

Computational Electromagnetics
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FDTD: Materials and Boundary Conditions
Lecture-13.16
Implementing PML into FDTD - Part 2

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Implementing into FDTD: Comparisons with lossy media

$$(\nabla \times \vec{H}) = \hat{x} \left(\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} \right) + \hat{y} \left(\frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} \right) + \hat{z} \left(\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} \right) \leftarrow (\text{unit vecs})$$

$$\hat{x} \times \vec{H} = \hat{x} \times [\hat{x} H_x + \hat{y} H_y + \hat{z} H_z] = \hat{z} H_y - \hat{y} H_z \quad \uparrow$$

$$\nabla \times \vec{H} = \frac{\partial (\hat{x} \times \vec{H})}{\partial x} + \frac{\partial (\hat{y} \times \vec{H})}{\partial y} + \frac{\partial (\hat{z} \times \vec{H})}{\partial z} \quad \text{--- (1) (partial derivatives)}$$

↳ lossy media (Ohm's Law)

$$\nabla \times \vec{H} = \vec{J} + \frac{\partial \vec{D}}{\partial t} = \sigma \vec{E} + j\omega \epsilon_r \epsilon_0 \vec{E}$$

↳ Not along $\hat{x}, \hat{y}, \hat{z}$

$$= j\omega \epsilon_0 \left[\epsilon_r - \frac{j\sigma}{\omega \epsilon_0} \right] \vec{E} = j\omega \epsilon_0 \epsilon' \left[\vec{E}_{\hat{x}} + \vec{E}_{\hat{y}} + \vec{E}_{\hat{z}} \right] \quad \text{--- (2)}$$

$$\vec{E}_{\hat{x}} \triangleq \frac{1}{j\omega \epsilon_0 \epsilon'} \left(\frac{\partial \hat{x} \times \vec{H}}{\partial x} \right) \quad \text{--- (3)}$$

So, let us have a look at that right.

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Implementing into FDTD: Setting parameters

Putting into PML.

For lossy media

$$\nabla_h \times \vec{H} = j\omega\epsilon_0 \vec{E}$$

↓ only 3rd comp

$$\frac{1}{s_z} \frac{\partial}{\partial z} (\hat{z} \times \vec{H}) = j\omega\epsilon_0 \vec{E}_{sz} \leftarrow \text{PML}$$

For lossy media

$$\frac{\partial}{\partial z} (\hat{z} \times \vec{H}) = j\omega\epsilon_0 \left[\epsilon_r - \frac{j\sigma}{\omega\epsilon_0} \right] \vec{E}_{sz}$$

So on for each comp.

How to implement?

$$\nabla \times \vec{H} = \epsilon \vec{E} + \sigma \vec{E}$$

$$= \epsilon \left(\frac{\vec{E}^n - \vec{E}^{n-1}}{\Delta t} \right) + \frac{\sigma}{2} \left(\frac{\vec{E}^n + \vec{E}^{n-1}}{2} \right)$$

$\sigma(x) = \left(\frac{x}{L} \right)^m, 0 < x < L$

So, putting into PML ok; so, in PML what are we started writing the Maxwell's equations in terms of $\nabla_h \times \vec{H}$ to give that coordinate stretching number right. So, that I wrote was equal to $j\omega\epsilon\vec{E}$ there is no current term over here and further let us just make it ϵ_0 because we had discussed previously that the between the interface I mean at the interface between vacuum and PML epsilon mu were the same right.

So, now I am talking about the PML region where I am going to write this Maxwell's equation. So now, let us just take one of these terms, for example, we can take the \vec{E}_{sz} term let just look at that. So, what is that going to be equal to? When I look at this side ok so, this is the equation and I want to look at this term ok. So, what should I write over there is going to be; obviously, $\partial/\partial z (\hat{z} \times \vec{H})$ anything else?

Students: 1 by s z.

Exactly $1/s_z \partial/\partial z (\hat{z} \times \vec{H})$, that is the left hand side ok. So, I am only taking the 3rd component right. So, only 3rd component you can take all, but I am just simplifying it right now and what happens to the right hand side?

Student: E s z.

$j\omega\epsilon_0\vec{E}_{sz}$ correct ok, like this there is one to one between all three. So, if you want we can; if you want we can write it all down should I understood right from each and so on, for each component fine.

This is what PML is telling us and seemingly unrelated this is what a lossy medium looks like. So, is there a similarity or something that we can use ok. So, this is for let us just write it this is for PML ok, let us write down for lossy; lossy medium has no relation so, far with PML right let just write down what the lossy medium says for us. So, it says that

$$\partial/\partial z (\hat{z} \times \vec{H}) = j\omega\epsilon_0[\epsilon_r - j\sigma/\omega\epsilon_0]\vec{E}_{sz}$$

This is I am just rewriting this equation number 3. I see a few blank faces, is it clear what I did. So, let us take one step back lossy.

So, Maxwell's equation were re-written in this no problem from here I wrote it in terms of 3 vectors 1 2 3. Now for example, I look at the 3rd component right so, this term over here.

Student: (Refer Time: 03:44).

Those three may or may not be, I mean, they should be orthogonal I should not say.

Student: Orthogonal.

Yeah, fine because this $\hat{x} \hat{y} \hat{z}$ are orthogonal. So, x hat cross some same vector all three I will just get it another set of orthogonal vectors. Now, I am looking at the 3rd component. So, the 3rd component is being written over here this equation over here right that is what I have written over here this is the 3rd component which is on both side we have the 3rd component ok.

So, now we have them both on the same page. So, this is for lossy media and this is for PML and what we want to do is compare these two characters. So, looking at this what?

Student: s z.

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Choice of coordinate stretch parameters

Reg 1: vacuum, $\mu = \mu_0, \epsilon = \epsilon_0$

$(\epsilon_x, \epsilon_y, \epsilon_z, \mu_x, \mu_y, \mu_z) = (1, 1, 1, 1, 1, 1)$

Reg 2: PML

$(\epsilon_{2x}, \epsilon_{2y}, \epsilon_{2z}, \mu_{2x}, \mu_{2y}, \mu_{2z}) = (1, 1, s_z, 1, 1, s_z)$ ✓

⇒ created an interface with 0 reflections

- both poles
- any inc angle

s_z is the only thing that I have to set right in when we did our PML if you go back to the summary of PML medium 1 was all the parameters $(1, 1, 1, 1, 1, 1)$. PML was all of them were one except for the z parts, here I call them s_2 and s_2 and they were both equal and the discussion had ended by saying there should be some s_2 . What should that s_2 to be?

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Summary of PML theory

$k_z = \omega \sqrt{\mu_0 \epsilon_0} \frac{s_z \cos \theta}{1}$ In our hand.

$e^{jk_z z} = e^{jk_0 \cos \theta z} e^{-k_0 z \cos \theta}$

→ decays

impose ABC

Time conv: $e^{-j\omega t}$
 $\Rightarrow s = p + j\beta$

Time conv: $e^{+j\omega t}$
 $\Rightarrow s = p - j\beta$

It should be complex, but we had not decided what that value is right. So, when we come down to implementing we have to say what is the value of that s right. So, after looking at

the comparison with lossy media we find out that the interpretation of s_z can be taken from that of a lossy media it is as though. So, if I had a lossy media where I set this epsilon r and sigma I get the value of s_z right. So, I can write down

$$s_z = \epsilon_r - j\sigma/\omega\epsilon_0$$

And remember that is what I wanted for a for a PML medium I needed a lossy thing. So, that the wave decays inside right that is what we saw over here I for time convention $e^{j\omega t}$ I needed $s = p - jq$ right.

So, that is what I get to set over here it is like $p - jq$, but the parameters in our hand are ϵ_r and σ we can decide what those numbers are ok. So, this is so, in terms of implementation why did I sort of take recourse to lossy media because we already know how to implement lossy media in FDTD is not it we will discuss that. I will write down the updated equation again if its not clear, but we already know how to implement lossy media therefore, we already know to implement PML.

Student: (Refer Time: 06:26).

Yeah, but if I make so that the remember that is this coordinate stretching way of understanding PML. So, we have understood PML and we have understood that the PML is the same as a lossy media.

But remember that this is s_z only right it is anisotropic its not be its not the it's not going to experience the same loss for example, and what are the values of s_x and s_y one right. So, that is not a purely lossy media right. So, that is it so, that is the difference let me write it over here $s_x = 1$, $s_y = 1$. If all of these guys were the same then I am right and remember what I have written here is only for the z component when I look at the $\partial/\partial z$ term what will I get over there?

Student: s_x .

s_x will be there which is one? So, that that interpretation is not of a lossy media right. So, let us we already know how to implement this how to implement. So, I just rewrite it over here. Our update equations for \vec{H} for example, were right

$$\nabla \times \vec{H} = \partial \vec{D} / \partial t + \vec{J}$$

\vec{J} I am writing as $\vec{J} = \sigma \vec{E}$ and \vec{D} I am writing as $\epsilon \vec{E}$ its inaccurate, but we will live with that. What are the time indices we had said that electric field is every integer time index and magnetic field every half integer right. So, this is $n - 0.5$ therefore, this is also $n - 0.5$ and this is also $n - 0.5$ right and the problem was of course, that with this term over here. I am not storing electric field at half time integer instances. So, in terms of implementation this became $(E^n - E^{n-1}) / \Delta t$. No problem the second term because I am not storing electric field at half integer time instance this became average?

Student: Average.

So, this became $(E^n + E^{n-1}) / 2$. So, we already, so we know how to implement this equation right. So, when I take the component wise you know which part is s_x which part is s_y which part is s_z I know how to implement this ok.

$$\nabla \times \vec{H}^{n-0.5} = \epsilon (E^n - E^{n-1}) / \Delta t + \sigma (E^n + E^{n-1}) / 2$$

So, I am not going to write down those very detailed equations, but you know the principle now I have to set these s parameters and I get my PML ok. One final sort of and very important take is.

Student: Sir.

Yeah.

Student: Where do the PML.

Yeah why don't you tell me?

Student: (Refer Time: 09:30).

So, I mean. So, σ is here and this is ϵ_r right. So, here is your ϵ_r here is your σ and that is your s_z . So, you get to implement your s parameters over here.

Student: (Refer Time: 09:51) automatically.

It automatically yeah you just have to implement the correct components do not do it for all x y and z otherwise you will be in trouble ok. But remember this s when I said this s_z over here right. So, let us go back to this equation over here this was if I wanted to decay a wave in the z direction right this was the z direction over here I chose an s_z to be different from 1 correct. So, if I want to observe a layer that is going into the z direction I choose s_z equal to whatever $s_x = s_y = 1$ right.

That is those are the parameters that we had chosen over here correct. Now let us look at a realistic 2D computational domain, I am exaggerating the PML thickness. So, this whole thing is PML and this is my computational domain my object ok.

I am purposely showing it very big and let us make a coordinate axis like this x y ok. So, this in practice what happens is you break up this there are these many distinct regions of the PML what is distinct about them? So, for example, this part over here what all should be in what direction should it observe the wave?

Student: x

x . So, what will be non-zero over here?

Student: s_x .

s_x right; so, the parameters for this part will be $(s_x, 1, 1)$ right make sense what about this part over here the left part again s_x same direction $(s_x, 1, 1)$ what about this guy over here?

$(1, s_y, 1)$ $(1, 1, s_y)$ that leaves out the corners what should the corner be?

Student: $s_x s_y$.

$(s_x, s_y, 1)$ right; so, the corners are slightly different because I want to absorb it in I mean it is a wave that needs to be absorbed in arbitrary direction.

Student: In the corner.

In the corner in the corner region if I have a 3D thing then in the corners I will have (s_x, s_y, s_z) .

Student: Sir in the corner region will there be exactly a lossy medium.

Yeah, but the loss yeah it will be exactly like a lossy medium, but for example, the intermediate once they will not be purely lossy medium they will anisotropic for example, here.

Student: We could advice that PML is for the normal incidence.

No. So, this PML is not for normal incidence this is this is going to absorb any wave that is incident on it.

Student: We have considered only (Refer Time: 12:56) beta wave.

No. So, this interpretation that we had over here this is absorbing at all angles that are incident on this interface, but I mean the axis of PML is defined by z . So, wave can come at any angle. So, this for this guy over here the parameter $(1, 1, s_z)$, but this absorbed a wave incident at any angle on the z interface.

It need not be travelling along the z , but the absorption I mean the parameters that I have to set is only the z parameter, but it's absorbing any direction incident on it.

Student: But the wave is travelling on it.

The wave is travelling in any direction no the wave is travelling is incident on it in any direction that is what we showed this reflection coefficient that we had.

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$\omega/c = k$

↓ ↗ ↘ ↑

Waves at an interface: tangential boundary conditions

Define: $k_{1z} = k_{iz}$, $k_{2z} = k_{tz}$, $k_{rz} = -k_{1z}$ ✓

1 → Region 1
2 → Region 2.


TM pol: $R = \frac{k_{1z} h_{2z} \epsilon_2 - k_{2z} h_{1z} \epsilon_1}{k_{1z} h_{2z} \epsilon_2 + k_{2z} h_{1z} \epsilon_1}$

Goal: Make R as small as possible.

Num: $(\omega \sqrt{\mu \epsilon_1} \sqrt{\epsilon_{2z} h_{2z} \cos \theta_1}) h_{1z} \epsilon_2 - (\omega \sqrt{\mu \epsilon_2} \sqrt{\epsilon_{1z} h_{1z} \cos \theta_2}) h_{1z} \epsilon_1$

$\propto (\epsilon_{1z} \epsilon_{2z} - \epsilon_{2z} \epsilon_{1z})$ TM

$= 0$



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$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \rightarrow j \vec{k} \times \vec{E} = -j \omega \mu \vec{H} \rightarrow \vec{k} \times \vec{E} = \omega \mu \vec{H}$

Waves at an interface: tangential boundary conditions


Recall: $\vec{k}_e \times \vec{E} = +\omega \mu \vec{H}$, $\vec{k}_h \times \vec{H} = -\omega \epsilon \vec{E}$, $\vec{k}_{ie} = (\frac{k_{ix}}{\epsilon_z}, \frac{k_{iy}}{\epsilon_z}, \frac{k_{iz}}{\epsilon_z})$, \vec{k}_{re} , \vec{k}_{te} similarly.

Reg 1: inc + ref = $\frac{\vec{k}_{ie} \times \vec{E}_0}{\omega \mu_1} e^{j \vec{k}_i \cdot \vec{r}} + R \frac{\vec{k}_{re} \times \vec{E}_0}{\omega \mu_1} e^{j \vec{k}_r \cdot \vec{r}}$ (inc + ref)

Reg 2: trans = $\frac{\vec{k}_{te} \times \vec{E}_0}{\omega \mu_2} e^{j \vec{k}_t \cdot \vec{r}}$

$\vec{H}_{\text{tot},1} = \vec{H}_{\text{tot},2}$ $k_{1z} \epsilon_{2z} \mu_2 [1 - R] = T k_{2z} \epsilon_{1z} \mu_1$ ①

$R^{TE} = \frac{k_{1z} \epsilon_{2z} \mu_2 - k_{2z} \epsilon_{1z} \mu_1}{k_{1z} \epsilon_{2z} \mu_2 + k_{2z} \epsilon_{1z} \mu_1}$



This R over here and this R over here this was 0 regardless of which angle the wave came at right you agree. The only parameter that I had to set over here was the z parameter this does not mean that the wave is travelling only along the z direction the wave is incident at any angle, but the parameter that I need to set is the z parameter. I should you should not interpret this as the wave is travelling only along the z direction.

The absorption is going to happen along this it is the exponential decay along the z direction yeah. So, let me draw what you are saying you are saying let us say I have an interface like this is my z axis let say now the wave come that it at some angle right. And what we find from this formulation is this $R = 0$.

Student: Is it 1 1 and so on.

Yeah I have said this is this is $(1, 1, 1)$. This is $(1, 1, s_z)$ on on what? On another interface.

Student: (Refer Time: 14:45).

So, let us take another interface here what differentiates ok. So, the question is I have interface I_1 and interface I_2 has coordinates $(1, s_y, 1)$ right. So, in I_1 I had $(1, 1, s_z)$ and in I_2 I had $(1, s_y, 1)$. So, what differentiates right. So, question so, if you look at the way we derived this.

For example, when you look at the reflection coefficient over here when I assume that the boundary was over along the $z = 0$ I got $k_{1z} k_{2z}$ that is why I needed to set s_z , but when I come to an interface like this I will not get $k_{1z} k_{2z}$ I will get $k_{1y} k_{2y}$ that is why I need to set s_y and then it is able to absorb any waves coming at it.

That is making the reflection coefficient 0, but the wave is travelling at any angle does not matter the trouble is I mean the interesting thing happening at this corner region over here right. So, corner region over here where will it get the wave from.

The wave, that has entered the PML and not yet fully absorbed, but travelling at some angle right. So, for example, something like this entered not fully absorbed and then it enters over here ok. So, it is a more cumbersome, but we can take.

Student: (Refer Time: 16:10).

It in the plane the k vector is in the plane in the 2 decays k vector is in the plane, the electric field polarization can be anywhere does not matter, but k is in the plane that is what makes it a 2D.

So this is where I mean implementation why is here the book keeping is a little bit more tedious because you have to keep track of x y z separately and this parameters (s_x , s_y , s_z) separately for each thing over here ok. And I think the final thing that I can say for example, if this is L over here a typical way of implementing this S parameter right now we are our interpretation is that s_z is like this sorry s_x is like this.

But what you want is usually done in practice is. So, by the way this ϵ_r can just be made 1 right because its adjacent to vacuum epsilon was the same on both sides, so this is 1. So, typically what you would do is that sigma you would make a function of x and you would do something like x by L to some power m ok.

And this is $0 \leq x \leq L$. So, the loss increases as, it does not become suddenly lossy it increases as some polynomial power of x. This is our implementation issue this is what gives the best performance. Theoretically you need do not need this, but when you get down to implementation this is what gives the best performance.

Student: Is there are some lossy medium.

Some lossy medium yeah in terms of implementation it is a kind of a lossy s z yeah.

Student: That is it.

That is that is it, but I have to rewrite my Maxwell's update equations to get that (s_x , s_y , s_z) parameters inside that is all you have to do and then set the correct value and this can be done and is done in FEM.

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Topics that were covered in this module

- 1 Failure of Absorbing Boundary Conditions
- 2 The remedy via Perfectly Matched Layers

References:

- * Ch 12 of Computational Methods for Electromagnetics - Peterson, Ray, Mitra
- * Computational Electrodynamics: The Finite-Difference Time-Domain Method – Allen Taflove (the 'Bible' for FDTD)
- * Chew, W. C. and Weedon, W. H. (1994), A 3D perfectly matched medium from modified maxwell's equations with stretched coordinates. Microw. Opt. Technol. Lett., 7: 599-604.



So, that brings us to an end of the discussion on PML.