Lecture Outline

- Review of Lecture 12
- Background Information
- The Uniaxial Perfectly Matched Layer (UPML)
- Calculating the PML parameters
- Convolutional PML (CPML)
- Incorporating a UPML into Maxwell’s equations
Review of Lecture 12

Effect of “Windowing” on FDTD Spectrum

- Long simulation time
- Wide window
- Narrow window spectrum
- Less “blurring”
- High frequency resolution

- Moderate simulation time
- Moderate window
- Moderate window spectrum
- More “blurring”
- Reduced frequency resolution

- Short simulation time
- Narrow window
- Wide window spectrum
- Much “blurring”
- Poor frequency resolution
Ensuring Sufficient Iterations to Resolve $\Delta f$

Given the time step $\Delta t$, the Nyquist sampling theorem quantifies the highest frequency that can be resolved.

$$f_{\text{max}} = \frac{1}{2\Delta t}$$

Note: In practice, you should set $\Delta t = \frac{1}{N_t f_{\text{max}}} \quad N_t \geq 10$

Given the FDTD simulation runs for $\text{STEPS}$ number of iterations, the frequency resolution is

$$\Delta f = \frac{2 f_{\text{max}}}{\text{STEPS}} = \frac{1}{\Delta t \cdot \text{STEPS}}$$

Therefore, to resolve the frequency response down to a resolution of $\Delta f$, the number of iterations required is

$$\text{STEPS} \geq \frac{1}{\Delta t \cdot \Delta f}$$

Notes:
1. This is related to the uncertainty principle.
2. You can calculate kernels for very finely spaced frequency points, but the actual frequency resolution is still limited by the windowing effect. Your data will be “blurred.”

Dielectric Smoothing

Physical Device

- Conventional Representation on Grid
- Representation on Grid with Dielectric Smoothing
Anisotropic Dielectric Smoothing

Given the simulation problem defined by

\[ \vec{D} = [\varepsilon] \vec{E} \]

We can improve the convergence rate by smoothing the dielectric function according to

\[ [\varepsilon_{\text{smooth}}] = \langle [\varepsilon] \rangle + \left( \langle [\varepsilon]^{-1} \rangle - \langle [\varepsilon] \rangle \right) \left[ \hat{N} \right] \]

\[ \left[ \hat{N} \right] = \begin{bmatrix} n_x^2 & n_x n_y & n_x n_z \\ n_y n_x & n_y^2 & n_y n_z \\ n_z n_x & n_z n_y & n_z^2 \end{bmatrix} \]

Dielectric Smoothing of a Sphere

Given a sphere with dielectric constant \( \varepsilon_r = 5.0 \) in air and in a grid with \( N_x = N_y = N_z = 25 \) cells, the dielectric tensor after smoothing is

xy cross section

xz cross section
2× Grid Technique

The 2× grid is only used for building devices on a Yee grid. It is not used anywhere else!

Concept of the 2× Grid

The Conventional 1× Grid

Due to the staggered nature of the Yee grid, we are effectively getting twice the resolution.

It now makes sense to talk about a grid that is at twice the resolution, the “2× grid.”

The 2× grid concept is useful because we can create devices (or PMLs) on the 2× grid without having to think about where the different field components are located. In a second step, we can easily pull off the values from the 2× grid where they exist for a particular field component.
Parsing the Materials From 2× to 1× Grid

Background
### Tensors

Tensors are a generalization of a scaling factor where the direction of a vector can be altered in addition to its magnitude.

Scalar Relation $\rightarrow \quad \vec{V} \quad \rightarrow \quad a\vec{V}$

Tensor Relation $\left[a\right]\vec{V}$

$[a]\vec{V} = \begin{bmatrix} a_{xx} & a_{xy} & a_{xz} \\ a_{yx} & a_{yy} & a_{yz} \\ a_{zx} & a_{zy} & a_{zz} \end{bmatrix} \begin{bmatrix} V_x \\ V_y \\ V_z \end{bmatrix}$

---

### Reflectance from a Surface with Loss

Complex refractive index

$$\tilde{n} = n + j\kappa$$

$n \equiv$ ordinary refractive index

$\kappa \equiv$ extinction coefficient

Reflectance from a lossy surface

$$R = \frac{(1 - n)^2 + \kappa^2}{(1 + n)^2 + \kappa^2}$$

**Loss contributes to reflections**
Reflection, Transmission and Refraction at an Interface: Isotropic Case

Angles
\[ \theta_{\text{inc}} = \theta_{\text{ref}} = \theta_1 \]
\[ n_1 \sin \theta_1 = n_2 \sin \theta_2 \quad \text{Snell’s Law} \]

TE Polarization
\[ r_{\text{TE}} = \frac{n_2 \cos \theta_2 - n_1 \cos \theta_1}{n_2 \cos \theta_2 + n_1 \cos \theta_1} \]
\[ t_{\text{TE}} = \frac{2n_2 \cos \theta_2}{n_2 \cos \theta_2 + n_1 \cos \theta_1} \]

TM Polarization
\[ r_{\text{TM}} = \frac{n_2 \cos \theta_2 - n_1 \cos \theta_1}{n_2 \cos \theta_2 + n_1 \cos \theta_1} \]
\[ t_{\text{TM}} = \frac{2n_2 \cos \theta_2}{n_2 \cos \theta_2 + n_1 \cos \theta_1} \]

\[ n_i = \text{refractive index in region } i \]
\[ \eta_i = \text{impedance in region } i \]

Maxwell’s Equations in Anisotropic Media

Maxwell’s curl equations in anisotropic media are:
\[ \nabla \times \vec{H} = j\omega\epsilon_0 \left[ \epsilon_r \right] \vec{E} \]
\[ \nabla \times \vec{E} = -j\omega\mu_0 \left[ \mu_r \right] \vec{H} \]

These can also be written in a matrix form that makes the tensor aspect of \( \mu \) and \( \epsilon \) more obvious.

\[
\begin{bmatrix}
0 & -\frac{\partial}{\partial x} & \frac{\partial}{\partial y} \\
\frac{\partial}{\partial x} & 0 & -\frac{\partial}{\partial z} \\
-\frac{\partial}{\partial y} & \frac{\partial}{\partial z} & 0
\end{bmatrix}
\begin{bmatrix}
H_x \\
H_y \\
H_z
\end{bmatrix}
= j\omega\epsilon_0
\begin{bmatrix}
\epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\
\epsilon_{yx} & \epsilon_{yy} & \epsilon_{yz} \\
\epsilon_{zx} & \epsilon_{zy} & \epsilon_{zz}
\end{bmatrix}
\begin{bmatrix}
E_x \\
E_y \\
E_z
\end{bmatrix}
\]

\[
\begin{bmatrix}
0 & -\frac{\partial}{\partial x} & \frac{\partial}{\partial y} \\
\frac{\partial}{\partial x} & 0 & -\frac{\partial}{\partial z} \\
-\frac{\partial}{\partial y} & \frac{\partial}{\partial z} & 0
\end{bmatrix}
\begin{bmatrix}
E_x \\
E_y \\
E_z
\end{bmatrix}
= -j\omega\mu_0
\begin{bmatrix}
\mu_{xx} & \mu_{xy} & \mu_{xz} \\
\mu_{yx} & \mu_{yy} & \mu_{yz} \\
\mu_{zx} & \mu_{zy} & \mu_{zz}
\end{bmatrix}
\begin{bmatrix}
H_x \\
H_y \\
H_z
\end{bmatrix}
\]
Types of Anisotropic Media

There are three basic types of anisotropic media:

- **Isotropic**
  \[
  \begin{bmatrix}
  \varepsilon_{\text{iso}} & 0 & 0 \\
  0 & \varepsilon_{\text{iso}} & 0 \\
  0 & 0 & \varepsilon_{\text{iso}}
  \end{bmatrix}
  \]

- **Uniaxial**
  \[
  \begin{bmatrix}
  \varepsilon_0 & 0 & 0 \\
  0 & \varepsilon_0 & 0 \\
  0 & 0 & \varepsilon_e
  \end{bmatrix}
  \]

- **Biaxial**
  \[
  \begin{bmatrix}
  \varepsilon_a & 0 & 0 \\
  0 & \varepsilon_b & 0 \\
  0 & 0 & \varepsilon_c
  \end{bmatrix}
  \]

Note: terms only arise in the off-diagonal positions when the tensor is rotated relative to the coordinate system.

(\(\varepsilon', \varepsilon''\)) Vs. (\(\varepsilon, \sigma\))

There are two ways to incorporate loss into Maxwell’s equations.

At very low frequencies and/or for time-domain analysis, the \((\varepsilon, \sigma)\) system is usually preferred.

\[
\nabla \times \vec{H} = \vec{J} + j\omega \vec{D} = \sigma \vec{E} + j\omega \varepsilon_0 \vec{E} = (\sigma + j\omega \varepsilon_0) \vec{E}
\]

We use this for FDTD.

At high frequencies and in the frequency-domain, \((\varepsilon', \varepsilon'')\) is usually preferred.

\[
\nabla \times \vec{H} = j\omega \vec{D} = j\omega \varepsilon_0 \vec{E}
\]

The parameters are related through

\[
\varepsilon' = \varepsilon_0 + \frac{\sigma}{j\omega}
\]

Note: It does not make sense to have a complex \(\varepsilon\) and a conductivity \(\sigma\).
Maxwell’s Equations in Doubly-Diagonally Anisotropic Media

Maxwell’s equations for diagonally anisotropic media can be written as

\[
\begin{bmatrix}
0 & -\frac{\varepsilon_x}{\mu_x} & 0 & 0 & 0 & 0 & 0 & 0 \\
-\frac{\varepsilon_y}{\mu_y} & 0 & -\frac{\varepsilon_z}{\mu_z} & 0 & 0 & 0 & 0 & 0 \\
-\frac{\varepsilon_y}{\mu_y} & 0 & 0 & -\frac{\varepsilon_z}{\mu_z} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -\frac{\mu_x}{\varepsilon_x} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -\frac{\mu_y}{\varepsilon_y} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\mu_z}{\varepsilon_z}
\end{bmatrix}
\begin{bmatrix}
H_x \\
H_y \\
H_z \\
E_x \\
E_y \\
E_z
\end{bmatrix}
= j\omega \varepsilon_x \begin{bmatrix} 0 & 0 & 0 \\
0 & \varepsilon_y + \sigma_y^E / j\omega & 0 \\
0 & 0 & \varepsilon_z + \sigma_z^E / j\omega
\end{bmatrix}
\begin{bmatrix} E_x \\
E_y \\
E_z \end{bmatrix}

\begin{align*}
\frac{\varepsilon_x + \sigma_x^E / j\omega}{\mu_x + \sigma_x^H / j\omega} & = 0 & 0 \\
\frac{\varepsilon_y + \sigma_y^E / j\omega}{\mu_y + \sigma_y^H / j\omega} & = 0 & 0 \\
\frac{\varepsilon_z + \sigma_z^E / j\omega}{\mu_z + \sigma_z^H / j\omega} & = 0 & 0
\end{align*}

We can generalize further by incorporating loss.

\[
\begin{bmatrix}
0 & -\frac{\varepsilon_x}{\mu_x} & 0 & 0 & 0 & 0 & 0 & 0 \\
-\frac{\varepsilon_y}{\mu_y} & 0 & -\frac{\varepsilon_z}{\mu_z} & 0 & 0 & 0 & 0 & 0 \\
-\frac{\varepsilon_y}{\mu_y} & 0 & 0 & -\frac{\varepsilon_z}{\mu_z} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -\frac{\mu_x}{\varepsilon_x} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -\frac{\mu_y}{\varepsilon_y} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\mu_z}{\varepsilon_z}
\end{bmatrix}
\begin{bmatrix}
H_x \\
H_y \\
H_z \\
E_x \\
E_y \\
E_z
\end{bmatrix}
= j\omega \varepsilon_x \begin{bmatrix} 0 & 0 & 0 \\
0 & \varepsilon_y + \sigma_y^E / j\omega & 0 \\
0 & 0 & \varepsilon_z + \sigma_z^E / j\omega
\end{bmatrix}
\begin{bmatrix} E_x \\
E_y \\
E_z \end{bmatrix}

\begin{align*}
\frac{\varepsilon_x + \sigma_x^E / j\omega}{\mu_x + \sigma_x^H / j\omega} & = 0 & 0 \\
\frac{\varepsilon_y + \sigma_y^E / j\omega}{\mu_y + \sigma_y^H / j\omega} & = 0 & 0 \\
\frac{\varepsilon_z + \sigma_z^E / j\omega}{\mu_z + \sigma_z^H / j\omega} & = 0 & 0
\end{align*}

Scattering at a Doubly-Diagonal Anisotropic Interface

Refraction into a diagonally anisotropic material is described by

\[ \sin \theta_1 = \sqrt{bc} \sin \theta_2 \]

Reflection from a diagonally anisotropic material is

\[
r_{TE} = \frac{\sqrt{a} \cos \theta_1 - \sqrt{b} \cos \theta_2}{\sqrt{a} \cos \theta_1 + \sqrt{b} \cos \theta_2} \\
r_{TM} = \frac{-\sqrt{a} \cos \theta_1 + \sqrt{b} \cos \theta_2}{\sqrt{a} \cos \theta_1 + \sqrt{b} \cos \theta_2}
\]

Notes on a Single Interface

- It is a change in impedance that causes reflections
- Snell’s Law quantifies the angle of transmission
- Angle of transmission and reflection does not depend on polarization
- The Fresnel equations quantify the amount of reflection and transmission
- Amount of reflection and transmission depends on the polarization

The Uniaxial Perfectly Matched Layer (UPML)

Boundary Condition Problem

If we model a wave hitting some device or object, it will scatter the applied wave into potentially many directions. We do NOT want these scattered waves to reflect from the boundaries of the grid. We also don’t want them to reenter from the other side of the grid (periodic boundaries).

No PAB in Two Dimensions

Waves at different angles travel at different speeds through a boundary. Therefore, the PAB condition can only be satisfied for one direction, not all directions.
How We Prevent Reflections in Lab

In the lab, we use anechoic foam to absorb outgoing waves.

Concept of a PML

STEP 2 of 500

- $y$-lo PML
- $y$-hi PML
- $x$-lo PML
- $x$-hi PML
Absorbing Boundary Conditions

We can introduce loss at the boundaries of the grid!

![Diagram showing Absorbing Boundary Conditions]

Oops!!

But if we introduce loss, we also introduce reflections from the lossy regions!!

![Diagram showing reflections from lossy regions]

\[ R = \frac{(1-n)^2 + \kappa^2}{(1+n)^2 + \kappa^2} \]
Match the Impedance

We need to introduce loss to absorb outgoing waves, but we also need to match the impedance of the problem space to prevent reflections.

\[ \tilde{\mathcal{E}}_r = \mathcal{E}'_r + j\mathcal{E}''_r \]

introduce loss here

adjust this to control impedance

More Trouble?

By examining the Fresnel equations, we see that we can only prevent reflections from the interface at one frequency, one angle of incidence, and one polarization.

\[ r_{\text{TE}} = \frac{\eta_2 \cos \theta_1 - \eta_1 \cos \theta_2}{\eta_2 \cos \theta_1 + \eta_1 \cos \theta_2} = 0 \quad \rightarrow \quad \eta_2 = \eta_1 \frac{\cos \theta_2}{\cos \theta_1} \]

\[ r_{\text{TM}} = \frac{\eta_2 \cos \theta_2 - \eta_1 \cos \theta_1}{\eta_1 \cos \theta_1 + \eta_2 \cos \theta_2} = 0 \quad \rightarrow \quad \eta_2 = \eta_1 \frac{\cos \theta_1}{\cos \theta_2} \]
Anisotropy to the Rescue!!

It turns out we can prevent reflections at all angles and for all polarizations if we allow our absorbing material to be doubly-diagonally anisotropic.

Problem Statement for the PML

Free Space $\mu_0, \varepsilon_0$

$\begin{bmatrix} \mu \end{bmatrix}, \begin{bmatrix} \varepsilon \end{bmatrix}$
Designing Anisotropy for Zero Reflection (1 of 3)

We need to perfectly match the impedance of the grid to the impedance of the absorbing region. For an absorbing boundary in air, this condition can be thought of as:

\[ \eta = \sqrt{\frac{\mu}{\varepsilon}} \text{ everywhere} \]

One easy way to ensure impedance is perfectly matched to air is:

\[
\begin{bmatrix}
\mu_r \\
\epsilon_r
\end{bmatrix}
= 
\begin{bmatrix}
a & 0 & 0 \\
0 & b & 0 \\
0 & 0 & c
\end{bmatrix}
\]

Designing Anisotropy for Zero Reflection (2 of 3)

If we choose \( \sqrt{bc} = 1 \), then the refraction equation reduces to:

\[ \sin \theta_1 = \sqrt{bc} \sin \theta_2 = \sin \theta_2 \quad \rightarrow \quad \theta_1 = \theta_2 \quad \text{No refraction!} \]

With this choice, the reflection coefficients reduce to:

\[
r_{TE} = \frac{\sqrt{a} \cos \theta_1 - \sqrt{b} \cos \theta_2}{\sqrt{a} \cos \theta_1 + \sqrt{b} \cos \theta_2} = \frac{\sqrt{a} - \sqrt{b}}{\sqrt{a} + \sqrt{b}}
\]

\[
r_{TM} = \frac{-\sqrt{a} \cos \theta_1 + \sqrt{b} \cos \theta_2}{\sqrt{a} \cos \theta_1 + \sqrt{b} \cos \theta_2} = \frac{-\sqrt{a} + \sqrt{b}}{\sqrt{a} + \sqrt{b}}
\]

These are no longer a function of angle!! 😊
Designing Anisotropy for Zero Reflection (3 of 3)

If we further choose \( a = b \), the reflection equations reduce to

\[
\begin{align*}
    r^\text{TE} &= \frac{\sqrt{a} - \sqrt{b}}{\sqrt{a} + \sqrt{b}} = 0 \\
    r^\text{TM} &= \frac{-\sqrt{a} + \sqrt{b}}{\sqrt{a} + \sqrt{b}} = 0
\end{align*}
\]

Reflection will always be zero regardless of frequency, angle of incidence, or polarization!! 😊

Recall the necessary conditions: \( \sqrt{bc} = 1 \) and \( a = b \)

The PML Parameters (1 of 4)

So far, we have

\[
\begin{bmatrix}
    \mu_r \\
    \varepsilon_r
\end{bmatrix} =
\begin{bmatrix}
    a & 0 & 0 \\
    0 & b & 0 \\
    0 & 0 & c
\end{bmatrix}
\]

Thus, we can write our PML in terms of just one parameter \( s_z \).

\[
\begin{bmatrix}
    S_z
\end{bmatrix} =
\begin{bmatrix}
    s_z & 0 & 0 \\
    0 & s_z & 0 \\
    0 & 0 & s_z^{-1}
\end{bmatrix}
\]

This is for a wave travelling in the \(+z\) direction incident on one boundary.
The PML Parameters (2 of 4)

Recall the complex permittivity $\tilde{\varepsilon}$ is related to the conductivity $\sigma$ and real-valued permittivity $\varepsilon$ through

$$\tilde{\varepsilon} = \varepsilon + \frac{\sigma}{j\omega} \quad \Rightarrow \quad \tilde{\varepsilon}_r = \varepsilon_r + \frac{\sigma}{j\omega \varepsilon_0}$$

We want the PML parameters to act like the complex relative permittivity $\tilde{\varepsilon}_r$ so that we will know more intuitively how to control it.

$$s_z = \varepsilon'_r + \frac{\sigma'}{j\omega \varepsilon_0} \quad \Rightarrow \quad \varepsilon' = \text{PML fictitious relative permittivity}$$

$$\sigma' = \text{PML fictitious conductivity}$$

For simplicity, we will set $\varepsilon'_r = 1$.

$$s_z = 1 + \frac{\sigma'}{j\omega \varepsilon_0} \quad \text{Many PML implementation use } \varepsilon'_r \neq 1 \text{ in order to better handle evanescent fields.}$$

The PML Parameters (3 of 4)

We potentially want a PML along all the borders.

$$[S_x] = \begin{bmatrix} s_x^{-1} & 0 & 0 \\ 0 & s_x & 0 \\ 0 & 0 & s_x \end{bmatrix} \quad [S_y] = \begin{bmatrix} s_y & 0 & 0 \\ 0 & s_y^{-1} & 0 \\ 0 & 0 & s_y \end{bmatrix} \quad [S_z] = \begin{bmatrix} s_z & 0 & 0 \\ 0 & s_z & 0 \\ 0 & 0 & s_z^{-1} \end{bmatrix}$$

These can be combined into a single tensor quantity.

$$[S] = [S_x][S_y][S_z] = \begin{bmatrix} \frac{s_y s_z}{s_x} & 0 & 0 \\ 0 & \frac{s_y s_z}{s_y} & 0 \\ 0 & 0 & \frac{s_y s_z}{s_z} \end{bmatrix}$$
The PML Parameters (4 of 4)

The 3D PML can be visualized this way...

\[
\begin{bmatrix}
  \frac{s_y s_z}{s_x} & 0 & 0 \\
  \frac{s_x s_z}{s_y} & 0 & 0 \\
  0 & 0 & \frac{s_x s_y}{s_z}
\end{bmatrix}
\]

The PML is Not a Boundary Condition

A numerical boundary condition is the rule you follow when a finite-difference equation references a field from outside the grid.

The PML does not address this issue.

It is simply a way of incorporating loss while preventing reflections so as to absorb outgoing waves.

Sometimes it is called an absorbing boundary condition, but this is still a misleading title because the PML is not a boundary condition.
Incorporating a UPML into Maxwell’s Equations

Before incorporating a PML, Maxwell’s equations in the frequency-domain are

\[ \nabla \times \tilde{E}(\omega) = -j\omega\mu_0 [\mu_r] \tilde{H}(\omega) \]
\[ \nabla \times \tilde{H}(\omega) = \sigma \tilde{E}(\omega) + j\omega \tilde{D}(\omega) \]
\[ \tilde{D}(\omega) = \varepsilon_0 [\varepsilon_r] \tilde{E}(\omega) \]

We can incorporate a PML independent of the actual materials on the grid as follows:

\[ \nabla \times \tilde{E}(\omega) = -j\omega\mu_0 [\mu_r][S] \tilde{H}(\omega) \]
\[ \nabla \times \tilde{H}(\omega) = \sigma \tilde{E}(\omega) + j\omega [S] \tilde{D}(\omega) \]
\[ \tilde{D}(\omega) = \varepsilon_0 [\varepsilon_r] \tilde{E}(\omega) \]
 Normalize Maxwell’s Equations with UPML

We normalize the electric field quantities according to

\[ \tilde{E} = \sqrt{\frac{\varepsilon_0}{\mu_0}} \tilde{E} = \frac{1}{\eta_0} \tilde{E} \]

\[ \tilde{D} = \frac{1}{\sqrt{\mu_0 \varepsilon_0}} \tilde{D} = c_0 \tilde{D} \]

Maxwell’s equations with the UPML and normalized fields are

\[ \nabla \times \tilde{E}(\omega) = -j \omega \left[ \frac{\mu_r}{c_0} \right] \left[ S \right] \tilde{H}(\omega) \]

\[ \nabla \times \tilde{H}(\omega) = \eta_0 \mu_0 \tilde{E}(\omega) + \frac{j \omega}{c_0} \left[ S \right] \tilde{D}(\omega) \]

Matrix Form of Maxwell’s Equations

Maxwell’s equations can be written in matrix form as

\[
\begin{bmatrix}
0 & -\frac{i}{\omega} & \frac{i}{\omega} & [\tilde{E}_x(\omega)] \\
\frac{i}{\omega} & 0 & -\frac{i}{\omega} & [\tilde{E}_y(\omega)] \\
-\frac{i}{\omega} & \frac{i}{\omega} & 0 & [\tilde{E}_z(\omega)]
\end{bmatrix} = -j \omega \left[ \frac{\mu_r}{c_0} \right] \left[ S \right] \begin{bmatrix}
\sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\
\sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\
\sigma_{zx} & \sigma_{zy} & \sigma_{zz}
\end{bmatrix} \begin{bmatrix}
\tilde{E}_x(\omega) \\
\tilde{E}_y(\omega) \\
\tilde{E}_z(\omega)
\end{bmatrix} + \frac{j \omega}{c_0} \begin{bmatrix}
s_x s_y s_z \\
s_x s_y s_z \\
s_x s_y s_z
\end{bmatrix} \begin{bmatrix}
\tilde{D}_x(\omega) \\
\tilde{D}_y(\omega) \\
\tilde{D}_z(\omega)
\end{bmatrix}
\]

\[
\begin{bmatrix}
\tilde{D}_x(\omega) \\
\tilde{D}_y(\omega) \\
\tilde{D}_z(\omega)
\end{bmatrix} = \begin{bmatrix}
\varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\
\varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\
\varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz}
\end{bmatrix} \begin{bmatrix}
\tilde{E}_x(\omega) \\
\tilde{E}_y(\omega) \\
\tilde{E}_z(\omega)
\end{bmatrix}
\]
Assume Only Diagonal Tensors

Here we assume that $[\mu]$, $[\varepsilon]$, and $[\sigma]$ contain only diagonal terms.

\[
\begin{bmatrix}
0 & -\frac{\sigma_{xx}}{c_0} & \frac{\sigma_{xz}}{c_0} \\
\frac{\sigma_{xx}}{c_0} & 0 & -\frac{\sigma_{zz}}{c_0} \\
-\frac{\sigma_{xz}}{c_0} & \frac{\sigma_{zz}}{c_0} & 0
\end{bmatrix}
\cdot
\begin{bmatrix}
\frac{\mu_{xx}}{c_0} & 0 & 0 \\
0 & \frac{\mu_{yy}}{c_0} & 0 \\
0 & 0 & \frac{\mu_{zz}}{c_0}
\end{bmatrix}
\cdot
\begin{bmatrix}
\frac{\omega}{c_0} & 0 & 0 \\
0 & \frac{\omega}{c_0} & 0 \\
0 & 0 & \frac{\omega}{c_0}
\end{bmatrix}
\cdot
\begin{bmatrix}
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{bmatrix}
\]

Vector Expansion of Maxwell’s Equations

\[
\nabla \times \vec{E}(\omega) = -j\omega \left[ \begin{array}{c} \mu_{xx} \frac{\partial}{\partial y} \vec{E}_{xx}(\omega) \\
\mu_{yy} \frac{\partial}{\partial z} \vec{E}_{yy}(\omega) \\
\mu_{zz} \frac{\partial}{\partial x} \vec{E}_{zz}(\omega)
\end{array} \right] + \begin{array}{c} \frac{\epsilon_{xx}}{c_0} \frac{\partial}{\partial y} \vec{E}_{xx}(\omega) \\
\frac{\epsilon_{yy}}{c_0} \frac{\partial}{\partial z} \vec{E}_{yy}(\omega) \\
\frac{\epsilon_{zz}}{c_0} \frac{\partial}{\partial x} \vec{E}_{zz}(\omega)
\end{array}
\]

\[
\nabla \times \vec{H}(\omega) = \begin{array}{c} \eta_{xx} \frac{\partial}{\partial y} \vec{H}_{xx}(\omega) \\
\eta_{yy} \frac{\partial}{\partial z} \vec{H}_{yy}(\omega) \\
\eta_{zz} \frac{\partial}{\partial x} \vec{H}_{zz}(\omega)
\end{array} + \begin{array}{c} \frac{j \omega}{c_0} \frac{\partial}{\partial y} \vec{H}_{xx}(\omega) \\
\frac{j \omega}{c_0} \frac{\partial}{\partial z} \vec{H}_{yy}(\omega) \\
\frac{j \omega}{c_0} \frac{\partial}{\partial x} \vec{H}_{zz}(\omega)
\end{array}
\]

\[
\vec{D}(\omega) = \left[ \begin{array}{c} \varepsilon_{xx} \vec{E}_{xx}(\omega) \\
\varepsilon_{yy} \vec{E}_{yy}(\omega) \\
\varepsilon_{zz} \vec{E}_{zz}(\omega)
\end{array} \right]
\]

\[
\vec{D}_{xx}(\omega) = \varepsilon_{xx} \vec{E}_{xx}(\omega) \\
\vec{D}_{yy}(\omega) = \varepsilon_{yy} \vec{E}_{yy}(\omega) \\
\vec{D}_{zz}(\omega) = \varepsilon_{zz} \vec{E}_{zz}(\omega)
\]
Final Form of Maxwell’s Equations with UPML

\[
\begin{align*}
\nabla \times \vec{E}(\omega) &= -j \omega \frac{\mu_0}{c_0} \sigma \vec{H}(\omega) \\
\nabla \times \vec{H}(\omega) &= \eta \sigma \vec{E}(\omega) + \frac{j \omega}{c_0} \frac{\rho}{c_0} \vec{D}(\omega)
\end{align*}
\]

\[
\begin{align*}
\vec{D}(\omega) &= \varepsilon_0 \vec{E}(\omega) \\
\vec{B}(\omega) &= \mu_0 \vec{H}(\omega)
\end{align*}
\]

Convolutional Perfectly Matched Layer (CPML)
The Uniaxial PML

Maxwell’s equations with uniaxial PML are:

\[ \nabla \times \vec{E} = k_0 \begin{bmatrix} S \end{bmatrix} \begin{bmatrix} \mu_r \end{bmatrix} \vec{H} \]
\[ \nabla \times \vec{H} = k_0 \begin{bmatrix} S \end{bmatrix} \begin{bmatrix} \varepsilon_r \end{bmatrix} \vec{E} \]

\[ [S] = \begin{bmatrix}
  s_x s_z & 0 & 0 \\
  s_x & 0 & s_y \\
  0 & 0 & s_z \\
\end{bmatrix} \]

Rearrange the Terms

We can bring the PML tensor to the left side of the equations and associate it with the curl operator.

\[ [S]^{-1} \nabla \times \vec{E} = k_0 \begin{bmatrix} \mu_r \end{bmatrix} \vec{H} \]
\[ [S]^{-1} \nabla \times \vec{H} = k_0 \begin{bmatrix} \varepsilon_r \end{bmatrix} \vec{E} \]

The curl operator is now

\[ [S]^{-1} \nabla \times = \begin{bmatrix}
  s_x^{-1} s_y^{-1} s_x & 0 & 0 \\
  0 & s_z s_x^{-1} s_y & 0 \\
  0 & 0 & s_z s_y^{-1} s_x \\
\end{bmatrix} \begin{bmatrix}
  \frac{\partial}{\partial x} & -\frac{\partial}{\partial y} & -\frac{\partial}{\partial z} \\
  \frac{\partial}{\partial y} & \frac{\partial}{\partial z} & \frac{\partial}{\partial x} \\
  \frac{\partial}{\partial z} & \frac{\partial}{\partial x} & \frac{\partial}{\partial y} \\
\end{bmatrix} \]

= \begin{bmatrix}
  0 & -\frac{\partial}{\partial y} \left( \frac{1}{\varepsilon_r} \right) & \frac{\partial}{\partial z} \left( \frac{1}{\varepsilon_r} \right) \\
  \frac{\partial}{\partial y} \left( \frac{1}{\varepsilon_r} \right) & 0 & -\frac{\partial}{\partial z} \left( \frac{1}{\varepsilon_r} \right) \\
  -\frac{\partial}{\partial z} \left( \frac{1}{\varepsilon_r} \right) & \frac{\partial}{\partial z} \left( \frac{1}{\varepsilon_r} \right) & 0 \\
\end{bmatrix} \]
**“Stretched” Coordinates**

Our new curl operator is

\[
[S]^{-1} \nabla \times = \begin{bmatrix}
0 & -\frac{s_x}{s_y} \left( \frac{1}{s_z} \frac{\partial}{\partial z} \right) & \frac{s_x}{s_z} \left( \frac{1}{s_y} \frac{\partial}{\partial y} \right) \\
-\frac{s_y}{s_x} \left( \frac{1}{s_z} \frac{\partial}{\partial z} \right) & 0 & -\frac{s_y}{s_z} \left( \frac{1}{s_x} \frac{\partial}{\partial x} \right) \\
-\frac{s_z}{s_y} \left( \frac{1}{s_x} \frac{\partial}{\partial x} \right) & \frac{s_z}{s_x} \left( \frac{1}{s_y} \frac{\partial}{\partial y} \right) & 0
\end{bmatrix}
\]

The factors \(s_x, s_y, s_z\) are effectively “stretching” the coordinates, but they are “stretching” into a complex space.

**Drop the Other Terms**

We drop the non-stretching terms.

\[
\nabla \times = \begin{bmatrix}
0 & -\frac{1}{s_x} \left( \frac{\partial}{\partial x} \right) & \frac{1}{s_y} \left( \frac{\partial}{\partial y} \right) \\
-\frac{1}{s_y} \left( \frac{\partial}{\partial y} \right) & 0 & -\frac{1}{s_z} \left( \frac{\partial}{\partial z} \right) \\
-\frac{1}{s_z} \left( \frac{\partial}{\partial z} \right) & \frac{1}{s_x} \left( \frac{\partial}{\partial x} \right) & 0
\end{bmatrix}
\]

**Justification**

\[
\frac{s_x}{s_y} \left( \frac{1}{s_z} \frac{\partial}{\partial z} \right) = \frac{1}{s_x} \frac{\partial}{\partial x}
\]

Inside the \(z\)-PML, \(s_x = s_y = 1\). This is valid everywhere except at the extreme corners of the grid where the PMLs overlap.

This also implies that the UPML and SC-PML have nearly identical performance in terms of reflections, sensitivity to angle of incidence, polarization, etc.
Maxwell’s Equations with a SC-PML

Maxwell’s equations before the PML is added are
\[
\nabla \times \vec{E} = k_0 [\mu_r] \vec{H}
\]
\[
\nabla \times \vec{H} = k_0 [\varepsilon_r] \vec{E}
\]

The SC-PML is incorporated as follows.
\[
\nabla_s \times \vec{E} = -j\omega [\mu] \vec{H}
\]
\[
\nabla_s \times \vec{H} = j\omega [\varepsilon] \vec{E}
\]

\[
\nabla_s \times = \begin{bmatrix}
0 & -\frac{1}{s_x} \frac{\partial}{\partial z} & \frac{1}{s_y} \frac{\partial}{\partial y} \\
\frac{1}{s_x} \frac{\partial}{\partial z} & 0 & -\frac{1}{s_x} \frac{\partial}{\partial x} \\
-\frac{1}{s_y} \frac{\partial}{\partial y} & \frac{1}{s_x} \frac{\partial}{\partial x} & 0
\end{bmatrix}
\]

Vector Expansion

Maxwell’s equations with a SC-PML expand to

**Fully Anisotropic**

\[
\frac{1}{s_y} \frac{\partial \vec{H}_y}{\partial z} - \frac{1}{s_z} \frac{\partial \vec{H}_z}{\partial y} = k_0 \left( \varepsilon_{ys} E_x + \varepsilon_{zy} E_y + \varepsilon_{zz} E_z \right)
\]
\[
\frac{1}{s_z} \frac{\partial \vec{H}_z}{\partial x} + \frac{1}{s_x} \frac{\partial \vec{H}_x}{\partial z} = k_0 \left( \varepsilon_{xz} E_x + \varepsilon_{zy} E_y + \varepsilon_{yz} E_z \right)
\]
\[
\frac{1}{s_x} \frac{\partial \vec{H}_x}{\partial y} - \frac{1}{s_y} \frac{\partial \vec{H}_y}{\partial x} = k_0 \left( \varepsilon_{xy} E_x + \varepsilon_{yx} E_y + \varepsilon_{xx} E_z \right)
\]

\[
\frac{1}{s_y} \frac{\partial \vec{E}_y}{\partial z} - \frac{1}{s_z} \frac{\partial \vec{E}_z}{\partial y} = k_0 \left( \mu_{ys} \vec{H}_x + \mu_{zy} \vec{H}_y + \mu_{zz} \vec{H}_z \right)
\]
\[
\frac{1}{s_z} \frac{\partial \vec{E}_z}{\partial x} + \frac{1}{s_x} \frac{\partial \vec{E}_x}{\partial z} = k_0 \left( \mu_{xz} \vec{H}_x + \mu_{zy} \vec{H}_y + \mu_{yz} \vec{H}_z \right)
\]
\[
\frac{1}{s_x} \frac{\partial \vec{E}_x}{\partial y} - \frac{1}{s_y} \frac{\partial \vec{E}_y}{\partial x} = k_0 \left( \mu_{xy} \vec{H}_x + \mu_{yx} \vec{H}_y + \mu_{xx} \vec{H}_z \right)
\]

**Diagonally Anisotropic**

\[
\frac{1}{s_y} \frac{\partial \vec{H}_y}{\partial z} - \frac{1}{s_z} \frac{\partial \vec{H}_z}{\partial y} = k_0 \varepsilon_{xx} E_x
\]
\[
\frac{1}{s_z} \frac{\partial \vec{H}_z}{\partial x} + \frac{1}{s_x} \frac{\partial \vec{H}_x}{\partial z} = k_0 \varepsilon_{yy} E_y
\]
\[
\frac{1}{s_x} \frac{\partial \vec{H}_x}{\partial y} - \frac{1}{s_y} \frac{\partial \vec{H}_y}{\partial x} = k_0 \varepsilon_{zz} E_z
\]

\[
\frac{1}{s_y} \frac{\partial \vec{E}_y}{\partial z} - \frac{1}{s_z} \frac{\partial \vec{E}_z}{\partial y} = k_0 \mu_{xx} \vec{H}_x
\]
\[
\frac{1}{s_z} \frac{\partial \vec{E}_z}{\partial x} + \frac{1}{s_x} \frac{\partial \vec{E}_x}{\partial z} = k_0 \mu_{yy} \vec{H}_y
\]
\[
\frac{1}{s_x} \frac{\partial \vec{E}_x}{\partial y} - \frac{1}{s_y} \frac{\partial \vec{E}_y}{\partial x} = k_0 \mu_{zz} \vec{H}_z
\]
**Convolutional PML**

A convolutional PML is a SC-PML that is solved efficiently in the time-domain.

We have a multiplication operation in the frequency-domain.
This becomes convolution in the time-domain.

\[
\begin{align*}
\frac{1}{s_y} \frac{\partial E_y}{\partial y} - \frac{1}{s_z} \frac{\partial E_z}{\partial z} &= k_0 \varepsilon_{xx} E_x, \\
\frac{1}{s_z} \frac{\partial E_z}{\partial z} - \frac{1}{s_x} \frac{\partial E_x}{\partial x} &= k_0 \varepsilon_{yy} E_y, \\
\frac{1}{s_y} \frac{\partial E_y}{\partial y} - \frac{1}{s_x} \frac{\partial E_x}{\partial x} &= k_0 \varepsilon_{zz} E_z.
\end{align*}
\]

\[
\begin{align*}
\frac{1}{s_y} \frac{\partial H_y}{\partial y} - \frac{1}{s_z} \frac{\partial H_z}{\partial z} &= k_0 \mu_{xx} H_x, \\
\frac{1}{s_z} \frac{\partial H_z}{\partial z} - \frac{1}{s_x} \frac{\partial H_x}{\partial x} &= k_0 \mu_{yy} H_y, \\
\frac{1}{s_y} \frac{\partial H_y}{\partial y} - \frac{1}{s_x} \frac{\partial H_x}{\partial x} &= k_0 \mu_{zz} H_z.
\end{align*}
\]

**UPML Vs. SC-PML**

- **Uniaxial PML**
  - Has a physical interpretation
  - Models can be formulated and implemented without considering the PML in the frequency-domain
  - **Benefits**
  - Less computationally intensive in time-domain
  - More efficient implementation in the time-domain
  - Matrices are better conditioned.

- **Drawbacks**
  - Can be more computationally intensive to implement in time-domain
  - Resulting matrices are less well conditioned in the frequency-domain

- **Stretched-Coordinate PML**
  - Must be accounted for in the formulation and implementation of the numerical method.
  - Not intuitive to understand

- **Benefits**
  - Has a physical interpretation
  - Models can be formulated and implemented without considering the PML in the frequency-domain
  - Less computationally intensive in time-domain
  - More efficient implementation in the time-domain
  - Matrices are better conditioned.
Why a UPML for This Course?

• A CPML (or SC-PML) is currently the state-of-the-art in FDTD.
• A UPML offers benefits to frequency-domain models that are useful for beginners.
  – The models can be formulated and implemented without considering the PML. The PML is incorporated simply by adjusting the values of permittivity and permeability at the edges of the grid.
• Implementing a UPML in this course offers better continuity going into the following course, *Computational Electromagnetics*.

Calculating the PML Parameters
The Perfectly Matched Layer (PML)

The perfectly matched layer (PML) is an absorbing boundary condition (ABC) where the impedance is perfectly matched to the problem space. Reflections entering the lossy regions are prevented because impedance is matched. Reflections from the grid boundaries are prevented because the outgoing waves are absorbed.

Calculating the PML Loss Terms

For best performance, the loss terms should increase gradually into the PMLs.

\[
\begin{align*}
    s_x(x) &= 1 + \frac{\sigma_x'(x)}{j\omega\varepsilon_0} \\
    s_y(y) &= 1 + \frac{\sigma_y'(y)}{j\omega\varepsilon_0} \\
    s_z(z) &= 1 + \frac{\sigma_z'(z)}{j\omega\varepsilon_0}
\end{align*}
\]

\[
\begin{align*}
    \sigma_x'(x) &= \frac{\varepsilon_0}{2\Delta t} \left( \frac{x}{L_x} \right)^3 \\
    \sigma_y'(y) &= \frac{\varepsilon_0}{2\Delta t} \left( \frac{y}{L_y} \right)^3 \\
    \sigma_z'(z) &= \frac{\varepsilon_0}{2\Delta t} \left( \frac{z}{L_z} \right)^3
\end{align*}
\]

\[L_y \equiv \text{length of the PML in the } ? \text{ direction}\]
Visualizing the PML Loss Terms – 2D

For best performance, the loss terms should increase gradually into the PMLs.

\[ \sigma'_x(x) \quad \text{and} \quad \sigma'_y(y) \]

Note About \( x/L_x \), \( y/L_y \), and \( z/L_z \)

The following ratios provide a single quantity that goes from 0 to 1 as you move through a PML region.

\[ \frac{x}{L_x} \text{ and } \frac{y}{L_y} \text{ and } \frac{z}{L_z} \]

\( x, y, z \equiv \) position within PML

\( L_x, L_y, L_z \equiv \) size of PML

We can calculate the same ratio using integer indices from our grid.

\[ \frac{x}{L_x} \approx \frac{nx}{NXLO} \text{ or } \frac{nx}{NXHI} \quad \text{nx} = 1, 2, \ldots, NXLO \]
\[ \frac{y}{L_y} \approx \frac{ny}{NYLO} \text{ or } \frac{ny}{NYHI} \quad \text{ny} = 1, 2, \ldots, NYLO \]
\[ \frac{z}{L_z} \approx \frac{nz}{NZLO} \text{ or } \frac{nz}{NZHI} \quad \text{nz} = 1, 2, \ldots, NZLO \]
Visualizing the Calculation of $\sigma_x$ in 2D

% ADD XLO PML
for nx = 1 : NXLO
    ox(NXLO-nx+1,:) = ...
end

% ADD XHI PML
for nx = 1 : NXHI
    ox(Nx-NXHI+nx,:) = ...
end

$\sigma_x(x) = \sigma_{max}(x/L_x)^3$

Visualizing the Calculation of $\sigma_y$ in 2D

% ADD YLO PML
for ny = 1 : NYLO
    oy(:,NYLO-ny+1) = ...
end

% ADD YHI PML
for ny = 1 : NYHI
    oy(:,Ny-NYHI+ny) = ...
end

$\sigma_y(y) = \sigma_{max}(y/L_y)^3$

$\sigma_x(x) = 0$

$\sigma_y(y) = 1$
Procedure for Calculating $\sigma_x$ and $\sigma_y$ on a 2D Grid

1. Initialize $\sigma_x$ and $\sigma_y$ to all zeros.
   
   $$\sigma_x(x,y) = \sigma_y(x,y) = 0$$

2. Fill in x-axis PML regions using two for loops.

3. Fill in y-axis PML regions using two for loops.