

Computational Electromagnetics
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FDTD: Materials and Boundary Conditions
Lecture - 13.04
Debye Model - Part 2

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Every Yee cell has its own value of $\epsilon_r(\omega)$

Plugging the dispersive relation into FDTD

$$\frac{D^n - D^{n-1}}{\Delta t} = \nabla \times H^{n-1/2}$$


$$D^n = \epsilon_0 \left[\epsilon_\infty E^n + \underbrace{E^n \bar{\beta}^0 + E^{n-1} \bar{\beta}^1 + \dots + E^1 \bar{\beta}^{n-1}}_{n \text{ terms}} \right]$$

$$D^{n-1} = \epsilon_0 \left[\epsilon_\infty E^{n-1} + \underbrace{E^{n-1} \bar{\beta}^0 + \dots + E^1 \bar{\beta}^{n-2}}_{(n-1) \text{ terms}} \right]$$

$$\Rightarrow D^n - D^{n-1} = \epsilon_0 \left[\epsilon_\infty (E^n - E^{n-1}) + E^n \bar{\beta}^0 + \sum_{m=0}^{n-2} E^{n-1-m} (\bar{\beta}^{m+1} - \bar{\beta}^m) \right] = \Delta t [\nabla \times H^{n-1/2}]$$

Update eqn: $E^n = \left[\frac{\epsilon_\infty}{\epsilon_\infty + \bar{\beta}^0} \right] \left[E^{n-1} - \frac{1}{\epsilon_\infty} \bar{\Psi}^{n-1} + \frac{\Delta t}{\epsilon_0 \epsilon_\infty} \nabla \times H^{n-1/2} \right]$

present past



So, we will continue our discussion of how to incorporate dispersive materials into FDTD. So, so far what we did was, we started with the Debye model and one thing I want to clarify is that every Yee cell has its own value of ϵ_r . ok. So, this has to be kept in mind in the data structures you need to have an elaborate data structure that stores.

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Dispersive materials - Debye model (approximation)

High freq static relaxation time.

$$\tilde{\epsilon}_r(\omega) = \epsilon_\infty + (\epsilon_s - \epsilon_\infty) \frac{1}{1 + j\omega\tau}$$

(approximation)

IFT

$$\epsilon_r(t) = \left\{ \epsilon_\infty \delta(t) + \left(\frac{\epsilon_s - \epsilon_\infty}{\tau} \right) e^{-t/\tau} U(t) \right\}$$

Unit step.

$$\beta(t) = \left(\frac{\epsilon_s - \epsilon_\infty}{\tau} \right) e^{-t/\tau} U(t)$$

Cocts.

$$D(t) = \epsilon_\infty \int_0^t E(t-\tau) \epsilon_r(\tau) d\tau$$

Discrete

$$D^n = \epsilon_\infty \left[\epsilon_\infty E^n + \sum_{m=0}^{n-1} E^{n-m} \int_{m\Delta t}^{(m+1)\Delta t} \beta(\tau) d\tau \right]$$

$\bar{\beta}^m$

So, for example, what all numbers will you have to store? For every Yee cell you will have to store $\epsilon_\infty, \epsilon_s, \tau$ ok. These are three it is a three parameter model. So, what we did was we took this Debye model we took its inverse Fourier transform and substituted it into the relation for D to obtain D in the time domain. Once I get D in the time domain, I can take finite differences and use Maxwell's equations over here. The whole reason that we were trying to do this is, somehow we want to avoid having to store the entire field history right; right now the expression that I have over here this expression does not avoid that.

Because electric field for all the past time instances is still being stored ok. So, let us see now, what we can do with this expression ok. So, what follows now is, little bit of algebra only ok. Now, to make this whole math a little bit easier, I am going to define a new auxiliary variable ok. So, this entire summation over here that you see ok, I am going to call it by new variable Ψ^{n-1} just for convenience ok.

$$\Psi^{n-1} = \sum_{m=0}^{n-2} E^{n-1-m} (\bar{\beta}^{m+1} - \bar{\beta}^m)$$

And then what I can do is, in an update equation, what do I want? I want the relation for E^n in terms of everything else, that has been the philosophy of FDTD right. So, this $D^n - D^{n-1}$, I am not interested in D, I want relation between E and H. So, I use Maxwell's equation and

what should I replace this by? So, this is $D^n - D^{n-1}$, it should get replaced by $\nabla \times H$ and a Δt right. So, this should be equal to $\Delta t \nabla \times H^{n-1/2}$ right.

So, it is just the difference $D^n - D^{n-1}$. So, from this entire expression, I can extract, what do I want to extract? E^n , I want a relation for E^n in terms of all past electric field and magnetic field. So, can I do that? I can how many in this expression over here, how many places does E^n appear? 1, 2, 3 or many times, only once because, the summation never reaches, the m summation never reaches E^n . So, I can pull out E^n on one side; move everything else to the right hand side right. So, I can, I will this is a fairly simple manipulation. So, I will move this $\epsilon_0 \epsilon_\infty$ to the right hand side.

So, I will write down the final expression that you get,

$$E^n = [\epsilon_\infty / (\epsilon_\infty + \tilde{\beta}^0)] [E^{n-1} - (1/\epsilon_\infty) \bar{\Psi}^{n-1} + (\Delta t / \epsilon_0 \epsilon_\infty) \nabla \times H^{n-1/2}]$$

So, you can see part of the reason why I introduce this Ψ , just to make this expression look a little bit compact. Otherwise, it will look very ugly. So, from the FDTD philosophy, I have let us say present and this whole thing is past. So, the philosophy in FDTD has been use the past to get to the present and time step.

So, still this is not something I can implement on code because, the term over here which is very difficult for me is, this guy Ψ^{n-1} right; Ψ^{n-1} is has the sum of all past electric field which I do not want. So, now, let us try a little bit more of algebra to see how we can simplify things further.

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So, let us see still need that is what we have. So, in Ψ^{n-1} , you notice that there is a $\bar{\beta}^{m+1} - \bar{\beta}^m$ correct this expression over here.

So, I am going to call this term over here as another there are many many simplifications that we need to do. So, I am going to call this $\Delta\beta^m$. why is it Ψ^{n-1} you mean.

Student: (Refer Time: 05:56) minus (Refer Time: 05:58) psi bar.

So, this $\Delta\beta^m$, we wrote it as this $\Delta\beta^m = \bar{\beta}^{m+1} - \bar{\beta}^m = \int_{(m+1)\Delta t}^{(m+2)\Delta t} \beta(t) dt - \int_{m\Delta t}^{(m+1)\Delta t} \beta(t) dt$

So, our $\beta(t)$ expression, which I will just write down from earlier was $\beta(t) = ((\epsilon_s - \epsilon_\infty)/\tau) e^{-t/\tau} U(t)$.

So, does this look like an integral that I can do? Looks straight forward right does not look very complicated at all. So, its just an exponential right. So, I can integrate it, how many terms do you expect will happen?

Student: Four.

Four terms each exponential when I integrate, I will get an exponential the two the limits will give me two terms.

Student: (Refer Time: 08:36).

And there will be one common.

Student: Yeah.

$m+1$ right. So, I should expect three terms right; in the when I evaluate this integral ok, this just to anticipate what happens. So, this expression let me write it.

$$\Delta\beta^m = -\tau((\epsilon_s - \epsilon_\infty)/\tau)(1 - 2e^{-\Delta t/\tau} + e^{-2\Delta t/\tau})e^{-m\Delta t/\tau}$$

So, I have taken care of all four terms combined into three terms ok. So, this is $\Delta\beta^m$. So, what after doing all of this what is interesting to note is where is m appearing in this expression? I have so many terms, but m is appearing only in only one term over here, this is the only place where m appears right. So, in other words if I look at this, if I look at $\Delta\beta^m$, the m term is only appearing here supposing I want to calculate $\Delta\beta^{m+1}$ then, what will happen? There will only be a $m+1$.

So, what do these $\Delta\beta$ s resemble? What kind of series does it look like? Geometric progression, every term is obtained by multiplying just one constant term to it right. So, in other words these $\Delta\beta^m$ s resemble a geometric progression and that is a thing that is going to help us a lot because, we know that the ratio of consecutive terms of a GP is constant right independent of m . So, if I look at $\Delta\beta^{m+1}/\Delta\beta^m$, what should this ratio be?

$$\Delta\beta^{m+1}/\Delta\beta^m = e^{-\Delta t/\tau}$$

Student: (Refer Time: 11:40).

Yeah, m should not be there ok. So now, I can write down the expression for Ψ^{n-1} I can write it as

$$\Psi^{n-1} = E^{n-1}\Delta\beta^0 + \sum_{m=1}^{n-2} E^{n-1-m}\Delta\beta^m$$

So, I want to utilize this observation that I have over here. I have not done anything great so far ok. Now, in this summation, what I can do is I can introduce a new summation variable instead of, see this in the summation for Ψ^{n-1} , my m is going from 0 to something and the way that I have written it over here now m is going from 1 to something.

If I want to bring it back down to 0, I need to introduce a new variable. So, let us call it $p = m - 1$ right.

$$\Psi^{n-1} = E^{n-1} \Delta\beta^0 + \sum_{p=0}^{n-3} E^{n-2-p} \Delta\beta^{p+1} = E^{n-1} \Delta\beta^0 + \sum_{p=0}^{n-3} E^{n-2-p} \Delta\beta^p (e^{-\Delta t/\tau})$$

So, this term can be taken outside the summation so, since it does not depend on p right. So, this guy can be taken out over here. Now, as the final step, I can go back to my supposing I go back to my, well I do not need to go back. So, now, over here I can replace, need not replace it. So, what does my expression become?

$$\Psi^{n-1} = E^{n-1} \Delta\beta^0 + (e^{-\Delta t/\tau}) \sum_{p=0}^{n-3} E^{n-2-p} \Delta\beta^p$$

Does anyone recognize what this expression on the right looks like particularly this expression. Look at this expression and this expression, is there something common? It is

$$\Psi^{n-2} = \sum_{p=0}^{n-3} E^{n-2-p} \Delta\beta^p$$

$$\Psi^{n-1} = E^{n-1} \Delta\beta^0 + e^{-\Delta t/\tau} \Psi^{n-2}$$

Is it clear what we did? And what was key to this was the geometric progression, it allowed me to just remove one term and make it look like the previous term Ψ^{n-2} ok.

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$$\Psi^{n-1} = \epsilon \Delta \beta^{n-1} + e^{-\Delta t/c} \Psi^{n-2}$$

update eqn for Ψ

Final simplifications


So far we were storing E, H at x, t grids
 Now E, H, Ψ at x, t grids

+ No need to store entire history of E, H !
 - Store one new Aux variable, Ψ

Reduced a convolution integral to a running summation.

→ Assumption: Debye model
 others: Lorentzian resonances

MEEP
 ↓
 Ab Initio group at MIT
 Scheme, C++



So, let us write down this final expression once again and then we can see the implications of it. So, after doing all of this algebra can, what have we gained? So, when I look at this expression, I needed Ψ to evaluate Ψ^{n-1} , I needed all past electric fields. Now, when I look at this expression that has something changed one past and one.

Student: (Refer Time: 18:19).

And one Ψ also yeah. So, is that an improvement? Yeah. So, I do not need to so, I do not need to store all the electric fields, but I need to store one new variable which is Ψ . To evaluate Ψ^{n-1} , I only need Ψ^{n-2} ; I do not need $\Psi^{n-3}, \Psi^{n-4}, \dots \Psi^0$.

Student: (Refer Time: 18:45).

No. So, see so far what was so far ok so, so far we were storing, what all were we storing? We were storing the E's and the H at space and time grids. Now, what we have to do E, H and psi at space time grids. So, I have my computational load has increased by one more variable that I have to store. Now, if I initialize this Ψ properly, then every time I want to evaluate psi, I just need one past value. It is just like the electric field update, I need one past value of electric field one past value of magnetic field to get the current E and H, same thing is happening now my price is store one more auxiliary variable right.

So, the plus point is, no need to store entire history of E and H and the minus point is store one new Aux variable auxiliary variable what which is Ψ .

Student: (Refer Time: 20:15).

Yeah well how well once you initialize it. So, I mean you have the definition of Ψ over here right. So, you can see Ψ^{n-1} . So, for example.

Student: (Refer Time: 20:31).

Yes. So, I will you there is an. So, this is your new this is your update equation for update equation for Ψ . Yeah well how do I, no his question is how do I get Ψ in the first place? Yeah so, to get psi in the first place, I need electric fields and this expression over here in the green arrow. Once I get it once then I am done then I need to use this equation right. So, you can call this the, instead of update we can call this the initialization equation for Ψ and then this becomes the update equation for Ψ ok. So, what we have done as a result of this is, we have reduced a convolution integral to a running sum ok. Did we do any approximations to arrive at this? No.

So, this is as accurate as if you wanted to store all the electric field histories, there is no approximation made in going from electric field history from convolution to this running summation ok. So, the only price we have to pay is store yeah store one new variable and of course the so, this was the assumption was Debye model ok. There are other kinds of resonances possible so, for example, there are others are more general are Lorentzian resonances. So, in fact, the Griffiths reference which I give you derives a Lorentzian resonance.

So, they have their own update equations to get I mean they have their own algebra to get an update equation, but we will not deal with that in this (Refer Time: 23:01). So, I think this is a sort of a good point to tell you about introduce at least the name to you, there is a popular open source software in which you can solve FDTD equations ok, it is written for 1-D, 2-D, 3-D it is called MEEP ok, this is by the Ab Initio group at MIT, where I mean it is a very flexible and its open source. So, you know you can go and see how they have implemented

various update equations and all and it can handle of quite a variety of different resonances ok.

So, I mean it is used extensively for research purposes so just Google this name and you will find out how to do it ok. It is written in the basic language in which it have implemented it, is something which is not very common ok. It is a very peculiar language called Scheme ok. It is not a compiled language. So, unlike C or C++, it is not that you can compile it and then run it is like a little bit like python right it will go step by step, interpretable right. They also have a C++ interface, if you wanted speed ok, have a look at this software.