Content of this lecture

1. Overview of numerical methods for nanophotonics
2. Finite difference time domain (FDTD) method
3. Finite element method (FEM)
4. Comparison of FDTD and FEM

Why rigorous numerical methods?

- To understand the fundamental physics of nanophotonic structures and phenomena, we need analytical theories (such as Mie theory) and models (such as Fano model), which are often only applicable to simple geometries or otherwise with many assumptions!

- To simulate the EM responses of nanostructures and perform designs and optimizations, we need rigorous numerical methods to implement "numerical experiments" (in analogy with the laboratory experiments), which are much cheaper, time-saving, convenient, reliable …

- There are various numerical methods for different categories of nanostructures (e.g., for photonic crystals, there are Plane Wave Expansion method, FDTD method, Transfer Matrix method, etc.)

- In this lecture, we introduce some commonly used numerical methods for nanophotonics. The principles and implementations of two most popular methods FDTD and FEM are presented in detail.

analytical: 解析的，simulate: 模拟，optimization: 优化，rigorous: 严格的，numerical: 数值的

1. Overview of the numerical methods

Classification of the numerical methods:

- Frequency-domain methods vs. time-domain methods
- Domain-discretization methods vs. boundary-discretization methods
- Methods for periodic structures vs. methods for aperiodic structures
- Near-field methods vs. far-field methods
- Fully-vectorial methods vs. approximate methods
- …

All the methods ***solve Maxwell's equations*** by certain techniques

- There are quite many methods and commercial softwares available
- However, <u>no a single method (software) can solve all problems!</u>
- Users are required to be very familiar with the software, the principle & limitations of the technique, and the problem being analyzed

frequency-domain: 频域，time-domain: 时域，discretization: 离散化，aperiodic: 非周期性的

Frequency-domain methods

Method of Moment (MoM)

Finite Element Methods (FEM)

Modal methods for gratings:
- Fourier Modal Method (FMM)
- Coordinate-transformation method (C Method)

Time-domain methods

Finite Difference Time Domain (FDTD)

Multi-Resolution Time Domain (MRTD)

Pseudo-Spectral Time Domain (PSTD)

Learn more about numerical methods for gratings in Prof. Lifeng Li's course: ***Electromagnetic theory of gratings***

Finite Element Method: 有限元法，Finite Difference Time Domain: 时域有限差分法

Domain-discretization methods

- Finite Element Methods (FEM)
- Finite Difference Time Domain (FDTD)

Boundary-discretization methods

- Multiple Multipole Program (MMP)
- Method of Auxiliary Sources (MAS)
- Meshless Boundary Integral Equation (BIE) Approach

Smajic et al., “Comparison of Numerical Methods for the Analysis of Plasmonic Structures”, Journal of Computational and Theoretical Nanoscience **6**, 763 (2009)

Methods for periodic structures

- Fourier Modal Method (FMM)
- Coordinate-transformation method (C Method)
- Differential Method
- Integral Method
- Rayleigh-Fourier Method
- Iterative Method

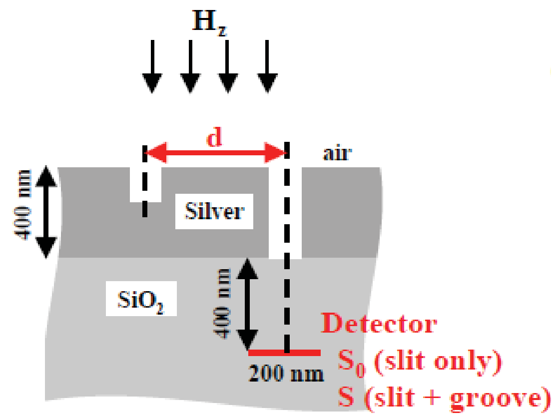
Methods for aperiodic structures

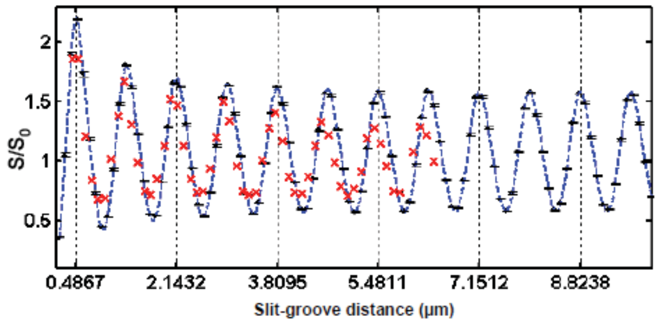
- Finite Difference Time Domain (FDTD)
- Finite Element Methods (FEM)
- Aperiodic FMM (a-FMM)
- Volume Integral Method (VIM)
- Method of Lines (MoL)
- Local Eigenmode-Modal Method (LEMM)

Loewen and Popov, *Diffraction Gratings and Applications* (Marcel Dekker, 1997)
Besbes et al., J. Eur. Opt. Soc.-Rapid Publ. **2**, 07022 (2007)

Benchmark of various methods

Numerical analysis of a slit-groove diffraction problem





Method category	Acronym	Institution
Aperiodic Fourier Modal Method (a-FMM)	MM1	Delft Univ. of Technol.
	MM2	LASMEA
	MM3	Institut d'Optique
Method of Lines (MOL)	MM4	Fern Univ.
Local Eigenmode-Modal method (CAMFR)	MM5	Ghent Univ.
FDTD method	FDTD1	Delft Univ. of Technol.
	FDTD2	Institut FEMTO-ST
	FDTD3	Northwestern Univ.
Finite Element Method	FEM1	Delft Univ. of Technol.
	FEM2	Institut d'Optique
Volume Integral method	VIM	Delft Univ. of Technol.
Hybrid a-FMM/FEM	HYB	Institut d'Optique

See Besbes et al., J. Eur. Opt. Soc.-Rapid Publ. **2**, 07022 (2007)

For other benchmark reports, see:

Mode solvers for waveguides: Bienstman et al., Opt. Quantum Electron. **38**, 731 (2006)

Numerical methods for gratings: Nevière and Popov, SPIE **3450**, 2 (1998)

benchmark: 基准对比试验

- According to my experience, FDTD and FEM are the most popular methods used for modeling complex (esp. aperiodic) nanostructures

  Advantages:
  - Flexible for modeling almost any arbitrary complex geometries
  - FDTD can easily show the temporal evolution of field
  - Strength on the modeling and representation of near-field response

  Disadvantages:
  - Heavy computation load: long computation time & huge memory cost (10+G)
  - Practically not suitable for far-field calculation

- FMM (or the so-called RCWA) is the most commonly used method for modeling periodic structures (gratings)

  Advantages:
  - Fast (a few seconds for a single calculation), accurate, and efficient
  - Computation resources cost-effective: low memory cost on desktop computer
  - Strength on the modeling of far-field response of gratings

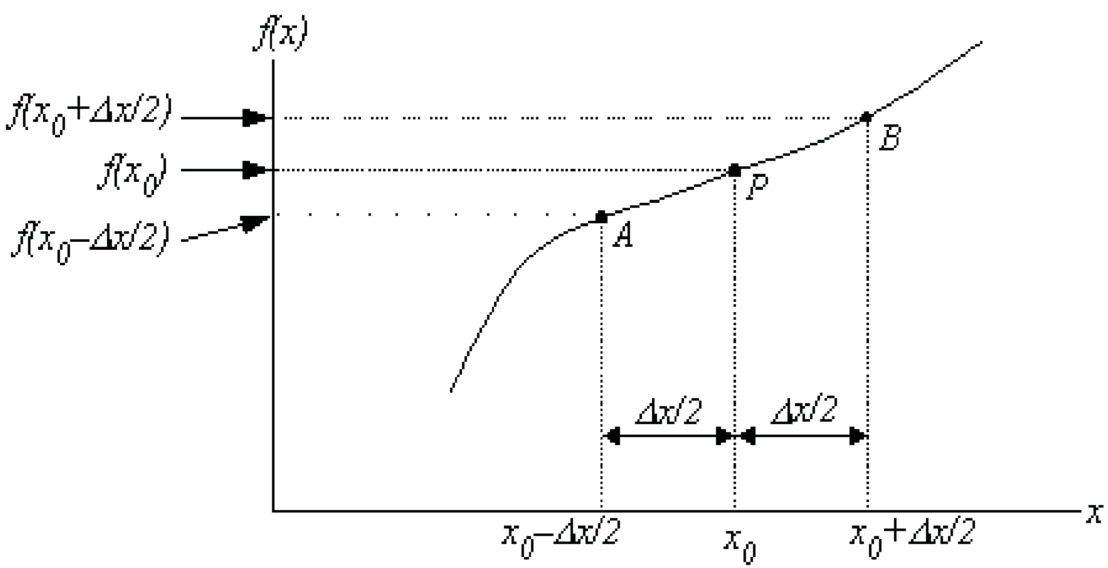
  Disadvantages:
  - Challenges in modeling complex-patterned structures (such as sphere array)
  - Not suitable for modeling aperiodic structures (although a-FMM is available)

temporal: 时间的， evolution: 演进

2. Finite difference time domain (FDTD) method

Principle of finite difference

$$\frac{df(x_0)}{dx} = f^{'}(x_0) \cong \frac{f(x_0 + \Delta x/2) - f(x_0 - \Delta x/2)}{\Delta x}$$



Derivative of $f(x)$ at point P is approximated by the ***finite difference***

derivative: 微分，finite difference: 有限差分

A more rigorous derivation by *Taylor series* expansion

- Taylor series expansion of $f(x_i, t_n) \equiv f_i^n$ around a given position x_i:

$$\frac{\partial f}{\partial x}\bigg|_i^n = \frac{1}{2\Delta x}\left\{f_{i+1}^n - f_{i-1}^n\right\} - \frac{1}{6}(\Delta x)^2 \frac{\partial^3 f}{\partial x^3}\bigg|_i^n - \ldots$$

- Therefore, for space derivative, we have:

$$\frac{\partial f}{\partial x}\bigg|_i^n \approx \frac{1}{2\Delta x}\left\{f_{i+1}^n - f_{i-1}^n\right\}$$

- Similarly, for time derivative, we have:

$$\frac{\partial f}{\partial t}\bigg|_i^n \approx \frac{1}{2\Delta t}\left\{f_i^{n+1} - f_i^{n-1}\right\}$$

Derivation of FDTD algorithm

- Starting from Maxwell's differential equations:

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

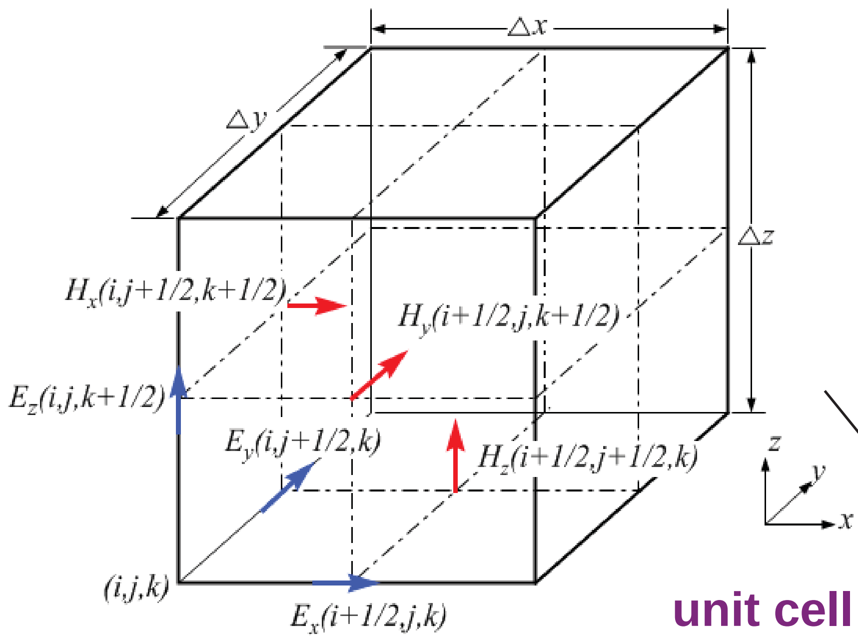
$$\begin{bmatrix} \frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} \\ \frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} \\ \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} \end{bmatrix} = \varepsilon \cdot \begin{bmatrix} \frac{\partial E_x}{\partial t} \\ \frac{\partial E_y}{\partial t} \\ \frac{\partial E_z}{\partial t} \end{bmatrix} \qquad\qquad \begin{bmatrix} \frac{\partial E_z}{\partial y} - \frac{\partial E_y}{\partial z} \\ \frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x} \\ \frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} \end{bmatrix} = -\mu \cdot \begin{bmatrix} \frac{\partial H_x}{\partial t} \\ \frac{\partial H_y}{\partial t} \\ \frac{\partial H_z}{\partial t} \end{bmatrix}$$

- All the partial derivatives of field components are to be approximated by finite differences

- For this purpose, the structure should first be discretized into meshes

derivation: 推导， algorithm: 算法， partial derivative: 偏微分， mesh: 网格

Mesh Structure for FDTD Algorithm

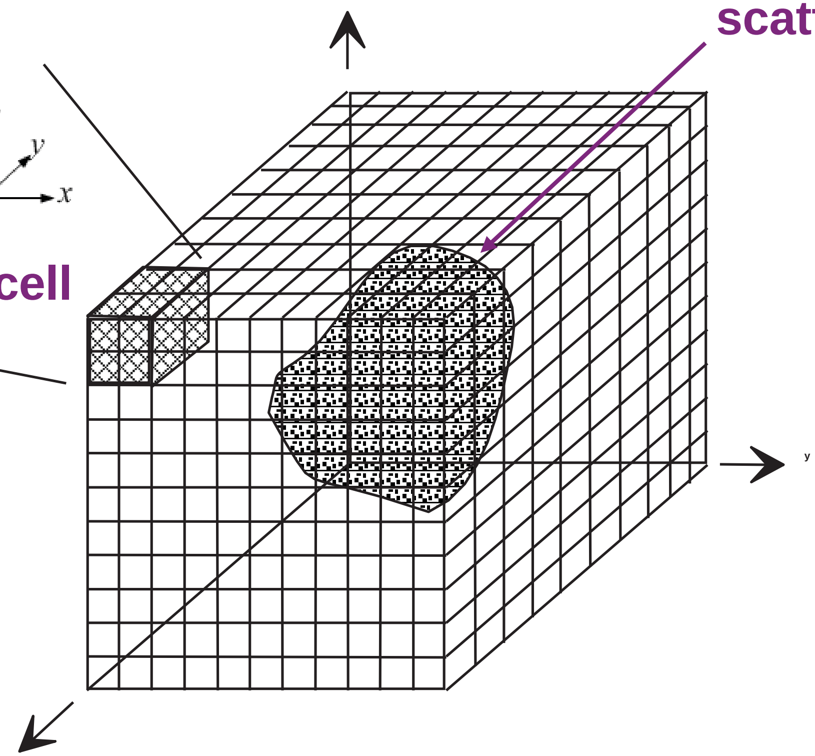


Standard Yee's lattice

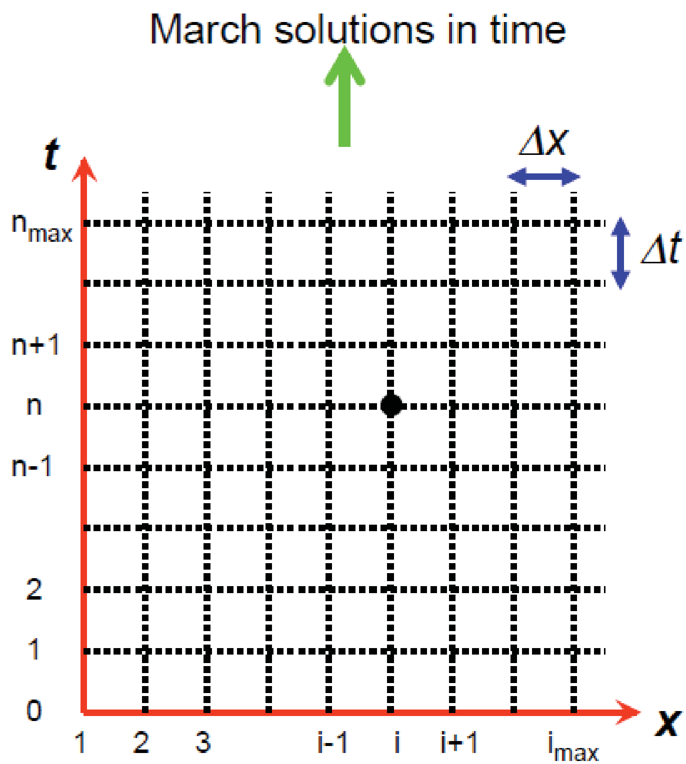
The **entire volume** (not just the scatter) is meshed!

scatterer

unit cell



scatterer: 散射体，unit cell: 单位元



Gridlines **in space**: $x_i = (i\text{-}1)\Delta x$

Gridlines **in time**: $t_n = n\Delta t$

- Solution is obtained by time-marching values of the physical quantity to determine its value at grid points corresponding to higher n
- Implement the finite difference by using Taylor series expansions of function around the grid points

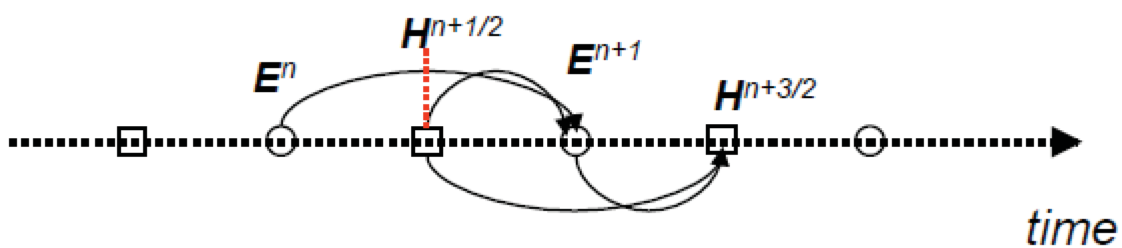
- Time derivatives of fields are solved with the updating of **E** and **H** staggered in time by one half time-step, i.e.,
  - write **H** field at half time steps *n*+1/2
  - write **E** field at integral time steps *n*

$$\left.\frac{\partial f}{\partial t}\right|_i^n \approx \frac{1}{2\Delta t}\left\{f_i^{n+1} - f_i^{n-1}\right\}$$

$$\left.\frac{\partial \boldsymbol{E}}{\partial t}\right|^{n+1/2} \approx \frac{\boldsymbol{E}^{n+1} - \boldsymbol{E}^{n}}{\Delta t} = \frac{1}{\varepsilon}[\nabla \times \boldsymbol{H}]^{n+1/2} \qquad \left.\frac{\partial \boldsymbol{H}}{\partial t}\right|^{n} \approx \frac{\boldsymbol{H}^{n+1/2} - \boldsymbol{H}^{n-1/2}}{\Delta t} = -\frac{1}{\mu}[\nabla \times \boldsymbol{E}]^{n}$$

$$\Downarrow \qquad\qquad \Downarrow$$

$$\boldsymbol{E}^{n+1} = \boldsymbol{E}^{n} + \frac{\Delta t}{\varepsilon}[\nabla \times \boldsymbol{H}]^{n+1/2} \qquad \boldsymbol{H}^{n+3/2} = \boldsymbol{H}^{n+1/2} - \frac{\Delta t}{\mu}[\nabla \times \boldsymbol{E}]^{n+1}$$



Also called the "Leap-Frog Algorithm"

stagger: 错开

- For spatial derivatives, we first consider 2D case where there is no variation in *z* direction, i.e., all derivatives with respect to *z* drop out.

$$-\mu\frac{\partial \boldsymbol{H}}{\partial t}=\nabla\times\boldsymbol{E} \quad\Rightarrow\quad \begin{aligned}\frac{\partial H_x}{\partial t}&=-\frac{1}{\mu}\frac{\partial E_z}{\partial y}\\ \frac{\partial H_y}{\partial t}&=\frac{1}{\mu}\frac{\partial E_z}{\partial x}\\ \frac{\partial H_z}{\partial t}&=\frac{1}{\mu}\left(\frac{\partial E_x}{\partial y}-\frac{\partial E_y}{\partial x}\right)\end{aligned}$$

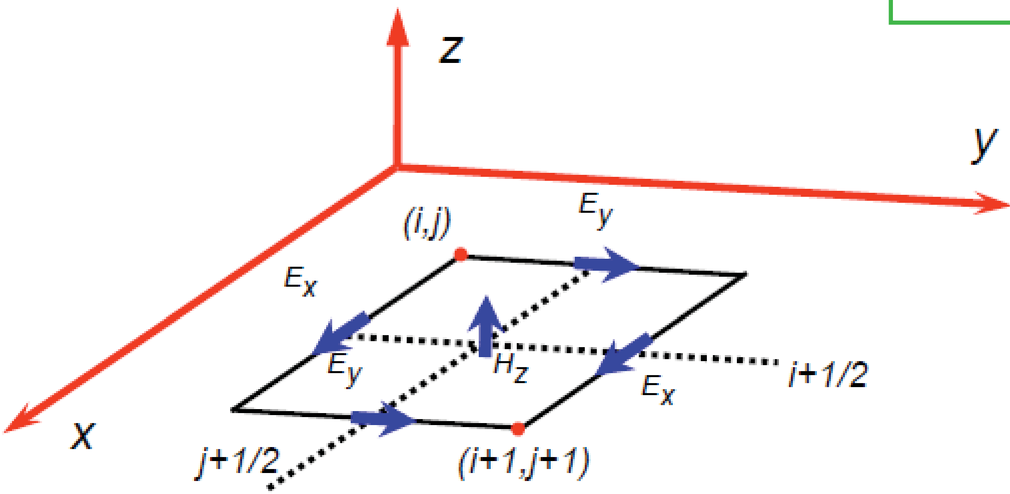
$$\varepsilon\frac{\partial \boldsymbol{E}}{\partial t}=\nabla\times\boldsymbol{H} \quad\Rightarrow\quad \begin{aligned}\frac{\partial E_x}{\partial t}&=\frac{1}{\varepsilon}\frac{\partial H_z}{\partial y}\\ \frac{\partial E_y}{\partial t}&=-\frac{1}{\varepsilon}\frac{\partial H_z}{\partial x}\\ \frac{\partial E_z}{\partial t}&=\frac{1}{\varepsilon}\left(\frac{\partial H_y}{\partial x}-\frac{\partial H_x}{\partial y}\right)\end{aligned}$$

TE problem

TM problem

For TM problem (H_z, E_x, E_y):

$$\left.\frac{\partial f}{\partial x}\right|_i^n \approx \frac{1}{2\Delta x}\left\{ f_{i+1}^n - f_{i-1}^n \right\}$$



Spatial meshes of E and H are also staggered!

E_x are stored at (i+1/2, j)
E_y are stored at (i, j+1/2)
H_z are stored at (i+1/2, j+1/2)

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

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

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

$\Rightarrow$

$$\left.\frac{\partial E_x}{\partial t}\right|_{i+1/2,j} = \frac{1}{\varepsilon}\left[\frac{H_z|_{i+1/2,j+1/2} - H_z|_{i+1/2,j-1/2}}{\Delta y}\right]$$

$$\left.\frac{\partial E_y}{\partial t}\right|_{i,j+1/2} = -\frac{1}{\varepsilon}\left[\frac{H_z|_{i+1/2,j+1/2} - H_z|_{i-1/2,j+1/2}}{\Delta x}\right]$$

$$\left.\frac{\partial H_z}{\partial t}\right|_{i+1/2,j+1/2} = \frac{1}{\mu}\left[\frac{E_x|_{i+1/2,j+1} - E_x|_{i+1/2,j}}{\Delta y} - \frac{E_y|_{i+1,j+1/2} - E_y|_{i,j+1/2}}{\Delta x}\right]$$

spatial: 空间的

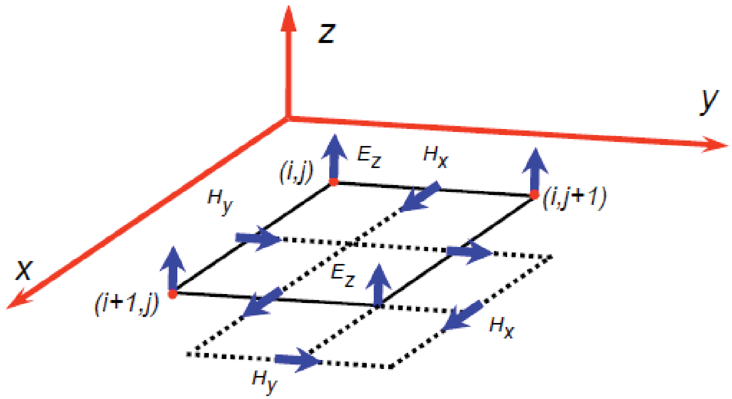
Rearrange and perform the finite difference of time derivative, we get:

$$H_z\Big|_{i+1/2,j+1/2}^{n+1/2} = H_z\Big|_{i+1/2,j+1/2}^{n-1/2} + \frac{\Delta t}{\mu_{i+1/2,j+1/2}}\left[\frac{E_x\big|_{i+1/2,j+1}^{n} - E_x\big|_{i+1/2,j}^{n}}{\Delta y} - \frac{E_y\big|_{i+1,j+1/2}^{n} - E_y\big|_{i,j+1/2}^{n}}{\Delta x}\right]$$

$$E_x\Big|_{i+1/2,j}^{n+1} = E_x\Big|_{i+1/2,j}^{n} + \frac{\Delta t}{\varepsilon_{i+1/2,j}\Delta y}\left[H_z\Big|_{i+1/2,j+1/2}^{n+1/2} - H_z\Big|_{i+1/2,j-1/2}^{n+1/2}\right]$$

$$E_y\Big|_{i,j+1/2}^{n+1} = E_y\Big|_{i,j+1/2}^{n} - \frac{\Delta t}{\varepsilon_{i,j+1/2}\,\Delta x}\left[H_z\Big|_{i+1/2,j+1/2}^{n+1/2} - H_z\Big|_{i-1/2,j+1/2}^{n+1/2}\right]$$

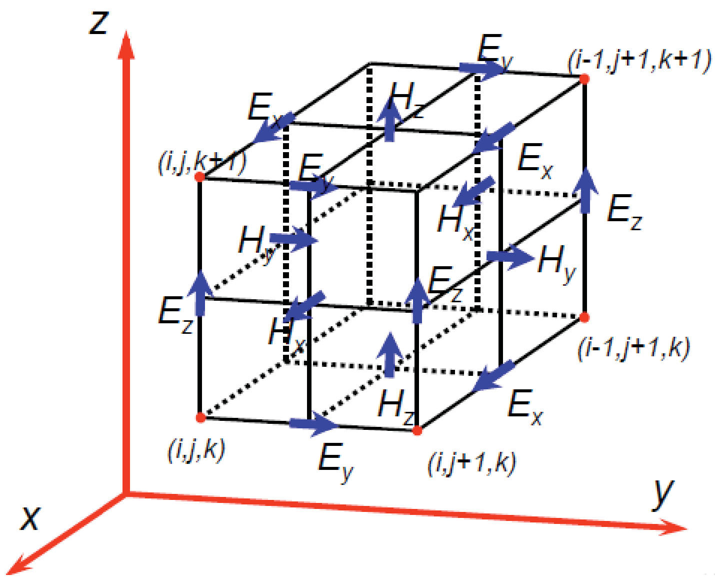
For TE problem (E_z, H_x, H_y):



H_x are stored at $(i, j+1/2)$
H_y are stored at $(i+1/2, j)$
E_z are stored at (i, j)

We just do the similar process for finite difference.

- Finite difference of spatial derivatives in 3D space:



Each **E** component is surrounded by four **H** components and vice versa

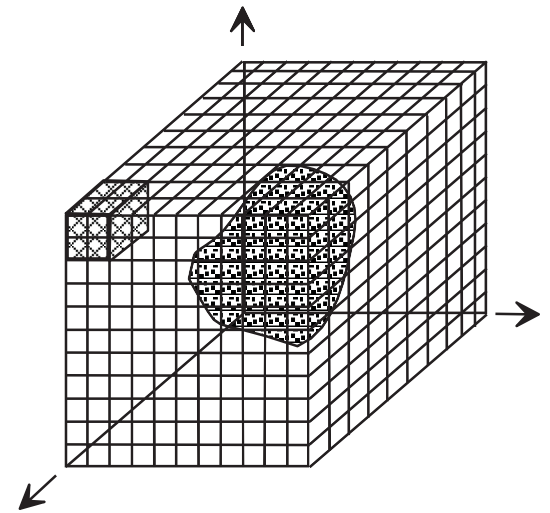
Similar can be done for H field

$$E_x\Big|_{i+1/2,j,k}^{n+1} = E_x\Big|_{i+1/2,j,k}^{n} + \frac{\Delta t}{\varepsilon_{i+1/2,j,k}}\left[\frac{H_z\Big|_{i+1/2,j+1/2,k}^{n+1/2} - H_z\Big|_{i+1/2,j-1/2,k}^{n+1/2}}{\Delta y} - \frac{H_y\Big|_{i+1/2,j,k+1/2}^{n+1/2} - H_y\Big|_{i+1/2,j,k-1/2}^{n+1/2}}{\Delta z}\right]$$

$$E_y\Big|_{i,j+1/2,k}^{n+1} = E_y\Big|_{i,j+1/2,k}^{n} + \frac{\Delta t}{\varepsilon_{i,j+1/2,k}}\left[\frac{H_x\Big|_{i,j+1/2,k+1/2}^{n+1/2} - H_x\Big|_{i,j+1/2,k-1/2}^{n+1/2}}{\Delta z} - \frac{H_z\Big|_{i+1/2,j+1/2,k}^{n+1/2} - H_z\Big|_{i-1/2,j+1/2,k}^{n+1/2}}{\Delta x}\right]$$

$$E_z\Big|_{i,j,k+1/2}^{n+1} = E_z\Big|_{i,j,k+1/2}^{n} + \frac{\Delta t}{\varepsilon_{i,j,k+1/2}}\left[\frac{H_y\Big|_{i+1/2,j,k+1/2}^{n+1/2} - H_y\Big|_{i-1/2,j,k+1/2}^{n+1/2}}{\Delta x} - \frac{H_x\Big|_{i,j+1/2,k+1/2}^{n+1/2} - H_x\Big|_{i,j-1/2,k+1/2}^{n+1/2}}{\Delta y}\right]$$

Boundary conditions



Shielded boundary:

- Perfect Electric Conductor (PEC)
- Perfect Magnetic Conductor (PMC)

(Used for, e.g., symmetry cases)

Open boundary:

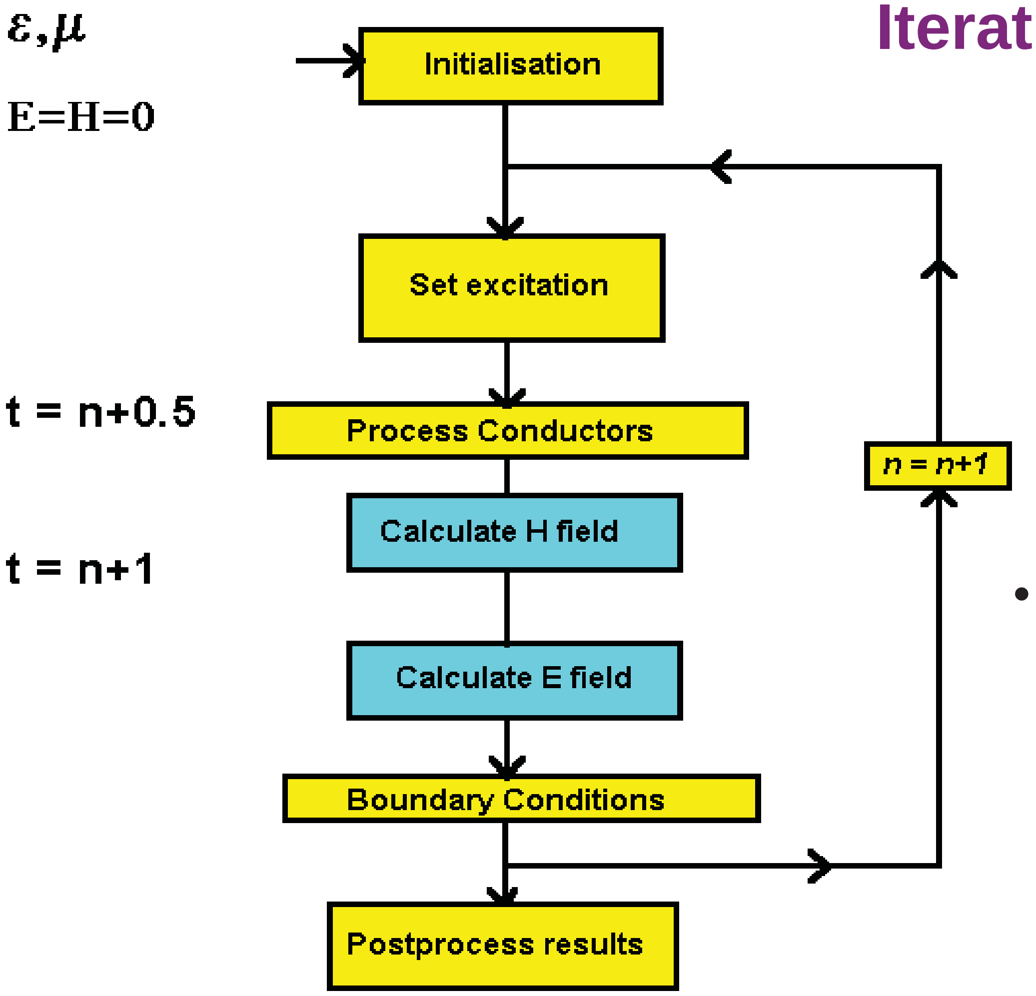
- Absorbing Boundary Condition (ABC)
- Perfectly Matched Layer (PML)

Commonly used for solving most practical problems

shield: 屏蔽

Implementation of FDTD (Yee) algorithm

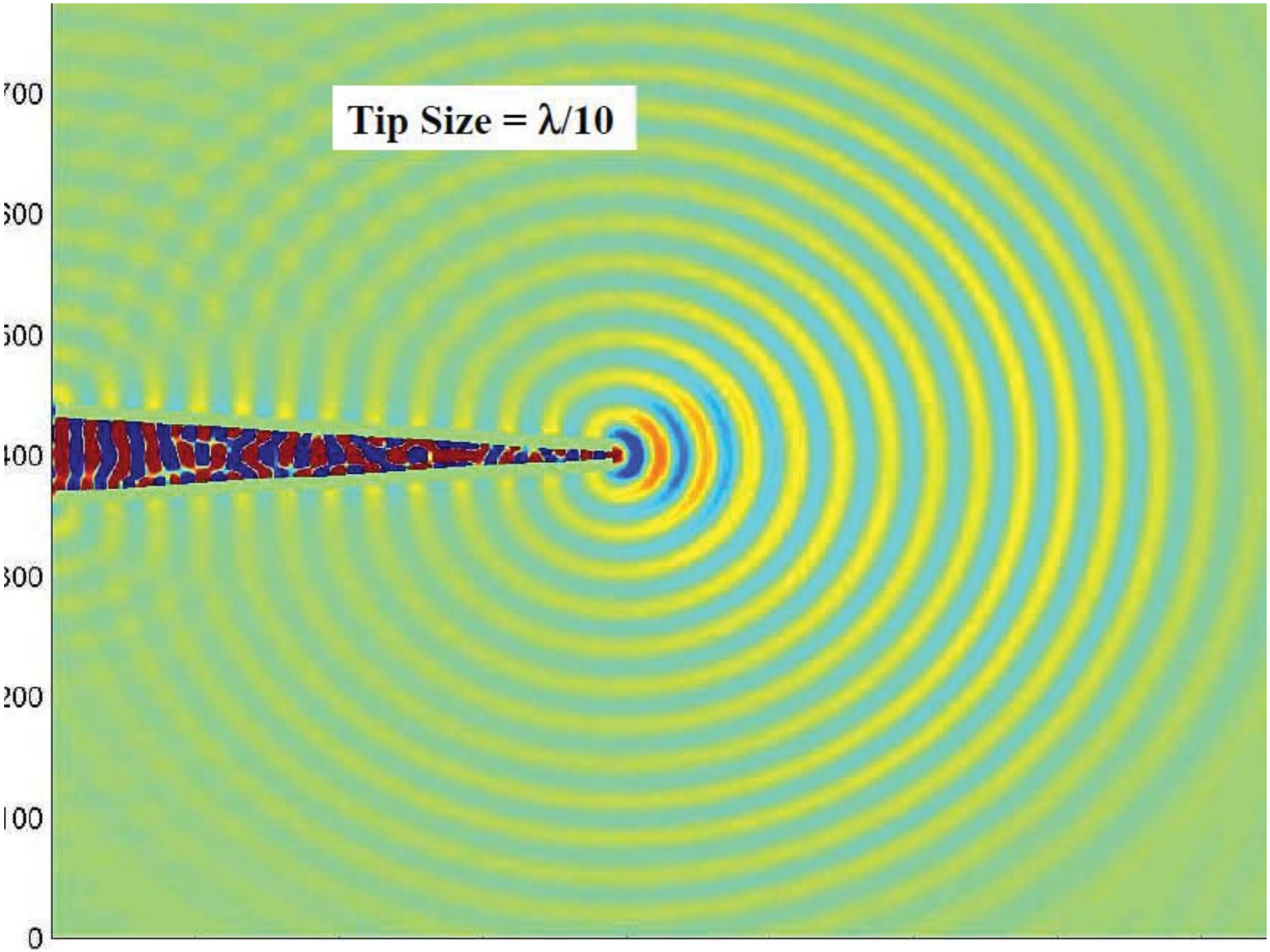
Iteration process in FDTD



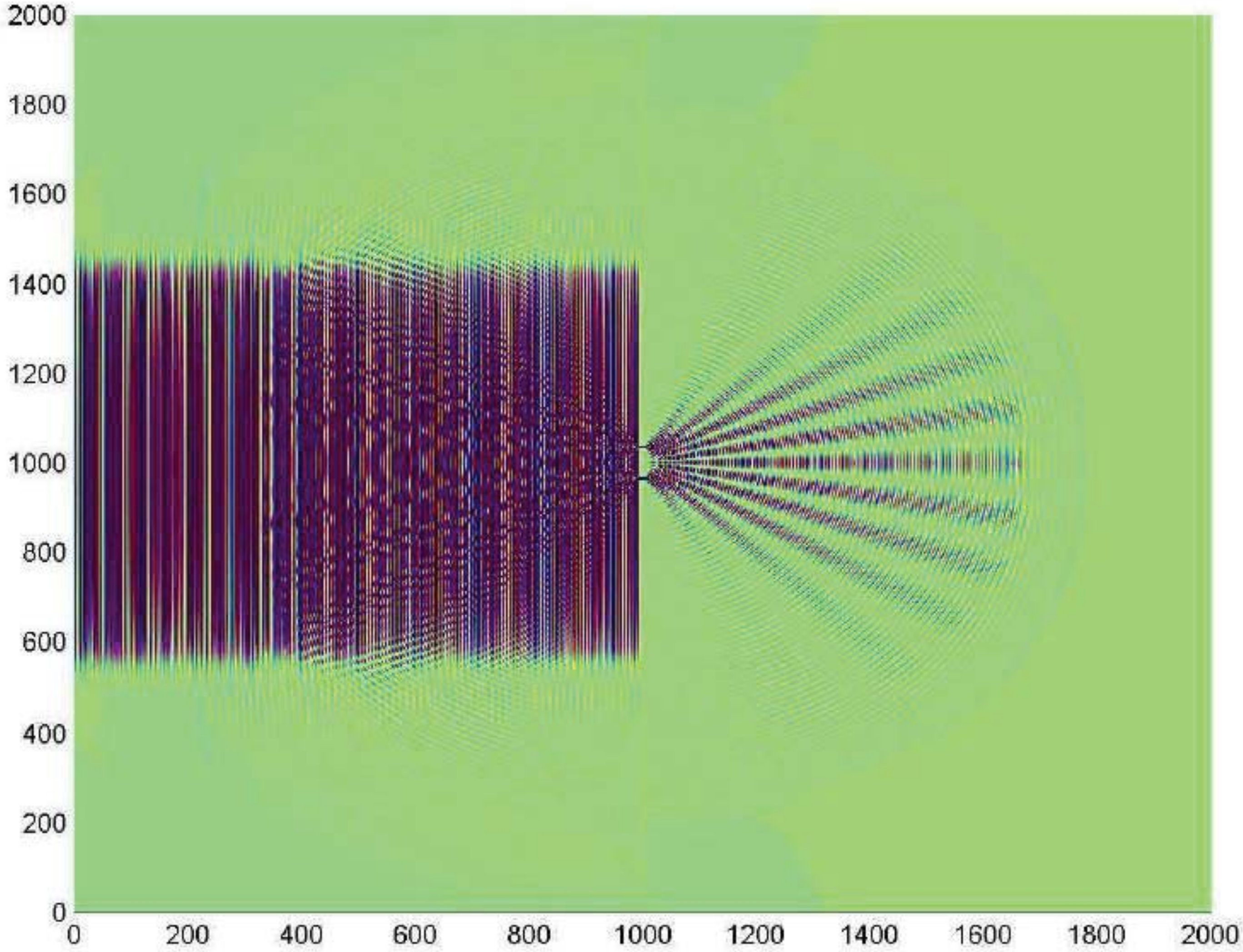
- Therefore, the spatial and temporal evolution of fields can be simulated

iteration: 迭代

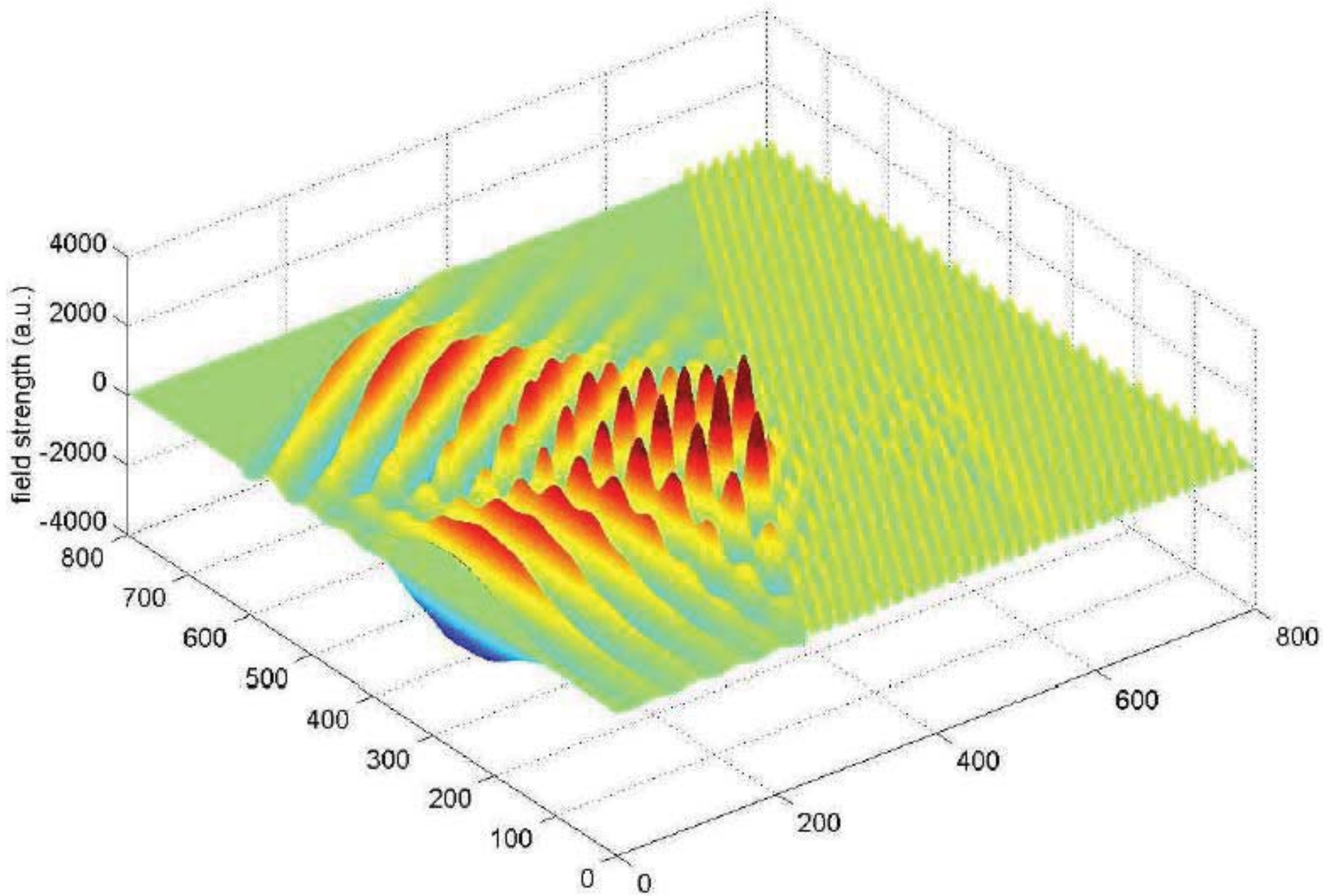
FDTD calculation example 1: focusing SPPs to the tip of a probe



FDTD calculation example 2: light going through double nanoslits



FDTD calculation example 3: light reflected by periodic nanolayers with alternating refractive indices



Summary of FDTD:

- A time-domain method, suitable for simulating spatial and time evolution of fields.
- Explicit: E (H) fields are obtained from previously calculated and stored H (E) fields; no need to solve a system of simultaneous equations (matrix).
- The dispersion of metals have to be approximated by suitable analytical expressions which introduce substantial error in broadband calculations.
- It is possible to obtain the entire frequency response with one single calculation by exciting a broadband pulse and calculating the Fourier transform.
- Computation load $\propto$ density and amount of spatial and temporal grid points
  - For structures with very small features, the spatial grids has to be very dense to resolve the fine structure → heavy computation load
  - For far-field calculation, large amount of grid points → heavy computation load
  - For accurate temporal evolution of fast light-matter interaction, small time step is required → heavy computation load

Some commercial softwares:

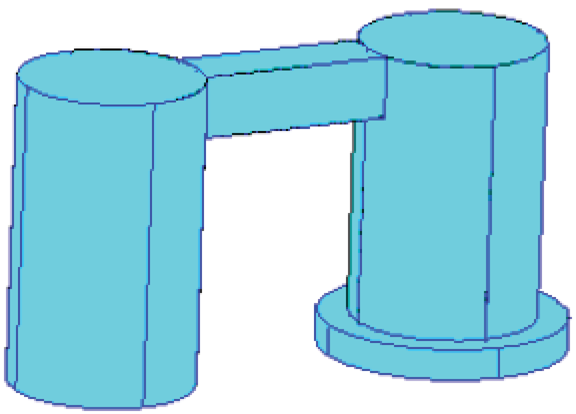
<u>FDTD Solutions</u>, OptiFDTD, Remcom XFDTD, Zeland Fidelity, APLAC, Empire, Microwave Studio, RM Associate CFDTD

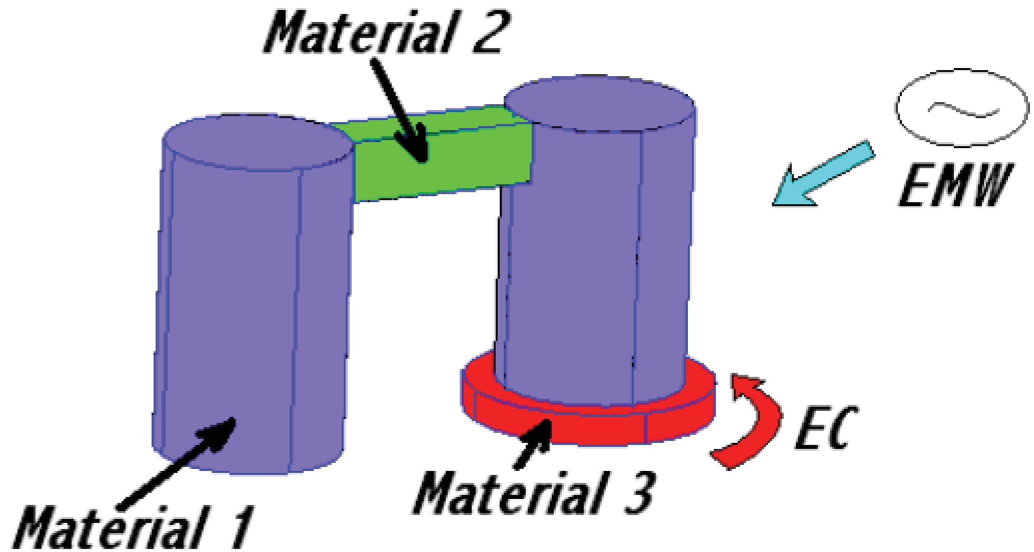
Fourier transform: 傅立叶变换，dense: 密集的，resolve: 分辨

3. Finite element method (FEM)

- FEM: a numerical method for solving systems of partial differential equations (PDEs)
- Initially used in structural mechanics and thermodynamics dating back to the 1950's
- First application in electromagnetism appeared in literature in the late 1960's but did not see widespread adoption until the 1980's (a problem of "spurious modes" was not solved until the 1980's)
- FEM starts with the partial differential form of Maxwell's equations.
- Basic idea: although the EM response is complex over a large region, a simple approximation may be sufficient for a small sub-region
- Main principle of FEM: divide a complex-shaped problem into smaller, simple-shaped problems where a solution is known and easy

partial differential equation: 偏微分方程





Mathematical description

$$D\vec{f}\,(\vec{x}) = 0,\ \vec{x} \in \Omega$$

$$B\vec{f}\,(\vec{x}) = 0,\ \vec{x} \in \partial\Omega$$

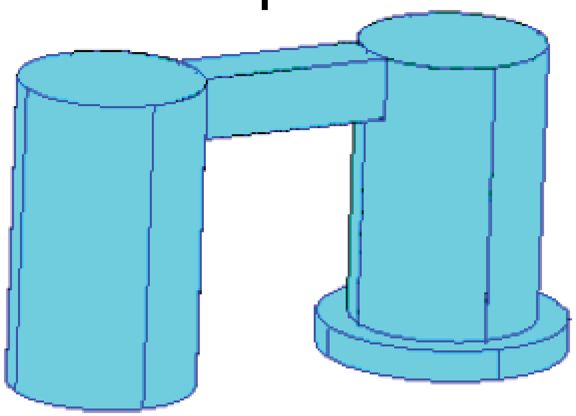
Model parameters

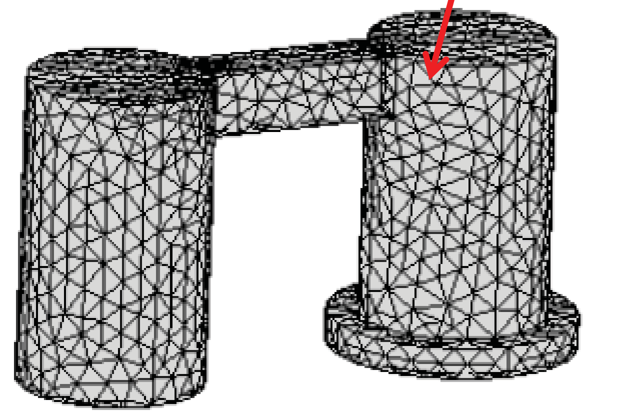
$$material:(\mu,\sigma,\varepsilon)$$

$$frequency:\quad (f)$$

$$sources:(\vec{E}_s,\vec{H}_s,\vec{J}_s)$$

Model discretization





PDE & Boundary Condition

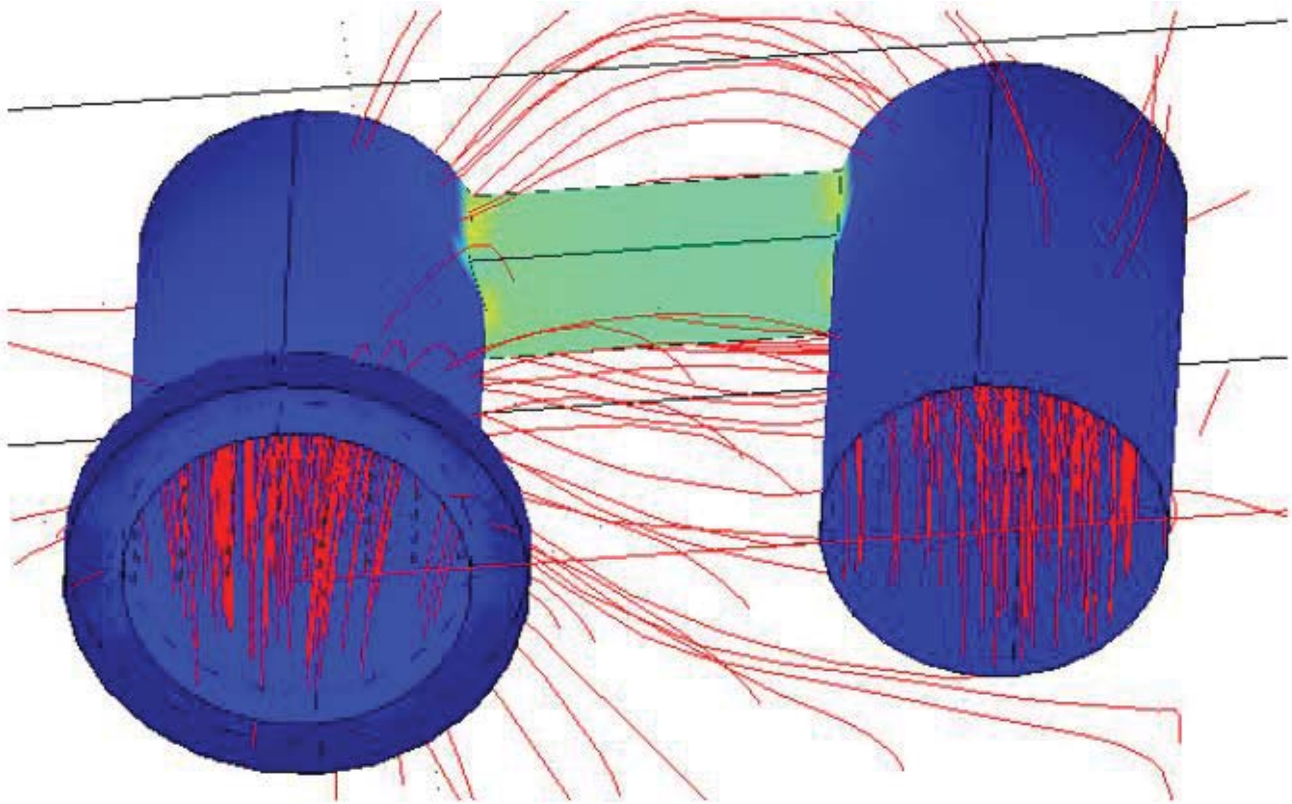
$$D\vec{f}(\vec{x}) = 0,\ \vec{x} \in \Omega$$
$$B\vec{f}(\vec{x}) = 0,\ \vec{x} \in \partial\Omega$$

FEM scheme

Large sparse linear system of equations

$$[A]\{x\} = \{b\}$$

sparse: 稀疏的， linear system of equations: 线性方程组



"Fancy" pictures as a final result of field calculation

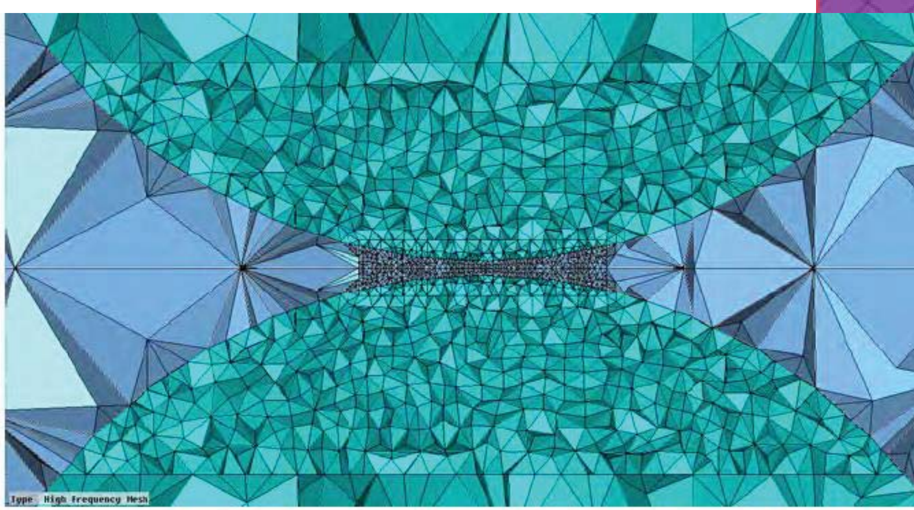
Magnetic, electric field, potential…

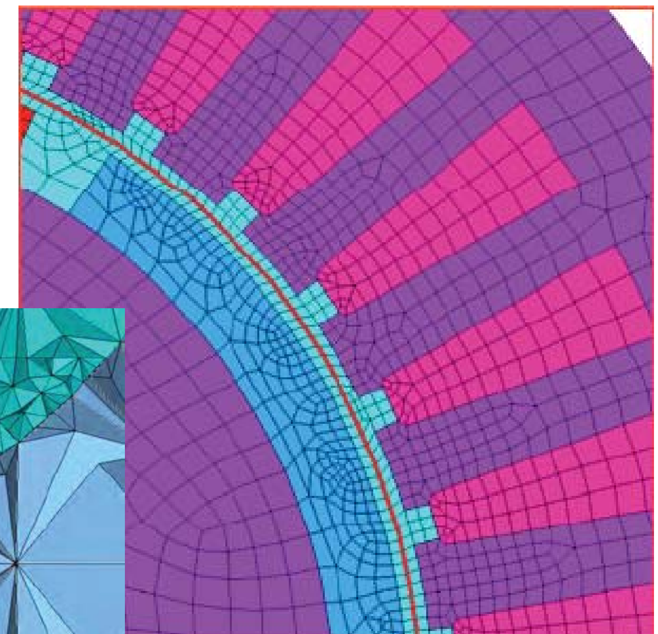
Electromagnetic energy, force …

Temperature, pressure, velocity…

Finite elements

- The whole region is meshed into elementary sub-domains, called finite elements, and the field equations are applied to each of them.
- Unlike FDTD, the unit cells of mesh (finite elements) are not necessarily rectangular, which may be triangular, etc.
- Again, unlike FDTD, the grids do not need to be uniform. Finer mesh is used in areas with larger field gradients.





rectangular: 矩形的，triangular: 三角形的，uniform: 均匀的，gradient: 梯度

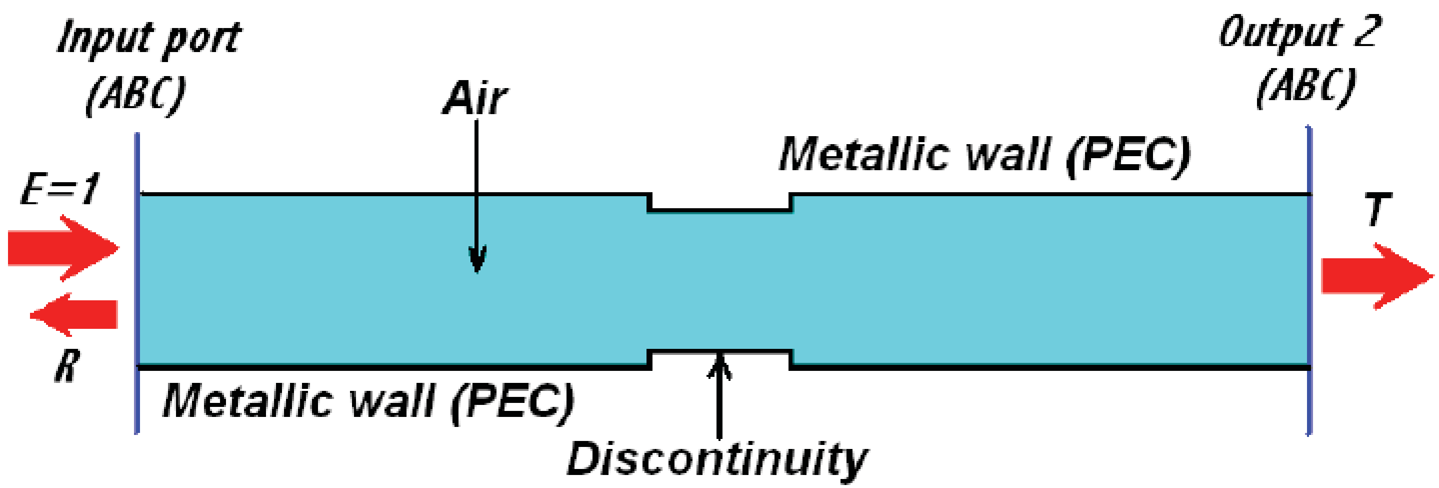
Implementation of FEM

- **Major steps:**
  - Discretize the whole region into a mesh of finite elements
  - Derive the variational equations for the individual finite elements
  - Relate the individual finite elements to the assembly of the elements
  - Obtain and solve the system of equations for the unknown quantity

Helmholtz equation – wave propagation example

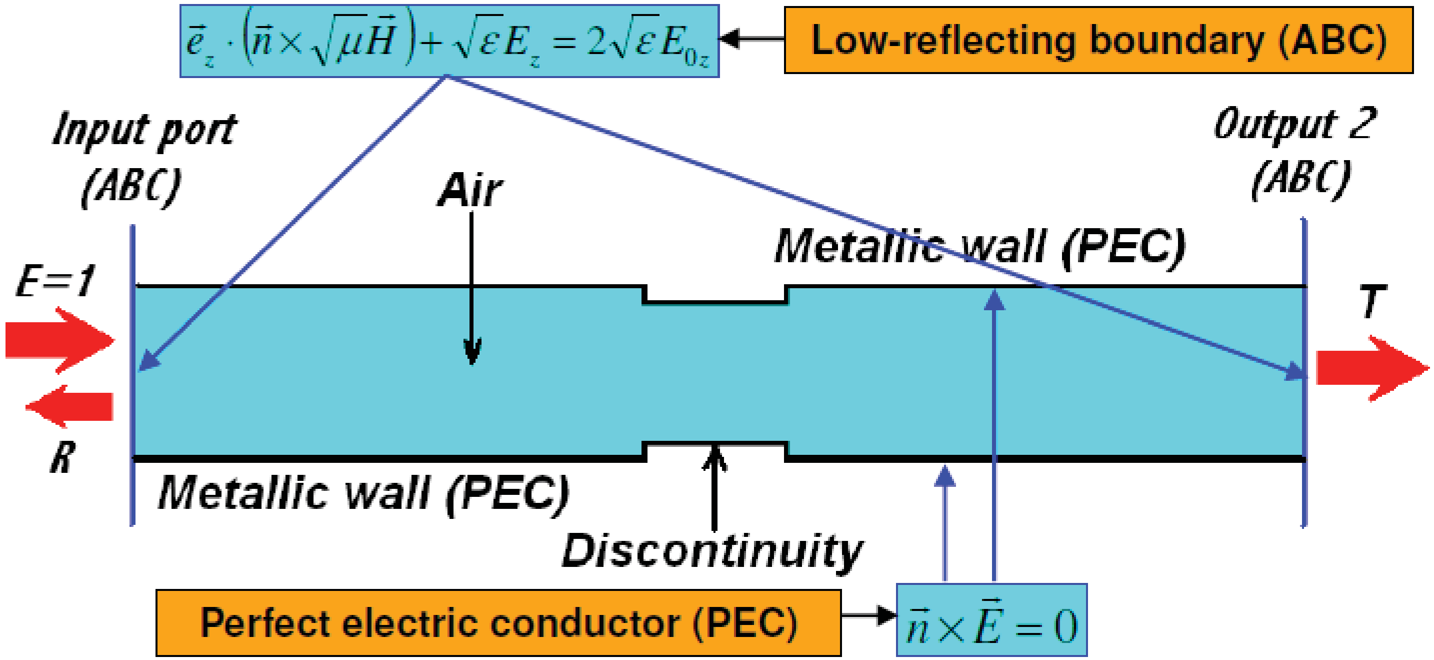
Example

$$\frac{\partial}{\partial x}\left(\frac{1}{\mu_r}\frac{\partial E_z}{\partial x}\right)-\frac{\partial}{\partial y}\left(\frac{1}{\mu_r}\frac{\partial E_z}{\partial y}\right)+k_0^2\varepsilon_r E_z=0$$

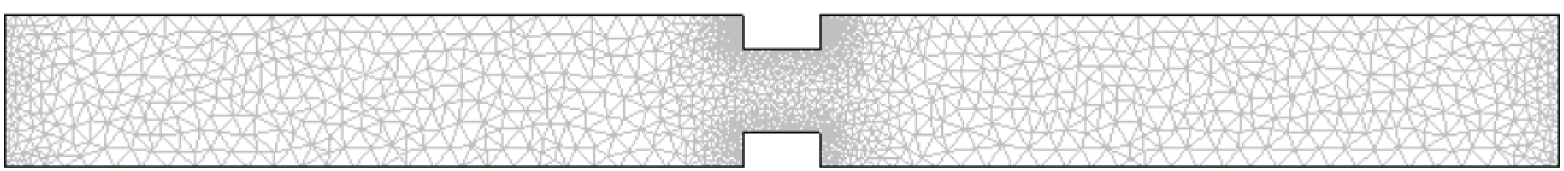


implementation: 执行，variational equation: 变分方程，assembly: 总体

Boundary condition:



Create the mesh of finite elements:



Derive the variational equation for each element:

$$F^e\left(E_z^e\right) = \frac{1}{2}\iint_{(\Omega^e)}\left[\left(\frac{\partial E_z^e}{\partial x}\right)^2 + \left(\frac{\partial E_z^e}{\partial y}\right)^2 + k^2 E_z^{e\,2}\right] d\Omega + \int_{(\partial\Omega_N^e)}\left(-\frac{jk}{2}E_z^{e\,2} + 2\,jkE_{0z}^e\right) d\Gamma$$

Sum up the elemental contribution:

$$F(\Phi) = \sum_{e=1}^{N_e} F^e\left(\Phi^e\right)$$

$$\left\{\frac{\partial F}{\partial \Phi}\right\} = \sum_{e=1}^{N^e}\left\{\frac{\partial F^e}{\partial \Phi^e}\right\} = \sum_{e=1}^{N^e}\left(\left[K^e\right]\left\{\Phi^e\right\} - \left\{b^e\right\}\right) = 0 \quad \Rightarrow \quad [K]\{\Phi\} = \{b\}$$

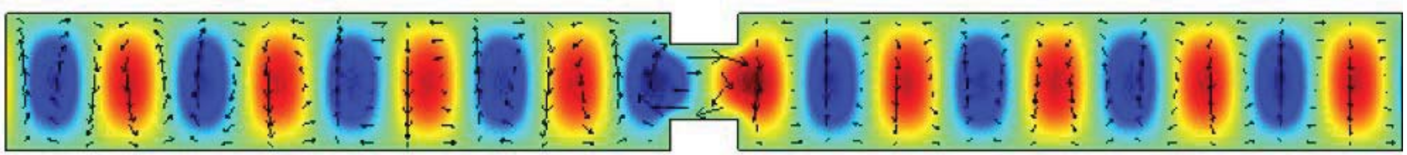
Solve this linear equation system to get the solution:

$$S_{11} = \frac{\int_{(Port_1)}\left(E_{zC} - E_{z1}\right)\cdot E_{z1}\cdot dA_1}{\int_{(Port_1)} E_{z1}\cdot E_{z1}\cdot dA_1}, \quad R = \left|S_{11}\right|^2$$

$$S_{12} = \frac{\int_{(Port_2)} E_{zC}\cdot E_{z2}\cdot dA_2}{\int_{(Port_2)} E_{z2}\cdot E_{z2}\cdot dA_2}, \quad T = \left|S_{12}\right|^2$$

F=0.78e9 (Hz), Fund. “even” mode

R=21.33%, T=78.67%, R+T=100%



Field results; Ez – color fill ; H vector - arrows

Another example

Wave equation - 3D analysis of photonic crystal waveguide

Governing PDE

$$\nabla\times\left(\frac{1}{\mu_r}\nabla\times\vec{E}\right)-k_0^2\varepsilon_r\vec{E}=0$$

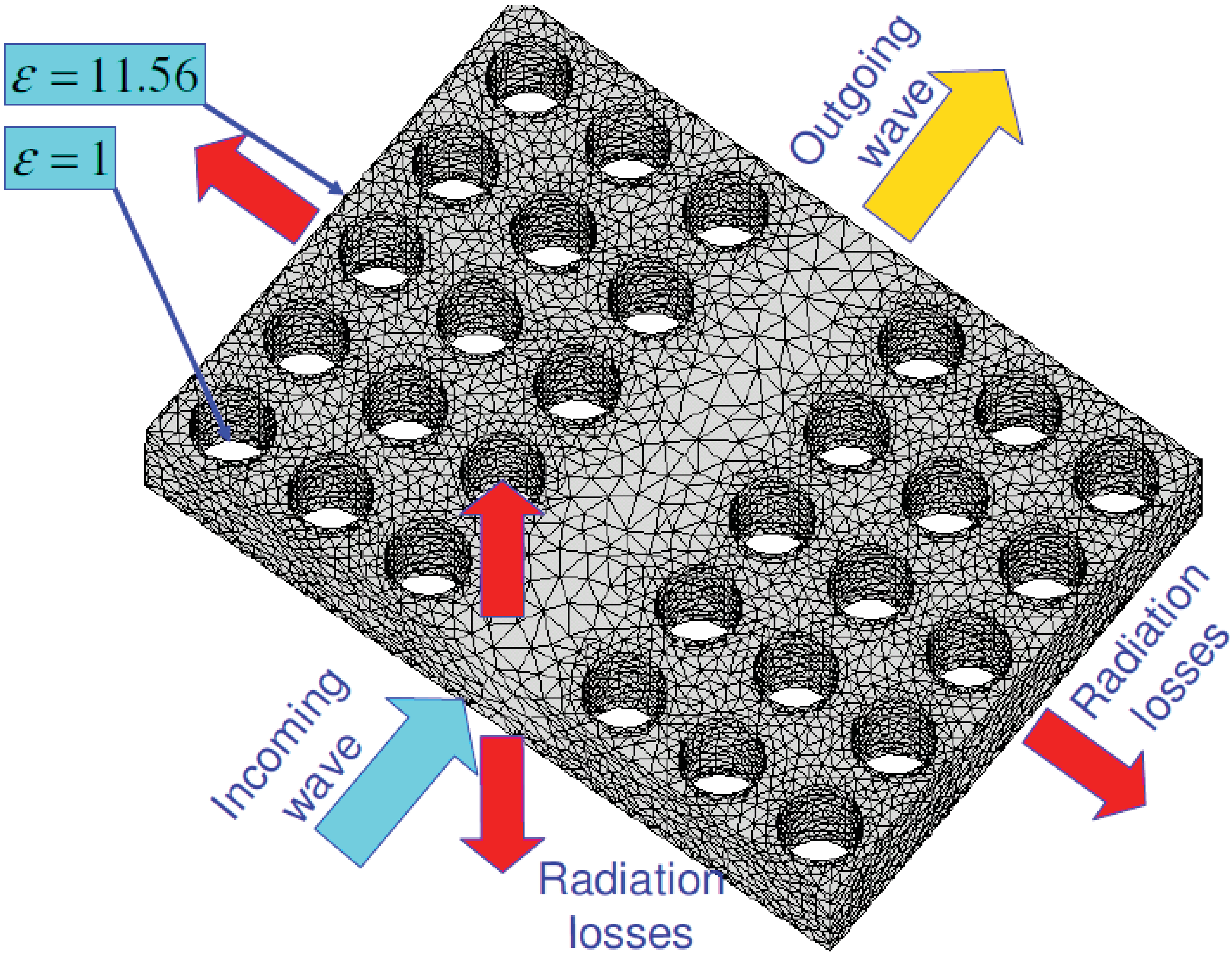
Boundary conditions

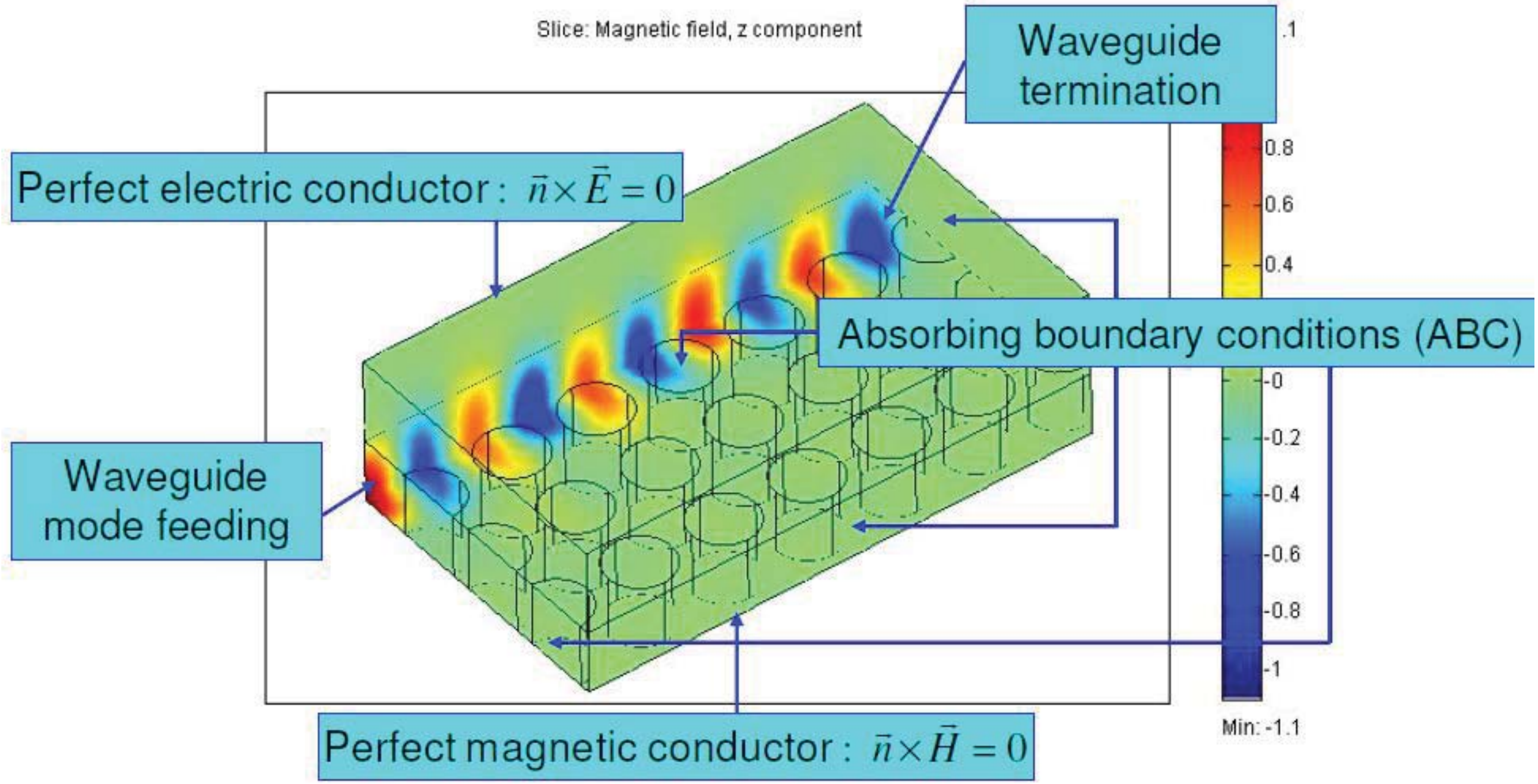
$$\vec{n}\times\vec{E}=0\,(PEC)\quad ;\quad \vec{n}\times\left(\nabla\times\vec{E}\right)=0\,(PMC)$$

$$\frac{1}{\mu_r}\vec{n}\times\left(\nabla\times\vec{E}\right)+\gamma_e\vec{n}\times\left(\vec{n}\times\vec{E}\right)=\vec{U}$$

Functional

$$F(\vec{E})=\frac{1}{2}\iiint\limits_{(V)}\left[\frac{1}{\mu_r}\left(\nabla\times\vec{E}\right)\cdot\left(\nabla\times\vec{E}\right)-k_0^2\varepsilon_r\vec{E}\cdot\vec{E}\right]dV+\iint\limits_{(S_2)}\left[\frac{\gamma_e}{2}\left(\vec{n}\times\vec{E}\right)\cdot\left(\vec{n}\times\vec{E}\right)+\vec{E}\cdot\vec{U}\right]dS$$


$\varepsilon = 11.56$
$\varepsilon = 1$
Outgoing wave
Incoming wave
Radiation losses
Radiation losses


Slice: Magnetic field, z component
Waveguide termination
Perfect electric conductor : $\vec{n}\times\vec{E}=0$
Absorbing boundary conditions (ABC)
Waveguide mode feeding
Perfect magnetic conductor : $\vec{n}\times\vec{H}=0$
.1
0.8
0.6
0.4
-0
-0.2
-0.4
-0.6
-0.8
-1
Min: -1.1

Summary of FEM:

Strengths of FEM

- Handles complex geometries and material inhomogeneities easily
- Handles dispersive or frequency-dependent materials easily
- Handles eigenproblems easily
- Easily applicable to "multi-physics" problems by coupling solutions in thermal or mechanical to the EM solution

Weaknesses of FEM

- FEM meshes become very complex for large 3-D structures
- More difficult to implement than FDTD thus limiting their use in commercial software. Little code development is done by engineers.
- Efficient preconditioned iterative solvers are required when higher-order elements are used.

Some commercial softwares:

Comsol, Ansoft Maxwell SV, ANSYS, FEM2000, FlexPDE, QuickField, Matlab PDE Toolbox, Ansoft HFSS, UGS FEMAP

inhomogeneity: 不均匀性，eigenproblem: 特征值问题

4. Comparison of FDTD and FEM

FEM	FDTD
Arbitrarily shaped 3D metals and dielectrics	Arbitrarily shaped 3D metals and dielectrics
Full wave (vectorial, rigorous)	Full wave (vectorial, rigorous)
Frequency domain, individual frequency points calculated with Fast Frequency Sweep	Time domain, frequency via Fourier transform, broadband response in one simulation
Multi-port simulations with no additional cost	Each port requires new simulation
Implicit scheme: requires solution of matrix equation with sparse matrix	Explicit scheme: does not require matrix solution, instead iterative time-stepping
Good for stationary field problems (e.g., mode analysis in high-Q structures)	Good for transient field problems (e.g., pulse propagation, antenna radiation)
Advantages: mature method, adaptive mesh	Advantages: simple, robust, versatile
Disadvantage: huge matrices (large memory)	Disadvantage: long computation time
Adaptive mesh refinement	
Better in handling multi-physics problems	Better in handling larger, higher complexity structures
	Hardware acceleration (GPU)

mature: 成熟的，adaptive: 适应性的，broadband: 宽带的

Summary

- Numerical methods are needed for the rigorous simulation, design, and optimization of EM response of optical nanostructures
- Overview of numerical methods for nanophotonics:
  Frequency-domain vs. time-domain, domain-discretization vs. boundary-discretization, periodic vs. aperiodic, near-field vs. far-field, importance of understanding the principles and limitations of different methods
- Finite difference time domain (FDTD) method:
  Applicable to arbitrary complex geometries, time-domain method, spatial and temporal evolution of field, broadband response in one calculation, explicit scheme, long computation time
- Finite element method (FEM):
  Applicable to arbitrary complex geometries, frequency-domain method, adaptive mesh, multi-port simulation, solution of large matrix needed (huge memory cost)