表面等离激元学

模拟仿真计算

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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, no a single method (software) can solve all problems!
- 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)

- 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)

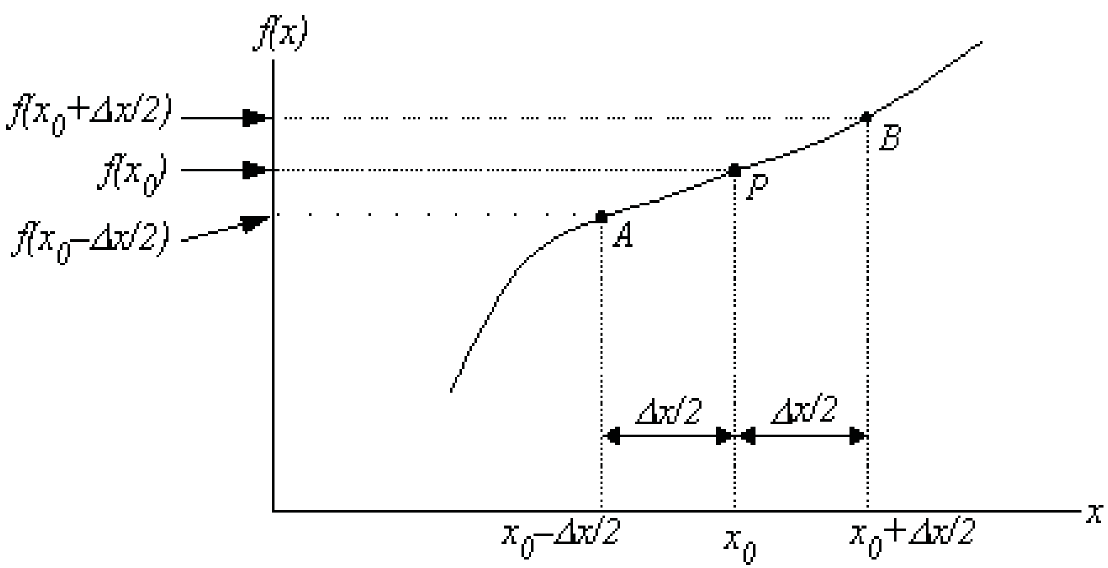
temporal: 时间的， evolution: 演进

2. Finite difference time domain (FDTD) method

Principle of finite difference

1966 K.S.Yee

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



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:

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

- Therefore, for space derivative, we have:

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

- Similarly, for time derivative, we have:

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

Derivation of FDTD algorithm

- Starting from Maxwell's differential equations:

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

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

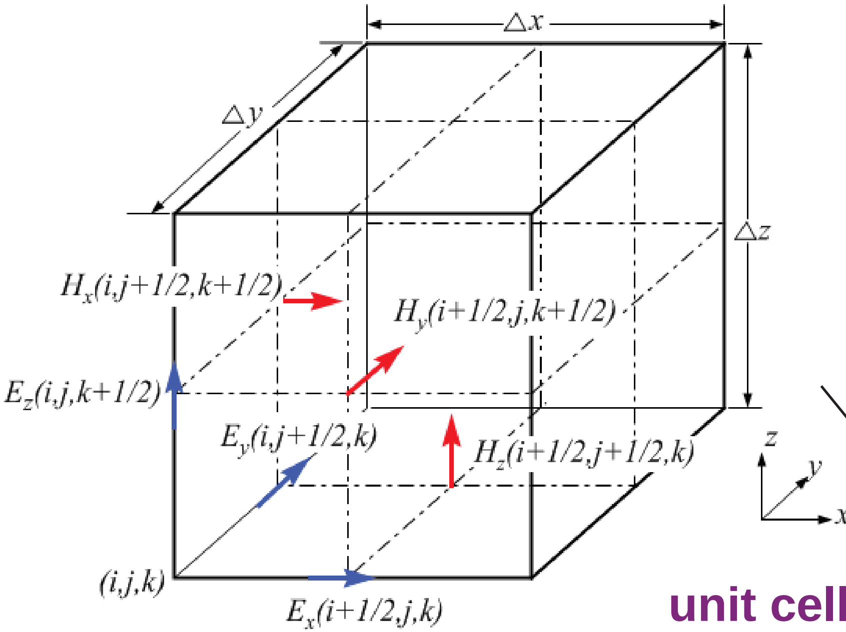
$$\begin{bmatrix} \dfrac{\partial H_z}{\partial y} - \dfrac{\partial H_y}{\partial z} \\ \dfrac{\partial H_x}{\partial z} - \dfrac{\partial H_z}{\partial x} \\ \dfrac{\partial H_y}{\partial x} - \dfrac{\partial H_x}{\partial y} \end{bmatrix} = \varepsilon \cdot \begin{bmatrix} \dfrac{\partial E_x}{\partial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

- 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

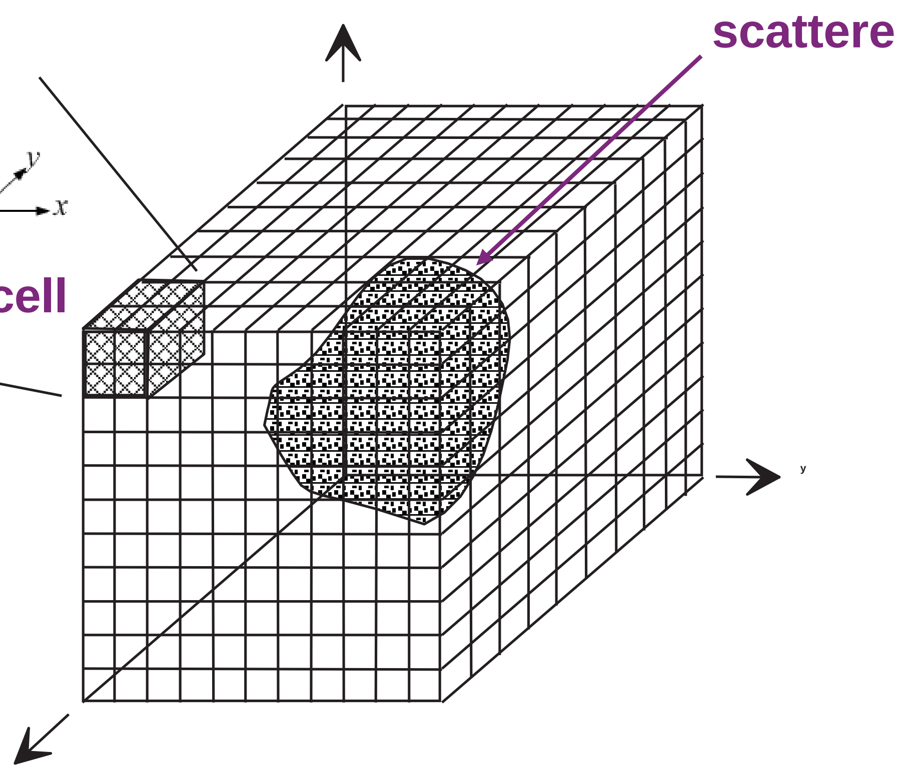
derivation: 推导， algorithm: 算法， partial derivative: 偏微分， mesh: 网格

Mesh Structure for FDTD Algorithm

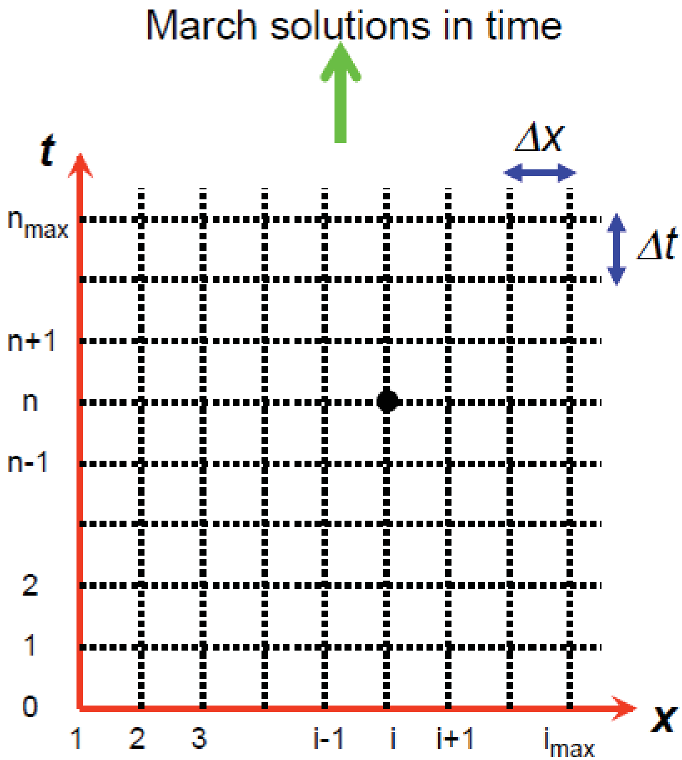


Standard Yee's lattice

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



scatterer: 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*

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

$$F(x,y,z,t) = F(i\Delta x, j\Delta y, k\Delta z, n\Delta t) = F^n(i,j,k)$$

for space derivative:

$$\left.\frac{\partial F(x,y,z,t)}{\partial x}\right|_{x=i\Delta x} \approx \frac{F^n(i+1/2,j,k) - F^n(i-1/2,j,k)}{\Delta x} + O\left[(\Delta x)^2\right]$$

$$\left.\frac{\partial F(x,y,z,t)}{\partial y}\right|_{y=j\Delta y} \approx \frac{F^n(i,j+1/2,k) - F^n(i,j-1/2,k)}{\Delta y} + O\left[(\Delta y)^2\right]$$

$$\left.\frac{\partial F(x,y,z,t)}{\partial z}\right|_{z=k\Delta z} \approx \frac{F^n(i,j,k+1/2) - F^n(i,j,k-1/2)}{\Delta z} + O\left[(\Delta z)^2\right]$$

for time derivative:

$$\left.\frac{\partial F(x,y,z,t)}{\partial t}\right|_{t=n\Delta t} \approx \frac{F^{n+1/2}(i,j,k) - F^{n-1/2}(i,j,k)}{\Delta t} + O\left[(\Delta t)^2\right]$$

$$E_x^{n+1}(i+1,j,k) = \frac{1 - \dfrac{\sigma(i+1/2,j,k)\Delta t}{2\varepsilon(i+1/2,j,k)}}{1 + \dfrac{\sigma(i+1/2,j,k)\Delta t}{2\varepsilon(i+1/2,j,k)}} E_x^n(i+1-/2,j,k)$$

$$+ \frac{\Delta t}{\varepsilon(i+1/2,j,k)} \cdot \frac{1}{1 + \dfrac{\sigma(i+1/2,j,k)\Delta t}{2\varepsilon(i+1/2,j,k)}} \cdot$$

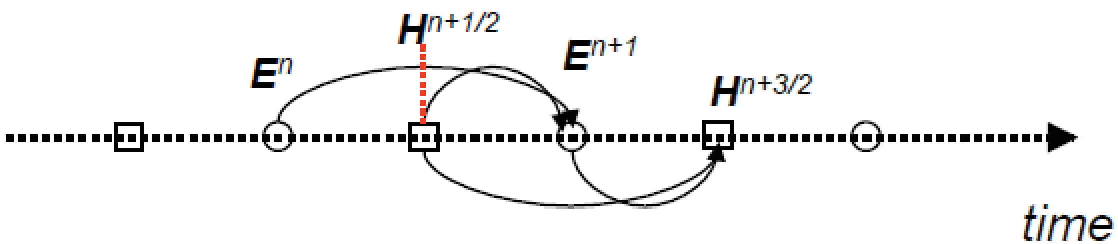
$$\left[\frac{H_z^{n+1/2}(i+1/2,j,k) - H_z^{n+1/2}(i+1/2,j-1/2,k)}{\Delta y} + \frac{H_y^{n+1/2}(i+1/2,j,k-1/2) - H_y^{n+1/2}(i+1/2,j,k+1/2)}{\Delta z}\right]$$

stagger: 错开

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

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

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



Also called the "Leap-Frog Algorithm"

- 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.

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

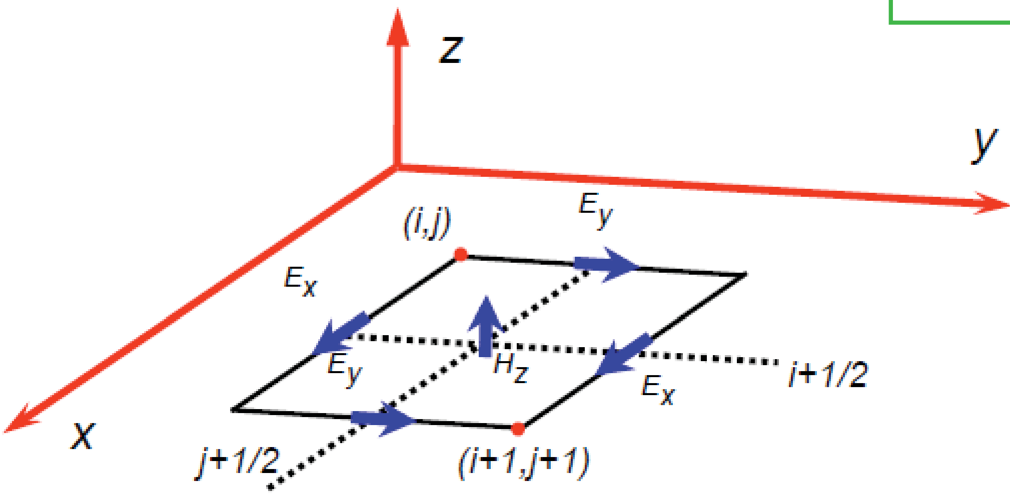
$$\varepsilon \frac{\partial \boldsymbol{E}}{\partial t} = \nabla \times \boldsymbol{H} \quad \Rightarrow \quad \frac{\partial E_x}{\partial t} = \frac{1}{\varepsilon}\frac{\partial H_z}{\partial y}, \quad \frac{\partial E_y}{\partial t} = -\frac{1}{\varepsilon}\frac{\partial H_z}{\partial x}, \quad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

TM problem

TE problem

For TE problem (H_z, E_x, E_y):

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



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

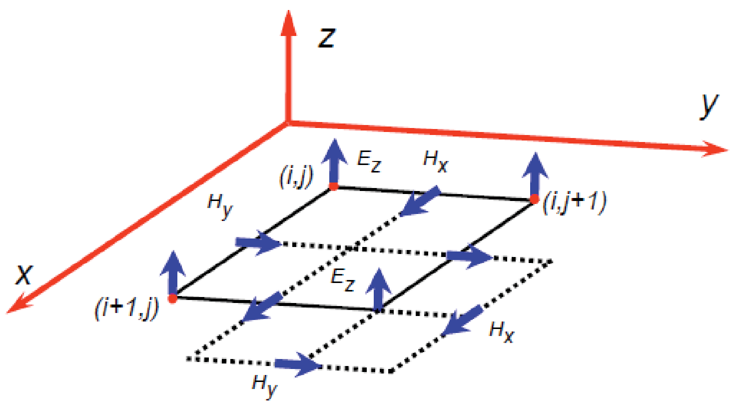
Rearrange and perform the finite difference of time derivative, we get:

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

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

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

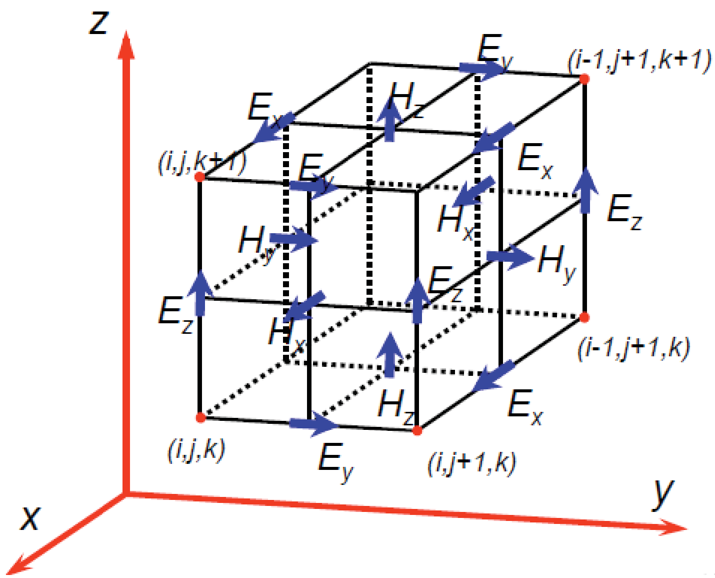
For TM problem (E_z, H_x, H_y):



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

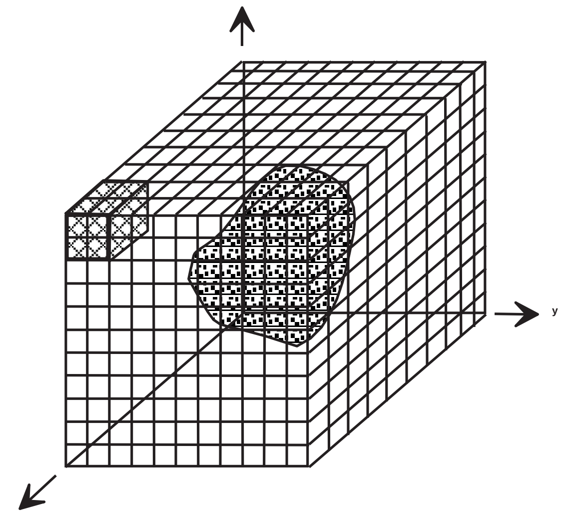
Similar can be done for H field

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

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

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

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)

在电磁场的辐射和散射问题中，边界总是开放的，然而计算机的内存是有限的，所以我们只能模拟有限的空间。

Commonly used for solving most practical problems

shield: 屏蔽

数值稳定性条件

时间步长△t，空间步长△x，△y，△z必须满足一定的关系，否则会使得数值表现不稳定，随着计算步数的增加，计算场量的数值会无限增大。
稳定性条件：

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

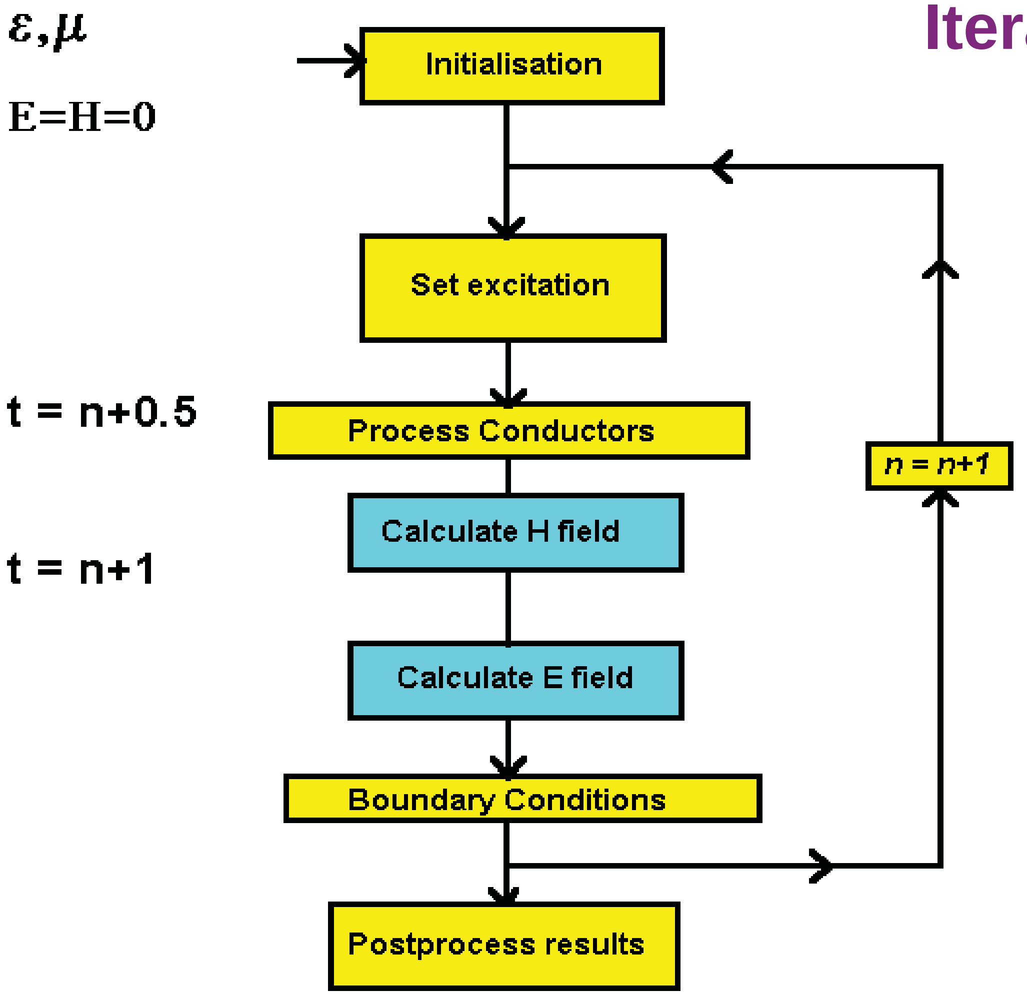
若采用均匀立方体网格，

$$\Delta t = \frac{\min(\Delta x, \Delta y, \Delta z)}{2c}$$

数值色散

在FDTD网格中，电磁波的相速度与频率相关，电磁波的相速度随波长、传播方向及变量离散化的情况不同而改变。色散将导致非物理因素引起的脉冲波形畸变、人为的各向异性和虚假的折射现象等。这是由于用近似差分替代连续微分引起的，当时间步长和空间步长都足够小时就能获得理想的色散关系，此时问题空间分割应按照小于正常网格的原则进行，一般选取的最大空间步长为$\triangle_{max}=\lambda_{min}/20$, λ_{min}为研究范围内的电磁波的最小波长。

Implementation of FDTD (Yee) algorithm



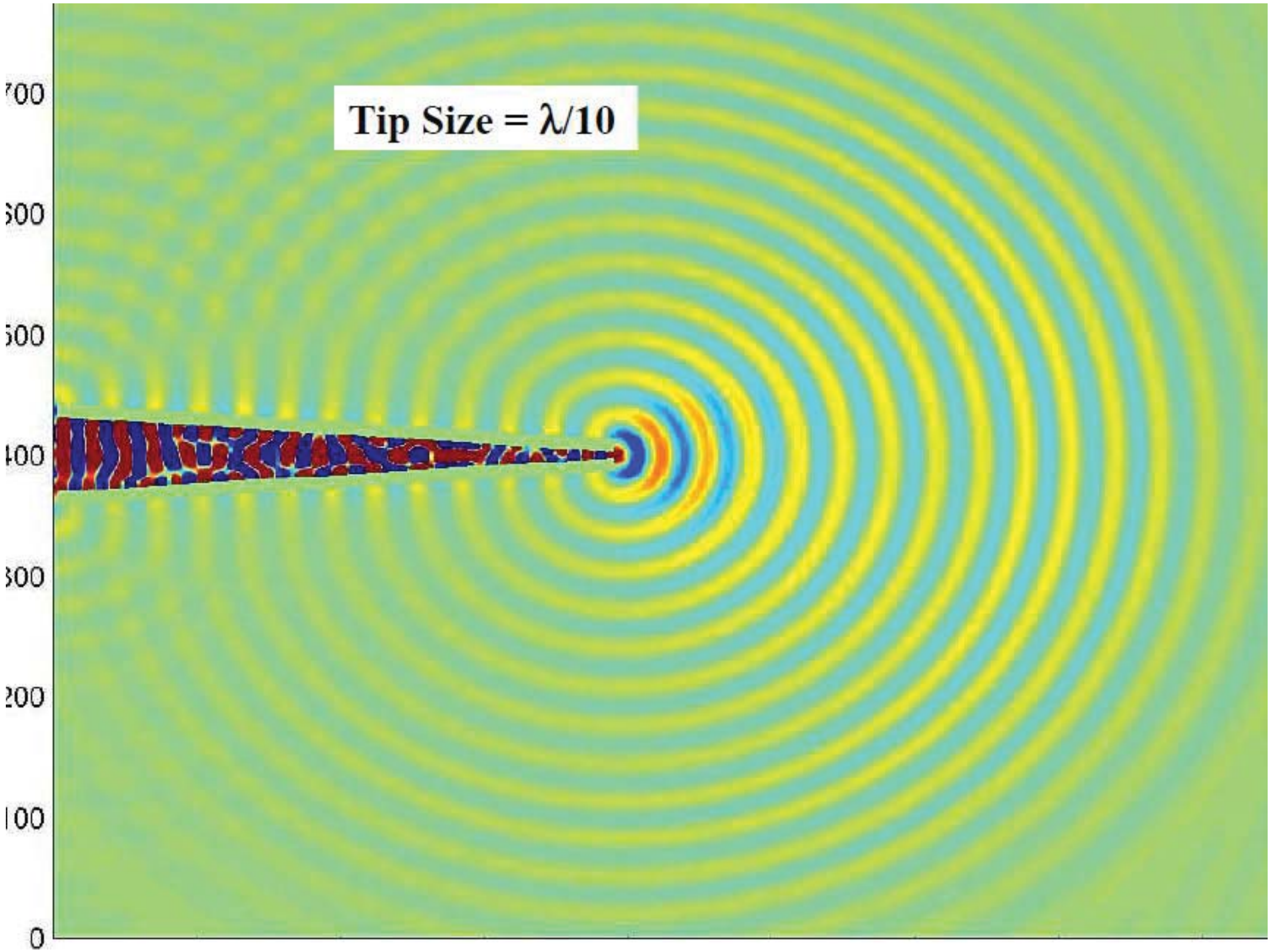
Iteration process in FDTD

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

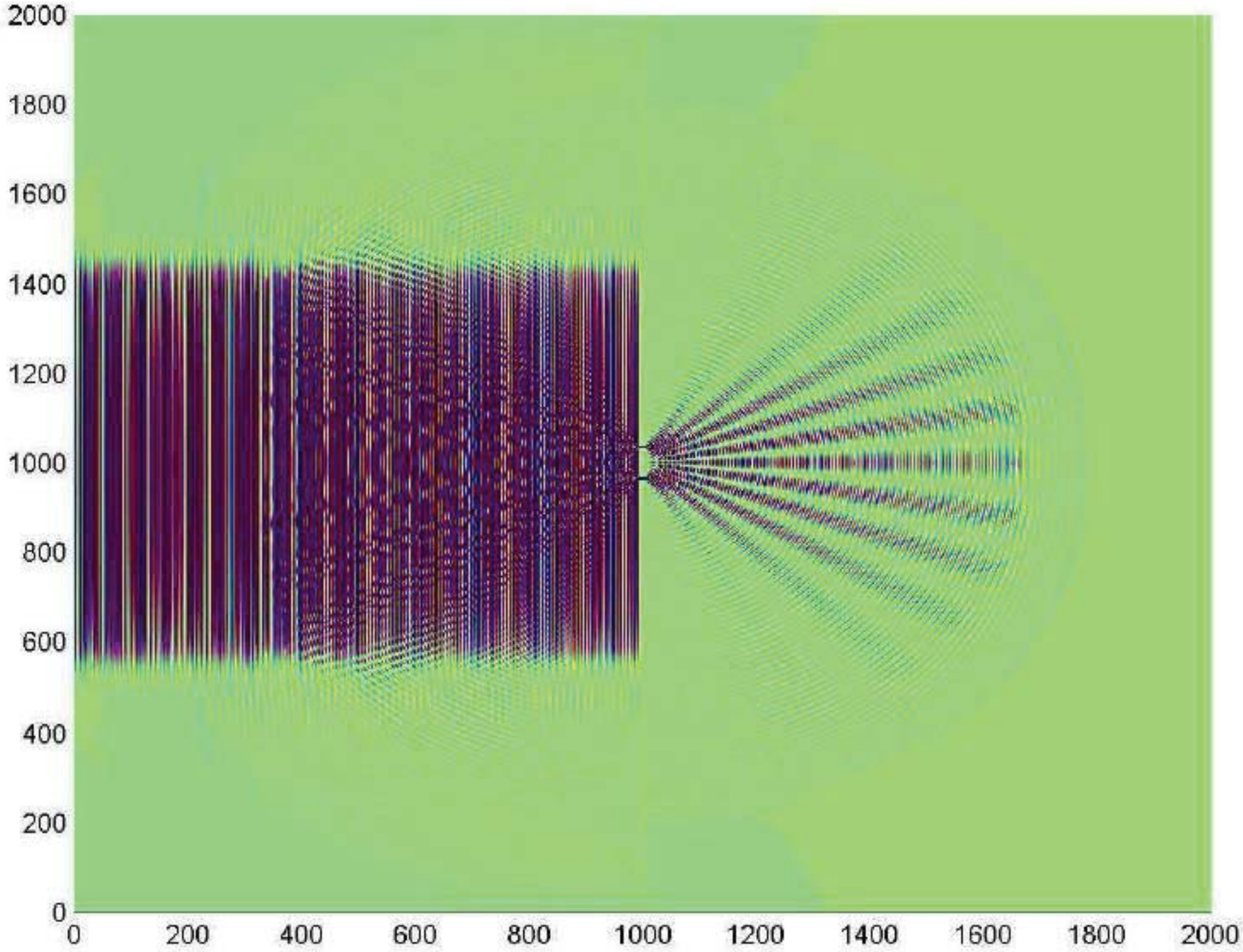
时域有限差分法是通过将**Maxwell**旋度方程进行差分后转化为显式的有限差分方程组，进而直接在时域进行求解，通过建立时间离散的递进序列，在相互交织的网格空间中交替计算电场和磁场。

iteration: 迭代

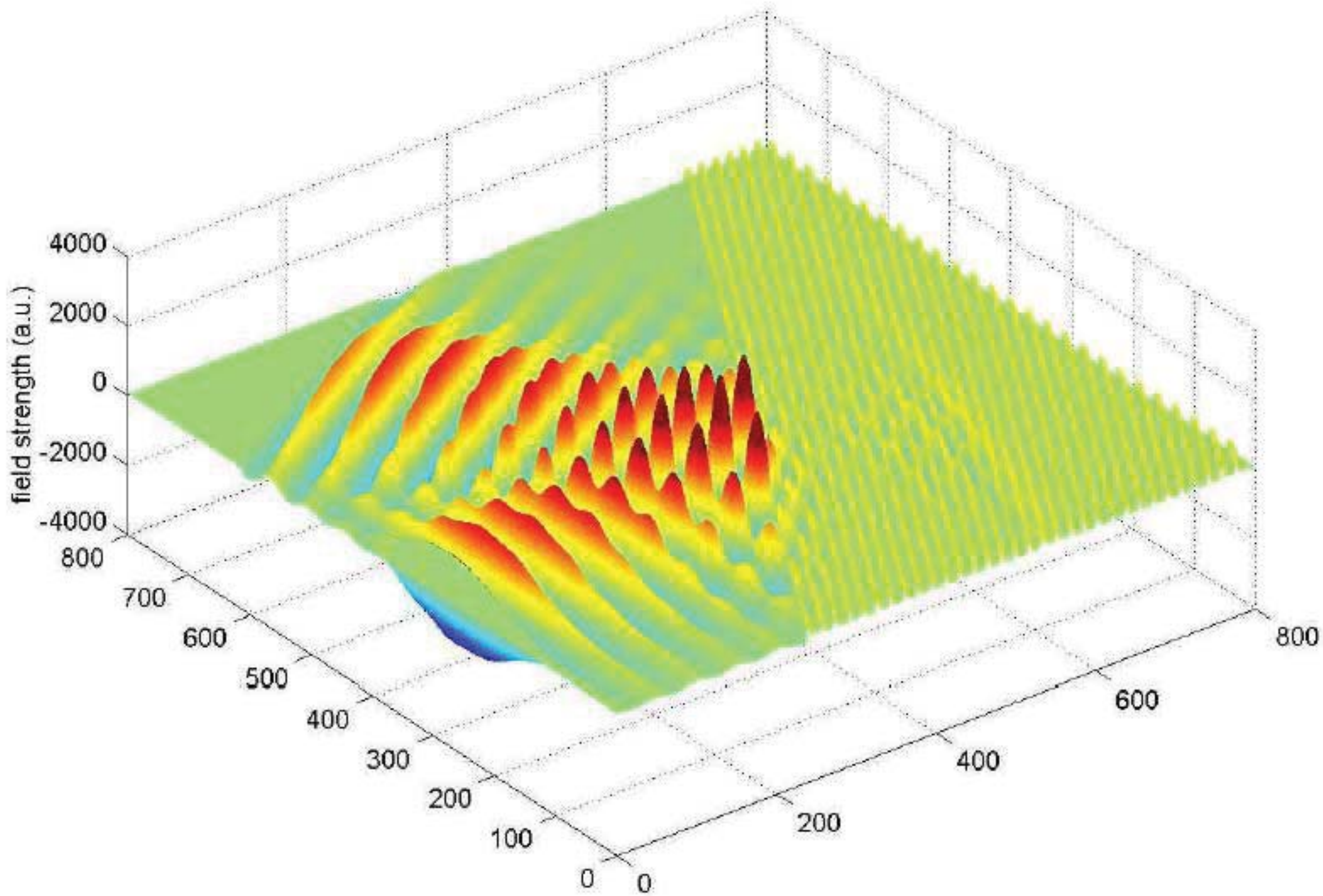
FDTD calculation example 1: focusing SPPs to the tip of a probe



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:

https://www.lumerical.com/cn/

- 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:

FDTD Solutions, OptiFDTD, Remcom XFDTD, Zeland Fidelity, APLAC, Empire, Microwave Studio, RM Associate CFDTD

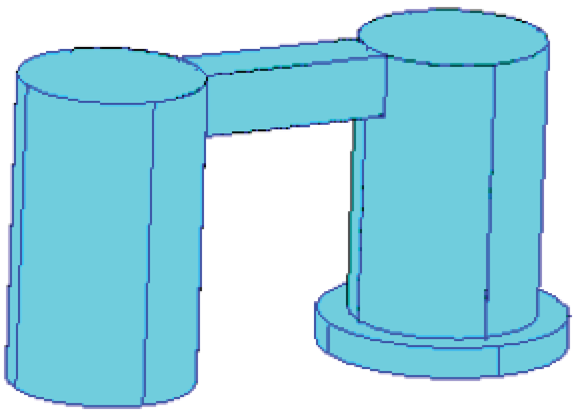
Fourier transform: 傅立叶变换，dense: 密集的，resolve: 分辨

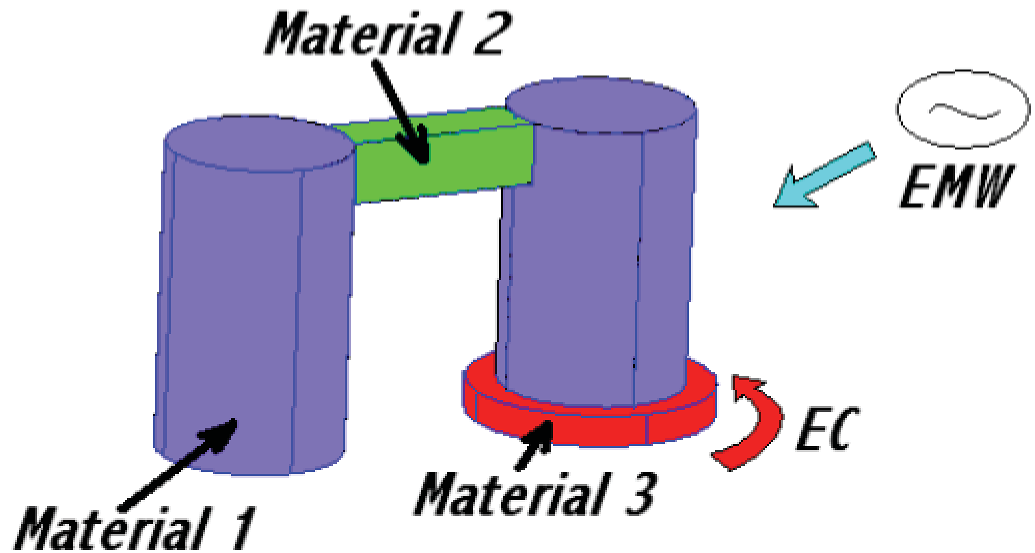
3. Finite element method (FEM)

- 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

圆的周长问题





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

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

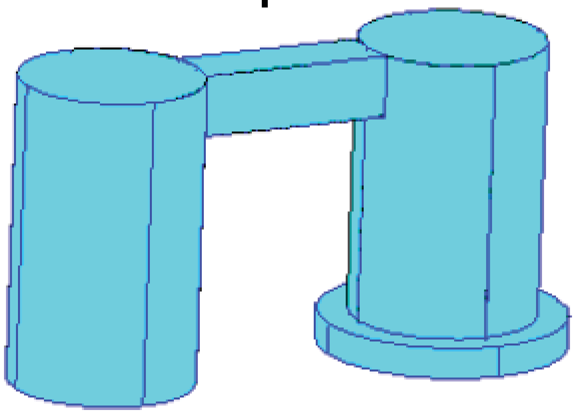
$$frequency : \quad (f)$$

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

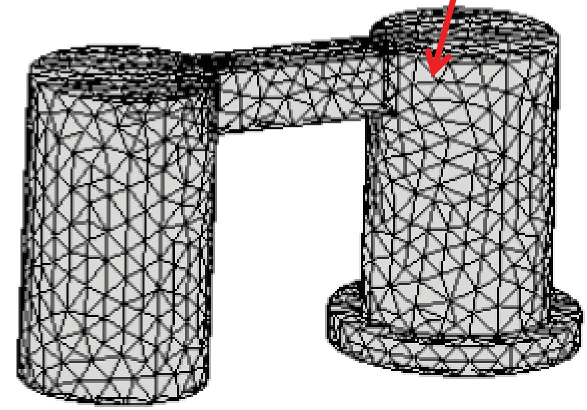
Clough:Rayleigh-Ritz法+分片函数

Finite element

Model discretization



不用考虑整个定义
域复杂的边界条件



PDE &
Boundary Condition

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

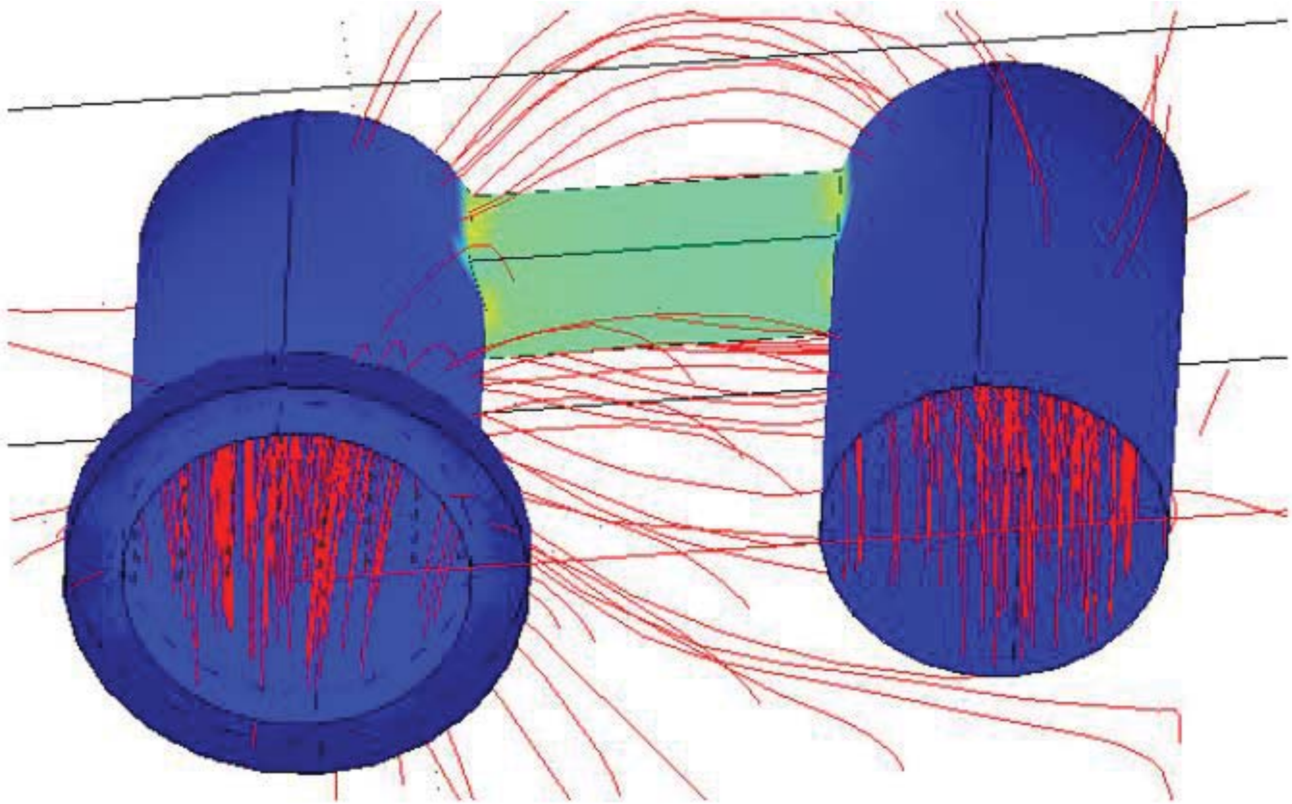
$$B\vec{f}(\vec{x}) = 0, \vec{x} \in \partial\Omega$$

FEM scheme

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

Large sparse linear system of equations

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

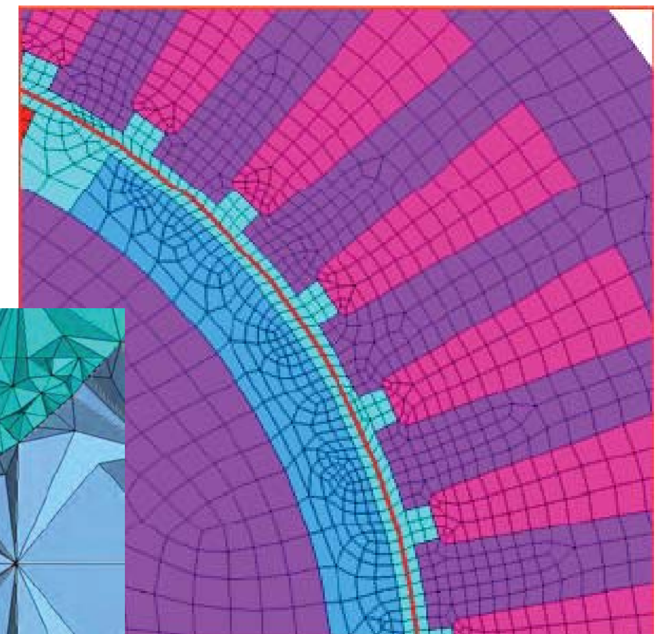


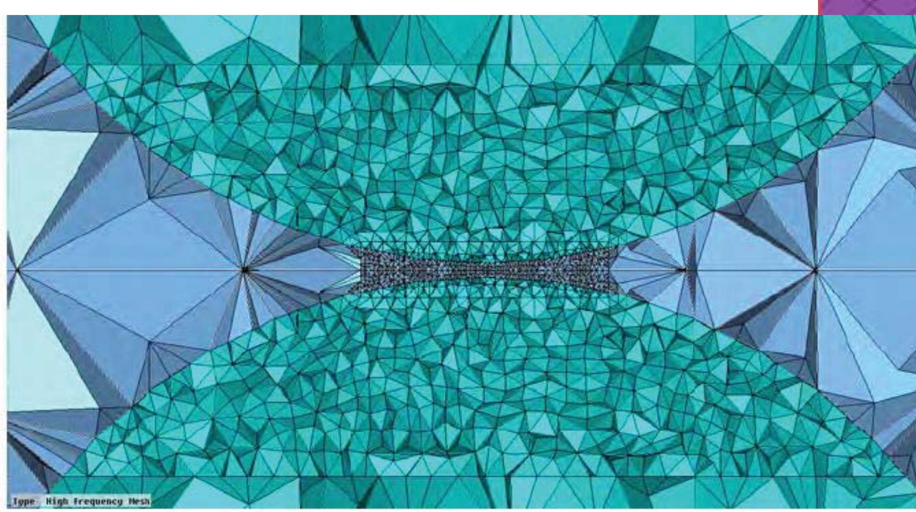
"Fancy" pictures as a final result of field calculation

- 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

前处理：

1：问题及求解域定义

根据实际问题近似确定求解域的物理性质和几何区域。

2：求解域离散化

将求解域近似为具有不同有限大小和形状且彼此相连的有限个单元组成的离散域，习惯上称为有限元网络划分。单元越小（网络越细）则离散域的近似程度越好，计算结果也越精确，但计算量及误差都将增大。

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

处理：

1：确定状态变量及控制方法

一个具体的物理问题通常可以用一组包含问题状态变量边界条件的微分方程式表示，为适合有限元求解，通常将微分方程化为等价的泛函形式。

2：单元推导

对单元构造一个适合的近似解，即推导有限单元的列式，其中包括选择合理的单元坐标系，建立单元试函数，以某种方法给出单元各状态变量的离散关系，从而形成单元矩阵(结构力学中称刚度阵或柔度阵)。

为保证问题求解的收敛性，单元推导有许多原则要遵循。对工程应用而言，重要的是应注意每一种单元的解题性能与约束。例如，单元形状应以规则为好，畸形时不仅精度低，而且有缺秩的危险，将导致无法求解。

3：总装求解

将单元总装形成离散域的总矩阵方程(联合方程组)，反映对近似求解域的离散域的要求，即单元函数的连续性要满足一定的连续条件。总装是在相邻单元结点进行，状态变量及其导数(可能的话)连续性建立在结点处。

4：联立方程组求解和结果解释

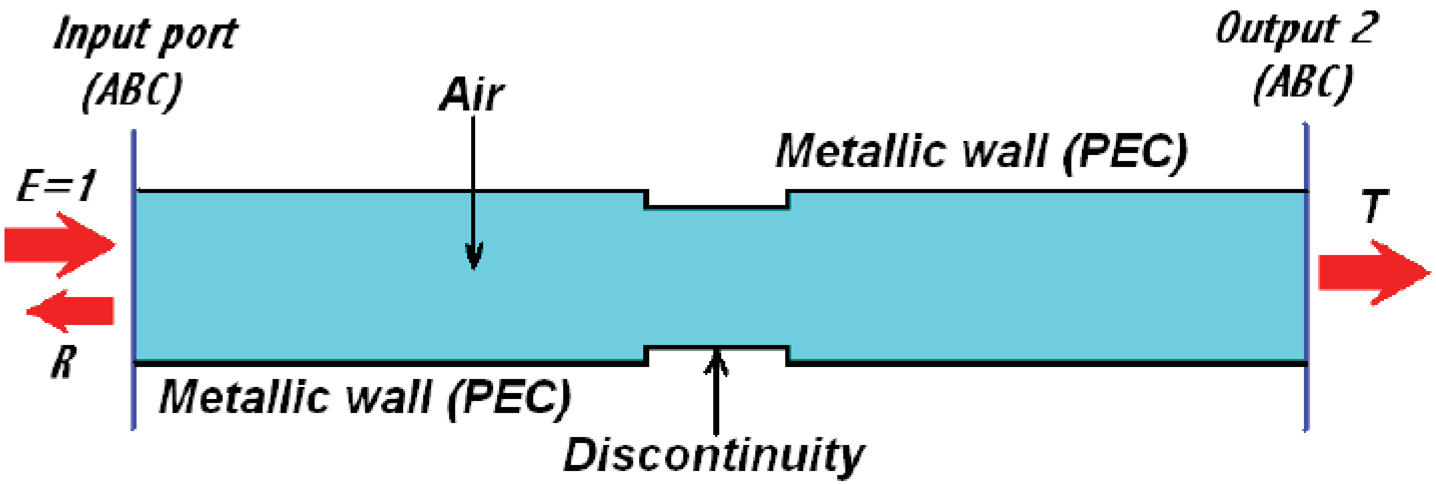
有限元法最终导致联立方程组。联立方程组的求解可用直接法、迭代法和随机法。求解结果是单元结点处状态变量的近似值。对于计算结果的质量，将通过与设计准则提供的允许值比较来评价并确定是否需要重复计算。

后处理：采集处理分析结果，使用户能简便提取信息，了解计算结果

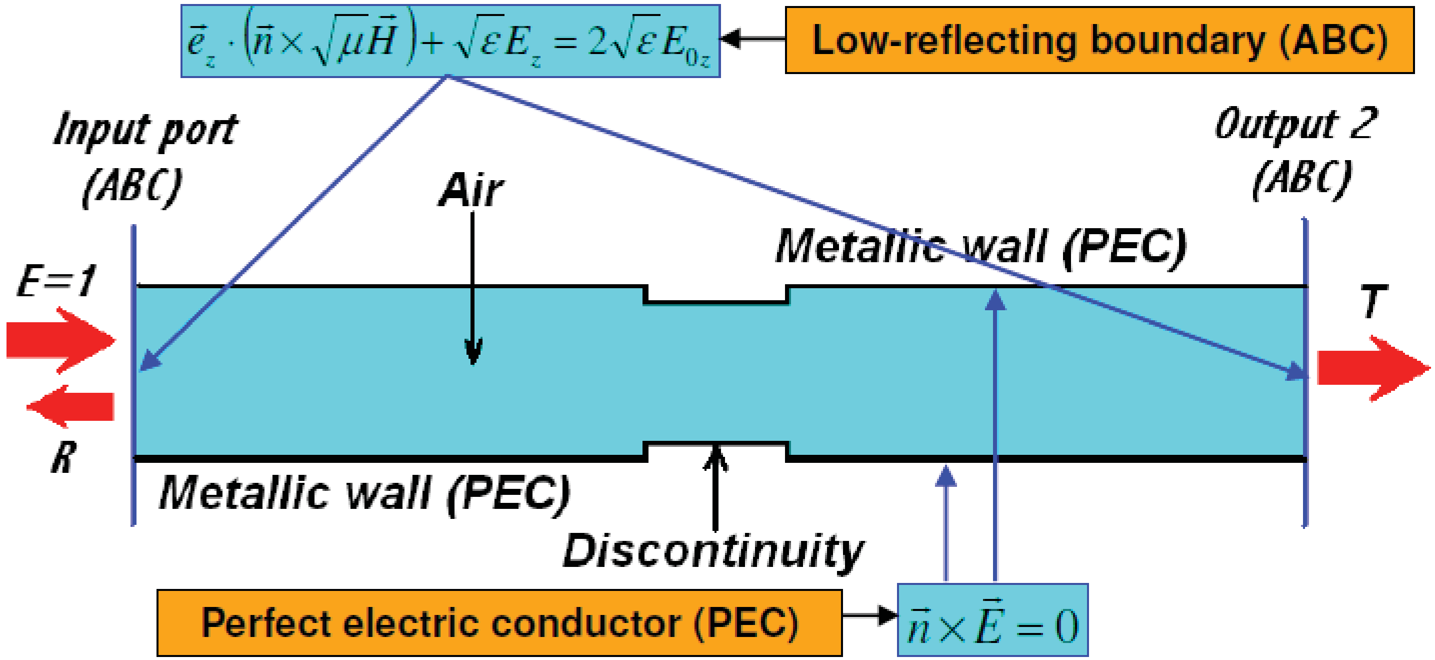
Helmholtz equation – wave propagation example

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

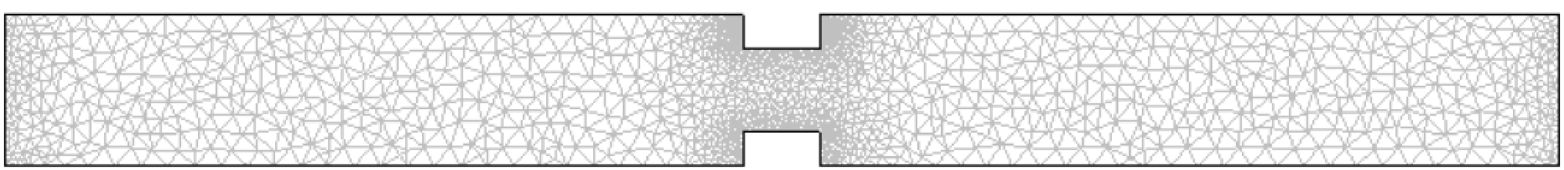
Example



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:

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

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

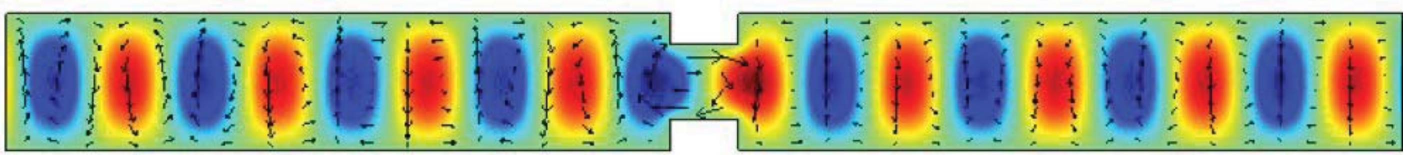
Solve this linear equation system to get the solution:

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

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

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

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

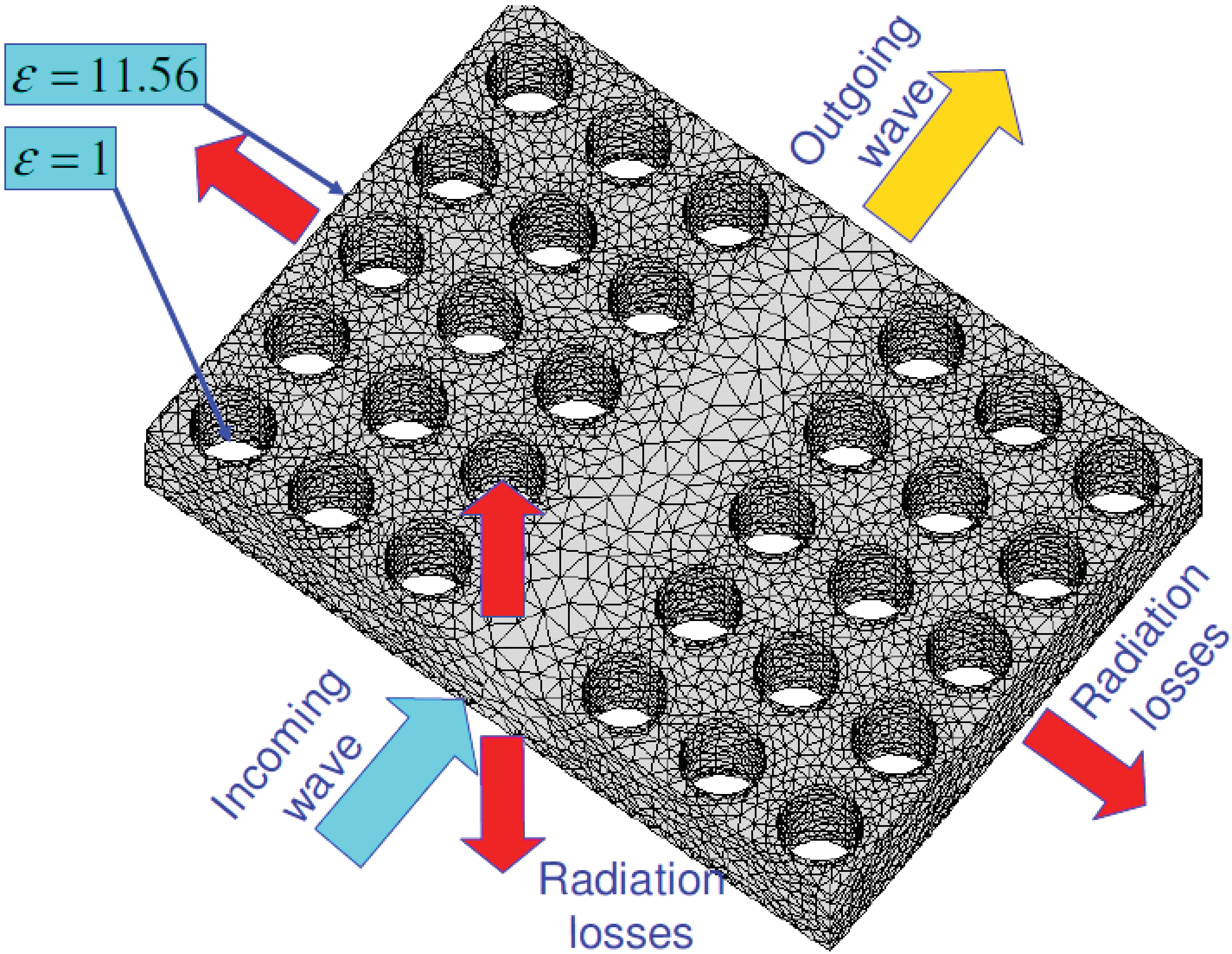
Boundary conditions

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

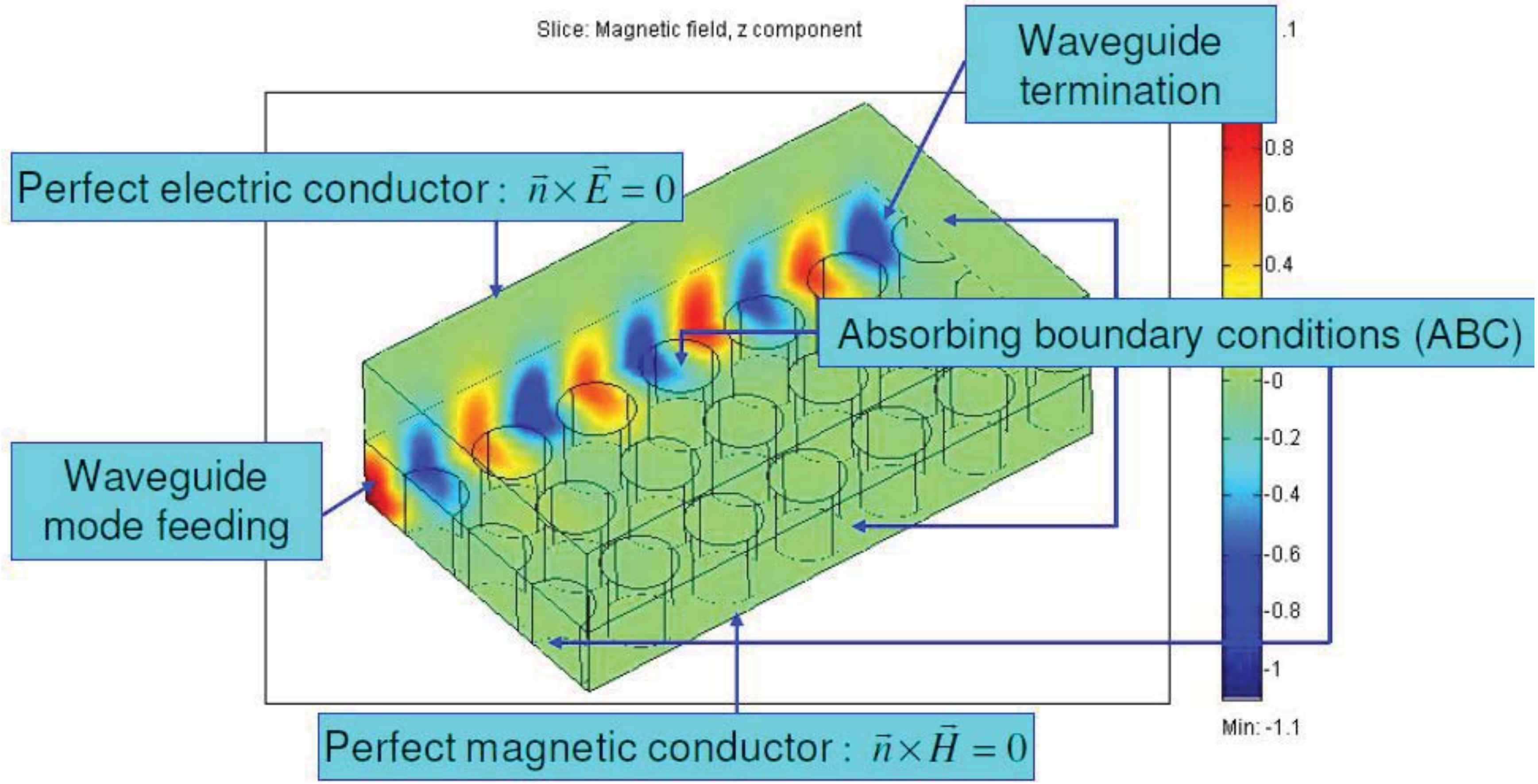
$$\frac{1}{\mu_r} \vec{n} \times \left(\nabla \times \vec{E} \right) + \gamma_e \vec{n} \times \left(\vec{n} \times \vec{E} \right) = \vec{U}$$

Functional

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



$\varepsilon = 11.56$
$\varepsilon = 1$
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

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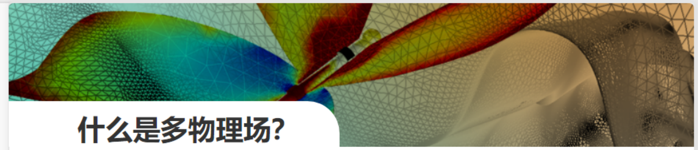
多物理场仿真百科



什么是多物理场?

多物理场（Multiphysics，mul·ti·phys·ics［mul-ti-fiz-iks］，*名词*）

1. 计算机仿真中研究的耦合物理现象。
2. 对多个相互作用的物理属性之间的研究。

理解什么是物理场

我们可以使用各种物理定律来描述万物的产生和变化。自 20 世纪 40 年代以来，人们就一直在致力于利用计算机来理解各种物理现象。最初的时候，由于计算资源非常稀缺，研究主要集中在各种孤立的物理效应。然而，我们现实世界中的物理现象并不是孤立发生的。

多物理场的世界

现实世界在本质上是一个多物理场的世界。

我们每个人用的手机就是这样一个例子。手机中的天线用来接收电磁波；触摸屏或按键是用来与使用者进行交互的机械和电子元件；电池会发生化学反应，并包含离子运动和电子流动等等。这样一个小小的设备，包含着多种物理现象的相互作用。

借助具有多物理场功能的仿真工具，我们可以准确地抓住产品设计工作中的关键因素。

浏览“多物理场百科”

http://cn.comsol.commultiphysics

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)