Numerical EM workshop

Tuesday, May 8, 2018 12:41 AM

Outline

1. Overview of numerical E&M
2. Revisit Maxwell's equations
3. Introduce finite difference, Yee's cell, and FDTD
4. Introduce FDFD
5. Modeling dispersive materials in FDTD
6. Adjoint variable method with FDFD
7. Brief introduction to other methods

Overview

FIRST RULE: No numerical method is omnipotent! ☆

Popular numerical methods

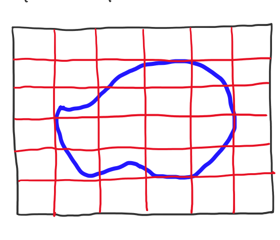
	Time domain	Frequency domain
Finite difference	FDTD Lumerical	FDFD Open source
Finite element	FETD Active research	FEM COMSOL

← simple in implementation

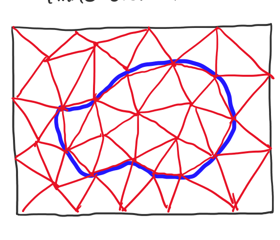
← good for curved surfaces

Consider a dielectric block:

Finite difference



Finite element



Finite difference methods

	FDTD	FDFD
Algorithm	simple	involved
Frequency response	one-shot	ω by ω
Steady state	slow	instant
Dispersive media	approximate	exact
Nonlinear optics	straight forward	recently developed

Revisit Maxwell's equations

$$\nabla \times E = -\mu \partial_t H$$
$$\nabla \times H = \epsilon \partial_t E + J$$

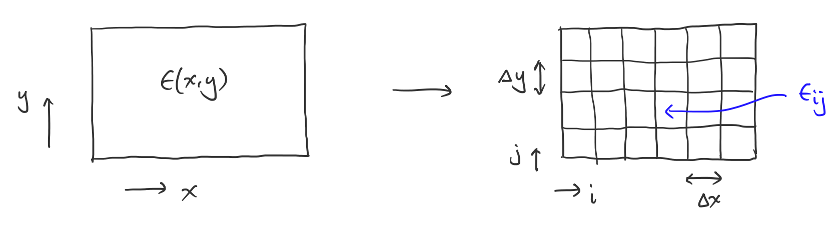
In 2D, we have TE, TM separation.

Consider TM (E_z, H_x, H_y).

$$\partial_t H_x = -\frac{1}{\mu} \partial_y E_z$$
$$\partial_t H_y = \frac{1}{\mu} \partial_x E_z$$
$$\partial_t E_z = \frac{1}{\epsilon}\left(\partial_x H_y - \partial_y H_x - J_z\right)$$

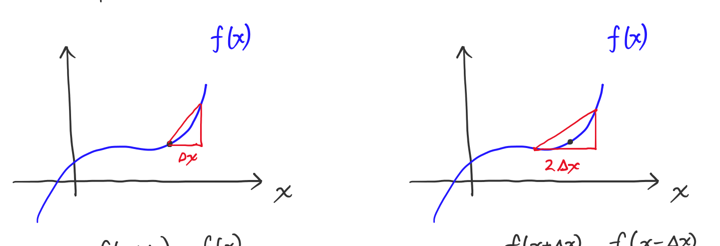
Finite difference

Continuous domain: $E_z, H_x, H_y \sim (x, y; t)$ Discrete domain: $E_z, H_x, H_y \sim [i, j; n]$



Next step: approximate $\partial_t, \partial_x, \partial_y$ with finite difference

Calc I: forward difference center difference



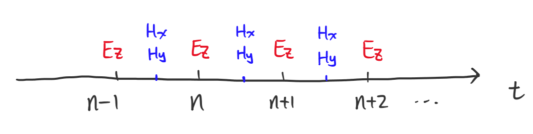
$$\partial_x f \approx \frac{f(x+\Delta x) - f(x)}{\Delta x} \qquad \partial_x f \simeq \frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x}$$

Converges as $\mathcal{O}(\Delta x)$ Converges as $\mathcal{O}(\Delta x^2)$

We would like to use center difference for $\partial_t, \partial_x, \partial_y$.

Center difference in time, ∂_t:

E_z and H_x, H_y are offset by HALF of a time step.



n-th time step:

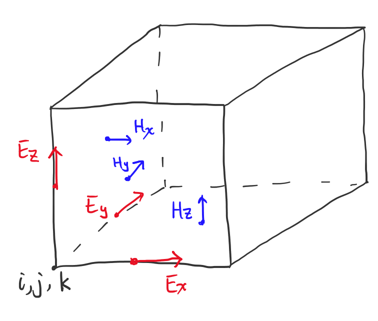
$$E_z|^n \,; \quad H_x|^{n+\frac{1}{2}}, \quad H_y|^{n+\frac{1}{2}}.$$

$$\partial_t E_z|^{n+\frac{1}{2}} = \frac{E_z|^{n+1} - E_z|^n}{\Delta t}$$

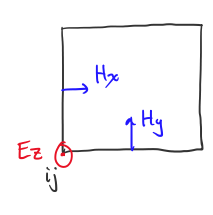
Update equations

$$E_z|^{n+1} = E_z|^n + \frac{\Delta t}{\epsilon}\left[\partial_x H_y - \partial_y H_x - J\right]^{n+\frac{1}{2}}$$
$$H_x|^{n+\frac{3}{2}} = H_x|^{n+\frac{1}{2}} + \frac{\Delta t}{\mu}\left[-\partial_y E_z\right]^{n+1}$$
$$H_y|^{n+\frac{3}{2}} = H_y|^{n+\frac{1}{2}} + \frac{\Delta t}{\mu}\left[\partial_x E_z\right]^{n+1}$$

Center difference in space – Yee's lattice



In 2D, the ij-th cell looks like



$E_z|_{ij}$ $H_x|_{i,j+\frac{1}{2}}$ $H_y|_{i+\frac{1}{2},j}$

Update equations:

$$E_z|^{n+1}_{ij} = E_z|^n_{ij} + \frac{\Delta t}{\epsilon}\left[\frac{H_y|^{n+\frac{1}{2}}_{i+\frac{1}{2},j} - H_y|^{n+\frac{1}{2}}_{i-\frac{1}{2},j}}{\Delta x} - \frac{H_x|^{n+\frac{1}{2}}_{i,j+\frac{1}{2}} - H_x|^{n+\frac{1}{2}}_{i,j-\frac{1}{2}}}{\Delta y} - J_z|^{n+\frac{1}{2}}_{ij}\right]$$

$$H_x|^{n+\frac{3}{2}}_{i,j+\frac{1}{2}} = H_x|^{n+\frac{1}{2}}_{i,j+\frac{1}{2}} - \frac{\Delta t}{\mu}\left[\frac{E_z|^{n+1}_{i,j+1} - E_z|^{n+1}_{i,j}}{\Delta y}\right]$$

$$H_y|^{n+\frac{3}{2}}_{i+\frac{1}{2},j} = H_y|^{n+\frac{1}{2}}_{i+\frac{1}{2},j} + \frac{\Delta t}{\mu}\left[\frac{E_z|^{n+1}_{i+1,j} - E_z|^{n+1}_{i,j}}{\Delta x}\right]$$

These are the internal update equations for FDTD!

Demonstration on MATLAB

Things that I will only briefly cover:

1. Boundary conditions:
   - PEC: set all $E_{\parallel} = 0$
   - PMC: set all $H_{\parallel} = 0$
   - Periodic: set $E_z(:, N_y) = E_z(:, 1)$
     $E_z(N_x, :) = E_z(1, :)$
     Likewise for H_x, H_y
   - Perfectly matched layers: pretty complicated
     - Developed in 1994
     - Absorbs waves with no reflection
2. Stability:
   $$\Delta t \leq \frac{1}{c_0} \cdot \frac{1}{\sqrt{\Delta x^{-2} + \Delta y^{-2}}} \quad \leftarrow \text{Courant stability condition}$$
3. Numerical dispersion.
   Take-away point: use at least about 20 cells / wavelength.
4. Sources
   - Point source
   - Line / modal source
   - Total-field scattered field: allows arbitrary incident waves.
5. Permittivity smoothing
   - results in intrinsically anisotropic permittivity grid.
6. Signal processing
   - Use Fourier transform to get spectral response.
7. Dispersive materials
   - Will be covered in part II of this session.

Alex will now cover the basics of FDFD

FDTD with dispersive materials

In nature, by necessity, materials exhibit refractive index dispersion.

$$D(\omega) = \epsilon(\omega) E(\omega) \quad \leftarrow \text{simple to model in FDFD}$$

However, how do we model this in FDTD?

$$D(t) = \epsilon(t) * E(t) = \int_{\tau=0}^{\infty} \epsilon(t-\tau) E(\tau)\, d\tau$$

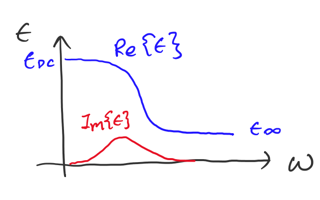
Requires the whole time history of E. Impractical.

Fortunately, there are efficient ways in numerical E&M to deal with them.

Common forms of dispersion:

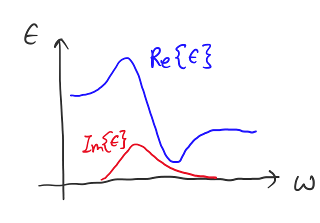
Debye model:

$$\epsilon(\omega) = \epsilon_0\left(\epsilon_\infty + \frac{\epsilon_{DC} - \epsilon_\infty}{1 + i\omega\tau_0}\right)$$



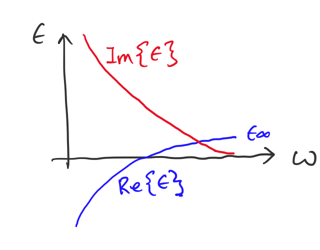
Lorentz model:

$$\epsilon(\omega) = \epsilon_0\epsilon_\infty + \epsilon_0 \frac{\omega_p^2}{\omega_0^2 - \omega^2 + i\omega\gamma_0}$$



Drude model:

$$\epsilon(\omega) = \epsilon_0\epsilon_\infty - \epsilon_0 \frac{\omega_p^2}{\omega^2 - i\omega\gamma_0}$$



Debye Model in FDTD

Instead of updating E, let us update D and see what happens

$$\nabla \times H = \frac{\partial D}{\partial t} + J$$
$$\nabla \times E = -\mu_0 \frac{\partial H}{\partial t}$$

n-th time step:

$$\left[\nabla \times H\right]^{n+\frac{1}{2}} = \frac{D|^{n+1} - D|^n}{\Delta t} + J|^{n+\frac{1}{2}}$$

$$D|^{n+1} = D|^n + \Delta t\left[\nabla \times H\right]^{n+\frac{1}{2}} - \Delta t\, J|^{n+\frac{1}{2}}$$

Now, we relate $D|^{n+1}$ to $E|^{n+1}$.

Note: in frequency domain,

$$D(\omega) = \epsilon(\omega) E(\omega) = \epsilon_0\epsilon_\infty E(\omega) + \epsilon_0 \frac{\epsilon_{DC} - \epsilon_\infty}{1 + i\omega\tau_0} E(\omega)$$

$$D(\omega) + i\omega\tau_0 D(\omega) = i\omega\tau_0\epsilon_0\epsilon_\infty E(\omega) + \epsilon_0\epsilon_{DC} E(\omega)$$

Fourier transform: $i\omega \leftrightarrow \partial_t$

$$D(t) + \tau_0 \frac{\partial D}{\partial t} = \tau_0\epsilon_0\epsilon_\infty \frac{\partial E}{\partial t} + \epsilon_0\epsilon_{DC} E(t)$$

Evaluate $\frac{\partial D}{\partial t}, \frac{\partial E}{\partial t}$ at the $n+\frac{1}{2}$ time step,

$$\frac{D|^{n+1} + D|^n}{2} + \tau_0 \frac{D|^{n+1} - D|^n}{\Delta t} = \tau_0\epsilon_0\epsilon_\infty \frac{E|^{n+1} - E|^n}{\Delta t} + \epsilon_0\epsilon_{DC} \frac{E|^{n+1} + E|^n}{2}$$

We already know $D|^{n+1}, D|^n, E|^n$, so we can solve for $E|^{n+1}$:

$$E|^{n+1} = \left[\frac{\Delta t + 2\tau_0}{2\tau_0\epsilon_0\epsilon_\infty + \epsilon_0\epsilon_{DC}\Delta t}\right] D|^{n+1} + \left[\frac{\Delta t - 2\tau_0}{2\tau_0\epsilon_0\epsilon_\infty + \epsilon_0\epsilon_{DC}\Delta t}\right] D|^n + \left[\frac{2\tau_0\epsilon_0\epsilon_\infty - \epsilon_0\epsilon_{DC}\Delta t}{2\tau_0\epsilon_0\epsilon_\infty + \epsilon_0\epsilon_{DC}\Delta t}\right] E|^n$$

Another example: Drude model.

Introduce auxillary fields – a more general way of treating dispersion.

$$D(t) = \epsilon_0\epsilon_\infty E(t) + P(t)$$

$$\left[\nabla \times H = \epsilon_0\epsilon_\infty \frac{\partial E}{\partial t} + J_p(t)\right]^{n+\frac{1}{2}}, \quad \text{where } J_p(t) = \frac{\partial P}{\partial t}$$

Freq domain:

$$P(\omega) = -\epsilon_0 \frac{\omega_p^2}{\omega^2 - i\omega\gamma_0} E(\omega)$$

$$J_p(\omega) = -i\omega\epsilon_0 \frac{\omega_p^2}{\omega^2 - i\omega\gamma_0} E(\omega)$$

$$\omega^2 J_p(\omega) - i\omega\gamma_0 J_p(\omega) = -i\omega\epsilon_0\omega_p^2 E(\omega)$$

$$i\omega J_p(\omega) + \gamma_0 J_p(\omega) = \epsilon_0\omega_p^2 E(\omega)$$

Time domain

$$\frac{\partial J_p}{\partial t} + \gamma_0 J_p(t) = \epsilon_0\omega_p^2 E(t)$$

$$\frac{J_p|^{n+1} - J_p|^n}{\Delta t} + \gamma_0 \frac{J_p|^{n+1} + J_p|^n}{2} = \epsilon_0\omega_p^2 \frac{E|^{n+1} + E|^n}{2}$$

Solve for $J_p|^{n+1}$:

$$J_p|^{n+1} = \left(\frac{2 - \Delta t\gamma_0}{2 + \Delta t\gamma_0}\right) J_p|^n + \left(\frac{\omega_p^2\epsilon_0\Delta t}{2 + \Delta t \cdot \gamma_0}\right)\left(\frac{E|^{n+1} + E|^n}{2}\right)$$
$$\equiv \alpha J_p|^n + \beta\left(\frac{E|^{n+1} + E|^n}{2}\right)$$

Need $J_p|^{n+\frac{1}{2}} = \frac{1}{2}\left(J_p|^{n+1} + J_p|^n\right)$:

$$J_p|^{n+\frac{1}{2}} = \frac{1}{2}\left((1+\alpha) J_p|^n + \beta\left(\frac{E|^{n+1} + E|^n}{2}\right)\right)$$

Now, we can explicitly write the update equation for $E|^{n+1}$ in the equation

$$\left[\nabla \times H\right]^{\frac{1}{2}} = \epsilon_0\epsilon_\infty \frac{E|^{n+1} - E|^n}{\Delta t} + J_p|^{n+\frac{1}{2}}$$

in other words, $E|^{n+1}$ is purely a function of the known quantities: $\left[\nabla \times H\right]^{\frac{1}{2}}, E|^n, J_p|^n$.