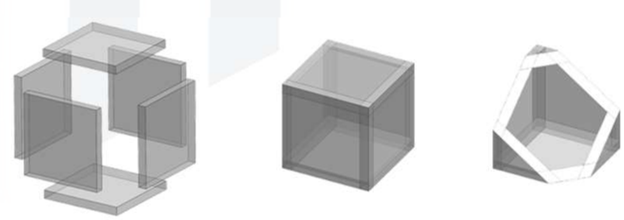
Advanced Computation:

Computational Electromagnetics

The Perfectly Matched Layer

Outline

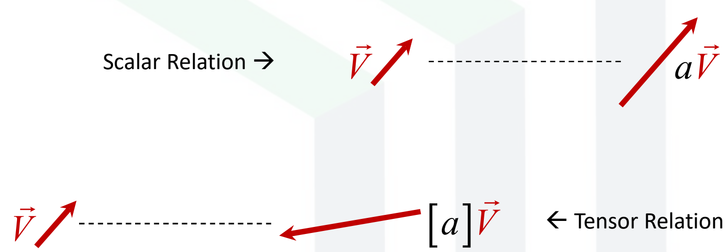
- Background Information
- The Uniaxial Perfectly Matched Layer (UPML)
- Incorporating a UPML into Maxwell's Equations
- Implementing the UPML
- Stretched Coordinate PML (SC-PML)
- PML Performance
- UPML vs SC-PML



Background Information

Tensors

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



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

Reflectance from a Surface with Loss

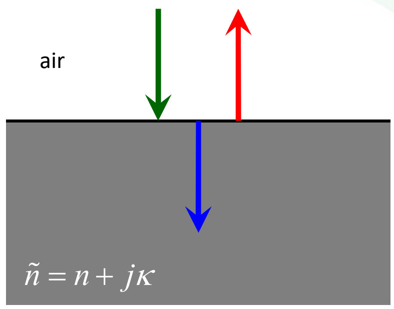
Complex Refractive Index

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

$n_o \equiv$ ordinary refractive index (oscillation)

$\kappa \equiv$ extinction coefficient (decay)

Reflectance from a lossy surface



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

** Loss contributes to reflections

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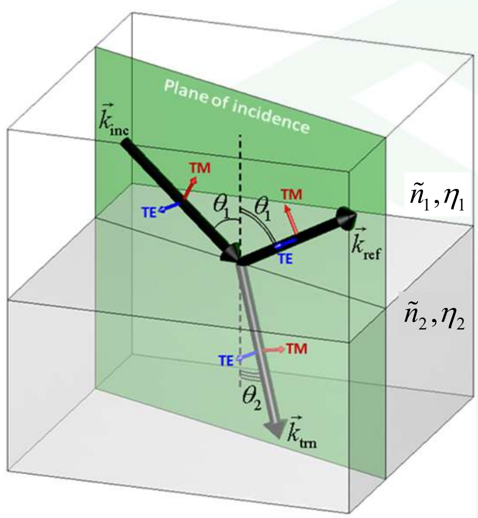
Reflection, Transmission and Refraction at an Interface: *Isotropic Case*



Angles

$$\theta_{inc} = \theta_{ref} = \theta_1$$

$$n_1 \sin\theta_1 = n_2 \sin\theta_2 \quad \text{Snell's Law}$$

TE Polarization

$$r_{TE} = \frac{\eta_2\cos\theta_1 - \eta_1\cos\theta_2}{\eta_2\cos\theta_1 + \eta_1\cos\theta_2} \qquad t_{TE} = \frac{2\eta_2\cos\theta_1}{\eta_2\cos\theta_1 + \eta_1\cos\theta_2}$$

TM Polarization

$$r_{TM} = \frac{\eta_2\cos\theta_2 - \eta_1\cos\theta_1}{\eta_1\cos\theta_1 + \eta_2\cos\theta_2} \qquad t_{TM} = \frac{2\eta_2\cos\theta_1}{\eta_1\cos\theta_1 + \eta_2\cos\theta_2}$$

$n_i \equiv$ refractive index in region i $\qquad \eta_i \equiv$ impedance in region i

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Maxwell's Equations in Anisotropic Media

Maxwell's curl equations in anisotropic media are:

$$\nabla \times \vec{H} = j\omega\varepsilon_0 \left[\varepsilon_{\mathrm{r}}\right]\vec{E} \qquad \nabla \times \vec{E} = -j\omega\mu_0 \left[\mu_{\mathrm{r}}\right]\vec{H}$$

These can also be written in a matrix form that makes the tensor aspect of μ and ε 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:

$$\begin{bmatrix} \varepsilon_{\mathrm{iso}} & 0 & 0 \\ 0 & \varepsilon_{\mathrm{iso}} & 0 \\ 0 & 0 & \varepsilon_{\mathrm{iso}} \end{bmatrix} \quad \text{isotropic}$$

$$\begin{bmatrix} \varepsilon_{\mathrm{o}} & 0 & 0 \\ 0 & \varepsilon_{\mathrm{o}} & 0 \\ 0 & 0 & \varepsilon_{\mathrm{e}} \end{bmatrix} \quad \text{uniaxial}$$

$$\begin{bmatrix} \varepsilon_{\mathrm{a}} & 0 & 0 \\ 0 & \varepsilon_{\mathrm{b}} & 0 \\ 0 & 0 & \varepsilon_{\mathrm{c}} \end{bmatrix} \quad \text{biaxial}$$

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

(ε_r' & ε_r'') Vs. (ε_r & σ)

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

At very low frequencies and/or for time-domain analysis, the (ε_r & σ) system is usually preferred.

$$\nabla \times \vec{H} = \vec{J} + j\omega\vec{D} = \sigma\vec{E} + j\omega\varepsilon_r\vec{E} = \left(\sigma + j\omega\varepsilon_r\right)\vec{E}$$

← We use this for FDTD

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

$$\nabla \times \vec{H} = j\omega\vec{D} = j\omega\tilde{\varepsilon}_r\vec{E}$$

The parameters are related through

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

Note: It does not make sense to have a complex $\tilde{\varepsilon}_r$ and a conductivity σ.

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Maxwell's Equations in Doubly-Diagonally Anisotropic Media

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

$$\begin{bmatrix} 0 & -\frac{\partial}{\partial z} & \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} & 0 & -\frac{\partial}{\partial x} \\ -\frac{\partial}{\partial y} & \frac{\partial}{\partial x} & 0 \end{bmatrix}\begin{bmatrix} H_x \\ H_y \\ H_z \end{bmatrix} = j\omega\varepsilon_0\begin{bmatrix} \varepsilon_{xx} & 0 & 0 \\ 0 & \varepsilon_{yy} & 0 \\ 0 & 0 & \varepsilon_{zz} \end{bmatrix}\begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix} \qquad \begin{bmatrix} 0 & -\frac{\partial}{\partial z} & \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} & 0 & -\frac{\partial}{\partial x} \\ -\frac{\partial}{\partial y} & \frac{\partial}{\partial x} & 0 \end{bmatrix}\begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix} = -j\omega\mu_0\begin{bmatrix} \mu_{xx} & 0 & 0 \\ 0 & \mu_{yy} & 0 \\ 0 & 0 & \mu_{zz} \end{bmatrix}\begin{bmatrix} H_x \\ H_y \\ H_z \end{bmatrix}$$

This can be generalized even further by incorporating loss.

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

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

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Scattering at a Doubly-Anisotropic Interface

Refraction into a diagonally anisotropic materials is described by

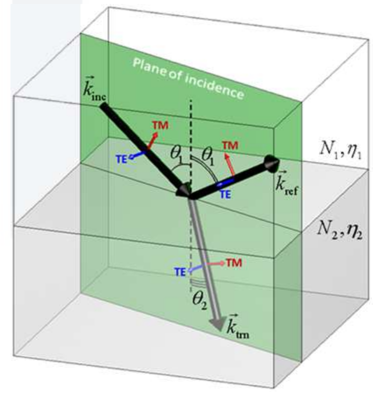
$$\sin\theta_1 = \sqrt{bc}\sin\theta_2$$

$$[\mu_\mathrm{r}] = [\varepsilon_\mathrm{r}] = \begin{bmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{bmatrix}$$

Reflection from a diagonally anisotropic material is

$$r_\mathrm{TE} = \frac{\sqrt{a}\cos\theta_1 - \sqrt{b}\cos\theta_2}{\sqrt{a}\cos\theta_1 + \sqrt{b}\cos\theta_2}$$

$$r_\mathrm{TM} = \frac{-\sqrt{a}\cos\theta_1 + \sqrt{b}\cos\theta_2}{\sqrt{a}\cos\theta_1 + \sqrt{b}\cos\theta_2}$$



Sacks, Zachary S., et al. "A perfectly matched anisotropic absorber for use as an absorbing boundary condition." IEEE Trans. Antennas and Propagation, Vol. 43, No. 12, pp. 1460-1463, 1995.

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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

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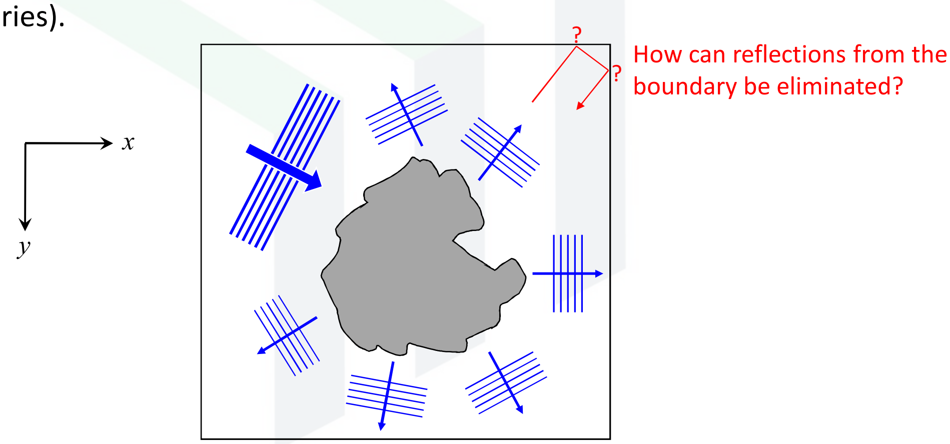
Uniaxial Perfectly Matched Layer (UPML)

S. Zachary, D. Kingsland, R. Lee, J. Lee, "A Perfectly Matched Anisotropic Absorber for Use as an Absorbing Boundary Condition," IEEE Trans. on Ant. and Prop., Vol. 43, No. 12, pp 1460–1463, 1995.

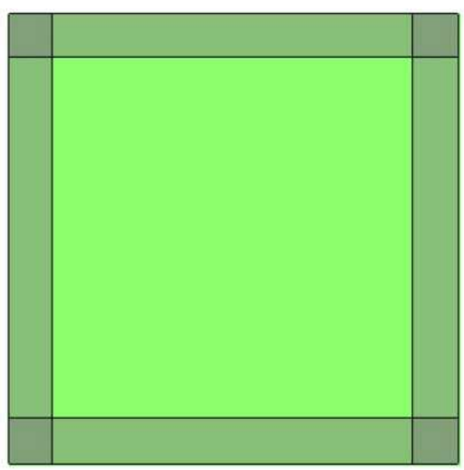
Boundary Condition Problem

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).



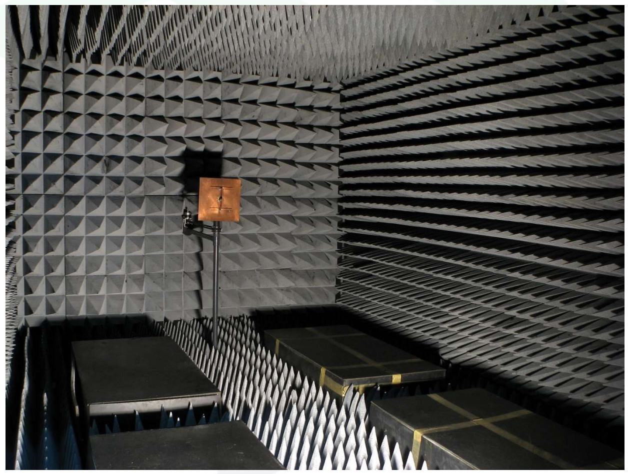
Simulation Without a PML

Simulation With a PML



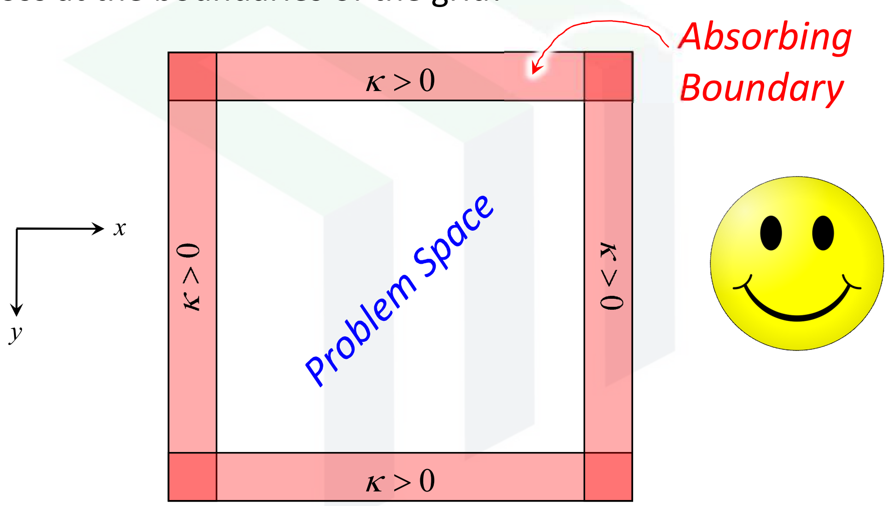
How To Prevent Reflections in Lab

In the lab, anechoic foam is used to absorb outgoing waves.



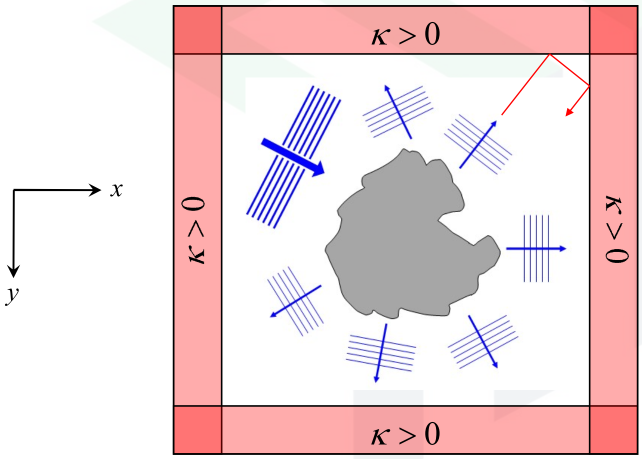
Absorbing Boundary Conditions

Introduce loss at the boundaries of the grid!



Oops!!

But if loss is introduced, reflections are also introduced from the lossy regions!!



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

Match the Impedance

Loss must be incorporated to absorb outgoing waves, but the impedance must also remain matched to the problem space to prevent reflections.

introduce loss here

$$\tilde{\varepsilon}_r = \varepsilon_r' + j\varepsilon_r''$$

adjust this to maintain constant impedance

More Trouble?

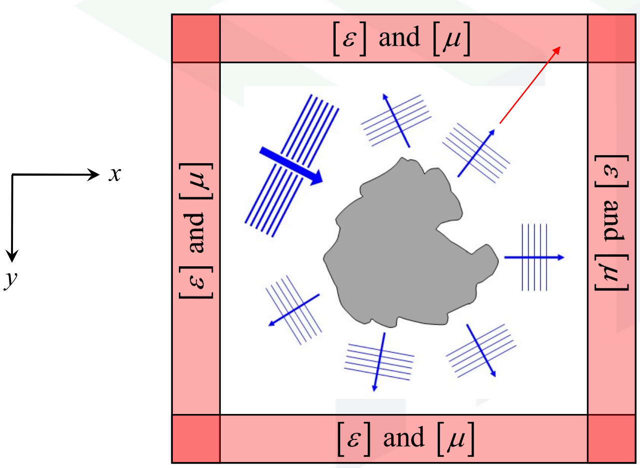
By examining the Fresnel equations, it is observed that reflections can only be eliminated from an interface at one frequency, one angle of incidence, and one polarization.

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

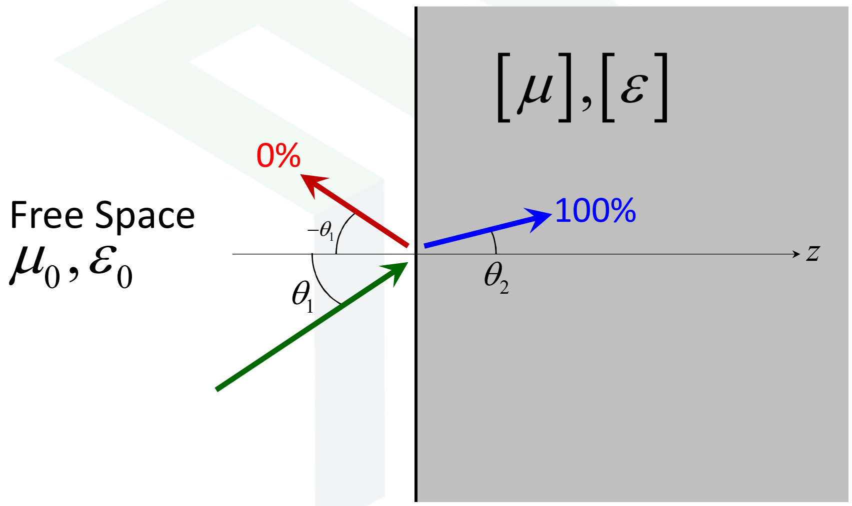
$$r_{\text{TM}} = \frac{\eta_2 \cos\theta_2 - \eta_1 \cos\theta_1}{\eta_1 \cos\theta_1 + \eta_2 \cos\theta_2} = 0 \quad \rightarrow \quad \eta_2 = \eta_1 \frac{\cos\theta_1}{\cos\theta_2}$$

Anisotropy to the Rescue!!

It turns out reflections can be eliminated at all angles and for all polarizations if the absorbing material is made to be doubly-diagonally anisotropic.



Problem Setup for the UPML



Designing Anisotropy for Zero Reflection (1 of 3)

The impedance of the PML must be perfectly matched to the impedance of the grid.

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

One easy way to ensure impedance is perfectly matched is:

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

For now, the elements along the diagonal are set to a, b, c.

Next, rules for these will be determined.

Designing Anisotropy for Zero Reflection (2 of 3)

If $\sqrt{bc} = 1$ is chosen, 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 reduce to

$$r_{\text{TE}} = \frac{\sqrt{a}\cos\theta_1 - \sqrt{b}\cos\theta_2}{\sqrt{a}\cos\theta_1 + \sqrt{b}\cos\theta_2} = \frac{\sqrt{a} - \sqrt{b}}{\sqrt{a} + \sqrt{b}}$$

$$r_{\text{TM}} = \frac{-\sqrt{a}\cos\theta_1 + \sqrt{b}\cos\theta_2}{\sqrt{a}\cos\theta_1 + \sqrt{b}\cos\theta_2} = \frac{-\sqrt{a} + \sqrt{b}}{\sqrt{a} + \sqrt{b}}$$

The amount of reflection is no longer a function of angle!! ☺

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Designing Anisotropy for Zero Reflection (3 of 3)

Further, if $a = b$ is chosen, the reflection equations reduce to

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

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

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

Recall the necessary conditions: $\boxed{\sqrt{bc} = 1 \quad \text{and} \quad a = b}$

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The PML Parameters (1 of 3)

So far, the tensors for the UPML are

$$[\mu_r] = [\varepsilon_r] = \begin{bmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{bmatrix} \qquad a = b = \frac{1}{c}$$

Thus, the PML in terms can be written in terms of just one parameter s_z.

$$[S_z] = \begin{bmatrix} s_z & 0 & 0 \\ 0 & s_z & 0 \\ 0 & 0 & s_z^{-1} \end{bmatrix} \qquad s_z = \alpha - j\beta$$

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

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

The PML Parameters (2 of 3)

A UPML is potentially needed along all the borders.

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

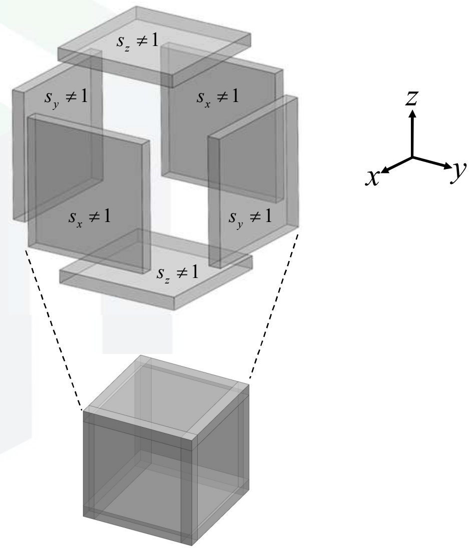
These can be combined into a single tensor quantity.

$$[S] = [S_x] \cdot [S_y] \cdot [S_z] = \begin{bmatrix} \frac{s_y s_z}{s_x} & 0 & 0 \\ 0 & \frac{s_x s_z}{s_y} & 0 \\ 0 & 0 & \frac{s_x s_y}{s_z} \end{bmatrix}$$

The PML Parameters (3 of 3)

The 3D PML can be visualized this way…

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



UPML in Cylindrical and Spherical Coordinates

Cylindrical Coordinates

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

Spherical Coordinates

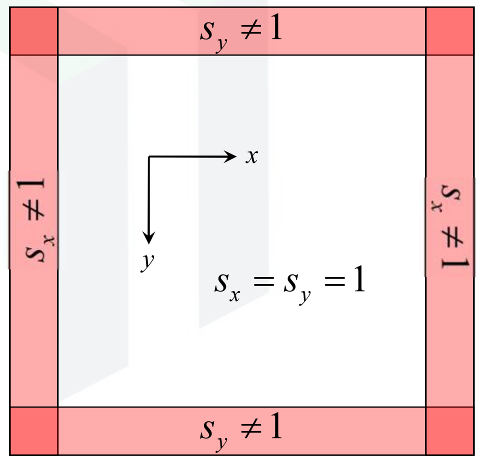
$$[S]=\begin{bmatrix} \left(\dfrac{\tilde{r}}{r}\right)^2 \dfrac{1}{s_r} & 0 & 0 \\ 0 & s_r & 0 \\ 0 & 0 & s_r \end{bmatrix}$$

F. L. Teixeira, W. C. Chew, "Systematic Derivation of Anisotropic PML Absorbing Media in Cylindrical and Spherical Coordiantes," IEEE Microwave and Guided Wave Letters, Vol. 7, No. 11, pp. 371-373, 1997.

Two-Dimensional UPML

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

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



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Incorporating a UPML into Maxwell's Equations

Incorporating the UPML Into Maxwell's Eqs.

Maxwell's Equations

The below set of equations does account for devices, but not a UPML at the boundary to absorb outgoing waves.

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

UPML

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

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

Maxwell's Equations with UPML

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

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.

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Maxwell's Equations with a UPML

Maxwell's equations with a UPML

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

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

The UPML can be incorporated into the material tensors directly.

$$\nabla \times \vec{E} = k_0 [\mu_r'] \vec{\tilde{H}} \qquad [\mu_r'] = [\mu_r][S]$$
$$\nabla \times \vec{\tilde{H}} = k_0 [\varepsilon_r'] \vec{E} \qquad [\varepsilon_r'] = [\varepsilon_r][S]$$

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

This allows a numerical algorithm to be formulated and implemented without having to explicitly consider the UPML. It is simply incorporated into the material tensors.

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Vector Expansion

Assuming only diagonal tensors

$$[\varepsilon_r]=\begin{bmatrix}\varepsilon_{xx} & 0 & 0\\ 0 & \varepsilon_{yy} & 0\\ 0 & 0 & \varepsilon_{zz}\end{bmatrix} \qquad [\mu_r]=\begin{bmatrix}\mu_{xx} & 0 & 0\\ 0 & \mu_{yy} & 0\\ 0 & 0 & \mu_{zz}\end{bmatrix}$$

Maxwell's equations expand to

$$\frac{\partial E_z}{\partial y}-\frac{\partial E_y}{\partial z}=k_0\mu_{xx}\frac{s_y s_z}{s_x}\tilde{H}_x \qquad \frac{\partial \tilde{H}_z}{\partial y}-\frac{\partial \tilde{H}_y}{\partial z}=k_0\varepsilon_{xx}\frac{s_y s_z}{s_x}E_x$$

$$\frac{\partial E_x}{\partial z}-\frac{\partial E_z}{\partial x}=k_0\mu_{yy}\frac{s_x s_z}{s_y}\tilde{H}_y \qquad \frac{\partial \tilde{H}_x}{\partial z}-\frac{\partial \tilde{H}_z}{\partial x}=k_0\varepsilon_{yy}\frac{s_x s_z}{s_y}E_y$$

$$\frac{\partial E_y}{\partial x}-\frac{\partial E_x}{\partial y}=k_0\mu_{zz}\frac{s_x s_y}{s_z}\tilde{H}_z \qquad \frac{\partial \tilde{H}_y}{\partial x}-\frac{\partial \tilde{H}_x}{\partial y}=k_0\varepsilon_{zz}\frac{s_x s_y}{s_z}E_z$$

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Absorb UPML into μ and ε (3D Grid)

The UPML parameters are incorporated directly into the material functions.

$$\mu'_{xx}=\mu_{xx}\frac{s_y s_z}{s_x} \qquad \varepsilon'_{xx}=\varepsilon_{xx}\frac{s_y s_z}{s_x}$$

$$\mu'_{yy}=\mu_{yy}\frac{s_x s_z}{s_y} \qquad \varepsilon'_{yy}=\varepsilon_{yy}\frac{s_x s_z}{s_y}$$

$$\mu'_{zz}=\mu_{zz}\frac{s_x s_y}{s_z} \qquad \varepsilon'_{zz}=\varepsilon_{zz}\frac{s_x s_y}{s_z}$$

Maxwell's equations can now be written in terms of the modified material functions.

$$\frac{\partial E_z}{\partial y}-\frac{\partial E_y}{\partial z}=k_0\mu'_{xx}\tilde{H}_x \qquad \frac{\partial \tilde{H}_z}{\partial y}-\frac{\partial \tilde{H}_y}{\partial z}=k_0\varepsilon'_{xx}E_x$$

$$\frac{\partial E_x}{\partial z}-\frac{\partial E_z}{\partial x}=k_0\mu'_{yy}\tilde{H}_y \qquad \frac{\partial \tilde{H}_x}{\partial z}-\frac{\partial \tilde{H}_z}{\partial x}=k_0\varepsilon'_{yy}E_y$$

$$\frac{\partial E_y}{\partial x}-\frac{\partial E_x}{\partial y}=k_0\mu'_{zz}\tilde{H}_z \qquad \frac{\partial \tilde{H}_y}{\partial x}-\frac{\partial \tilde{H}_x}{\partial y}=k_0\varepsilon'_{zz}E_z$$

This means a code can be formulated as if there was no UPML. All that must be done is to modify the materials being modeled near the boundaries.

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Absorb UPML into μ and ε (2D Grid)

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

The UPML parameters are still incorporated into the material functions.

$$\mu'_{xx} = \mu_{xx}\frac{s_y}{s_x} \qquad \varepsilon'_{xx} = \varepsilon_{xx}\frac{s_y}{s_x}$$

$$\mu'_{yy} = \mu_{yy}\frac{s_x}{s_y} \qquad \varepsilon'_{yy} = \varepsilon_{yy}\frac{s_x}{s_y}$$

$$\mu'_{zz} = \mu_{zz}s_x s_y \qquad \varepsilon'_{zz} = \varepsilon_{zz}s_x s_y$$

Maxwell's equations for 2D grids reduce to

E Mode

$$\frac{\partial\tilde{H}_y}{\partial x} - \frac{\partial\tilde{H}_x}{\partial y} = k_0\varepsilon'_{zz}E_z$$

$$\frac{\partial E_z}{\partial y} = k_0\mu'_{xx}\tilde{H}_x$$

$$-\frac{\partial E_z}{\partial x} = k_0\mu'_{yy}\tilde{H}_y$$

H Mode

$$\frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} = k_0\mu'_{zz}\tilde{H}_z$$

$$\frac{\partial\tilde{H}_z}{\partial y} = k_0\varepsilon'_{xx}E_x$$

$$-\frac{\partial\tilde{H}_z}{\partial x} = k_0\varepsilon'_{yy}E_y$$

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Implementing the UPML

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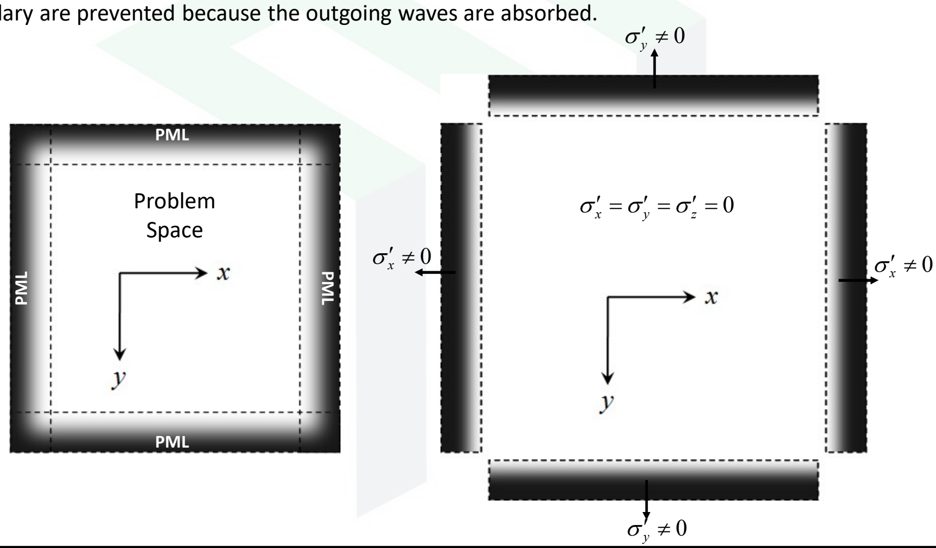
The Perfectly Matched Layer (PML)

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.



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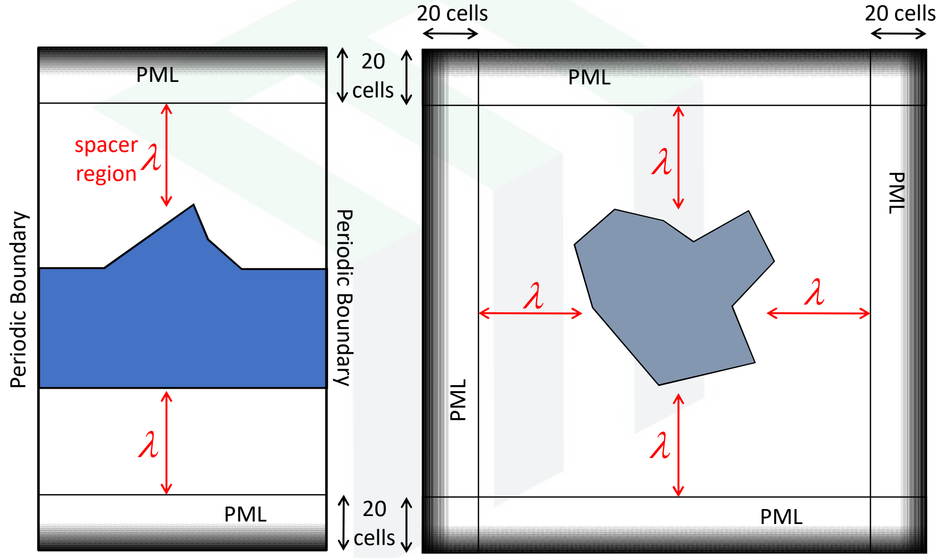
Typical Grid Schemes



Periodic Devices

Finite Devices

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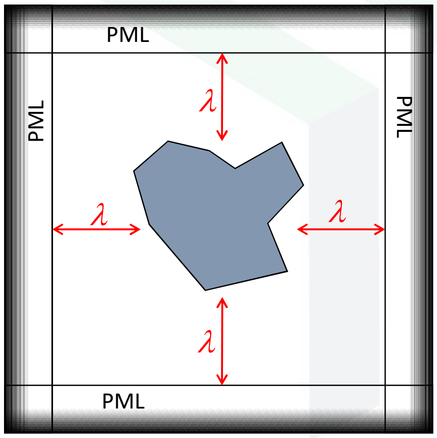
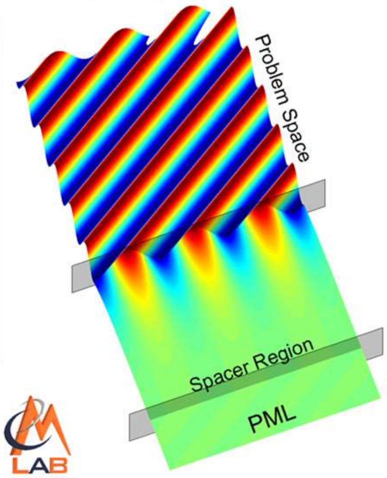
Justification for the Spacer Regions

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





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How to Calculate the PML Parameters

<u>Maxwell's Eqs. with PML</u>

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

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

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

```
NGRID   = [Nx Ny];
NPML    = [0 0 20 20];
[sx,sy] = calcpml2d(NGRID,NPML);
```

Writing this function will be in homework ☺

<u>Computing PML Parameters</u>

$$s_x(x) = a_x(x)\left[1 + j\eta_0 \sigma'_x(x)\right]$$

$$s_y(y) = a_y(y)\left[1 + j\eta_0 \sigma'_y(y)\right]$$

$$s_z(z) = a_z(z)\left[1 + j\eta_0 \sigma'_z(z)\right]$$

$$\eta_0 = 376.73\ldots \equiv \text{free space impedance}$$

$$a_x(x) = 1 + a_{\max} \cdot (x/L_x)^p$$

$$a_y(y) = 1 + a_{\max} \cdot (y/L_y)^p$$

$$a_z(z) = 1 + a_{\max} \cdot (z/L_z)^p$$

$$0 \le a_{\max} \le 5$$

$$3 \le p \le 5$$

$$\sigma'_{\max} \approx 1$$

$$\sigma'_x(x) = \sigma'_{\max} \sin^2\left(\frac{\pi x}{2L_x}\right)$$

$$\sigma'_y(y) = \sigma'_{\max} \sin^2\left(\frac{\pi y}{2L_y}\right)$$

$$\sigma'_z(z) = \sigma'_{\max} \sin^2\left(\frac{\pi z}{2L_z}\right)$$

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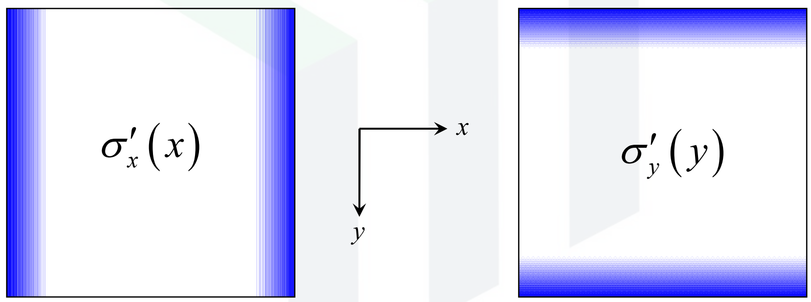
Visualizing the PML Loss Terms – 2D

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

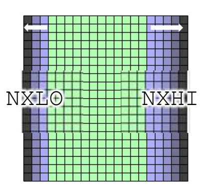


Procedure for Calculating s_x and s_y on a 2D Grid

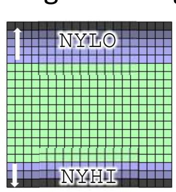
1. Initialize s_x and s_y to all ones.

$$s_x(x,y) = s_y(x,y) = 1$$

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 a function of distance into the PML.

$$\frac{x}{L_x} \quad \text{and} \quad \frac{y}{L_y} \quad \text{and} \quad \frac{z}{L_z}$$

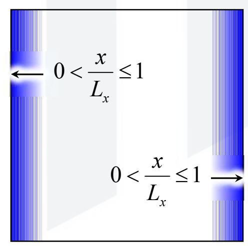
$$x, y, z \equiv \text{position within PML}$$
$$L_x, L_y, L_z \equiv \text{size of PML}$$

The same ratio can be calculated using integer indices from our grid.

$$\frac{x}{L_x} \approx \frac{\text{nx}}{\text{NXLO}} \text{ or } \frac{\text{nx}}{\text{NXHI}} \qquad \begin{array}{l} \text{nx} = 1, 2, \ldots, \text{NXLO} \\ \text{nx} = 1, 2, \ldots, \text{NXHI} \end{array}$$

$$\frac{y}{L_y} \approx \frac{\text{ny}}{\text{NYLO}} \text{ or } \frac{\text{ny}}{\text{NYHI}} \qquad \begin{array}{l} \text{ny} = 1, 2, \ldots, \text{NYLO} \\ \text{ny} = 1, 2, \ldots, \text{NYHI} \end{array}$$

$$\frac{z}{L_z} \approx \frac{\text{nz}}{\text{NZLO}} \text{ or } \frac{\text{nz}}{\text{NZHI}} \qquad \begin{array}{l} \text{nz} = 1, 2, \ldots, \text{NZLO} \\ \text{nz} = 1, 2, \ldots, \text{NZHI} \end{array}$$



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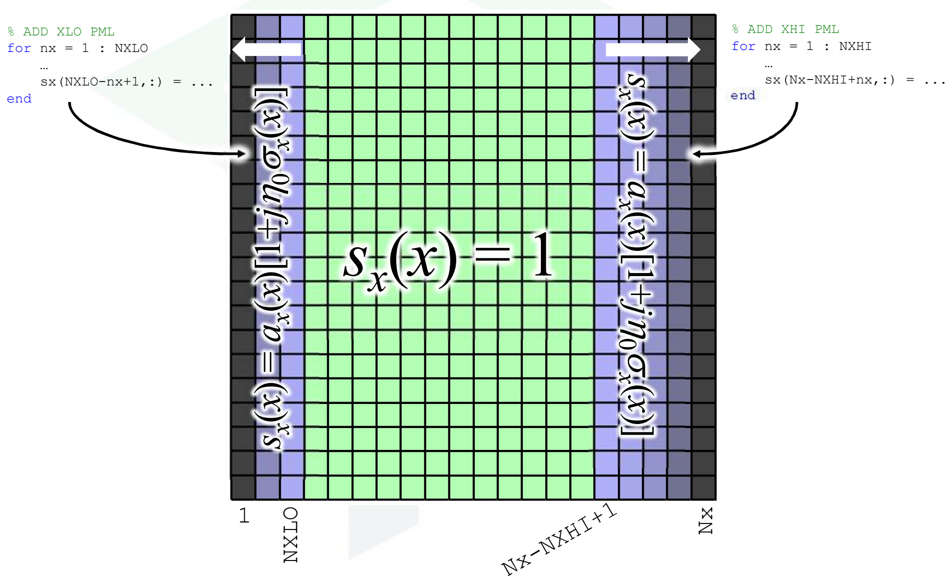
Visualizing s_x in 2D



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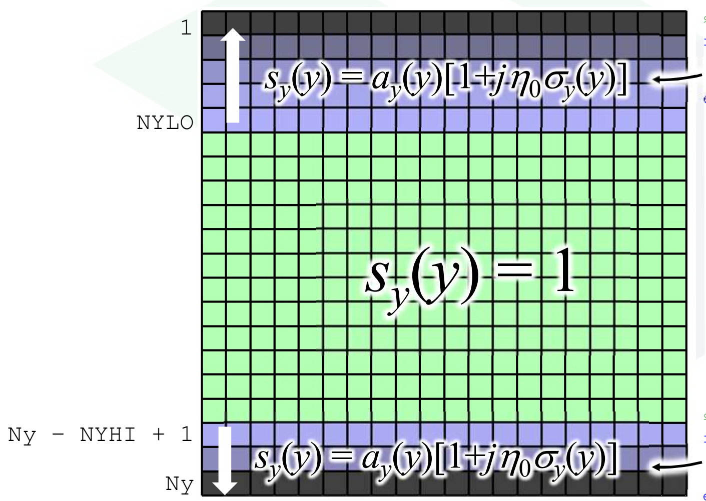
Visualizing s_y in 2D




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

```
% ADD YHI PML
for ny = 1 : NYHI
    …
    sy(:,Ny-NYHI+ny) = …
end
```


Example Data for 2D

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

$a_{max} = 3$
$p = 3$
$\sigma'_{max} = 1$

```
sx =  1.0e+03 *

   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
   0.0010             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
   0.0019 + 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


sy =  1.0e+03 *

   0.0040 + 1.5069i   0.0010             0.0014 + 0.2590i   0.0040 + 1.5069i
   0.0040 + 1.5069i   0.0010             0.0014 + 0.2590i   0.0040 + 1.5069i
   0.0040 + 1.5069i   0.0010             0.0014 + 0.2590i   0.0040 + 1.5069i
   0.0040 + 1.5069i   0.0010             0.0014 + 0.2590i   0.0040 + 1.5069i
   0.0040 + 1.5069i   0.0010             0.0014 + 0.2590i   0.0040 + 1.5069i
   0.0040 + 1.5069i   0.0010             0.0014 + 0.2590i   0.0040 + 1.5069i
   0.0040 + 1.5069i   0.0010             0.0014 + 0.2590i   0.0040 + 1.5069i
```

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:

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

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

Rearrange the Terms

The PML tensor can be brought to the left side of the equations and be associated with the curl operator.

$$[S]^{-1} \nabla \times \vec{E} = k_0 [\mu_r]\vec{\tilde{H}} \qquad [S]^{-1} \nabla \times \vec{\tilde{H}} = k_0 [\varepsilon_r]\vec{E}$$

The curl operator is now

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

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

"Stretched" Coordinates

The new curl operator is

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

The factors s_x, s_y, and s_z are effectively "stretching" the coordinates, but they are "stretching" into a complex space. Weird, huh?

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Drop the Other Terms

Drop the non-stretching terms.

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

<u>Justification</u>

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

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Maxwell's Equations with a SC-PML

Maxwell's equations before the PML is added are

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

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

The SC-PML is incorporated as follows.

$$\nabla_s \times \vec{E} = k_0 [\mu_r] \tilde{\vec{H}} \qquad \nabla_s \times \tilde{\vec{H}} = k_0 [\varepsilon_r] \vec{E}$$

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

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Vector Expansion

Maxwell's equations with a SC-PML expand to

Fully Anisotropic

$$\frac{1}{s_y}\frac{\partial \tilde{H}_z}{\partial y} - \frac{1}{s_z}\frac{\partial \tilde{H}_y}{\partial z} = k_0\left(\varepsilon_{xx}E_x + \varepsilon_{xy}E_y + \varepsilon_{xz}E_z\right)$$

$$\frac{1}{s_z}\frac{\partial \tilde{H}_x}{\partial z} - \frac{1}{s_x}\frac{\partial \tilde{H}_z}{\partial x} = k_0\left(\varepsilon_{yx}E_x + \varepsilon_{yy}E_y + \varepsilon_{yz}E_z\right)$$

$$\frac{1}{s_x}\frac{\partial \tilde{H}_y}{\partial x} - \frac{1}{s_y}\frac{\partial \tilde{H}_x}{\partial y} = k_0\left(\varepsilon_{zx}E_x + \varepsilon_{zy}E_y + \varepsilon_{zz}E_z\right)$$

$$\frac{1}{s_y}\frac{\partial E_z}{\partial y} - \frac{1}{s_z}\frac{\partial E_y}{\partial z} = k_0\left(\mu_{xx}\tilde{H}_x + \mu_{xy}\tilde{H}_y + \mu_{xz}\tilde{H}_z\right)$$

$$\frac{1}{s_z}\frac{\partial E_x}{\partial z} - \frac{1}{s_x}\frac{\partial E_z}{\partial x} = k_0\left(\mu_{yx}\tilde{H}_x + \mu_{yy}\tilde{H}_y + \mu_{yz}\tilde{H}_z\right)$$

$$\frac{1}{s_x}\frac{\partial E_y}{\partial x} - \frac{1}{s_y}\frac{\partial E_x}{\partial y} = k_0\left(\mu_{zx}\tilde{H}_x + \mu_{zy}\tilde{H}_y + \mu_{zz}\tilde{H}_z\right)$$

Diagonally Anisotropic

$$\frac{1}{s_y}\frac{\partial \tilde{H}_z}{\partial y} - \frac{1}{s_z}\frac{\partial \tilde{H}_y}{\partial z} = k_0\varepsilon_{xx}E_x$$

$$\frac{1}{s_z}\frac{\partial \tilde{H}_x}{\partial z} - \frac{1}{s_x}\frac{\partial \tilde{H}_z}{\partial x} = k_0\varepsilon_{yy}E_y$$

$$\frac{1}{s_x}\frac{\partial \tilde{H}_y}{\partial x} - \frac{1}{s_y}\frac{\partial \tilde{H}_x}{\partial y} = k_0\varepsilon_{zz}E_z$$

$$\frac{1}{s_y}\frac{\partial E_z}{\partial y} - \frac{1}{s_z}\frac{\partial E_y}{\partial z} = k_0\mu_{xx}\tilde{H}_x$$

$$\frac{1}{s_z}\frac{\partial E_x}{\partial z} - \frac{1}{s_x}\frac{\partial E_z}{\partial x} = k_0\mu_{yy}\tilde{H}_y$$

$$\frac{1}{s_x}\frac{\partial E_y}{\partial x} - \frac{1}{s_y}\frac{\partial E_x}{\partial y} = k_0\mu_{zz}\tilde{H}_z$$

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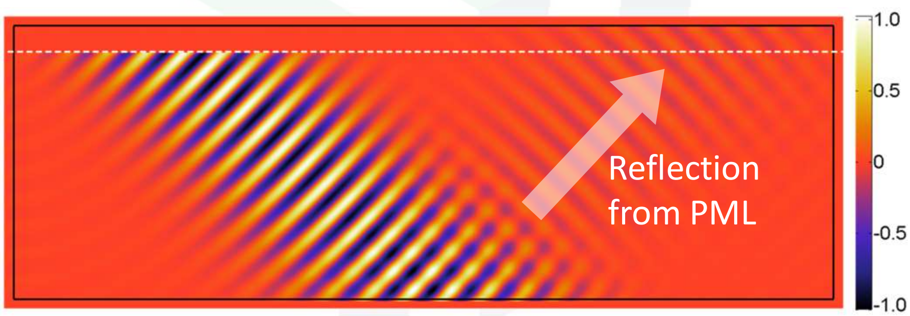
PML Performance

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

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

$$s_x(x) = 1 + j\frac{\sigma_x(x)}{\omega\varepsilon_0} \qquad \sigma_x(x) = \sigma_{x,\max}\cdot\left(\frac{x}{L_x}\right)^m$$

$$s_y(y) = 1 + j\frac{\sigma_y(y)}{\omega\varepsilon_0} \qquad \sigma_y(y) = \sigma_{y,\max}\cdot\left(\frac{y}{L_y}\right)^m$$

$$s_z(z) = 1 + j\frac{\sigma_z(z)}{\omega\varepsilon_0} \qquad \sigma_z(z) = \sigma_{z,\max}\cdot\left(\frac{z}{L_z}\right)^m$$

Choose $\sigma_{i,\max}$ to achieve a target maximum reflectance R at normal incidence according to

$$\sigma_{i,\max} = -\frac{(m+1)\ln R}{2\eta_0 L_i}$$

Typical choice for this course

$$3 \le m \le 4 \qquad \sigma_{i,\max} \approx \frac{4}{\eta_0 \Delta_i}$$

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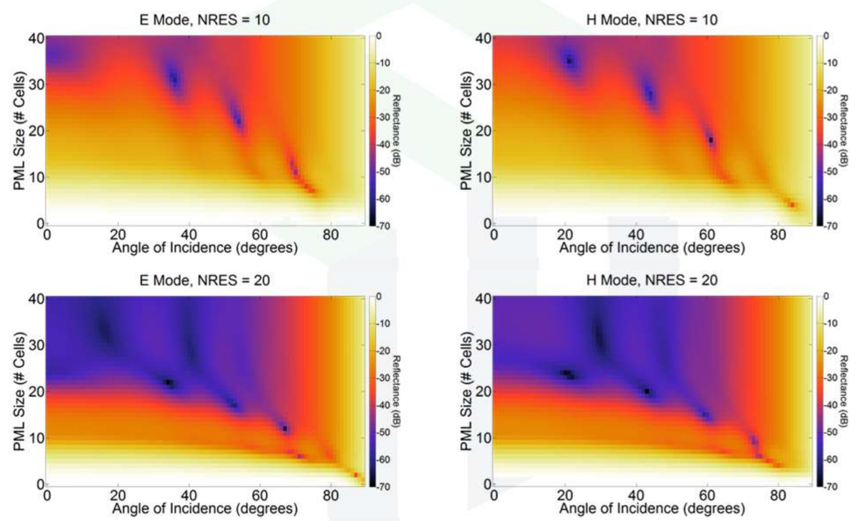
UPML Performance in FDFD



$a_{\max} = 3$

$p = 3$

$\sigma'_{\max} = 1$

UPML performance is affected by `NRES` and its size.
H mode UPML exhibits slightly poorer performance.

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UPML Vs. SC-PML

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