EE 5337
Computational Electromagnetics

Lecture #9
Perfectly Matched Layer

Outline

• Background Information
• The Uniaxial Perfectly Matched Layer (UPML)
• Incorporating a UPML into Maxwell’s Equations
• Implementing the UPML
• Stretched Coordinate PML (SC-PML)
• PML Performance
• UPML vs SC-PML
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 \( \vec{V} \rightarrow a\vec{V} \)

Tensor Relation \( [a][\vec{V}] \)

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

Complex Refractive Index

\[ \tilde{n} = n + j \kappa \]

- \( n \) is the ordinary refractive index (oscillation)
- \( \kappa \) is the extinction coefficient (decay)

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

- \( \theta_{\text{inc}} = \theta_{\text{ref}} = \theta_1 \)
- \( n_1 \sin \theta_1 = n_2 \sin \theta_2 \)  
  Snell’s Law

**TE Polarization**

- Reflectance:
  \[ r_{\text{TE}} = \frac{\eta_2 \cos \theta_1 - \eta_1 \cos \theta_2}{\eta_2 \cos \theta_1 + \eta_1 \cos \theta_2} \]
- Transmission:
  \[ t_{\text{TE}} = \frac{2\eta_2 \cos \theta_1}{\eta_2 \cos \theta_1 + \eta_1 \cos \theta_2} \]

**TM Polarization**

- Reflectance:
  \[ r_{\text{TM}} = \frac{\eta_2 \cos \theta_2 - \eta_1 \cos \theta_1}{\eta_2 \cos \theta_1 + \eta_1 \cos \theta_2} \]
- Transmission:
  \[ t_{\text{TM}} = \frac{2\eta_2 \cos \theta_1}{\eta_2 \cos \theta_1 + \eta_1 \cos \theta_2} \]
Maxwell’s Equations in Anisotropic Media

Maxwell’s curl equations in anisotropic media are:

\[ \nabla \times \vec{H} = j \omega \varepsilon_0 [\varepsilon_r] \vec{E} \]
\[ \nabla \times \vec{E} = -j \omega \mu_0 [\mu_r] \vec{H} \]

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

\[
\begin{bmatrix}
0 & -\frac{\partial}{\partial z} & \frac{\partial}{\partial y} \\
\frac{\partial}{\partial z} & 0 & -\frac{\partial}{\partial x} \\
-\frac{\partial}{\partial y} & \frac{\partial}{\partial x} & 0
\end{bmatrix}
\begin{bmatrix}
H_x \\
H_y \\
H_z
\end{bmatrix}
= j \omega \varepsilon_0
\begin{bmatrix}
\varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\
\varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\
\varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz}
\end{bmatrix}
\begin{bmatrix}
E_x \\
E_y \\
E_z
\end{bmatrix}
\]

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

Types of Anisotropic Media

There are three basic types of anisotropic media:

\[
\begin{bmatrix}
\varepsilon_{iso} & 0 & 0 \\
0 & \varepsilon_{iso} & 0 \\
0 & 0 & \varepsilon_{iso}
\end{bmatrix}
\text{ isotropic}
\]

\[
\begin{bmatrix}
\varepsilon_o & 0 & 0 \\
0 & \varepsilon_o & 0 \\
0 & 0 & \varepsilon_e
\end{bmatrix}
\text{ uniaxial}
\]

\[
\begin{bmatrix}
\varepsilon_a & 0 & 0 \\
0 & \varepsilon_b & 0 \\
0 & 0 & \varepsilon_c
\end{bmatrix}
\text{ biaxial}
\]

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

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

We use this for FDTD

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

\[
\nabla \times \vec{H} = j \omega \varepsilon_r \varepsilon \vec{E}
\]

The parameters are related through

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

Note: It does not make sense to have a complex \(\varepsilon_r\) and a conductivity \(\sigma\).

Maxwell’s Equations in Doubly-Diagonally Anisotropic Media

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

\[
\begin{bmatrix}
0 & -\frac{\partial}{\partial x} & \frac{\partial}{\partial y} \\
\frac{\partial}{\partial x} & 0 & -\frac{\partial}{\partial z} \\
-\frac{\partial}{\partial y} & \frac{\partial}{\partial z} & 0
\end{bmatrix}
\begin{bmatrix}
H_x \\
H_y \\
H_z
\end{bmatrix}
= j \omega \varepsilon_0 \begin{bmatrix}
\varepsilon_x + \sigma_x^E / j \omega \\
\varepsilon_y + \sigma_y^E / j \omega \\
\varepsilon_z + \sigma_z^E / j \omega
\end{bmatrix}
\begin{bmatrix}
E_x \\
E_y \\
E_z
\end{bmatrix}
\]

We can generalize further by incorporating loss.

\[
\begin{bmatrix}
0 & -\frac{\partial}{\partial x} & \frac{\partial}{\partial y} \\
\frac{\partial}{\partial x} & 0 & -\frac{\partial}{\partial z} \\
-\frac{\partial}{\partial y} & \frac{\partial}{\partial z} & 0
\end{bmatrix}
\begin{bmatrix}
H_x \\
H_y \\
H_z
\end{bmatrix}
= j \omega \mu_0 \begin{bmatrix}
\sigma_x^H / j \omega \\
\sigma_y^H / j \omega \\
\sigma_z^H / j \omega
\end{bmatrix}
\begin{bmatrix}
E_x \\
E_y \\
E_z
\end{bmatrix}
\]

\[
\begin{bmatrix}
0 & -\frac{\partial}{\partial x} & \frac{\partial}{\partial y} \\
\frac{\partial}{\partial x} & 0 & -\frac{\partial}{\partial z} \\
-\frac{\partial}{\partial y} & \frac{\partial}{\partial z} & 0
\end{bmatrix}
\begin{bmatrix}
H_x \\
H_y \\
H_z
\end{bmatrix}
= j \omega \mu_0 \begin{bmatrix}
\mu_x + \sigma_x^H / j \omega \\
\mu_y + \sigma_y^H / j \omega \\
\mu_z + \sigma_z^H / j \omega
\end{bmatrix}
\begin{bmatrix}
H_x \\
H_y \\
H_z
\end{bmatrix}
\]
Scattering at a Doubly-Anisotropic Interface

Refraction into a diagonally anisotropic materials is described by

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

Reflection from a diagonally anisotropic material is

\[
\begin{align*}
    r_{TE} &= \frac{\sqrt{a} \cos \theta_1 - \sqrt{b} \cos \theta_2}{\sqrt{a} \cos \theta_1 + \sqrt{b} \cos \theta_2} \\
    r_{TM} &= \frac{-\sqrt{a} \cos \theta_1 + \sqrt{b} \cos \theta_2}{\sqrt{a} \cos \theta_1 + \sqrt{b} \cos \theta_2}
\end{align*}
\]


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
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).

How do we prevent this?
How We Prevent Reflections in Lab

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

Absorbing Boundary Conditions

We can introduce loss at the boundaries of the grid!
Oops!!

But if we introduce loss, we also introduce reflections from the 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 to the problem space to prevent reflections.

\[ \tilde{\varepsilon}_r = \varepsilon'_r + j\varepsilon''_r \]

introduce loss here

adjust this to control impedance
By examining the Fresnel equations, we see that we can only prevent reflections from the interface at one frequency, one angle of incident, and one polarization.

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

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

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 $\mu_0, \varepsilon_0$

$\theta_1$ $\theta_2$

$0\%$ $100\%$

$\begin{bmatrix} \mu, \varepsilon \end{bmatrix}$

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.

$$\eta = \sqrt{\frac{\mu}{\varepsilon}} \quad \text{everywhere}$$

One easy way to ensure impedance is perfectly matched is:

$$\begin{bmatrix} \mu_r \end{bmatrix} = \begin{bmatrix} \varepsilon_r \end{bmatrix} = \begin{bmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{bmatrix}$$
Designing Anisotropy for Zero Reflection (2 of 3)

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

$$\sin \theta_1 = \sqrt{bc} \sin \theta_2 = \sin \theta_2 \quad \rightarrow \quad \theta_1 = \theta_2$$

No refraction!

The reflection coefficients now 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

$$r_{TE} = \frac{\sqrt{a} - \sqrt{b}}{\sqrt{a} + \sqrt{b}} = 0$$

$$r_{TM} = \frac{-\sqrt{a} + \sqrt{b}}{\sqrt{a} + \sqrt{b}} = 0$$

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 3)

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 \(s_z\).

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

This is for a wave travelling in the \(+z\) direction incident on a \(z\)-axis boundary.

This form of tensor is why we call this a uniaxial PML.

The PML Parameters (2 of 3)

We potentially want a PML along all the borders.

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

These can be combined into a single tensor quantity.

\[
\begin{bmatrix}
\frac{s_y s_z}{s_x} & 0 & 0 \\
0 & \frac{s_y s_z}{s_y} & 0 \\
0 & 0 & \frac{s_y s_z}{s_z}
\end{bmatrix}
\]
The PML Parameters (3 of 3)

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

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

UPML in Cylindrical and Spherical Coordinates

Cylindrical Coordinates

\[
[S] = \begin{bmatrix}
  \tilde{\rho} s_z & 0 & 0 \\
  \rho s_\rho & 0 & \tilde{\rho} s_z s_\rho \\
  0 & 0 & \tilde{\rho} s_\rho
\end{bmatrix}
\]

Spherical Coordinates

\[
[S] = \begin{bmatrix}
  (\tilde{\rho}/r)^2 & 1 & 0 & 0 \\
  0 & s_r & 0 & 0 \\
  0 & 0 & s_r
\end{bmatrix}
\]

Two-Dimensional UPML

For 2D simulations in the x-y plane, $s_z = 1$ and the UPML tensor reduces to

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

Incorporating a UPML into Maxwell’s Equations
Incorporating the UPML Into Maxwell’s Eqs.

Maxwell’s Equations
This set of equations does include devices, but no UPML at the boundary to absorb outgoing waves.

\[ \nabla \times \vec{E} = k_0 [\mu_r] \vec{H} \]
\[ \nabla \times \vec{H} = k_0 [\varepsilon_r] \vec{E} \]

UPML
This set of equations includes the UPML to absorb outgoing waves, but does not include devices or real materials.

\[ \nabla \times \vec{E} = k_0 [S] \vec{H} \]
\[ \nabla \times \vec{H} = k_0 [S] \vec{E} \]

Maxwell’s Equations with UPML
This approach incorporates the PML in a way that is independent of the materials. It keeps the PML impedance matched to the background materials automatically.

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

Maxwell’s Equations with a UPML

The UPML can be incorporated into the material tensors directly.

\[ \nabla \times \vec{E} = k_0 [\mu_r'] \vec{H} \]
\[ \nabla \times \vec{H} = k_0 [\varepsilon_r'] \vec{E} \]

This let’s us formulate and implement a numerical algorithm without having to explicitly consider the PML. It is simply incorporated into the material tensors.
Vector Expansion

Assuming only diagonal tensors

\[
\begin{bmatrix}
\varepsilon_{xx} & 0 & 0 \\
0 & \varepsilon_{yy} & 0 \\
0 & 0 & \varepsilon_{zz}
\end{bmatrix}
\quad \begin{bmatrix}
\mu_{xx} & 0 & 0 \\
0 & \mu_{yy} & 0 \\
0 & 0 & \mu_{zz}
\end{bmatrix}
\]

Maxwell's equations expand to

\[
\frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial x} = k_0 \varepsilon_{xx} \frac{s_z}{s_y} H_x \\
\frac{\partial E_z}{\partial z} - \frac{\partial E_x}{\partial y} = k_0 \mu_{zz} \frac{s_z}{s_y} H_y \\
\frac{\partial E_x}{\partial x} - \frac{\partial E_y}{\partial y} = k_0 \mu_{yy} \frac{s_z}{s_y} H_z
\]

Absorb UPML into \( \mu \) and \( \varepsilon \) (3D Grid)

We can absorb the UPML parameters into the material functions.

\[
\begin{align*}
\mu'_{xx} &= \mu_{xx} \frac{s_z}{s_y} \\
\mu'_{yy} &= \mu_{yy} \frac{s_z}{s_y} \\
\mu'_{zz} &= \mu_{zz} \frac{s_z}{s_y} \\
\varepsilon'_{xx} &= \varepsilon_{xx} \frac{s_z}{s_y} \\
\varepsilon'_{yy} &= \varepsilon_{yy} \frac{s_z}{s_y} \\
\varepsilon'_{zz} &= \varepsilon_{zz} \frac{s_z}{s_y}
\end{align*}
\]

We can now write Maxwell's equations as

\[
\begin{align*}
\frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial x} &= k_0 \mu'_{xx} H_x \\
\frac{\partial E_z}{\partial z} - \frac{\partial E_x}{\partial y} &= k_0 \mu'_{yy} H_y \\
\frac{\partial E_x}{\partial x} - \frac{\partial E_y}{\partial y} &= k_0 \mu'_{zz} H_z
\end{align*}
\]

This means we can formulate a code as if there was no PML. All we have to do is modify the materials being modeled near the boundaries.
Absorb UPML into $\mu$ and $\varepsilon$ (2D Grid)

Let $z$ be the uniform direction, then $d/dz = 0$ and $s_z = 1$.

We can still absorb the UPML parameters into the material functions.

\[
\begin{align*}
\mu'_xx &= \mu_{xx} \frac{s_x}{s_z} \\
\mu'_yy &= \mu_{yy} \frac{s_y}{s_z} \\
\mu'_zz &= \mu_{zz} s_z s_y \\
\varepsilon'_xx &= \varepsilon_{xx} \frac{s_x}{s_z} \\
\varepsilon'_yy &= \varepsilon_{yy} \frac{s_y}{s_z} \\
\varepsilon'_zz &= \varepsilon_{zz} s_z s_y
\end{align*}
\]

We can now write Maxwell’s equations as

**E Mode**
\[
\begin{align*}
\frac{\partial \vec{H}_x}{\partial x} - \frac{\partial \vec{H}_y}{\partial y} &= k_0 \varepsilon'_x \vec{E}_x \\
\frac{\partial \vec{E}_x}{\partial y} &= k_0 \mu'_x \vec{H}_z \\
-\frac{\partial \vec{E}_x}{\partial x} &= k_0 \mu'_z \vec{H}_y
\end{align*}
\]

**H Mode**
\[
\begin{align*}
\frac{\partial \vec{E}_x}{\partial x} - \frac{\partial \vec{E}_y}{\partial y} &= k_0 \mu'_x \vec{H}_z \\
\frac{\partial \vec{H}_x}{\partial y} &= k_0 \varepsilon'_x \vec{E}_x \\
\frac{\partial \vec{H}_x}{\partial x} &= k_0 \varepsilon'_y \vec{E}_y
\end{align*}
\]
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 boundary are prevented because the outgoing waves are absorbed.

Typical Grid Schemes

Periodic Devices

Periodic Boundary

Finite Devices

Periodic Boundary

Spacer region

20 cells

20 cells

20 cells

20 cells

λ

λ

λ

λ
**Justification for the Spacer Regions**

The refractive index is high inside the PML so evanescent waves can become propagating waves, giving an escape path for power.

**How to Calculate the PML Parameters**

Maxwell's Eqs. with PML

\[ \nabla \times \vec{E} = k_0 [\mu_r] [s] \tilde{H} \]
\[ \nabla \times \vec{H} = k_0 c [\varepsilon_r] [s] \tilde{E} \]

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

Computing PML Parameters

\[ s_x (x) = a_x (x) \left[ 1 + j \eta_0 \sigma'_x (x) \right] \]
\[ s_y (y) = a_y (y) \left[ 1 + j \eta_0 \sigma'_y (y) \right] \]
\[ s_z (z) = a_z (z) \left[ 1 + j \eta_0 \sigma'_z (z) \right] \]

\[ \eta_0 = 376.73... = \text{free space impedance} \]

\[ a_x (x) = 1 + a_{\text{max}}^{-1} \left( x/L_x \right) \]
\[ a_y (y) = 1 + a_{\text{max}}^{-1} \left( y/L_y \right) \]
\[ a_z (z) = 1 + a_{\text{max}}^{-1} \left( z/L_z \right) \]

\[ \sigma'_x (x) = \sigma'_{\text{max}} \sin^2 \left( \frac{\pi x}{2L_x} \right) \]
\[ \sigma'_y (y) = \sigma'_{\text{max}} \sin^2 \left( \frac{\pi y}{2L_y} \right) \]
\[ \sigma'_z (z) = \sigma'_{\text{max}} \sin^2 \left( \frac{\pi z}{2L_z} \right) \]

\[ 0 \leq a_{\text{max}} \leq 5 \]
\[ 3 \leq p \leq 5 \]
\[ \sigma'_{\text{max}} = 1 \]

NGRID = [Nx Ny];
NPML  = [0 0 20 20];
[nx, ny] = calcpml2d(NGRID, NPML);

Writing this function will be in homework 😊
Visualizing the PML Loss Terms – 2D

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

\[
\sigma'_x(x) \quad \sigma'_y(y)
\]

Procedure for Calculating \(s_x\) and \(s_y\) on a 2D Grid

1. Initialize \(s_x\) and \(s_y\) to all ones.
   \[s_x(x, y) = s_y(x, y) = 1\]

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

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

$$\frac{x}{L_x} \approx \frac{nx}{NXLO} \text{ or } \frac{nx}{NXHI} \quad nx = 1, 2, \ldots, NXLO$$

$$\frac{y}{L_y} \approx \frac{ny}{NYLO} \text{ or } \frac{ny}{NYHI} \quad ny = 1, 2, \ldots, NYLO$$

$$\frac{z}{L_z} \approx \frac{nz}{NZLO} \text{ or } \frac{nz}{NZHI} \quad nz = 1, 2, \ldots, NZLO$$

Visualizing $s_x$ in 2D

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

% ADD XHI PML
for nx = 1 : NXHI
    % sx(nx-NXHI+nx,:) = ...
end
```
Visualizing $s_y$ in 2D

\[ s_y(y) = 1 \]

\[ s_y(y) = a_y(y)[1 + j\eta_0\sigma_y(y)] \]

Example Data for 2D

NGRID = [7 4];
NPML = [2 3 1 2];
[sx, sy] = calcpml2d(NGRID, NPML);

\[
\begin{align*}
\sigma_{\text{max}} &= 3 \\
p &= 3 \\
\sigma'_{\text{max}} &= 1
\end{align*}
\]

\[
\begin{array}{cccccccc}
sx &= 1.0e+03 & * \\
0.0040 + 1.5069i & 0.0040 + 1.5069i & 0.0040 + 1.5069i & 0.0040 + 1.5069i & 0.0040 + 1.5069i & 0.0040 + 1.5069i & 0.0040 + 1.5069i & 0.0040 + 1.5069i \\
0.0014 + 0.2590i & 0.0014 + 0.2590i & 0.0014 + 0.2590i & 0.0014 + 0.2590i & 0.0014 + 0.2590i & 0.0014 + 0.2590i & 0.0014 + 0.2590i & 0.0014 + 0.2590i \\
0.0010 & 0.0010 & 0.0010 & 0.0010 & 0.0010 & 0.0010 & 0.0010 & 0.0010 \\
0.0010 & 0.0010 & 0.0010 & 0.0010 & 0.0010 & 0.0010 & 0.0010 & 0.0010 \\
0.0011 + 0.1046i & 0.0011 + 0.1046i & 0.0011 + 0.1046i & 0.0011 + 0.1046i & 0.0011 + 0.1046i & 0.0011 + 0.1046i & 0.0011 + 0.1046i & 0.0011 + 0.1046i \\
0.0019 + 0.5337i & 0.0019 + 0.5337i & 0.0019 + 0.5337i & 0.0019 + 0.5337i & 0.0019 + 0.5337i & 0.0019 + 0.5337i & 0.0019 + 0.5337i & 0.0019 + 0.5337i \\
0.0040 + 1.5069i & 0.0040 + 1.5069i & 0.0040 + 1.5069i & 0.0040 + 1.5069i & 0.0040 + 1.5069i & 0.0040 + 1.5069i & 0.0040 + 1.5069i & 0.0040 + 1.5069i \\
\end{array}
\]

\[
\begin{array}{cccccccc}
sy &= 1.0e+03 & * \\
0.0040 + 1.5069i & 0.0010 & 0.0014 + 0.2590i & 0.0040 + 1.5069i & 0.0040 + 1.5069i & 0.0040 + 1.5069i & 0.0040 + 1.5069i & 0.0040 + 1.5069i \\
0.0040 + 1.5069i & 0.0010 & 0.0014 + 0.2590i & 0.0040 + 1.5069i & 0.0040 + 1.5069i & 0.0040 + 1.5069i & 0.0040 + 1.5069i & 0.0040 + 1.5069i \\
0.0040 + 1.5069i & 0.0010 & 0.0014 + 0.2590i & 0.0040 + 1.5069i & 0.0040 + 1.5069i & 0.0040 + 1.5069i & 0.0040 + 1.5069i & 0.0040 + 1.5069i \\
0.0040 + 1.5069i & 0.0010 & 0.0014 + 0.2590i & 0.0040 + 1.5069i & 0.0040 + 1.5069i & 0.0040 + 1.5069i & 0.0040 + 1.5069i & 0.0040 + 1.5069i \\
0.0040 + 1.5069i & 0.0010 & 0.0014 + 0.2590i & 0.0040 + 1.5069i & 0.0040 + 1.5069i & 0.0040 + 1.5069i & 0.0040 + 1.5069i & 0.0040 + 1.5069i \\
0.0040 + 1.5069i & 0.0010 & 0.0014 + 0.2590i & 0.0040 + 1.5069i & 0.0040 + 1.5069i & 0.0040 + 1.5069i & 0.0040 + 1.5069i & 0.0040 + 1.5069i \\
\end{array}
\]
PML is Not a Boundary Condition

A numerical boundary condition is the rule you follow when an 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 misleading as the PML is not a true boundary condition.

Stretched Coordinate
Perfectly Matched Layer
(SC-PML)
The Uniaxial PML

Maxwell’s equations with uniaxial PML are:

\[ \nabla \times \vec{E} = k_0 \left[ \mu_r \right] [S] \vec{H} \]
\[ \nabla \times \vec{H} = k_0 \left[ \epsilon_r \right] [S] \vec{E} \]

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

Rearrange the Terms

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

\[ [S]^{-1} \nabla \times \vec{E} = k_0 \left[ \mu_r \right] \vec{H} \]
\[ [S]^{-1} \nabla \times \vec{H} = k_0 \left[ \epsilon_r \right] \vec{E} \]

The curl operator is now

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

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

Our new curl operator is

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

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

Drop the Other Terms

We drop the non-stretching terms.

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

Justification

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

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

\[ \nabla \times \vec{E} = k_0 \left[ \mu_r \right] \vec{H} \]
\[ \nabla \times \vec{H} = k_0 \left[ \varepsilon_r \right] \vec{E} \]

\[ [\varepsilon_r] = \begin{bmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{bmatrix} \]
\[ [\mu_r] = \begin{bmatrix} \mu_{xx} & \mu_{xy} & \mu_{xz} \\ \mu_{yx} & \mu_{yy} & \mu_{yz} \\ \mu_{zx} & \mu_{zy} & \mu_{zz} \end{bmatrix} \]

The SC-PML is incorporated as follows.

\[ \nabla_s \times \vec{E} = -j\omega [\mu] \vec{H} \]
\[ \nabla_s \times \vec{H} = j\omega [\varepsilon] \vec{E} \]

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

Vector Expansion

Maxwell’s equations with a SC-PML expand to

**Fully Anisotropic**

\[ \frac{1}{s_z} \frac{\partial H_y}{\partial z} - \frac{1}{s_y} \frac{\partial H_z}{\partial y} = k_0 \left( \varepsilon_{xx} E_x + \varepsilon_{xy} E_y + \varepsilon_{xz} E_z \right) \]
\[ \frac{1}{s_x} \frac{\partial H_z}{\partial x} - \frac{1}{s_y} \frac{\partial H_z}{\partial y} = k_0 \left( \varepsilon_{xx} E_x + \varepsilon_{xy} E_y + \varepsilon_{xz} E_z \right) \]
\[ \frac{1}{s_y} \frac{\partial H_z}{\partial y} - \frac{1}{s_z} \frac{\partial H_z}{\partial z} = k_0 \left( \varepsilon_{xx} E_x + \varepsilon_{xy} E_y + \varepsilon_{xz} E_z \right) \]

**Diagonally Anisotropic**

\[ \frac{1}{s_z} \frac{\partial H_y}{\partial z} - \frac{1}{s_y} \frac{\partial H_z}{\partial y} = k_0 \varepsilon_{xx} E_x \]
\[ \frac{1}{s_x} \frac{\partial H_z}{\partial x} - \frac{1}{s_y} \frac{\partial H_z}{\partial y} = k_0 \varepsilon_{xx} E_x \]
\[ \frac{1}{s_y} \frac{\partial H_z}{\partial y} - \frac{1}{s_z} \frac{\partial H_z}{\partial z} = k_0 \varepsilon_{xx} E_x \]

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PMLs Are Not Perfect

PML absorbing boundary conditions are not perfect absorbers. They still reflect waves!
Theoretical Performance

Given the following choice of PML parameters

\[
\nabla_s = \frac{1}{s_x} \frac{\partial}{\partial x} \hat{a}_x + \frac{1}{s_y} \frac{\partial}{\partial y} \hat{a}_y + \frac{1}{s_z} \frac{\partial}{\partial z} \hat{a}_z
\]

\[
s_x(x) = 1 + j \sigma_x(x) \quad \sigma_x(x) = \sigma_{x,\text{max}} \left( \frac{x}{L_x} \right)^m
\]

\[
s_y(y) = 1 + j \sigma_y(y) \quad \sigma_y(y) = \sigma_{y,\text{max}} \left( \frac{y}{L_y} \right)^m
\]

\[
s_z(z) = 1 + j \sigma_z(z) \quad \sigma_z(z) = \sigma_{z,\text{max}} \left( \frac{z}{L_z} \right)^m
\]

We choose \( \sigma_{i,\text{max}} \) to achieve a target maximum reflectance \( R \) at normal incidence according to

\[
\sigma_{i,\text{max}} = -\left( m + 1 \right) \ln R \quad \frac{2\eta_i L_i}{m}
\]

We typically choose

\[
3 \leq m \leq 4
\]

\[
\sigma_{i,\text{max}} \approx \frac{4}{\eta_i L_i}
\]

UPML Performance in FDFD

UPML performance if affected by \( \eta_i \) and its size. H mode UPML exhibits slightly poorer performance.

\[
a_{\text{max}} = 3
\]

\[
p = 3
\]

\[
\sigma_{i,\text{max}}' = 1
\]
UPML Vs. SC-PML

Uniaxial PML

Benefits
- Has a physical interpretation
- Models can be formulated and implemented without considering the PML in the frequency-domain

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

Stretched-Coordinate PML

Benefits
- Less computationally intensive in time-domain
- More efficient implementation in the time-domain
- Matrices are better conditioned.

Drawbacks
- Must be accounted for in the formulation and implementation of the numerical method.
- Not intuitive to understand