

(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

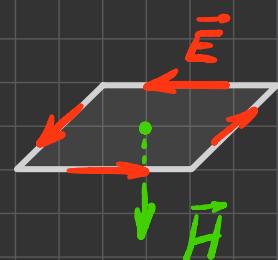
this is a
multiplication
in frequency
domain

Assume that our material is

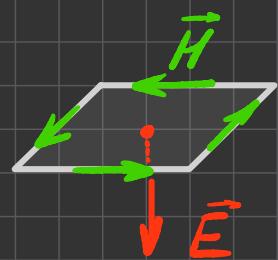
linear
isotropic
non-dispersive

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

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



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



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

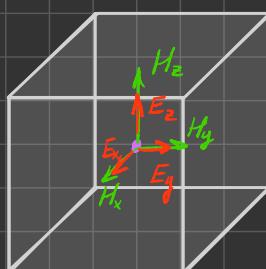
$$\vec{H}^{t+\frac{\Delta t}{2}} = \vec{H}^{t-\frac{\Delta t}{2}} - \frac{\Delta t}{\mu} \left[\vec{\nabla} \times \vec{E} \right]^t$$

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

$\frac{\Delta t}{\epsilon}$, $\frac{\Delta t}{\mu}$ 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



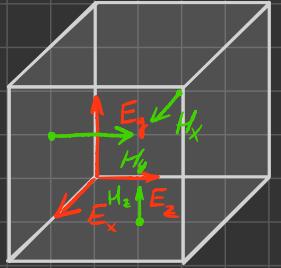
Staggered grids (Yee cell)

Physical

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

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

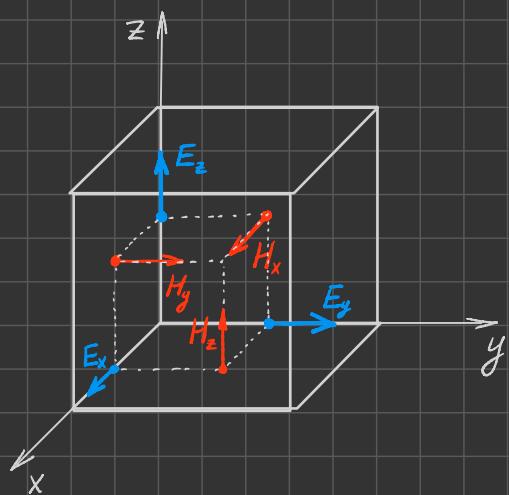
$$\nabla \cdot \vec{B} = 0$$



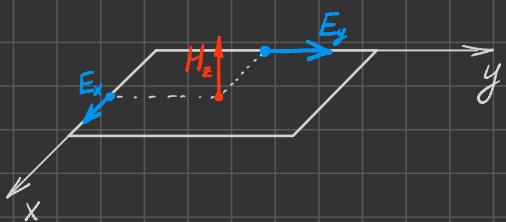
for divergence - free medium

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

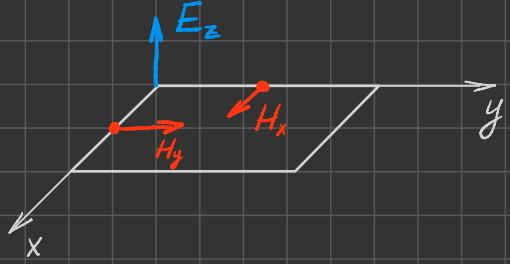
3D



2D



H_z mode

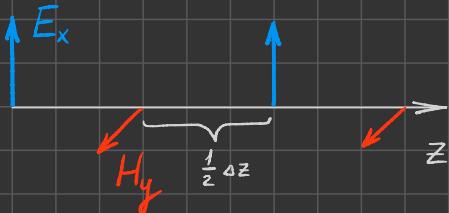


E_z mode

1D



E_y mode

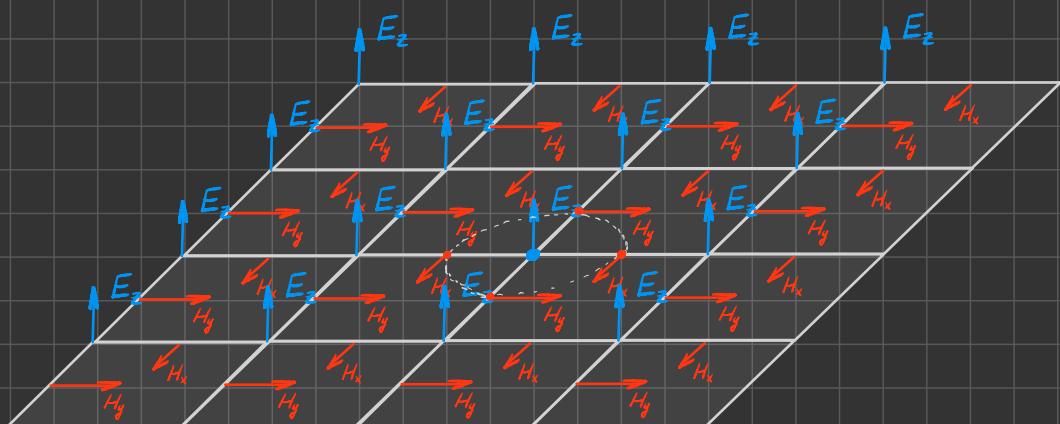


E_x mode

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.

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

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

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

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

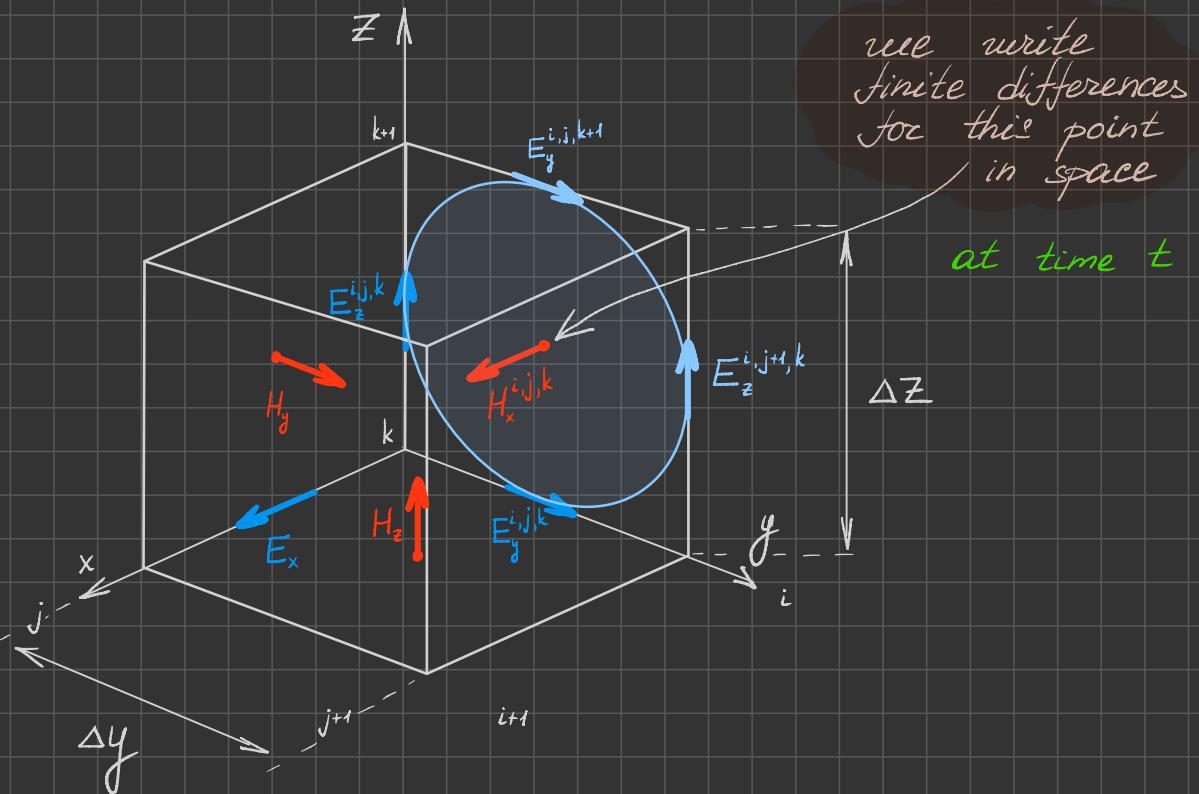
$$5 \quad \partial_z H_x - \partial_x H_z = \frac{1}{C_0} \epsilon_{yy} \partial_t E_y + \gamma_0 J_y$$

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

We will approximate these 6 equalities on the grid.
 (next 6 pages)

1

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



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

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

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

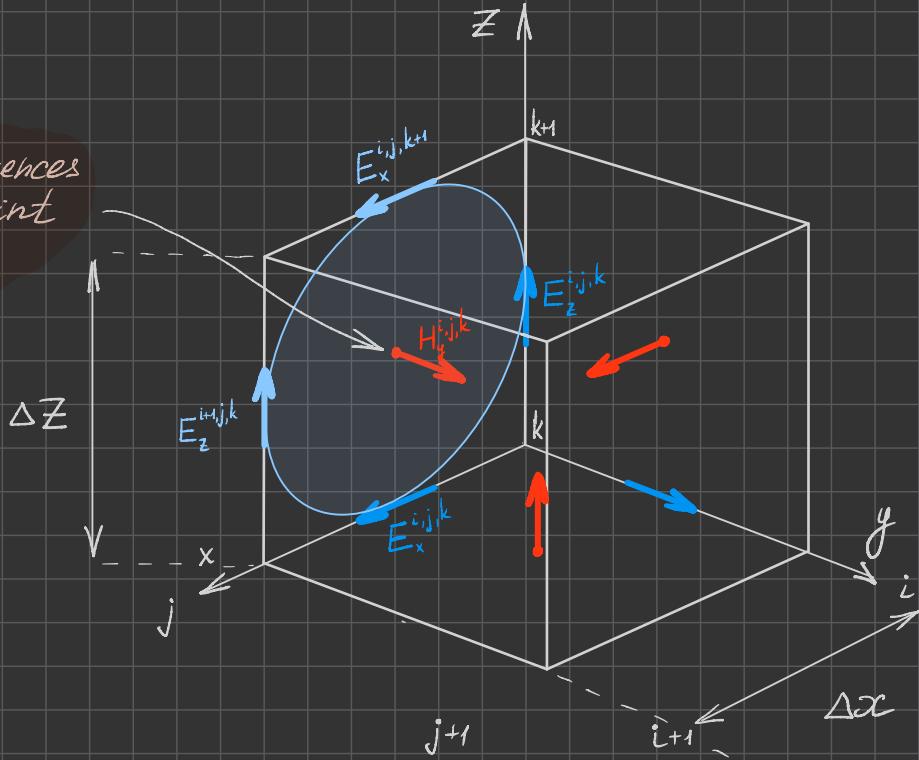
For the electric field derivative we need to reach to the next cells in space

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

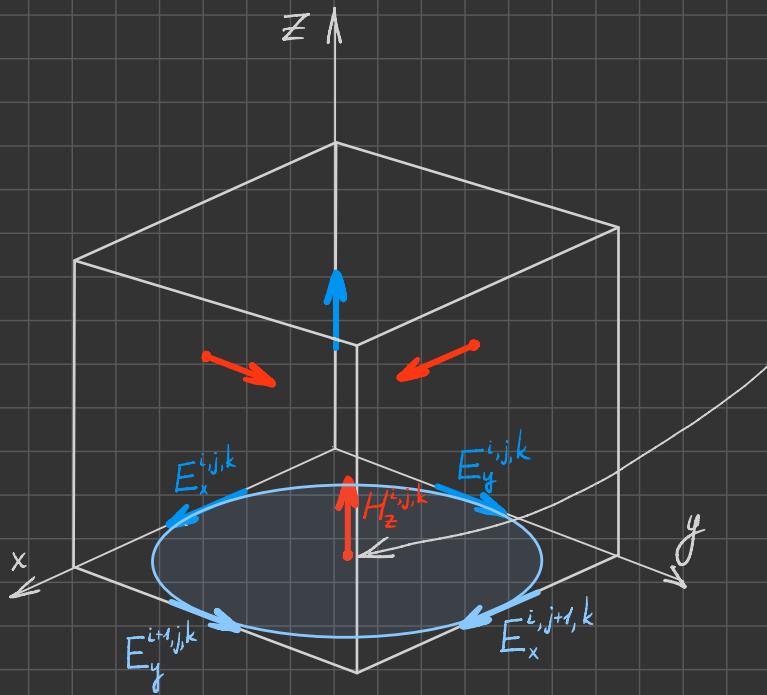
at time t



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

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

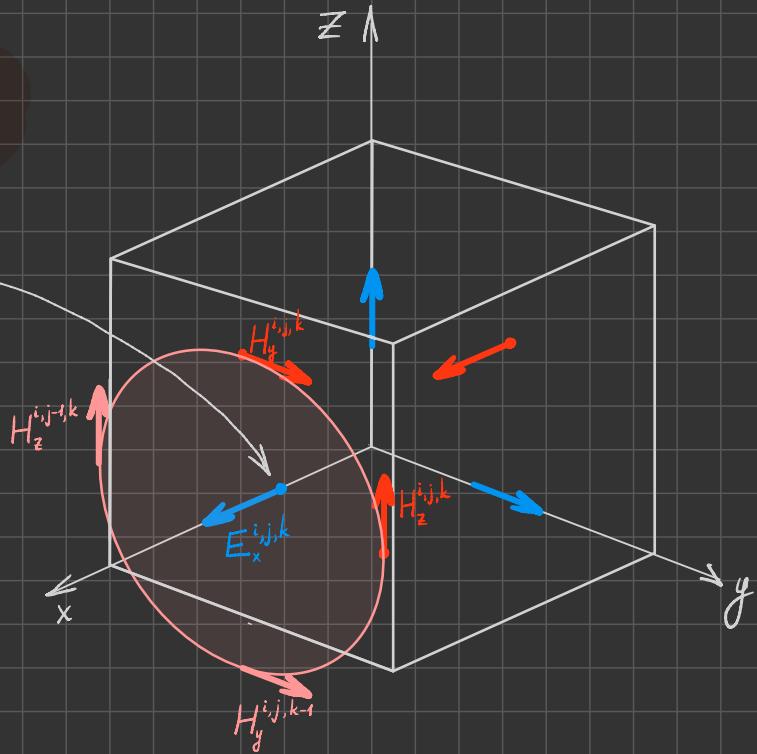
$$\frac{E_y^{i+1,j,k}|_t - E_y^{i,j,k}|_t}{\Delta x} - \frac{E_x^{i,j+1,k}|_t - E_x^{i,j,k}|_t}{\Delta y} = -\frac{1}{C_0} / \mu_{zz}^i \frac{H_z^{i,j,k}|_{t+\frac{\Delta t}{2}} - H_z^{i,j,k}|_{t-\frac{\Delta t}{2}}}{\Delta t} - M_z^{i,j,k}|_t$$

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

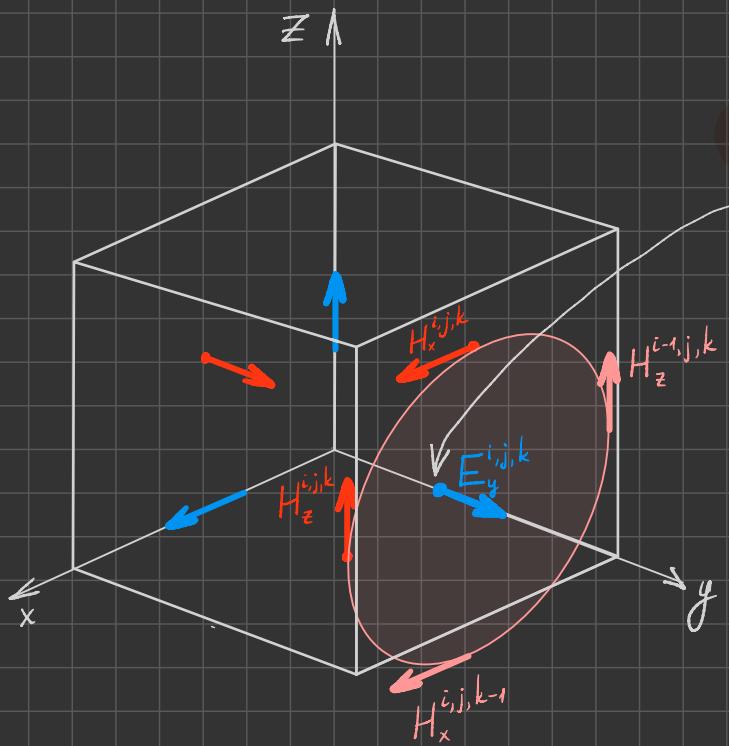


$$\frac{H_z^{i,j,k}|_{t+\frac{\Delta t}{2}} - H_z^{i,j-1,k}|_{t+\frac{\Delta t}{2}}}{\Delta y} - \frac{H_y^{i,j,k}|_{t+\frac{\Delta t}{2}} - H_y^{i,j,k-1}|_{t+\frac{\Delta t}{2}}}{\Delta z} = \frac{1}{C_0} \epsilon_{xx}^{i,j,k} \frac{E_x^{i,j,k}|_{t+\Delta t} - E_x^{i,j,k}|_t}{\Delta t} + \gamma_0 J_x^{i,j,k}|_{t+\frac{\Delta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

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

5

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



rewriting finite difference equations
for this point

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

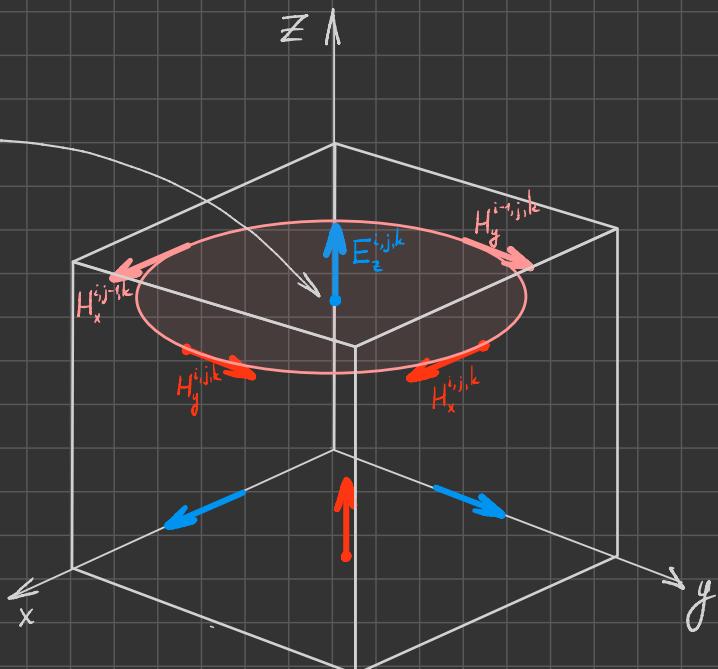
$$\frac{H_x^{i,j,k} \Big|_{t+\frac{\Delta t}{2}} - H_x^{i,j,k-1} \Big|_{t+\frac{\Delta t}{2}}}{\Delta z} - \frac{H_z^{i,j,k} \Big|_{t+\frac{\Delta t}{2}} - H_z^{i-1,j,k} \Big|_{t+\frac{\Delta t}{2}}}{\Delta x} = \frac{1}{C_0} \epsilon_{yy}^{i,j,k} \frac{E_y^{i,j,k} \Big|_{t+\Delta t} - E_y^{i,j,k} \Big|_t}{\Delta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

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)

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

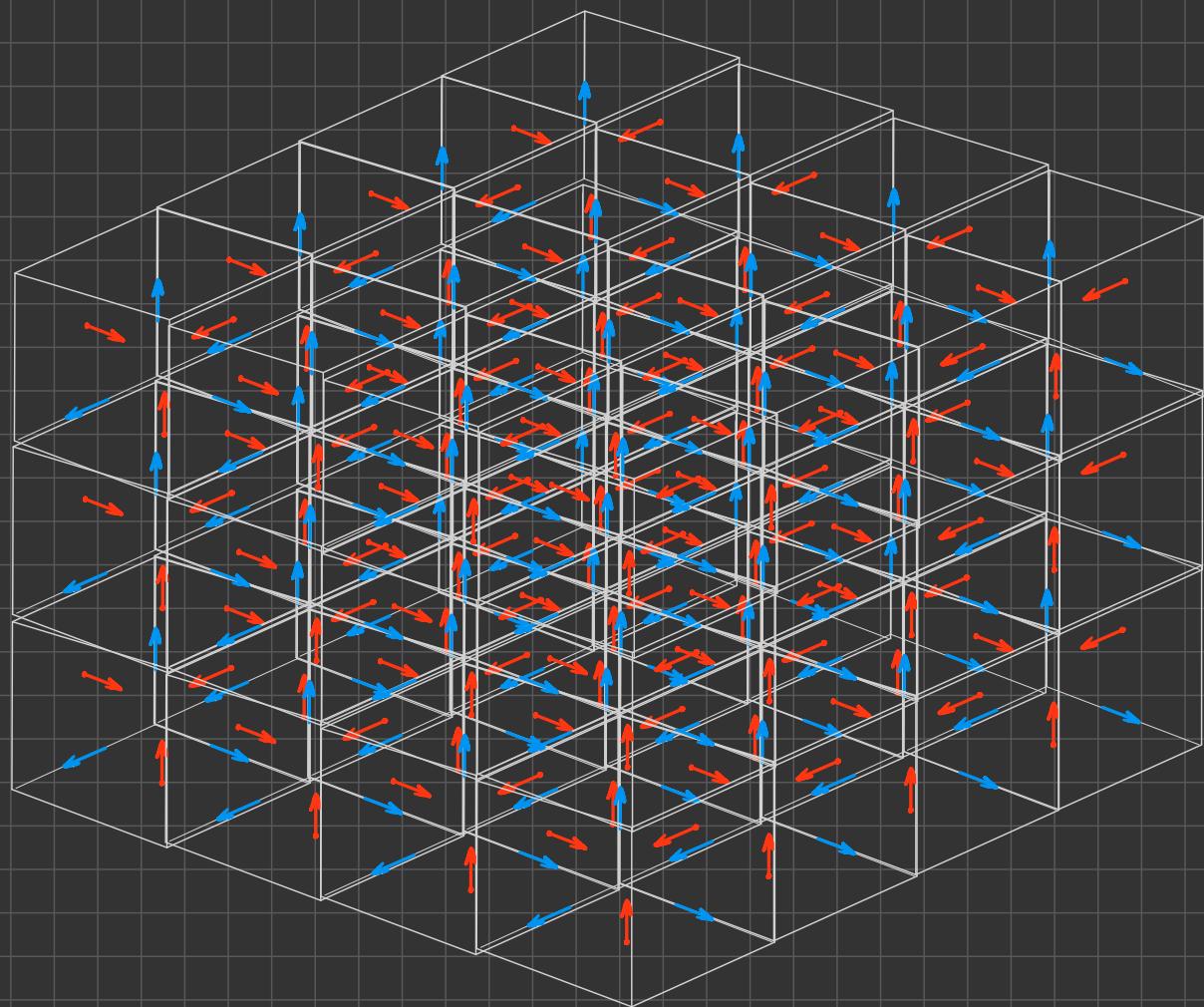
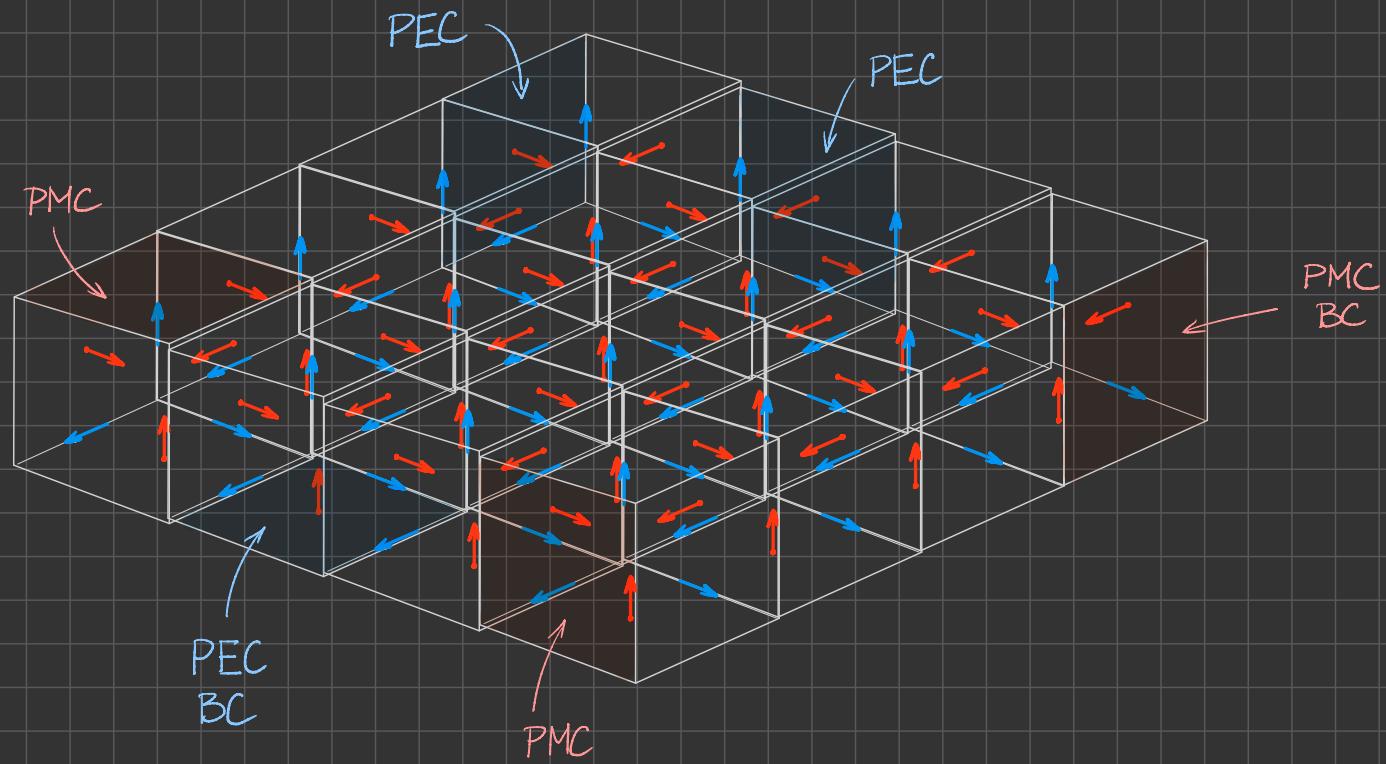
$$\frac{E_x^{i,j,k+1} - E_x^{i,j,k}}{\Delta z} - \frac{E_z^{i+1,j,k} - E_z^{i,j,k}}{\Delta x} = -\frac{1}{C_0} \mu_{yy}^{i,j,k} \frac{H_y^{i,j,k} \Big|_{t+\frac{\Delta t}{2}} - H_y^{i,j,k} \Big|_{t-\frac{\Delta t}{2}}}{\Delta t} - \mathcal{M}_y^{i,j,k} \Big|_t$$

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

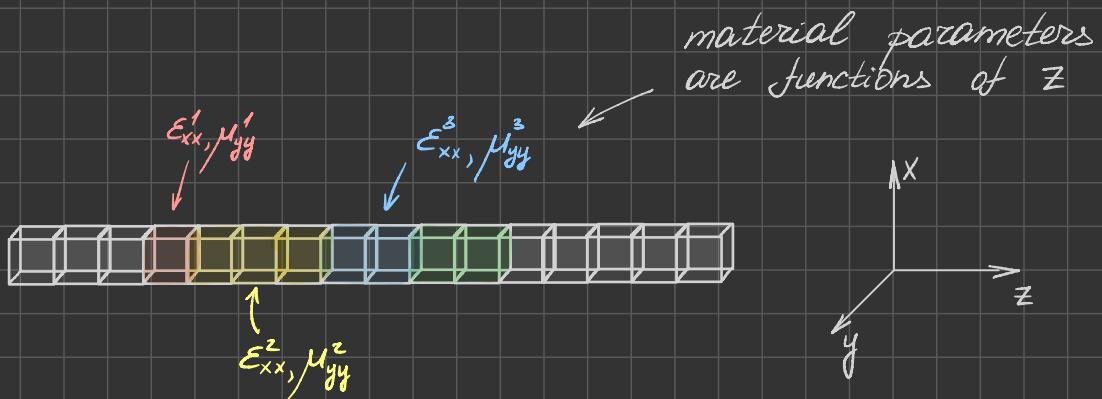
$$\frac{H_z^{i,j,k} \Big|_{t+\frac{\Delta t}{2}} - H_z^{i,j-1,k} \Big|_{t+\frac{\Delta t}{2}}}{\Delta y} - \frac{H_y^{i,j,k} \Big|_{t+\frac{\Delta t}{2}} - H_y^{i,j,k-1} \Big|_{t+\frac{\Delta t}{2}}}{\Delta z} = \frac{1}{C_0} \epsilon_{xx}^{i,j,k} \frac{E_x^{i,j,k} \Big|_{t+\Delta t} - E_x^{i,j,k} \Big|_t}{\Delta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

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

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



1D case



$$\partial_x = \partial_y = 0$$

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

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

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

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

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

E_x / H_y
mode

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

E_y / H_x
mode

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

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

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

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

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

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.

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

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

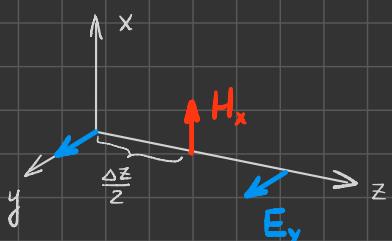
Let's derive update equations. (omit indices i and j)

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

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



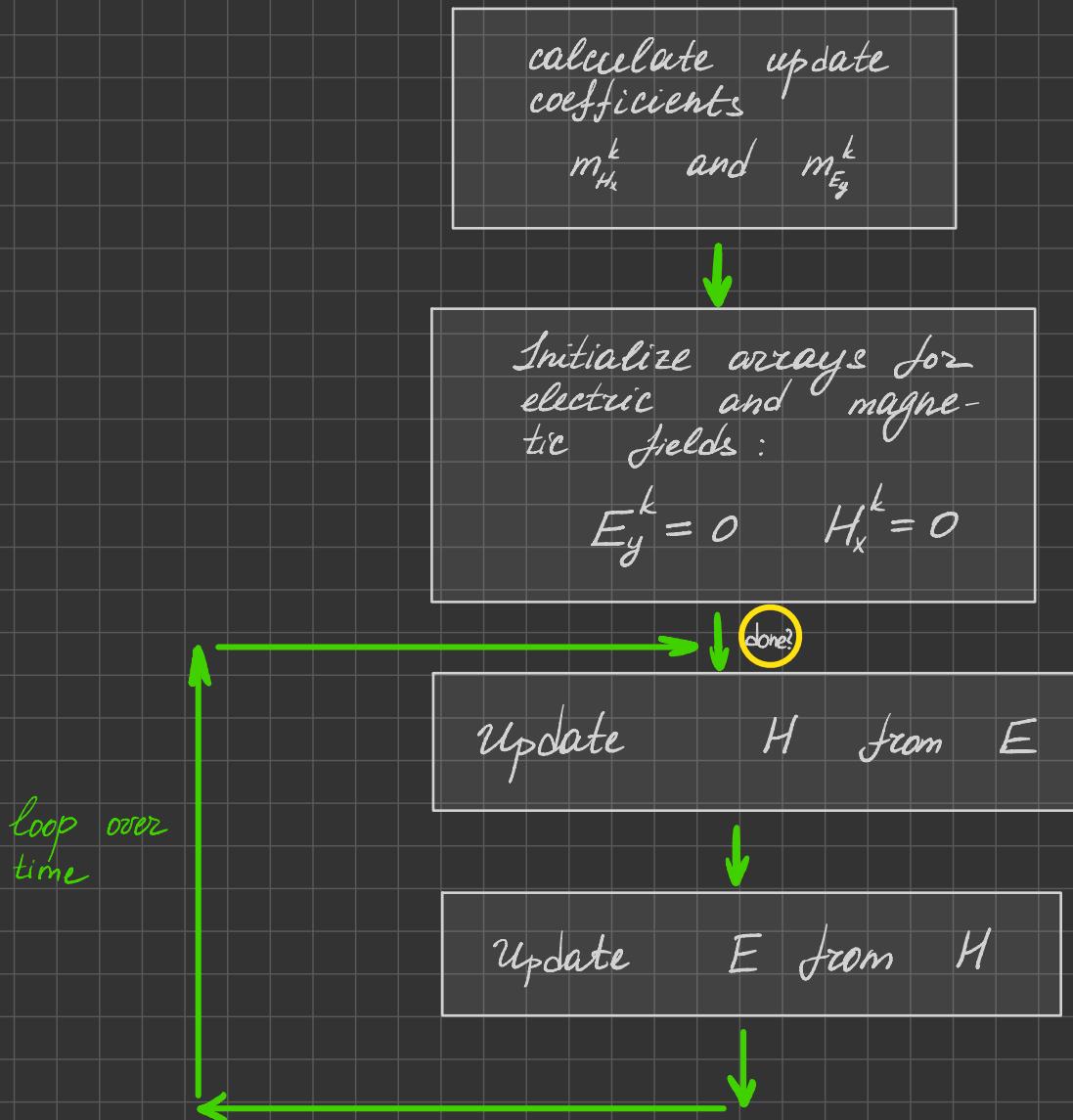
Implementation

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

} 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.

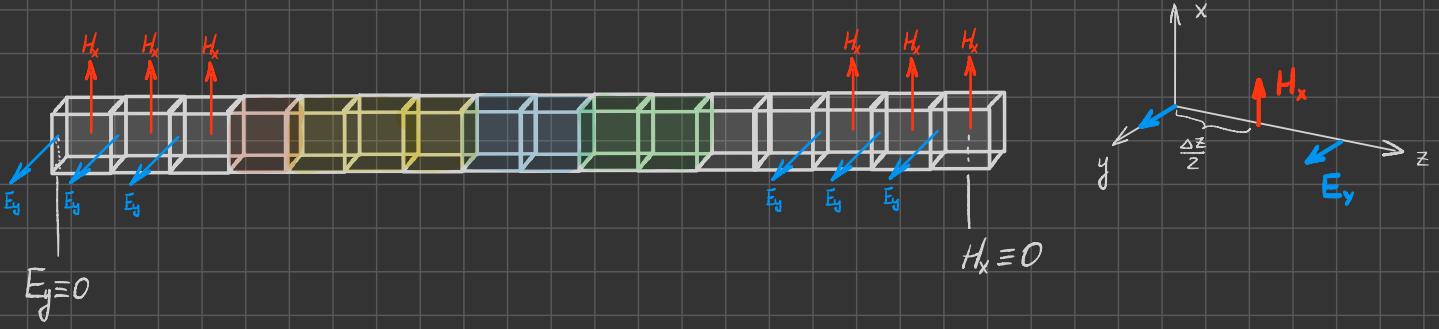
Force the values outside the grid to be zero

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

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



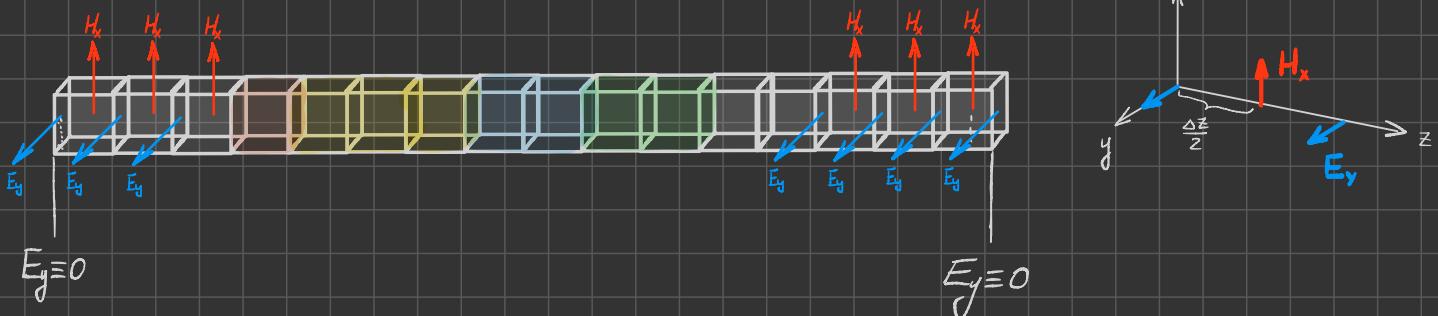
Sizes of arrays for E_y and H_x are the same :

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

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

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



$$H_x = \text{array}(N_z + 1)$$

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

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

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

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

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

Gaussian pulse

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

(base form)

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

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

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

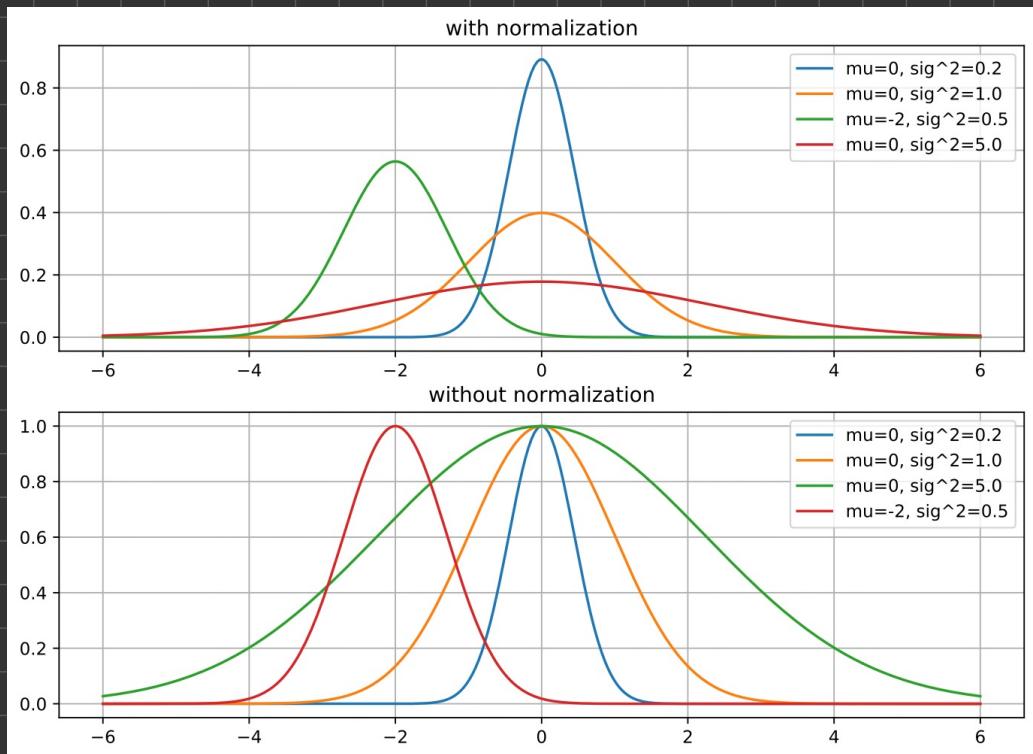
$$a = \frac{1}{c \sqrt{2\pi}}$$

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

$b = \mu$ — expected value

$c = \sigma$ — variance

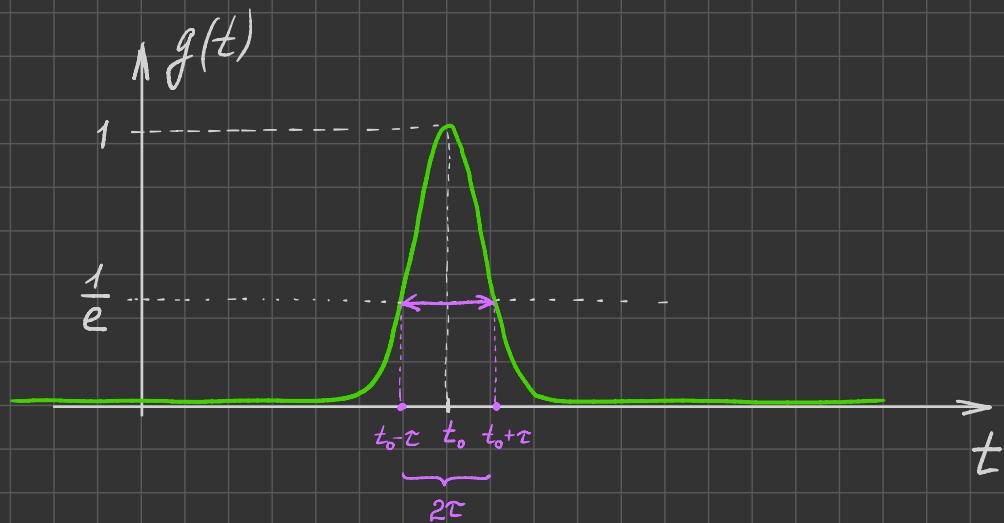
$$g(x) = \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$



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

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 (\approx 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

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

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

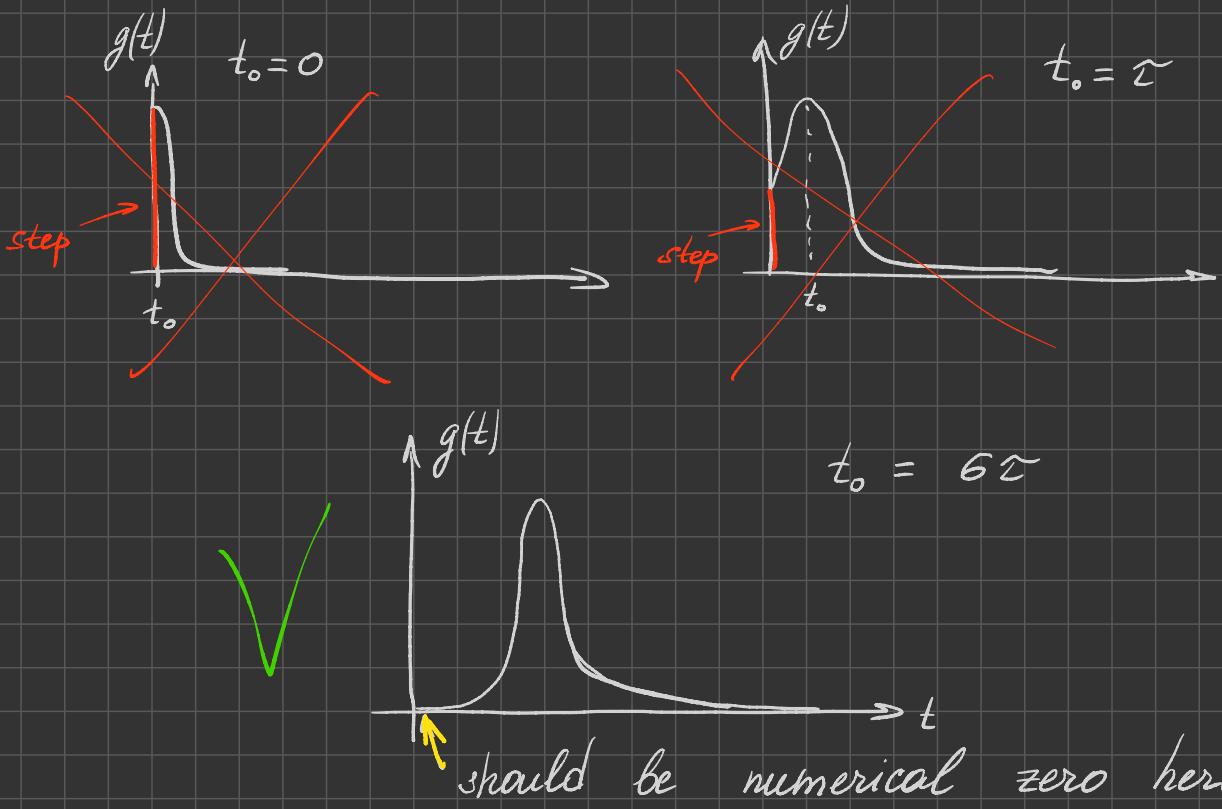
Then determine Δt_2 based on resolving

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

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

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

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

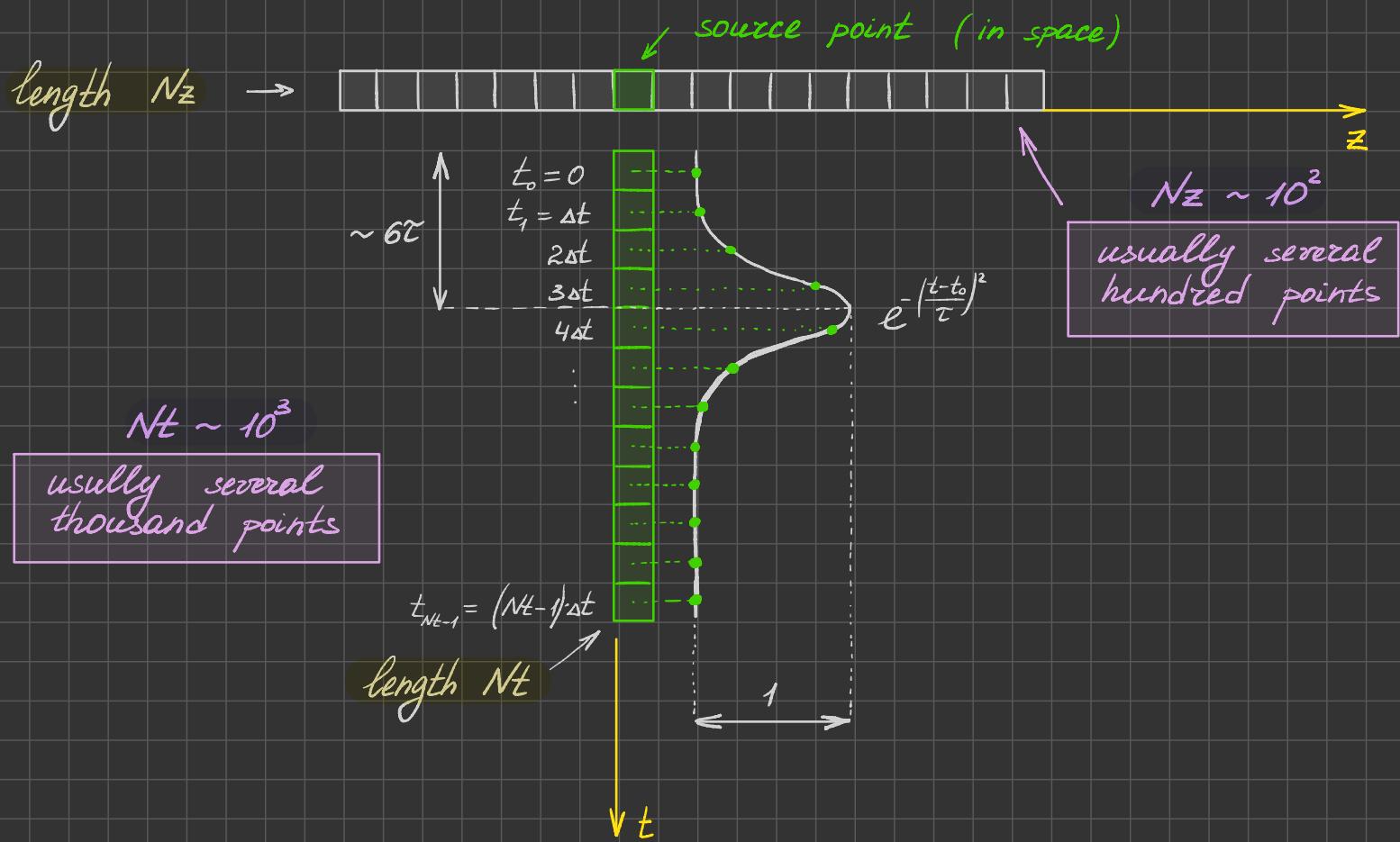
$$E_y^k \Big|_{t+\Delta t} + = g_E \Big|_t$$

- 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 Nt

Δt

Time resolution at

Courant - Friderich - Levy stability condition

over the duration of one time step Δt EM 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

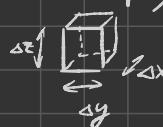
$$\Delta t < \frac{\Delta Z}{(C_0/n)}$$

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?

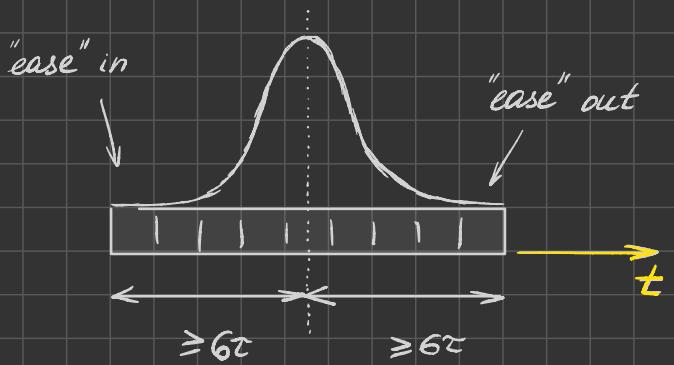
$$t_{\text{prop.}} = \frac{n_{\max} N_z \cdot \Delta z}{c_0}$$

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_{λ}	material
10 - 20	low contrast dielectric
20 - 30	high contrast dieel.
40 - 60	most metallic structures
100 - 200	plasmonic devices

2. Mechanical features

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



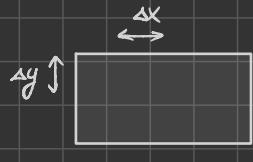
→ want to resolve this mechanical feat. d_{\min} with

1 to 4 cells Δ_d

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

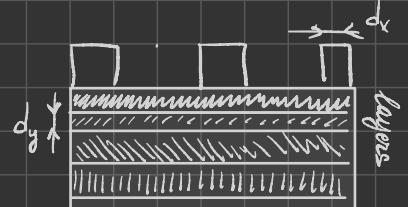
3. Adjust init. resolution Δz

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



4. "Snap" grid to critical dimensions

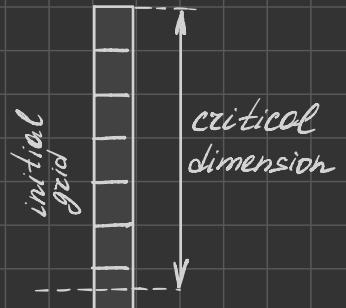
→ decide what dimensions along each axis are critical : d_x and d_y



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

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

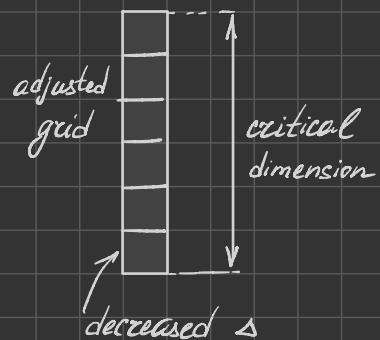
$$M_y \equiv \text{ceil} \left(\frac{d_y}{\Delta_y} \right)$$



→ 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

