

(lecture 4)

Flow of MEs

update \mathcal{B}

$$\vec{\nabla} \times \vec{E}(t) = -\frac{\partial}{\partial t} \vec{B}(t)$$

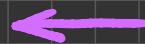
update H

$$\vec{B}(t) = \bar{\mu}(t) * \vec{H}(t)$$



$$\vec{D}(t) = \bar{\epsilon}(t) * \vec{E}(t)$$

update E



update D

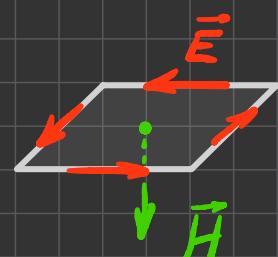
this is a
multiplication
in frequency
domain

Assume that our material is

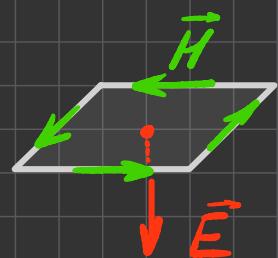
linear
isotropic
non-dispersive

$$\begin{aligned}\bar{\mu}^* &\rightarrow \mu \\ \bar{\epsilon}^* &\rightarrow \epsilon\end{aligned}$$

$$\vec{\nabla} \times \vec{E}(t) = -\mu \cdot \frac{\partial}{\partial t} \vec{H}(t)$$



$$\vec{\nabla} \times \vec{H}(t) = \epsilon \cdot \frac{\partial}{\partial t} \vec{E}(t) + \vec{J}(t)$$



Approximating time derivative

$$\vec{\nabla} \times \vec{E} = -\mu \frac{\partial}{\partial t} \vec{H} \longrightarrow -\frac{1}{\mu} \vec{\nabla} \times \vec{E}(t) \approx \frac{\vec{H}(t + \frac{\Delta t}{2}) - \vec{H}(t - \frac{\Delta t}{2})}{\Delta t}$$

$$\vec{\nabla} \times \vec{H} = \epsilon \frac{\partial}{\partial t} \vec{E} + \vec{J} \longrightarrow \frac{1}{\epsilon} \vec{\nabla} \times \vec{H}(t + \frac{\Delta t}{2}) \approx \frac{\vec{E}(t + \Delta t) - \vec{E}(t)}{\Delta t} + \vec{J}\left(t + \frac{\Delta t}{2}\right)$$

Update equations

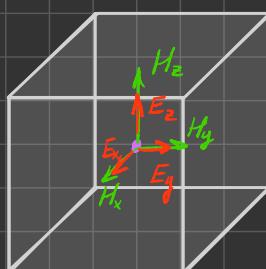
$$\vec{H}^{t+\frac{\Delta t}{2}} = \vec{H}^{t-\frac{\Delta t}{2}} - \frac{\Delta t}{\mu} \left[\vec{\nabla} \times \vec{E} \right]^t$$

$$\vec{E}^{t+\Delta t} = \vec{E}^t + \frac{\Delta t}{\epsilon} \left[\vec{\nabla} \times \vec{H} \right]^{t+\frac{\Delta t}{2}} - \frac{\Delta t}{\epsilon} \vec{J}^{t+\frac{\Delta t}{2}}$$

$\frac{\Delta t}{\epsilon}$, $\frac{\Delta t}{\mu}$ are update coefficients = const - will be calculated ahead of simulation.

lecture 5

Collocated grids - when \vec{E} and \vec{H} are defined at the same point in a grid cell



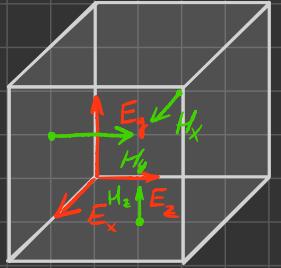
Staggered grids (Yee cell)

Physical

- BCs are naturally satisfied
- Gauss (\vec{D} and \vec{B}) laws are satisfied

$$\nabla \cdot \vec{D} = 0$$

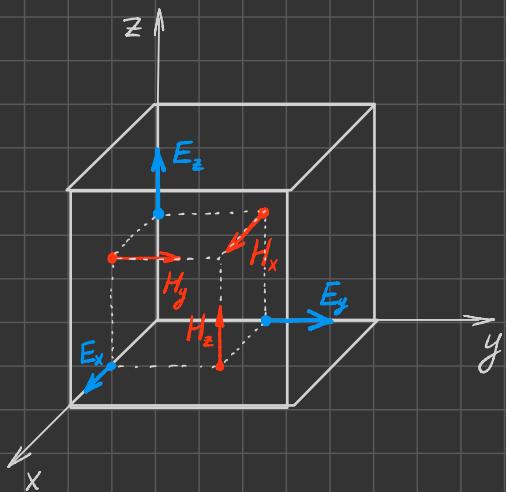
$$\nabla \cdot \vec{B} = 0$$



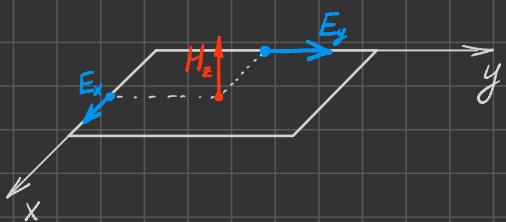
for divergence - free medium

Yee cell for 1D, 2D, and 3D

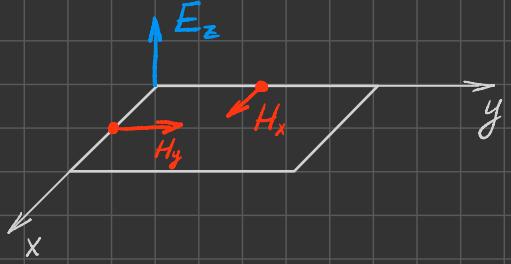
3D



2D



H_z mode

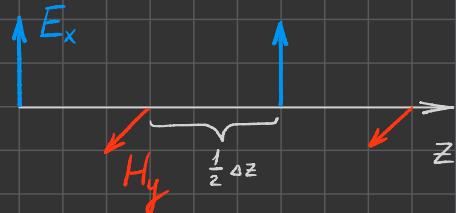


E_z mode

1D



E_y mode

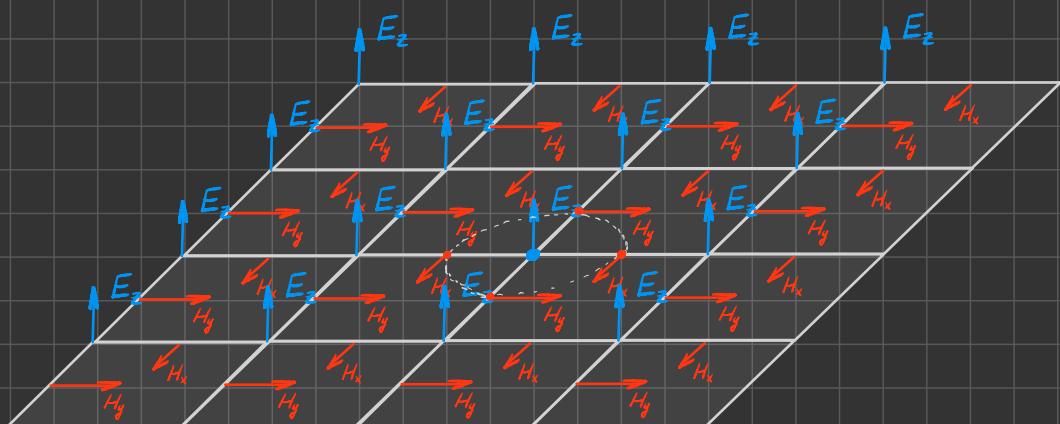


E_x mode

Consequences of Yee grid

- Field components E_x, E_y, E_z may reside in different materials even being in one cell.
- ! • Field components will be out of phase.

Example for 2D : 4×4 grid. E_z mode



FD approximation to MEs

1. We satisfied the divergence equations (Gauss's laws) automatically by adopting Yee's grid.

2. Normalization

$$H = \frac{1}{\gamma_0} E \quad , \quad \gamma_0 \equiv \sqrt{\frac{\mu_0}{\epsilon_0}} \simeq 377 \Omega$$

$$\Rightarrow E \simeq 377 H$$

i.e. magnitude of H is always 2-3 orders lower than of E . Thus, we will lose 2-3 digits of accuracy in numerical simulations.

Remedy is to normalize magnetic field H :

$$\tilde{H} \equiv \sqrt{\frac{\mu_0}{\epsilon_0}} H = \gamma_0 H$$

$$\vec{E} = \gamma_0 \vec{H} \equiv \tilde{H} \Rightarrow$$

\vec{E} and \tilde{H} have the same magnitude

Original magn. field

$$H \equiv \frac{1}{\gamma_0} \tilde{H}$$

Substitute it into Faraday's & Ampere's laws:

$$\left\{ \begin{array}{l} \vec{\nabla} \times \left(\frac{1}{\mu_0} \vec{H} \right) = \epsilon_0 \bar{\epsilon}_z \frac{\partial}{\partial t} \vec{E} + \vec{J} \\ \vec{\nabla} \times \vec{E} = -\mu_0 \bar{\mu}_z \frac{\partial}{\partial t} \left(\frac{1}{\mu_0} \vec{H} \right) - \vec{M} \end{array} \right.$$

$$\left\{ \begin{array}{l} \frac{1}{C_0} = \sqrt{\mu_0 \epsilon_0} \\ \vec{\nabla} \times \vec{H} = \frac{1}{C_0} \bar{\epsilon}_z \frac{\partial}{\partial t} \vec{E} + \gamma_0 \vec{J} \\ \vec{\nabla} \times \vec{E} = -\frac{1}{C_0} \bar{\mu}_z \frac{\partial}{\partial t} \vec{H} - \vec{M} \end{array} \right.$$

?

maybe this multiplication will be better included into Gaussian ?

We will omit \sim above \vec{H} keeping in mind that it's normalized and it will be denormalized for quantitative analysis.

$$\vec{\nabla} \times \vec{E} = -\frac{1}{C_0} \bar{\mu}_z \frac{\partial}{\partial t} \vec{H} - \vec{M}$$

$$\vec{\nabla} \times \vec{H} = \frac{1}{C_0} \bar{\epsilon}_z \frac{\partial}{\partial t} \vec{E} + \gamma_0 \vec{J}$$

Component-wise:

$$x: \partial_y E_z - \partial_z E_y = -\frac{1}{C_0} (\mu_{xx} \partial_t H_x + \mu_{xy} \partial_t H_y + \mu_{xz} \partial_t H_z) - M_x$$

$$y: \partial_z E_x - \partial_x E_z = -\frac{1}{C_0} (\mu_{yx} \partial_t H_x + \mu_{yy} \partial_t H_y + \mu_{yz} \partial_t H_z) - M_y$$

$$z: \partial_x E_y - \partial_y E_x = -\frac{1}{C_0} (\mu_{zx} \partial_t H_x + \mu_{zy} \partial_t H_y + \mu_{zz} \partial_t H_z) - M_z$$

$$x: \partial_y H_z - \partial_z H_y = \frac{1}{C_0} (\epsilon_{xx} \partial_t E_x + \epsilon_{xy} \partial_t E_y + \epsilon_{xz} \partial_t E_z) + \gamma_0 J_x$$

$$y: \partial_z H_x - \partial_x H_z = \frac{1}{C_0} (\epsilon_{yx} \partial_t E_x + \epsilon_{yy} \partial_t E_y + \epsilon_{yz} \partial_t E_z) + \gamma_0 J_y$$

$$z: \partial_x H_y - \partial_y H_x = \frac{1}{C_0} (\epsilon_{zx} \partial_t E_x + \epsilon_{zy} \partial_t E_y + \epsilon_{zz} \partial_t E_z) + \gamma_0 J_z$$

Assume we have only diagonally - anisotropic materials.

$$1 \quad \partial_y E_z - \partial_z E_y = -\frac{1}{C_0} \mu_{xx} \partial_t H_x - m_x$$

$$2 \quad \partial_z E_x - \partial_x E_z = -\frac{1}{C_0} \mu_{yy} \partial_t H_y - m_y$$

$$3 \quad \partial_x E_y - \partial_y E_x = -\frac{1}{C_0} \mu_{zz} \partial_t H_z - m_z$$

$$4 \quad \partial_y H_z - \partial_z H_y = \frac{1}{C_0} \epsilon_{xx} \partial_t E_x + \gamma_0 J_x$$

$$5 \quad \partial_z H_x - \partial_x H_z = \frac{1}{C_0} \epsilon_{yy} \partial_t E_y + \gamma_0 J_y$$

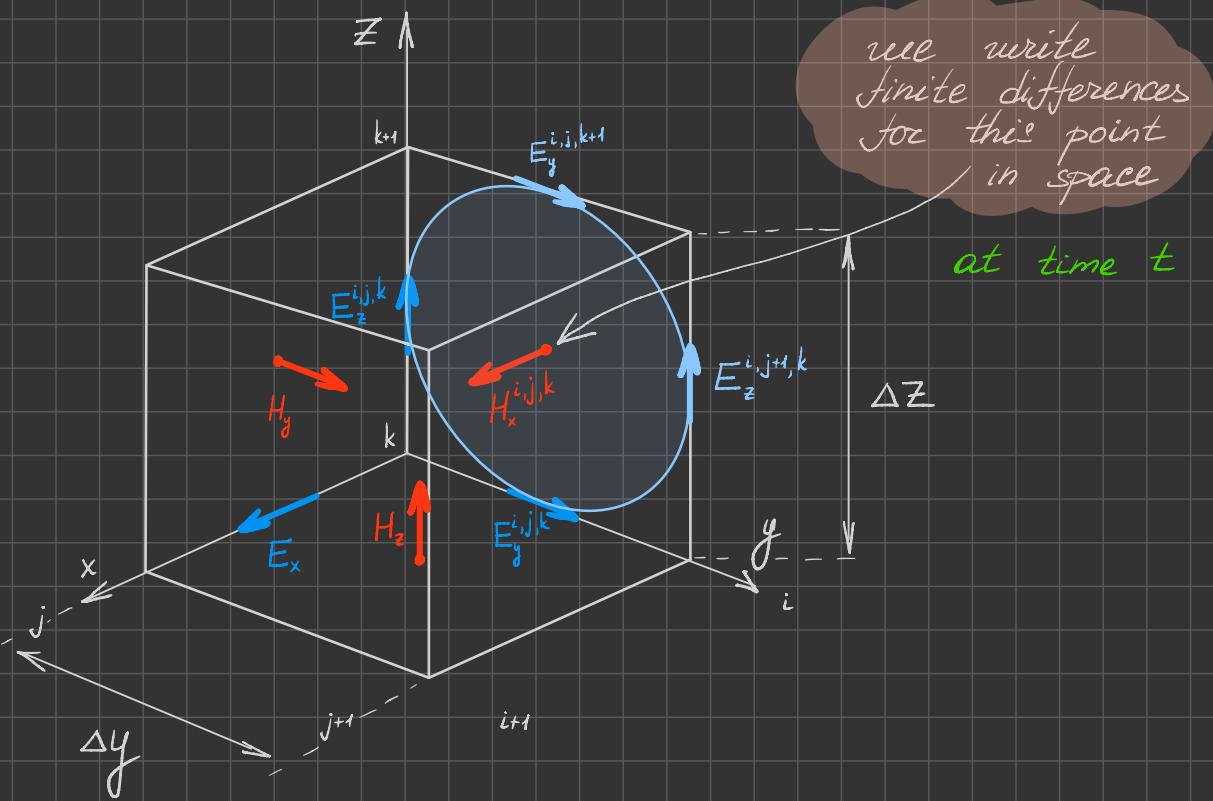
$$6 \quad \partial_x H_y - \partial_y H_x = \frac{1}{C_0} \epsilon_{zz} \partial_t E_z + \gamma_0 J_z$$

We will approximate these 6 equalities on the grid.

(next 6 pages)

1

$$\frac{\partial E_z}{\partial y} - \frac{\partial E_y}{\partial z} = -\frac{1}{c_0} \mu_{xx} \frac{\partial H_x}{\partial t} - m_x$$



we write
finite differences
for this point
in space

at time t

$$\frac{E_z^{i,j+1,k}|_t - E_z^{i,j,k}|_t}{\Delta y} - \frac{E_y^{i,j,k+1}|_t - E_y^{i,j,k}|_t}{\Delta z} = -\frac{1}{c_0} \mu_{xx}^{i,j,k} \frac{H_x^{i,j,k}|_{t+\frac{\Delta t}{2}} - H_x^{i,j,k}|_{t-\frac{\Delta t}{2}}}{\Delta t} - m_x^{i,j,k}|_t$$

μ components may also vary in space: $\mu_{xx} \rightarrow \mu_{xx}^{i,j,k}$

$$E_{xx} \rightarrow E_{xx}^{i,j,k}$$

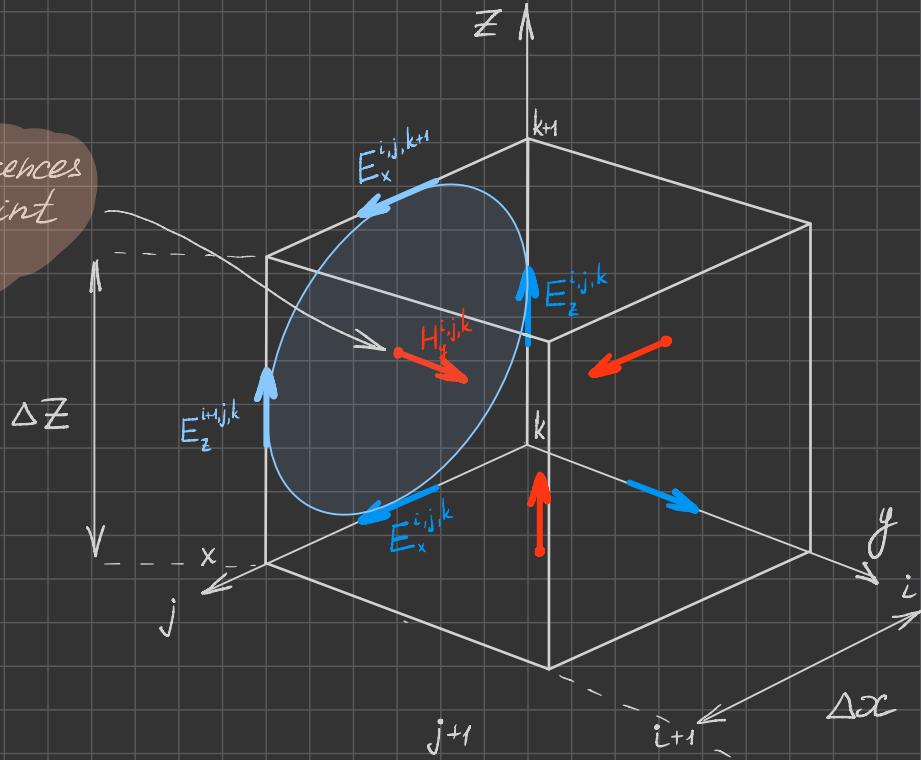
For the electric field derivative we need to reach to the next cells in space

2

$$\frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x} = -\frac{1}{C_0} M_{yy} \frac{\partial H_y}{\partial t} - M_y$$

finite differences
at this point
in space

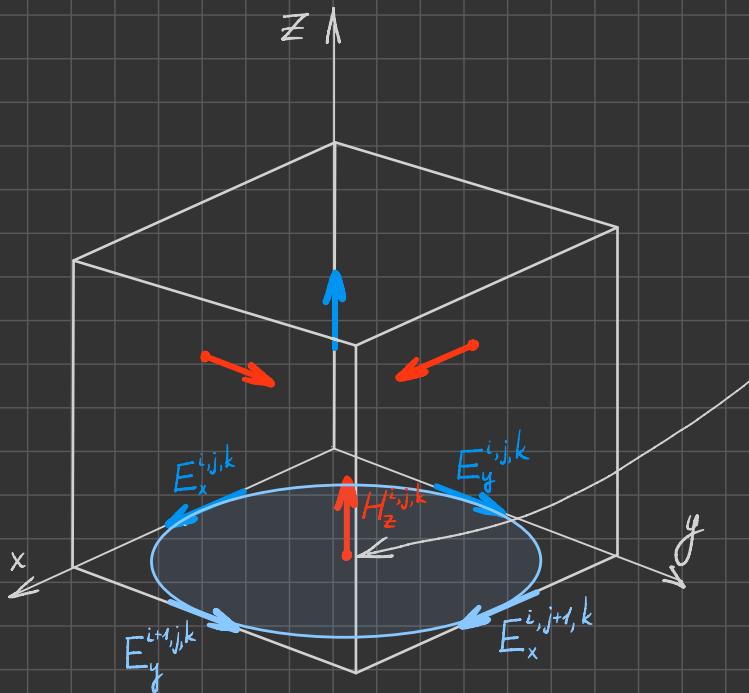
at time t



$$\frac{E_x^{i,j,k+1}|_t - E_x^{i,j,k}|_t}{\Delta z} - \frac{E_z^{i+1,j,k}|_t - E_z^{i,j,k}|_t}{\Delta x} = -\frac{1}{C_0} M_{yy}^{i,j,k} \frac{H_y^{i,j,k}|_{t+\frac{\Delta t}{2}} - H_y^{i,j,k}|_{t-\frac{\Delta t}{2}}}{\Delta t} - M_y^{i,j,k}|_t$$

3

$$\frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} = -\frac{1}{C_0} / \mu_{zz} \frac{\partial H_z}{\partial t} - M_z$$



we are approximating spatial derivatives at this point

at time t

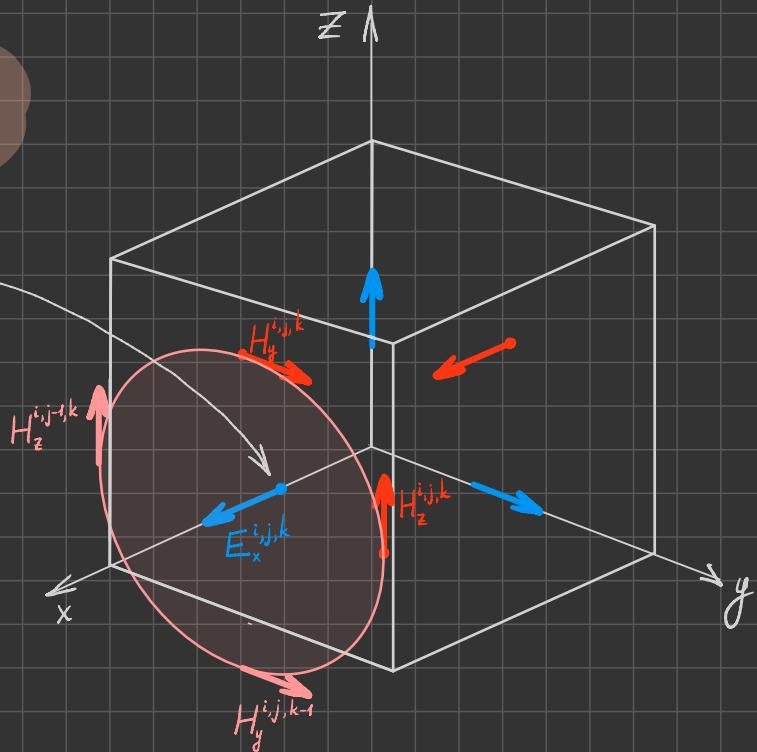
$$\frac{E_y^{i+1,j,k}|_t - E_y^{i,j,k}|_t}{\Delta x} - \frac{E_x^{i,j+1,k}|_t - E_x^{i,j,k}|_t}{\Delta y} = -\frac{1}{C_0} / \mu_{zz}^i \frac{H_z^{i,j,k}|_{t+\frac{\Delta t}{2}} - H_z^{i,j,k}|_{t-\frac{\Delta t}{2}}}{\Delta t} - M_z^{i,j,k}|_t$$

4

$$\partial_y H_z - \partial_z H_y = \frac{1}{C_0} \epsilon_{xx} \partial_z E_x + \gamma_0 J_x$$

finite difference equation is written for this point

at time $t + \frac{\Delta t}{2}$

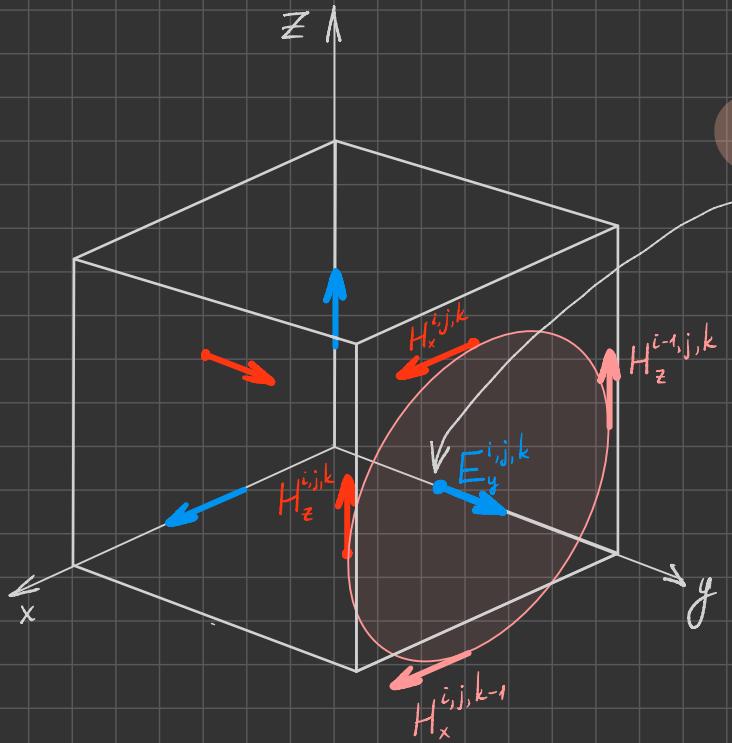


$$\frac{H_z^{i,j,k} \Big|_{t+\frac{\Delta t}{2}} - H_z^{i,j-1,k} \Big|_{t+\frac{\Delta t}{2}}}{\Delta y} - \frac{H_y^{i,j,k} \Big|_{t+\frac{\Delta t}{2}} - H_y^{i,j,k-1} \Big|_{t+\frac{\Delta t}{2}}}{\Delta z} = \frac{1}{C_0} \epsilon_{xx}^{i,j,k} \frac{E_x^{i,j,k} \Big|_{t+\frac{\Delta t}{2}} - E_x^{i,j,k} \Big|_t}{\Delta t} + \gamma_0 J_x^{i,j,k} \Big|_{t+\frac{\Delta t}{2}}$$

For magnetic field derivative we have to reach to the previous cell in space

5

$$\partial_z H_x - \partial_x H_z = \frac{1}{C_0} \epsilon_{yy} \partial_t E_y + \gamma_0 J_y$$



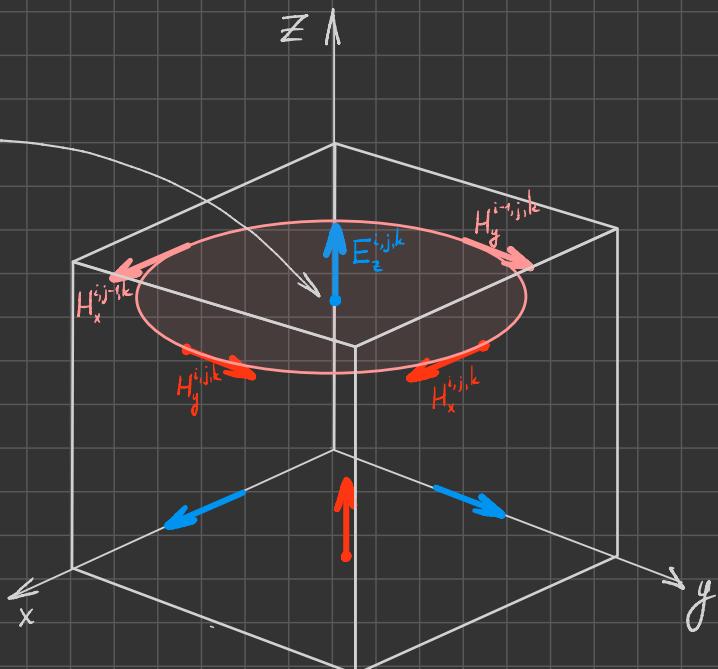
$$\frac{H_x^{i,j,k} \Big|_{t+\frac{\Delta t}{2}} - H_x^{i,j,k-1} \Big|_{t+\frac{\Delta t}{2}}}{\Delta z} - \frac{H_z^{i,j,k} \Big|_{t+\frac{\Delta t}{2}} - H_z^{i-1,j,k} \Big|_{t+\frac{\Delta t}{2}}}{\Delta x} = \frac{1}{C_0} \epsilon_{yy}^{i,j,k} \frac{E_y^{i,j,k} \Big|_{t+\Delta t} - E_y^{i,j,k} \Big|_t}{\Delta t} + \gamma_0 J_y^{i,j,k} \Big|_{t+\frac{\Delta t}{2}}$$

6

$$\partial_x H_y - \partial_y H_x = \frac{1}{C_0} \epsilon_{zz} \partial_z E_z + \gamma_0 J_z$$

we write
finite difference
equations at
this point

at time $t + \frac{\Delta t}{2}$



$$\frac{H_y^{i,j,k}|_{t+\frac{\Delta t}{2}} - H_y^{i-j,j,k}|_{t+\frac{\Delta t}{2}}}{\Delta x} - \frac{H_x^{i,j,k}|_{t+\frac{\Delta t}{2}} - H_x^{i,j-1,k}|_{t+\frac{\Delta t}{2}}}{\Delta y} = \frac{1}{C_0} \epsilon_{zz}^{i,j,k} \frac{E_z^{i,j,k}|_{t+\frac{\Delta t}{2}} - E_z^{i,j,k}|_t}{\Delta t} + \gamma_0 J_z^{i,j,k}|_{t+\frac{\Delta t}{2}}$$

For the same spatial cell electric J and magnetic H currents are also staggered in time $\frac{\Delta t}{2}$ apart. (J is $\frac{\Delta t}{2}$ ahead of H)

$$\frac{E_z^{i,j+1,k} - E_z^{i,j,k}}{\Delta y} - \frac{E_y^{i,j,k+1} - E_y^{i,j,k}}{\Delta z} = -\frac{1}{C_0} \mu_{xx}^{i,j,k} \frac{H_x^{i,j,k} \Big|_{t+\frac{\Delta t}{2}} - H_x^{i,j,k} \Big|_{t-\frac{\Delta t}{2}}}{\Delta t} - \mathcal{M}_x^{i,j,k} \Big|_t$$

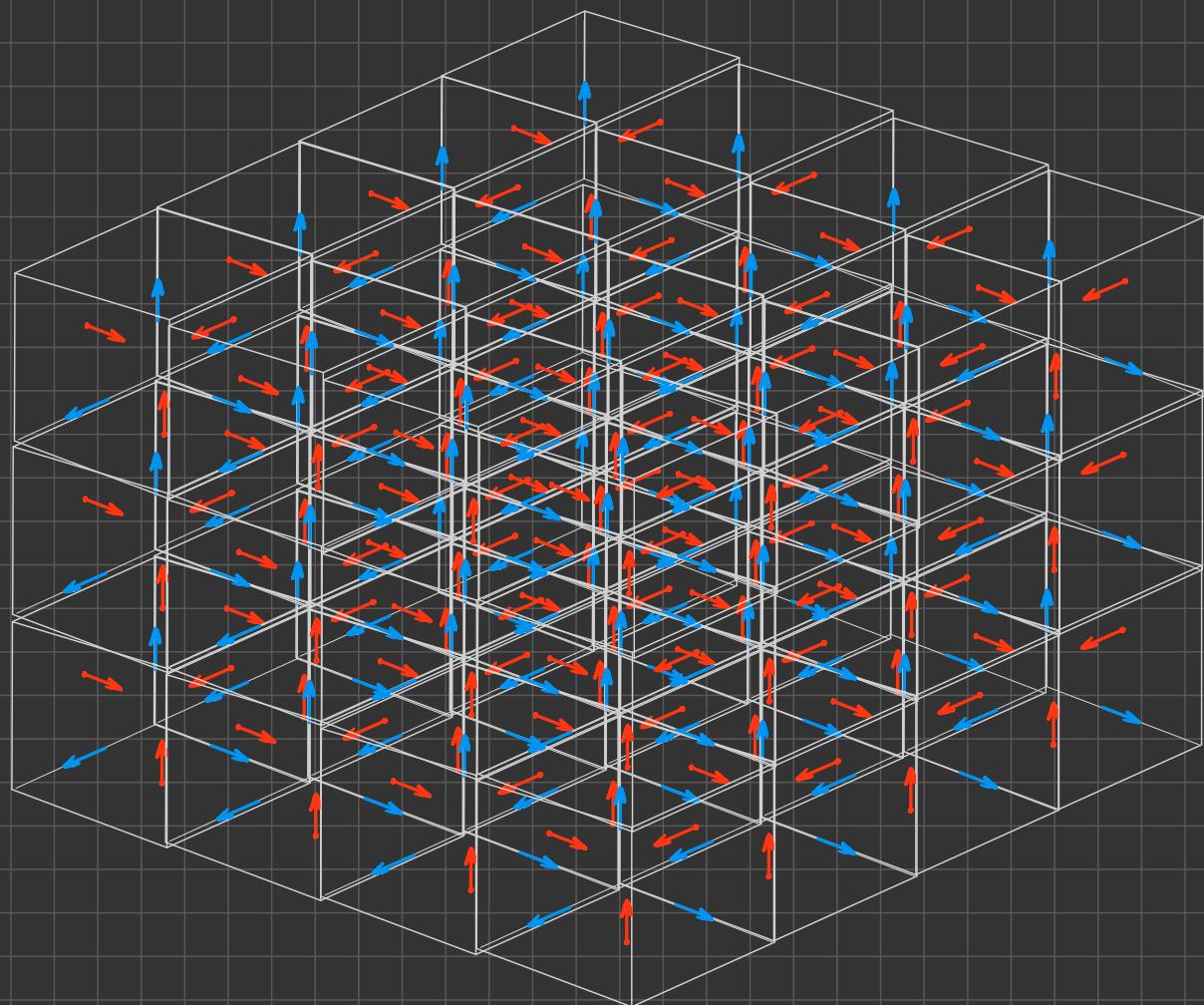
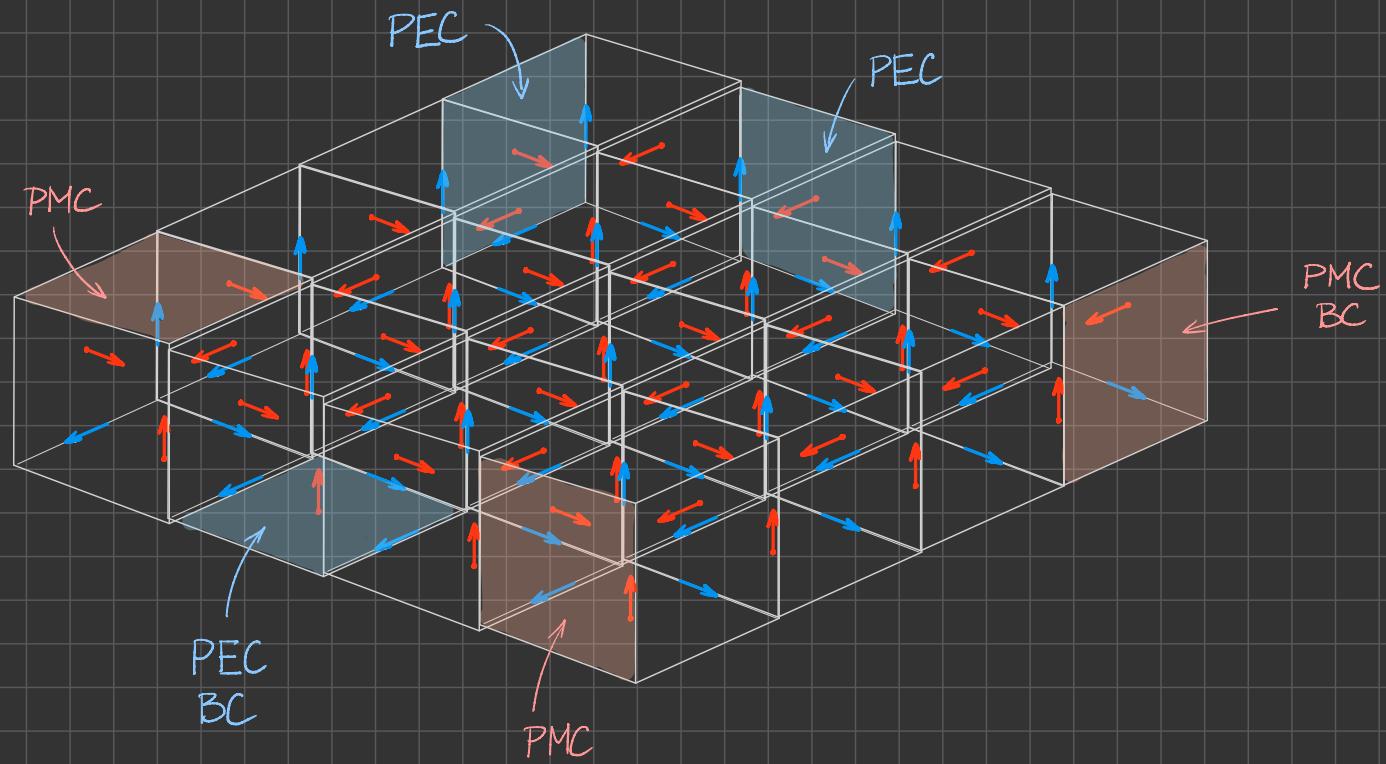
$$\frac{E_x^{i,j,k+1} - E_x^{i,j,k}}{\Delta z} - \frac{E_z^{i+1,j,k} - E_z^{i,j,k}}{\Delta x} = -\frac{1}{C_0} \mu_{yy}^{i,j,k} \frac{H_y^{i,j,k} \Big|_{t+\frac{\Delta t}{2}} - H_y^{i,j,k} \Big|_{t-\frac{\Delta t}{2}}}{\Delta t} - \mathcal{M}_y^{i,j,k} \Big|_t$$

$$\frac{E_y^{i+1,j,k} - E_y^{i,j,k}}{\Delta x} - \frac{E_x^{i,j+1,k} - E_x^{i,j,k}}{\Delta y} = -\frac{1}{C_0} \mu_{zz}^{i,j,k} \frac{H_z^{i,j,k} \Big|_{t+\frac{\Delta t}{2}} - H_z^{i,j,k} \Big|_{t-\frac{\Delta t}{2}}}{\Delta t} - \mathcal{M}_z^{i,j,k} \Big|_t$$

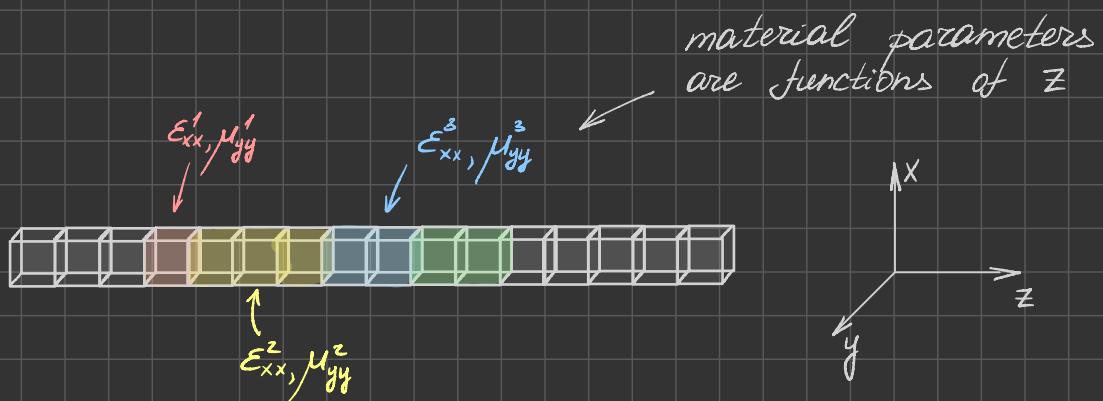
$$\frac{H_z^{i,j,k} \Big|_{t+\frac{\Delta t}{2}} - H_z^{i,j-1,k} \Big|_{t+\frac{\Delta t}{2}}}{\Delta y} - \frac{H_y^{i,j,k} \Big|_{t+\frac{\Delta t}{2}} - H_y^{i,j,k-1} \Big|_{t+\frac{\Delta t}{2}}}{\Delta z} = \frac{1}{C_0} \epsilon_{xx}^{i,j,k} \frac{E_x^{i,j,k} \Big|_{t+\Delta t} - E_x^{i,j,k} \Big|_t}{\Delta t} + \eta_0 \mathcal{J}_x^{i,j,k} \Big|_{t+\frac{\Delta t}{2}}$$

$$\frac{H_x^{i,j,k} \Big|_{t+\frac{\Delta t}{2}} - H_x^{i,j,k-1} \Big|_{t+\frac{\Delta t}{2}}}{\Delta z} - \frac{H_z^{i,j,k} \Big|_{t+\frac{\Delta t}{2}} - H_z^{i-1,j,k} \Big|_{t+\frac{\Delta t}{2}}}{\Delta x} = \frac{1}{C_0} \epsilon_{yy}^{i,j,k} \frac{E_y^{i,j,k} \Big|_{t+\Delta t} - E_y^{i,j,k} \Big|_t}{\Delta t} + \eta_0 \mathcal{J}_y^{i,j,k} \Big|_{t+\frac{\Delta t}{2}}$$

$$\frac{H_y^{i,j,k} \Big|_{t+\frac{\Delta t}{2}} - H_y^{i-1,j,k} \Big|_{t+\frac{\Delta t}{2}}}{\Delta x} - \frac{H_x^{i,j,k} \Big|_{t+\frac{\Delta t}{2}} - H_x^{i,j-1,k} \Big|_{t+\frac{\Delta t}{2}}}{\Delta y} = \frac{1}{C_0} \epsilon_{zz}^{i,j,k} \frac{E_z^{i,j,k} \Big|_{t+\Delta t} - E_z^{i,j,k} \Big|_t}{\Delta t} + \eta_0 \mathcal{J}_z^{i,j,k} \Big|_{t+\frac{\Delta t}{2}}$$



1D case



$$\partial_x = \partial_y = 0$$

\Rightarrow we cross out corresponding terms from our finite difference equations:

$$-\frac{E_y^{i,j,k+1}|_t - E_y^{i,j,k}|_t}{\Delta z} = -\frac{1}{C_0} \mu_{xx}^{i,j,k} \frac{H_x^{i,j,k}|_{t+\frac{\Delta t}{2}} - H_x^{i,j,k}|_{t-\frac{\Delta t}{2}}}{\Delta t}$$

$- \mathcal{M}_x^{i,j,k}|_t$

decoupled

$$\frac{E_x^{i,j,k+1}|_t - E_x^{i,j,k}|_t}{\Delta z} = -\frac{1}{C_0} \mu_{yy}^{i,j,k} \frac{H_y^{i,j,k}|_{t+\frac{\Delta t}{2}} - H_y^{i,j,k}|_{t-\frac{\Delta t}{2}}}{\Delta t}$$

$- \mathcal{M}_y^{i,j,k}|_t$

$H_z^{i,j,k} = 0$

E_x / H_y mode

E_y / H_x mode

$$-\frac{H_y^{i,j,k}|_{t+\frac{\Delta t}{2}} - H_y^{i,j,k-1}|_{t+\frac{\Delta t}{2}}}{\Delta z} = \frac{1}{C_0} \epsilon_{xx}^{i,j,k} \frac{E_x^{i,j,k}|_{t+\Delta t} - E_x^{i,j,k}|_t}{\Delta t} +$$

$+ \eta_0 \mathcal{T}_x^{i,j,k}|_{t+\frac{\Delta t}{2}}$

decoupled

$$\frac{H_x^{i,j,k}|_{t+\frac{\Delta t}{2}} - H_x^{i,j,k-1}|_{t+\frac{\Delta t}{2}}}{\Delta z} = \frac{1}{C_0} \epsilon_{yy}^{i,j,k} \frac{E_y^{i,j,k}|_{t+\Delta t} - E_y^{i,j,k}|_t}{\Delta t} +$$

$+ \eta_0 \mathcal{T}_y^{i,j,k}|_{t+\frac{\Delta t}{2}}$

$E_z^{i,j,k} = 0$

If there's no anisotropy in the model, those modes have the same numerical behavior; they are physical modes and propagate independently.

We will consider E_y / H_x mode.

$$-\frac{E_y^{i,j,k+1}|_t - E_y^{i,j,k}|_t}{\Delta z} = -\frac{1}{C_0} \mu_{xx}^{i,j,k} \frac{H_x^{i,j,k}|_{t+\frac{\Delta t}{2}} - H_x^{i,j,k}|_{t-\frac{\Delta t}{2}}}{\Delta t} - m_x^{i,j,k}|_t$$

$$\frac{H_x^{i,j,k}|_{t+\frac{\Delta t}{2}} - H_x^{i,j,k-1}|_{t+\frac{\Delta t}{2}}}{\Delta z} = \frac{1}{C_0} \epsilon_{yy}^{i,j,k} \frac{E_y^{i,j,k}|_{t+\Delta t} - E_y^{i,j,k}|_t}{\Delta t} + \eta_0 J_y^{i,j,k}|_{t+\frac{\Delta t}{2}}$$

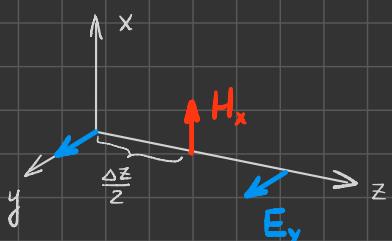
Let's derive update equations. (omit indices i and j)

Ampere's law:

$$E_y^k|_{t+\Delta t} = E_y^k|_t + \frac{1}{\Delta z} \cdot \Delta t \cdot \underbrace{\frac{C_0}{\epsilon_{yy}^k} \left(H_x^k|_{t+\frac{\Delta t}{2}} - H_x^{k-1}|_{t+\frac{\Delta t}{2}} \right)}_{\equiv m_{E_y}^k} - \Delta t \cdot \underbrace{\frac{C_0}{\epsilon_{yy}^k} \eta_0 J_y^k|_{t+\frac{\Delta t}{2}}}_{m_{J_y}^k}$$

Faraday's law

$$H_x^k|_{t+\frac{\Delta t}{2}} = H_x^k|_{t-\frac{\Delta t}{2}} + \frac{1}{\Delta z} \cdot \Delta t \cdot \underbrace{\frac{C_0}{\mu_{xx}^k} \cdot (E_y^{k+1}|_t - E_y^k|_t)}_{\equiv m_{E_y}^k} - \Delta t \cdot \underbrace{\frac{C_0}{\mu_{xx}^k} m_x^k|_t}_{m_{H_x}^k}$$



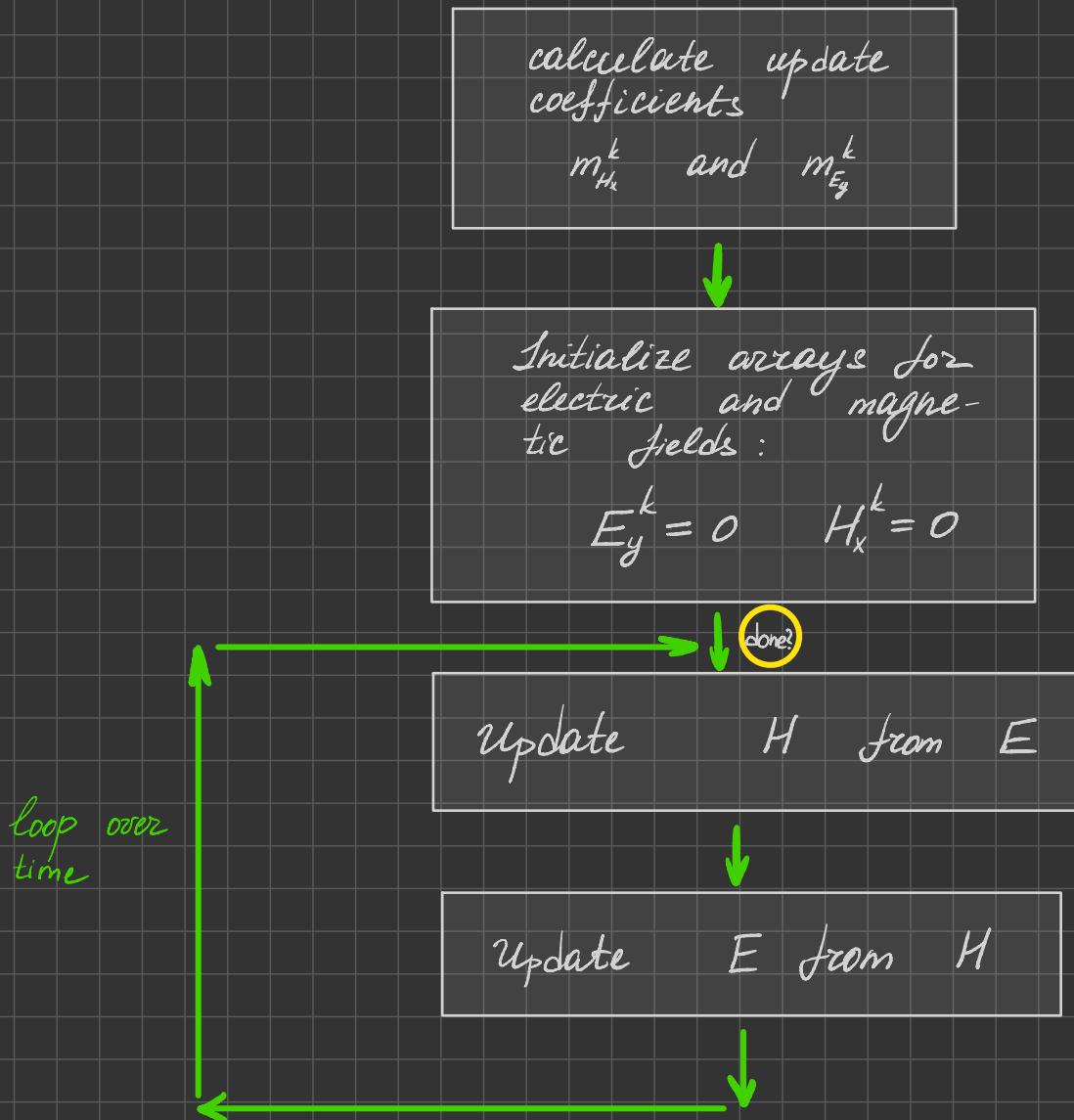
Implementation

$$m_{E_y}^k \equiv \frac{C_0 \Delta t}{\epsilon_{yy}^k} \quad m_{H_x}^k \equiv \frac{C_0 \Delta t}{\mu_{xx}^k}$$

} 1D arrays since ϵ_{yy}^k and μ_{xx}^k are the functions of $z = k \cdot \Delta z$

precomputed before the simulation

Workflow :



Numerical boundary conditions.

Dirichlet BC.

Faraday's law

$$H_x^k|_{t+\frac{\Delta t}{2}} = H_x^k|_{t-\frac{\Delta t}{2}} + \frac{1}{\Delta z} \cdot m_{H_x}^k \left(E_y^{k+1}|_t - E_y^k|_t \right) - m_{H_x}^k M_x^k|_t$$

what do we do at

$k = N_z$: $E_y^{N_z+1}$ does ?
not exist.

Ampere's law :

$$E_y^k|_{t+\Delta t} = E_y^k|_t + \frac{1}{\Delta z} \cdot m_{E_y}^k \left(H_x^k|_{t+\frac{\Delta t}{2}} - H_x^{k-1}|_{t+\frac{\Delta t}{2}} \right) - m_{E_y}^k \gamma_0 J_y^k|_{t+\frac{\Delta t}{2}}$$

what do we do at

$k = 0$: H_x^{-1} does ?
not exist.

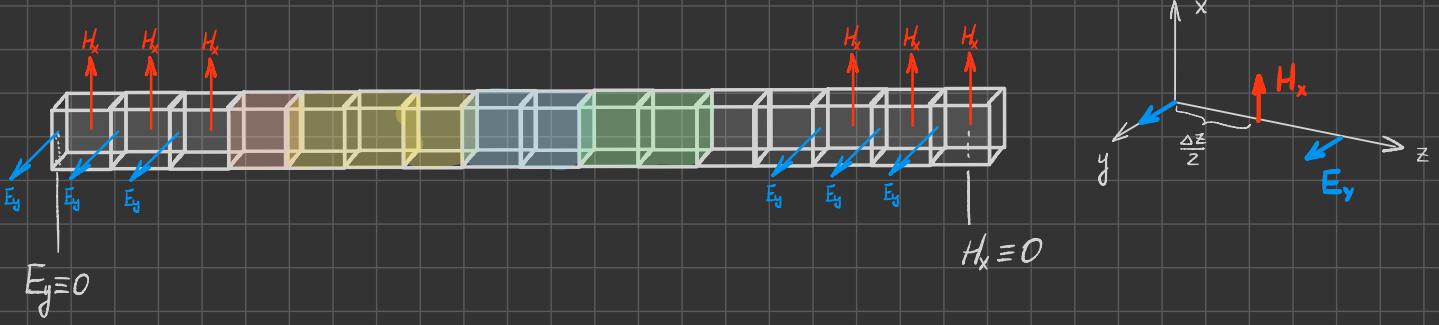
Force the values outside the grid to be zero

$$k = \overline{0, N_z-1} \quad H_x^k|_{t+\frac{\Delta t}{2}} = H_x^k|_{t-\frac{\Delta t}{2}} + \frac{1}{\Delta z} \cdot m_{H_x}^k \left(E_y^{k+1}|_t - E_y^k|_t \right) - m_{H_x}^k M_x^k|_t$$

$k = N_z$ right boundary $H_x^k|_{t+\frac{\Delta t}{2}} = H_x^k|_{t-\frac{\Delta t}{2}} + \frac{1}{\Delta z} \cdot m_{H_x}^k \left(0 - E_y^k|_t \right) - m_{H_x}^k M_x^k|_t$ PEC

$k = \overline{1, N_z}$ $E_y^k|_{t+\Delta t} = E_y^k|_t + \frac{1}{\Delta z} \cdot m_{E_y}^k \left(H_x^k|_{t+\frac{\Delta t}{2}} - H_x^{k-1}|_{t+\frac{\Delta t}{2}} \right) - m_{E_y}^k \gamma_0 J_y^k|_{t+\frac{\Delta t}{2}}$ PMLC

$k = 0$ left boundary $E_y^k|_{t+\Delta t} = E_y^k|_t + \frac{1}{\Delta z} \cdot m_{E_y}^k \left(H_x^k|_{t+\frac{\Delta t}{2}} - 0 \right) - m_{E_y}^k \gamma_0 J_y^k|_{t+\frac{\Delta t}{2}}$



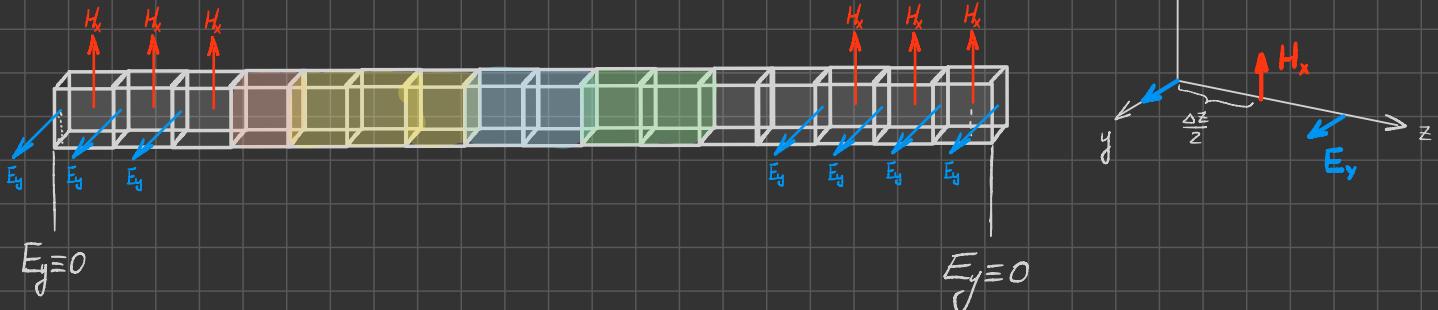
Sizes of arrays for E_y and H_x are the same :

$$E_y = \text{array}(Nz)$$

$$H_x = \text{array}(Nz)$$

PEC boundary condition

- values of E_y are set to zero at the boundaries
- we have an extra value of electric field at the right boundary



$$E_y = \text{array}(Nz + 1)$$

$$H_x = \text{array}(Nz)$$

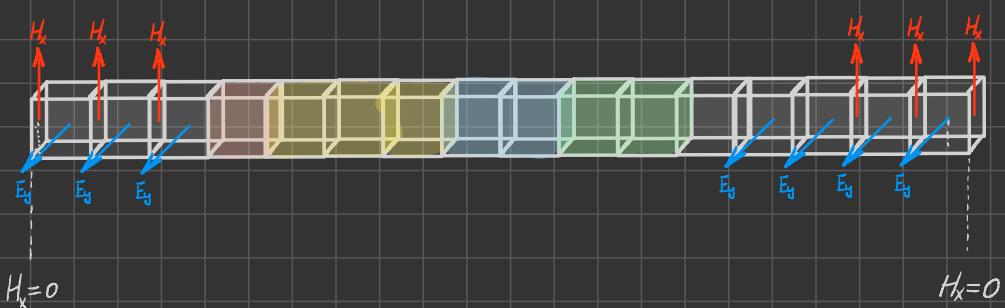
$$k = 1, \dots, N_z - 1 \quad H_x^k|_{t+\frac{\Delta t}{2}} = H_x^k|_{t-\frac{\Delta t}{2}} + \frac{1}{\Delta z} \cdot m_{H_x}^k \left(E_y^{k+1}|_t - E_y^k|_t \right) - m_{H_x}^k \mathcal{M}_x^k|_t$$

$$k = 0, \dots, N_z - 1 \quad E_y^k|_{t+\Delta t} = E_y^k|_t + \frac{1}{\Delta z} \cdot m_{E_y}^k \left(H_x^k|_{t+\frac{\Delta t}{2}} - H_x^{k-1}|_{t+\frac{\Delta t}{2}} \right) - m_{E_y}^k \gamma_0 \mathcal{Y}_y^k|_{t+\frac{\Delta t}{2}}$$

$$k = 0 \quad E_y^0|_{t+\Delta t} \equiv 0$$

$$k = N_z \quad E_y^{N_z}|_{t+\Delta t} \equiv 0$$

PMC Boundary condition



$$\boxed{\begin{aligned} H_x &= \text{array}(N_z + 1) \\ E_y &= \text{array}(N_z) \end{aligned}}$$

$$k = 0, \dots, N_z - 1 \quad H_x^k|_{t+\frac{\Delta t}{2}} = H_x^k|_{t-\frac{\Delta t}{2}} + \frac{1}{\Delta z} \cdot m_{H_x}^k \left(E_y^{k+1}|_t - E_y^k|_t \right) - m_{H_x}^k \mathcal{M}_x^k|_t$$

$$k = 1, \dots, N_z - 1 \quad E_y^k|_{t+\Delta t} = E_y^k|_t + \frac{1}{\Delta z} \cdot m_{E_y}^k \left(H_x^k|_{t+\frac{\Delta t}{2}} - H_x^{k-1}|_{t+\frac{\Delta t}{2}} \right) - m_{E_y}^k \gamma_0 \mathcal{Y}_y^k|_{t+\frac{\Delta t}{2}}$$

$$k = 0 \quad H_x^0|_{t+\Delta t} \equiv 0$$

$$k = N_z \quad H_x^{N_z}|_{t+\Delta t} \equiv 0$$

Gaussian pulse

$$f(x) = e^{-x^2} \quad - \text{Gaussian Function}$$

(base form)

$$\int_{-\infty}^{+\infty} \underbrace{e^{-x^2}}_{f(x)} dx = \sqrt{\pi}$$

$$f(x) = a \cdot \exp\left(-\frac{(x-b)^2}{2c^2}\right) \quad - \text{with parametric extension}$$

$$\int_{-\infty}^{+\infty} a \cdot e^{-\frac{(x-b)^2}{2c^2}} dx = a \cdot c \cdot \sqrt{2\pi} \quad = 1$$

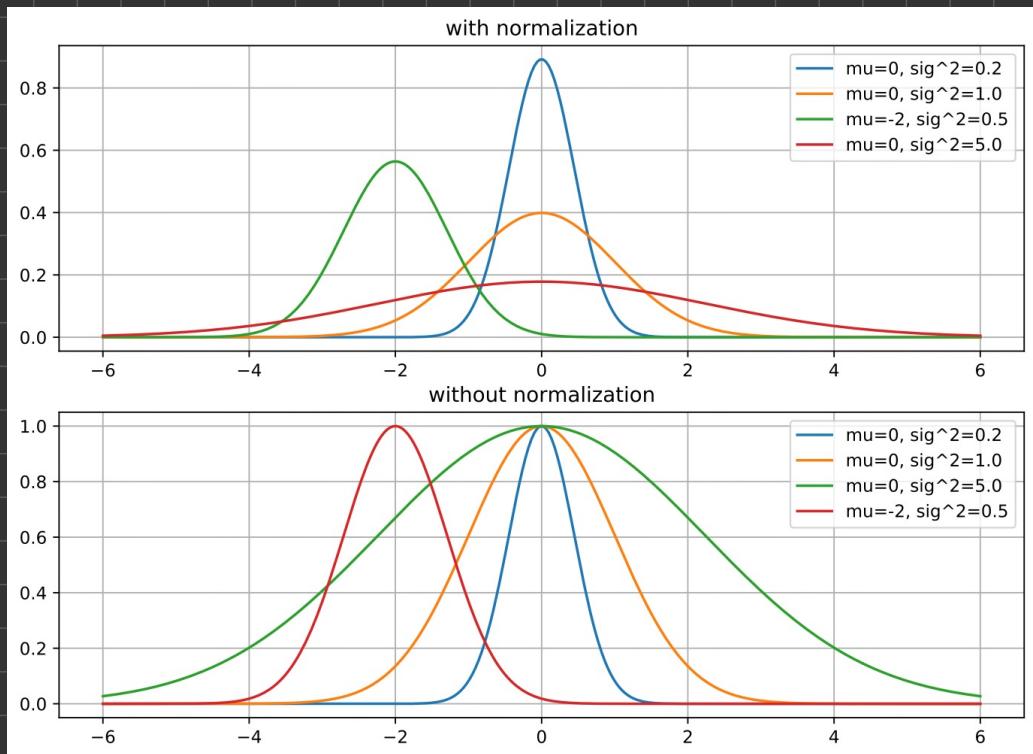
$$a = \frac{1}{c \sqrt{2\pi}}$$

$$a = \frac{1}{6 \cdot \sqrt{2\pi}}$$

$b = \mu$ — expected value

$c = \sigma$ — variance

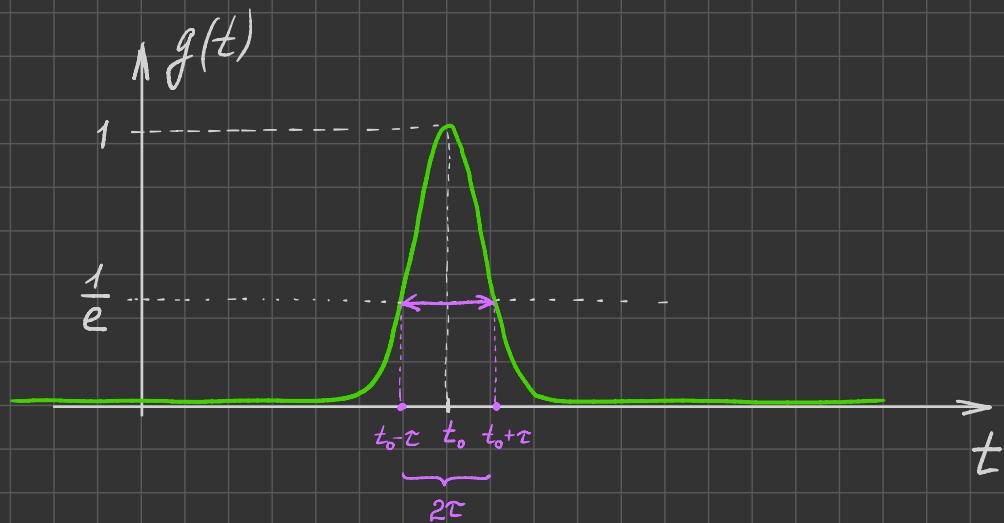
$$g(x) = \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$



$$g(x) = e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

In the code I used

$$g(t) = e^{-\left(\frac{t-t_0}{\tau}\right)^2}$$



Implementation of the Gaussian source

Frequency content of Gaussian pulse.

Fourier transform of a Gaussian is a Gaussian:

$$g(t) = e^{-\frac{t^2}{\tau^2}} \longleftrightarrow G(f) = \frac{1}{\sqrt{\pi} B} e^{-\frac{f^2}{B^2}}$$

The frequency content of the Gaussian pulse extends from DC (0 Hz) up to around B

$$B = \frac{1}{\pi \tau}$$

- ✓ → the narrower the pulse (τ smaller) the more frequencies are captured \Rightarrow we choose τ according to the frequencies we want to have in the simulation
- ✗ → The higher the frequency the shorter the time step Δt will be.

Designing the pulse source.

Step 1: determine max freq. you're interested in simulating.

$$f_{\max}$$

Step 2: compute pulse width considering copper frequency limit

$$B = f_{\max} = \frac{1}{\pi \tau} \rightarrow \tau \leq \frac{1}{\pi f_{\max}} ;$$

$$\tau \approx \frac{0.5}{f_{\max}}$$

Step 3: check the time step. May need to reduce it. Gaussian pulse should be resolved by at least 10 - 20 time steps.

$$\Delta t = \frac{\tau}{N_t}$$

$$N_t \geq 10$$

Everything is automatically satisfied if

$$\Delta t = \frac{n \Delta z}{2 c_0} ABC$$

Typically you determine a first Δt_1 , based on CFL stability condition.

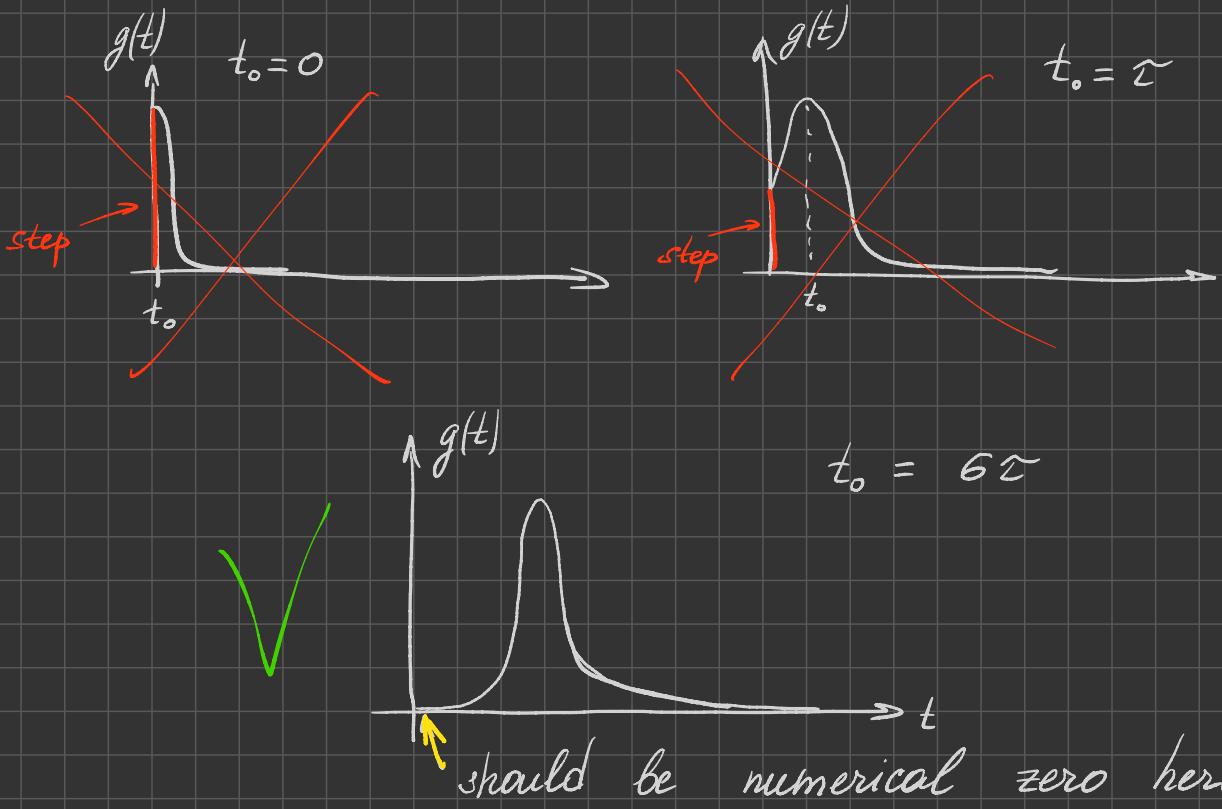
Then determine Δt_2 based on resolving

the maximum frequency f_{\max} .

Then choose the smallest value.

$$\Delta t = \min(\Delta t_1, \Delta t_2)$$

Step 4 : compute time delay t_0



The source must start at zero and gradually increase. NO STEP FUNCTIONS.

$$t_0 \geq 6\tilde{\tau}$$

why $6\tilde{\tau}$? what's the value $g(0)$ when $t_0 = 6\tilde{\tau}$?

$$g(0) \Big|_{t_0=6\tilde{\tau}} = e^{-\left(\frac{0-6\tilde{\tau}}{\tilde{\tau}}\right)^2} = e^{-36} \sim 2^{36} \sim 10^{-12}$$

Types of sources (see my notes on sources)

hard (voltage)

soft (current)

- overwrite
- source cell is felt by the fields as either PEC or PML
- add to parent to scattered waves passing through it
- injects energy into both directions
- great for testing boundary conditions

$$H_x^k \Big|_{t+\frac{\Delta t}{2}} = g_H \Big|_t$$

$$E_y^k \Big|_{t+\Delta t} = g_E \Big|_t$$

$$H_x^k \Big|_{t+\frac{\Delta t}{2}} + = g_H \Big|_t$$

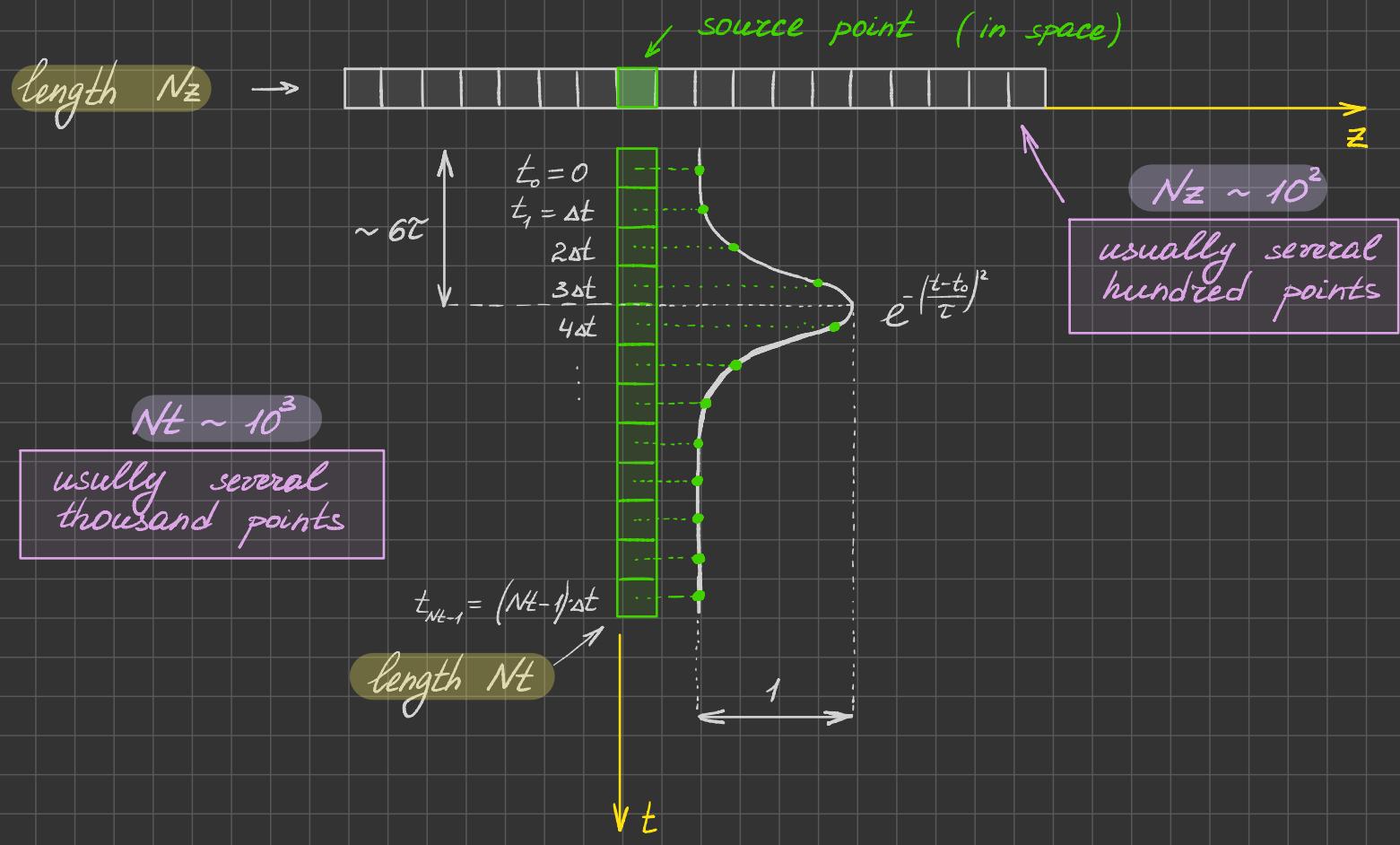
$$E_y^k \Big|_{t+\Delta t} + = g_E \Big|_t$$

- not usually a practical source
- rarely used. Use until learn SF / TF source.

* see Kuniaki Tashitomi's paper on this account.

Visualizing the arrays

E_y , H_x , (ER, UR) , mE_y , mH_x are stored in the arrays of length Nz .



g_E and g_H are stored in the arrays of length N_t

Time resolution at

Courant - Friderich - Levy stability condition

over the duration of one time step Δt all disturbance will travel

- numerical distance covered in Δt : ΔZ
- physical dist. covered in Δt : $C_0 \cdot \frac{\Delta t}{n}$

In numerical algorithm it's impossible for a disturbance to travel farther than one cell ΔZ in a single time step Δt .

For this reason we need to make sure that the physical wave would not propagate farther than a unit cell ΔZ in one time step Δt .

$$\underbrace{\frac{C_0}{n} \cdot \Delta t}_{\text{physical}} < \underbrace{\Delta Z}_{\text{numerical}}$$

\Rightarrow upper limit on time step Δt

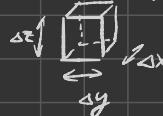
$$\Delta t < \frac{\Delta Z}{(C_0/n)}$$

n - smallest refractive idx ; $n \geq 1 \Rightarrow$ usually n is set to 1 and dropped from the ineq.

For 2D and 3D cases:

$$\Delta t < \frac{1}{C_0 \sqrt{\frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2} + \frac{1}{(\Delta z)^2}}}$$

CFL stability condition

This condition will be most restrictive along the shortest dimension of the unit cell 

$$\Delta_{\min} = \min \{ \Delta x, \Delta y, \Delta z \}$$

$$\Delta t < \frac{\Delta_{\min}}{2C_0} \quad \frac{1}{2} - \text{safety margin}$$

More general case:

$$\Delta t < \frac{1}{2} \frac{n_{\min} \Delta_{\min}}{C_0}$$

- grid filled with dielectric \Rightarrow wave travels slower everywhere
- model includes materials with $n < 1$

For perfect boundary condition

$$\Delta t = \frac{n_{\infty} \cdot \Delta z}{2C_0}$$

n_{∞} - refr. idx at the boundaries ; materials should be the same at both boundaries

Total number of iterations N_t

Nz

Depends mainly on:

- device we model
- properties of device we calculate

device

information

- highly resonant devices typically require more iterations
 - purely scattering devices require very few iterations
 - more iterations needed the more waves bounce around in the grid
 - calculating spectral shapes requires the most iterations: reflectance, transmittance, line shapes ..
 - calculating positions of resonances requires fewer iterations
- This might be very difficult in frequency domain.

Rule of thumb

1. How long it takes a ^{slowest} wave to propagate across the grid?

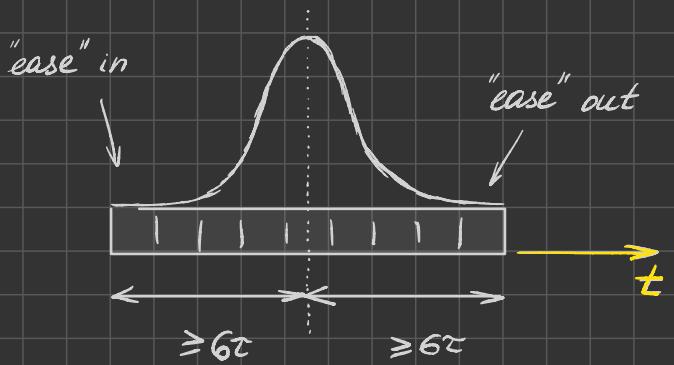
$$t_{\text{prop.}} = \frac{n_{\max} N_z \cdot \Delta z}{c_0}$$

physical size of the grid

2. Simulation time T must include the entire pulse

of duration τ

$$T \geq 6\tau + 6\tau$$



3. Simulation time should allow for ~ 5 bounces

$$T \geq 5t_{prop}$$

4. Rule of thumb for total simulation time

$$T \gtrsim 12\tau + 5t_{prop}$$

* for highly resonant devices this time is **NOT** enough

5. Given time step Δt , the total # of iterations is

$$Nt \equiv \text{round}^1 \left[\frac{T}{\Delta t} \right] \text{ (ceil)}$$

this is in context of `for (1, ..., Nt) loop`.

Another approach is to set a `while (...) loop` and keep running until the power is stuck in the grid and stop iterations when the power in the domain drops below some threshold.

Grid resolution Δz

1. Wavelength

- Δz should be sufficient to resolve the shortest wavelength

→ determine

$$\lambda_{\min} = \frac{c_0}{f_{\max} \cdot n_{\max}}$$

n_{\max} - largest refractive idx found in the grid

→ resolve wave with at least $N_{\lambda} = 10$ cells

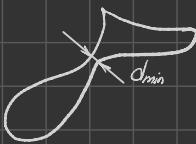
$$\Delta_{\lambda} \approx \frac{\lambda_{\min}}{N_{\lambda}}$$

$$N_{\lambda} \geq 10$$

N_i	material
10 - 20	low contrast dielectric
20 - 30	high contrast dielectric
40 - 60	most metallic structures
100 - 200	plasmonic devices

2. Mechanical features

- Δz should be sufficient to resolve the smallest mechanical feature d_{\min}



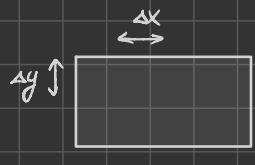
→ want to resolve this mechanical feat. d_{\min} with

1 to 4 cells Δ_d

$$\Delta_d \approx \frac{d_{\min}}{N_d}, \quad N_d \geq 1$$

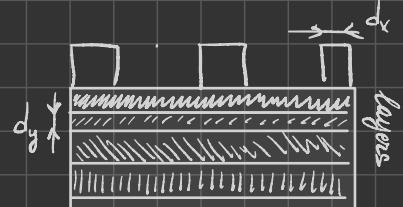
3. Adjust init. resolution Δz

$$\Delta x = \Delta y = \Delta z = \min [\Delta_\lambda, \Delta_d]$$



4. "Snap" grid to critical dimensions

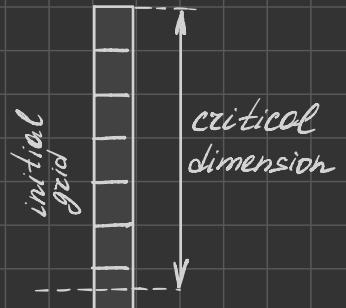
→ decide what dimensions along each axis are critical : d_x and d_y



→ compute how many grid cells comprise $d_x/d_y/d_z$ and round up

$$M_x \equiv \text{ceil} \left(\frac{d_x}{\Delta_x} \right)$$

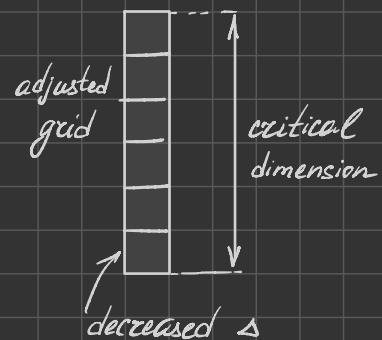
$$M_y \equiv \text{ceil} \left(\frac{d_y}{\Delta_y} \right)$$



→ adjust grid resolution to fit this dimension
 d_x/d_y in grid exactly

$$\Delta_x \equiv \frac{d_x}{M_x}$$

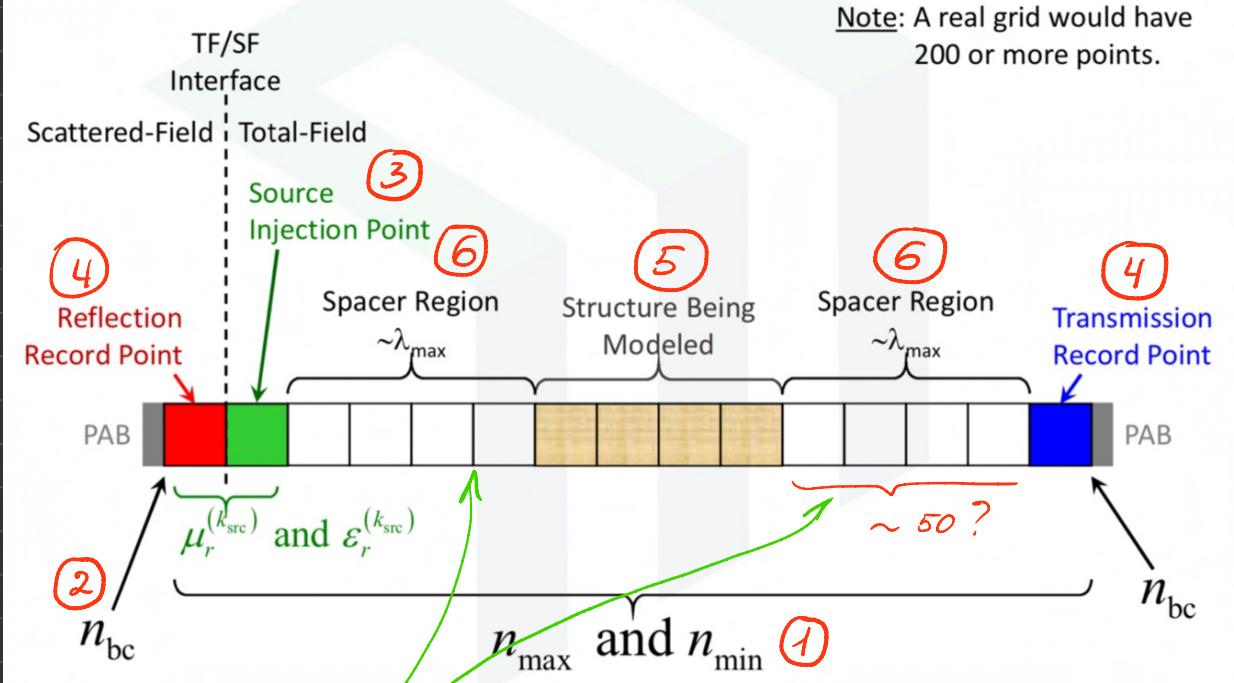
$$\Delta_y \equiv \frac{d_y}{M_y}$$



Total number of space cells N_z

N_z

1D-FDTD Grid

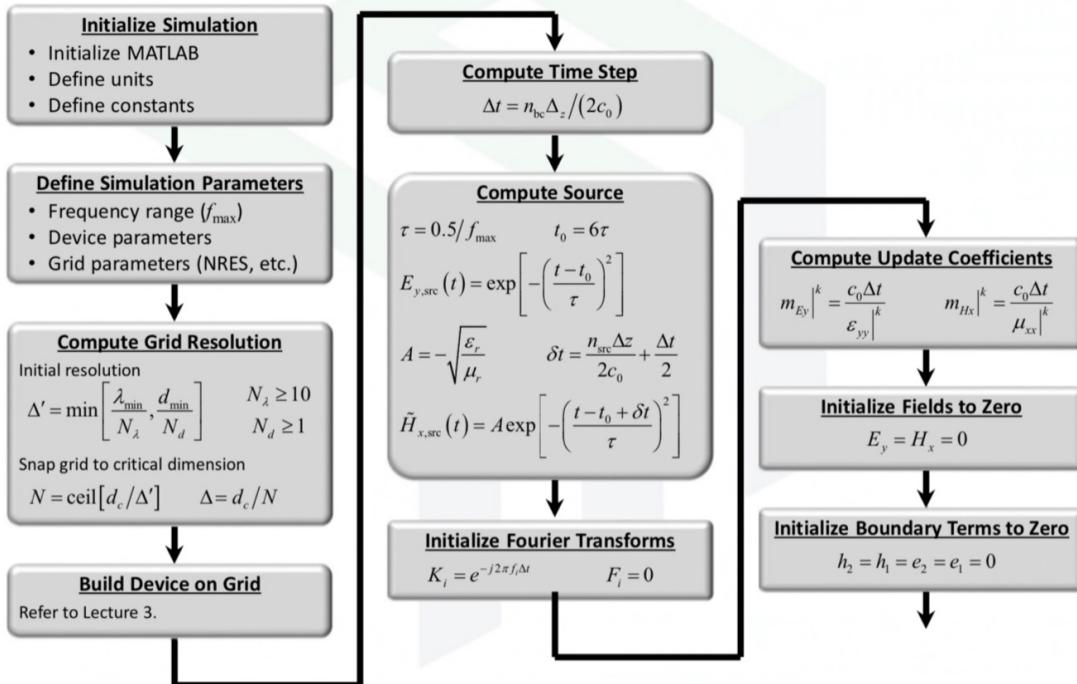


Note: A real grid would have 200 or more points.

In 2D and 3D for resonant devices we will have evanescent fields around device which should not reach PML, otherwise we will have reflections.
 \Rightarrow need spacer regions.

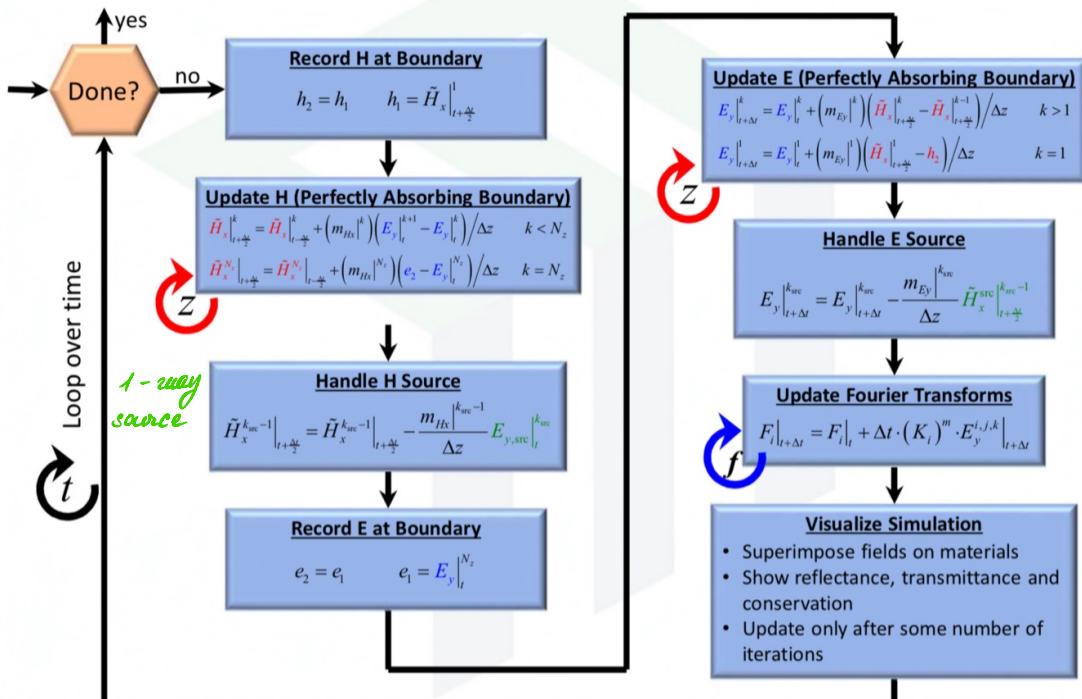
Sequence of initialization for simulation

Initializing the FDTD Simulation



Main loop

The Main FDTD Loop

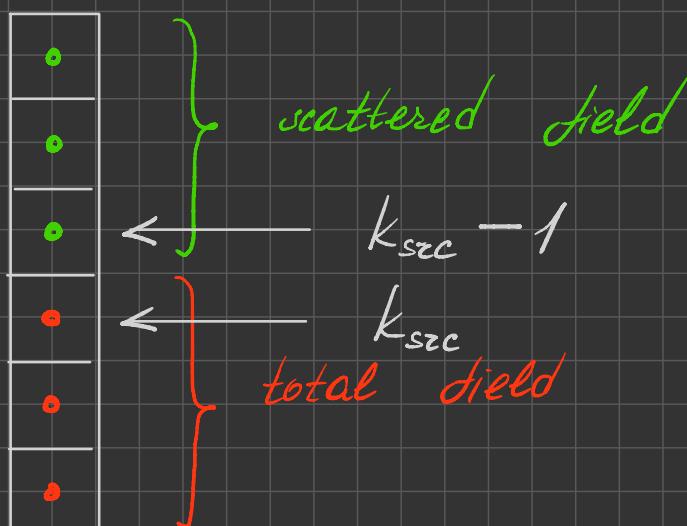


Total field / Scattered field source

1D grid

1 eq has term from total field \rightarrow 2 upd eq-s \rightarrow 2 upd eq-s

1 eq has term from scattered field



1. On the scattered field side

update equation for H_x :

Faraday's law

$$H_x \Big|_{t+\frac{\Delta t}{2}}^{k_{src}-1} = H_x \Big|_{t-\frac{\Delta t}{2}}^{k_{src}-1} + \underbrace{\frac{1}{\Delta z} \Delta t \cdot \frac{C_0}{\mu_{xx}^k}}_{\equiv m_{H_x}^k} \cdot \left(E_y \Big|_{t}^{k_{src}} - E_y \Big|_{t}^{k_{src}-1} \right) - \underbrace{\Delta t \cdot \frac{C_0}{\mu_{xx}^k} M_x \Big|_{t}}_{m_{H_x}^k}$$

↑
on the total field side

$$E_y \Big|_t^{k_{src}} = \text{total} = \text{source} + \text{scattered}$$

\Rightarrow we need to subtract source for it to be purely scattered on the scattered field side.

Update equation with correction

$$H_x \Big|_{t+\frac{\Delta t}{2}}^{k_{src}-1} = H_x \Big|_t^{k_{src}-1} + \frac{1}{\Delta z} \cdot \Delta t \cdot \frac{C_0}{\mu_{xx}^k} \cdot \left[\underbrace{\left(E_y \Big|_t^{k_{src}} - E_y \Big|_t^{k_{src}-1} \right)}_{\equiv m_{H_x}^k} - \underbrace{E_y \Big|_t^{k_{src}-1}}_{E_y^{\text{scat}} \Big|_t^{k_{src}}} - \underbrace{\Delta t \cdot \frac{C_0}{\mu_{xx}^k} M_x \Big|_t}_{m_{H_x}^k} \right]$$

Let's bring this source term E_y^{src} outside the brackets:

$$H_x \Big|_{t+\frac{\Delta t}{2}}^{k_{src}-1} = H_x \Big|_t^{k_{src}-1} + \frac{1}{\Delta z} \cdot m_{H_x}^{k-1} \cdot \left[\underbrace{\left(E_y \Big|_t^{k_{src}} - E_y \Big|_t^{k_{src}-1} - m_{H_x}^{k-1} \cdot M_x \Big|_t^{k_{src}-1} \right)}_{\text{original equation}} - m_{H_x}^{k-1} \cdot \frac{E_y^{\text{src}} \Big|_t^{k_{src}}}{\Delta z} \right]$$

correction

can be implemented after

2. On total field side: $k = k_{src}$

$$E_y \Big|_{t+\frac{\Delta t}{2}}^{k_{src}} = E_y \Big|_t^{k_{src}} + \frac{1}{\Delta z} \cdot m_{E_y}^{k_{src}} \left(H_x \Big|_{t+\frac{\Delta t}{2}}^{k_{src}} - H_x \Big|_{t+\frac{\Delta t}{2}}^{k_{src}-1} \right) - \underbrace{m_{E_y}^k \gamma_0 J_y \Big|_{t+\frac{\Delta t}{2}}^k}_{\text{this term is from scattered field side}}$$

$$H_x \Big|_{t+\frac{\Delta t}{2}}^{k_{src}-1} = \text{total} - \text{source}$$

$$\Rightarrow \text{total} = H_x^{\text{scat}} \Big|_{t+\frac{\Delta t}{2}}^{k_{\text{src}}-1} + H_x^{\text{src}} \Big|_{t+\frac{\Delta t}{2}}^{k_{\text{src}}-1}$$

Correct Ampere's law accordingly.

$$E_y^{\text{k}_{\text{src}}} = E_y^{\text{k}_{\text{src}}} + \frac{1}{\Delta z} \cdot m_{E_y}^{\text{k}_{\text{src}}} \left[H_x^{\text{k}_{\text{src}}} \Big|_{t+\frac{\Delta t}{2}} - \left(H_x^{\text{k}_{\text{src}}-1} \Big|_{t+\frac{\Delta t}{2}} + H_x^{\text{k}_{\text{src}}} \Big|_{t+\frac{\Delta t}{2}} \right) \right] - m_{E_y}^k \gamma_0 J_y^k \Big|_{t+\frac{\Delta t}{2}}$$

take it out of the brackets:

$$E_y^{\text{k}_{\text{src}}} = E_y^{\text{k}_{\text{src}}} + \frac{1}{\Delta z} \cdot m_{E_y}^{\text{k}_{\text{src}}} \left[H_x^{\text{k}_{\text{src}}} \Big|_{t+\frac{\Delta t}{2}} - H_x^{\text{k}_{\text{src}}-1} \Big|_{t+\frac{\Delta t}{2}} \right] - m_{E_y}^k \gamma_0 J_y^k \Big|_{t+\frac{\Delta t}{2}} - \frac{1}{\Delta z} m_{E_y}^{\text{k}_{\text{src}}} H_x^{\text{k}_{\text{src}}} \Big|_{t+\frac{\Delta t}{2}}$$

will be added after the regular update equation

3. We need to calculate 2 source functions before main (time) FDTD loop.

normalized \rightarrow	$H_x^{\text{src}} \Big _{t+\frac{\Delta t}{2}}^{k_{\text{src}}-1}$	- for scattered field side
	$E_y^{\text{src}} \Big _t^{k_{\text{src}}}$	- for total field side

- ! exist
 - at different time moments
 - at different locations
 - H^{src} should be normalized before adding.

$$\tilde{H} = \gamma_0 H$$

For E_y / H_x mode:

$$E_y^{src} \Big|_{t}^{k_{src}} = g(t) - \text{gaussian}$$

Then normalized magn. field:

$$\tilde{H}_x^{src} \Big|_{t+\frac{\Delta t}{2}}^{k_{src}-1} = (-) \sqrt{\frac{\epsilon_z^{k_{src}}}{\mu_z^{k_{src}}}} \cdot g\left(t + \frac{n_{src} \cdot \Delta z}{2c_0} + \frac{\Delta t}{2}\right)$$

ahead of
 E_y in time

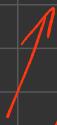
because of
different phase

amplitude
to satisfy
Maxwell's eq-s

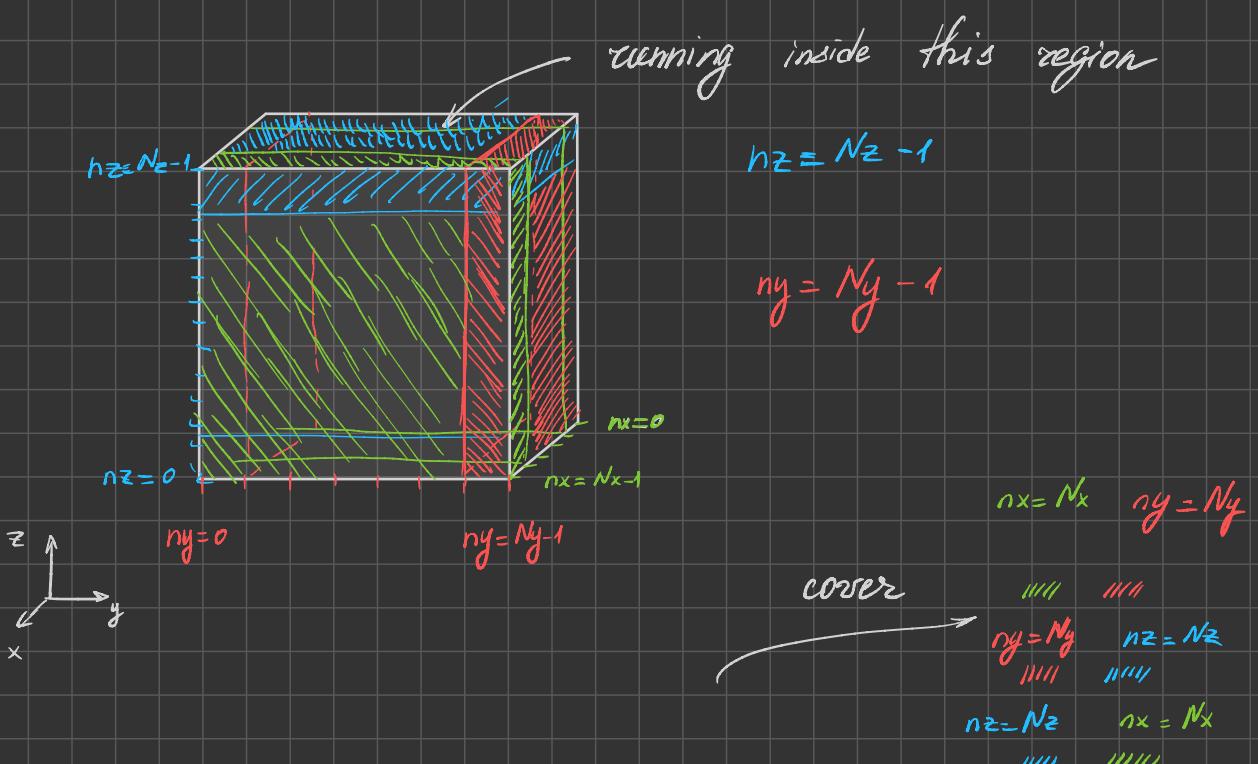
delay through
half of a
grid cell

half
time
step
difference

$\mu_z^{k_{src}}$, $\epsilon_z^{k_{src}}$, n_{src} — where the source is injected.



this implementation doesn't work = (

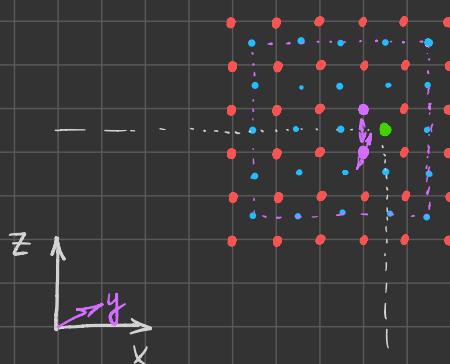


then // // //

nx	ny
n_x	n_z
ny	n_z

E field H-field

1 upd. magnetic field



$$k=2 \quad i=3 \quad j=1 \quad \frac{c_0 \Delta t}{\mu_{xx}^{3,1,2}} \left(E_z^{3,4,1,2} - E_z^{3,1,2} \right) \frac{E_y^{3,1,2+1} - E_y^{3,1,2}}{\Delta z} =$$

$$= H_x^{3,1,2} \left| - H_x^{3,1,2} \right|_{t+\frac{\Delta t}{2}} \Big|_{t-\frac{\Delta t}{2}}$$

FFT

$$E_x(x, y, z)$$

$$E_y(x, y, z)$$

$$E_z(x, y, z)$$

need ; variation of E_z is
X direction :

$$E_z \left[: , \underbrace{y_{-\text{src}}, z_{-\text{src}}} \right]$$

at the

source point

need to store this for
every time step:

$$E_z - \text{fft} = \left[\begin{array}{c} E_z(0) \\ E_z(1) \\ E_z(2) \\ E_z(3) \\ \vdots \end{array} \right] \left[\begin{array}{c} E_z(0) \\ E_z(1) \\ E_z(2) \\ E_z(3) \\ \vdots \end{array} \right] \left[\begin{array}{c} \cdot \\ \vdots \\ \cdot \\ \vdots \\ \cdot \end{array} \right] \cdots \left[\begin{array}{c} \cdot \\ \vdots \\ \cdot \\ \vdots \\ \cdot \end{array} \right] \right]_{Nt}$$

$$\text{FFT}(g) = \int_{-\infty}^{+\infty} g(t) e^{-j2\pi f_a t} dt$$

$E_z - \text{fft}$ $[121, 300]$ $g(t)$ - has dt vectors

$K [10]$

$E_f [122]$

exponential kernel

$$E_z - \text{fft} = K^{n_{dt}} \cdot E_z [: , y_s, z_s]$$

length of frequency

$E_z - \text{fft}$ - what is its size ?

same spatial dimensions but

now # frequencies

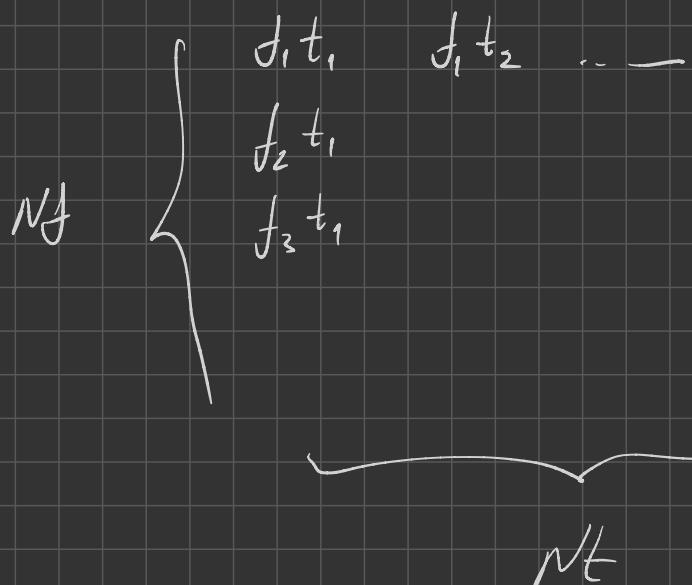
E_z - spatial dim \times # of time steps

$\Rightarrow K$ should be # time steps \times
 \times # of frequencies

$$K = e^{-j \cdot 2\pi \cdot \underbrace{[f_{\text{req}}]}_{Nf} \cdot \underbrace{\frac{m}{Nt}}_{Nt}}$$

sample it for
each time step
and for each
freq.

$$\tilde{E}_{z,f} = K \cdot \frac{E_z}{Nf \times Nx} \quad Nf \times Nt \quad Nt \times Nx$$



$$\frac{\partial E_z(x, y)}{\partial t} = \frac{1}{\epsilon} \left(\frac{\partial H_y(x, y)}{\partial x} - \frac{\partial H_x(x, y)}{\partial y} \right)$$

$$\frac{1}{\Delta t} (E_z^{n+1}|_{i,j} - E_z^n|_{i,j})$$

$$\frac{H_y^{t+\frac{1}{2}}|_{i+\frac{1}{2}, j} - H_y^{t+\frac{1}{2}}|_{i-\frac{1}{2}, j}}{\Delta x}$$

$$\frac{H_x^{t+\frac{1}{2}}|_{i, j+\frac{1}{2}} - H_x^{t+\frac{1}{2}}|_{i, j-\frac{1}{2}}}{\Delta y}$$

From this we can write an update eq. for E_z :

$$E_z^{n+1} = E_z^n + \dots$$

Avoiding DC offset in current source.

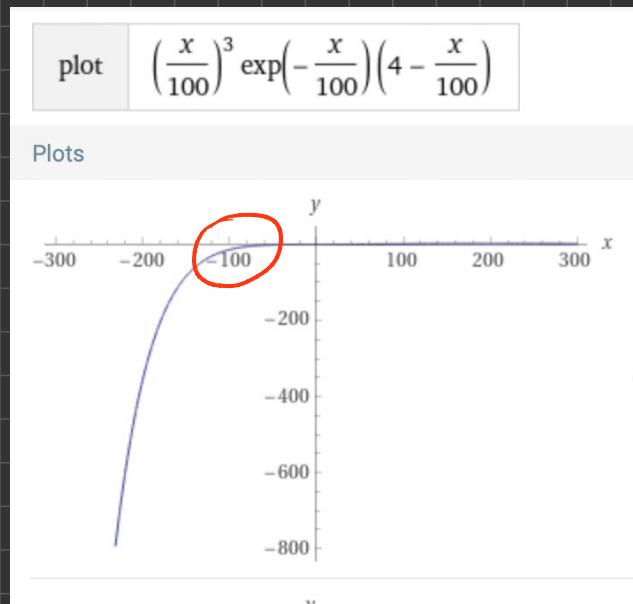
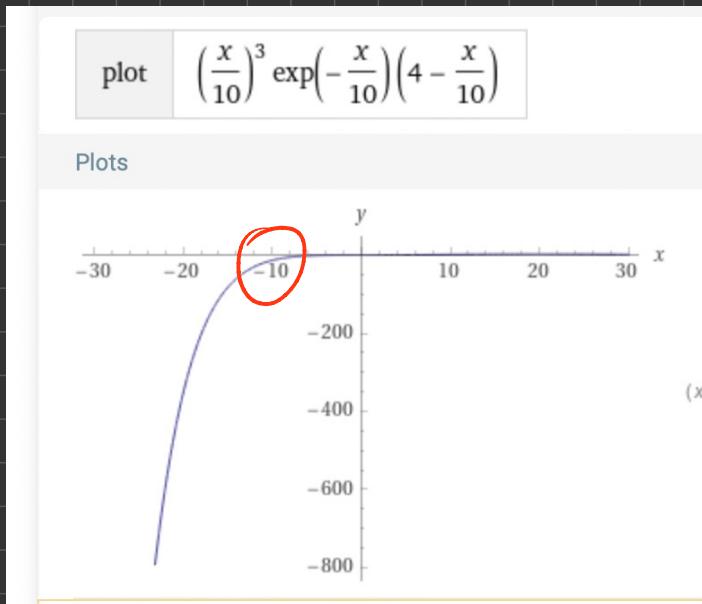
$$I(t) = \tau \frac{d}{dt} \left(\left(\frac{t}{\tau}\right)^4 e^{-\frac{t}{\tau}} \right) =$$

$$= \cancel{\tau} \left[4 \left(\frac{t}{\tau}\right)^3 \cdot \cancel{\frac{1}{\tau}} \cdot e^{-\frac{t}{\tau}} + \left(-\frac{1}{\tau}\right) \cdot e^{-\frac{t}{\tau}} \cdot \left(\frac{t}{\tau}\right)^4 \right] =$$

$$= \boxed{\left(\frac{t}{\tau}\right)^3 e^{-\frac{t}{\tau}} \left(4 - \frac{t}{\tau} \right)}$$

$$\tau = 10$$

$$\tau = 100$$



Ref.: Cheru, Moghaddam "Model of subsurface Interf. Radar"