

Computational Electromagnetics
Prof. Uday Khankhoje
Department of Electrical Engineering
Indian Institute of Technology, Madras

FDTD: Materials and Boundary Conditions
Lecture - 13.02
Dealing with dispersive dielectric media

(Refer Slide Time: 00:13)

Dealing with PECs

$$E^n = \left[\frac{1 - \sigma \Delta t / 2\epsilon}{1 + \sigma \Delta t / 2\epsilon} \right] E^{n-1} + \left[\frac{1}{1 + \frac{\sigma \Delta t}{2\epsilon}} \right] \frac{\Delta t}{\epsilon} [\nabla \times H^{n-1/2}]$$

to be evaluated. known

↳ dielectric materials: finite σ .

↳ PEC $\rightarrow \sigma \rightarrow \infty$

Update Eqn: $E^n = -E^{n-1}$

If we initialize E to be zero on the PEC boundary, it stays zero.

So, now let us take a, this is a dielectric material; dielectric material has finite conductivity right. So, for dielectric material. So a special case that often arises that in your simulation domain you have metal perfect metal: metallic waveguide, metallic aircraft, whatever right. So, that is a what conductivity will be associate with it infinity right.

So, this is a dielectric material now PEC: Perfect Electric Conductor sigma tends to infinity right. Putting numerically something has infinity is a problem, so we need to work out the limit before we put it into the code right. So, what happens to this expression?

Student: (Refer Time: 01:07).

Divide by sigma I mean you will divide the numerator and denominator by sigma and take the limit correct, what will you get update equation?

Student: (Refer Time: 01:16).

Is equal to.

Student: (Refer Time: 01:21).

Student: (Refer Time: 01:22).

That is I have, so at the position of the metal the electric field should be 0 as per the boundary conditions, but our update equation should also give me that. It should not be that the update equations are taking in some different directions. So, let us have a look at, so supposing I at some time instant time I put the electric field equal to 0 let us say at $t = 0$. I start my simulation, I put $t = 0$. It had better remain 0, right, to respect physics. Let us see if that is happening over here. So, what is the first term simply to?

Student: Minus (Refer Time: 02:00).

Minus.

Student: Minus.

Minus yeah right, so I will get $E^n = -E^{n-1}$ and that is it the term goes to 0 alright and so that I mean that is very helpful for me because if I initialize it at 0 on a PEC which is what it should be it continuous to be 0.

Student: So.

I do not need to explicitly.

Student: (Refer Time: 02:25).

Yeah, the update equation is automatically doing it for me right. So, in some sense what I am saying is that I do not need to explicitly keep running the update equations on the PEC locations, I can set it to 0 either I can set it to 0 at each step explicitly or I let the update equations run they will keep it at 0 ok. So, if we initialize E to be 0 on the PEC boundary it stays that way right.

So, PEC the PEC boundary condition is very trivially being satisfied. So, what we have looked at is two very very simple cases dielectric material plane I mean without loss and with loss. You know what to do we get an update equation and PEC also very simple to do ok.

(Refer Slide Time: 03:44)

2

Dealing with dielectric materials – simplistic

$\frac{\partial \vec{D}}{\partial t} = \nabla \times \vec{H}$, $\vec{D} = \epsilon \vec{E}$
 $\epsilon \vec{E} = \nabla \times \vec{H}$ → fixed appropriately in each Yee cell.

usual update equations.

deal with conductivity? $\nabla \times \vec{H} = \frac{\partial \vec{D}}{\partial t} + \vec{J}$

Ohm's law: $\vec{J} = \sigma \vec{E}$ $\nabla \times \vec{H} = \epsilon \frac{\partial \vec{E}}{\partial t} + \sigma \vec{E}$

Say want to update \underline{E}^n
Need E^{n-1} , $H^{n-1/2}$.

$\nabla \times H^{n-1/2} = \epsilon \frac{E^{n-1/2} - E^{n-3/2}}{\Delta t} + \sigma \frac{E^{n-1/2} + E^{n-3/2}}{2}$
 As before $\left(\frac{E^n - E^{n-1}}{\Delta t} \right)$ $\left(\frac{E^n + E^{n-1}}{2} \right)$
 FD Average

Yee cell, time & space update.

So, now let us let us actually ask I mean what I was hinting and that was at this equation over here that is something wrong with it ok. So now let us go a little bit deeper into that.

(Refer Slide Time: 03:49)

4

Dealing with dispersive dielectric materials

$\vec{D} \rightarrow$ time domain
 $\vec{D} \rightarrow$ freq domain.

$\vec{D}(\omega) = \vec{\epsilon}_r(\omega) \epsilon_0 \vec{E}(\omega)$ (freq domain). ← [x ch 9 of Griffiths book (FD)]

time domain $\left[D(t) = \epsilon_0 \int_{-\infty}^t E(t-\tau) \epsilon_r(\tau) d\tau \right]$ time picture. Now, I need full time history of \vec{E} to get \vec{D} .

0 due to causality

$\forall D(t) = \epsilon_r \otimes E(t)$, what is $\epsilon_r(t)$?
 $\epsilon_r(t) = \epsilon_r \delta(t)$
 \Rightarrow Instantaneous response (Unrealistic)

Yee cell, time & space update.

So, we all know that most natural materials are dispersive right. So, there is a part of this which I am not going to be able to derive over here its I will give you a reference for it. So, chapter 9 of Griffiths book on electrodynamics right, everyone has seen that, the blue color book right.

So, here he describes very properly what how do you model the dispersive medium using a simple spring and mass attached to it models. So, what is the spring and what is the mass? It is for example, an atom and the nucleus and the electrons or model has the mass right. So, there is a positively charged nucleus is an electron right there is some spring constant between them when an electromagnetic field falls on it there is a polarization there was slight going to as a force that is exerted on this mass.

So, when you put all the force equations together and work through it is a very elegant derivation which shows you that frequency, the frequency dependence of the refractive index it comes out over there. So, I will recommend that you read through it is just a few pages of a simple derivation, we will start with the conclusion of that the conclusion of this modeling the, so what is the spring model? Spring models resonances a spring is the most simplest model for a resonance we have all studied this for. For example, if a spring has no damping coefficient and if I excited once, so what happens? It keeps going on forever right, so the resonance.

So, the interaction of an electromagnetic wave with the material is also. There are various resonances, for example, in a microwave oven, what is the principle and there is water molecule it has a certain resonance I send an EM wave at that frequency and that resonance condition being met it excites that resonance and heats up the whatever material is there.

So, after having done all of that what you get? So the convention is, so far we have been using symbols like D we will say that this is the time domain picture and if I want to talk about its Fourier transform that is a spectral component I will write it as \tilde{D} ok, so this is the frequency domain ok. So, as a conclusion of this discussion in Griffiths what you get is that \tilde{D} , so it has to be as a function of ω is going is actually $\epsilon_0 \epsilon_r$ is vacuum right.

So, this relation that we have been blindly writing every time the $D = \epsilon E$ strictly speaking is true, but in the frequency domain not in the time domain ok. So, that is I mean because I am

not showing you the derivation from Griffiths it seems like where did this come from, but I mean we will assume it for now the moment you said dealing with realistic materials this relation $D = \epsilon E$ is incorrect to write in the time domain, the correct relation is only in the frequency domain ok.

$$\tilde{D}(\omega) = \tilde{\epsilon}_r(\omega) \epsilon_0 \tilde{E}(\omega)$$

So, this is just a fact that we will have to take it and go back and read this part. So, now, these are all so this is in the frequency domain. So, as a result of this what is actually our time domain relation then?

Student: Convolution.

Convolution right this is a product in frequency domain, so in time domain it is convolution. If I go over here to time domain this will become

$$D(t) = \epsilon_0 \int_{-\infty}^t E(t - \tau) \epsilon_r(\tau) d\tau$$

Convolution will go from $-\infty$ to some t right same t over here, I have $E(t - \tau) \epsilon_r(\tau) d\tau$, the simple signal and systems.

Student: (Refer Time: 08:22).

Well we will keep it t . So, for example, what about the fact that our material is causal? This causality has to be respected right, the D at a certain time should not depend on E at future time instance obviously. So, will any of these limits change?

Student: 0.

Right so, due to causality this will become 0 due to causality and for the same reason we are going to limit our upper limit to t right otherwise this will like E at future time instance will also come over here right. So, this is; so this is the true picture. So, when we have been writing that $D(t) = \epsilon_r \epsilon_0 E(t)$ in time domain what does it imply, what kind of ϵ_r satisfies that?

So, if $D(t) = \epsilon_r \epsilon_0 E(t)$, what is this value of $\epsilon_r(t)$ is it, under what condition will I get this very simple relation? Look at the convolution relation, rather we are just writing it like this right we have been writing it like this.

Student: Delta.

Delta function right. So,

$$\epsilon_r(t) = \epsilon_r \delta(t)$$

then this convolution gives me the simple relation right. So, in other words, this is a material that reacts instantaneously to the incident radiation because the response is. So, you can look at this convolution has also you know the convolution of an impulse response with the input right and so if the impulse response is a delta function; that means, the response is instantaneous right which is unrealistic.

Student: (Refer Time: 11:06).

No material can respond instantaneously to even a springs supposing you apply some force to it does not in one I mean there is no instantly start oscillating it take some time. Similarly, when you remove the forcing function it does not instantaneously stop it goes for a while and then stops right, so nothing is instantaneous in nature right. So, so this is what we have been using all along and we will now build a theory of what happens in realistic materials, this was not an issue for our case of yours integral equations because there I was dealing with single frequency.

So, I was anyway assuming $e^{j\omega t}$. So, I was implicitly working in the frequency domain and at I was using this relation without really realizing it and putting the value of epsilon at that frequency, so there was no problem there. The problem comes in now when I am explicitly in time domain I have to worry about what is the relation of D and E in time because our Maxwell's equations the way in the differential form they need time yeah.

So, this is let us assume that this is the main equation that we have to work with. So, let us try to just think of what are the challenges that will come when we are trying to implement this

equation in FDTD. So, you remember your Yee cell there is an update in time, there is an update in space right.

So, there is Yee cell time and space update. So, for example, in this previous here this equation over here to calculate E^n , how many passed values of E^i do I need to store only one previous time instant and only one previous time instant of magnetic field, you do not see E^0 , E^1 , R^2 , E^3 over here in this relation.

So, what does that tell you in terms of the memory requirements of my computation? I do not need to store the history of fields I just need even if I wanted to for some plotting or something then yes, but I do not need it to calculate future time instance right; however, does this now tell you something else?

So, if I were to just discretize this equation over here τ is going from 0 to t , so if I want D at a certain time t I need electric field not only at that time instant, but I need the entire history otherwise how will I calculate D at that time instant right. So, now, I need full time history of electric field to get displacement field.

Student: (Refer Time: 14:00).

I need everything before otherwise how will I calculate this integral right. So, is that a problem? That is a huge problem because this is needed not just I mean this is needed at every point on the Yee grid not just at one point you need it in all points has space you need to store the entire electric field history for all time right, so that is that is impractical. So, just looking at this you would just give up on FDTD because it is not possible to store so much, you will only be able to run your simulation for so much time and then you will run out of time right.

So, so what you do in you have faced with such a situation? As an engineer, what would you do?

Student: Reduce the number (Refer Time: 23:00).

Reduce the number of time history.

Student: The time.

That is one way of dealing with it. So, you will face some approximation error, anything else that you can do deal with?

Student: (Refer Time: 15:38).

It looks like a numerical.

Student: (Refer Time: 15:42).

Numerical quadrature is a way of implementing this integral, but that is not gone help you this integration is not challenging.

Student: (Refer Time: 15:409).

Yeah.

Student: (Refer Time: 15:54).

So you can think of applying quadrature rule over here.

Student: (Refer Time: 16:00).

Yeah, but then that works quadrature rule works when the polynomial or function that you are trying to integrate is well behaved right, it should be it will be accurate up to polynomial degree of so much depending on how many points and you do not know you do not know how jumpy this electric field is going to be.

Student: The error increase.

The error will keep increasing right. For example, if an electric field is a sine wave how many polynomials you need to represent a sine wave right a very large amount and finally, it does not converge. So, what we will do is we will assume a simplistic model rather than compromising on the calculation we will assume a simplistic model of this frequency dependence of permittivity and see if we can if that saves us from saving the entire time history. So, our objective is to model a dispersive material realistically at the same time not

have to store the entire field history, if we can achieve these then I can apply FDTD to dispersive materials.

So, the entire field of things like plasmonics and all where then they critically depends on frequency dependence of permittivity needs us to be able to model it right. So, general a very general model of this epsilon r as a function of frequency is what is discussed in this chapter 9 as a summation of various resonances. So, after this class please go back and have a look at it what we will do is we will assume a simple version of that and it is something which you will all have studied. If you put epsilon r of tau equal to 0, but I mean.

Student: (Refer Time: 17:44).

The material the electric field is always there. ϵ_r is telling you the response of the material to that field you cannot.

Student: So if its non zero and only are expressed by.

It will be not be non zero anywhere because as long as there is a field this response is always going to be there. So, it is not going to be 0 its not in your hand its physical, its nature property, so on my hand. So, the simplest model is actually something that you have seen you have heard of Drude model.

Student: Lorentzian

You have heard of Lorentzian models, you heard of Debye models.