of magnitude compared to classical second-order formulations.

References

Festa, G. and Vilotte, J.P. [2005] The Newmark scheme as velocity-stress time-staggering: an efficient PML implementation for spectral-element simulations of elastodynamics. *Geophys. J. Int.*, **161**, 789–812, doi: 10.1111/j.1365-246X.2005.02601.x.

Komatitsch, D. and Martin, R. [2007] An unsplit convolutional Perfectly Matched Layer improved at grazing incidence for the seismic wave equation. *Geophysics*, **72**(5), SM155–SM167, doi:10.1190/1.2757586.

Martin, R. and Komatitsch, D. [2009] An unsplit convolutional perfectly matched layer technique improved at grazing incidence for the viscoelastic wave equation. *Geophys. J. Int.*, **179**(1), 333–344, doi:10.1111/j.1365-246X.2009.04278.x.

Martin, R., Komatitsch, D. and Ezziani, A. [2008a] An unsplit convolutional perfectly matched layer improved at grazing incidence for seismic wave equation in poroelastic media. *Geophysics*, **73**(4), T51–T61, doi:10.1190/1.2939484.

Martin, R., Komatitsch, D., Gedney, S. and Bruthiaux, E. [2010] A high-order time and space formulation of the unsplit perfectly matched layer for the seismic wave equation. *Comput. Model. Eng. Sci.*, submitted.

Martin, R., Komatitsch, D. and Gedney, S.D. [2008b] A variational formulation of a stabilized unsplit convolutional perfectly matched layer for the isotropic or anisotropic seismic wave equation. *Comput. Model. Eng. Sci.*, **37**(3), 274–304.

Meza-Fajardo, K.C. and Papageorgiou, A.S. [2008] A nonconvolutional, split-field, perfectly matched layer for wave propagation in isotropic and anisotropic elastic media; stability analysis. *Bull. Seismol. Soc. Am.*, **98**(4), 1811–1836.