Chapter 8
Perfectly Matched Layers

One common problem in computational electromagnetics is how to simulate wave propagation on an unbounded domain accurately and efficiently. One typical technique is to use the absorbing boundary conditions (ABCs) to truncate the unbounded domain to a bounded domain. The solution computed with an ABC on a bounded domain should be a good approximation to the solution originally given on the unbounded domain. Hence constructing a good ABC is quite challenging.

Over the years various ABCs have been developed in computational electromagnetics, and the most effective ABC seems to be the perfectly matched layer (PML) introduced by Berenger in 1994 [34]. Since 1994, the PML has been intensively investigated, and many interesting results have been obtained (cf. [10], [276, Chap. 7] and references therein).

In this chapter, we present some interesting PMLs developed over the last 20 years. More specifically, in Sect. 8.1, we discuss three ways for obtaining the PMLs matched to the free space. Then in Sect. 8.2, we extend the discussion to lossy media. Finally, we describe some PMLs developed for the dispersive media and metamaterials in Sect. 8.3.

8.1 PMLs Matched to the Free Space

8.1.1 Berenger Split PMLs

In 1994, Berenger [34] proposed the first time-domain perfectly matched layer for modeling electromagnetic wave propagation in unbounded free space. The basic idea is to introduce a specially designed layer to absorb the electromagnetic waves without any reflection from the interfaces between the free space and the special layer. Later in 1996, Berenger [35] extended the PML medium technique to 3-D. Below we shall introduce the 3-D Berenger PML, since the 2-D PML can be directly obtained from the 3-D model as special cases. Following [35], Berenger's PML is

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based on a splitted form of Maxwell's equations: the six field components are split into 12 subcomponents (i.e., $\mathbf{E}_x = E_{xy} + E_{xz}, \mathbf{E}_y = E_{yx} + E_{yz}, \mathbf{E}_z = E_{zx} + E_{zy}$, $\mathbf{H}_x = H_{xy} + H_{xz}, \mathbf{H}_y = H_{yx} + H_{yz}, \mathbf{H}_z = H_{zx} + H_{zy}$), in which case the original six Cartesian equations are split into 12 subequations as follows:

$$\epsilon_0 \frac{\partial E_{xy}}{\partial t} + \sigma_y E_{xy} = \frac{\partial (H_{zx} + H_{zy})}{\partial y} \tag{8.1a}$$

$$\epsilon_0 \frac{\partial E_{xz}}{\partial t} + \sigma_z E_{xz} = -\frac{\partial (H_{yz} + H_{yx})}{\partial z} \tag{8.1b}$$

$$\epsilon_0 \frac{\partial E_{yz}}{\partial t} + \sigma_z E_{yz} = \frac{\partial (H_{xy} + H_{xz})}{\partial z} \tag{8.1c}$$

$$\epsilon_0 \frac{\partial E_{yx}}{\partial t} + \sigma_x E_{yx} = -\frac{\partial (H_{zx} + H_{zy})}{\partial x} \tag{8.1d}$$

$$\epsilon_0 \frac{\partial E_{zx}}{\partial t} + \sigma_x E_{zx} = \frac{\partial (H_{yz} + H_{yx})}{\partial x} \tag{8.1e}$$

$$\epsilon_0 \frac{\partial E_{zy}}{\partial t} + \sigma_y E_{zy} = -\frac{\partial (H_{xy} + H_{xz})}{\partial y} \tag{8.1f}$$

$$\mu_0 \frac{\partial H_{xy}}{\partial t} + \sigma_y^* H_{xy} = -\frac{\partial (E_{zx} + E_{zy})}{\partial y} \tag{8.1g}$$

$$\mu_0 \frac{\partial H_{xz}}{\partial t} + \sigma_z^* H_{xz} = \frac{\partial (E_{yz} + E_{yx})}{\partial z} \tag{8.1h}$$

$$\mu_0 \frac{\partial H_{yz}}{\partial t} + \sigma_z^* H_{yz} = -\frac{\partial (E_{xy} + E_{xz})}{\partial z} \tag{8.1i}$$

$$\mu_0 \frac{\partial H_{yx}}{\partial t} + \sigma_x^* H_{yx} = \frac{\partial (E_{zx} + E_{zy})}{\partial x} \tag{8.1j}$$

$$\mu_0 \frac{\partial H_{zx}}{\partial t} + \sigma_x^* H_{zx} = -\frac{\partial (E_{yx} + E_{yz})}{\partial x} \tag{8.1k}$$

$$\mu_0 \frac{\partial H_{zy}}{\partial t} + \sigma_y^* H_{zy} = \frac{\partial (E_{xy} + E_{xz})}{\partial y} \tag{8.1l}$$

where parameters $\sigma_i, \sigma_i^*, i = x, y, z$, are the homogeneous electric and magnetic conductivities in the i direction.

Replacing each component of (8.1) by a plane wave solution, for example,

$$E_{xy} = \tilde{E}_{xy} e^{j(\omega t - \mathbf{k} \cdot \mathbf{r})}, \tag{8.2}$$

we can obtain 12 equations expressed in terms of the angular frequency ω, the wave number $\mathbf{k} = (k_x, k_y, k_z)$, the position vector $\mathbf{r} = (x, y, z)$, and 12 components $\tilde{E}_{xy}, \tilde{E}_{xz}, \cdots, \tilde{H}_{zx}, \tilde{H}_{zy}$. By introducing stretching parameters s_i and s_i^* [35]:

$$s_i = 1 + \frac{\sigma_i}{j\omega\epsilon_0}, \quad s_i^* = 1 + \frac{\sigma_i^*}{j\omega\mu_0}, \quad i = x, y, z, \tag{8.3}$$

we can further reduce the resulting 12 equations into just 6 equations:

$$\omega\epsilon_0 \tilde{E}_x = -\frac{k_y}{s_y}\tilde{H}_z + \frac{k_z}{s_z}\tilde{H}_y \tag{8.4a}$$

$$\omega\epsilon_0 \tilde{E}_y = -\frac{k_z}{s_z}\tilde{H}_x + \frac{k_x}{s_x}\tilde{H}_z \tag{8.4b}$$

$$\omega\epsilon_0 \tilde{E}_z = -\frac{k_x}{s_x}\tilde{H}_y + \frac{k_y}{s_y}\tilde{H}_x \tag{8.4c}$$

$$\omega\mu_0 \tilde{H}_x = \frac{k_y}{s_y^*}\tilde{E}_z - \frac{k_z}{s_z^*}\tilde{E}_y \tag{8.4d}$$

$$\omega\mu_0 \tilde{H}_y = \frac{k_z}{s_z^*}\tilde{E}_x - \frac{k_x}{s_x^*}\tilde{E}_z \tag{8.4e}$$

$$\omega\mu_0 \tilde{H}_z = \frac{k_x}{s_x^*}\tilde{E}_y - \frac{k_y}{s_y^*}\tilde{E}_x, \tag{8.4f}$$

where we denote

$$\tilde{E}_x = \tilde{E}_{xy} + \tilde{E}_{xz},\ \tilde{E}_y = \tilde{E}_{yx} + \tilde{E}_{yz},\ \tilde{E}_z = \tilde{E}_{zx} + \tilde{E}_{zy}, \tag{8.5}$$

$$\tilde{H}_x = \tilde{H}_{xy} + \tilde{H}_{xz},\ \tilde{H}_y = \tilde{H}_{yx} + \tilde{H}_{yz},\ \tilde{H}_z = \tilde{H}_{zx} + \tilde{H}_{zy}. \tag{8.6}$$

Note that (8.4) can be rewritten in vector form as

$$\epsilon_0\omega\tilde{\mathbf{E}} = -\mathbf{k}_s \times \tilde{\mathbf{H}},\ \ \mu_0\omega\tilde{\mathbf{H}} = \mathbf{k}_s^* \times \tilde{\mathbf{E}}, \tag{8.7}$$

where we denote

$$\tilde{\mathbf{E}} = (\tilde{E}_x, \tilde{E}_y, \tilde{E}_z)', \quad \tilde{\mathbf{H}} = (\tilde{H}_x, \tilde{H}_y, \tilde{H}_z)'.$$

and

$$\mathbf{k}_s = (k_x/s_x, k_y/s_y, k_z/s_z)',\ \ \mathbf{k}_s^* = (k_x/s_x^*, k_y/s_y^*, k_z/s_z^*)'.$$

It is interesting to note that if applying (8.2) to the Maxwell's equations in vaccum

$$\epsilon_0\frac{\partial \mathbf{E}}{\partial t} = \nabla \times \mathbf{H}, \quad -\mu_0\frac{\partial \mathbf{H}}{\partial t} = \nabla \times \mathbf{E}, \tag{8.8}$$

we have

$$\epsilon_0 \omega \tilde{\mathbf{E}} = -\mathbf{k} \times \tilde{\mathbf{H}}, \quad \mu_0 \omega \tilde{\mathbf{H}} = \mathbf{k} \times \tilde{\mathbf{E}}, \tag{8.9}$$

which is a special case of the PML equations (8.7). This fact is not surprising, since (8.8) is a special case of (8.1) with $\sigma_i = \sigma_i^* = 0, \ i = x, y, z$.

To make the PML work properly, the electric and magnetic conductivities have to be choosen carefully. In the PML region matched to a vacuum, the transverse conductivities equal zero and the longitudinal conductivities satisfy the impedance matching condition

$$\frac{\sigma_i}{\epsilon_0} = \frac{\sigma_i^*}{\mu_0}, \quad i = x, y, z. \tag{8.10}$$

For example, consider an inner vacuum domain surrounded by an absorbing PML medium. On the six walls of the computational domain, the transverse conductivities of the PML media are set to zero in order to cancel the reflection from the vacuum-PML interfaces. For example, $(0, 0, 0, 0, \sigma_z, \sigma_z^*)$ should be used in the upper and lower walls (i.e., the interfaces normal to the z-direction). Along the 12 interface edges, the longitudinal conductivities are equal to zero, and the transverse conductivities are equal to those of the adjacent side media. Hence, no reflection is produced theoretically from side-edge interfaces. In the eight corner regions, the conductivities are chosen to match those of the adjacent edges, i.e., the transverse conductivities match at interfaces between edge layers and corner layers, which makes zero reflection from all the edge-corner interfaces. Detailed specifications of conductivities in the edge and corner regions of PML are depicted in Fig. 8.1 (cf. Fig. 3 of [35]). Many experiments ([276]) show that the PML conductivities (either σ_i or σ_i^*) can be simply chosen as a polynomial:

$$\sigma_\rho(\rho) = \sigma_* (\frac{\rho}{\delta})^n, \tag{8.11}$$

where $n \geq 2$ is the polynomial degree, δ is the PML thickness, ρ is the distance from the interface, σ_* is the conductivity on the outer side of the PML (at $\rho = \delta$). Note that given a reflection goal $R(0)$, σ_* is often chosen as

$$\sigma_* = -\frac{(n+1)\epsilon_0 C_v}{2\delta} \ln R(0). \tag{8.12}$$

Recall that $C_v = 1/\sqrt{\epsilon_0 \mu_0}$ denotes the wave propagation speed in vacuum.

Finally, we want to mention that in 2-D cases, the above 3-D PML equations (8.1) are reduced to a set of four equations by splitting only one component. More specifically, in the TE_z (transverse electric to z) case, only the magnetic component is split, which results the PML equations for the TE_z case as:

$$\epsilon_0 \frac{\partial E_x}{\partial t} + \sigma_y E_x = \frac{\partial (H_{zx} + H_{zy})}{\partial y} \tag{8.13a}$$

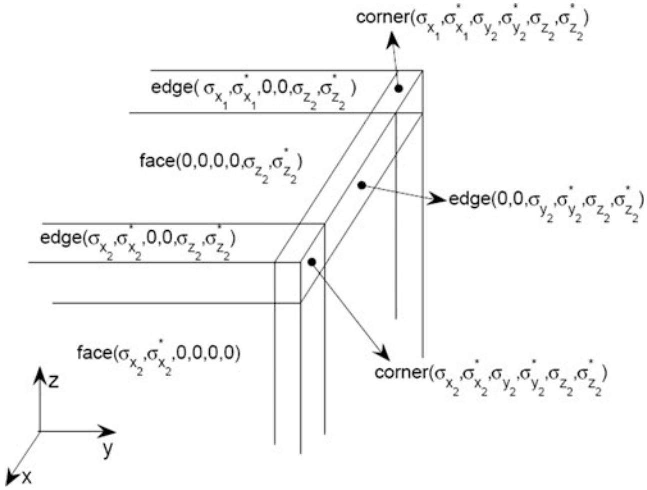

Fig. 8.1 Illustration of the 3-D PML

$$\epsilon_0 \frac{\partial E_y}{\partial t} + \sigma_x E_y = -\frac{\partial (H_{zx} + H_{zy})}{\partial x} \tag{8.13b}$$

$$\mu_0 \frac{\partial H_{zx}}{\partial t} + \sigma_x^* H_{zx} = -\frac{\partial E_y}{\partial x} \tag{8.13c}$$

$$\mu_0 \frac{\partial H_{zy}}{\partial t} + \sigma_y^* H_{zy} = \frac{\partial E_x}{\partial y}. \tag{8.13d}$$

Similarly in the TM case, only the electric component is split. For example, the PML equations for TM_z (transverse magnetic to z) case are:

$$\mu_0 \frac{\partial H_x}{\partial t} + \sigma_y^* H_x = -\frac{\partial (E_{zx} + E_{zy})}{\partial y} \tag{8.14a}$$

$$\mu_0 \frac{\partial H_y}{\partial t} + \sigma_x^* H_y = \frac{\partial (E_{zx} + E_{zy})}{\partial x} \tag{8.14b}$$

$$\epsilon_0 \frac{\partial E_{zx}}{\partial t} + \sigma_x E_{zx} = \frac{\partial H_y}{\partial x} \tag{8.14c}$$

$$\epsilon_0 \frac{\partial E_{zy}}{\partial t} + \sigma_y E_{zy} = -\frac{\partial H_x}{\partial y}. \tag{8.14d}$$

Detailed specifications of conductivities in the face and corner regions of PML are depicted in Fig. 8.2.

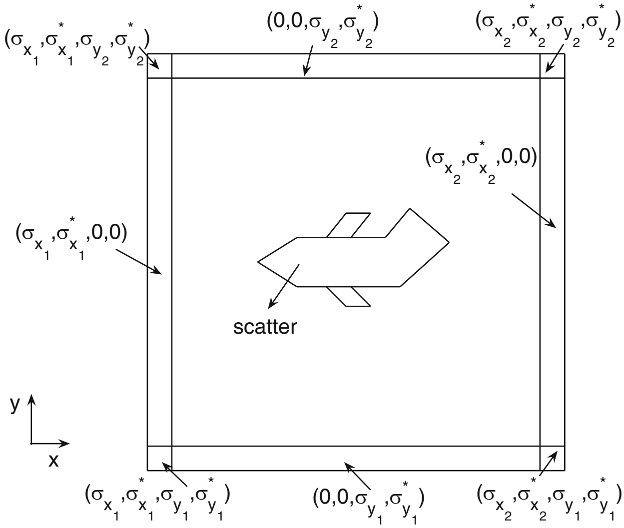

Fig. 8.2 Illustration of the 2-D PML

8.1.1.1 The PML Medium and Stretched Coordinates

Soon after Berenger's PML propoosal, researchers [74, 213, 246] found that the Berenger PML equations can be derived using a stretched coordinate approach.

Substituting the plane wave solution (8.2) into (8.1) and adding every two subequations together, we obtain the following six equations which are equivalent to (8.1):

$$j\omega\epsilon_0\tilde{E}_x = \frac{1}{s_y}\frac{\partial \tilde{H}_z}{\partial y} - \frac{1}{s_z}\frac{\partial \tilde{H}_y}{\partial z}, \tag{8.15a}$$

$$j\omega\epsilon_0\tilde{E}_y = \frac{1}{s_z}\frac{\partial \tilde{H}_x}{\partial z} - \frac{1}{s_x}\frac{\partial \tilde{H}_z}{\partial x}, \tag{8.15b}$$

$$j\omega\epsilon_0\tilde{E}_z = \frac{1}{s_x}\frac{\partial \tilde{H}_y}{\partial x} - \frac{1}{s_y}\frac{\partial \tilde{H}_x}{\partial y}, \tag{8.15c}$$

$$j\omega\mu_0\tilde{H}_x = -\frac{1}{s_y^*}\frac{\partial \tilde{E}_z}{\partial y} + \frac{1}{s_z^*}\frac{\partial \tilde{E}_y}{\partial z}, \tag{8.15d}$$

$$j\omega\mu_0\tilde{H}_y = -\frac{1}{s_z^*}\frac{\partial \tilde{E}_x}{\partial z} + \frac{1}{s_x^*}\frac{\partial \tilde{E}_z}{\partial x}, \tag{8.15e}$$

$$j\omega\mu_0\tilde{H}_z = -\frac{1}{s_x^*}\frac{\partial \tilde{E}_y}{\partial x} + \frac{1}{s_y^*}\frac{\partial \tilde{E}_x}{\partial y}, \tag{8.15f}$$

where the stretching parameters s_i and s_i^* are the same as (8.3).

Assuming that coefficients s_x, s_y, s_z vary with x, y, z, respectively, and introducing the following change of variables

$$dx' = s_x(x)dx, \;\; dy' = s_y(y)dy, \;\; dz' = s_z(z)dz, \tag{8.16}$$

we can rewrite the first three equations of (8.15) as:

$$j\omega\epsilon_0 \tilde{E}_x = \frac{\partial \tilde{H}_z}{\partial y'} - \frac{\partial \tilde{H}_y}{\partial z'} \tag{8.17a}$$

$$j\omega\epsilon_0 \tilde{E}_y = \frac{\partial \tilde{H}_x}{\partial z'} - \frac{\partial \tilde{H}_z}{\partial x'} \tag{8.17b}$$

$$j\omega\epsilon_0 \tilde{E}_z = \frac{\partial \tilde{H}_y}{\partial x'} - \frac{\partial \tilde{H}_x}{\partial y'}. \tag{8.17c}$$

Changed into time domain with the stretched coordinates (8.16) and (8.17) becomes $\epsilon_0 \frac{\partial \mathbf{E}}{\partial t} = \nabla' \times \mathbf{H}$, which has the same form as Ampere equations in vacuum.

By the same technique, the last three equations of (8.15) can be rewritten as:

$$j\omega\mu_0 \tilde{H}_x = -\frac{\partial \tilde{E}_z}{\partial y''} + \frac{\partial \tilde{E}_y}{\partial z''} \tag{8.18a}$$

$$j\omega\mu_0 \tilde{H}_y = -\frac{\partial \tilde{E}_x}{\partial z''} + \frac{\partial \tilde{E}_z}{\partial x''} \tag{8.18b}$$

$$j\omega\mu_0 \tilde{H}_z = -\frac{\partial \tilde{E}_y}{\partial x''} + \frac{\partial \tilde{E}_x}{\partial y''}. \tag{8.18c}$$

In time domain, (8.18) can be rewritten as $\mu_0 \frac{\partial \mathbf{H}}{\partial t} = -\nabla'' \times \mathbf{E}$ in the stretched coordinates $dx'' = s_x^*(x)dx, \;\; dy'' = s_y^*(y)dy, \;\; dz'' = s_z^*(z)dz$, and have exactly the same form as the Faraday equations in vacuum.

Hence, the original Berenger's split PML can be recast in a nonsplit form, which makes manipulating the PML equations easy and simplifies the understanding of the behavior of the PML. Furthermore, Berenger's split PML also offers an easy way to map the PML into other coordinate systems such as cylindrical and spherical coordinates [278].

8.1.2 *The Convolutional PML*

From the frequency domain equations (8.4), we can obtain the so-called convolutional PML, which was introduced by Roden and Gedney [248]. One important feature of the convolutional PML equations is that it is easy to generalize to any physical medium, be it inhomogeneous, lossy, anisotropic, dispersive, or even nonlinear.

Transforming (8.15a) into time domain, we obtain [248]:

$$\epsilon_0 \frac{\partial E_x}{\partial t} = \overline{s_y}(t) * \frac{\partial H_z}{\partial y} - \overline{s_z}(t) * \frac{\partial H_y}{\partial z}, \tag{8.19}$$

where $*$ denotes the convolution product, and $\overline{s_y}(t)$ and $\overline{s_z}(t)$ are the inverse Laplace transforms of $\frac{1}{s_y(\omega)}$ and $\frac{1}{s_z(\omega)}$, respectively. For example, when the stretching factors $s_y(\omega)$ and $s_z(\omega)$ are given by (8.3), we have

$$\overline{s_i}(t) = \delta(t) + \xi_i(t), \quad i = y, z, \tag{8.20}$$

where $\delta(t)$ is the Dirac function, and

$$\xi_i(t) = -\frac{\sigma_i}{\epsilon_0} e^{-\frac{\sigma_i}{\epsilon_0} t} u(t), \quad i = y, z, \tag{8.21}$$

where $u(t)$ is the unit step function. Hence (8.19) can be rewritten as

$$\epsilon_0 \frac{\partial E_x}{\partial t} = \frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} + \xi_y(t) * \frac{\partial H_z}{\partial y} - \xi_z(t) * \frac{\partial H_y}{\partial z}. \tag{8.22}$$

Other five equations similar to (8.22) can be obtained from (8.4b)–(8.4f). Hence the convolutional PML is equivalent to the standard Maxwell's equations in vacuum, plus 12 convolutional terms.

8.1.3 The Uniaxial PML

Note that the split PML equations (8.1) differ from the standard Maxwell's equations, hence the split PML is often termed as non-Maxwellian in the literature. It renders implementation difficult and shows long term unstability [1,29,30], which prompted the development of other PMLs. The uniaxial PML [125,249] is one type of unsplit PMLs, and it can be derived from (8.4).

Let us introduce the following change of variables:

$$\hat{E}_x = s_x \tilde{E}_x, \quad \hat{E}_y = s_y \tilde{E}_y, \quad \hat{E}_z = s_z \tilde{E}_z, \tag{8.23}$$

$$\hat{H}_x = s_x^* \tilde{H}_x, \quad \hat{H}_y = s_y^* \tilde{H}_y, \quad \hat{H}_z = s_z^* \tilde{H}_z, \tag{8.24}$$

using which we can rewrite (8.4a) as

$$\omega\epsilon_0 \frac{1}{s_x}\hat{E}_x = -\frac{1}{s_y s_z^*}k_y \hat{H}_z + \frac{1}{s_z s_y^*}k_z \hat{H}_y. \tag{8.25}$$

Assume that the matching condition (8.10) holds, i.e., $s_x = s_x^*, s_y = s_y^*, s_z = s_z^*$, then (8.25) can be rewritten as

$$\omega\epsilon_0 \frac{s_y s_z}{s_x}\hat{E}_x = -k_y \hat{H}_z + k_z \hat{H}_y. \tag{8.26}$$

Similar equations can be obtained for the rest five equations of (8.4). The final system for the uniaxial PML in frequency domain can be written as [125]:

$$\omega\epsilon_0 \tilde{\epsilon_s}\hat{\mathbf{E}} = -\mathbf{k}\times\hat{\mathbf{H}}, \quad \omega\mu_0\tilde{\mu_s}\hat{\mathbf{H}} = \mathbf{k}\times\hat{\mathbf{E}}, \tag{8.27}$$

where the tensors $\tilde{\epsilon_s}$ and $\tilde{\mu_s}$ are

$$\tilde{\epsilon_s} = \tilde{\mu_s} = \mathrm{diag}(\frac{s_y s_z}{s_x}, \frac{s_z s_x}{s_y}, \frac{s_x s_y}{s_z}). \tag{8.28}$$

To simplify the derivation for the uniaxial PML in time domain, below we drop the hat for all fields in (8.27). The first subequation of (8.27) can be written as

$$j\omega\epsilon_0 \frac{s_y s_z}{s_x}E_x = \frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z}, \tag{8.29}$$

which can be rewritten into a system of two equations:

$$j\omega s_y D_x = \frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z}, \quad D_x = \epsilon_0 \frac{s_z}{s_x}E_x. \tag{8.30}$$

Recall the explicit expressions (8.3) for $s_i, i = x, y, z$, we can transform (8.30) into time domain as:

$$\frac{\partial D_x}{\partial t} + \frac{\sigma_y}{\epsilon_0}D_x = \frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z}, \tag{8.31}$$

$$\epsilon_0 \frac{\partial E_x}{\partial t} + \sigma_z E_x = \frac{\partial D_x}{\partial t} + \frac{\sigma_x}{\epsilon_0}D_x. \tag{8.32}$$

Similarly, from the second and third subequations of (8.27), we have

$$\frac{\partial D_y}{\partial t} + \frac{\sigma_z}{\epsilon_0}D_y = \frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x}, \tag{8.33}$$

$$\epsilon_0 \frac{\partial E_y}{\partial t} + \sigma_x E_y = \frac{\partial D_y}{\partial t} + \frac{\sigma_y}{\epsilon_0}D_y. \tag{8.34}$$

and

$$\frac{\partial D_z}{\partial t} + \frac{\sigma_x}{\epsilon_0} D_z = \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y}, \tag{8.35}$$

$$\epsilon_0 \frac{\partial E_z}{\partial t} + \sigma_y E_z = \frac{\partial D_z}{\partial t} + \frac{\sigma_z}{\epsilon_0} D_z. \tag{8.36}$$

where we denote $D_y = \epsilon_0 \frac{s_x}{s_y} E_y$ and $D_z = \epsilon_0 \frac{s_y}{s_z} E_z$.

By the same technique, we can obtain another group of six time domain equations resulting from the second equation of (8.27). Note that (8.31), (8.33) and (8.35) can be written in vector form as

$$\frac{\partial \mathbf{D}}{\partial t} + \mathrm{diag}(\frac{\sigma_y}{\epsilon_0}, \frac{\sigma_z}{\epsilon_0}, \frac{\sigma_x}{\epsilon_0})\mathbf{D} = \nabla \times \mathbf{H},$$

which is the Ampere equation in a lossy medium. Hence the uniaxial PML can be regarded as a lossy medium plus a set of six differential equations.

8.2 PMLs for Lossy Media

8.2.1 Split PML

A PML for lossy media was presented in [115]. Following [115], the PML equations for a lossy medium $(\epsilon, \mu, \sigma_0, \sigma_0^*)$ in a stretched coordinate can be written as (cf. (8.15) and (8.18)):

$$\nabla_s \times \tilde{\mathbf{H}} = j\omega\epsilon' \tilde{\mathbf{E}} \tag{8.37}$$

$$\nabla_{s^*} \times \tilde{\mathbf{E}} = -j\omega\mu' \tilde{\mathbf{H}} \tag{8.38}$$

where

$$\mu' = \mu + \frac{\sigma_0^*}{j\omega}, \quad \epsilon' = \epsilon + \frac{\sigma_0}{j\omega}, \tag{8.39}$$

and $\nabla_s = \hat{\mathbf{x}} \frac{1}{s_x} \frac{\partial}{\partial x} + \hat{\mathbf{y}} \frac{1}{s_y} \frac{\partial}{\partial y} + \hat{\mathbf{z}} \frac{1}{s_z} \frac{\partial}{\partial z}$. The stretching parameters are chosen as

$$s_i(i) = 1 + \frac{\sigma_i(i)}{j\omega\epsilon}, \quad s_i^*(i) = 1 + \frac{\sigma_i^*(i)}{j\omega\mu}, \quad i = x, y, z. \tag{8.40}$$

We can write the x component of (8.37) as

$$j\omega\epsilon(1+\frac{\sigma_0}{j\omega\epsilon})\tilde{E}_x = \frac{1}{s_y}\frac{\partial \tilde{H}_z}{\partial y} - \frac{1}{s_z}\frac{\partial \tilde{H}_y}{\partial z}, \tag{8.41}$$

which can be split into two subequations:

$$j\omega\epsilon(1+\frac{\sigma_0}{j\omega\epsilon})\tilde{E}_{xy} = \frac{1}{s_y}\frac{\partial \tilde{H}_z}{\partial y} \tag{8.42a}$$

$$j\omega\epsilon(1+\frac{\sigma_0}{j\omega\epsilon})\tilde{E}_{xz} = -\frac{1}{s_z}\frac{\partial \tilde{H}_y}{\partial z} \tag{8.42b}$$

where $\tilde{E}_{xy}$ and $\tilde{E}_{xz}$ are the two split components of $\tilde{E}_x$, i.e., $\tilde{E}_x = \tilde{E}_{xy} + \tilde{E}_{xz}$.

Substituting the definition (8.40) for s_y into (8.42a), we obtain

$$(j\omega\epsilon + \sigma_0 + \sigma_y + \frac{\sigma_0\sigma_y}{j\omega\epsilon})\tilde{E}_{xy} = \frac{\partial \tilde{H}_z}{\partial y},$$

which can be rewritten in time domain as follows:

$$\epsilon\frac{\partial E_{xy}}{\partial t} + (\sigma_0+\sigma_y)E_{xy} + \frac{\sigma_0\sigma_y}{\epsilon}\int_{-\infty}^{t} E_{xy}dt' = \frac{\partial H_z}{\partial y}. \tag{8.43}$$

Similarly, from (8.37) we can obtain the rest five PML equations in frequency domain:

$$(j\omega\epsilon + \sigma_0 + \sigma_z + \frac{\sigma_0\sigma_z}{j\omega\epsilon})\tilde{E}_{xz} = -\frac{\partial \tilde{H}_y}{\partial z}$$

$$(j\omega\epsilon + \sigma_0 + \sigma_x + \frac{\sigma_0\sigma_x}{j\omega\epsilon})\tilde{E}_{yx} = -\frac{\partial \tilde{H}_z}{\partial x}$$

$$(j\omega\epsilon + \sigma_0 + \sigma_z + \frac{\sigma_0\sigma_z}{j\omega\epsilon})\tilde{E}_{yz} = \frac{\partial \tilde{H}_x}{\partial z}$$

$$(j\omega\epsilon + \sigma_0 + \sigma_x + \frac{\sigma_0\sigma_x}{j\omega\epsilon})\tilde{E}_{zx} = \frac{\partial \tilde{H}_y}{\partial x}$$

$$(j\omega\epsilon + \sigma_0 + \sigma_y + \frac{\sigma_0\sigma_y}{j\omega\epsilon})\tilde{E}_{zy} = -\frac{\partial \tilde{H}_x}{\partial y}.$$

On the other hand, the x component of (8.38) yields

$$-j\omega(\mu + \frac{\sigma_0^*}{j\omega})\tilde{H}_x = \frac{1}{s_y^*}\frac{\partial \tilde{E}_z}{\partial y} - \frac{1}{s_z^*}\frac{\partial \tilde{E}_y}{\partial z}, \tag{8.44}$$

which can be split into two subequations:

$$-j\omega(\mu + \frac{\sigma_0^*}{j\omega})\tilde{H}_{xy} = \frac{1}{s_y^*}\frac{\partial \tilde{E}_z}{\partial y} \tag{8.45a}$$

$$-j\omega(\mu + \frac{\sigma_0^*}{j\omega})\tilde{H}_{xz} = -\frac{1}{s_z^*}\frac{\partial \tilde{E}_y}{\partial z} \tag{8.45b}$$

where $\tilde{H}_{xy}$ and $\tilde{H}_{xz}$ are the two components of $\tilde{H}_x$.

Substituting the stretching parameters into (8.45a) and (8.45b), respectively, we obtain

$$(j\omega\mu + \sigma_0^* + \sigma_y^* + \frac{\sigma_0^*\sigma_y^*}{j\omega})\tilde{H}_{xy} = -\frac{\partial \tilde{E}_z}{\partial y}$$

$$(j\omega\mu + \sigma_0^* + \sigma_z^* + \frac{\sigma_0^*\sigma_z^*}{j\omega})\tilde{H}_{xz} = \frac{\partial \tilde{E}_y}{\partial z}.$$

Similarly, the y and z components of (8.38) lead to the following four PML equations in frequency domain:

$$(j\omega\mu + \sigma_0^* + \sigma_z^* + \frac{\sigma_0^*\sigma_z^*}{j\omega})\tilde{H}_{yz} = -\frac{\partial \tilde{E}_x}{\partial z}$$

$$(j\omega\mu + \sigma_0^* + \sigma_x^* + \frac{\sigma_0^*\sigma_x^*}{j\omega})\tilde{H}_{yx} = \frac{\partial \tilde{E}_z}{\partial x}$$

$$(j\omega\mu + \sigma_0^* + \sigma_x^* + \frac{\sigma_0^*\sigma_x^*}{j\omega})\tilde{H}_{zx} = -\frac{\partial \tilde{E}_y}{\partial x}$$

$$(j\omega\mu + \sigma_0^* + \sigma_y^* + \frac{\sigma_0^*\sigma_y^*}{j\omega})\tilde{H}_{zy} = \frac{\partial \tilde{E}_x}{\partial y}.$$

Note that the PML parameters should satisfy the impedance matching conditions

$$\frac{\sigma_i}{\epsilon} = \frac{\sigma_i^*}{\mu}, \quad i = x, y, z,$$

but σ_0 and σ_0^* do not need to satisfy $\frac{\sigma_0}{\epsilon} = \frac{\sigma_0^*}{\mu}$. Furthermore, if $\sigma_0 = \sigma_0^* = 0$, the PML equations obtained here reduce to the original Berenger PML. The corresponding time domain PML equations can be obtained similar to (8.43).

8.2.2 The Convolutional PML

The PML equation (8.41) can be rewritten in time domain as

$$\epsilon \frac{\partial E_x}{\partial t} + \sigma_0 E_x = \overline{s_y}(t) * \frac{\partial H_z}{\partial y} - \overline{s_z}(t) * \frac{\partial H_y}{\partial z}, \tag{8.46}$$

where (p. 335 of [248])

$$\overline{s_i}(t) = \frac{\delta(t)}{k_i} + \xi_i(t), \quad \xi_i(t) = -\frac{\sigma_i}{\epsilon k_i^2} e^{-\frac{1}{\epsilon}(\frac{\sigma_i}{k_i}+\alpha_i)t} u(t), \tag{8.47}$$

which is the inverse Laplace transform of the complex stretching factor proposed by Kuzuoglu and Mittra [173]:

$$s_i = k_i + \frac{\sigma_i}{\alpha_i + j\omega\epsilon}, \quad i = x, y, z, \tag{8.48}$$

where parameters $\sigma_i, \alpha_i > 0$ and $k_i \geq 1$.

Substituting (8.47) into (8.46) yields

$$\epsilon \frac{\partial E_x}{\partial t} + \sigma_0 E_x = \frac{1}{k_y}\frac{\partial H_z}{\partial y} - \frac{1}{k_z}\frac{\partial H_y}{\partial z} + \xi_y(t) * \frac{\partial H_z}{\partial y} - \xi_z(t) * \frac{\partial H_y}{\partial z}. \tag{8.49}$$

Similar equations can be obtained for the evolution of components E_y and E_z. The three equations for H components are the same as the convolutional PML matched to a vacuum.

8.2.3 The Uniaxial PML

A uniaxial PML for isotropic lossy media was presented in [125]. In frequency domain, the PML equations are

$$\omega\epsilon_0(1 + \frac{\sigma}{j\omega\epsilon_0})\tilde{\epsilon}_s \tilde{\mathbf{E}} = -\mathbf{k} \times \tilde{\mathbf{H}}, \quad \omega\mu_0\tilde{\mu}_s \tilde{\mathbf{H}} = \mathbf{k} \times \tilde{\mathbf{E}}, \tag{8.50}$$

where the tensors $\tilde{\epsilon}_s$ and $\tilde{\mu}_s$ are still defined by (8.28).

The x component of (8.50) can be written as

$$j\omega\epsilon_0(1 + \frac{\sigma}{j\omega\epsilon_0})\frac{s_y s_z}{s_x}\tilde{E}_x = \frac{\partial \tilde{H}_z}{\partial y} - \frac{\partial \tilde{H}_y}{\partial z}, \tag{8.51}$$

Introducing two new variables

$$\tilde{D}'_x = s_y \tilde{D}_x, \quad \tilde{D}_x = \epsilon_0 \frac{s_z}{s_x} \tilde{E}_x, \tag{8.52}$$

we can transform (8.51) into time domain equation as:

$$\frac{\partial D'_x}{\partial t} + \frac{\sigma}{\epsilon_0} D'_x = \frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z}, \tag{8.53}$$

plus the following two equations for the new variables:

$$\frac{\partial D_x}{\partial t} + \frac{\sigma_y}{\epsilon_0} D_x = \frac{\partial D'_x}{\partial t} \tag{8.54a}$$

$$\epsilon_0 \frac{\partial E_x}{\partial t} + \sigma_z E_x = \frac{\partial D_x}{\partial t} + \frac{\sigma_x}{\epsilon_0} D_x. \tag{8.54b}$$

Similarly, we can obtain two other groups of equations for components E_y and E_z. The magnetic field equation in the lossy uniaxial PML is exactly the same as that in the uniaxial PML matched to a vacuum.

8.2.4 Time Derivative Lorentz Material Model

In 1999, Ziolkowski [310] presented the time-derivative Lorentz material (TDLM) model as absorbing boundary conditions. Following the notation of [310], we assume that the PML fills a cubical simulation domain, the face regions have absorbing layers with only one normal direction; the edge regions are the joins of two face regions; and the corners are the overlapping parts of three face regions.

The corner region is reflectionless if both the relative permittivity and permeability tensor there are chosen to be

$$\Lambda_{xyz}(\omega) = \text{diag}(\frac{a_y(\omega)a_z(\omega)}{a_x(\omega)}, \frac{a_z(\omega)a_x(\omega)}{a_y(\omega)}, \frac{a_x(\omega)a_y(\omega)}{a_z(\omega)}), \tag{8.55}$$

where the coefficients

$$a_i(\omega) = 1 + \chi_i(\omega), \quad \chi_i(\omega) = \frac{\sigma_i}{j\omega}, \quad i = x, y, z.$$

Here $\sigma_i \geq 0$ represents the damping variation along the i-direction, where $i = x, y, z$.

Hence we have

$$\frac{a_y(\omega)a_z(\omega)}{a_x(\omega)} - 1 = \frac{[\chi_y(\omega) + \chi_z(\omega) - \chi_x(\omega)] + \chi_y(\omega)\chi_z(\omega)}{1 + \chi_x(\omega)}$$
$$= \frac{(j\omega)[(\sigma_y + \sigma_z) - \sigma_x] + \sigma_y\sigma_z}{-\omega^2 + j\omega\sigma_x} = \frac{P_x}{\epsilon_0 E_x}, \tag{8.56a}$$
$$\frac{a_z(\omega)a_x(\omega)}{a_y(\omega)} - 1 = \frac{[\chi_z(\omega) + \chi_x(\omega) - \chi_y(\omega)] + \chi_z(\omega)\chi_x(\omega)}{1 + \chi_y(\omega)}$$
$$= \frac{(j\omega)[(\sigma_z + \sigma_x) - \sigma_y] + \sigma_z\sigma_x}{-\omega^2 + j\omega\sigma_y} = \frac{P_y}{\epsilon_0 E_y}, \tag{8.56b}$$
$$\frac{a_x(\omega)a_y(\omega)}{a_z(\omega)} - 1 = \frac{[\chi_x(\omega) + \chi_y(\omega) - \chi_z(\omega)] + \chi_x(\omega)\chi_y(\omega)}{1 + \chi_z(\omega)}$$
$$= \frac{(j\omega)[(\sigma_x + \sigma_y) - \sigma_z] + \sigma_x\sigma_y}{-\omega^2 + j\omega\sigma_z} = \frac{P_z}{\epsilon_0 E_z}. \tag{8.56c}$$

Here P_i denotes the polarization component in the i-direction, where $i = x, y, z$.

Thus, the corresponding time domain equations for the polarizations in the PML corner region are

$$\frac{\partial^2 P_x}{\partial t^2} + \sigma_x \frac{\partial P_x}{\partial t} = \epsilon_0[(\sigma_y + \sigma_z) - \sigma_x]\frac{\partial E_x}{\partial t} + \epsilon_0\sigma_y\sigma_z E_x, \tag{8.57a}$$
$$\frac{\partial^2 P_y}{\partial t^2} + \sigma_y \frac{\partial P_y}{\partial t} = \epsilon_0[(\sigma_z + \sigma_x) - \sigma_y]\frac{\partial E_y}{\partial t} + \epsilon_0\sigma_z\sigma_x E_y, \tag{8.57b}$$
$$\frac{\partial^2 P_z}{\partial t^2} + \sigma_z \frac{\partial P_z}{\partial t} = \epsilon_0[(\sigma_x + \sigma_y) - \sigma_z]\frac{\partial E_z}{\partial t} + \epsilon_0\sigma_x\sigma_y E_z. \tag{8.57c}$$

Let us choose the x polarization current

$$J_x = \frac{\partial P_x}{\partial t} - \epsilon_0[(\sigma_y + \sigma_z) - \sigma_x]E_x. \tag{8.58}$$

Then using (8.57a), we obtain

$$\frac{\partial J_x}{\partial t} = \frac{\partial^2 P_x}{\partial t^2} - \epsilon_0[(\sigma_y + \sigma_z) - \sigma_x]\frac{\partial E_x}{\partial t} = -\sigma_x[J_x + \epsilon_0(\sigma_y + \sigma_z - \sigma_x)E_x] + \epsilon_0\sigma_y\sigma_z E_x,$$

i.e.,

$$\frac{\partial J_x}{\partial t} + \sigma_x J_x = \epsilon_0[-\sigma_x(\sigma_y + \sigma_z - \sigma_x) + \sigma_y\sigma_z]E_x = \epsilon_0(\sigma_y - \sigma_x)(\sigma_z - \sigma_x)E_x. \tag{8.59}$$

Substituting (8.58) into the Maxwell's equation

$$\frac{\partial E_x}{\partial t} = \frac{1}{\epsilon_0}(\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z}) - \frac{1}{\epsilon_0}\frac{\partial P_x}{\partial t}$$

yields

$$\frac{\partial E_x}{\partial t} + (\sigma_y + \sigma_z - \sigma_x)E_x = \frac{1}{\epsilon_0}(\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z}) - \frac{1}{\epsilon_0}J_x. \tag{8.60}$$

We can treat y and z directions similarly. In summary, we have

$$\frac{\partial J_x}{\partial t} + \sigma_x J_x = \epsilon_0(\sigma_y - \sigma_x)(\sigma_z - \sigma_x)E_x, \tag{8.61a}$$

$$\frac{\partial E_x}{\partial t} + (\sigma_y + \sigma_z - \sigma_x)E_x = \frac{1}{\epsilon_0}(\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z}) - \frac{1}{\epsilon_0}J_x, \tag{8.61b}$$

$$\frac{\partial J_y}{\partial t} + \sigma_y J_y = \epsilon_0(\sigma_x - \sigma_y)(\sigma_z - \sigma_y)E_y, \tag{8.61c}$$

$$\frac{\partial E_y}{\partial t} + (\sigma_z + \sigma_x - \sigma_y)E_y = \frac{1}{\epsilon_0}(\frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x}) - \frac{1}{\epsilon_0}J_y, \tag{8.61d}$$

$$\frac{\partial J_z}{\partial t} + \sigma_z J_z = \epsilon_0(\sigma_x - \sigma_z)(\sigma_y - \sigma_z)E_z, \tag{8.61e}$$

$$\frac{\partial E_z}{\partial t} + (\sigma_x + \sigma_y - \sigma_z)E_z = \frac{1}{\epsilon_0}(\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y}) - \frac{1}{\epsilon_0}J_z. \tag{8.61f}$$

Similarly, for the magnetization M_x in the x direction we have

$$\frac{\partial^2 M_x}{\partial t^2} + \sigma_x \frac{\partial M_x}{\partial t} = \mu_0[(\sigma_y + \sigma_z) - \sigma_x]\frac{\partial H_x}{\partial t} + \mu_0(\sigma_y \sigma_z)H_x.$$

Choosing the magnetization current K_x in the x direction as:

$$K_x = \frac{\partial M_x}{\partial t} - \mu_0[(\sigma_y + \sigma_z) - \sigma_x]H_x,$$

we obtain

$$\frac{\partial K_x}{\partial t} + \sigma_x K_x = \mu_0(\sigma_y - \sigma_x)(\sigma_z - \sigma_x)H_x. \tag{8.62}$$

Then coupling (8.62) with the Maxwell's equation

$$-\nabla \times \mathbf{E} = \frac{\partial}{\partial t}(\mu_0 \mathbf{H}) + \frac{\partial \mathbf{M}}{\partial t},$$

we finally have

$$\frac{\partial H_x}{\partial t} + (\sigma_y + \sigma_z - \sigma_x)H_x = -\frac{1}{\mu_0}(\frac{\partial E_z}{\partial y} - \frac{\partial E_y}{\partial z}) - \frac{1}{\mu_0}K_x.$$

Similar equations can be derived in the y and z directions.

In all, the complete PML governing equations for the corner region are

$$\frac{\partial \mathbf{E}}{\partial t} + D_1\mathbf{E} = \frac{1}{\epsilon_0}\nabla \times \mathbf{H} - \frac{1}{\epsilon_0}\mathbf{J} \tag{8.63}$$

$$\frac{\partial \mathbf{J}}{\partial t} + D_2\mathbf{J} = \epsilon_0 D_3\mathbf{E} \tag{8.64}$$

$$\frac{\partial \mathbf{H}}{\partial t} + D_1\mathbf{H} = -\frac{1}{\mu_0}\nabla \times \mathbf{E} - \frac{1}{\mu_0}\mathbf{K} \tag{8.65}$$

$$\frac{\partial \mathbf{K}}{\partial t} + D_2\mathbf{K} = \mu_0 D_3\mathbf{H} \tag{8.66}$$

where $D_i, i = 1, 2, 3$, are 3×3 diagonal matrices shown below:

$$D_1 = \mathrm{diag}(\sigma_y + \sigma_z - \sigma_x, \sigma_z + \sigma_x - \sigma_y, \sigma_x + \sigma_y - \sigma_z),$$
$$D_2 = \mathrm{diag}(\sigma_x, \sigma_y, \sigma_z),$$
$$D_3 = \mathrm{diag}((\sigma_x - \sigma_y)(\sigma_x - \sigma_z), (\sigma_y - \sigma_x)(\sigma_y - \sigma_z), (\sigma_z - \sigma_x)(\sigma_z - \sigma_y)).$$

Usually, quadratic profiles are chosen for the damping functions σ_x, σ_y and σ_z.

This TDLM PML model has a very nice feature: the governing equations for the corner region automatically reduces to those equations for the face and edge regions when the corresponding material coefficients become zero. For example, setting $\sigma_y = 0$ and the y-component of $\mathbf{J}$ zero in Eqs. (8.63)–(8.66) yields the PML equations in the xz edge region; setting $\sigma_y = \sigma_x = 0$ and $\mathbf{J} = (0, 0, \mathbf{J}_z)'$ (i.e., only z-component of $\mathbf{J}$ is nonzero) in Eqs. (8.63)–(8.66) gives the PML equations in the z-directed face region. Hence the set of PML equations (8.63)–(8.66) covers all PML regions. Furthermore, the set of PML equations (8.63)–(8.66) automatically reduces to the standard Maxwell's equations on a bounded domain by setting $D_1 = D_2 = D_3 = 0$ and interpreting $\mathbf{J}$ and $\mathbf{K}$ as given current sources. Hence the analysis of this PML model is very interesting, since the results derived from the TDLM PML model automatically cover the Maxwell's equations in free space. Some finite element schemes for solving this PML model were developed in [152].

8.3 PMLs for Dispersive Media and Metamaterials

The absorbing boundary condition is required to truncate the computational domain without reflection in simulating wave propagation in metamaterials. However, the standard PML is inherently unstable when it is extended to truncate the boundary of metamaterials without modification [88, 95, 102]. In this section, we present some PMLs developed for modeling wave propagation in dispersive media and metamaterials.

8.3.1 *Complex Frequency-Shifted Technique*

The complex frequency-shifted PML (CFS-PML) was introduced in [173], and its main idea is to shift poles off the real axis. Many experiments have shown that CFS-PML is quite general when applied to various dispersive media, and is also very efficient in attenuating evanescent waves and reducing late-time reflections [36, 248]. The material for this subsection is essentially from [241].

In frequency domain, the PML Maxwell's equations can be written as:

$$\nabla \times \tilde{\mathbf{H}} = j\omega\epsilon_0[\frac{\sigma(\mathbf{r})}{j\omega\epsilon_0} + \epsilon_r(\mathbf{r},\omega)]A \cdot \tilde{\mathbf{E}}, \tag{8.67}$$

$$\nabla \times \tilde{\mathbf{E}} = -j\omega\mu_0\mu_r(\mathbf{r},\omega)A \cdot \tilde{\mathbf{H}}, \tag{8.68}$$

where $A = \mathrm{diag}\{\frac{\xi_x}{\xi_y\xi_z}, \frac{\xi_y}{\xi_z\xi_x}, \frac{\xi_z}{\xi_x\xi_y}\}$ is the material tensor. For dispersive media such as Debye, Drude, and Lorentz types, we define a general stretching parameter

$$\xi_i = 1/(k_i + \frac{\sigma_i}{\gamma + j\omega}), \quad i = x, y, z. \tag{8.69}$$

Here parameters k_i and σ_i provide additional attenuation to both propagating and evanescent waves.

8.3.1.1 Debye Media

First we consider the case of Debye medium of order N, whose relative permittivity in the frequency domain is defined as

$$\epsilon_r(\omega) = \epsilon_{r,\infty} + \sum_{p=1}^{N} \frac{\epsilon_{r,sp} - \epsilon_{r,\infty}}{1 + j\omega\tau_p}, \tag{8.70}$$

where $\epsilon_{r,\infty}$ and $\epsilon_{r,sp}$ are the relative permittivities at infinite and zero frequencies for the p-th pole, respectively, and τ_p is the relaxation time of the p-th pole.

Note that the Ampere's law (8.67) can be written as

$$\nabla \times \tilde{\mathbf{H}} = j\omega\epsilon_0\epsilon_{r,\infty}A \cdot \tilde{\mathbf{E}} + \sigma A \cdot \tilde{\mathbf{E}} + j\omega \sum_{p=1}^{N} \tilde{\mathbf{Q}}_{e,p}, \tag{8.71}$$

where $\tilde{\mathbf{Q}}_{e,p}$ (subscripts e and p stand for the electric dispersion and pole p, respectively) is defined as

$$\tilde{\mathbf{Q}}_{e,p} = \frac{\epsilon_0(\epsilon_{r,sp} - \epsilon_{r,\infty})}{1 + j\omega\tau_p} A \cdot \tilde{\mathbf{E}}. \tag{8.72}$$

We define a new variable $\tilde{\mathbf{R}} = A \cdot \tilde{\mathbf{E}}$, and rewrite (8.71) as

$$\nabla \times \tilde{\mathbf{H}} = j\omega\epsilon_0\epsilon_{r,\infty}\tilde{\mathbf{R}} + \sigma\tilde{\mathbf{R}} + j\omega \sum_{p=1}^{N} \tilde{\mathbf{Q}}_{e,p}, \tag{8.73}$$

which in time domain is equivalent to

$$\nabla \times \mathbf{H} = \epsilon_0\epsilon_{r,\infty}\frac{d\mathbf{R}}{dt} + \sigma\mathbf{R} + \sum_{p=1}^{N} \frac{d\mathbf{Q}_{e,p}}{dt}. \tag{8.74}$$

Similarly, we can transform (8.72) into time domain as

$$\mathbf{Q}_{e,p} + \tau_p \frac{d\mathbf{Q}_{e,p}}{dt} = \epsilon_0(\epsilon_{r,sp} - \epsilon_{r,\infty})\mathbf{R}. \tag{8.75}$$

By the definition of $\tilde{\mathbf{R}}$, we have

$$\tilde{R}_x = \frac{\xi_x}{\xi_y\xi_z}\tilde{E}_x, \quad \tilde{R}_y = \frac{\xi_y}{\xi_z\xi_x}\tilde{E}_y, \quad \tilde{R}_z = \frac{\xi_z}{\xi_x\xi_y}\tilde{E}_z. \tag{8.76}$$

We introduce a new variable $\tilde{\mathbf{S}}$, whose components are

$$\tilde{S}_x = \frac{\xi_x}{\xi_y}\tilde{E}_x, \quad \tilde{S}_y = \frac{\xi_y}{\xi_z}\tilde{E}_y, \quad \tilde{S}_z = \frac{\xi_z}{\xi_x}\tilde{E}_z. \tag{8.77}$$

Transforming (8.76) and (8.77) into time domain yields

$$k_x\frac{dS_x}{dt} + (k_x\gamma + \sigma_x)S_x = k_y\frac{dE_x}{dt} + (k_y\gamma + \sigma_y)E_x, \tag{8.78}$$

$$\frac{dR_x}{dt} + \gamma R_x = k_z\frac{dS_x}{dt} + (k_z\gamma + \sigma_z)S_x. \tag{8.79}$$

Similar equations can be obtained for other components.

To consider the magnetic components, we assume that $\mu_r = 1$ and $\gamma = 0$ in (8.69). Hence, the x-component of Faraday's law (8.68) can be written as

$$(\nabla \times \tilde{\mathbf{E}})_x = -j\omega\frac{\tilde{B}_x}{\xi_z}, \quad \tilde{B}_x = \mu_0\frac{\xi_x}{\xi_y}\tilde{H}_x, \tag{8.80}$$

which in time domain become

$$(\nabla \times \mathbf{E})_x = -k_z \frac{dB_x}{dt} - \sigma_z B_x, \tag{8.81}$$

$$\sigma_x B_x + k_x \frac{dB_x}{dt} = \mu_0 (k_y \frac{dH_x}{dt} + \sigma_y H_x). \tag{8.82}$$

Similar equations can be obtained for other components.

In [241], Prokopidis developed a FDTD method to solve the Debye PML model in the following order: $R \to Q_{e,p} \to S \to E \to B \to H$.

8.3.1.2 Drude Media

The Drude media can be described by the complex permittivity:

$$\epsilon_r(\omega) = 1 + \frac{\omega_p^2}{j\omega\nu - \omega^2}, \tag{8.83}$$

where ω_p is the plasma frequency and ν is the collision frequency.

For Drude media, the corresponding Ampere's law (8.67) can be written as

$$\nabla \times \tilde{\mathbf{H}} = j\omega\epsilon_0 A \cdot \tilde{\mathbf{E}} + \sigma A \cdot \tilde{\mathbf{E}} + \tilde{\mathbf{Q}}, \quad \tilde{\mathbf{Q}} = \frac{\epsilon_0 \omega_p^2}{j\omega + \nu} A \cdot \tilde{\mathbf{E}}. \tag{8.84}$$

By introducing the new variable $\tilde{\mathbf{R}} = A \cdot \tilde{\mathbf{E}}$, we can transform (8.84) into time domain as follows:

$$\nabla \times \mathbf{H} = \epsilon_0 \frac{d\mathbf{R}}{dt} + \sigma \mathbf{R} + \mathbf{Q}, \tag{8.85}$$

$$\frac{d\mathbf{Q}}{dt} + \nu \mathbf{Q} = \epsilon_0 \omega_p^2 \mathbf{R}. \tag{8.86}$$

The rest governing equations are the same as those described above for the Debye model.

8.3.1.3 Lorentz Media

For the Lorentz medium of order N, the relative permittivity in the frequency domain is described by

$$\epsilon_r(\omega) = \epsilon_{r,\infty} + (\epsilon_{r,s} - \epsilon_{r,\infty}) \sum_{p=1}^{N} \frac{G_p \omega_p^2}{\omega_p^2 + 2j\omega\nu_p - \omega^2}, \tag{8.87}$$

where $G_p \geq 0$ and $\sum_{p=1}^{N} G_p = 1$.

If we define a new variable

$$\tilde{\mathbf{Q}}_p = \epsilon_0(\epsilon_{r,s} - \epsilon_{r,\infty})\frac{G_p\omega_p^2}{\omega_p^2 + 2j\omega\nu_p - \omega^2}A \cdot \tilde{\mathbf{E}}, \tag{8.88}$$

then Ampere's law (8.67) can be written as

$$\nabla \times \tilde{\mathbf{H}} = \sigma A \cdot \tilde{\mathbf{E}} + j\omega\epsilon_0\epsilon_{r,\infty}A \cdot \tilde{\mathbf{E}} + j\omega\sum_{p=1}^{N}\tilde{\mathbf{Q}}_p, \tag{8.89}$$

which in time domain becomes

$$\nabla \times \mathbf{H} = \sigma\mathbf{R} + \epsilon_0\epsilon_{r,\infty}\frac{d\mathbf{R}}{dt} + \sum_{p=1}^{N}\frac{d\mathbf{Q}_p}{dt}. \tag{8.90}$$

Transforming (8.88) into time domain, we have

$$\frac{d^2\mathbf{Q}_p}{dt^2} + 2\nu_p\frac{d\mathbf{Q}_p}{dt} + \omega_p^2\mathbf{Q}_p = \epsilon_0(\epsilon_{r,s} - \epsilon_{r,\infty})G_p\omega_p^2\mathbf{R}. \tag{8.91}$$

The rest PML equations are the same as those for the Debye model.

8.3.2 *Complex-Coordinate Stretching*

Here we introduce a modified PML for metamaterials [262] obtained by the complex-coordinate stretching technique [74]. For simplicity, below we present the derivation for 2-D TMz Maxwell's equations in metamaterials described by the Lorentz medium model:

$$\epsilon(\omega) = \epsilon_0(1 + \frac{\omega_{pe}^2}{\omega_{0e}^2 - \omega^2 + j\Gamma_e\omega}), \tag{8.92}$$

$$\mu(\omega) = \mu_0(1 + \frac{\omega_{pm}^2}{\omega_{0m}^2 - \omega^2 + j\Gamma_m\omega}). \tag{8.93}$$

The rest of this subsection is mainly based on [262].

8.3.2.1 Derivation of TMz Maxwell's Equations in Metamaterials

Since only three nonzero fields H_x, H_y, E_z exist in TMz case, from Maxwell's equations

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}, \quad \frac{\partial \mathbf{D}}{\partial t} = \nabla \times \mathbf{H},$$

we can obtain the TMz Maxwell's equations in frequency domain:

$$j\omega B_x = -\frac{\partial E_z}{\partial y} \tag{8.94}$$

$$j\omega B_y = \frac{\partial E_z}{\partial x} \tag{8.95}$$

$$j\omega D_z = \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} \tag{8.96}$$

where the constitutive equations are

$$D_z = \epsilon(\omega)E_z, \quad B_x = \mu(\omega)H_x, \quad B_y = \mu(\omega)H_y.$$

Substituting (8.93) into (8.94), we obtain

$$j\omega H_x + K_x = -\frac{1}{\mu_0}\frac{\partial E_z}{\partial y}, \tag{8.97}$$

where $K_x = \frac{j\omega\omega_{pm}^2}{\omega_{0m}^2 - \omega^2 + j\Gamma_m\omega} H_x$, which can be rewritten as

$$\left(\frac{\omega_{0m}^2}{j\omega} + j\omega + \Gamma_m\right)K_x = \omega_{pm}^2 H_x,$$

or equivalent to

$$j\omega K_x + \Gamma_m K_x = \omega_{pm}^2 H_x - \omega_{0m}^2 F_x, \tag{8.98}$$

where F_x is a new auxiliary variable defined as

$$F_x = \frac{1}{j\omega} K_x. \tag{8.99}$$

By the same technique, from (8.95) we have

$$j\omega H_y + K_y = \frac{1}{\mu_0}\frac{\partial E_z}{\partial x} \tag{8.100}$$

$$j\omega K_y + \Gamma_m K_y = \omega_{pm}^2 H_y - \omega_{0m}^2 F_y \tag{8.101}$$

$$j\omega F_y = K_y. \tag{8.102}$$

Similarly, substituting (8.92) into (8.96), we obtain

$$j\omega E_z + J_z = \frac{1}{\epsilon_0}\left(\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y}\right), \tag{8.103}$$

where $J_z = \frac{j\omega\omega_{pe}^2}{\omega_{0e}^2 - \omega^2 + j\Gamma_e\omega} E_z$, which can be rewritten as

$$\left(\frac{\omega_{0e}^2}{j\omega} + j\omega + \Gamma_e\right) J_z = \omega_{pe}^2 E_z,$$

or

$$j\omega J_z + \Gamma_e J_z = \omega_{pe}^2 E_z - \omega_{0e}^2 R_z, \tag{8.104}$$

where the auxiliary variable R_z is defined as

$$R_z = \frac{1}{j\omega} J_z. \tag{8.105}$$

Changing the above equations into time domain, we have the TMz Maxwell's equations in metamaterials:

$$\frac{\partial H_x}{\partial t} = -\frac{1}{\mu_0}\frac{\partial E_z}{\partial y} - K_x, \tag{8.106}$$

$$\frac{\partial H_y}{\partial t} = \frac{1}{\mu_0}\frac{\partial E_z}{\partial x} - K_y, \tag{8.107}$$

$$\frac{\partial E_z}{\partial t} = \frac{1}{\epsilon_0}\left(\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y}\right) - J_z, \tag{8.108}$$

supplemented by the following auxiliary constitutive equations:

$$\frac{\partial K_x}{\partial t} + \Gamma_m K_x = \omega_{pm}^2 H_x - \omega_{0m}^2 F_x \tag{8.109}$$

$$\frac{\partial F_x}{\partial t} = K_x \tag{8.110}$$

$$\frac{\partial K_y}{\partial t} + \Gamma_m K_y = \omega_{pm}^2 H_y - \omega_{0m}^2 F_y \tag{8.111}$$

$$\frac{\partial F_y}{\partial t} = K_y \tag{8.112}$$

$$\frac{\partial J_z}{\partial t} + \Gamma_e J_z = \omega_{pe}^2 E_z - \omega_{0e}^2 R_z \tag{8.113}$$

$$\frac{\partial R_z}{\partial t} = J_z. \tag{8.114}$$

8.3.2.2 The PML Equations for Metamaterials

Now we want to derive a stable non-split PML model for metamaterials. Following [262], we introduce the following complex-coordinate stretching variables:

$$\frac{\partial}{\partial x} \Rightarrow 1/[1+\frac{\sigma_x}{j\omega(1+\frac{\omega_{pe}^2}{\omega_{0e}^2-\omega^2+j\Gamma_e\omega})}]\frac{\partial}{\partial x}, \tag{8.115}$$

$$\frac{\partial}{\partial y} \Rightarrow 1/[1+\frac{\sigma_y}{j\omega(1+\frac{\omega_{pe}^2}{\omega_{0e}^2-\omega^2+j\Gamma_e\omega})}]\frac{\partial}{\partial y}, \tag{8.116}$$

and define the magnetic and electric field variables for the metamaterial PML region:

$$\tilde{H}_x = 1/[1+\frac{\sigma_y}{j\omega(1+\frac{\omega_{pe}^2}{\omega_{0e}^2-\omega^2+j\Gamma_e\omega})}]H_x \tag{8.117}$$

$$\tilde{H}_y = 1/[1+\frac{\sigma_x}{j\omega(1+\frac{\omega_{pe}^2}{\omega_{0e}^2-\omega^2+j\Gamma_e\omega})}]H_y \tag{8.118}$$

$$\tilde{E}_{z1} = 1/[1+\frac{\sigma_y}{j\omega(1+\frac{\omega_{pe}^2}{\omega_{0e}^2-\omega^2+j\Gamma_e\omega})}]E_z \tag{8.119}$$

$$\tilde{E}_{z2} = 1/[1+\frac{\sigma_x}{j\omega(1+\frac{\omega_{pe}^2}{\omega_{0e}^2-\omega^2+j\Gamma_e\omega})}]E_z. \tag{8.120}$$

With these definitions, we can easily obtain the unsplit PML equations for metamaterials:

$$\frac{\partial H_x}{\partial t} = -\frac{1}{\mu_0}\frac{\partial \tilde{E}_{z1}}{\partial y} - K_x \tag{8.121}$$

$$\frac{\partial H_y}{\partial t} = \frac{1}{\mu_0}\frac{\partial \tilde{E}_{z2}}{\partial x} - K_y \tag{8.122}$$

$$\frac{\partial E_z}{\partial t} = \frac{1}{\epsilon_0}(\frac{\partial \tilde{H}_y}{\partial x} - \frac{\partial \tilde{H}_x}{\partial y}) - J_z, \tag{8.123}$$

plus many constitutive equations we shall derive below.

Note that (8.117) is same as $[1+\frac{\sigma_y}{j\omega(1+\frac{\omega_{pe}^2}{\omega_{0e}^2-\omega^2+j\Gamma_e\omega})}]\tilde{H}_x = H_x$, which can be written as

$$\tilde{H}_x + \sigma_y P_x = H_x. \tag{8.124}$$

If we introduce a new variable $P_x = \frac{1}{j\omega(1+\frac{\omega_{pe}^2}{\omega_{0e}^2-\omega^2+j\Gamma_e\omega})}\tilde{H}_x$, which is same as

$$j\omega(1+\frac{\omega_{pe}^2}{\omega_{0e}^2-\omega^2+j\Gamma_e\omega})P_x = \tilde{H}_x,$$

or equivalently

$$j\omega P_x + \omega_{pe}^2 Q_x = \tilde{H}_x, \tag{8.125}$$

if we introduce another new variable $Q_x = \frac{j\omega}{\omega_{0e}^2-\omega^2+j\Gamma_e\omega}P_x$, which is same as

$$(\frac{\omega_{0e}^2}{j\omega} + j\omega + \Gamma_e)Q_x = P_x,$$

or

$$(j\omega + \Gamma_e)Q_x = P_x - \omega_{0e}^2 U_x,\ \ U_x = \frac{1}{j\omega}Q_x. \tag{8.126}$$

We can write (8.125) and (8.126) in time domain as:

$$\frac{\partial P_x}{\partial t} + \omega_{pe}^2 Q_x = \tilde{H}_x \tag{8.127}$$

$$\frac{\partial Q_x}{\partial t} + \Gamma_e Q_x = P_x - \omega_{0e}^2 U_x \tag{8.128}$$

$$\frac{\partial U_x}{\partial t} = Q_x. \tag{8.129}$$

By similar techniques, we can obtain the rest auxiliary time domain equations:

$$\tilde{H}_y = H_y - \sigma_x P_y \tag{8.130}$$

$$\frac{\partial P_y}{\partial t} = \tilde{H}_y - \omega_{pe}^2 Q_y \tag{8.131}$$

$$\frac{\partial Q_y}{\partial t} = P_y - \omega_{0e}^2 U_y - \Gamma_e Q_y \tag{8.132}$$

$$\frac{\partial U_y}{\partial t} = Q_y \tag{8.133}$$

$$\tilde{E}_{z1} = E_z - \sigma_y D_{z1} \tag{8.134}$$

$$\frac{\partial D_{z1}}{\partial t} = \tilde{E}_{z1} - \omega_{pe}^2 B_{z1} \tag{8.135}$$

$$\frac{\partial B_{z1}}{\partial t} = D_{z1} - \omega_{0e}^2 C_{z1} - \Gamma_e B_{z1} \tag{8.136}$$

$$\frac{\partial C_{z1}}{\partial t} = B_{z1} \tag{8.137}$$

$$\tilde{E}_{z2} = E_z - \sigma_x D_{z2} \tag{8.138}$$

$$\frac{\partial D_{z2}}{\partial t} = \tilde{E}_{z2} - \omega_{pe}^2 B_{z2} \tag{8.139}$$

$$\frac{\partial B_{z2}}{\partial t} = D_{z2} - \omega_{0e}^2 C_{z2} - \Gamma_e B_{z2} \tag{8.140}$$

$$\frac{\partial C_{z2}}{\partial t} = B_{z2}. \tag{8.141}$$

Note that in the above non-split metamaterial PML model, those terms involving temporal and spatial derivatives are exactly the same as those from the standard Maxwell's equations, which makes the PML implementation quite simple. Furthermore, when $\sigma_x = \sigma_y = 0$, the metamaterial PML equations reduce to the standard Maxwell's equations.

8.4 Bibliographical Remarks

In this chapter, we reviewed many PML models developed since Berenger introduced the PML concept in 1994. Considering the technicality of mathematical analysis of PMLs, we didn't cover the theoretical analysis of those PML models. Interested readers can consult Sect. 13.5 of Monk's book [217] for works published before 2002. More recent works on finite element analysis of PMLs can be found in [26, 49, 69] and references cited therein. Some interesting topics worth further exploration are rigorous mathematical analysis and finite element applications of those PML models coupled to metamaterials.