Alternate Forms of the PML Metric Tensor

o Berenger Originally proposed:

$$s_x = 1 + \frac{\sigma_x}{j\omega\varepsilon_o}$$

• We found that for a plane wave incident on the boundary with normal dependence $e^{-j\beta_x^i x}$, the propagation constant in the PML will be

$$e^{-j\beta_x^i s_x x} = e^{-j\beta_x^i \left(1 + \frac{\sigma_x}{j\omega \varepsilon_o}\right) x} = e^{-j\beta_x^i x} e^{-\sigma_x \eta \sqrt{\varepsilon_r} \cos \theta^i x}$$

- O Now consider a wave impinging on the boundary that has a complex wave number (e.g., lossy medium, guided mode below cutoff, or the evanescent part of a wave expansion): $e^{-\gamma_x^i x} = e^{-(\alpha_x^i + j\beta_x^i)x}$.
- o If the wave is incident on the PML boundary, it can be shown that the wave transmitted in the PML is still perfectly matched with propagate along the normal direction as:

$$e^{-\gamma_x^i s_x x} = e^{-\left(\alpha_x^i + j\beta_x^i\right) s_x x} = e^{-\left(\alpha_x^i + j\beta_x^i\right) \left(1 + \frac{\sigma_x}{j\omega \varepsilon_o}\right) x} = e^{-\alpha_x^i x} e^{j\alpha_x^i \frac{\sigma_x}{\omega \varepsilon_o} x} e^{-j\beta_x^i x} e^{-\sigma_x \eta \sqrt{\varepsilon_r} \cos \theta^i x}$$

o What if the wave was purely evanescent ($\beta_x^i = 0$)? The transmitted wave is:

$$e^{-\alpha_x^i x} e^{j\alpha_x^i \frac{\sigma_x}{\omega \varepsilon_o} x}$$

which has no additional attenuation!

o Propose instead:

$$s_{x} = \kappa_{x} + \frac{\sigma_{x}}{j\omega\varepsilon_{o}}$$

where $\kappa_r \ge 1$.

o Then, the transmitted wave behaves as:

$$e^{-\gamma_x^i s_x x} = e^{-\left(\alpha_x^i + j\beta_x^i\right) s_x x} = e^{-\left(\alpha_x^i + j\beta_x^i\right) \left(\kappa_x + \frac{\sigma_x}{j\omega\varepsilon_o}\right) x} = e^{-\alpha_x^i \kappa_x x} e^{j\alpha_x^i \frac{\sigma_x}{\omega\varepsilon_o} x} e^{-j\kappa_x \beta_x^i x} e^{-\sigma_x \eta \sqrt{\varepsilon_r} \cos\theta^i x}$$

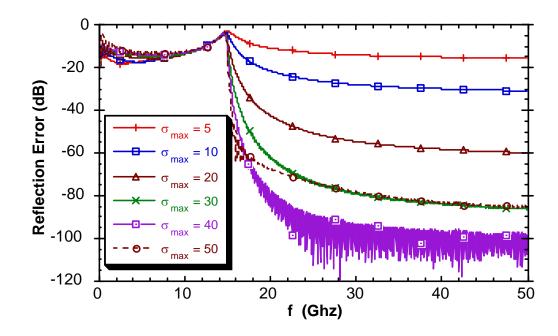
Now, the attenuation is amplified by κ_x . Also note that the wave speed is effectively reduced. Once again, κ_x cannot be increased indiscriminately. In fact, if κ_x becomes too large, it can actually degrade the reflection coefficient of a propagating wave impinging on the boundary, since it increases the time interaction with the PML medium.

o In practice, κ_x must be scaled to reduce discretization error. A recommended scaling is between 1 (at the front boundary) and κ_x^{max} at the PEC wall. For a PML of depth d with boundary interface x = 0, set:

$$\kappa_x(x) = 1 + (\kappa_{\text{max}} - 1) \left(\frac{x}{d}\right)^m$$

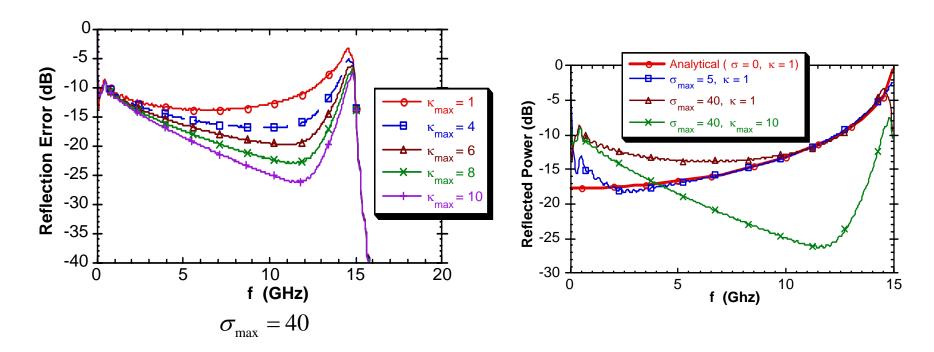
Example – Rectangular Waveguide

- o Consider a lossless rectangular waveguide with a height of 0.5 cm and a width of 1.0 cm. For these dimensions, the cutoff frequency of the TE_{10} mode is 15 GHz.
- The FDTD lattice has the uniform dimensions $\Delta x = \Delta y = \Delta z = 0.25$ mm.
- o The TE₁₀ mode is excited in a rectangular waveguide. The time-dependent source was a modulated Gaussian pulse, with center frequency of 20 GHz and half bandwidth of 30 GHz. The field was measured 20 cells from the source (0.5 cm) and three cells from the PML interface. The PML medium was 10 cells thick.
- \circ Reflection error (relative) as σ_{max} is varied between 5 and 50 and $\kappa_{\text{max}} = 1$.



o Above cutoff, the mode is well absorbed. Below cutoff, only attenuation is due to the waveguide mode.

o Now increase κ



PML for Lossy (Conducting) Media

o Consider the application of PML in a Lossy medium:

$$\begin{bmatrix} \frac{\partial}{\partial y} H_z - \frac{\partial}{\partial z} H_y \\ \frac{\partial}{\partial z} H_x - \frac{\partial}{\partial x} H_z \\ \frac{\partial}{\partial x} H_y - \frac{\partial}{\partial y} H_x \end{bmatrix} = j\omega \varepsilon_o \left(\varepsilon_r + \frac{\sigma}{j\omega \varepsilon_o} \right) \begin{bmatrix} \frac{s_y s_z}{s_x} & 0 & 0 \\ 0 & \frac{s_x s_z}{s_y} & 0 \\ 0 & 0 & \frac{s_x s_y}{s_z} \end{bmatrix} \begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix}$$

o Previously, we introduced the constitutive relation for the lossless medium:

$$D_z = \varepsilon_o \varepsilon_r \frac{s_x}{s_z} E_z$$
. For a lossy medium, this would be: $D_z = \varepsilon_o \varepsilon_r (1 + \frac{\sigma}{j\omega \varepsilon_o}) \frac{s_x}{s_z} E_z$. This

would lead to a second-order auxiliary equation.

o Rather, use the constitutive relations:

$$P_z = \frac{S_x}{S_z} E_z, \quad Q_z = S_y P_z$$

o Given $s_i = \kappa_i + \frac{\sigma_i}{j\omega\varepsilon_o}$, we can rewrite these as:

$$s_{z}P_{z} = s_{x}E_{z} \Rightarrow \left(\kappa_{z} + \frac{\sigma_{z}}{j\omega\varepsilon_{o}}\right)P_{z} = \left(\kappa_{x} + \frac{\sigma_{x}}{j\omega\varepsilon_{o}}\right)E_{z} \Rightarrow \left(j\omega\varepsilon_{o}\kappa_{z} + \sigma_{z}\right)P_{z} = \left(j\omega\varepsilon_{o}\kappa_{x} + \sigma_{x}\right)E_{z}$$

$$Q_{z} = \left(\kappa_{y} + \frac{\sigma_{y}}{j\omega\varepsilon_{o}}\right)P_{z} \Rightarrow j\omega\varepsilon_{o}Q_{z} = \left(j\omega\varepsilon_{o}\kappa_{y} + \sigma_{y}\right)P_{z}$$

o In the time domain, these are expressed as:

$$\varepsilon_{o} \kappa_{z} \frac{\partial P_{z}}{\partial t} + \sigma_{z} P_{z} = \varepsilon_{o} \kappa_{x} \frac{\partial E_{z}}{\partial t} + \sigma_{x} E_{z}$$
$$\varepsilon_{o} \frac{\partial Q_{z}}{\partial t} = \varepsilon_{o} \kappa_{y} \frac{\partial P_{z}}{\partial t} + \sigma_{y} P_{z}$$

o Update procedure (z-projection):

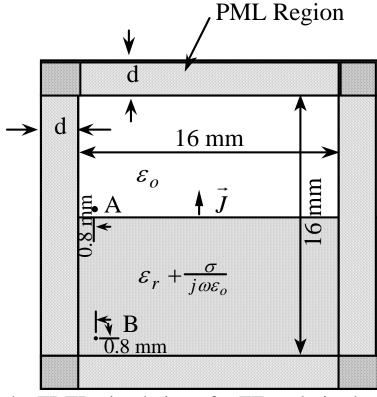
$$Q_{z_{i,j,k+1/2}}^{n+1/2} = \frac{2\varepsilon_o - \Delta t\sigma}{2\varepsilon_o + \Delta t\sigma_y} Q_{z_{i,j,k+1/2}}^{n-1/2} + \frac{2\varepsilon_o \Delta t}{2\varepsilon_o + \Delta t\sigma} \cdot \left\{ \left(H_{y_{i+\frac{1}{2},j,k+\frac{1}{2}}}^{n} - H_{y_{i-\frac{1}{2},j,k+\frac{1}{2}}}^{n} \right) \middle/ \Delta x - \left(H_{x_{i,j+\frac{1}{2},k+\frac{1}{2}}}^{n} - H_{x_{i,j-\frac{1}{2},k+\frac{1}{2}}}^{n} \right) \middle/ \Delta y \right\}$$

$$\begin{split} & \varepsilon_{o} \kappa_{y} \frac{P_{z_{i,j,k+1/2}}^{n+1/2} - P_{z_{i,j,k+1/2}}^{n-1/2}}{\Delta t} + \sigma_{y} \frac{P_{z_{i,j,k+1/2}}^{n+1/2} + P_{z_{i,j,k+1/2}}^{n-1/2}}{2} = \varepsilon_{o} \frac{Q_{z_{i,j,k+1/2}}^{n+1/2} - Q_{z_{i,j,k+1/2}}^{n-1/2}}{\Delta t} \\ \Rightarrow & P_{z_{i,j,k+1/2}}^{n+1/2} = \frac{2\varepsilon_{o} \kappa_{y} - \Delta t \sigma_{y}}{2\varepsilon_{o} \kappa_{y} + \Delta t \sigma_{y}} P_{z_{i,j,k+1/2}}^{n-1/2} + \frac{2\varepsilon_{o}}{2\varepsilon_{o} \kappa_{y} + \Delta t \sigma_{y}} \left(Q_{z_{i,j,k+1/2}}^{n+1/2} - Q_{z_{i,j,k+1/2}}^{n-1/2}\right) \end{split}$$

$$\begin{split} & \mathcal{E}_{o} \kappa_{z} \frac{P_{z_{i,j,k+1/2}}^{n+1/2} - P_{z_{i,j,k+1/2}}^{n-1/2}}{\Delta t} + \sigma_{z} \frac{P_{z_{i,j,k+1/2}}^{n+1/2} + P_{z_{i,j,k+1/2}}^{n-1/2}}{2} = \mathcal{E}_{o} \kappa_{x} \frac{E_{z_{i,j,k+1/2}}^{n+1/2} - E_{z_{i,j,k+1/2}}^{n-1/2}}{\Delta t} + \sigma_{x} \frac{E_{z_{i,j,k+1/2}}^{n+1/2} + E_{z_{i,j,k+1/2}}^{n-1/2}}{2} \\ \Rightarrow & E_{z_{i,j,k+1/2}}^{n+1/2} = \frac{2\mathcal{E}_{o} \kappa_{x} - \sigma_{x} \Delta t}{2\mathcal{E}_{o} \kappa_{x} + \sigma_{x} \Delta t} E_{z_{i,j,k+1/2}}^{n-1/2} + \frac{1}{2\mathcal{E}_{o} \kappa_{x} + \sigma_{x} \Delta t} \left(\left(2\mathcal{E}_{o} \kappa_{z} + \sigma_{z} \Delta t \right) P_{z_{i,j,k+1/2}}^{n+1/2} - \left(2\mathcal{E}_{o} \kappa_{z} - \sigma_{z} \Delta t \right) P_{z_{i,j,k+1/2}}^{n-1/2} \right) \end{split}$$

- o Repeated for the rest of the E and H-field projections.
- o Note that the conductivity requires an additional auxiliary variable.
- o Three-step update process for each field projection
- o Nevertheless, medium is perfectly matched. The κ terms aide in the absorption of the attenuating and evanescent waves.

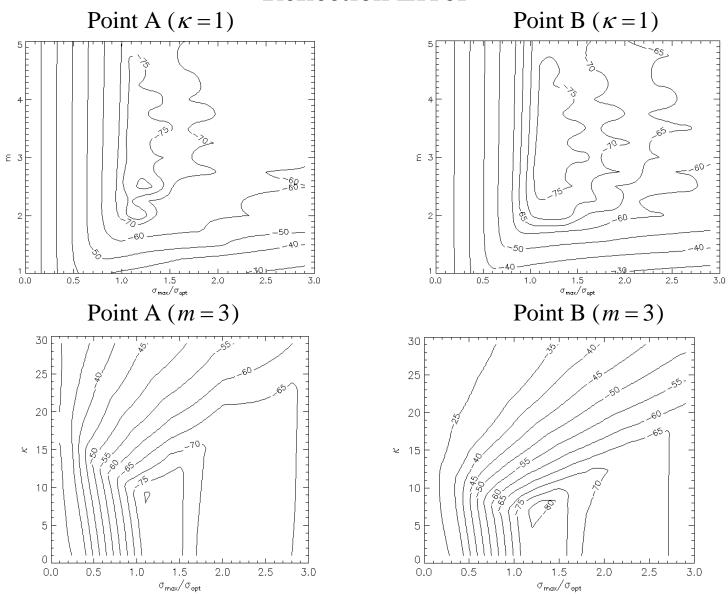




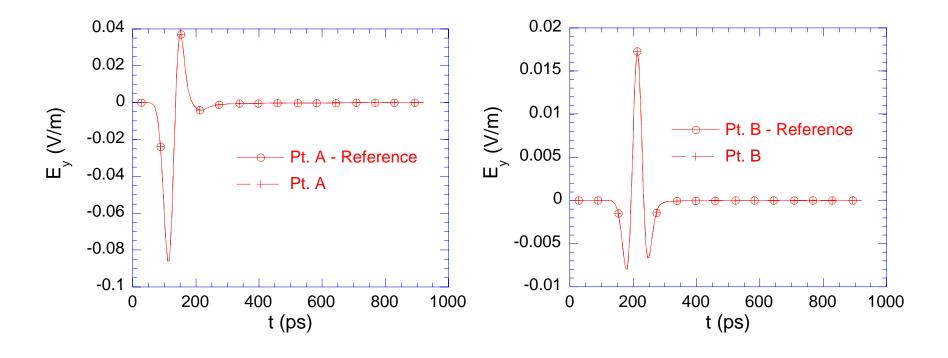
Geometry for the FDTD simulation of a TE_z polarized wave excited by a vertical electric current source above a lossy half space. The working volume was 40 cells by 40 cells ($\Delta x = \Delta y = 0.4$ mm), and the PML layers are 10 cells thick (d = 4 mm). ($\varepsilon_r = 10$, $\sigma = 0.3$ S/m). (Lossy medium extends thru PML to PEC boundaries)

$$J_{y}(x_{o}, y_{o}, t) = -2\frac{t - t_{o}}{t_{w}}e^{-\left(\frac{t - t_{o}}{t_{w}}\right)^{2}}$$
, with $t_{w} = 2.65258 \times 10^{-11} \text{ s & } t_{o} = 4 t_{w}$

Reflection Error



o Vertical electric field at points *A* and *B* due to the electric current dipole radiating above the lossy half space computed with the PML termination as compared with a reference solution computed on an extremely large grid. 10 cell PML, $\sigma_{max} = 1.1 \ \sigma_{opt}$, m = 3.5, $\kappa_{max} = 7$.



Complex-Frequency Shifted PML Tensor

- o The PML still suffers from
 - o Large reflections for very slowly varying wave (low frequency, large evanescence, highly-oblique angles of incidence)
 - o The majority of the reflection error comes from the front boundary interface c.f., [J. P. Berenger, "Evanescent waves in PML's: Origin of the numerical reflection in wave-structure interaction problems," *IEEE Transactions on Antennas and Propagation*, vol. 47, pp. 1497-1503, 1999.]
 - o This is partly related to the pole in the metric tensor at the origin ($\omega = 0$).
 - o We can circumvent this by introducing a metric tensor coefficient of the form:

$$S_{x} = \kappa_{x} + \frac{\sigma_{x}}{\alpha_{x} + j\omega\varepsilon_{o}}$$

o This is referred to as the Complex-Frequency-Shifted (CFS) PML tensor coefficient. First proposed by M. Kuzuoglu and R. Mittra, in "Frequency dependence of the constitutive parameters of causal perfectly matched anisotropic absorbers," *IEEE Microwave and Guided Wave Letters*, vol. 6, pp. 447-449, 1996, for frequency dependent FEM.

First proposed for FDTD, with implementation, by Gedney in Chapter 7 of *Advances* in Computational Electrodynamics: The Finite-Difference Time-Domain Method, Allen Taflove, Ed., Artech House, Boston, 1998.

o Consider a wave that is incident on the PML with a complex wave-number:

$$e^{-\gamma_x^i s_x x} = e^{-\left(\alpha_x^i + j\beta_x^i\right) s_x x} = e^{-\left(\alpha_x^i + j\beta_x^i\right)\left(\kappa_x + \frac{\sigma_x}{\alpha_x + j\omega\varepsilon_o}\right) x} = e^{-\kappa_x \alpha_x^i x} e^{-\frac{\sigma_x}{\alpha_x + j\omega\varepsilon_o} \alpha_x^i x} e^{-j\kappa_x \beta_x^i x} e^{-j\omega\sqrt{\mu\varepsilon}\cos\theta^i \frac{\sigma_x}{\alpha_x + j\omega\varepsilon_o} x}$$

o At very low frequency $(\omega \rightarrow 0)$:

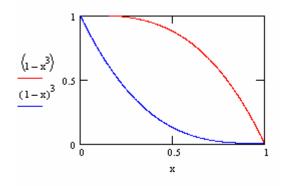
$$\approx e^{-\kappa_x \alpha_x^i x} e^{-\frac{\sigma_x}{\alpha_x} \alpha_x^i x}$$

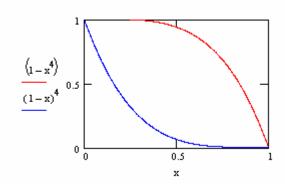
- \circ Which is purely attenuating. In fact, now both κ_x and σ_x attenuate the wave.
- o At higher frequencies, where $\omega \varepsilon_o >> \alpha_x$, the CFS PML behaves as the original PML.
- The consequence of this is that we can better attenuate low-frequency interactions with the PML. A rigorous study of this was presented by Berenger in: "Numerical reflection from FDTD-PMLs: A comparison of the split PML with the unsplit and CFSPML," IEEE TRANSACTIONS ON ANTENNAS AND PROPAGATION, vol. 50 (3): pp. 258-265 MAR 2002

o Caveat: For a purely propagating wave, the CFS PML tensor can provide little to no attenuation. Consider a TEM mode with propagation $e^{-j\beta x}$, where $\beta = \omega \sqrt{\mu \varepsilon}$.

- o In the CFS PML, the wave propagate as: $e^{-j\kappa_x\beta x}e^{-j\beta\frac{\sigma_x}{\alpha_x+j\omega\varepsilon_o}x}$.
- o In the limit $\omega \to 0$, this becomes: $e^{-j\kappa_x\beta x}e^{-j\beta\frac{\sigma_x}{\alpha_x}}$, which has no attenuation at all!
- o To circumvent this, we need to scale α_x . It is recommended to scale α_x to be maximum at the interface, and minimum at the back wall.
- o Two different polynomial scalings:

$$\alpha_x(x) = \alpha_x^{\max} \left(1 - \left(\frac{x}{d} \right)^m \right), \quad \alpha_x(x) = \alpha_x^{\max} \left(1 - \frac{x}{d} \right)^m$$





Implementing the CFS PML

Method 1: Auxiliary Equation Approach

o Given the CFS tensor coefficients:

$$s_x = \kappa_x + \frac{\sigma_x}{\alpha_x + j\omega\varepsilon_o}, \ s_y = \kappa_y + \frac{\sigma_y}{\alpha_y + j\omega\varepsilon_o}, \ s_z = \kappa_z + \frac{\sigma_z}{\alpha_z + j\omega\varepsilon_o}$$

o Lets work with the x-projection of Ampere's Law:

$$j\omega\varepsilon\overline{\overline{s}}E_{x} = \frac{\partial H_{z}}{\partial y} - \frac{\partial H_{y}}{\partial z}$$
, where $\overline{\overline{s}} = \begin{bmatrix} s_{y}s_{z}/s_{x} & 0 & 0\\ 0 & s_{z}s_{x}/s_{y} & 0\\ 0 & 0 & s_{x}s_{y}/s_{z} \end{bmatrix}$

O Make the substitution:

$$P_x = \frac{1}{s_x} E_x$$
, $P_x^z = s_z P_x$, $P_x^y = s_y P_x^z$

o Then, from $P_x^y = s_y P_x^z$

$$P_{x}^{y} = \left(\kappa_{y} + \frac{\sigma_{y}}{\alpha_{y} + j\omega\varepsilon_{o}}\right)P_{x}^{z} \Rightarrow \left(\alpha_{y} + j\omega\varepsilon_{o}\right)P_{x}^{y} = \left[\kappa_{y}\left(\alpha_{y} + j\omega\varepsilon_{o}\right) + \sigma_{y}\right]P_{x}^{z}$$

o Transforming this to the time domain:

$$\alpha_{y}P_{x}^{y} + \varepsilon_{o}\frac{\partial}{\partial t}P_{x}^{y} = \left(\kappa_{y}\alpha_{y} + \sigma_{y}\right)P_{x}^{z} + \kappa_{t}\varepsilon_{o}\frac{\partial}{\partial t}P_{x}^{z}$$

o Therefore, to write down the CFS equations, we can use the following procedure:

1.
$$j\omega\varepsilon P_x^y = \frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z}$$

2.
$$(\kappa_{y}\alpha_{y} + \sigma_{y})P_{x}^{z} + \kappa_{y}\varepsilon_{o}\frac{\partial}{\partial t}P_{x}^{z} = \alpha_{y}P_{x}^{y} + \varepsilon_{o}\frac{\partial}{\partial t}P_{x}^{y}$$

3.
$$(\kappa_z \alpha_z + \sigma_z) P_x + \kappa_z \varepsilon_o \frac{\partial}{\partial t} P_x = \alpha_z P_x^z + \varepsilon_o \frac{\partial}{\partial t} P_x^z$$

4.
$$\alpha_x E_x + \varepsilon_o \frac{\partial}{\partial t} E_x = (\kappa_x \alpha_x + \sigma_x) P_x + \kappa_x \varepsilon_o \frac{\partial}{\partial t} P_x$$

- We can discretize this in a second-order accurate manner as before.
- o Problem: We've increased to 4 unknowns per field projection! In 3D, this increases the number of base field vectors from 6 to 24!
- o A more efficient procedure was introduced in: [Roden JA, Gedney SD, "Convolution PML (CPML): An efficient FDTD implementation of the CFS-PML for arbitrary media", Microwave and Optical Technology Letters, vol. 27, no. 6, pp. 334-339, Dec. 5, 2000]
- o Note that the CPML procedure improves efficiency of the algorithm, but exactly the same reflection properties.

Method 1: Convolutional PML - CPML

o If we combine the split field projections of Berenger, we can express Maxwell's equations in the PML region in a "stretched coordinate form". Thus,

$$j\omega\varepsilon E_{x} = \frac{1}{s_{y}}\frac{\partial H_{z}}{\partial y} - \frac{1}{s_{z}}\frac{\partial H_{y}}{\partial z}, \qquad -j\omega\mu H_{x} = \frac{1}{s_{y}}\frac{\partial E_{z}}{\partial y} - \frac{1}{s_{z}}\frac{\partial E_{y}}{\partial z}$$

$$j\omega\varepsilon E_{y} = \frac{1}{s_{z}}\frac{\partial H_{x}}{\partial z} - \frac{1}{s_{z}}\frac{\partial H_{z}}{\partial x}, \qquad -j\omega\mu H_{y} = \frac{1}{s_{z}}\frac{\partial E_{x}}{\partial z} - \frac{1}{s_{x}}\frac{\partial E_{z}}{\partial x}$$

$$j\omega\varepsilon E_{z} = \frac{1}{s_{x}}\frac{\partial H_{y}}{\partial x} - \frac{1}{s_{y}}\frac{\partial H_{x}}{\partial y}, \qquad -j\omega\mu H_{z} = \frac{1}{s_{x}}\frac{\partial E_{y}}{\partial x} - \frac{1}{s_{y}}\frac{\partial E_{x}}{\partial y}$$

- \circ Note, this is derived by first dividing both sides by s_k , then adding split fields.
- We can then express this in the time domain as:

$$\varepsilon \frac{\partial}{\partial t} E_x = \overline{s}_y(t) * \frac{\partial}{\partial y} H_z - \overline{s}_z(t) * \frac{\partial}{\partial z} H_y$$

- o Where $\overline{s}_y(t)$ is the inverse Fourier transform of $1/s_y$, and similarly for $\overline{s}_z(t)$
- o Given that $s_i = \kappa_i + \frac{\sigma_i}{\alpha_i + j\omega\varepsilon_o}$, (i = x, y, or z), we can show that

$$\overline{s}_{i}(t) = \frac{\delta(t)}{\kappa_{i}} - \frac{\sigma_{i}}{\varepsilon_{o}\kappa_{i}^{2}} e^{-\left(\frac{\sigma_{i}}{\varepsilon_{o}\kappa_{i}} + \frac{\alpha_{i}}{\varepsilon_{o}}\right)^{t}} u(t) = \frac{\delta(t)}{\kappa_{i}} + \zeta_{i}(t)$$

$$\overline{s_i}(t) = \frac{\delta(t)}{\kappa_i} - \frac{\sigma_i}{\varepsilon_o \kappa_i^2} e^{-\left(\frac{\sigma_i}{\varepsilon_o \kappa_i} + \frac{\alpha_i}{\varepsilon_o}\right)^t} u(t) = \frac{\delta(t)}{\kappa_i} + \zeta_i(t)$$

o Now, we can rewrite the *x*-projection of Ampere's law as:
$$\varepsilon \frac{\partial}{\partial t} E_x = \frac{1}{\kappa_y} \frac{\partial}{\partial y} H_z - \frac{1}{\kappa_z} \frac{\partial}{\partial z} H_y + \zeta_y(t) * \frac{\partial}{\partial y} H_z - \zeta_z(t) * \frac{\partial}{\partial z} H_y$$

- At this point, we need to compute the convolutions efficiently.
- o Define the "Discrete Impulse Response" for $\zeta_i(t)$ as:

$$\begin{split} Z_{0_{i}}\left(m\right) &= \int_{m\Delta_{t}}^{(m+1)\Delta_{t}} \zeta_{i}(\tau) d\tau = -\frac{\sigma_{i}}{\varepsilon_{o} \kappa_{i}^{2}} \int_{m\Delta_{t}}^{(m+1)\Delta_{t}} e^{-\left(\frac{\sigma_{i}}{\varepsilon_{o} \kappa_{i}} + \frac{\alpha}{\varepsilon_{o}}\right)^{\tau}} d\tau \\ &= a_{i} e^{-\left(\frac{\sigma_{i}}{\kappa_{i}} + \alpha\right) \frac{m\Delta_{t}}{\varepsilon_{o}}} \end{split}$$
 where $a_{i} = \frac{\sigma_{i}}{\left(\sigma_{i} \kappa_{i} + \kappa_{i}^{2} \alpha_{i}\right)} \left(e^{-\left(\frac{\sigma_{i}}{\kappa_{i}} + \alpha_{i}\right) \frac{\Delta_{t}}{\varepsilon_{o}}} - 1.0\right)$

 \circ Then, the discrete convolution of $\zeta_i(t)$ with a discrete function f(t) sampled at $n\Delta t$ is:

$$f(t) * \zeta_i(t) = \sum_{m=0}^{N-1} Z_{o_i}(m) f(n-m)$$

o Inserting this into Ampere's law, and discretizing in time leads to:

0

$$\varepsilon_{r}\varepsilon_{0} \frac{E_{x_{i+\frac{1}{2},j,k}}^{n+1} - E_{x_{i+\frac{1}{2},j,k}}^{n}}{\Delta_{t}} = \frac{H_{z_{i+\frac{1}{2},j+\frac{1}{2},k}}^{n+\frac{1}{2}} - H_{z_{i+\frac{1}{2},j-\frac{1}{2},k}}^{n+\frac{1}{2}}}{\kappa_{y}\Delta_{y}} - \frac{H_{y_{i+\frac{1}{2},j,k+\frac{1}{2}}}^{n+\frac{1}{2}} - H_{y_{i+\frac{1}{2},j,k-\frac{1}{2}}}^{n+\frac{1}{2}}}{\kappa_{z}\Delta_{z}} + \sum_{m=0}^{N-1} Z_{o_{y}}(m) \frac{H_{z_{i+\frac{1}{2},j+\frac{1}{2},k}}^{n-m+\frac{1}{2}} - H_{z_{i+\frac{1}{2},j-\frac{1}{2},k}}^{n-m+\frac{1}{2}}}{\Delta_{y}} - \sum_{m=0}^{N-1} Z_{o_{z}}(m) \frac{H_{y_{i+\frac{1}{2},j,k+\frac{1}{2}}}^{n-m+\frac{1}{2}} - H_{y_{i+\frac{1}{2},j,k-\frac{1}{2}}}^{n-m+\frac{1}{2}}}{\Delta_{z}}$$

o This is still too expensive, since it requires a full summation at every time step!

o Fortunately, given the properties of $Z_{o_i}(m)$, this can be performed in a simplified manner using the "Recursive Convolution Method" [R. J. Luebbers and F. Hunsberger, "FDTD for Nth-Order Dispersive Media," *IEEE Transactions on Antennas and Propagation*, vol. 40, pp. 1297-1301, 1992.]. Thus, the update can be re-written as:

$$\varepsilon_{r}\varepsilon_{0}\frac{E_{x_{i+\frac{1}{2},j,k}}^{n+1}-E_{x_{i+\frac{1}{2},j,k}}^{n}}{\Delta_{t}}=\frac{H_{z_{i+\frac{1}{2},j+\frac{1}{2},k}}^{n+\frac{1}{2}}-H_{z_{i+\frac{1}{2},j-\frac{1}{2},k}}^{n+\frac{1}{2}}}{\kappa_{y}\Delta_{y}}-\frac{H_{y_{i+\frac{1}{2},j,k+\frac{1}{2}}}^{n+\frac{1}{2}}-H_{y_{i+\frac{1}{2},j,k-\frac{1}{2}}}^{n+\frac{1}{2}}}{\kappa_{z}\Delta_{z}}+\psi_{e_{xy_{i+\frac{1}{2},j,k}}}^{n+\frac{1}{2}}-\psi_{e_{xz_{i+\frac{1}{2},j,k}}}^{n+\frac{1}{2}}$$

where

$$\psi_{e_{xy_{i+\frac{1}{2},j,k}}}^{n+\frac{1}{2}} = b_{y}\psi_{e_{xy_{i+\frac{1}{2},j,k}}}^{n-\frac{1}{2}} + a_{y}\left(H_{z_{i+\frac{1}{2},j+\frac{1}{2},k}}^{n+\frac{1}{2}} - H_{z_{i+\frac{1}{2},j-\frac{1}{2},k}}^{n+\frac{1}{2}}\right) / \Delta_{y}$$

$$\psi_{e_{xz_{i+\frac{1}{2},j,k}}}^{n+\frac{1}{2}} = b_z \psi_{e_{xz_{i+\frac{1}{2},j,k}}}^{n-\frac{1}{2}} + a_z \left(H_{y_{i+\frac{1}{2},j,k+\frac{1}{2}}}^{n+\frac{1}{2}} - H_{y_{i+\frac{1}{2},j,k-\frac{1}{2}}}^{n+\frac{1}{2}} \right) / \Delta_z$$

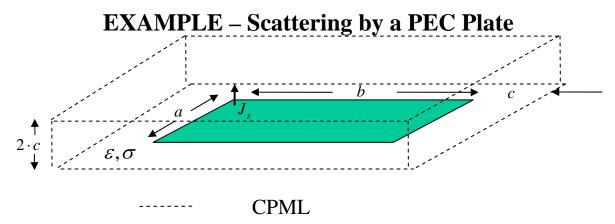
$$b_i = e^{-\left(\frac{\sigma_i}{\kappa_i} + \alpha_i\right)\frac{\Delta_t}{\varepsilon_o}}, \ (i = x, y, \text{ or } z)$$

- o Advantages of the CPML formulation:
 - 1. Reduced the number of auxiliary variables from 3 to 2
 - 2. Lossy medium is similarly treated. Updates do not require additional terms!:

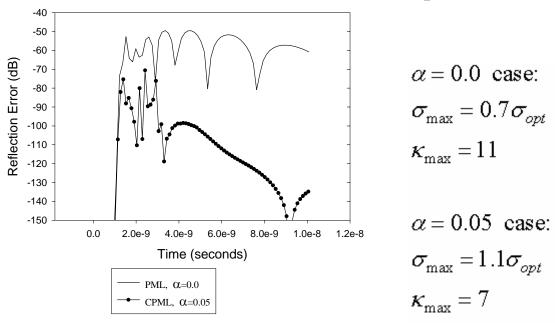
$$\varepsilon_{r}\varepsilon_{0} \frac{E_{x_{i+\frac{1}{2},j,k}}^{n+1} - E_{x_{i+\frac{1}{2},j,k}}^{n}}{\Delta_{t}} + \sigma \frac{E_{x_{i+\frac{1}{2},j,k}}^{n+1} - E_{x_{i+\frac{1}{2},j,k}}^{n}}{2} = \frac{H_{z_{i+\frac{1}{2},j+\frac{1}{2},k}}^{n+\frac{1}{2}} - H_{z_{i+\frac{1}{2},j-\frac{1}{2},k}}^{n+\frac{1}{2}}}{\kappa_{y}\Delta_{y}} - \frac{H_{y_{i+\frac{1}{2},j,k+\frac{1}{2}}}^{n+\frac{1}{2}} - H_{y_{i+\frac{1}{2},j,k-\frac{1}{2}}}^{n+\frac{1}{2}}}{\kappa_{z}\Delta_{z}} + \psi_{e_{xy_{i+\frac{1}{2},j,k}}}^{n+\frac{1}{2}} - \psi_{e_{xz_{i+\frac{1}{2},j,k}}}^{n+\frac{1}{2}}$$

- 3. No more expensive than standard PML terminating a lossy medium
- 4. The convolutional terms ψ are simply added in as soft source terms standard FDTD update loops are not corrupted.
- 5. Very easy to implement in a standard FDTD code with inhomogeneous and lossy medium.
- o In practice, $\alpha_i, \kappa_i, \sigma_i$ are scaled along the *i*-direction. The same rule applies to CPML as PML. You sample $\alpha_i, \kappa_i, \sigma_i$ at the *edge-centers* for E-field updates, and you sample $\alpha_i, \kappa_i, \sigma_i$ at the *face-centers* for H-field updates.
- o The update coefficients can them be pre-calculated and stored as *one-dimensional* vectors

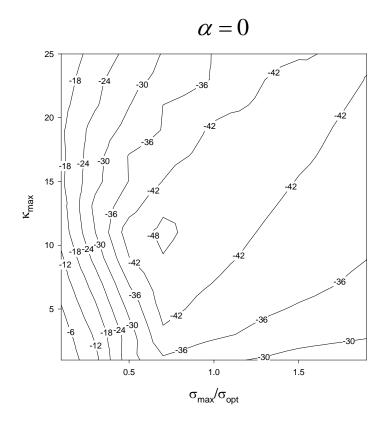
S. Gedney

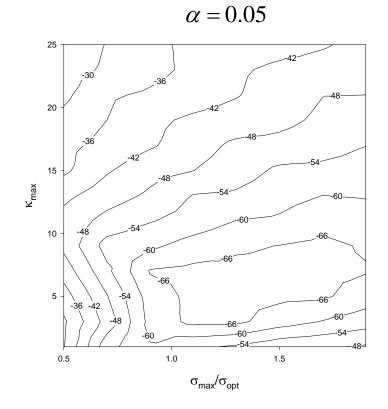


a=25 mm, b=100 mm, PML is 10 cells thick, and 3 cells from plate in all dimensions Maximum relative reflection error over 2,000 time steps for 10 cell thick PML



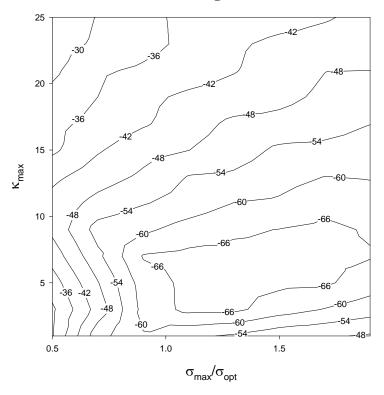
o A significant improvement is the late time reflection error.



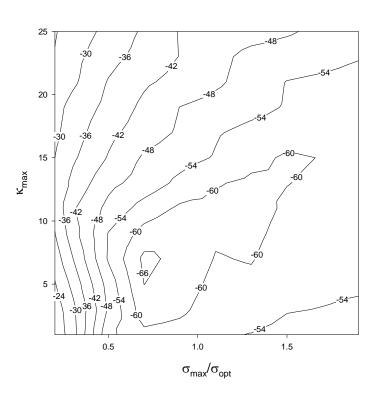


Maximum relative reflection error over 2,000 time steps for 10 cell PML

PML 3 cells from plate & $\alpha = 0.05$



PML 17 cells from plate & $\alpha = 0$



(note PML boundary is equidistant from plate on all sides)

Lattice 1: $126 \times 51 \times 26$ Lattice 2: $154 \times 79 \times 54$

Memory Savings Factor: $2 \times 154 \times 79 \times 54/3 \times 126 \times 51 \times 26 = 2.6$

Late Time-Stability of PML

- o Consider a PML termination of a single boundary with no overlapping corner regions (a bounded wave guide would be an example).
- o For simplicity, assume a lossless, homogeneous region, with a *z*-normal:

$$\begin{bmatrix} \frac{\partial}{\partial y} H_z - \frac{\partial}{\partial z} H_y \\ \frac{\partial}{\partial z} H_x - \frac{\partial}{\partial x} H_z \\ \frac{\partial}{\partial x} H_y - \frac{\partial}{\partial y} H_x \end{bmatrix} = j\omega\varepsilon_o \begin{bmatrix} s_z & 0 & 0 \\ 0 & s_z & 0 \\ 0 & 0 & 1/s_z \end{bmatrix} \begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix}, \begin{bmatrix} \frac{\partial}{\partial y} E_z - \frac{\partial}{\partial z} E_y \\ \frac{\partial}{\partial z} E_x - \frac{\partial}{\partial x} E_z \\ \frac{\partial}{\partial x} E_y - \frac{\partial}{\partial y} E_x \end{bmatrix} = -j\omega\mu_o \begin{bmatrix} s_z & 0 & 0 \\ 0 & s_z & 0 \\ 0 & 0 & 1/s_z \end{bmatrix} \begin{bmatrix} H_x \\ H_y \\ H_z \end{bmatrix}$$

o The PML updates for the transverse fields appear in the form of a lossy medium. The normal fields, as a Debye medium. We write these in a two step update process:

$$\frac{\partial}{\partial x}H_{y} - \frac{\partial}{\partial y}H_{x} = j\omega\varepsilon_{o}P_{z} \& E_{z} = s_{z}P_{z}$$

o In the time-domain:

$$\frac{\partial}{\partial x}H_{y} - \frac{\partial}{\partial y}H_{x} = \varepsilon_{o}\frac{\partial P_{z}}{\partial t} \& \frac{\partial E_{z}}{\partial t} = \frac{\partial P_{z}}{\partial t} + \frac{\sigma_{z}}{\varepsilon_{o}}P_{z}$$

o Comparing these two equations, we recognize that $\frac{\partial P_z}{\partial t}$ is proportional to the transverse derivatives of the transverse magnetic field. We have a dual situation from Faradays law

o In the very late time, as the fields reach steady state, the transverse derivatives of the transverse fields will tend to zero.

- As a consequence $\frac{\partial}{\partial x}H_y \frac{\partial}{\partial y}H_x = 0 = \varepsilon_o \frac{\partial P_z}{\partial t}$
- o Therefore, the auxiliary equation reduces: $\frac{\partial E_z}{\partial t} = \frac{\sigma_z}{\varepsilon_o} P_z$.
- o Where, since $\frac{\partial P_z}{\partial t} = 0$, then P_z is a constant in time. Thus, the solution to the ODE $\frac{\partial E_z}{\partial t} = \frac{\sigma_z}{\varepsilon_o} P_z$ is simply: $E_z = \frac{\sigma_z}{\varepsilon_o} P_z t + E_{z_0}$, which is a linear function in time! Similarly,

for the dual field $H_z = \frac{\sigma_z}{\varepsilon_o} Q_z t + H_{z_0}$. Therefore, in the event that the transverse gradient of the fields is zero, the normal fields in the PML can grow linearly in time!

- o This has been the topic of some publications:
- S. Abarbanel, D. Gottlieb, and J. S. Hesthaven, "Long time behavior of the PML equations in computational electromagnetics," *Journal of Scientific Computing*, vol. 17, no. 1-4, pp. 405-422, 2002.
- E. Becache, P. Petropoulos, & S. D. Gedney, "On the long-time behavior of unsplit perfectly matched layers," *IEEE Transactions on Antennas and Propagation*, to appear.
- S. J. Yakura, D. Dietz, and A. D. Greenwood, "A dynamic stability analysis of the PML method," Interaction Note Series Note 582, Kirtland Air Force Base, Albuquerque, NM, November 1, 2002

Consequences of the late time instability:

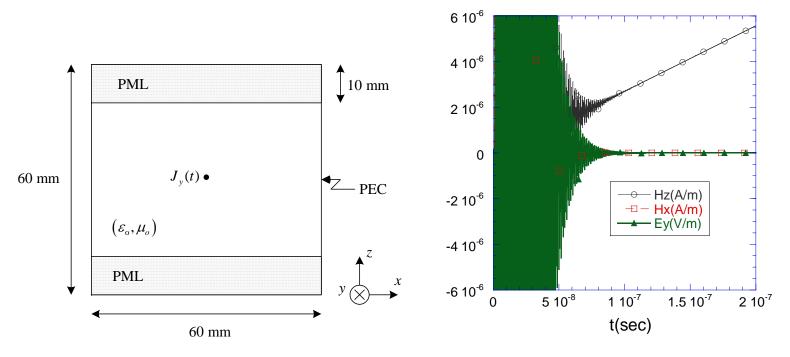
- 1. The late time instability does not occur until after the fields in the working volume are ~ zero, which is beyond steady state for a radiation/scattering problem
- 2. The linear growth of the fields only occurs *in* the PML, when using the UPML formulation. : it does not corrupt the fields in the working volume. For the split-field PML, the linear growth can affect the fields in the working volume.
- 3. If the PML boundaries are overlapping, this problem does not occur. .
- 4. Late time instability does not occur for CFS PML. Why? The late time-stability is related to the weakly causal nature of the constitutive parameters.

Examples from Bécache, Petropoulos & Gedney

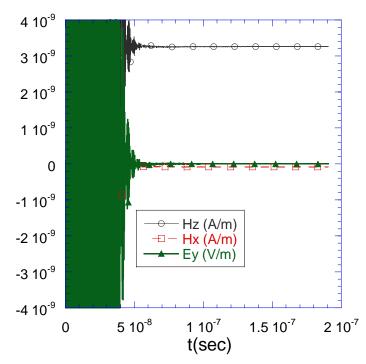
TM_z polarization. $\Delta x = \Delta y = 1mm$, $\Delta t = 2.35 \times 10^{-12} \text{ s.}$ $J_y(t) = -2\frac{t}{t_w} e^{\frac{-(t-t_o)}{t_w^2}} \sin(2\pi f_c t)$,

with $t_w = 3.183 \times 10^{-10}$ s, $t_o = 4t_w$, and $f_c = 3 \times 10^9$ Hz. Standard PML with m = 4, $\sigma_{\rm max} = 10.61$ S/m, $\kappa_{\rm max} = 1$.

We are monitoring the fields *inside* the PML in the very late time (~100,000 time steps).



Normal field shows linear growth in the late time as predicted!



Repeat the same experiment with CFS PML, with $\alpha = 0.08$. The field remains constant – no linear growth. Here we have:

$$H_{z} = s_{z}Q_{z} = \left(\kappa_{z} + \frac{\sigma_{z}}{\alpha_{z} + j\omega\varepsilon_{o}}\right)Q_{z} \Rightarrow \alpha_{z}H_{z} + \varepsilon_{o}\frac{\partial H_{z}}{\partial t} = \left(\kappa_{z}\alpha_{z} + \sigma_{z}\right)\frac{\partial Q_{z}}{\partial t} + \sigma_{z}Q_{z}$$

 $H_z = s_z Q_z = \left(\kappa_z + \frac{\sigma_z}{\alpha_z + j\omega\varepsilon_o}\right) Q_z \Rightarrow \alpha_z H_z + \varepsilon_o \frac{\partial H_z}{\partial t} = \left(\kappa_z \alpha_z + \sigma_z\right) \frac{\partial Q_z}{\partial t} + \sigma_z Q_z$ In the late time, if $\frac{\partial Q_z}{\partial t} = 0$, then $\alpha_z H_z + \varepsilon_o \frac{\partial H_z}{\partial t} = \sigma_z Q_z$, which has solution: $H_z = \frac{\sigma_z}{\alpha_z} Q_z$.

Therefore, H_z is a non-zero constant in the late time. Nevertheless, it is quite small.