

# Chapter 11

## Perfectly Matched Layer

### 11.1 Introduction

The perfectly matched layer (PML) is generally considered the state-of-the-art for the termination of FDTD grids. There are some situations where specially designed ABC's can outperform a PML, but this is very much the exception rather than the rule. The theory behind a PML is typically pertinent to the continuous world. In the continuous world the PML should indeed work “perfectly” (as its name implies) for all incident angles and for all frequencies. However, when a PML is implemented in the discretized world of FDTD, there are always some imperfections (i.e., reflections) present.

There are several different PML formulations. However, all PML's essentially act as a lossy material. The lossy material, or lossy layer, is used to absorb the fields traveling away from the interior of the grid. The PML is anisotropic and constructed in such a way that there is no loss in the direction tangential to the interface between the lossless region and the PML (actually there can be loss in the non-PML region too, but we will ignore that fact for the moment). However, in the PML there is always loss in the direction normal to the interface.

The PML was originally proposed by J.-P. Bérenger in 1994. In that original work he split each field component into two separate parts. The actual field components were the sum of these two parts but by splitting the field Bérenger could create an (non-physical) anisotropic medium with the necessary phase velocity and conductivity to eliminate reflections at an interface between a PML and non-PML region. Since Bérenger first paper, others have described PML's using different approaches such as the complex coordinate-stretching technique put forward by Chew and Weedon, also in 1994.

Arguably the best PML formulation today is the Convolutional-PML (CPML). CPML constructs the PML from an anisotropic, dispersive material. CPML does not require the fields to be split and can be implemented in a relatively straightforward manner.

Before considering CPML, it is instructive to first consider a simple lossy layer. Recall that a lossy layer provided an excellent ABC for 1D grids. However, a traditional lossy layer does not work in higher dimensions where oblique incidence is possible. We will discuss this and show how the split-field PML fixes this problem.

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<sup>†</sup>Lecture notes by John Schneider. `fdtd-pml.tex`

## 11.2 Lossy Layer, 1D

A lossy layer was previously introduced in Sec. 3.12. Here we will revisit lossy material but initially focus of the continuous world and time-harmonic fields. For continuous, time-harmonic fields, the governing curl equations can be written

$$\nabla \times \mathbf{H} = j\omega\epsilon\mathbf{E} + \sigma\mathbf{E} = j\omega\left(\epsilon - j\frac{\sigma}{\omega}\right)\mathbf{E} = j\omega\tilde{\epsilon}\mathbf{E}, \quad (11.1)$$

$$\nabla \times \mathbf{E} = -j\omega\mu\mathbf{H} - \sigma_m\mathbf{H} = -j\omega\left(\mu - j\frac{\sigma_m}{\omega}\right)\mathbf{H} = -j\omega\tilde{\mu}\mathbf{H}, \quad (11.2)$$

where the complex permittivity and permeability are given by

$$\tilde{\epsilon} = \epsilon - j\frac{\sigma}{\omega}, \quad (11.3)$$

$$\tilde{\mu} = \mu - j\frac{\sigma_m}{\omega}. \quad (11.4)$$

For now, let us restrict consideration to a 1D field that is  $z$ -polarized so that the electric field is given by

$$\mathbf{E} = \hat{\mathbf{a}}_z e^{-\gamma x} = \hat{\mathbf{a}}_z E_z(x) \quad (11.5)$$

where the propagation constant  $\gamma$  is yet to be determined. Given the electric field, the magnetic field is given by

$$\mathbf{H} = -\frac{1}{j\omega\tilde{\mu}}\nabla \times \mathbf{E} = -\hat{\mathbf{a}}_y \frac{\gamma}{j\omega\tilde{\mu}} E_z(x). \quad (11.6)$$

Thus the magnetic field only has a  $y$  component, i.e.,  $\mathbf{H} = \hat{\mathbf{a}}_y H_y(x)$ .

The characteristic impedance of the medium  $\eta$  is the ratio of the electric field to the magnetic field (actually, in this case, the negative of that ratio). Thus,

$$\eta = -\frac{E_z(x)}{H_y(x)} = \frac{j\omega\tilde{\mu}}{\gamma}. \quad (11.7)$$

Since  $\gamma$  has not yet been determined, we have not actually specified the characteristic impedance yet. To determine  $\gamma$  we use the other curl equation where we solve for the electric field in terms of the magnetic field we just obtained:

$$\mathbf{E} = \frac{1}{j\omega\tilde{\epsilon}}\nabla \times \mathbf{H} = \frac{1}{j\omega\tilde{\epsilon}} \frac{\gamma^2}{j\omega\tilde{\mu}} e^{-\gamma x} \hat{\mathbf{a}}_z. \quad (11.8)$$

However, we already know the electric field since we started with that as a given, i.e.,  $\mathbf{E} = \exp(-\gamma x)\hat{\mathbf{a}}_z$ . Thus, in order for (11.8) to be true, we must have

$$\frac{\gamma^2}{(j\omega)^2\tilde{\mu}\tilde{\epsilon}} = 1, \quad (11.9)$$

or, solving for  $\gamma$  (and only keeping the positive root)

$$\gamma = j\omega\sqrt{\tilde{\mu}\tilde{\epsilon}}. \quad (11.10)$$

Because  $\tilde{\mu}$  and  $\tilde{\epsilon}$  are complex,  $\gamma$  will be complex and we write  $\gamma = \alpha + j\beta$  where  $\alpha$  is the attenuation constant and  $\beta$  is the phase constant (or wave number).

Returning to the characteristic impedance as given in (11.7), we can now write

$$\eta = \frac{j\omega\tilde{\mu}}{j\omega\sqrt{\tilde{\mu}\tilde{\epsilon}}} = \sqrt{\frac{\tilde{\mu}}{\tilde{\epsilon}}}. \quad (11.11)$$

Alternatively, we can write

$$\eta = \sqrt{\frac{\mu \left(1 - j\frac{\sigma_m}{\omega\mu}\right)}{\epsilon \left(1 - j\frac{\sigma}{\omega\epsilon}\right)}}. \quad (11.12)$$

Let us now consider a  $z$ -polarized plane wave normally incident from a lossless material to a lossy material. There is a planar interface between the two media at  $x = 0$ . The (known) incident field is given by

$$E_z^i = e^{-j\beta_1 x} \quad H_y^i = -\frac{1}{\eta_1} e^{-j\beta_1 x} \quad (11.13)$$

where  $\beta_1 = \omega\sqrt{\mu_1\epsilon_1}$ . The reflected field is given by

$$E_z^r = \Gamma e^{j\beta_1 x} \quad H_y^r = \frac{\Gamma}{\eta_1} e^{j\beta_1 x} \quad (11.14)$$

where the only unknown is the reflection coefficient  $\Gamma$ . The transmitted field is given by

$$E_z^t = T e^{-\gamma_2 x} \quad H_y^t = -\frac{T}{\eta_2} e^{-\gamma_2 x} \quad (11.15)$$

where the only unknown is the transmission coefficient  $T$ .

Both the electric field and the magnetic field are tangential to the interface at  $x = 0$ . Thus, the boundary conditions dictate that the sum of the incident and reflected field must equal the transmitted field at  $x = 0$ . Matching the electric fields at the interface yields

$$1 + \Gamma = T. \quad (11.16)$$

Matching the magnetic fields yields

$$-\frac{1}{\eta_1} + \frac{\Gamma}{\eta_1} = -\frac{T}{\eta_2} \quad (11.17)$$

or, rearranging slightly,

$$1 - \Gamma = \frac{\eta_1}{\eta_2} T. \quad (11.18)$$

Adding (11.16) and (11.18) and rearranging yields

$$T = \frac{2\eta_2}{\eta_2 + \eta_1}. \quad (11.19)$$

Plugging this back into (11.16) yields

$$\Gamma = \frac{\eta_2 - \eta_1}{\eta_2 + \eta_1}. \quad (11.20)$$

Consider the case where the media are related by

$$\frac{\mu_2}{\epsilon_2} = \frac{\mu_1}{\epsilon_1} \quad \text{and} \quad \frac{\sigma_m}{\mu_2} = \frac{\sigma}{\epsilon_2}. \quad (11.21)$$

We will call these conditions the “matching conditions.” Under these conditions the impedances equal:

$$\eta_2 = \sqrt{\frac{\mu_2 \left(1 - j \frac{\sigma_m}{\omega \mu_2}\right)}{\epsilon_2 \left(1 - j \frac{\sigma}{\omega \epsilon_2}\right)}} = \sqrt{\frac{\mu_1 \left(1 - j \frac{\sigma}{\omega \epsilon_2}\right)}{\epsilon_1 \left(1 - j \frac{\sigma}{\omega \epsilon_2}\right)}} = \sqrt{\frac{\mu_1}{\epsilon_1}} = \eta_1. \quad (11.22)$$

When the impedances are equal, from (11.20) we see that the reflection coefficient must be zero (and the transmission coefficient is unity). We further note that this is true independent of the frequency.

As we have seen previously, this type of lossy layer can be implemented in an FDTD grid. To minimize numeric artifacts it is best to gradually increase the conductivity within the lossy region. Any field that makes it to the end of the grid will be reflected, but, because of the loss, this reflected field can be greatly attenuated. Furthermore, as the field propagates back through the lossy region toward the lossless region, it is further attenuated. Thus the reflected field from this lossy region (and the termination of the grid) can be made relatively inconsequential.

## 11.3 Lossy Layer, 2D

Since a lossy layer works so well in 1D and is so easy to implement, it is natural to ask if it can be used in 2D. The answer, we shall see, is that a simple lossy layer cannot be matched to the lossless region for obliquely traveling waves.

Consider a  $\text{TM}^z$  field where the incident electric field is given by

$$\mathbf{E}^i = \hat{\mathbf{a}}_z e^{-j\mathbf{k}_1 \cdot \mathbf{r}}, \quad (11.23)$$

$$= \hat{\mathbf{a}}_z e^{-j\beta_1 \cos(\theta_i)x - j\beta_1 \sin(\theta_i)y}, \quad (11.24)$$

$$= \hat{\mathbf{a}}_z e^{-j\beta_{1x}x - j\beta_{1y}y}. \quad (11.25)$$

Knowing that the angle of incidence equals the angle of reflection (owing to the required phase matching along the interface), the reflected field is given by

$$\mathbf{E}^r = \hat{\mathbf{a}}_z \Gamma e^{j\beta_{1x}x - j\beta_{1y}y}. \quad (11.26)$$

Combining the incident and reflected field yields

$$\mathbf{E}_1 = \hat{\mathbf{a}}_z \left( e^{-j\beta_{1x}x} + \Gamma e^{j\beta_{1x}x} \right) e^{-j\beta_{1y}y} = \hat{\mathbf{a}}_z E_{1z}. \quad (11.27)$$

The magnetic field in the first medium is given by

$$\mathbf{H}_1 = -\frac{1}{j\omega\mu_1} \nabla \times \mathbf{E}_1, \quad (11.28)$$

$$= \hat{\mathbf{a}}_x \frac{\beta_{1y}}{\omega\mu_1} \left( e^{-j\beta_{1x}x} + \Gamma e^{j\beta_{1x}x} \right) e^{-j\beta_{1y}y} + \hat{\mathbf{a}}_y \frac{\beta_{1x}}{\omega\mu_1} \left( -e^{-j\beta_{1x}x} + \Gamma e^{j\beta_{1x}x} \right) e^{-j\beta_{1y}y}. \quad (11.29)$$

The transmitted electric field is

$$\mathbf{E}^t = \hat{\mathbf{a}}_z T e^{-\gamma_2 \cdot \mathbf{r}} \quad (11.30)$$

$$= \hat{\mathbf{a}}_z T e^{-\gamma_{2x}x - \gamma_{2y}y}, \quad (11.31)$$

$$= \hat{\mathbf{a}}_z E_z^t. \quad (11.32)$$

Plugging this expression into Maxwell's equations (or, equivalently, the wave equation) ultimately yields the constraint equation

$$\gamma_{2x}^2 + \gamma_{2y}^2 = -\omega^2 \tilde{\mu}_2 \tilde{\epsilon}_2. \quad (11.33)$$

Owing to the boundary condition that the fields must match at the interface, the propagation in the  $y$  direction (i.e., tangential to the boundary) must be the same in both media. Thus,  $\gamma_{2y} = j\beta_{1y}$ . Plugging this into (11.33) and solving for  $\gamma_{2x}$  yields

$$\gamma_{2x} = \sqrt{\beta_{1y}^2 - \omega^2 \tilde{\mu}_2 \tilde{\epsilon}_2} = \alpha_{2x} + j\beta_{2x}. \quad (11.34)$$

Note that when  $\beta_{1y} = 0$ , i.e., there is no propagation in the  $y$  direction and the field is normally incident on the interface, this reduces to  $\gamma_{2x} = j\omega\sqrt{\tilde{\mu}_2\tilde{\epsilon}_2}$  which is what we had for the 1D case. On the other hand, when  $\sigma = \sigma_m = 0$  we obtain  $\gamma_{2x} = j(\omega^2\mu_2\epsilon_2 - \beta_{1y}^2)^{1/2}$  where the term in parentheses is purely real (so that  $\gamma_{2x}$  will either be purely real or purely imaginary). The transmitted magnetic field is given by

$$\mathbf{H}^t = -\frac{1}{j\omega\tilde{\mu}_2} \nabla \times \mathbf{E}^t, \quad (11.35)$$

$$= \hat{\mathbf{a}}_x \frac{\beta_{1y}}{\omega\tilde{\mu}_2} E_z^t - \hat{\mathbf{a}}_y \frac{\gamma_{2x}}{j\omega\tilde{\mu}_2} E_z^t. \quad (11.36)$$

Enforcing the boundary condition on the electric field and the  $y$ -component of the magnetic field at  $x = 0$  yields

$$1 + \Gamma = T, \quad (11.37)$$

$$\frac{\beta_{1x}}{\omega\mu_1} (-1 + \Gamma) = -\frac{\gamma_{2x}}{j\omega\tilde{\mu}_2} T, \quad (11.38)$$

or, rearranging the second equation,

$$1 - \Gamma = \frac{\mu_1 \gamma_{2x}}{j\tilde{\mu}_2 \beta_{1x}} T. \quad (11.39)$$

Adding (11.37) and (11.39) and rearranging yields

$$T = \frac{j^2 \tilde{\mu}_2}{j \frac{\tilde{\mu}_2}{\gamma_{2x}} + \frac{\mu_1}{\beta_{1x}}}. \quad (11.40)$$

Using this in (11.37) yields the reflection coefficient

$$\Gamma = \frac{j \frac{\tilde{\mu}_2}{\gamma_{2x}} - \frac{\mu_1}{\beta_{1x}}}{j \frac{\tilde{\mu}_2}{\gamma_{2x}} + \frac{\mu_1}{\beta_{1x}}}. \quad (11.41)$$

The reflection coefficient will be zero only if the terms in the numerator cancel. Let us consider these terms individually. Additionally, let us enforce a more restrictive form of the matching conditions where now  $\mu_2 = \mu_1$ ,  $\epsilon_2 = \epsilon_1$  and, as before,  $\sigma/\epsilon_2 = \sigma_m/\mu_2$ . The first term in the numerator can be written

$$j \frac{\tilde{\mu}_2}{\gamma_{2x}} = \frac{\tilde{\mu}_2}{\sqrt{\omega^2 \tilde{\mu}_2 \tilde{\epsilon}_2 - \beta_{1y}^2}}, \quad (11.42)$$

$$= \frac{\mu_1 \left(1 - j \frac{\sigma}{\omega \epsilon_1}\right)}{\sqrt{\omega^2 \mu_1 \epsilon_1 \left(1 - j \frac{\sigma}{\omega \epsilon_1}\right)^2 - \beta_{1y}^2}}, \quad (11.43)$$

$$= \frac{\mu_1}{\sqrt{\omega^2 \mu_1 \epsilon_1 - \frac{\beta_{1y}^2}{\left(1 - j \frac{\sigma}{\omega \epsilon_1}\right)^2}}}. \quad (11.44)$$

The second term in the numerator of the reflection coefficient is

$$\frac{\mu_1}{\beta_{1x}} = \frac{\mu_1}{\sqrt{\omega^2 \mu_1 \epsilon_1 - \beta_{1y}^2}}. \quad (11.45)$$

Clearly (11.44) and (11.45) are not equal (unless we further require that  $\sigma = 0$ , but then the lossy layer is not lossy). Thus, for oblique incidence, the numerator of the reflection coefficient cannot be zero and there will always be some reflection from this lossy medium.

## 11.4 Split-Field Perfectly Matched Layer

To obtain a perfect match between the lossless and lossy regions, Bérenger proposed a non-physical anisotropic material known as a perfectly matched layer (PML). In a PML there is no loss in the direction tangential to the interface but there is loss normal to the interface.

First, consider the governing equations for the components of the magnetic fields for TM<sup>z</sup> polarization. We have

$$j\omega\mu_2 H_y + \sigma_{mx} H_y = \frac{\partial E_z}{\partial x} \quad (11.46)$$

$$j\omega\mu_2 H_x + \sigma_{my} H_x = -\frac{\partial E_z}{\partial y} \quad (11.47)$$

where  $\sigma_{mx}$  and  $\sigma_{my}$  are the magnetic conductivities associated *not* with the  $x$  and  $y$  components of the magnetic field, but rather with propagation in the  $x$  or  $y$  direction. (Note that for 1D propagation in the  $x$  direction the non-zero fields are  $H_y$  and  $E_z$  while for 1D propagation in the  $y$  direction they are  $H_x$  and  $E_z$ .)

For the electric field the governing equation is

$$j\omega\epsilon_2 E_z + \sigma E_z = \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} \quad (11.48)$$

Here there is a single conductivity and no possibility to have explicitly anisotropic behavior of the electrical conductivity. Thus, it would still be impossible to match the lossy region to the lossless one.

Bérenger's fix was to split the electric field into two (non-physical) components. To get the "actual" field, we merely sum these components. Thus we write

$$E_z = E_{zx} + E_{zy} \quad (11.49)$$

These components are governed by

$$j\omega\epsilon_2 E_{zx} + \sigma_x E_{zx} = \frac{\partial H_y}{\partial x}, \quad (11.50)$$

$$j\omega\epsilon_2 E_{zy} + \sigma_y E_{zy} = -\frac{\partial H_x}{\partial y}. \quad (11.51)$$

Note that there are now two electrical conductivities:  $\sigma_x$  and  $\sigma_y$ . If we set  $\sigma_x = \sigma_y = \sigma$  and add these two equations together, we recover the original equation (11.48). Further note that if  $\sigma_y = \sigma_{my} = 0$  but  $\sigma_x \neq 0$  and  $\sigma_{mx} \neq 0$ , then a wave with components  $H_x$  and  $E_{zy}$  would not attenuate while a wave with components  $H_y$  and  $E_{zx}$  would attenuate.

Let us define the terms  $S_w$  and  $S_{mw}$  as

$$S_w = 1 + \frac{\sigma_w}{j\omega\epsilon_2} \quad (11.52)$$

$$S_{mw} = 1 + \frac{\sigma_{mw}}{j\omega\mu_2} \quad (11.53)$$

where  $w$  is either  $x$  or  $y$ . We can then write the governing equations as

$$j\omega\epsilon_2 S_x E_{zx} = \frac{\partial H_y}{\partial x}, \quad (11.54)$$

$$j\omega\epsilon_2 S_y E_{zy} = -\frac{\partial H_x}{\partial y}, \quad (11.55)$$

$$j\omega\mu_2 S_{mx} H_y = \frac{\partial}{\partial x} (E_{zx} + E_{zy}), \quad (11.56)$$

$$j\omega\mu_2 S_{my} H_x = -\frac{\partial}{\partial y} (E_{zx} + E_{zy}). \quad (11.57)$$

Taking the partial of (11.56) with respect to  $x$  and then substituting in the left-hand side of (11.54) yields

$$-\omega^2 \mu_2 \epsilon_2 S_x S_{mx} E_{zx} = \frac{\partial^2}{\partial x^2} (E_{zx} + E_{zy}). \quad (11.58)$$

Taking the partial of (11.57) with respect to  $y$  and then substituting in the left-hand side of (11.55) yields

$$-\omega^2 \mu_2 \epsilon_2 S_y S_{my} E_{zy} = \frac{\partial^2}{\partial y^2} (E_{zx} + E_{zy}). \quad (11.59)$$

Adding these two expressions together after dividing by the  $S$  terms yields

$$-\omega^2 \mu_2 \epsilon_2 (E_{zx} + E_{zy}) = \left( \frac{1}{S_{mx} S_x} \frac{\partial^2}{\partial x^2} + \frac{1}{S_{my} S_y} \frac{\partial^2}{\partial y^2} \right) (E_{zx} + E_{zy}) \quad (11.60)$$

or, after rearranging and recalling that  $E_{zx} + E_{zy} = E_z$ ,

$$\left( \frac{1}{S_{mx}S_x} \frac{\partial^2}{\partial x^2} + \frac{1}{S_{my}S_y} \frac{\partial^2}{\partial y^2} + \omega^2 \mu_2 \epsilon_2 \right) E_z = 0. \quad (11.61)$$

To satisfy this equation the transmitted field in the PML region would be given by

$$E_z^t = T e^{-j\sqrt{S_{mx}S_x}\beta_{2x}x - j\sqrt{S_{my}S_y}\beta_{2y}y} \quad (11.62)$$

where we must also have

$$\beta_{2x}^2 + \beta_{2y}^2 = \omega^2 \mu_2 \epsilon_2. \quad (11.63)$$

Using (11.56), the  $y$  component of the magnetic field in the PML is given by

$$H_y^t = \frac{1}{j\omega\mu_2 S_{mx}} \frac{\partial E_z^t}{\partial x} \quad (11.64)$$

$$= -\frac{\sqrt{S_{mx}S_x}\beta_{2x}}{\omega\mu_2 S_{mx}} E_z^t, \quad (11.65)$$

$$= -\frac{\beta_{2x}}{\omega\mu_2} \sqrt{\frac{S_x}{S_{mx}}} E_z^t. \quad (11.66)$$

As always, the tangential fields must match at the interface. Matching the electric fields again yields (11.37). Matching the  $y$  component of the magnetic fields yields

$$1 - \Gamma = \frac{\mu_1 \beta_{2x}}{\mu_2 \beta_{1x}} \sqrt{\frac{S_x}{S_{mx}}} T. \quad (11.67)$$

Using this and (11.37) to solve for the transmission and reflection coefficients yields

$$T = \frac{2\frac{\beta_{1x}}{\mu_1}}{\frac{\beta_{1x}}{\mu_1} + \frac{\beta_{2x}}{\mu_2} \sqrt{\frac{S_x}{S_{mx}}}}, \quad (11.68)$$

$$\Gamma = \frac{\frac{\beta_{1x}}{\mu_1} - \frac{\beta_{2x}}{\mu_2} \sqrt{\frac{S_x}{S_{mx}}}}{\frac{\beta_{1x}}{\mu_1} + \frac{\beta_{2x}}{\mu_2} \sqrt{\frac{S_x}{S_{mx}}}}. \quad (11.69)$$

It is now possible to match the PML to the non-PML region so that  $\Gamma$  is zero. We begin by setting  $\mu_2 = \mu_1$  and  $\epsilon_2 = \epsilon_1$ . Thus we have  $\omega^2 \mu_2 \epsilon_2 = \omega^2 \mu_1 \epsilon_1$  and

$$\beta_{2x} = (\omega^2 \mu_2 \epsilon_2 - \beta_{2y}^2)^{1/2}, \quad (11.70)$$

$$= (\omega^2 \mu_1 \epsilon_1 - \beta_{2y}^2)^{1/2}. \quad (11.71)$$

Recall that within the PML the propagation in the  $y$  direction is not given by  $\beta_{2y}$  but rather by  $\sqrt{S_y S_{my}} \beta_{2y}$ . Phase matching along the interface requires that

$$\sqrt{S_y S_{my}} \beta_{2y} = \beta_{1y}. \quad (11.72)$$



If we let  $S_y = S_{my} = 1$ , which can be realized by setting  $\sigma_y = \sigma_{my} = 0$ , then the phase matching condition reduces to

$$\beta_{2y} = \beta_{1y}. \quad (11.73)$$

Then, from (11.71), we have

$$\beta_{2x} = (\omega^2 \mu_1 \epsilon_1 - \beta_{1y}^2)^{1/2}, \quad (11.74)$$

$$= \beta_{1x}. \quad (11.75)$$

Returning to (11.69), we now have

$$\Gamma = \frac{\frac{\beta_{1x}}{\mu_1} - \frac{\beta_{1x}}{\mu_1} \sqrt{\frac{S_x}{S_{mx}}}}{\frac{\beta_{1x}}{\mu_1} + \frac{\beta_{1x}}{\mu_1} \sqrt{\frac{S_x}{S_{mx}}}}, \quad (11.76)$$

$$= \frac{1 - \sqrt{\frac{S_x}{S_{mx}}}}{1 + \sqrt{\frac{S_x}{S_{mx}}}}. \quad (11.77)$$

The last remaining requirement to achieve a perfect match is to have  $S_x = S_{mx}$ . This can be realized by having  $\sigma_x/\epsilon_2 = \sigma_{mx}/\mu_2$ .

To summarize, the complete set of matching conditions for a constant- $x$  interface are

$$\epsilon_2 = \epsilon_1 \quad (11.78)$$

$$\mu_2 = \mu_1 \quad (11.79)$$

$$\sigma_y = \sigma_{my} = 0 \quad (11.80)$$

$$\frac{\sigma_x}{\epsilon_2} = \frac{\sigma_{mx}}{\mu_2}. \quad (11.81)$$

Under these conditions propagation in the PML is governed by

$$e^{-jS_x\beta_{1x}x - j\beta_{1y}y} = \exp\left(-j\left(1 + \frac{\sigma}{j\omega\epsilon_1}\right)\beta_{1x}x - j\beta_{1y}y\right), \quad (11.82)$$

$$= \exp\left(-\frac{\beta_{1x}\sigma}{\omega\epsilon_1}x\right) e^{-j\beta_{1x}x - j\beta_{1y}y}. \quad (11.83)$$

This shows that there is exponential decay in the  $x$  direction but otherwise the phase propagates in exactly the same way as it does in the non-PML region.

## 11.5 Un-Split PML

In the previous section we had  $S_w$  and  $S_{mw}$  where  $w \in \{x, y\}$ . However, once the matching condition has been applied, i.e.,  $\sigma_w/\epsilon_2 = \sigma_{mw}/\mu_2$ , then we have  $S_w = S_{mw}$ . Hence we will drop the  $m$  from the subscript. Additionally, with the understanding that we are talking about the PML region, we will drop the subscript 2 from the material constants. We thus write

$$S_w = 1 + \frac{\sigma_w}{j\omega\epsilon}. \quad (11.84)$$

The conductivity in the PML is not dictated by underlying parameters in the physical space being modeled. Rather, this conductivity is set so as to minimize the reflections from the termination of the grid. In that sense  $\sigma_w$  is somewhat arbitrary. Therefore let us normalize the conductivity by the relative permittivity that pertains at that particular location, i.e.,

$$S_w = 1 + \frac{\sigma'_w}{j\omega\epsilon_0} \quad (11.85)$$

where  $\sigma'_w = \sigma_w/\epsilon_r$ . However, since the conductivity has not yet been specified, we drop the prime and merely write

$$S_w = 1 + \frac{\sigma_w}{j\omega\epsilon_0} \quad (11.86)$$

Note that there could potentially be a problem with  $S_w$  when the frequency goes to zero. In practice, in the curl equations this term is also multiplied by  $\omega$  and in that sense this is not a major problem. However, if we want to move these  $S_w$  terms around, low frequencies may cause problems. To fix this, we add an additional factor to ensure that  $S_w$  remains finite as the frequency goes to zero.

We can further generalize  $S_w$  by allowing the leading term to take on values other than unity. This is effectively equivalent to allowing the relative permittivity in the PML to change. The general expression for  $S_w$  we will use is

$$S_w = \kappa_w + \frac{\sigma_w}{a_w + j\omega\epsilon_0}. \quad (11.87)$$

For the sake of considering 3D problems we also assume  $w \in \{x, y, z\}$ .

Dividing by the  $S$  terms, the governing equations for TM<sup>z</sup> polarization are

$$j\omega\epsilon E_{zx} = \frac{1}{S_x} \frac{\partial H_y}{\partial x}, \quad (11.88)$$

$$j\omega\epsilon E_{zy} = -\frac{1}{S_y} \frac{\partial H_x}{\partial y}, \quad (11.89)$$

$$j\omega\mu H_y = \frac{1}{S_x} \frac{\partial E_z}{\partial x}, \quad (11.90)$$

$$j\omega\mu H_x = -\frac{1}{S_y} \frac{\partial E_z}{\partial y}. \quad (11.91)$$

Adding the first two equations together we obtain

$$j\omega\epsilon E_z = \frac{1}{S_x} \frac{\partial H_y}{\partial x} - \frac{1}{S_y} \frac{\partial H_x}{\partial y}. \quad (11.92)$$

Note that in all these equations each  $S_w$  term is always paired with the derivative in the “ $w$ ” direction.

Let us define a new del operator  $\tilde{\nabla}$  that incorporates this pairing

$$\tilde{\nabla} \equiv \hat{\mathbf{a}}_x \frac{1}{S_x} \frac{\partial}{\partial x} + \hat{\mathbf{a}}_y \frac{1}{S_y} \frac{\partial}{\partial y} + \hat{\mathbf{a}}_z \frac{1}{S_z} \frac{\partial}{\partial z}. \quad (11.93)$$

Using this operator Maxwell's curl equations become

$$j\omega\epsilon\mathbf{E} = \tilde{\nabla} \times \mathbf{H}, \quad (11.94)$$

$$-j\omega\mu\mathbf{H} = \tilde{\nabla} \times \mathbf{E}. \quad (11.95)$$

Note that these equations pertain to the general 3D case. This is known as the stretch-coordinate PML formulation since, as shown in (11.93), the complex  $S$  terms scale the various coordinate directions. Additionally, note there is no explicit mention of split fields in these equations. If we can find a way to implement these equations directly in the FDTD algorithm, we can avoid splitting the fields.

From these curl equations we obtain scalar equations such as (using the  $x$ -component of (11.94) and (11.95) as examples)

$$j\omega\epsilon E_x = \frac{1}{S_y} \frac{\partial H_z}{\partial y} - \frac{1}{S_z} \frac{\partial H_y}{\partial z}, \quad (11.96)$$

$$j\omega\mu H_x = -\frac{1}{S_y} \frac{\partial E_z}{\partial y} + \frac{1}{S_z} \frac{\partial E_y}{\partial z}. \quad (11.97)$$

Converting these to the time-domain yields

$$\epsilon \frac{\partial E_x}{\partial t} = \bar{S}_y \star \frac{\partial H_z}{\partial y} - \bar{S}_z \star \frac{\partial H_y}{\partial z}, \quad (11.98)$$

$$\mu \frac{\partial H_x}{\partial t} = -\bar{S}_y \star \frac{\partial E_z}{\partial y} + \bar{S}_z \star \frac{\partial E_y}{\partial z}, \quad (11.99)$$

where “ $\star$ ” indicates convolution and  $\bar{S}_w$  is the inverse Fourier transform of  $1/S_w$ , i.e.,

$$\bar{S}_w = \mathcal{F}^{-1} \left[ \frac{1}{S_w} \right]. \quad (11.100)$$

The reciprocal of  $S_w$  is given by

$$\frac{1}{S_w} = \frac{1}{\kappa_w + \frac{\sigma_w}{a_w + j\omega\epsilon_0}} = \frac{a_w + j\omega\epsilon_0}{a_w\kappa_w + \sigma_w + j\omega\kappa_w\epsilon_0}. \quad (11.101)$$

This is of the form  $(a + j\omega b)/(c + j\omega d)$  and we cannot do a partial fraction expansion since the order of the numerator and denominator are the same. Instead, we can divide the denominator into the numerator to obtain

$$\frac{a + j\omega b}{c + j\omega d} = \frac{b}{d} + \frac{a - c\frac{b}{d}}{c + j\omega d} = \frac{b}{d} + \frac{\frac{a}{c} - \frac{b}{d}}{1 + j\omega\frac{d}{c}}. \quad (11.102)$$

Recall the following Fourier transform pairs:

$$1 \Leftrightarrow \delta(t), \quad (11.103)$$

$$\frac{1}{1 + j\omega\tau} \Leftrightarrow \frac{1}{\tau} e^{-t/\tau} u(t), \quad (11.104)$$

where  $\delta(t)$  is the Dirac delta function and  $u(t)$  is the unit step function. Thus, we have

$$\mathcal{F}^{-1} \left[ \frac{b}{d} + \frac{\frac{a}{c} - \frac{b}{d}}{1 + j\omega \frac{d}{c}} \right] = \frac{b}{d} \delta(t) + \frac{ad - bc}{d^2} e^{-ct/d} u(t). \quad (11.105)$$

For the problem at hand, we have  $a = a_w$ ,  $b = \epsilon_0$ ,  $c = a_w \kappa_w + \sigma_w$ , and  $d = \kappa_w \epsilon_0$ . Using these values in (11.105) yields

$$\bar{S}_w = \frac{1}{\kappa_w} \delta(t) - \frac{\sigma_w}{\kappa_w^2 \epsilon_0} \exp \left( -t \left[ \frac{a_w}{\epsilon_0} + \frac{\sigma_w}{\kappa_w \epsilon_0} \right] \right) u(t). \quad (11.106)$$

Let us define  $\zeta_w(t)$  as

$$\zeta_w(t) = -\frac{\sigma_w}{\kappa_w^2 \epsilon_0} \exp \left( -t \left[ \frac{a_w}{\epsilon_0} + \frac{\sigma_w}{\kappa_w \epsilon_0} \right] \right) u(t) \quad (11.107)$$

so that

$$\bar{S}_w = \frac{1}{\kappa_w} \delta(t) + \zeta_w(t). \quad (11.108)$$

Recall that the convolution of a Dirac delta function with another function yields the original function, i.e.,

$$\delta(t) \star f(t) = f(t). \quad (11.109)$$

Incorporating this fact into (11.98) yields

$$\begin{aligned} \epsilon \frac{\partial E_x}{\partial t} &= \frac{1}{\kappa_y} \frac{\partial H_z}{\partial y} - \frac{1}{\kappa_z} \frac{\partial H_y}{\partial z} \\ &+ \zeta_y(t) \star \frac{\partial H_z}{\partial y} - \zeta_z(t) \star \frac{\partial H_y}{\partial z}. \end{aligned} \quad (11.110)$$

Note that the first line of this equation is almost the usual governing equation. The only differences are the  $\kappa$ 's. However, these are merely real constants. In the FDTD algorithm it is trivial to incorporate these terms in the update-equation coefficients. The second line again involves convolutions. Fortunately, these convolution are rather “benign” and, as we shall see, can be calculated efficiently using recursive convolution.

## 11.6 FDTD Implementation of Un-Split PML

We now wish to develop an FDTD implementation of the PML as formulated in the previous section. We start by defining the function  $\Psi_{E_u w}^q$  as

$$\Psi_{E_u w}^q = \zeta_w(t) \star \left. \frac{\partial H_v}{\partial w} \right|_{t=q\Delta_t} \quad (11.111)$$

$$= \int_{\tau=0}^{q\Delta_t} \zeta_w(\tau) \frac{\partial H_v(q\Delta_t - \tau)}{\partial w} d\tau \quad (11.112)$$

where  $E_u w$  in the subscript indicates this function will appear in the update of the  $E_u$  component of the electric field and it is concerned with the spatial derivative in the  $w$  direction. In (11.112) the derivative is of the  $H_v$  component of the magnetic field where  $w, u,$  and  $v$  are such that  $\{w, u, v\} \in \{x, y, z\}$  and  $w \neq u \neq v$ .

In (11.112) note that  $\zeta_w(\tau)$  is zero for  $\tau < 0$  hence the integrand would be zero for  $\tau < 0$ . This fixes the lower limit of integration to zero. On the other hand, we assume the fields are zero prior to  $t = 0$ , i.e.,  $H_v(t)$  is zero for  $t < 0$ . In the convolution the argument of the magnetic field is  $q\Delta_t - \tau$ . This argument will be negative when  $\tau > q\Delta_t$ . Thus the integrand will be zero for  $\tau > q\Delta_t$  and this fixes the upper limit of integration to  $q\Delta_t$ .

Let us assume the integration variable  $\tau$  in (11.112) varies continuously but, since we are considering fields in the FDTD method,  $H_v$  varies discretely. We can still express  $H_v$  in terms of a continuously varying argument  $t$ , but it takes on discrete values. Specifically  $\partial H_v(t)/\partial w$  can be represented by

$$\frac{\partial H_v(t)}{\partial w} = \sum_{i=0}^{I_{\max}} \frac{\partial H_v(i\Delta_t)}{\partial w} p_i(t) \quad (11.113)$$

where  $p_i(t)$  is the unit pulse function given by

$$p_i(t) = \begin{cases} 1 & \text{if } i\Delta_t \leq t < (i+1)\Delta_t, \\ 0 & \text{otherwise.} \end{cases} \quad (11.114)$$

To illustrate this further, for notational convenience let us write  $f(t) = \partial H_v(t)/\partial w$ . The stepwise representation of this function is shown in Fig. 11.1(a). Although not necessary, as is typical with FDTD simulations, this function is assumed to be zero for the first time-step. At  $t = \Delta_t$  the function is  $f_1$  and it remains constant until  $t = 2\Delta_t$  when it changes to  $f_2$ . At  $t = 3\Delta_t$  the function is  $f_3$ , and so on.

The convolution contains the function  $f(q\Delta_t - \tau)$ . At time-step zero (i.e.,  $q = 0$ ), this is merely  $f(-\tau)$  which is illustrated in Fig. 11.1(b). Here all the sample points  $f_n$  are flipped symmetrically about the origin. We assume that the function is constant to the right of these sample points so that the function is  $f_1$  for  $-\Delta_t \leq \tau < 0$ , it is  $f_2$  for  $-2\Delta_t \leq \tau < -\Delta_t$ ,  $f_3$  for  $-3\Delta_t \leq \tau < -2\Delta_t$ , and so on.

Fig. 11.1(c) shows an example of  $f(q\Delta_t - \tau)$  when  $q \neq 0$ , specifically for  $q = 4$ . Recall that in (11.112) the limits of integration are from zero to  $q\Delta_t$ —we do not need to concern ourselves with  $\tau$  less than zero nor greater than  $q\Delta_t$ . As shown in Fig. 11.1(c), the first “pulse” extending to the right of  $\tau = 0$  has a value of  $f_q$ , the pulse extending to the right of  $\tau = \Delta_t$  has a value of  $f_{q-1}$ , the one to the right of  $\tau = 2\Delta_t$  has a value of  $f_{q-2}$ , and so on. Thus, this shifted function can be written as

$$f(q\Delta_t - \tau) = \sum_{i=0}^{q-1} f_{q-i} p_i(\tau). \quad (11.115)$$

Returning to the derivative of the magnetic field, we write

$$\frac{\partial H_v(q\Delta_t - \tau)}{\partial w} = \sum_{i=0}^{q-1} \frac{\partial H_v^{q-i}}{\partial w} p_i(\tau) \quad (11.116)$$

where  $H_v^{q-i}$  is the magnetic field at time-step  $q-i$  and, when implemented in the FDTD algorithm, the spatial derivative will be realized as a spatial finite difference.

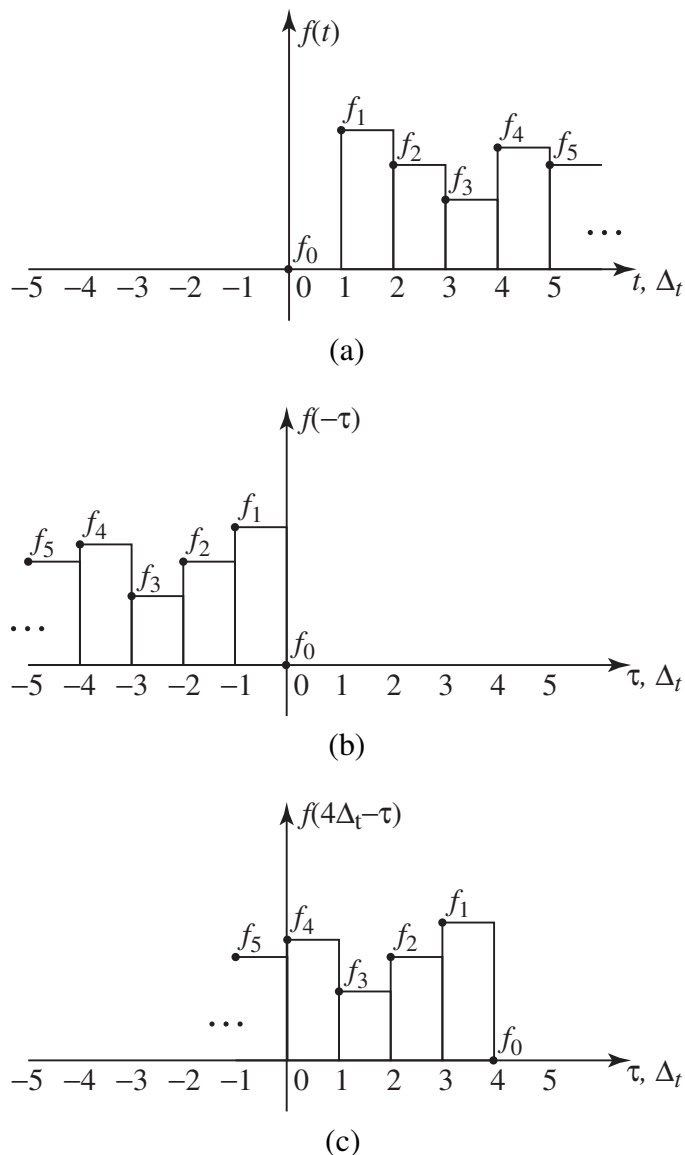


Figure 11.1: (a) Stepwise representation of a function  $f(t)$ . The function is a constant  $f_0$  for  $0 \leq t < \Delta_t$ ,  $f_1$  for  $\Delta_t \leq t < 2\Delta_t$ ,  $f_2$  for  $2\Delta_t \leq t < 3\Delta_t$ , and so on. (b) Stepwise representation of a function  $f(-\tau)$ . Here the constants  $f_n$  are flipped about the origin but the pulses still extend for one time-step to the right of the corresponding point. Hence the function is a constant  $f_1$  for  $-\Delta_t \leq \tau < 0$ ,  $f_2$  for  $-2\Delta_t \leq \tau < -\Delta_t$ , etc. (c) Stepwise representation of the function  $f(q\Delta_t - \tau)$  when  $q = 4$ .

At time-step  $q$ ,  $\Psi_{E_u w}$  is given by

$$\Psi_{E_u w}^q = \int_{\tau=0}^{q\Delta t} \zeta_w(\tau) \sum_{i=0}^{q-1} \frac{\partial H_v^{q-i}}{\partial w} p_i(\tau) d\tau \quad (11.117)$$

Interchanging the order of summation and integration yields

$$\Psi_{E_u w}^q = \sum_{i=0}^{q-1} \frac{\partial H_v^{q-i}}{\partial w} \int_{\tau=0}^{q\Delta t} \zeta_w(\tau) p_i(\tau) d\tau, \quad (11.118)$$

$$= \sum_{i=0}^{q-1} \frac{\partial H_v^{q-i}}{\partial w} \int_{\tau=i\Delta t}^{(i+1)\Delta t} \zeta_w(\tau) d\tau, \quad (11.119)$$

where, in going from (11.118) to (11.119), the pulse function was used to establish the limits of integration.

Consider the following integral

$$- \int_{i\Delta}^{(i+1)\Delta} e^{-at} dt = \frac{1}{a} e^{-at} \Big|_{i\Delta}^{(i+1)\Delta} \quad (11.120)$$

$$= \frac{1}{a} (e^{-a(i+1)\Delta} - e^{-ai\Delta}) \quad (11.121)$$

$$= \frac{1}{a} (e^{-a\Delta} - 1) e^{-ai\Delta} \quad (11.122)$$

$$= \frac{1}{a} (e^{-a\Delta} - 1) (e^{-a\Delta})^i \quad (11.123)$$

Keeping this in mind, the integration in (11.119) can be written as

$$\int_{\tau=i\Delta t}^{(i+1)\Delta t} \zeta_w(\tau) d\tau = -\frac{\sigma_w}{\kappa_w^2 \epsilon_0} \int_{\tau=i\Delta t}^{(i+1)\Delta t} \exp\left(-\tau \left[\frac{a_w}{\epsilon_0} + \frac{\sigma_w}{\kappa_w \epsilon_0}\right]\right) d\tau \quad (11.124)$$

$$= C_w (b_w)^i \quad (11.125)$$

where

$$b_w = \exp\left(-\left[\frac{a_w}{\epsilon_0} + \frac{\sigma_w}{\kappa_w \epsilon_0}\right] \Delta t\right), \quad (11.126)$$

$$C_w = \frac{\sigma_w}{\sigma_w \kappa_w + \kappa_w^2 a_w} (b_w - 1). \quad (11.127)$$

Note that in (11.125)  $b_w$  is raised to the power  $i$  which is an integer index. It is now possible to express  $\Psi_{E_u w}^q$  as

$$\Psi_{E_u w}^q = \sum_{i=0}^{q-1} \frac{\partial H_v^{q-i}}{\partial w} C_w (b_w)^i. \quad (11.128)$$

Let us explicitly separate the  $i = 0$  term from the rest of the summation:

$$\Psi_{E_u w}^q = C_w \frac{\partial H_v^q}{\partial w} + \sum_{i=1}^{q-1} \frac{\partial H_v^{q-i}}{\partial w} C_w (b_w)^i. \quad (11.129)$$

Replacing the index  $i$  with  $i' = i - 1$  (so that  $i = i' + 1$ ), this becomes

$$\Psi_{E_u w}^q = C_w \frac{\partial H_v^q}{\partial w} + \sum_{i'=0}^{q-2} \frac{\partial H_v^{q-i'-1}}{\partial w} C_w (b_w)^{i'+1}. \quad (11.130)$$

Dropping the prime from the index and rearranging slightly yields

$$\Psi_{E_u w}^q = C_w \frac{\partial H_v^q}{\partial w} + b_w \sum_{i=0}^{[q-1]-1} \frac{\partial H_v^{[q-1]-i}}{\partial w} C_w (b_w)^i. \quad (11.131)$$

Comparing the summation in this expression to the one in (11.128) one sees that this expression can be written as

$$\Psi_{E_u w}^q = C_w \frac{\partial H_v^q}{\partial w} + b_w \Psi_{E_u w}^{q-1}. \quad (11.132)$$

Note that  $\Psi_{E_u w}$  at time-step  $q$  is a function of  $\Psi_{E_u w}$  at time-step  $q - 1$ . Thus  $\Psi_{E_u w}$  can be updated recursively—there is no need to store the entire history of  $\Psi_{E_u w}$  to obtain the next value. As is typical with FDTD, one merely needs to know  $\Psi_{E_u w}$  at the previous time step.

We now have all the pieces in place to implement a PML in the FDTD method. The algorithm to update the electric fields is

1. Update the  $\Psi_{E_u w}$  terms employing the recursive update equation given by (11.132). Recall that these  $\Psi_{E_u w}$  functions represent the convolutions given in the second line of (11.110).
2. Update the electric fields in the standard way. However, incorporate the  $\kappa$ 's where appropriate. Essentially one employs the update equation implied by the top line of (11.110) (where that equation applies to  $E_x$  and similar equations apply to  $E_y$  and  $E_z$ ).
3. Apply, i.e., add or subtract,  $\Psi_{E_u w}$  to the electric field as indicated by the second line of (11.110).

This completes the update of the electric field.

The magnetic fields are updated in a completely analogous manner. First the  $\Psi$  functions that pertain to the magnetic fields are updated (in this case there are  $\Psi_{H_u w}$  functions that involve the spatial derivatives of the electric fields), then the magnetic fields are updated in the usual way (accounting for any  $\kappa$ 's), and finally the  $\Psi$  functions are applied to the magnetic fields (i.e., added or subtracted).