Computational Electromagnetics : Finite Difference Time Domain Methods – Materials and Boundary Conditions

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Topics in this module

1. Dealing with dielectric materials
2. Absorbing boundary conditions

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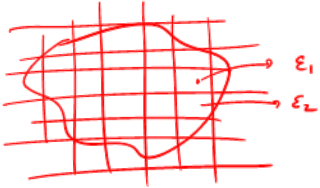
Dealing with dielectric materials – simplistic

↳ $\frac{\partial \bar{D}}{\partial t} = \nabla \times \bar{H}$, $\boxed{\vec{D} = \varepsilon \vec{E}}$

↳ $\varepsilon \dot{\vec{E}} = \nabla \times \bar{H}$

fixed appropriately in each Yee cell.

usual updat equations.



and μ's per Yee cell.

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

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

Say want to update E^n

Need E^{n-1}, $H^{n-1/2}$.

FDTD

↳ $$\underbrace{\nabla \times H^{n-\frac{1}{2}}}_{\text{as before}} = \varepsilon \underbrace{\dot{E}^{n-1/2}}_{\left(\frac{E^n - E^{n-1}}{\Delta t}\right)\ \text{FD}} + \sigma \underbrace{E^{n-1/2}}_{\left(\frac{E^n + E^{n-1}}{2}\right)\ \text{average}}$$

Dealing with PECs

to be evaluated. known

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

↳ 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.

Dealing with dispersive dielectric materials

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

$$\tilde{D}(\omega) = \tilde{\varepsilon}_r(\omega)\, \varepsilon_0\, \tilde{E}(\omega) \quad \text{(freq domain)}.$$

$\leftarrow$ [x ch 9 of Griffiths book (ED)]

Yee cell, time & space update.

time domain

$$\left[\, D(t) = \varepsilon_0 \int_{-\infty}^{t} E(t-\tau)\, \varepsilon_r(\tau)\, d\tau \,\right]$$

true picture.

Now, I need full time history of $\vec{E}$ to get $\vec{D}$.

$\dot{D} = \nabla \times \vec{H}$

$-\infty \rightarrow$ 0 due to causality

If $D(t) = \varepsilon_r\, \varepsilon_0\, E(t)$, what is $\varepsilon_r(t)$?

$$\varepsilon_r(t) = \varepsilon_r\, \delta(t)$$

$\Rightarrow$ Instantaneous response
(Unrealistic)

Dispersive materials – Debye model

(approximation)

High freq   static

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

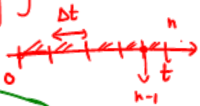
relaxation time.

IFT

$$\varepsilon_r(t) = \left\{ \varepsilon_\infty \delta(t) + \left[\left(\frac{\varepsilon_s - \varepsilon_\infty}{\tau}\right) e^{-t/\tau} u(t) \right] \right\}$$

$$\beta(t) = \frac{(\varepsilon_s - \varepsilon_\infty)}{\tau} e^{-t/\tau} u(t)$$

Unit step.



Conts. $\rightarrow$ $D(t) = \varepsilon_0 \int_0^t E(t-\tau)\, \varepsilon_r(\tau)\, d\tau$

Discrete $D^n = \varepsilon_0 \left[\varepsilon_\infty E^n + \sum_{m=0}^{n-1} E^{n-m} \underbrace{\int_{m\Delta t}^{(m+1)\Delta t} \beta(\tau)\, d\tau}_{\bar{\beta}^m} \right]$

Every Yee cell has it's own value of $\tilde{\varepsilon}_r(\omega)$

Plugging the dispersive relation into FDTD

$$\dot{D}^{n-1/2} = \nabla \times H^{n-1/2}$$

$$\frac{D^n - D^{n-1}}{\Delta t}$$

Subst

$$D^n = \varepsilon_0 \Big[\varepsilon_\infty E^n + \underbrace{E^n \bar{\beta}^0 + E^{n-1} \bar{\beta}^1 + \cdots + E^1 \bar{\beta}^{n-1}}_{n \text{ terms}} \Big]$$

$$D^{n-1} = \varepsilon_0 \Big[\varepsilon_\infty E^{n-1} + \text{—} + \underbrace{E^{n-1} \bar{\beta}^0 + \cdots + E^1 \bar{\beta}^{n-2}}_{(n-1) \text{ terms}} \Big]$$

$$\Rightarrow D^n - D^{n-1} = \varepsilon_0 \Big[\varepsilon_\infty (E^n - E^{n-1}) + E^n \bar{\beta}^0 + \underbrace{\sum_{m=0}^{n-2} E^{n-1-m} (\underbrace{\bar{\beta}^{m+1} - \bar{\beta}^m}_{\Delta\beta^m})}_{\Psi^{n-1}} \Big] = \Delta t \left[\nabla \times H^{n-1/2} \right]$$

Update eqn:

$$\underbrace{E^n}_{\text{present}} = \underbrace{\left[\frac{\varepsilon_\infty}{\varepsilon_\infty + \bar{\beta}^0} \right] \left[E^{n-1} - \frac{1}{\varepsilon_\infty} \Psi^{n-1} + \frac{\Delta t}{\varepsilon_0 \varepsilon_\infty} \nabla \times H^{n-1/2} \right]}_{\text{past}}$$

Final simplifications

Still need: $\bar{\Psi}^{n-1} = \sum_{m=0}^{n-2} E^{n-1-m} \Delta\beta^{m}$ ✓ Init eqn for Ψ

$$\Delta\beta^{m} = \bar{\beta}^{m+1} - \bar{\beta}^{m} = \int_{(m+1)\Delta t}^{(m+2)\Delta t} \beta(t)\,dt - \int_{m\Delta t}^{(m+1)\Delta t} \beta(t)\,dt$$

. Use $\beta(t) = \frac{\varepsilon_s - \varepsilon_\infty}{\tau} e^{-t/\tau} U(t)$

$$\Delta\beta^{m} = -\tau\left(\frac{\varepsilon_s - \varepsilon_\infty}{\tau}\right)\left(1 - 2e^{-\Delta t/\tau} + e^{-2\Delta t/\tau}\right)e^{-m\Delta t/\tau}$$

↑ where m appears

$\Delta\beta^{m}$'s resemble a geometric progression.

$$\left(\frac{\Delta\beta^{m+1}}{\Delta\beta^{m}} = e^{-\Delta t/\tau}\right) \Rightarrow \bar{\Psi}^{n-1} = E^{n-1}\Delta\beta^{0} + \underbrace{\sum_{m=1}^{n-2} E^{n-1-m}\Delta\beta^{m}}$$

$m-1 = p$

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

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

Final simplifications

$$\underline{\Psi}^{n-1} = \underline{E}^{n-1} \Delta\beta^{0} + e^{-\Delta t/\tau}\, \underline{\Psi}^{n-2}$$ ← update eqn for $\underline{\Psi}$

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

Now $E, H, \underline{\Psi}$ at x, t grids

+ No need to store entire history of E, H!

− Store one new Aux variable, $\underline{\Psi}$

Reduced a convolution integral to a running summation.

→ Assumption : Debye model.

others : Lorentzian resonances

MEEP

↓

Ab Initio group at MIT

Scheme, C++

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Introduction and 1D situation

ABC's come in 3 varieties (CEM in general)

1) Local ABC
2) Global ABC
3) Absorbing $\boxed{\text{media}}$ (PML - perfectly matched layers)

Engquist - Majda → 1st & 2nd order ABCs (1977)

G. Mur → FDTD (1981)

wave eqn $\quad \dfrac{\partial^2 E}{\partial x^2} = \dfrac{1}{c^2}\dfrac{\partial^2 E}{\partial t^2}$ ① $\rightarrow E \propto e^{j(kx \pm \omega t)}$

② $\left(\dfrac{\partial E}{\partial x} + \dfrac{1}{c}\dfrac{\partial E}{\partial t}\right) = 0$ and $\left(\dfrac{\partial E}{\partial x} - \dfrac{1}{c}\dfrac{\partial E}{\partial t}\right) = 0$ ③

$\downarrow$ $\qquad\qquad\qquad\qquad$ $\downarrow$

$E = e^{j(kx - \omega t)}$ ✓ $\qquad$ $E = e^{j(kx + \omega t)}$ ✓

$\downarrow$

Right hand side boundary

B

impose

$$\frac{\partial E}{\partial x} + \frac{1}{c}\frac{\partial E}{\partial t} = 0$$

perfect for 1D.

What happens in 2D?

2D wave

$e^{j(\omega t - k_x x - k_y y)}$

Impose $\frac{\partial E}{\partial x} + \frac{1}{c}\frac{\partial E}{\partial t} = 0$

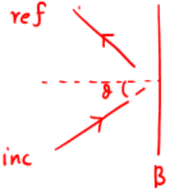
$-jk_x + j\frac{\omega}{c} \neq 0$

$\because k_x^2 + k_y^2 = (\omega/c)^2$

(numerical) —— unwanted.

$k_x = k\cos\theta$

$k_y = k\sin\theta$



Numerical

What is R?

(Refl coefficient)

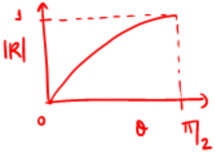
✓ inc: $e^{j(\omega t - k\cos\theta\, x - k\sin\theta\, y)}$

✓ ref: $Re^{j(\omega t + k\cos\theta\, x - k\sin\theta\, y)}$

tot = inc + ref. → BC → $\left(\frac{\partial}{\partial x} + \frac{1}{c}\frac{\partial}{\partial t}\right)(tot) = 0$

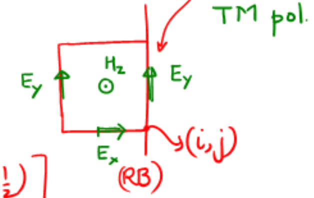
$(-k\cos\theta + Rk\cos\theta) + \frac{1}{c}(\omega + R\omega) = 0$

$\Rightarrow R = \frac{\cos\theta - 1}{\cos\theta + 1}$



Implementing in FDTD

Want to impose $\left[\frac{\partial}{\partial z} + \frac{1}{c}\frac{\partial}{\partial t}\right] E_y = 0$ in



↳ Could do BKWD differences, but error high.

↳ Compromise: use centre differences, but impose half a cell inside boundary.

$$\frac{\partial E_y}{\partial x} = \frac{1}{2}\left[\frac{E_y^{n+1}(i,j+\tfrac{1}{2}) - E_y^{n+1}(i-1,j+\tfrac{1}{2})}{\Delta x} + \frac{E_y^{n}(i,j+\tfrac{1}{2}) - E_y^{n}(i-1,j+\tfrac{1}{2})}{\Delta x}\right]$$

and

$$\frac{\partial E_y}{\partial t} = \frac{1}{2}\left[\frac{E_y^{n+1}(i,j+\tfrac{1}{2}) - E_y^{n}(i,j+\tfrac{1}{2})}{\Delta t} + \frac{E_y^{n+1}(i-1,j+\tfrac{1}{2}) - E_y^{n}(i-1,j+\tfrac{1}{2})}{\Delta t}\right]$$

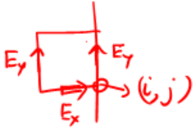
Adv: accurate to 2^{nd} order

Implementing in FDTD

Substituting to get update eqn for $E_y^{n+1}(i,j+1/2)$

$$E_y^{n+1}(i,j+1/2) = \gamma\, E_y^{n}(i,j+1/2) - \gamma\, \underbrace{E_y^{n+1}(i-1,j+1/2) + E_y^{n}(i-1,j+1/2)}_{\text{from usual update eqns.}}, \quad \gamma = \frac{1-\alpha}{1+\alpha}, \quad \alpha = \frac{c\Delta t}{\Delta x}$$

to get this, I need



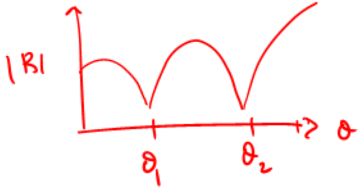
set $E_y^0 = 0$ initial condns.

reasonable in most cases.

Generalizing to higher order ABC? (Higdon)

$$\left(\frac{\partial}{\partial z} + \frac{1}{c}\frac{\partial}{\partial t}\right) E_y = 0 \quad \text{— } 1^{st} \text{ order ABC}$$

$$\left(\frac{\partial}{\partial z} + \frac{\cos\theta_1}{c}\frac{\partial}{\partial t}\right)\left(\frac{\partial}{\partial z} + \frac{\cos\theta_2}{c}\frac{\partial}{\partial t}\right) E_y = 0 \quad \text{— } 2^{nd} \text{ order ABC}$$



Topics that were covered in this module

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2. Absorbing boundary conditions

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)
* Interesting interview by Taflove on Maxwell's equations and FDTD: http://www.eecs.northwestern.edu/images/nphoton.2014.305.pdf