Absorbing boundary conditions and perfectly matched layers in wave propagation problems

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Abstract. In this article we discuss different techniques to solve numerically wave propagation phenomena in unbounded domains. We present in a unified and simple way the two ways to restrict the computation to a finite domain: absorbing (or artificial) boundary conditions (ABC) and perfectly matched layers (PML). The intent is to give the possibility to the reader to grasp easily similarities and differences between these two truncation techniques. It should also allow the reader to adapt a truncation technique to the peculiarities of his physical modeling.

Keywords. artificial boundary condition, perfectly matched layer.

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1 Introduction

To model numerically a wave propagation phenomena in a domain which extends to infinity, it is common practice to truncate the computational domain to a finite domain. The newly formed external boundary is somewhat artificial. To reduce undesired numerical reflections, there is a need for a special treatment at these boundaries. The solution must be as close as possible to the restriction of the solution that would have been computed in the original physical infinite domain. The most commonly used grid truncation techniques are so-called ABC, Artificial (or Absorbing) Boundary Conditions, and perfectly matched layer, PML, formulations. ABC technique was first formalized by B. Engquist and E. Majda in a seminal 1977 paper in [7]. The PML concept was introduced by J.-P. Berenger in a 1994 paper, see [13]. ABC techniques are more general than PML. However, PML (which is an absorbing region rather than a boundary condition per se) can provide orders-of-magnitude lower reflections. Both methods are widely used in acoustic, electromagnetic or elastodynamic simulation software codes. Their precise formulations and efficiency depend strongly on the underlying partial differential equations that are discretized. For example, a stable and quite efficient PML for the non dissipative wave equation may surprisingly lead to unstable computations if used in conjunction with a damped wave equation. We present in this article, a unified and simple approach to the design and study of both ABC and PML formulations. The intent is to give the possibility to the reader to grasp easily similarities and differences between these two techniques. It should also allow the reader to adapt a truncation technique to the peculiarities of his physical modeling.

2 ABC

Homogeneous Dirichlet or Neumann boundary conditions for the wave equation lead to a total reflection of an impinging wave on the artificial boundary of a computational domain. We present here the method introduced by B. Engquist and A. Majda in 1977 (see [7]) to design absorbing conditions that are easy to implement and yield a small reflection coefficient on the truncation boundary. The wave equation is solved in a domain exterior to an open bounded subset Ω of $\mathbf{R}^2$ denoted by Ω^c :

$$\begin{aligned} \frac{\partial^2 u}{\partial t^2} - c^2 \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) &= f(t, x, y), \quad (x, y) \in \Omega^c, \quad t > 0 \\ u(0, x, y) &= u_0(x, y) \text{ in } \Omega^c \\ \frac{\partial u}{\partial t}(0, x, y) &= u_1(x, y) \text{ in } \Omega^c \\ u &= 0 \text{ on } \partial\Omega \\ u &\text{ satisfies a radiation boundary condition at infinity} \end{aligned} \tag{2.1}$$

The origin of the coordinate system is such that Ω is a subset of the half-space of negative x . We assume that the initial conditions u_0 and u_1 and the right hand side f have a compact support in this half space. The computational domain is truncated on its right by the artificial boundary $x = 0$, denoted Γ . It is not possible to use as an ABC a Dirichlet boundary condition on Γ since the solution is not known on Γ . The idea to design the ABC by finding a relation satisfied by the solution on Γ that does not depend on the values of the right hand sides. This integrodifferential relation defines an exact ABC which will be approximated by a partial differential equation.

2.1 Exact ABC

We first study the solution u in the right half space $x \geq 0$ independently of the boundary condition satisfied at $x = 0$. We have:

$$\begin{aligned} \frac{\partial^2 u}{\partial t^2} - c^2 \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) &= 0, \quad x \geq 0, y \in \mathbf{R}, \quad t > 0 \\ u(0, x, y) &= 0, \quad x \geq 0, y \in \mathbf{R} \\ \frac{\partial u}{\partial t}(0, x, y) &= 0, \quad x \geq 0, y \in \mathbf{R} \end{aligned}$$

In order to use the Fourier transform in time, we first prolongate u by zero for negative times. Since the initial conditions are zero for $x \geq 0$, the prolonged function $\tilde{u}$ still satisfies the homogeneous wave equation

$$\frac{\partial^2 \tilde{u}}{\partial t^2} - c^2 \left(\frac{\partial^2 \tilde{u}}{\partial x^2} + \frac{\partial^2 \tilde{u}}{\partial y^2} \right) = 0, \quad x > 0, \quad t, y \in \mathbf{R}.$$

Figure 1. Truncation of the computational domain to a half-plane

We take the Fourier transform in t and y (dual variables are ω and k respectively) of this equation:

$$-\omega^2 \hat{u} - c^2 \frac{\partial^2 \hat{u}}{\partial x^2} + c^2 k^2 \hat{u} = 0.$$

For a given (ω, k) , it is an ordinary differential equation whose solution may be sought in the form $\hat{u}(\omega, x, k) = \sum_j \alpha_j(\omega, k) \exp(\lambda_j(\omega, k)x)$. We have

$$\lambda^2 = k^2 - \frac{\omega^2}{c^2}.$$

We have two possibilities:

- **evanescent waves**, $|k| > \frac{\omega}{c}$: $\lambda^\pm = \pm \sqrt{k^2 - \frac{\omega^2}{c^2}}$
- **propagative waves**, $|k| < \frac{\omega}{c}$: $\lambda^\pm = \pm i \frac{\omega}{c} \sqrt{1 - \frac{c^2 k^2}{\omega^2}}$ ($i^2 = -1$)

By using inverse Fourier transform, the general form for $\tilde{u}$ is:

$$\tilde{u}(t, x, y) = \int \int_{|k| > \frac{\omega}{c}} \alpha_-(\omega, k) e^{-\sqrt{k^2 - \frac{\omega^2}{c^2}} x} e^{i(\omega t + k y)} dk d\omega \quad (2.2)$$

$$+ \int \int_{|k| < \frac{\omega}{c}} \alpha_-(\omega, k) e^{i(\omega t - \frac{\omega}{c} \sqrt{1 - \frac{c^2 k^2}{\omega^2}} x + k y)} dk d\omega \quad (2.3)$$

$$+ \int \int_{|k| > \frac{\omega}{c}} \alpha_+(\omega, k) e^{\sqrt{k^2 - \frac{\omega^2}{c^2}} x} e^{i(\omega t + k y)} dk d\omega \quad (2.4)$$

$$+ \int \int_{|k| < \frac{\omega}{c}} \alpha_+(\omega, k) e^{i(\omega t + \frac{\omega}{c} \sqrt{1 - \frac{c^2 k^2}{\omega^2}} x + k y)} dk d\omega \quad (2.5)$$

Next, we show that $\alpha_+(\omega, k) \equiv 0$ for all (ω, k) . In (2.4) indeed, the term $e^{\sqrt{k^2 - \frac{\omega^2}{c^2}} x}$ tends to infinity as x tends to infinity. Solution $\tilde{u}$ is bounded, we must have $\alpha_+(\omega, k) = 0$ for $|k| > \frac{\omega}{c}$. Moreover, integral (2.5) corresponds to a linear combination of waves

propagating in the direction of negative x . It is impossible that waves originate from infinity, only the boundary Γ creates waves. As a result, we have $\alpha_+(\omega, k) = 0$ for $|k| < \frac{\omega}{c}$. Thus we have:

$$\begin{aligned} \tilde{u}(t, x, y) = & \int \int_{|k| > \frac{\omega}{c}} \alpha_-(\omega, k) e^{-\sqrt{k^2 - \frac{\omega^2}{c^2}} x} e^{i(\omega t + ky)} dk d\omega \\ & + \int \int_{|k| < \frac{\omega}{c}} \alpha_-(\omega, k) e^{i(\omega t - \frac{\omega}{c} \sqrt{1 - \frac{c^2 k^2}{\omega^2}} x + ky)} dk d\omega \end{aligned} \quad (2.6)$$

By taking $x = 0$ in this expression, we see that $\alpha_-(\omega, k) = \hat{u}(\omega, 0, k)$.

By differentiating (2.6) with respect to x , we have thus at $x = 0$

$$\frac{\partial \tilde{u}}{\partial x}(t, 0, y) - \int \int \hat{u}(\omega, 0, k) \lambda^-(\omega, k) e^{i(\omega t + ky)} dk d\omega = 0. \quad (2.7)$$

where

$$\lambda^-(\omega, k) = \begin{cases} -\sqrt{k^2 - \frac{\omega^2}{c^2}} & \text{for } |k| > \frac{\omega}{c} \\ -i\frac{\omega}{c} \sqrt{1 - \frac{c^2 k^2}{\omega^2}} & \text{for } |k| < \frac{\omega}{c}. \end{cases}$$

We assume that relation (2.7) can be used as a boundary condition. It is then an exact ABC since solution u to problem (2.1) has a unique solution and satisfies (2.7) as well.

2.2 Approximation of the exact ABC

The exact ABC (2.7) involves inverse and direct Fourier transforms in both time t and y through the multiplication by a non polynomial function in the Fourier variables ω and k . Due to the square root in the formula for λ^- , the inverse Fourier transform of (2.7) is not a differential equation. Its implementation would be thus costly. Moreover, for a varying velocity field $c(x, y)$ or a curved boundary, the previous computation is not valid and the analytic form for the exact absorbing boundary condition is not known. For these reasons, integrodifferential equation (2.7) is approximated by a partial differential equation. They are easy to implement and have a straightforward extension to variable coefficients and/or curved boundaries.

In the Fourier space, (2.7) reads

$$\frac{\partial \hat{u}}{\partial x}(\omega, 0, k) - \lambda^-(\omega, k) \hat{u}(\omega, 0, k) = 0. \quad (2.8)$$

For reasons that will be given later (see § 3), small values of $c \frac{k}{\omega}$ correspond to waves whose propagation direction is close to the normal to the artificial boundary, see figure 2. We approximate (2.8) by a Taylor expansion in $c \frac{k}{\omega}$ of order zero and centered at zero:

$$\frac{\partial \hat{u}}{\partial x}(\omega, 0, k) + i\frac{\omega}{c} \sqrt{1 - \frac{c^2 k^2}{\omega^2}} \hat{u}(\omega, 0, k) = 0 \approx \frac{\partial \hat{u}}{\partial x}(\omega, 0, k) + i\frac{\omega}{c} \hat{u}(\omega, 0, k) = 0.$$

The inverse Fourier transform yields a zero-order approximation to the exact ABC (2.7):

$$\frac{\partial u}{\partial t}(t, 0, y) + c \frac{\partial u}{\partial n}(t, 0, y) = 0 \quad (\text{zero-order ABC}) \quad (2.9)$$

where we replaced x by the outward normal to the boundary n in order to have a more intrinsic form. This is a partial differential equation which enables the dropping of the superscript $\sim$. It is easy to check that (2.9) is an exact ABC for the one dimensional constant coefficient wave equation.

A higher order ABC is obtained with a Taylor expansion of order two ($\sqrt{1 - \epsilon^2} \approx 1 - \frac{\epsilon^2}{2}$):

$$\frac{\partial \hat{u}}{\partial x}(\omega, 0, k) + i \frac{\omega}{c} \sqrt{1 - \frac{c^2 k^2}{\omega^2}} \hat{u}(\omega, 0, k) = 0 \quad (2.10)$$

$$\approx \frac{\partial \hat{u}}{\partial x}(\omega, 0, k) + i \frac{\omega}{c} \hat{u}(\omega, 0, k) + c \frac{k^2}{2i\omega} \hat{u}(\omega, 0, k) = 0. \quad (2.11)$$

The term $c \frac{k^2}{2i\omega}$ is not polynomial in ω and thus does not correspond (under inverse Fourier Transform) to a partial differential equation on the artificial boundary. In order to fix this difficulty, we have two possibilities. The first one consists simply in multiplying relation (2.11) by $i\omega$ before taking an inverse Fourier transform:

$$\frac{1}{c} \frac{\partial^2 u}{\partial t \partial n} + \frac{1}{c^2} \frac{\partial^2 u}{\partial t^2} - \frac{1}{2} \frac{\partial^2 u}{\partial \tau^2} = 0 \quad (\text{Order 2}) \quad (2.12)$$

where τ is the tangential direction on the artificial boundary. The second possibility is to introduce an auxiliary function $\hat{\phi} = c \frac{k^2}{2i\omega} \hat{u}(\omega, 0, k)$ or equivalently, $i\omega \hat{\phi} = c \frac{k^2}{2} \hat{u}(\omega, 0, k)$. We take the inverse Fourier transform and get:

$$\begin{cases} \frac{1}{c} \frac{\partial u}{\partial t} + \frac{\partial u}{\partial n} + \phi = 0 \\ \frac{1}{2} \frac{\partial^2 u}{\partial \tau^2} = \frac{1}{c} \frac{\partial \phi}{\partial t} \end{cases} \quad (\text{Order 2}) \quad (2.13)$$

For $\phi = 0$, this is equivalent to condition (2.9). Condition (2.13) is thus an incremental modification of (2.9) and is easier to implement than (2.12), see [12] for more details.

In order to get higher order ABCs a natural idea consists in using Taylor expansions of higher and higher orders. For instance, one could use a fourth order expansion $\sqrt{1 - \epsilon^2} \approx 1 - \frac{\epsilon^2}{2} - \frac{\epsilon^4}{8}$. The corresponding ABC would read in the Fourier space:

$$\frac{\partial \hat{u}}{\partial x}(\omega, 0, k) + i \frac{\omega}{c} \hat{u}(\omega, 0, k) + c \frac{k^2}{2i\omega} \hat{u}(\omega, 0, k) + \frac{c^3 k^4}{8i\omega^3} \hat{u}(\omega, 0, k) = 0. \quad (2.14)$$

As a matter of fact, the boundary value problem for the wave equation with the inverse Fourier transform of this boundary condition is not well-posed. It does not satisfy

Kreiss condition [14] or Shapiro-Lopatinski condition. In order to write stable high order ABCs it was proposed in [7] to use Padé approximations:

$$\sqrt{1 - \epsilon^2} \approx \frac{1 - \frac{3\epsilon^2}{4}}{1 - \frac{\epsilon^2}{4}},$$

see [12] as well for more details.

3 Plane waves analysis of an ABC

The analysis consists in computing for the various interface conditions the reflection of a plane wave as a function of its angle of incidence with respect to the normal to the interface. This gives an intuitive insight into the behavior of the ABCs we have introduced in the previous section. It enables to quantify the superiority of the ABC of order 2 (2.12) over the zeroth order one (2.9). It is also justified by the fact that both the incident wave and the scattered one can be decomposed into a linear combination of plane waves as in formula (2.2)-(2.5). The same kind of analysis will be performed in section 5 for the PML method. The incident wave is written as follows:

Figure 2. Incident wave with an angle θ with respect to the normal to the artificial boundary

$$u^I = e^{-i(\omega t - \frac{\omega}{c} \sqrt{1 - \frac{c^2 k^2}{\omega^2}} x + ky)}.$$

The angle of incidence θ with respect to the normal of the artificial boundary is such that:

$$\tan \theta = \frac{\frac{ck}{\omega}}{\sqrt{1 - \frac{c^2 k^2}{\omega^2}}} \text{ and } \cos \theta = \sqrt{1 - \frac{c^2 k^2}{\omega^2}}.$$

The reflected wave reads

$$u^R = R(\theta)e^{-i(\omega t + \frac{\omega}{c}\sqrt{1 - \frac{c^2 k^2}{\omega^2}}x + ky)}.$$

Function $u^I + R(\theta)u^R$ solves the homogeneous wave equation. The reflection coefficient $R(\theta)$ is computed by inserting the expression of $u^I + R(\theta)u^R$ in conditions (2.9) or (2.12).

For the zero-th order ABC (2.9), we have

$$R_0(\theta) = \frac{\cos \theta - 1}{\cos \theta + 1}; \quad R < 10^{-2} \text{ for } |\theta| \leq 11.45^\circ$$

and for the second order ABC (2.12):

$$R_2(\theta) = -\left(\frac{\cos \theta - 1}{\cos \theta + 1}\right)^2; \quad R < 10^{-2} \text{ for } |\theta| \leq 35^\circ.$$

The reflection coefficient for the first order ABC is smaller than one percent for a cone of angle 11.45° whereas the reflection of the second order reaches this magnitude for a larger cone of angle 35° . The latter ABC is sometimes referred to as a wide angle ABC.

4 PML

Historically, the first idea was to border the computational by a dissipative zone where the waves are damped. The dissipative equations were imposed a priori. The problem with this approach lies in the interface between the physical zone and the “sponge” layer. It led to reflection. This matching problem was first solved by Berenger in 1994 [5]. He introduced perfectly matched layers (PML) for use with Maxwell’s equations, and since that time there have been several related reformulations of PML for both Maxwell’s equations and for other wave equations. Berenger’s original formulation is based on a splitting of the electromagnetic fields into two unphysical fields in the PML region. In [6] PMLs were shown to correspond to a coordinate transformation in which the coordinate normal to the artificial boundary is mapped to complex numbers. This is actually an analytic continuation of the wave equation into complex coordinates, replacing propagating (oscillating) waves by exponentially decaying waves. The idea also consists in imposing the behavior of the solution in the PML and then retrieve the corresponding equations and interface conditions. In this way, it is possible to design a reflectionless PML. Thus key property of a PML that distinguishes it from an ordinary absorbing material is that it is designed so that waves incident upon the PML from a non-PML medium do not reflect at the interface. This property allows the PML to strongly absorb outgoing waves from the interior of a computational region without reflecting them back into the interior.

4.1 Helmholtz equation

Let $f : \mathbf{R}^2 \rightarrow \mathbf{C}$ be a function with a compact support in the half-space of negative x , $c > 0$ the speed of sound and ω a non zero real number. We start with a Helmholtz problem defined in the whole space with f as the right hand-side:

$$(-\omega^2 - c^2 \Delta)(u) = f \text{ in } \mathbf{R}^2$$

with Sommerfeld radiation condition at infinity. We consider a PML that will be located in the positive x half-space. Let u_0 be the solution at $x = 0$, $u_0(y) := u(0, y)$. We know from formula (2.6) that the solution to the Helmholtz equation in the right half-space $x > 0$ has the form:

$$u(x, y) = \int_{\mathbf{R}} \hat{u}_0(k) \exp(-i \frac{\omega}{c} \sqrt{1 - \frac{c^2 k^2}{\omega^2}} x) \exp(iky) dk \quad (4.1)$$

The PML must damp the propagative modes of the solution which correspond to the zone $c|k| \leq |\omega|$. For this, we first consider an analytic continuation of the solution with respect to the x coordinate. The complex variable will be denoted by $z \in \mathbf{C}$. The analytic continuation is formally defined as:

$$\tilde{u}(z, y) = \int_{\mathbf{R}} \hat{u}_0(k) \exp(-i \frac{\omega}{c} \sqrt{1 - \frac{c^2 k^2}{\omega^2}} z) \exp(iky) dk \quad (4.2)$$

We now make a change of coordinate w.r.t to the first coordinate. Let $\sigma(x)$ be a function such that $\sigma(x) \geq 0$ for $x \geq 0$. We define a path in the complex plane $s : \mathbf{R} \rightarrow \mathbf{C}$:

$$s(x) := x + \frac{c}{i\omega} \int_0^x \sigma(a) da \quad (4.3)$$

and the function $U : \mathbf{R}^2 \rightarrow \mathbf{C}$:

$$U(x, y) := \begin{cases} u(x, y) & \text{if } x < 0 \\ \tilde{u}(s(x), y) & \text{if } x > 0 \end{cases}$$

We first investigate the behavior of $U(x, y)$ for positive x . Let

$$\hat{u}(x, k) := \hat{u}_0(k) \exp(-i \frac{\omega}{c} \sqrt{1 - \frac{c^2 k^2}{\omega^2}} x).$$

We have with this notation:

$$U(x, y) = \int_{\mathbf{R}} \hat{u}(x, k) \exp\left(-\sqrt{1 - \frac{c^2 k^2}{\omega^2}} \int_0^x \sigma(a) da\right) \exp(iky) dk$$

We see that U is exponentially decreasing for $c|k| < |\omega|$ as x goes to infinity. The propagative modes of u have been turned into vanishing modes. As for the vanishing modes of u ($c|k| > |\omega|$), they are still exponentially decreasing as x goes to infinity although now with a sinusoidal modulation. In summary, U contains only vanishing modes as $x \rightarrow \infty$.

We now have to find out the equations satisfied by U . First of all, since $U(x, y) = u(x, y)$ for $x < 0$, we have:

$$(-\omega^2 - c^2 \Delta)(U) = f \text{ if } x < 0. \quad (4.4)$$

We now determine the equation satisfied by u in the right half-space $x > 0$. We have:

$$\frac{\partial U}{\partial x}(x, y) = s'(x) \frac{\partial \tilde{u}}{\partial z}(s(x), y).$$

This yields:

$$\frac{1}{s'(x)} \frac{\partial U}{\partial x}(x, y) = \frac{\partial \tilde{u}}{\partial z}(s(x), y).$$

Derivating again with respect to x , we get:

$$\frac{1}{s'(x)} \frac{\partial}{\partial x} \left(\frac{1}{s'(x)} \frac{\partial U}{\partial x} \right)(x, y) = \frac{\partial^2 \tilde{u}}{\partial z^2}(s(x), y).$$

As for the y derivatives, we have for any integer m :

$$\frac{\partial^m U}{\partial y^m}(x, y) = \frac{\partial^m \tilde{u}}{\partial y^m}(s(x), y).$$

From formula (4.2), $\tilde{u}$ satisfies the equation:

$$(-\omega^2 - c^2 \frac{\partial^2}{\partial z^2} - c^2 \frac{\partial^2}{\partial y^2})(\tilde{u}) = 0.$$

Therefore, the last three equations yield the equation on U on $x > 0$:

$$(-\omega^2 - c^2 \frac{1}{s'(x)} \frac{\partial}{\partial x} \left(\frac{1}{s'(x)} \frac{\partial}{\partial x} \right) - c^2 \frac{\partial^2}{\partial y^2})(U) = 0 \text{ if } x > 0. \quad (4.5)$$

We introduce the x -pml derivative:

$$\partial_x^{pml} := \frac{1}{s'(x)} \frac{\partial}{\partial x} = \frac{i\omega}{i\omega + c\sigma(x)} \frac{\partial}{\partial x}.$$

We now turn to the interface conditions at $x = 0$. Since U satisfies a second order equation both half-spaces, we need two matching conditions on the interface $x = 0$.

By definition of U and since $s(0) = 0$, we have that U is continuous along the interface $x = 0$:

$$U(0^-, y) = U(0^+, y). \quad (4.6)$$

We consider now the derivative with respect to x . We know that

$$\partial_x^{pml} U(0, y) = \frac{\partial \tilde{u}}{\partial z}(s(0), y).$$

By formula (4.2), we have $\frac{\partial \tilde{u}}{\partial z}(s(0), y) = \frac{\partial u}{\partial x}(0, y)$. Finally, since $s(0) = 0$, we get:

$$\frac{\partial u}{\partial x}(0, y) = \partial_x^{pml} U(0, y),$$

which yields the interface condition at $x = 0$ for U

$$\partial_x U(0^-, y) = \partial_x^{pml} U(0^+, y). \quad (4.7)$$

In practice, it is necessary to consider a bounded PML zone, for instance a vertical slab $(0, \delta) \times \mathbf{R}$. On the new boundary $x = \delta$, we have to impose a boundary condition, for instance a homogeneous boundary condition. Finally, we get the following boundary value problem:

$$\begin{aligned} (-\omega^2 - c^2 \Delta)(v) &= f \text{ in } \mathbf{R}_- \times \mathbf{R} \\ (-\omega^2 - c^2 \frac{i\omega}{i\omega + c\sigma(x)} \frac{\partial}{\partial x} (\frac{i\omega}{i\omega + c\sigma(x)} \frac{\partial}{\partial x} \cdot) - c^2 \frac{\partial^2}{\partial y^2})(v) &= 0, \quad 0 < x < \delta \\ v(0^-, y) &= v(0^+, y) \quad \forall y \in \mathbf{R} \\ \partial_x(v)(0^-, y) &= \frac{i\omega}{i\omega + c\sigma(x)} \frac{\partial}{\partial x} (v)(0^+, y) \quad \forall y \in \mathbf{R} \\ v(\delta, y) &= 0 \quad \forall y \in \mathbf{R} \end{aligned} \quad (4.8)$$

4.2 The wave equation

In order to design a PML for the wave equation, we should take the inverse Fourier transform of the PML of the Helmholtz equation (4.8). The terms in $(i\omega + c\sigma(x))^{-1}$ correspond to non differential operators. The way to bypass this difficulty is, similarly to what is done in (2.13), to introduce two auxiliary unknowns in the PML region: $\hat{w}(\omega, x, y)$ and $\hat{\phi}(\omega, x, y)$ defined as:

$$\begin{aligned} \hat{w}(\omega, x, y) &= \frac{i\omega}{i\omega + c\sigma(x)} \frac{\partial \hat{u}}{\partial x}(\omega, x, y) \\ \hat{\phi}(\omega, x, y) &= \frac{i\omega}{i\omega + c\sigma(x)} \frac{\partial \hat{w}}{\partial x}(\omega, x, y) \end{aligned} \quad (4.9)$$

or equivalently:

$$\begin{aligned} (i\omega + c\sigma(x))\hat{w}(\omega, x, y) &= i\omega \frac{\partial \hat{u}}{\partial x}(\omega, x, y) \\ (i\omega + c\sigma)\hat{\phi}(\omega, x, y) &= i\omega \frac{\partial \hat{w}}{\partial x}(\omega, x, y) \end{aligned} \quad (4.10)$$

At this point, an inverse Fourier transform in time yields partial differential equations. The time dependent counterpart of equation (4.8) reads:

$$\begin{aligned}
 \frac{\partial^2 v}{\partial t^2} - c^2(x, y) \Delta v &= f(t, x, y), & t > 0, x < 0, y \in \mathbf{R} \\
 \frac{\partial w}{\partial t} + c\sigma(x)w &= \frac{\partial^2 v}{\partial t \partial x}, & t > 0, 0 < x < \delta, y \in \mathbf{R} \\
 \frac{\partial \phi}{\partial t} + c\sigma(x)\phi &= \frac{\partial^2 w}{\partial t \partial x}, & t > 0, 0 < x < \delta, y \in \mathbf{R} \\
 -\frac{1}{c^2(x, y)} \frac{\partial^2 v}{\partial t^2} + \phi - \frac{\partial^2 v}{\partial y^2} &= 0, & t > 0, 0 < x < \delta, y \in \mathbf{R} \\
 v(t, 0^-, y) &= v(t, 0^+, y) & t > 0, y \in \mathbf{R} \\
 \frac{\partial v}{\partial x}(t, 0^-, y) &= w(t, 0^+, y) & t > 0, y \in \mathbf{R}
 \end{aligned} \tag{4.11}$$

together with initial conditions at $t = 0$: $v(0, x, y) = u_0(x, y)$, $\partial v / \partial t(0, x, y) = u_1(x, y)$ and since u_0 has compact support in $\mathbf{R}_- \times \mathbf{R}$, we can take zero initial conditions on the auxiliary unknowns in the PML region w and ϕ .

5 Computation of the reflection coefficient of a PML

The analysis consists in computing the reflection of a plane wave as a function of its angle of incidence with respect to the normal to the interface. This gives an intuitive insight into the behavior of the PML and the impact of the damping parameter σ and the thickness of the PML. It is also justified by the fact that both the incident wave and the scattered one can be decomposed into a linear combination of plane waves as in formula (2.2)-(2.5). The same kind of analysis was performed in section 3 for the ABCs. It enables thus to compare quantitatively ABCs with the PML technique.

In this section, the function σ takes a constant value still denoted by σ . As in (4.8), the Helmholtz domain is the left half-space $x < 0$. The PML is a band of width δ , $(0, \delta) \times \mathbf{R}$. We compute the reflection coefficient for a PML with a homogeneous Dirichlet at the boundary $x = \delta$ of the PML. We make a planar wave analysis by considering homogeneous equations but instead of having a radiation condition at minus infinity, we consider a planar wave “coming” from minus infinity.

Let

$$\begin{aligned}
 \lambda_H &= \frac{i\omega}{c} \sqrt{1 - \frac{c^2 k^2}{\omega^2}} \\
 \lambda_H^{pml} &= \left(1 + \frac{c\sigma}{i\omega}\right) \lambda_H
 \end{aligned}$$

It can be checked that the functions $e^{\pm \lambda_H x}$ are solutions to the homogeneous Helmholtz equations and $e^{\pm \lambda_H^{pml} x}$ are solutions to the homogeneous PML equations. We shall

make use of the following formulas:

$$\begin{cases} \partial_x(e^{\lambda_H x}) = \lambda_H e^{\lambda_H x} \\ \partial_x^{pml}(e^{\lambda_H^{pml} x}) = \frac{i\omega}{i\omega + c\sigma} \lambda_H^{pml} e^{\lambda_H^{pml} x} = \lambda_H e^{\lambda_H^{pml} x} \end{cases} \quad (5.1)$$

The solution u_H to the homogeneous Helmholtz equation in the left domain has the form

$$\hat{u}_H = \alpha_H e^{\lambda_H x} + \beta_H e^{-\lambda_H x}$$

and in the PML zone:

$$\hat{u}_{pml} = \alpha_{pml} e^{\lambda_H^{pml} x} + \beta_{pml} e^{-\lambda_H^{pml} x}$$

Using (5.1), the coupling conditions (4.6)-(4.7) at the interface between the Helmholtz and the PML yield:

$$\begin{cases} \alpha_H + \beta_H = \alpha_{pml} + \beta_{pml} \\ \lambda_H(\alpha_H - \beta_H) = \lambda_H(\alpha_{pml} - \beta_{pml}) \end{cases} \quad (5.2)$$

The homogeneous Dirichlet boundary condition in the PML at $x = \delta$ yields:

$$\alpha_{pml} e^{\lambda_H^{pml} \delta} + \beta_{pml} e^{-\lambda_H^{pml} \delta} = 0 \quad (5.3)$$

We study the damping of the PML by considering β_H to be given. This corresponds to an ingoing wave from the physical (in space) medium and moving towards the interface between the physical medium and the PML medium. The three other quantities ($\alpha_H, \alpha_{pml}, \beta_{pml}$) are determined by the interface conditions. The reflection caused by a finite width PML is given by the ratio $R := |\alpha_H/\beta_H|$. A direct computation shows that:

$$R = e^{-2\sqrt{1 - \frac{c^2 k^2}{\omega^2}} \sigma \delta} \quad (5.4)$$

Using the physical meaning of $\sqrt{1 - \frac{c^2 k^2}{\omega^2}}$ as the cosine of the angle θ between the ingoing wave and the normal to the boundary, R reads:

$$R = (e^{-2\sigma\delta})^{\cos(\theta)} \quad (5.5)$$

We see here the main advantage of the PML approach over the ABC approach. In order to decrease the reflection coefficient, it is sufficient to increase the width of the PML and/or to take a large damping coefficient σ whereas for the ABC approach, it is necessary to implement more and more complex absorbing boundary conditions. At this point, one could think that it is enough to take a very large damping parameter σ . Actually, it creates a numerical reflection that is proportional to $\sigma \Delta x$. A remedy consists in taking a variable damping $\sigma(x) = Cx^2/\delta$ and tune the parameters C and δ . In practice, δ is roughly a wavelength $2\pi c/\omega$ and C is 20 – 40. Of course, taking a smaller Δx (finer mesh) will improve the results as well since we come closer to the continuous limit.

6 Conclusion

We have designed absorbing boundary conditions and perfectly matched layers for some scalar second order partial differential operators: the Helmholtz equation and the wave equation. The construction of the ABC is based on Fourier symbol computations of an exact ABC which is then approximated by a rational fraction. By introducing auxiliary unknowns, this approximation yields, in the physical space, a system of partial differential equations. This technique is quite general and can be applied to systems of partial differential equations, like the isotropic or anisotropic elasticity system with or without anisotropy, Oseen equations (linearized Navier-Stokes equations), Maxwell system, . . . As for PML, their designs rely on a complex coordinate coordinate change that will be stable in the sense that propagative modes are turned into evanescent ones and that evanescent modes remain evanescent. For complex systems of PDEs with anisotropy, it is not always easy to find such a change of coordinates. Thus, although PMLs are usually better fitted to numerical computations than ABCs, their designs are not always feasible and are still an active area of research.

We have considered the design of absorbing boundary conditions and perfectly matched layers in a common Fourier framework and thus restricted ourselves to rectilinear boundaries for scalar equations. Actually, these concepts are also valid for curved boundaries and/or systems of partial differential equations, see for example [3, 9, 2, 15, 11, 10] and references therein.

An appealing feature of ABCs and PMLs is that these notions are building blocks for apparently unrelated applications such as domain decomposition methods [4], approximate factorizations preconditioners for Helmholtz type problems [8] or inverse problems via time reversal techniques [1]. From a general point of view, it is due to the fact that ABCs or PMLs are cheap approximations to non local operators.

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