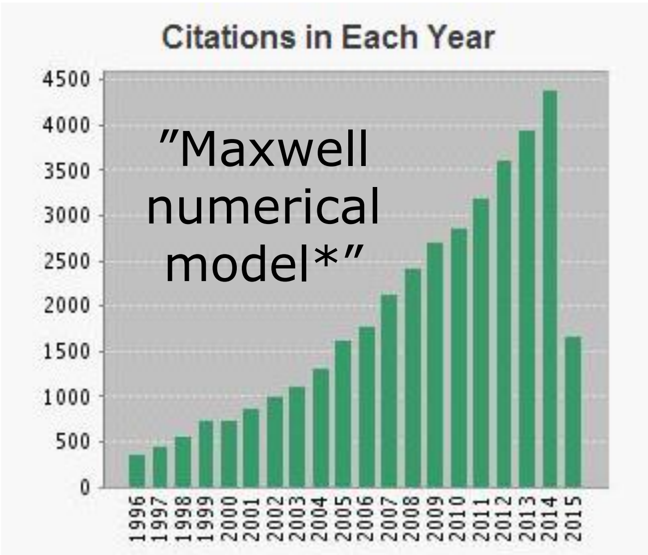
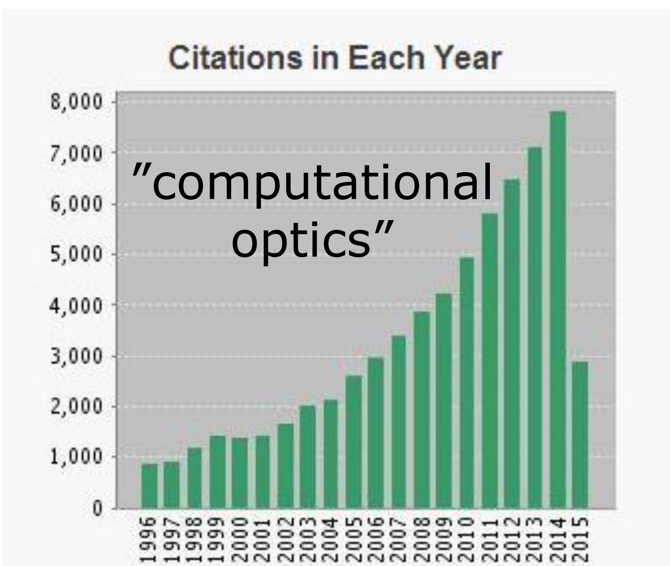
Finite-difference frequency-domain (FDFD) method

1. Introduction: computational electrodynamics





SWISS MADE speag

OptiFDTD

CST

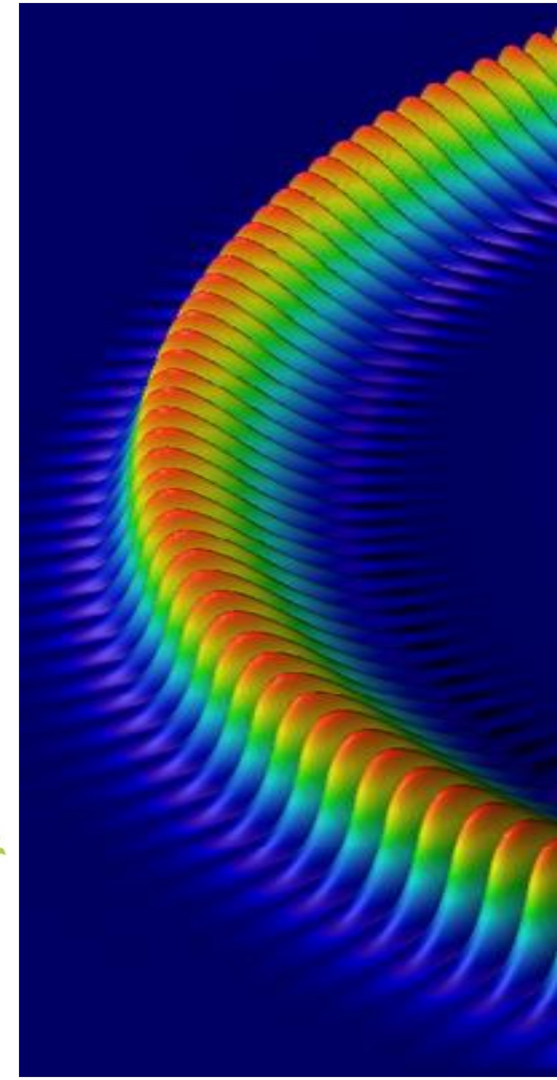
COMSOL

JCMwave

Photon Design®

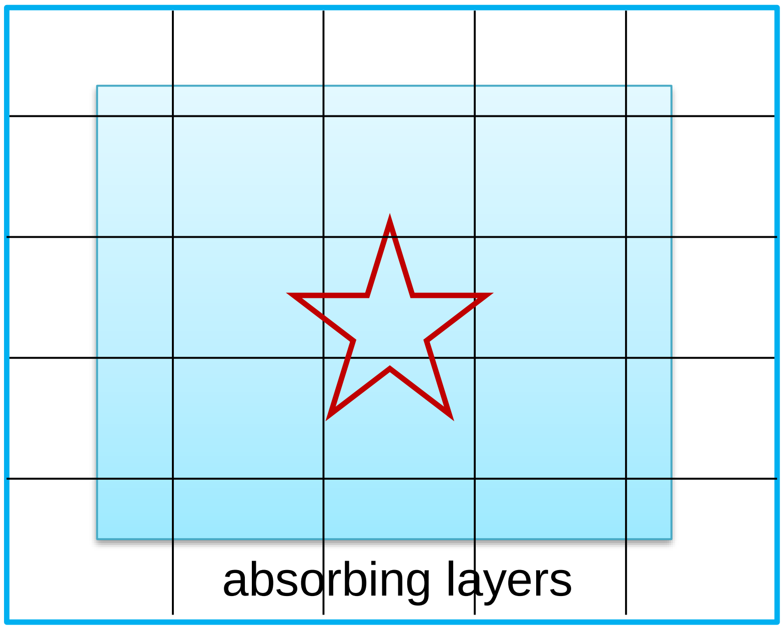
FEKO
Comprehensive Electromagnetic Solutions

ANSYS®



1. Introduction: numerical methods overview

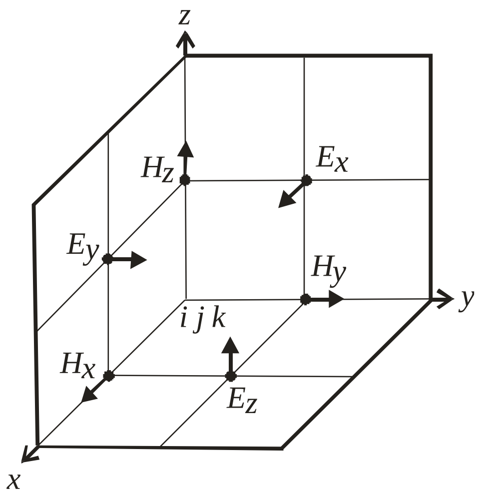
FDTD, FEM,
volume integral methods (VIM),
FDFD, DGTD,
method of lines (MoL),
Fourier modal method,
local eigenmode-modal method,
hybrid methods, Green functions



	Time Domain	Frequency Domain
Mesh generation effort	+	−
Transient simulation	+	−
Broadband solutions	+	0
Cosimulation	+	0
Low-frequency problems	−	+
Gigantic problems > 10^{10} unknowns	+	−
Nonlinear materials	+	−
Nonlinear cosimulation	+	−
Field and particle beam simulation	+	−
EMC simulations	+	0
Eigenmode calculations	−	+
Highly resonant structures	−	+
Periodic structures	0	+

[I. Munteanu, M. Timm, T. Weiland, 2010]

1. FDFD formulation: eigenproblem vs wave transmission



Maxwell's equations

$$\nabla \times \mathbf{E} = -\mu \frac{\partial \mathbf{H}}{\partial t} \qquad \nabla \times \mathbf{H} = \varepsilon \frac{\partial \mathbf{E}}{\partial t} + \mathbf{j}$$

$$\nabla \cdot \varepsilon \mathbf{E} = 0 \qquad \nabla \cdot \mu \mathbf{H} = 0$$

$$\frac{\partial}{\partial t} \rightarrow -i\omega$$

The eigenmode problem:

$$\frac{1}{\sqrt{\mu}} \nabla \times \frac{1}{\varepsilon} \nabla \times \frac{1}{\sqrt{\mu}} \sqrt{\mu}\mathbf{H} = \omega_{eig}{}^{2} \sqrt{\mu}\mathbf{H}$$

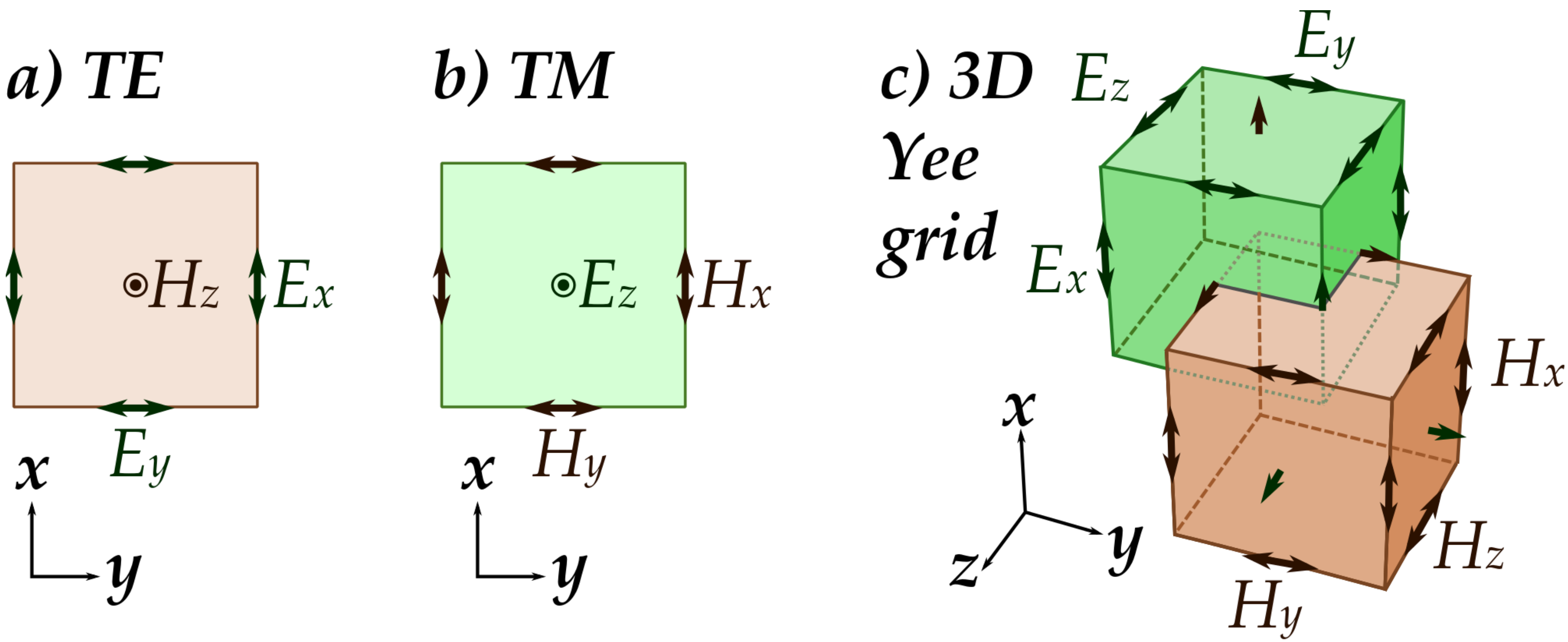
$$\omega_0 = \Re(\omega_{eig}), \quad Q = \frac{\omega_0}{2\Im(\omega_{eig})}$$

The wave scattering problem:

$$\left(\frac{1}{\sqrt{\mu}} \nabla \times \frac{1}{\varepsilon} \nabla \times \frac{1}{\sqrt{\mu}} - \omega^2 \right) \sqrt{\mu}\mathbf{H} = \mathbf{S}$$

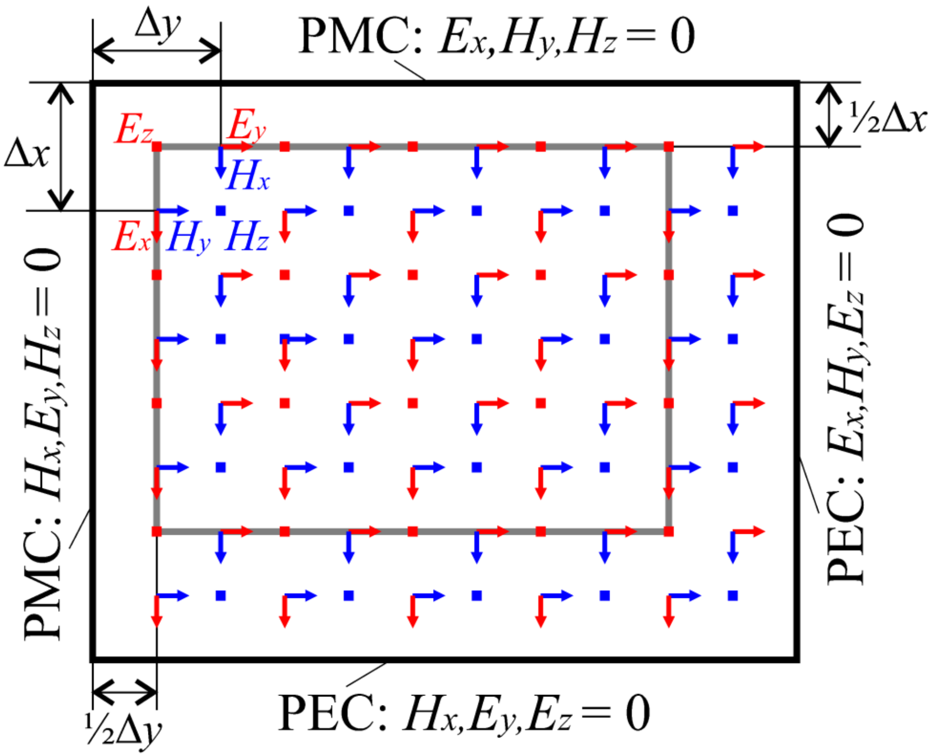
where $\mathbf{S} = \omega \sqrt{\mu^{-1}} \nabla \times \varepsilon^{-1} \mathbf{J}$

2. FDFD formulation: eigenproblem vs wave transmission



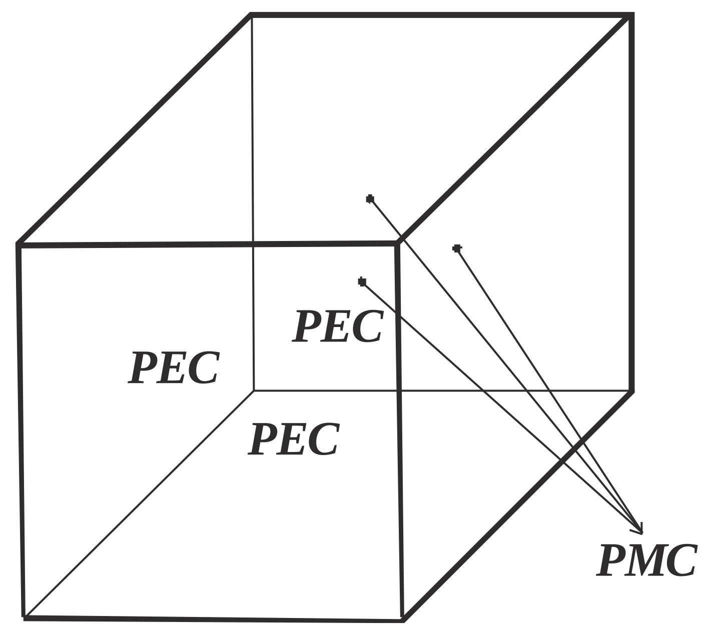
$$\nabla \times \mathbf{E} = -\mu \frac{\partial \mathbf{H}}{\partial t} \qquad \nabla \times \mathbf{H} = \varepsilon \frac{\partial \mathbf{E}}{\partial t} + \mathbf{j}$$

2. FDFD formulation: FDFD eigenproblem



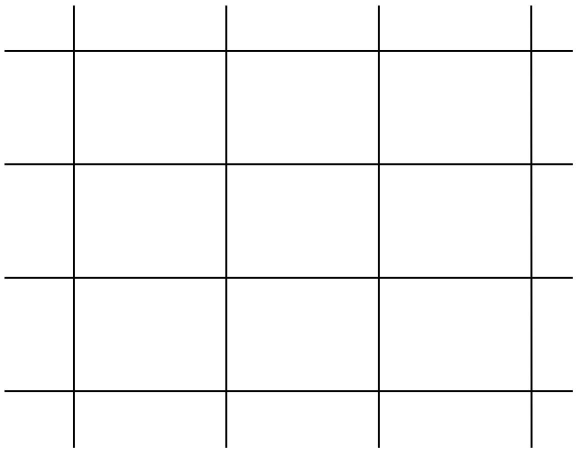
Forward differential:

$$f = \frac{1}{\Delta h} \cdot \begin{bmatrix} -1 & 1 & & \\ & \ddots & & \\ & & -1 & 1 \\ & & & -1 \end{bmatrix}$$

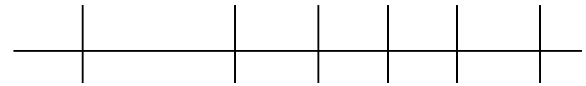


2. FDFD formulation: Non-uniform Meshes

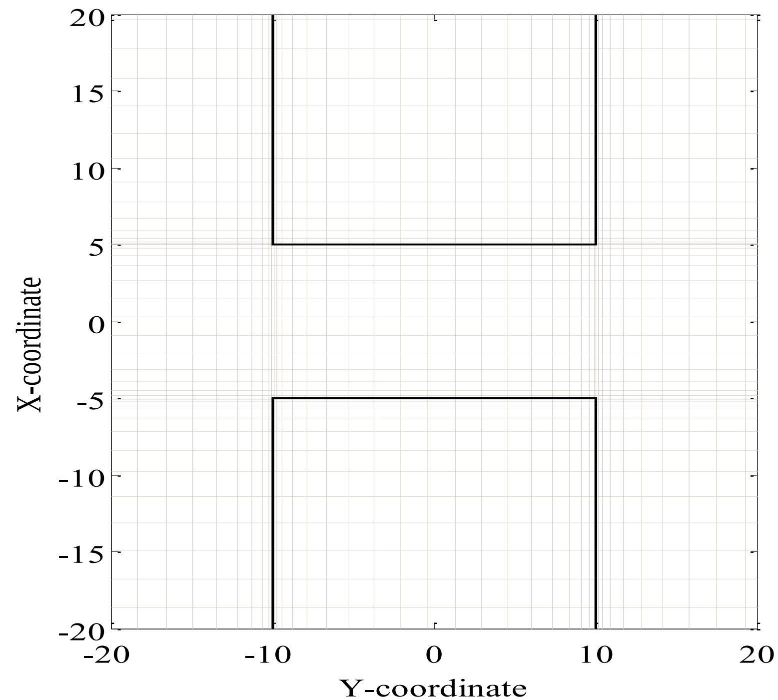
initial mesh



sub-gridding



alternative: uniformly varying grid density



1D FDFD: METAL CAVITY

3. 1D PROBLEM

Maxwell's equations

$$\nabla \times \mathbf{E} = -\mu\mu_0 \frac{\partial \mathbf{H}}{\partial t}$$

$$\nabla \times \mathbf{H} = \varepsilon\varepsilon_0 \frac{\partial \mathbf{E}}{\partial t}$$

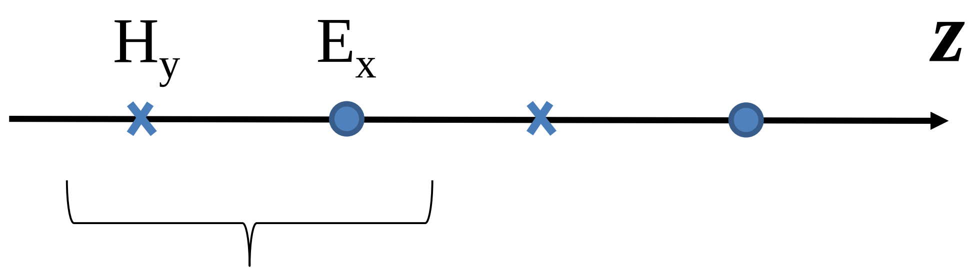
$$\frac{\partial}{\partial t} \rightarrow -i\omega$$

$$\frac{\partial E_x}{\partial z} = i\omega\mu\mu_0 H_y$$

$$\frac{\partial H_y}{\partial z} = -i\omega\varepsilon\varepsilon_0 E_x$$

$$\boxed{\frac{1}{\varepsilon}\frac{\partial}{\partial z}\frac{1}{\mu}\frac{\partial}{\partial z}E_x = -\left(\frac{\omega}{c}\right)^2 E_x}$$

$$\boxed{\frac{1}{\mu}\frac{\partial}{\partial z}\frac{1}{\varepsilon}\frac{\partial}{\partial z}H_y = -\left(\frac{\omega}{c}\right)^2 H_y}$$



Yee unit cell
staggered mesh

3. 1D FORWARD AND BACKWARD DIFFERENCES

Backward differential:

$$B = \frac{1}{\Delta z} \cdot \begin{bmatrix} 1 & & & 0 \\ -1 & \ddots & & \\ & -1 & 1 & \\ & & -1 & 1 \end{bmatrix} \qquad \begin{bmatrix} H_1 \\ H_2 \\ H_3 \\ \vdots \end{bmatrix}$$

Forward differential:

$$F = \frac{1}{\Delta z} \cdot \begin{bmatrix} -1 & 1 & & \\ & \ddots & & \\ & & -1 & 1 \\ 0 & & & -1 \end{bmatrix} \qquad \begin{bmatrix} E_1 \\ E_2 \\ E_3 \\ \vdots \end{bmatrix}$$

$$\boxed{\underbrace{\frac{1}{\varepsilon\mu} \mathrm{B\,F}}_{\text{eigenmatrix}} E_x = -\left(\frac{\omega_{eig}}{c}\right)^2 E_x}$$

$$\boxed{\lambda = \frac{2\pi c}{\Re(\omega_{eig})}, \qquad Q = \frac{\Re(\omega_{eig})}{2\Im(\omega_{eig})}}$$

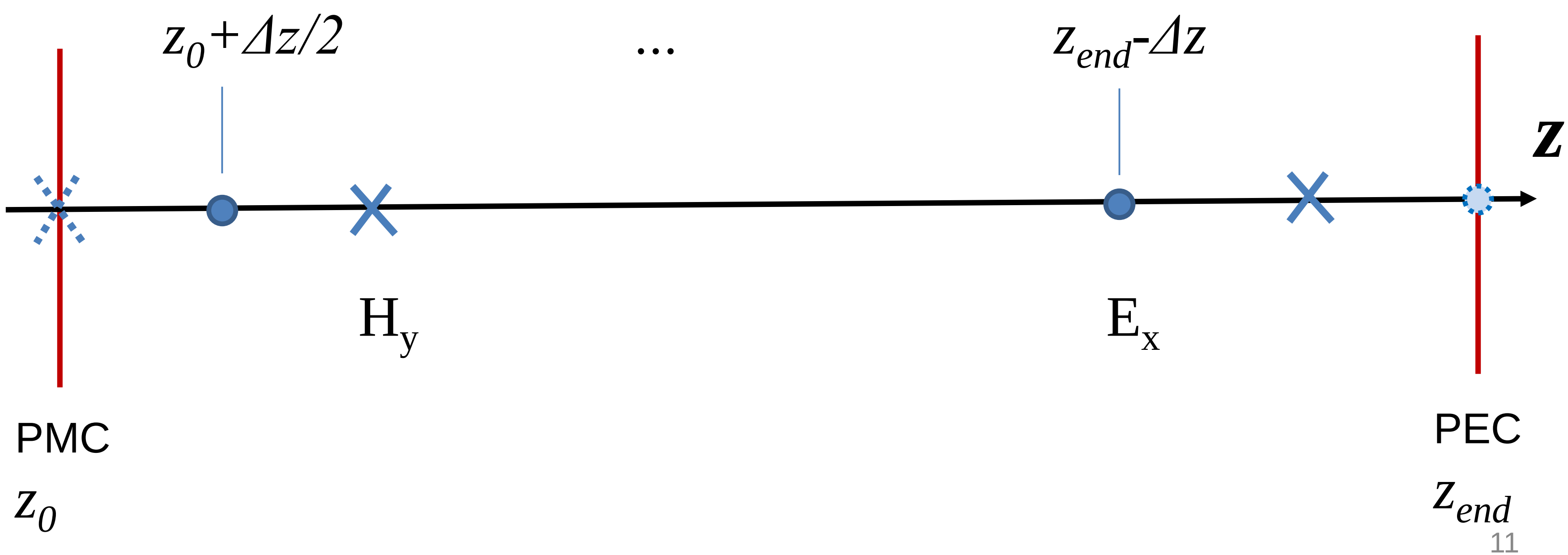
3. 1D FORWARD AND BACKWARD DIFFERENCES

Backward differential:

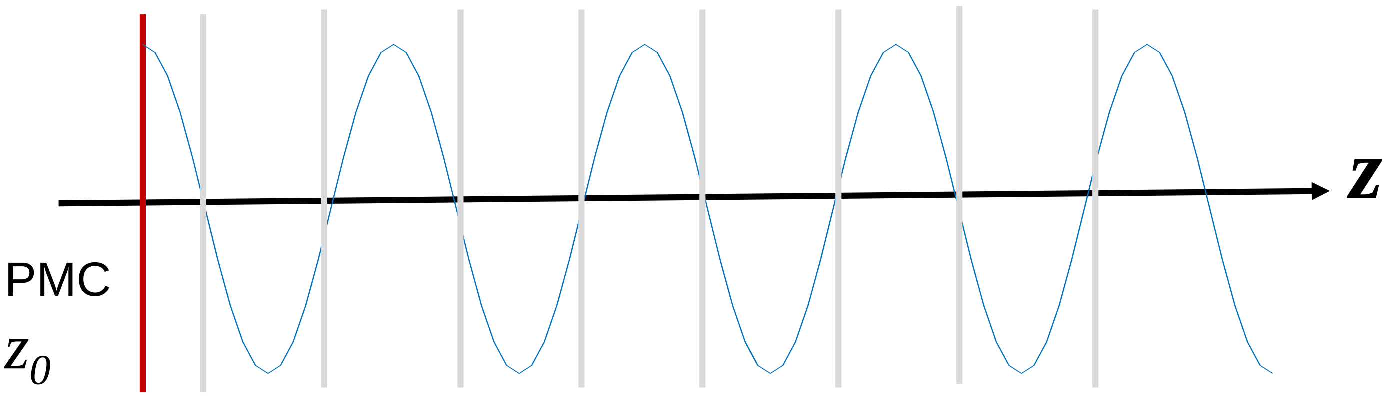
$$B = \frac{1}{\Delta z} \cdot \begin{bmatrix} 1 & & & 0 \\ -1 & \ddots & & \\ & -1 & 1 & \\ & & -1 & 1 \end{bmatrix} \qquad \begin{bmatrix} H_1 \\ H_2 \\ H_3 \\ \vdots \end{bmatrix}$$

Forward differential:

$$F = \frac{1}{\Delta z} \cdot \begin{bmatrix} -1 & 1 & & \\ & \ddots & & \\ & & -1 & 1 \\ 0 & & & -1 \end{bmatrix} \qquad \begin{bmatrix} E_1 \\ E_2 \\ E_3 \\ \vdots \end{bmatrix}$$



3. 1D PMC-PEC CAVITY



$$\frac{\lambda}{4} \quad \frac{3\lambda}{4} \quad \frac{5\lambda}{4} \quad \frac{7\lambda}{4} \quad \frac{9\lambda}{4}$$

=a (domain size)

$$\frac{\partial^2 E_x}{\partial z^2} + k_z{}^2 E_x = 0$$

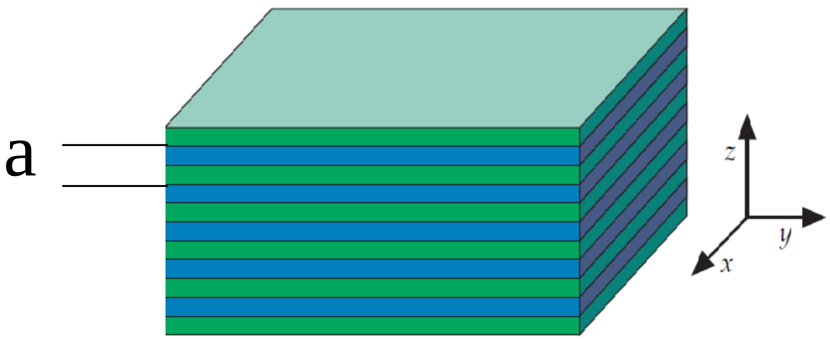
$$k_z = \frac{2\pi}{\lambda}$$

$$E_x = c_1 \cos(k_z z) + \cancel{c_2 \sin(k_z z)}$$

$$\lambda = \frac{4a}{2n+1}, n = 0, 1, 2, \ldots$$

1D FDFD: PERIODIC SOLUTION

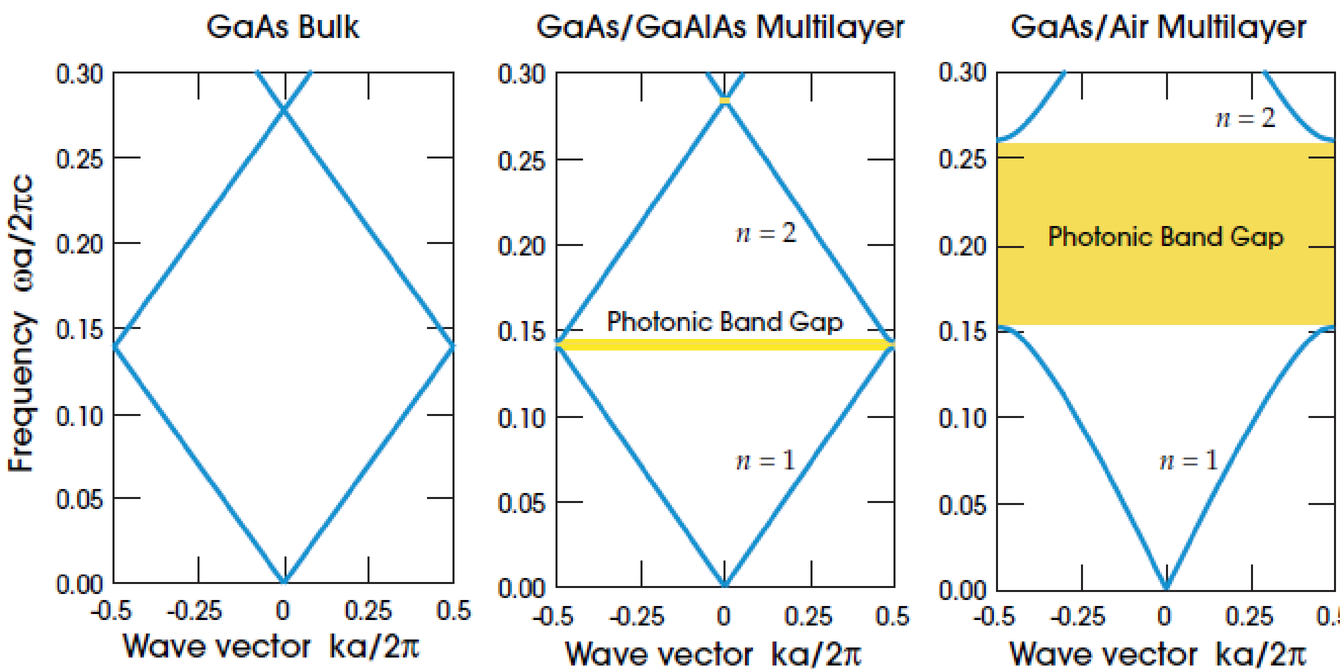
4. Band gap diagrams: multilayers



$$E_x(z) = e^{ik_z z}u(z)$$

$$u(z+a) = u(z)$$

$\varepsilon=13$ $\varepsilon_1=13,\ \varepsilon_2=12$ $\varepsilon_1=13,\ \varepsilon_2=1$



4. Band gap diagrams: 1st formulation

Forward differential:

$$\mathrm{F} = \frac{1}{\Delta z} \cdot \begin{bmatrix} -1 & 1 & & \\ & \ddots & & \\ & & -1 & 1 \\ e^{ik_z a} & & & -1 \end{bmatrix} \begin{bmatrix} E_1 \\ E_2 \\ E_3 \\ \vdots \end{bmatrix}$$

Backward differential:

$$\mathrm{B} = \frac{1}{\Delta z} \cdot \begin{bmatrix} 1 & & & -e^{ik_z a} \\ -1 & \ddots & & \\ & -1 & 1 & \\ & & -1 & 1 \end{bmatrix} \begin{bmatrix} H_1 \\ H_2 \\ H_3 \\ \vdots \end{bmatrix}$$

$$E_x(z+a) = e^{ik_z a} E_x(z)$$

$$\boxed{\underbrace{\frac{1}{\varepsilon\mu} \mathrm{B}\,\mathrm{F}}_{\text{eigenmatrix for particular } k_z} E_x = -\left(\frac{\omega_{eig}}{c}\right)^2 E_x}$$

eigenmatrix
for particular k_z

eigensolution

4. Band gap diagrams : 2nd formulation

Forward differential:

$$F = \frac{1}{\Delta z} \cdot \begin{bmatrix} -1 & 1 & & \\ & \ddots & & \\ & & -1 & 1 \\ 1 & & & -1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \end{bmatrix}$$

Backward differential:

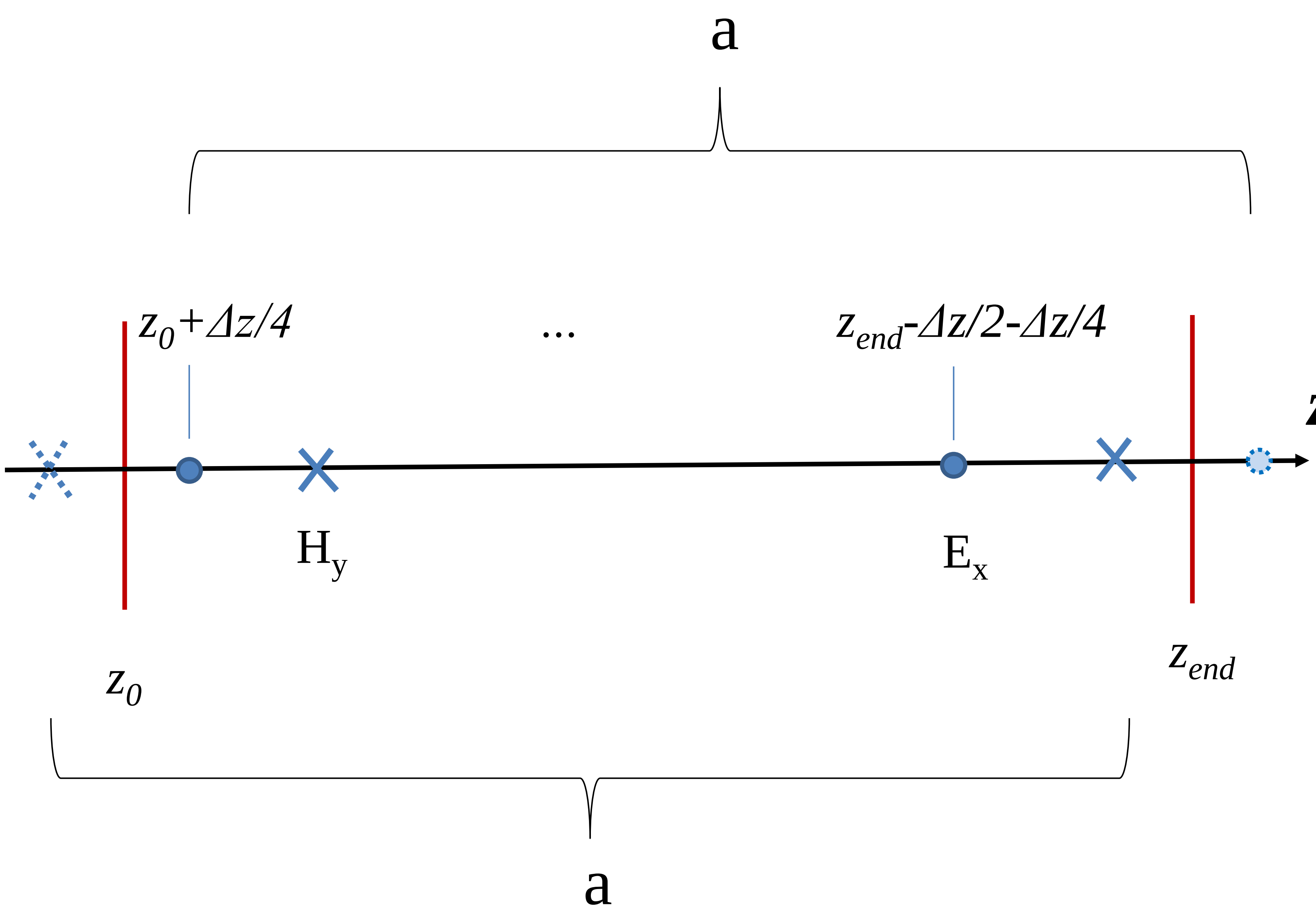
$$B = \frac{1}{\Delta z} \cdot \begin{bmatrix} 1 & & & 1 \\ -1 & \ddots & & \\ & -1 & 1 & \\ & & -1 & 1 \end{bmatrix}$$

$$u(z+a) = u(z)$$

$$E_x(z) = e^{ik_z z} u(z)$$

$$\frac{1}{\varepsilon\mu}(ik_z + B)(ik_z + F)u = -\left(\frac{\omega_{eig}}{c}\right)^2 u$$

4. Band gap diagrams : mesh and domain size



TASK ASSIGNMENT

5. Assignment

Task1:

- Find the modes of the PMC-PEC cavity.
- Check how solution improves as discretization becomes finer.
- Visualize the field inside the cavity.

Task2:

- Build 1D BG diagrams using 1st formulation. For particular k_z find several first eigenfrequencies ω_{eig}. (Do not pay attention to peculiarities of mesh generation at domain boundaries, use F and B from previous task. To impose periodicity use cosine fuction.)
- Construct the eigenmatrix for a multilayer consisting of two dielectrics of ε_1 and ε_2. Assume the layers have equal thickness. See how BG opens as contrast between ε_1 and ε_2 increases.

5. CHARTFLOW TO PROGRAMMING

1. Choose the domain size, for example, a=1.
2. Set the number of grid nodes n_{grid}.
3. Define the discretization unit $\Delta z = a / n_{grid}$.
4. For periodic conditions define k_z.
5. Define the differential operators F,B, each of size $[n_{grid}, n_{grid}]$.
6. Define the permittivity array. You will obtain matrix of size $[n_{grid}, n_{grid}]$ with inverse permittivity $1/\varepsilon$ on the main diagonal.
7. Assemble eigenmatrix. Find eigensolution.

Relevant Matlab functions:

spdiags
ones, repmat
eigs

Relevant Python functions:

numpy.ones
numpy.vstack
scipy.sparse.spdiags
sp.sparse.lil_matrix
scipy.sparse.lil_matrix.transpose
scipy.sparse.linalg.eigs

3D FDFD

6. 3D FDFD FORMULATION

$$\left(\frac{\omega}{c}\right)^2 \begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix} = \begin{bmatrix} \epsilon_{xx}^{-1} & & \\ & \epsilon_{yy}^{-1} & \\ & & \epsilon_{zz}^{-1} \end{bmatrix} \begin{bmatrix} 0 & -V_z & V_y \\ V_z & 0 & -V_x \\ -V_y & V_x & 0 \end{bmatrix}$$

$$\begin{bmatrix} \mu_{xx}^{-1} & & \\ & \mu_{yy}^{-1} & \\ & & \mu_{zz}^{-1} \end{bmatrix} \begin{bmatrix} 0 & -U_z & U_y \\ U_z & 0 & -U_x \\ -U_y & U_x & 0 \end{bmatrix} \begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix}$$

$$U_x = \frac{1}{dx} \hat{I}_{nz} \otimes \hat{I}_{ny} \otimes F_{nx}$$

$$U_y = \frac{1}{dy} \hat{I}_{nz} \otimes F_{ny} \otimes \hat{I}_{nx}$$

$$U_z = \frac{1}{dz} F_{nz} \otimes \hat{I}_{ny} \otimes \hat{I}_{nx}$$

$$\hat{V} = -\hat{U}^T$$

I_{n_x,n_y,n_z} unit matrix

$\otimes$ Kronecker product