Perfectly Matched Layer for scalar and vector waves: some notes

Vincent Laude

December 2020; revised 26/09/2022

Abstract

This document summarizes my understanding of the Perfectly Matched Layer (PML) in the frequency domain as a complex coordinate transformation method for arbitrary domains.

1 PML as complex coordinate transformation

The PML is introduced to transform an infinite (open) problem into a finite problem. The idea is to seek a solution to the dynamical equations by using a coordinate transformation that transforms the real infinite space to a complex space (that will admit evanescent waves as eigenfunctions instead of plane waves) and then to truncate the complex space to some finite size. If there are only evanescent waves and they have sufficiently decayed, then the additional boundary condition terminating the PML becomes less important (a Dirichlet BC is usually enforced).

Given coordinates $\boldsymbol{x}$ of real space, we introduce coordinates $\boldsymbol{y}$ of complex space via a transformation $y_i = y_i(\boldsymbol{x})$. Introduce the Jacobian matrix

$$J_{ij} = \frac{\partial y_i}{\partial x_j}.$$

In an integral, the integration element (volume) changes proportionaly to $\det(J)$. Consider a function $u(\boldsymbol{x}) = \tilde{u}(\boldsymbol{y})$. Then the gradient transforms as

$$\nabla \tilde{u} = \frac{\partial \tilde{u}}{\partial y_i} = \frac{\partial x_j}{\partial y_i} \frac{\partial u}{\partial x_j} = J^{-t} \nabla u.$$

The inverse Jacobian has elements

$$J^{-1}_{ij} = \frac{\partial x_i}{\partial y_j}.$$

Note the transpose operator when transforming the gradient.

1.1 Scalar case

Consider a scalar unknown $u(\boldsymbol{x}) = \tilde{u}(\boldsymbol{y})$. A mass integral transforms as

$$M = -\omega^2 \int_{\tilde{\Omega}} \rho \tilde{u} \tilde{v} = -\omega^2 \int_{\Omega} \rho u v \det(J). \tag{1}$$

A stiffness integral transforms as

$$K = \int_{\tilde{\Omega}} c \, \nabla \tilde{u} \nabla \tilde{v} = \int_{\Omega} c \, \nabla u J^{-1} J^{-t} \nabla v \det(J). \tag{2}$$

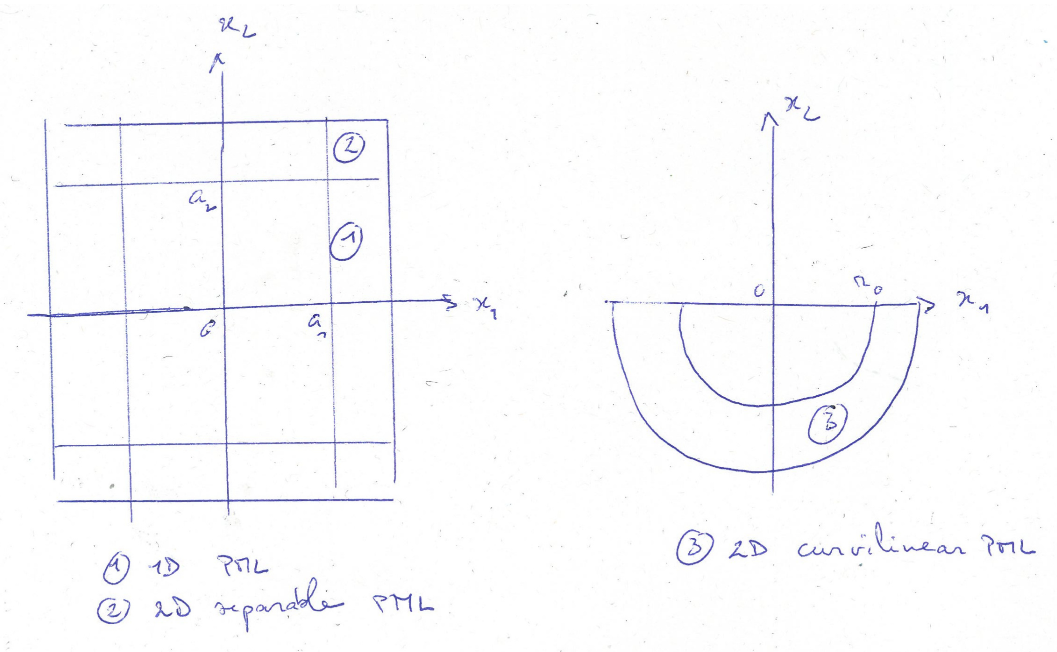

Figure 1: Three different PML definitions.

Matrix-vector notations have been used because they are found more often, but the tensor notation is even clearer

$$K = \int_\Omega c\; J^{-1}_{j,i} u_{,j} J^{-1}_{k,i} v_{,k} \det(J). \tag{3}$$

1.2 Vector case

Consider a vector unknown $u_i(\boldsymbol{x}) = \tilde{u}_i(\boldsymbol{y})$. A mass integral transforms as

$$M = -\omega^2 \int_\Omega \rho u_i v_i \det(J) = -\omega^2 \int_\Omega \hat{\rho} u_i v_i \tag{4}$$

with $\hat{\rho} = \rho \det(J)$. A stiffness integral transforms as (only tensor notation makes sense)

$$K = \int_\Omega c_{ijkl}\; J^{-1}_{m,j} u_{i,m} J^{-1}_{n,l} v_{k,n} \det(J). \tag{5}$$

Thus we can define the transformed stiffness tensor as

$$\hat{c}_{imkn} = c_{ijkl}\; J^{-1}_{m,j} J^{-1}_{n,l} \det(J), \tag{6}$$

so that

$$K = \int_\Omega \hat{c}_{imkn}\; u_{i,m} v_{k,n}. \tag{7}$$

This presentation, however, breaks the symmetries of the strain tensor[1], and is hence not really useful. It is better to write the strains as

$$\hat{S}_{ij} = \hat{S}_I \tag{8}$$

[1] If J is not itself symmetrical.

with

$$\hat{S}_1 = J^{-1}_{m,1} u_{1,m}, \tag{9}$$
$$\hat{S}_2 = J^{-1}_{m,2} u_{2,m}, \tag{10}$$
$$\hat{S}_3 = J^{-1}_{m,3} u_{3,m}, \tag{11}$$
$$\hat{S}_4 = J^{-1}_{m,2} u_{3,m} + J^{-1}_{m,3} u_{2,m}, \tag{12}$$
$$\hat{S}_5 = J^{-1}_{m,1} u_{3,m} + J^{-1}_{m,3} u_{1,m}, \tag{13}$$
$$\hat{S}_6 = J^{-1}_{m,1} u_{2,m} + J^{-1}_{m,2} u_{1,m}, \tag{14}$$
$$\tag{15}$$

and to factor $\det(J)$ globally (which makes sense since this term measures the variation of the volume element of integration). Finally,

$$K = \int_\Omega c_{IJ}\ \hat{S}(u)_I \hat{S}(v)_J \det(J). \tag{16}$$

In summary, the PML does not modify the material constants, but instead transforms the definition of strain and local volume.

In order to avoid reflections, the coordinate transformation and its first derivative should be continuous at the separation between the main domain and the PML. Physically, this is similar to continuity of the fields and their derivatives (displacement and strain).

2 The 1D PML in a 2D domain

Let us suppose we wish to attenuate waves in only one direction, e.g.

$$y_1 = x_1 + \frac{i}{\omega} \int_a^{x_1} \sigma(s) \mathrm{d}s, \tag{17}$$
$$y_2 = x_2. \tag{18}$$

This coordinate transformation is obviously continuous at $x_1 = a$. The derivative

$$y_{1,1} = 1 + \frac{i}{\omega} \sigma(x_1)$$

is furthermore continuous if $\sigma(a) = 0$. The simplest possible choice satisfying this condition is $\sigma(x_1) = \beta|x_1 - a|$, but this choice is in no way unique. The choice of dividing by the angular frequency is made in order to obtain a PML that works whatever the frequency. The choice of the value of the coefficient β is discussed later on.

In any case, we have

$$J = \begin{pmatrix} y_{1,1} & 0 \\ 0 & 1 \end{pmatrix}, \tag{19}$$
$$\det(J) = y_{1,1}, \tag{20}$$
$$J^{-1} = \begin{pmatrix} y_{1,1}^{-1} & 0 \\ 0 & 1 \end{pmatrix}, \tag{21}$$
$$J^{-1} J^{-t} \det(J) = \begin{pmatrix} y_{1,1}^{-1} & 0 \\ 0 & y_{1,1} \end{pmatrix} \tag{22}$$

This is exactly the traditional PML that can be found in most papers and was first introduced by Bérenger [1]. This choice is suitable for a domain terminated by a single straight boundary defined by $x_1 = a$. Generalization to 3D space is obvious.

The explanation of the choice of the coordinate transform is as follows. We limit the analysis to a scalar 2D version of the partial differential equation, that describes propagation in a homogeneous medium:

$$\frac{\partial}{\partial x_1}\left(\frac{\partial u}{\partial x_1}\right) + \frac{\partial}{\partial x_2}\left(\frac{\partial u}{\partial x_2}\right) + \frac{\omega^2}{c^2}u = 0 \tag{23}$$

Inside the PML, this equation becomes

$$\frac{\partial}{\partial x_1}\left(y_{1,1}^{-1}\frac{\partial u}{\partial x_1}\right) + y_{1,1}\frac{\partial}{\partial x_2}\left(\frac{\partial u}{\partial x_2}\right) + y_{1,1}\frac{\omega^2}{c^2}u = 0 \tag{24}$$

As is easily verified, a general solution can be obtained by superposition of the family of functions

$$u(x_1, x_2) = \exp\left(\pm\imath\frac{\omega\cos\theta}{c}y_1 \pm \imath\frac{\omega\sin\theta}{c}x_2\right) \tag{25}$$

where θ is an angle of incidence on the PML boundary. At the end of the PML, we have $y_1(x_1 = a+L) = a + L + \imath\frac{\beta L^2}{2\omega}$. Hence, the amplitude of the solution is there

$$u(a+L, x_2) = \exp\left(\mp\frac{\beta L^2\cos\theta}{2c} \pm \imath\frac{\omega\cos\theta}{c}(a+L) \pm \imath\frac{\omega\sin\theta}{c}x_2\right) \tag{26}$$

The Dirichlet boundary condition at the end of the PML eliminates the exponentially increasing solutions. After reflection on the end of the PML, the amplitude of the reflected wave that would exit the PML back into the incident medium is then

$$\exp\left(-\frac{\beta L^2\cos\theta}{c}\right)$$

In practice, I have used

$$\beta = 20\frac{c}{L^2}$$

with good results. Note that the value of L has no direct relation with the attenuation, but it still has to be comparable to the wavelength, since we need to represent the oscillating part of the solution. In practice, I have used a PML with a 'sufficient' number of elements in the depth (say, 20), to avoid numerical reflections arising from a coarse mesh, and the element size is simply taken as similar to the main computation domain.

3 2D separable PML

Let us suppose we wish to attenuate waves independently in only two direction, e.g.

$$y_1 = x_1 + \frac{i}{\omega}\int_{a_1}^{x_1}\sigma_1(s)\mathrm{d}s, \tag{27}$$

$$y_2 = x_2 + \frac{i}{\omega}\int_{a_2}^{x_2}\sigma_2(s)\mathrm{d}s. \tag{28}$$

This coordinate transformation is obviously continuous at $x_1 = a_1$ and $x_2 = a_2$. The derivatives $y_{1,1}$ and $y_{2,2}$ are furthermore continuous if $\sigma_1(a_1) = 0$ and $\sigma_2(a_2) = 0$.

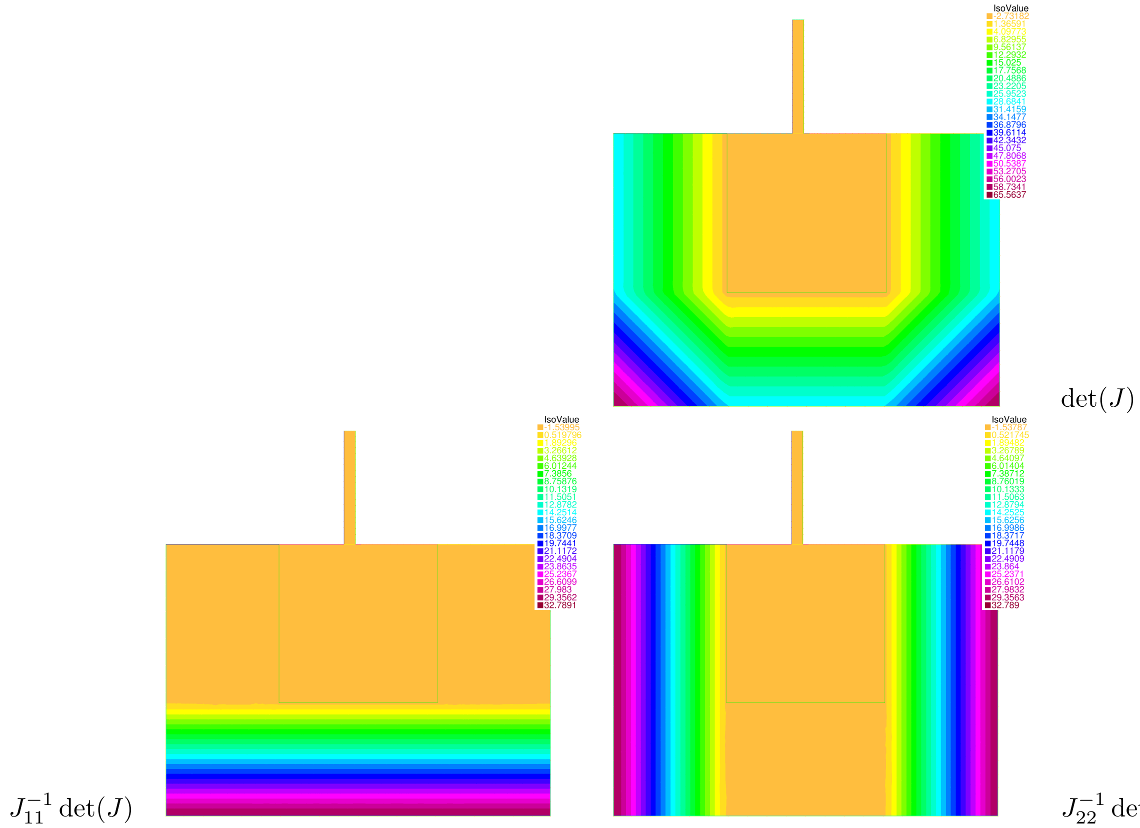

Figure 2: Example of a 2D separable PML. The function σ is set so that the PML width is half a wavelength.

In any case, we have

$$J = \begin{pmatrix} y_{1,1} & 0 \\ 0 & y_{2,2} \end{pmatrix}, \tag{29}$$

$$\det(J) = y_{1,1}y_{2,2} = \left(1 + \frac{i}{\omega}\sigma_1(x_1)\right)\left(1 + \frac{i}{\omega}\sigma_2(x_2)\right), \tag{30}$$

$$J^{-1} = \begin{pmatrix} y_{1,1}^{-1} & 0 \\ 0 & y_{2,2}^{-1} \end{pmatrix} = \frac{1}{\det(J)}\begin{pmatrix} y_{2,2} & 0 \\ 0 & y_{1,1} \end{pmatrix}, \tag{31}$$

$$J^{-1}J^{-t}\det(J) = \begin{pmatrix} y_{1,1}^{-1}y_{2,2} & 0 \\ 0 & y_{1,1}y_{2,2}^{-1} \end{pmatrix} \tag{32}$$

This is the traditional form for 2D domains with rectangular shape with only corner (a_1, a_2) connex to the main region, e.g. [2]. Generalization to 3D space is again straightforward.

4 2D curvilinear PML

Let us suppose we want to attenuate waves in an angular sector. The PML is enterred at the circular boundary satisfying $r = \sqrt{x_1^2 + x_2^2} = r_0$. We consider a sequence of three coordinate transforms:

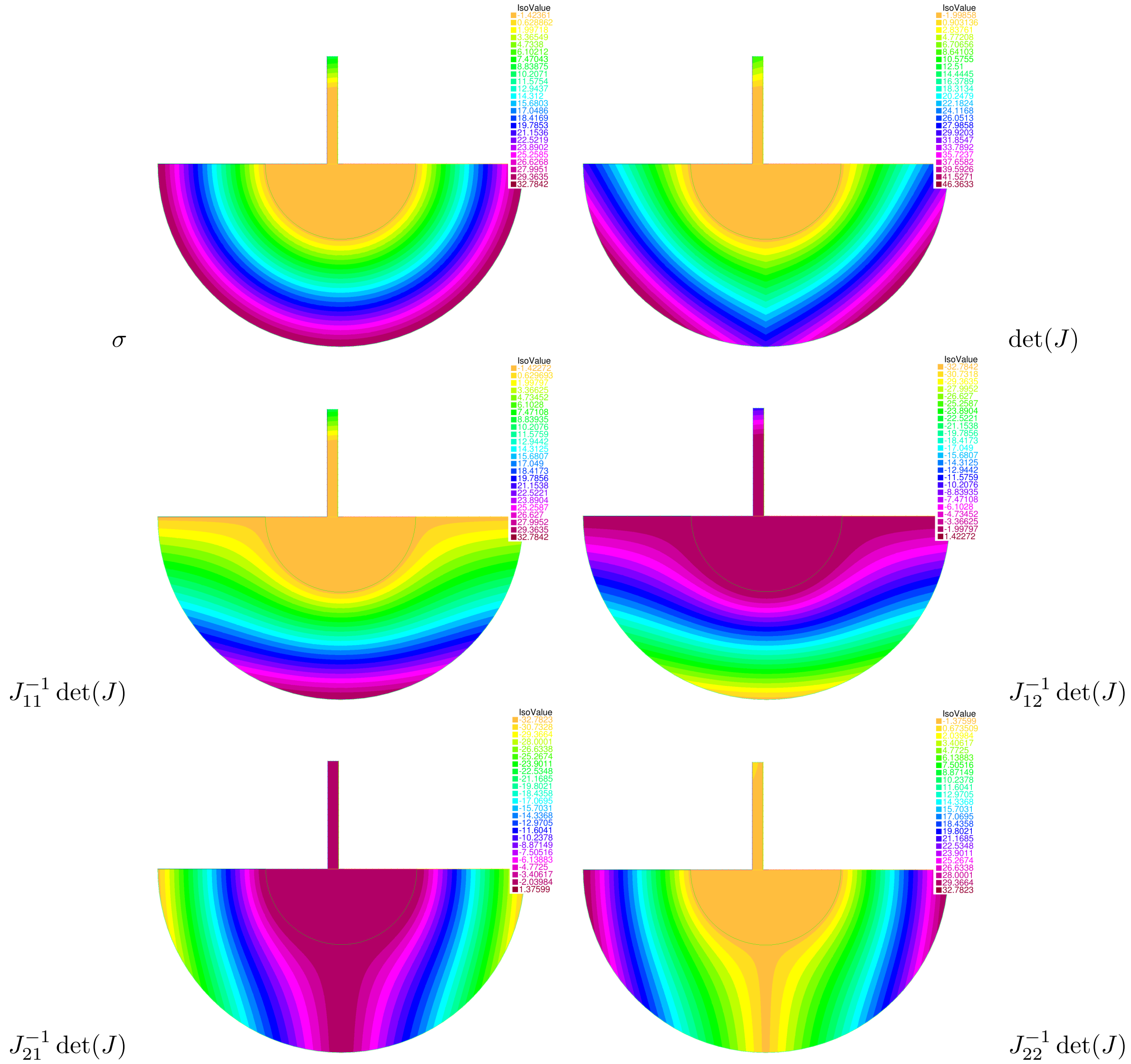

Figure 3: Example of a 2D curvilinear PML.

- Cartesian to polar coordinates,
- Complexification of the radial coordinate,
- Polar to Cartesian coordinates.

Polar to Cartesian coordinates is the easiest. We use $x = r\cos\phi$, $y = r\sin\phi$ and hence

$$J_{pc} = \begin{pmatrix} \cos\phi & -r\sin\phi \\ \sin\phi & r\cos\phi \end{pmatrix} = \begin{pmatrix} x/r & -y \\ y/r & x \end{pmatrix} \tag{33}$$

$$J_{pc}^{-t} = \begin{pmatrix} x/r & -y/r^2 \\ y/r & x/r^2 \end{pmatrix} \tag{34}$$

$$\det(J_{pc}) = r \tag{35}$$

The Cartesian to polar transform is then simply

$$J_{cp} = \begin{pmatrix} x/r & y/r \\ -y/r^2 & x/r^2 \end{pmatrix} \tag{36}$$

$$J_{cp}^{-t} = \begin{pmatrix} x/r & y/r \\ -y & x \end{pmatrix} \tag{37}$$

$$\det(J_{cp}) = 1/r \tag{38}$$

The complex polar transform is obviously similar to the 1D Cartesian case

$$r' = r + \frac{i}{\omega} \int_{r_0}^{r} \sigma(s) \mathrm{d}s \tag{39}$$

Gathering all contributions, we have

$$J = J_{cp} J_{pp'} J_{p'c'} \tag{40}$$

$$\det(J) = (1 + \frac{i}{\omega}\sigma(r))\frac{r'}{r} = \alpha^{-1}\frac{r'}{r} \tag{41}$$

$$\nabla_{c'} = J_{p'c'}^{-t} J_{pp'}^{-t} J_{cp}^{-t} \nabla_c \tag{42}$$

$$\nabla_{c'} = \begin{pmatrix} \alpha c^2 + \frac{r}{r'} s^2 & (\alpha - \frac{r}{r'})sc \\ (\alpha - \frac{r}{r'})sc & \alpha s^2 + \frac{r}{r'} c^2 \end{pmatrix} \nabla_c \tag{43}$$

Notice the symmetrical form of the transform.

References

[1] J.-P. Berenger. A perfectly matched layer for the absorption of electromagnetic waves. *J. Comput. Phys.*, 114:185, 1994.

[2] Isaac Harari, Michael Slavutin, and Eli Turkel. Analytical and numerical studies of a finite element PML for the Helmholtz equation. *J. Comp. Acoust.*, 8(01):121–137, 2000.