FDTD: Advances

- 2-D CN FDTD
- Let us consider TE^z case ($E_z=0$)

$$\frac{\partial E_x}{\partial t} = \frac{1}{\varepsilon}\frac{\partial H_z}{\partial y}$$

$$\frac{\partial E_y}{\partial t} = -\frac{1}{\varepsilon}\frac{\partial H_z}{\partial x}$$

$$\frac{\partial H_z}{\partial t} = \frac{1}{\mu}\left(\frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x}\right)$$

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$$\frac{\partial E_x}{\partial t} = \frac{1}{\varepsilon}\frac{\partial H_z}{\partial y}$$

Conventional FDTD

$$E_x^{n+1}\left(i+1/2,j\right) = E_x^{n}\left(i+1/2,j\right) + \frac{\Delta t}{\varepsilon \Delta y}\times$$

$$\left[H_z^{n+1/2}\left(i+1/2,j+1/2\right) - H_z^{n+1/2}\left(i+1/2,j-1/2\right)\right]$$

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$$\frac{\partial E_x}{\partial t} = \frac{1}{\varepsilon}\frac{\partial H_z}{\partial y}$$

$$E_x^{n+1}(i+1/2,j) = E_x^{n}(i+1/2,j) + \frac{\Delta t}{\varepsilon \Delta y}\times$$

$$\left[H_z^{n+1/2}(i+1/2,j+1/2) - H_z^{n+1/2}(i+1/2,j-1/2)\right]$$

CN FDTD

$$E_x^{n+1}(i+1/2,j) = E_x^{n}(i+1/2,j) + \frac{\Delta t}{2\varepsilon \Delta y}\times$$

$$\left[\begin{array}{l} H_z^{n+1}(i+1/2,j+1/2) + H_z^{n}(i+1/2,j+1/2) \\ -\left\{H_z^{n+1}(i+1/2,j-1/2) + H_z^{n}(i+1/2,j-1/2)\right\} \end{array}\right] \quad (1)$$

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$$\frac{\partial E_y}{\partial t} = -\frac{1}{\varepsilon}\frac{\partial H_z}{\partial x}$$

Conventional FDTD

$$E_y^{n+1}\left(i, j+1/2\right) = E_y^{n}\left(i, j+1/2\right) - \frac{\Delta t}{\varepsilon \Delta x} \times$$

$$\left[H_z^{n+1/2}\left(i+1/2, j+1/2\right) - H_z^{n+1/2}\left(i-1/2, j-1/2\right)\right]$$

FDTD: Advances

$$\frac{\partial E_y}{\partial t} = -\frac{1}{\varepsilon}\frac{\partial H_z}{\partial x}$$

$$E_y^{n+1}(i, j+1/2) = E_y^{n}(i, j+1/2) - \frac{\Delta t}{\varepsilon \Delta x} \times$$

$$\left[H_z^{n+1/2}(i+1/2, j+1/2) - H_z^{n+1/2}(i-1/2, j-1/2)\right]$$

CN FDTD

$$E_y^{n+1}(i, j+1/2) = E_y^{n}(i, j+1/2) - \frac{\Delta t}{2\varepsilon \Delta x} \times$$

$$\left[\begin{array}{l} H_z^{n+1}(i+1/2, j+1/2) + H_z^{n}(i+1/2, j+1/2) \\ -\left\{H_z^{n+1}(i-1/2, j-1/2) + H_z^{n}(i-1/2, j-1/2)\right\} \end{array}\right] \quad (2)$$

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$$\frac{\partial H_z}{\partial t} = \frac{1}{\mu}\left(\frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x}\right)$$

Conventional FDTD

$$H_z^{n+1}\left(i+1/2, j+1/2\right) = H_z^{n}\left(i+1/2, j+1/2\right)$$

$$+\frac{\Delta t}{\mu \Delta y}\left[E_x^{n+1/2}\left(i+1/2, j+1\right) - E_x^{n+1/2}\left(i+1/2, j\right)\right]$$

$$-\frac{\Delta t}{\mu \Delta x}\left[E_y^{n+1/2}\left(i+1, j+1/2\right) - E_y^{n+1/2}\left(i, j+1/2\right)\right]$$

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$$H_z^{n+1}\left(i+1/2, j+1/2\right) = H_z^{n}\left(i+1/2, j+1/2\right)$$
$$+\frac{\Delta t}{\mu \Delta y}\left[E_x^{n+1/2}\left(i+1/2, j+1\right) - E_x^{n+1/2}\left(i+1/2, j\right)\right]$$
$$-\frac{\Delta t}{\mu \Delta x}\left[E_y^{n+1/2}\left(i+1, j+1/2\right) - E_y^{n+1/2}\left(i, j+1/2\right)\right]$$

CN FDTD

$$H_z^{n+1}\left(i+1/2, j+1/2\right) = H_z^{n}\left(i+1/2, j+1/2\right)$$
$$+\frac{\Delta t}{2\mu \Delta y}\left[E_x^{n+1}\left(i+1/2, j+1\right) + E_x^{n}\left(i+1/2, j+1\right) - \left\{E_x^{n+1}\left(i+1/2, j\right) + E_x^{n}\left(i+1/2, j\right)\right\}\right]$$
$$-\frac{\Delta t}{2\mu \Delta x}\left[E_y^{n+1}\left(i+1, j+1/2\right) + E_y^{n}\left(i+1, j+1/2\right) - \left\{E_y^{n+1}\left(i, j+1/2\right) + E_y^{n}\left(i, j+1/2\right)\right\}\right]$$

(3)

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- In the CN update equations (1), (2) and (3),
  - the field components $E_x^{n+1}, E_y^{n+1}, H_z^{n+1}$ are coupled implicitly
- To decouple,
  - substitute equations (1) and (2) into equation (3)
- Denote

$$a_1 = \frac{\Delta t}{2\varepsilon}, a_2 = \frac{\Delta t}{2\mu}$$

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$$\left\{1-b^2\left(D_{2x}^{n+1}+D_{2y}^{n+1}\right)\right\}H_z^{n+1}\left(i+1/2,j+1/2\right)$$
$$=\left\{1+b^2\left(D_{2x}^{n}+D_{2y}^{n}\right)\right\}H_z^{n}\left(i+1/2,j+1/2\right)+f\left(E_x^n,E_y^n\right)$$

where

$$b=\frac{c\Delta t}{2}$$

$$D_{2x}^{i}=\frac{H_z^{n+1}\left(i+3/2,j+1/2\right)+H_z^{n+1}\left(i-1/2,j+1/2\right)-2H_z^{n+1}\left(i+1/2,j+1/2\right)}{\Delta x^2}$$

$$D_{2y}^{i}=\frac{H_z^{n+1}\left(i+1/2,j+3/2\right)+H_z^{n+1}\left(i+1/2,j-1/2\right)-2H_z^{n+1}\left(i+1/2,j+1/2\right)}{\Delta y^2}$$

$$f\left(E_x^n,E_y^n\right)=2a_2\frac{E_x^n\left(i+1/2,j+1\right)-E_x^n\left(i+1/2,j\right)}{\Delta y}-\frac{E_y^n\left(i+1,j+1/2\right)-E_y^n\left(i,j+1/2\right)}{\Delta x}$$

FDTD: Advances

- 3D CN FDTD (https://ieeexplore.ieee.org/document/1710457)
- Auxiliary Differential Equation (ADE) FDTD
- ***Digression:***
- The most well known material model is the **Lorentz model**
- Electron motion is described in terms of a
  - *driven, damped harmonic oscillator*
- We will assume that the charges are allowed to move
  - *in the same direction as the electric field*

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- The **Lorentz model** then describes the ***temporal response*** of a *component of the polarization field of the medium* to the *same component of the electric field* as

$$\frac{d^2}{dt^2}P_i + \Gamma_L \frac{d}{dt}P_i + \omega_0^2 P_i = \varepsilon_0 \chi_L E_i$$

- 1^{st} term: acceleration of charges
- 2^{nd} term: damping mechanism of the system with damping coefficient Γ_L (subscript L is for Lorentz)
- 3^{rd} term: restoring forces with the characteristic frequency $f_0=\omega_0/2\pi$

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- RHS term: driving term exhibits a coupling coefficient χ_L
- Frequency response for time harmonic fields with time dependence exp(+jωt) is given by

$$\frac{d^2}{dt^2}P_i + \Gamma_L \frac{d}{dt}P_i + \omega_0^2 P_i = \varepsilon_0 \chi_L E_i$$

$$P_i(\omega) = \frac{\chi_L}{-\omega^2 + j\Gamma_L\omega + \omega_0^2}\varepsilon_0 E_i(\omega)$$

- For small losses $\Gamma_L/\omega_0 << 1$, the response is clearly resonant at the natural frequency f_0

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- The polarization and electric fields are related to the ***electric susceptibility***

$$P_i(\omega)=\frac{\chi_L}{-\omega^2+j\Gamma_L\omega+\omega_0^2}\varepsilon_0 E_i(\omega)$$

$$\chi_{e,Lorentz}(\omega)=\frac{P_i(\omega)}{\varepsilon_0 E_i(\omega)}=\frac{\chi_L}{-\omega^2+j\Gamma_L\omega+\omega_0^2}$$

- Electric permittivity is obtained from electric susceptibility as

$$\varepsilon_{Lorentz}(\omega)=\varepsilon_0\left(1+\chi_{e,Lorentz}(\omega)\right)$$

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$$\frac{d^2}{dt^2}P_i + \Gamma_L \frac{d}{dt}P_i + \omega_0^2 P_i = \varepsilon_0 \chi_L E_i$$

- Special cases:
- **Debye model:** Acceleration term is small compared to others (subscript d is for Debye)

$$\Gamma_d \frac{d}{dt}P_i + \omega_0^2 P_i = \varepsilon_0 \chi_d E_i \qquad \chi_{e,Debye}(\omega) = \frac{P_i(\omega)}{\varepsilon_0 E_i(\omega)} = \frac{\chi_d}{j\Gamma_d \omega + \omega_0^2}$$

- **Drude model:** Restoring force is negligible (subscript d is for Debye)

$$\frac{d^2}{dt^2}P_i + \Gamma_D \frac{d}{dt}P_i = \varepsilon_0 \chi_D E_i \qquad \chi_{e,Drude}(\omega) = \frac{P_i(\omega)}{\varepsilon_0 E_i(\omega)} = \frac{\chi_L}{-\omega^2 + j\Gamma_D \omega}$$

- where the coupling frequency is generally represented by ***plasma frequency*** $\chi_D = \omega_p^2$

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- In all these models, at high frequency limit permittivity
  - reduces to that of the free space
- For linear materials, relationship between the *electric flux density* and *electric field phasor*,
  - valid at each frequency and at each point in space is

$$\mathbf{D}(\mathbf{r},\omega)=\varepsilon_c(\mathbf{r},\omega)\mathbf{E}(\mathbf{r},\omega)$$

- where complex permittivity ε_c may vary in space
- It is also often written as

$$\mathbf{D}(\mathbf{r},\omega)=\varepsilon_0\varepsilon_\infty\mathbf{E}(\mathbf{r},\omega)+\mathbf{P}(\mathbf{r},\omega)$$
$$\mathbf{D}(\mathbf{r},\omega)=\varepsilon_0\varepsilon_\infty\mathbf{E}(\mathbf{r},\omega)+\varepsilon_0\chi_e(\mathbf{r},\omega)\mathbf{E}(\mathbf{r},\omega)$$

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- where **P** is the polarization phasor
- χe is the electric susceptibility of the material
- ε_∞ is the relative permittivity at the upper end of the frequency band (usually 1 for all real materials, but FDTD simulation it may be taken as non-unit for artificial materials)
- ε_{dc} is the relative permittivity at the lower end of the frequency band
- Hence complex electric permittivity is related to electric susceptibility

$$\varepsilon_c(\omega) = \varepsilon_0 \left[\varepsilon_\infty + \chi_e(\omega) \right]$$

FDTD: Advances

- Debye materials

$$\varepsilon_c(\omega) = \varepsilon_0\left[\varepsilon_\infty + \chi_e(\omega)\right]$$

- which can be expressed as

$$\varepsilon_c(\omega) = \varepsilon_0\left[\varepsilon_\infty + \int_0^\infty \chi_e(t) e^{-j\omega t} dt\right]$$

- where $\chi_e(t)$ is some kind of decay factor
- Note that $\chi_e(t)$ should tends to zero for ω tending to infinity
- Since ω tending to infinity

$$\varepsilon_c(\omega) = \varepsilon_0[\varepsilon_\infty]$$

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- P. Debye gave a simple exponential model for decay factor as

$$\chi_e(t) = \chi_e(0) e^{-\frac{t}{\tau_0}} u(t)$$

- where *u(t)* is unit step function and τ_0 is the Debye relaxation time constant
- Hence, $\varepsilon_c(\omega) = \varepsilon_0 \left[\varepsilon_\infty + \int_0^\infty \chi_0(0) e^{\left(-j\omega - \frac{1}{\tau_0}\right)t} dt \right]$
- Therefore,

$$\varepsilon_c(\omega) = \varepsilon_0 \left[\varepsilon_\infty + \frac{\chi_e(0)}{\left(\frac{1}{\tau_0} + j\omega\right)} \right]$$

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- Therefore,

$$\chi_e(\omega)=\varepsilon_0\left[\varepsilon_\infty+\frac{\chi_e(0)\tau_0}{(1+j\omega\tau_0)}\right]$$

- We also have

$$\varepsilon_c(0)=\varepsilon_{dc}\varepsilon_0=\varepsilon_0\varepsilon_\infty+\varepsilon_0\chi_e(0)\tau_0 \qquad \varepsilon_c(\omega)=\varepsilon_0\left[\varepsilon_\infty+\frac{\chi_e(0)}{\left(\frac{1}{\tau_0}+j\omega\right)}\right]$$

- So,

$$\chi_e(0)=\frac{(\varepsilon_{dc}-\varepsilon_\infty)}{\tau_0}$$

- Finally,

$$\chi_{e,Debye}(\omega)=\varepsilon_0\left[\varepsilon_\infty+\frac{(\varepsilon_{dc}-\varepsilon_\infty)}{(1+j\omega\tau_0)}\right]$$

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- Therefore

$$\mathbf{D} = \varepsilon_c \mathbf{E}$$

$$\mathbf{D} = \varepsilon_0 \left[\varepsilon_\infty + \chi_e(\omega) \right] \mathbf{E}$$

$$\mathbf{D} = \varepsilon_0 \left[\varepsilon_\infty + \frac{\varepsilon_0 \left(\varepsilon_{dc} - \varepsilon_\infty \right)}{1 + j\omega\tau_0} \right] \mathbf{E}$$

- Simplifying

$$(1 + j\omega\tau_0)\mathbf{D} = \left(\varepsilon_0\varepsilon_\infty(1 + j\omega\tau_0) + \varepsilon_0(\varepsilon_{dc} - \varepsilon_\infty)\right)\mathbf{E}$$

- Finally

$$(1 + j\omega\tau_0)\mathbf{D} = \left(\varepsilon_0\varepsilon_\infty \times \quad j\omega\tau_0 + \varepsilon_0\varepsilon_{dc}\right)\mathbf{E}$$