纳米光子学及其应用

第13讲：数值模拟计算方法1

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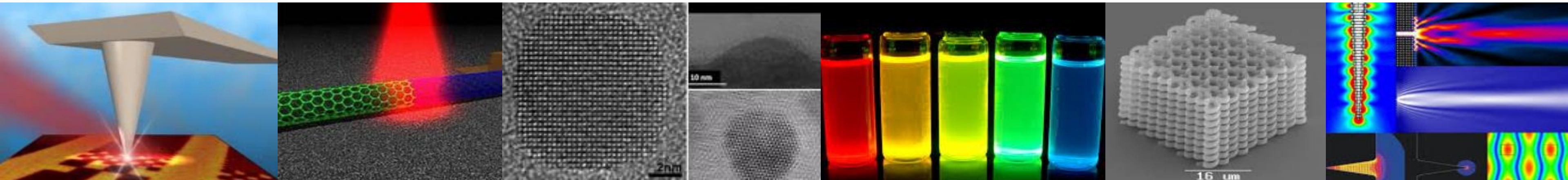


扫描近场光学显微镜(SNOM)

➢优势与劣势

	OM	SNOM	AFM	STM	SEM	TEM
相互作用	光与物质	光与物质	原子与原子	原子与原子	电子与物质	电子与物质
极限分辨率(nm)	200	5	0.1	0.1	1	0.01
检测效率	很快	慢	慢	慢	较快	慢
样品要求	无要求	较为平坦，光学效应	较为平坦	较为平坦，导电	导电，任意形状	特殊制样品
环境要求	大气	大气	大气	高真空	高真空	高真空

纳米光子学内容

课程知识点

1. 研究内容

纳米光子学基础

电子与光子异同

纳米尺度下光与物质相互作用

- 量子材料：电子的限域引起光学效应
- 表面等离子体光学：金属光学
- 光子晶体：周期性介质光学
- 亚波长共振：在远场影响光传播和偏振的周期性光学结构
- 超材料：人工设计电磁材料

2. 研究方法

特性描述：近场光学

计算方法：电磁场数值模拟

制备方法：纳米加工

本讲内容

- 纳米光学数值方法综述
- 时域有限差分法(FDTD) （重点）
- 有限元法(FEM) （理解）
- 平面波展开法 （PWM） （理解）
- 傅立叶模态法(FMM) （了解）

目的:

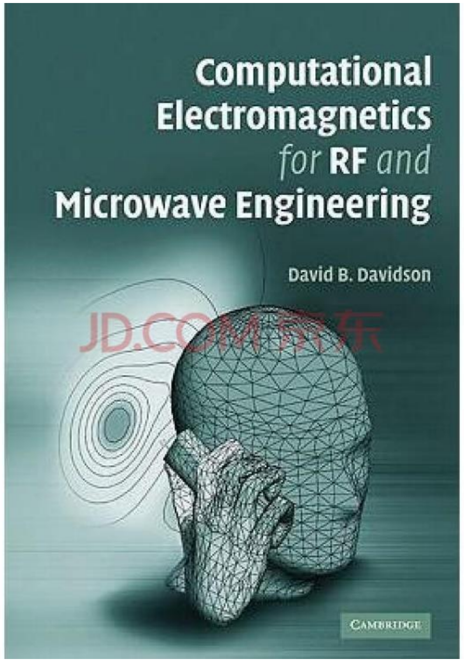
1. 为什么需要进行严格的数值模拟计算?
2. 有哪些常用的数值模拟计算方法?
3. 怎样选择计算方法?

为什么需要严格的数值方法?

- 为了解纳米光学现象的物理本质，往往针对简单几何体进行建模和分析(如Mie理论、Drude等模型)——物理图像
- 实际面临的情况是复杂的几何构型和物质组成，难以采用理论获得解析的结果。为了模拟纳米结构的电磁响应，需要采用数值方法开展“数值实验”，即计算机仿真，进而指导设计，优化相应的结构
- 介绍纳米光子学中最常用的数值计算方法：时域有限差分法(FDTD)，有限元法(FEM)，平面波展开法(PWM)——基本原理和应用
- 不同类型的纳米结构适用不同的数值方法(例如，光子晶体、有平面波法、时域有限差分法(FDTD)、传输矩阵等)

数值方法分类

- 频域方法&时域方法
- 域内的离散方法&边界离散方法
- 周期性结构法&非周期性结构法
- 近场法&远场法
- 全矢量法&近似法
- 、、、

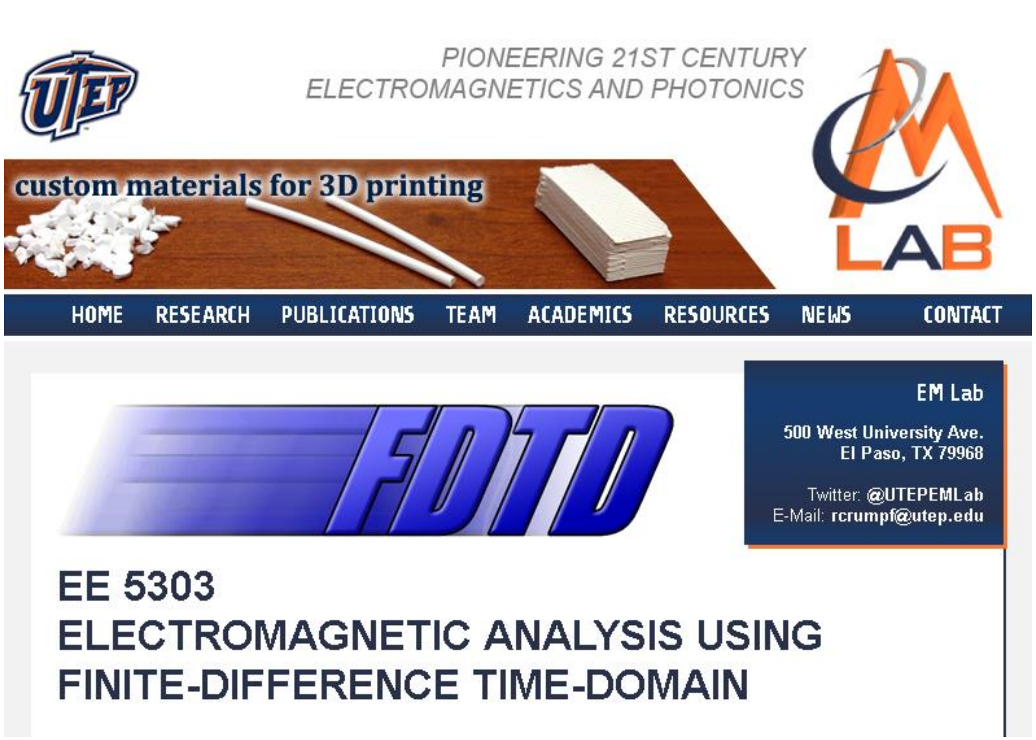


所有方法都是通过一定的技巧或近似解Maxwell方程——计算电磁学

•有很多方法和有用的商业软件，但是没有一种方法(软件)可以解决所有的问题！
•用户需要很熟悉这些软件、数值方法的原理和局限性，以及需要分析的问题。

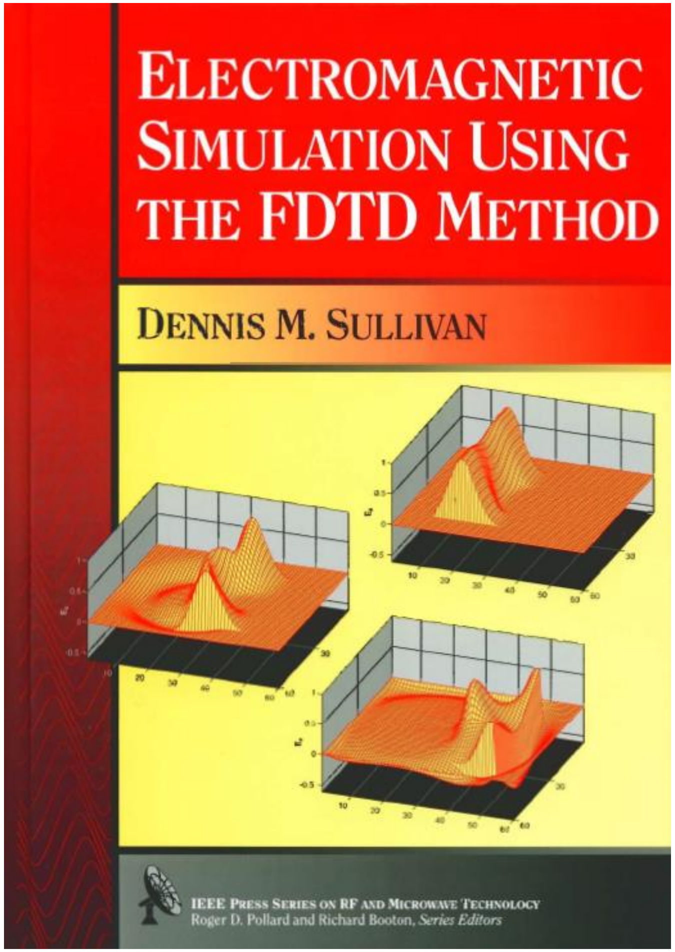
时域有限差分法
Finite-difference time-domain(FDTD)

Resources



The University of Texas at El Paso

http://emlab.utep.edu/ee5390fdtd.htm

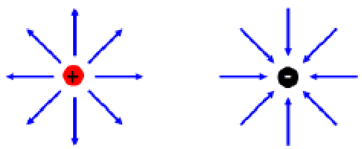


Maxwell方程组-有源空间

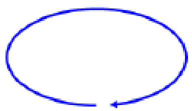
Gauss' Law

$$\boxed{\nabla \bullet \vec{D} = \rho_v} \qquad \nabla \bullet \vec{D} = \frac{\partial D_x}{\partial x} + \frac{\partial D_y}{\partial y} + \frac{\partial D_z}{\partial z}$$

Electric fields diverge from positive charges and converge on negative charges.



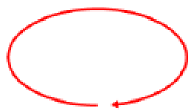
If there are no charges, electric fields must form loops.



Gauss' Law for Magnetic Fields

$$\boxed{\nabla \bullet \vec{B} = 0} \qquad \nabla \bullet \vec{B} = \frac{\partial B_x}{\partial x} + \frac{\partial B_y}{\partial y} + \frac{\partial B_z}{\partial z}$$

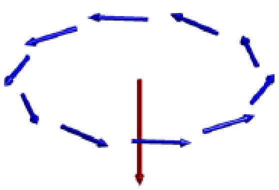
Magnetic fields always form loops.



Faraday'sLaw

$$\boxed{\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}} \qquad \nabla \times \vec{E} = \left(\frac{\partial E_z}{\partial y} - \frac{\partial E_y}{\partial z}\right)\hat{a}_x + \left(\frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x}\right)\hat{a}_y + \left(\frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y}\right)\hat{a}_z$$

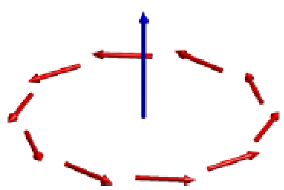
Circulating electric fields induce time varying magnetic fields.
Time varying magnetic fields induce circulating electric fields.



Ampere's Circuit Law

$$\boxed{\nabla \times \vec{H} = \vec{J} + \frac{\partial \vec{D}}{\partial t}} \qquad \nabla \times \vec{H} = \left(\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z}\right)\hat{a}_x + \left(\frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x}\right)\hat{a}_y + \left(\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y}\right)\hat{a}_z$$

Circulating magnetic fields induce currents and/or time varying electric fields.
Currents and/or time varying electric fields induce circulating magnetic fields.



Maxwell方程组-无源空间

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

A circulating ***E*** field induces a change in the ***B*** field at the center of circulation.

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

A ***B*** field induces an ***H*** field in proportion to the permeability.

$$\vec{D}(t) = [\varepsilon(t)] * \vec{E}(t)$$

A ***D*** field induces an ***E*** field in proportion to the permittivity.

$$\nabla \times \vec{H}(t) = \frac{\partial \vec{D}(t)}{\partial t}$$

A circulating ***H*** field induces a change in the ***D*** field at the center of circulation.

有旋电场诱导磁场的变化，有旋磁场诱导电场的变换 --> 电磁波的传播

时域有限差分法(FDTD)的提出

Numerical Solution of Initial Boundary Value Problems Involving Maxwell's Equations in Isotropic Media

KANE S. YEE

Abstract—**Maxwell's equations are replaced by a set of finite difference equations. It is shown that if one chooses the field points appropriately, the set of finite difference equations is applicable for a boundary condition involving perfectly conducting surfaces. An example is given of the scattering of an electromagnetic pulse by a perfectly conducting cylinder.**

Introduction

SOLUTIONS to the time-dependent Maxwell's equations in general form are unknown except for a few special cases. The difficulty is due mainly to the imposition of the boundary conditions. We shall show in this paper how to obtain the solution numerically when the boundary condition is that appropriate for a perfect conductor. In theory, this numerical attack can be employed for the most general case. However, because of the limited memory capacity of present day computers, numerical solutions to a scattering problem for which the ratio of the characteristic linear dimension of the obstacle to the wavelength is large still seem to be impractical. We shall show by an example that in the case of two dimensions, numerical solutions are practical even when the characteristic length of the obstacle is moderately large compared to that of an incoming wave.

A set of finite difference equations for the system of partial differential equations will be introduced in the early part of this paper. We shall then show that with an appropriate choice of the points at which the various field components are to be evaluated, the set of finite difference equations can be solved and the solution will satisfy the boundary condition. The latter part of this paper will specialize in two-dimensional problems, and an example illustrating scattering of an incoming pulse by a perfectly conducting square will be presented.

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Maxwell's Equation and the Equivalent Set of Finite Difference Equations

Maxwell's equations in an isotropic medium [1] are:[1]

$$\frac{\partial \boldsymbol{B}}{\partial t} + \nabla \times \boldsymbol{E} = 0, \quad \text{(1a)}$$

$$\frac{\partial \boldsymbol{D}}{\partial t} - \nabla \times \boldsymbol{H} = \boldsymbol{J}, \quad \text{(1b)}$$

$$\boldsymbol{B} = \mu \boldsymbol{H}, \quad \text{(1c)}$$

$$\boldsymbol{D} = \epsilon \boldsymbol{E}, \quad \text{(1d)}$$

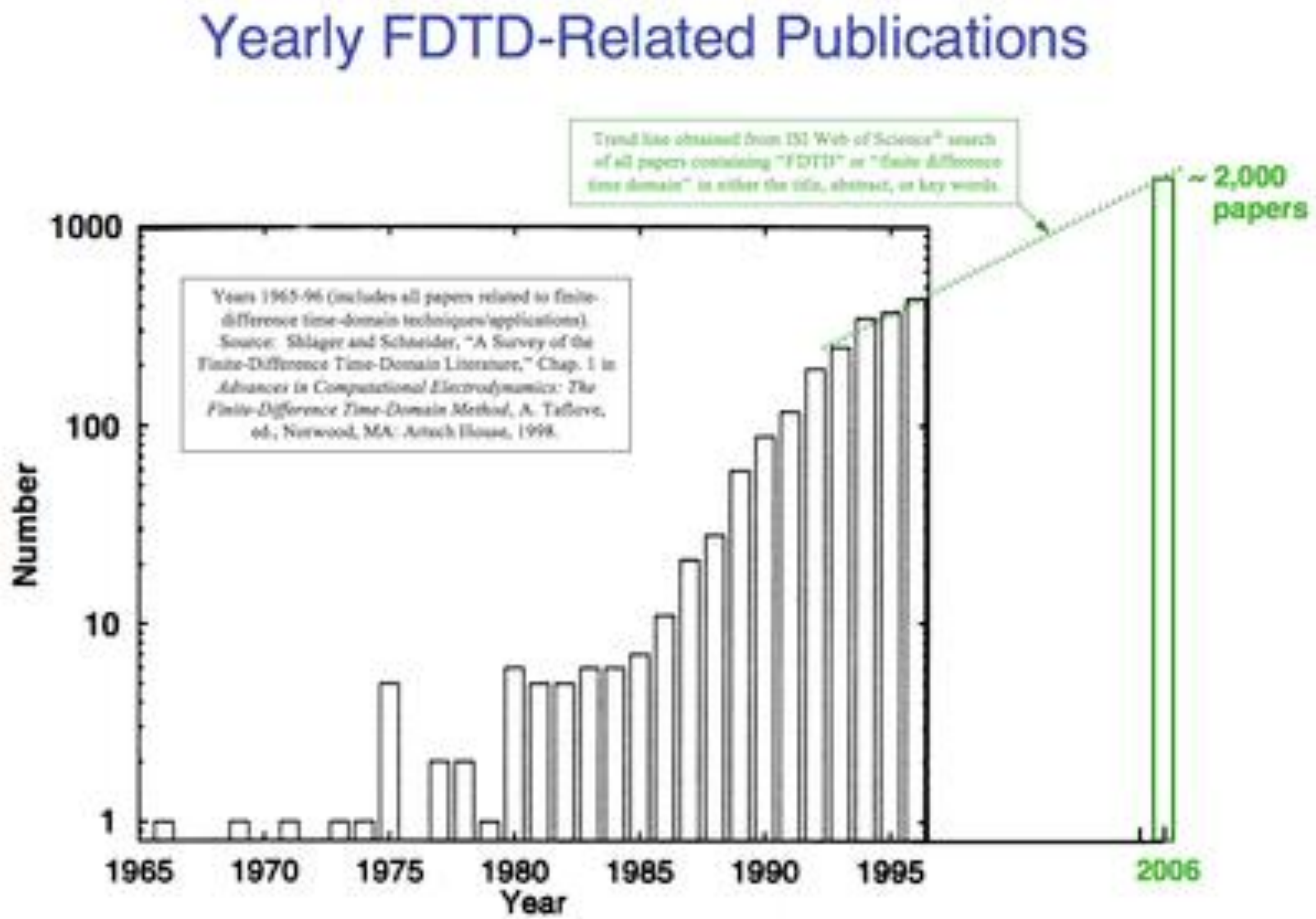
[1] In MKS system of units.

Kane Shee-Gong Yee
美籍华裔

IEEE Transactions on Antennas and Propagation

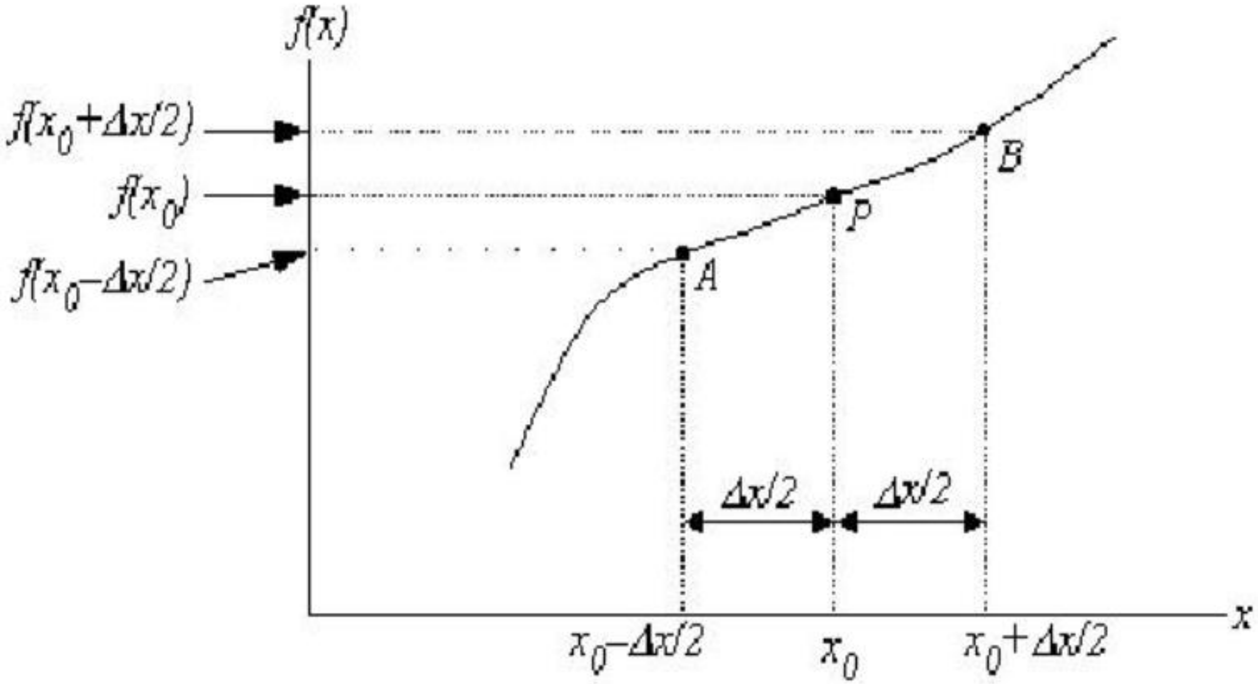
K.S. Yee, *IEEE Trans. Antennas Propagation*, 14, 302 (1966)

时域有限差分法(FDTD)



有限差分原理

$$\frac{\mathrm{d}f(x_0)}{dx}=f'(x_0)\cong\frac{f(x_0+\triangle x/2)-f(x_0-\triangle x/2)}{\triangle x}$$



$f(x)$在点x_0的微分用有限差分近似公式替代

时间离散

$$\nabla\times\boldsymbol{E}(t)=-\mu\frac{\partial\boldsymbol{H}(t)}{\partial t}\quad\Longrightarrow\quad\nabla\times\boldsymbol{E}\Big|_{t}=-\mu\frac{\boldsymbol{H}\Big|_{t+\frac{\Delta t}{2}}-\boldsymbol{H}\Big|_{t-\frac{\Delta t}{2}}}{\Delta t}$$

$$\nabla\times\boldsymbol{H}(t)=\varepsilon\frac{\partial\boldsymbol{E}(t)}{\partial t}\quad\Longrightarrow\quad\boxed{\nabla\times\boldsymbol{H}\Big|_{t+\frac{\Delta t}{2}}=\varepsilon\frac{\boldsymbol{E}\Big|_{t+\Delta t}-\boldsymbol{E}\Big|_{t}}{\Delta t}}$$

对时间的微分用有限差分近似替代

注意：电场和磁场的时间点是错开的

时间离散—物理意义

Update coefficient

为加速计算，这些量在迭代之前已经计算好

$$\vec{E}\Big|_{t+\Delta t} = \vec{E}\Big|_{t} + \frac{\Delta t}{\varepsilon}\left(\nabla \times \vec{H}\Big|_{t+\Delta t/2}\right)$$

Field at the next time step.

Field at the previous time step.

Curl of the “other” field at an intermediate time step

空间中任意一个时刻的电(磁)场只与邻近时刻的电(磁)场相关

时间离散—蛙跳运算

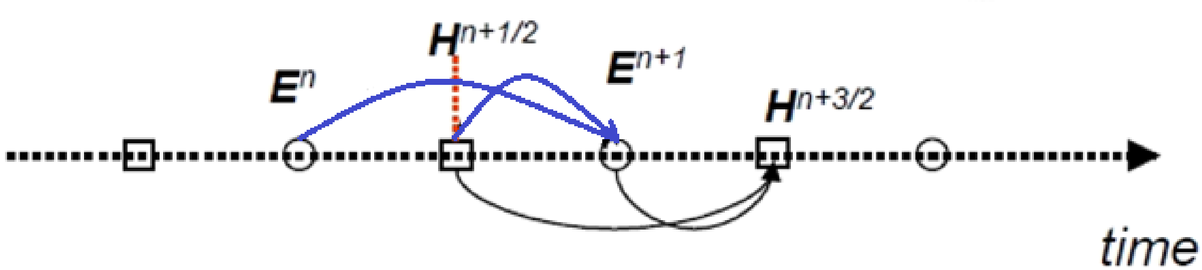
为满足精度要求，按半步长时间交错进行 $\boldsymbol{E}$ 和 $\boldsymbol{H}$ 的更新，解得场的时间微分，即：

——在时间半步长 n+1/2 处写 $\boldsymbol{H}$ 场

——在时间整步长 n 处写 $\boldsymbol{E}$ 场

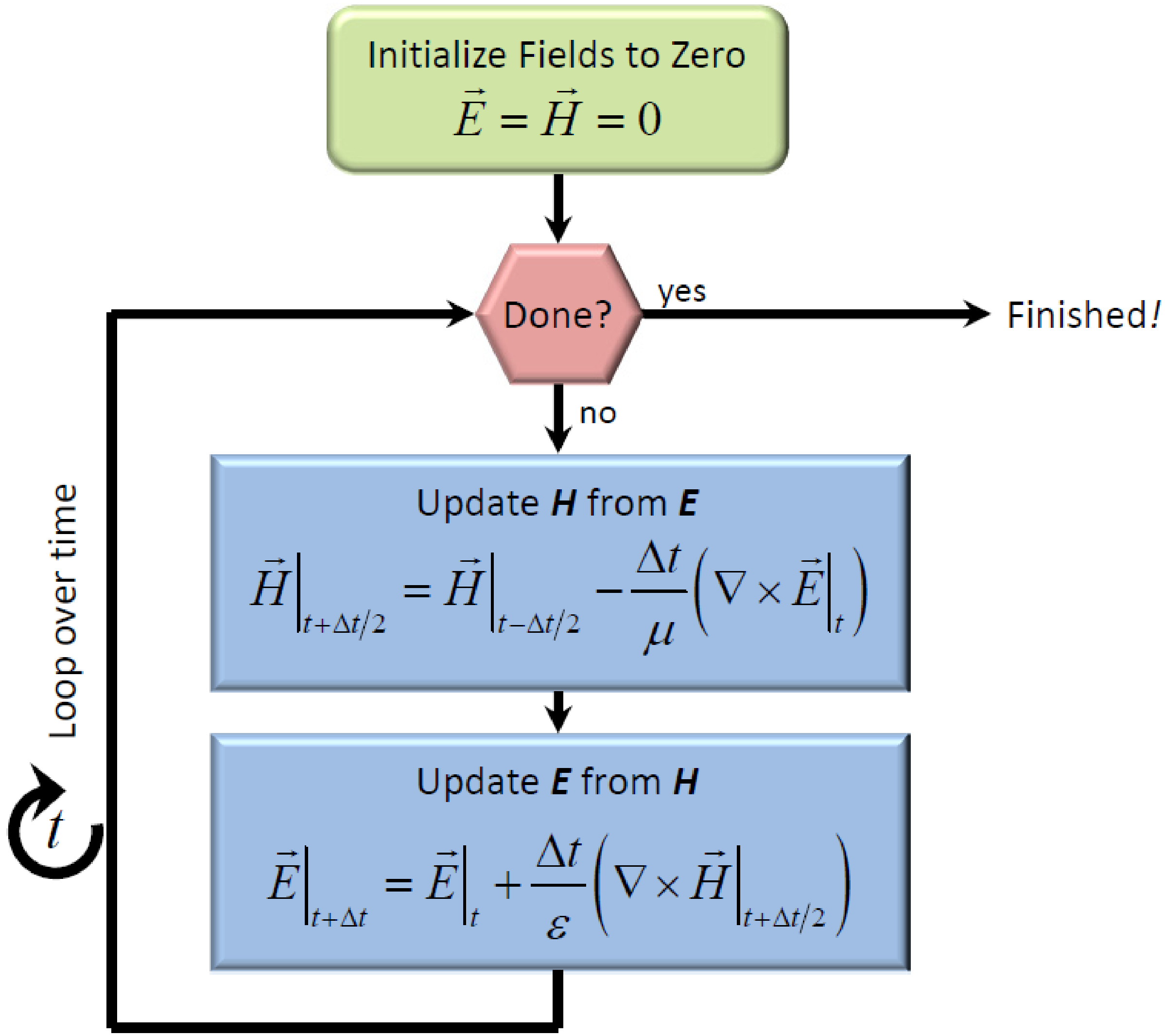
$$\frac{\partial \boldsymbol{E}}{\partial t}\Big|^{n+1/2} \approx \frac{\boldsymbol{E}^{n+1}-\boldsymbol{E}^{n}}{\Delta t} = \frac{1}{\varepsilon}[\nabla\times\boldsymbol{H}]^{n+1/2} \qquad \frac{\partial \boldsymbol{H}}{\partial t}\Big|^{n} \approx \frac{\boldsymbol{H}^{n+\frac{1}{2}}-\boldsymbol{H}^{n+\frac{1}{2}}}{\Delta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

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



也被称为“蛙跳运算法则”

时间离散—*E*、*H*交叠更新



$$\vec{H}\Big|_{t-\frac{\Delta t}{2}}=0 \qquad \vec{E}\Big|_{t}=0$$

$$\vec{H}\Big|_{t+\frac{\Delta t}{2}}\Leftarrow\vec{E}\Big|_{t}$$
$$\vec{E}\Big|_{t+\Delta t}\Leftarrow\vec{H}\Big|_{t+\frac{\Delta t}{2}}$$
$$\vec{H}\Big|_{t+\frac{3\Delta t}{2}}\Leftarrow\vec{E}\Big|_{t+\Delta t}$$
$$\vec{E}\Big|_{t+2\Delta t}\Leftarrow\vec{H}\Big|_{t+\frac{3\Delta t}{2}}$$
$$\vec{H}\Big|_{t+\frac{5\Delta t}{2}}\Leftarrow\vec{E}\Big|_{t+2\Delta t}$$
$$\vec{E}\Big|_{t+3\Delta t}\Leftarrow\vec{H}\Big|_{t+\frac{5\Delta t}{2}}$$
$$\vdots$$

空间离散化

从麦克斯韦的微分方程出发：

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

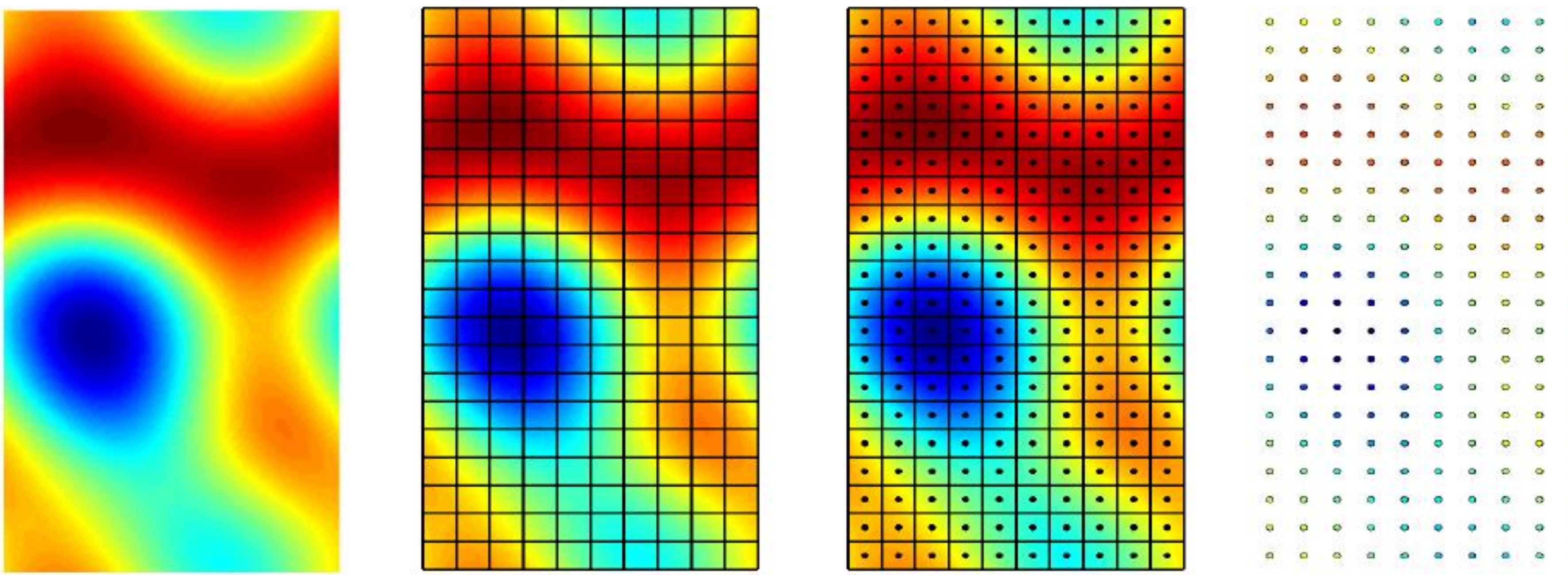
$$\begin{bmatrix} \dfrac{\partial H_z}{\partial y} - \dfrac{\partial H_y}{\partial z} \\ \dfrac{\partial H_x}{\partial z} - \dfrac{\partial H_z}{\partial x} \\ \dfrac{\partial H_y}{\partial x} - \dfrac{\partial H_x}{\partial y} \end{bmatrix} = \varepsilon \cdot \begin{bmatrix} \dfrac{\partial E_x}{\partial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

- 除了时间之外，空间结构也应该被离散成有限格点组成网络
- 所有场分量的偏微分方程都用一阶有限差分近似表示

Yee网格—空间离散化

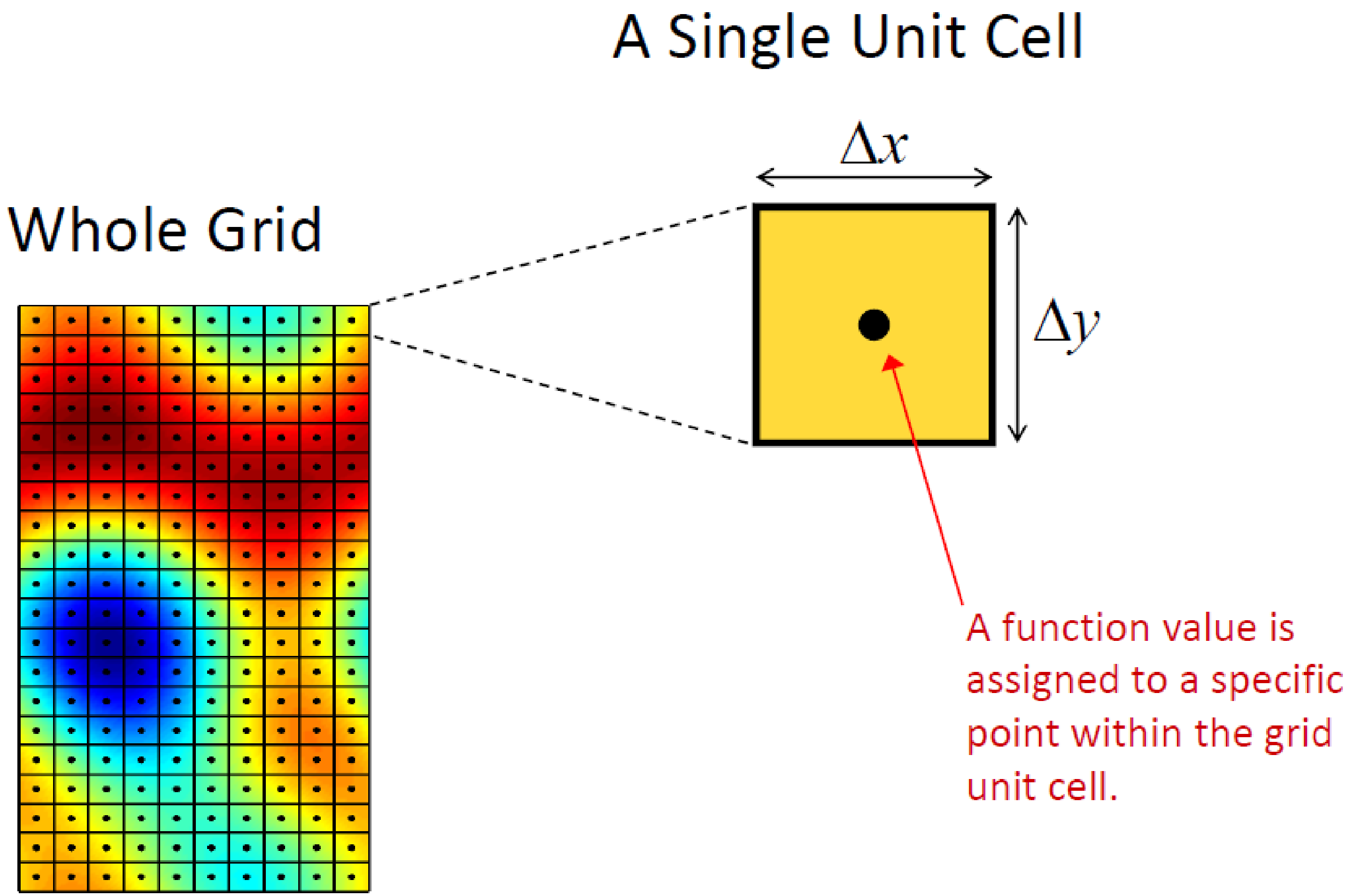
电脑存储数据只能是离散化的

Example physical (continuous) field profile	A grid is constructed by dividing space into discrete cells	Field is known only at discrete points	Representation of what is actually stored in memory



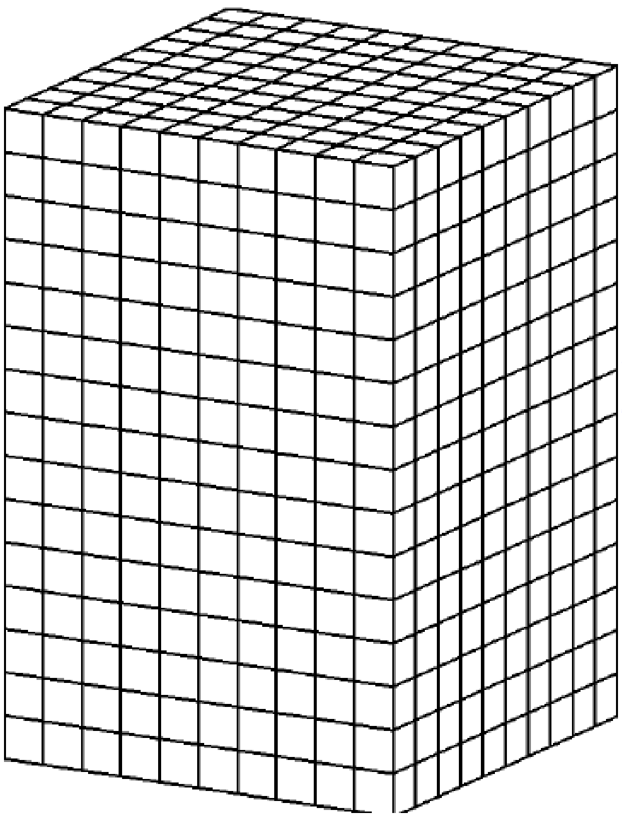
Yee’s grid

Yee网格—空间离散化


A Single Unit Cell
Δx
Δy
Whole Grid
A function value is
assigned to a specific
point within the grid
unit cell.

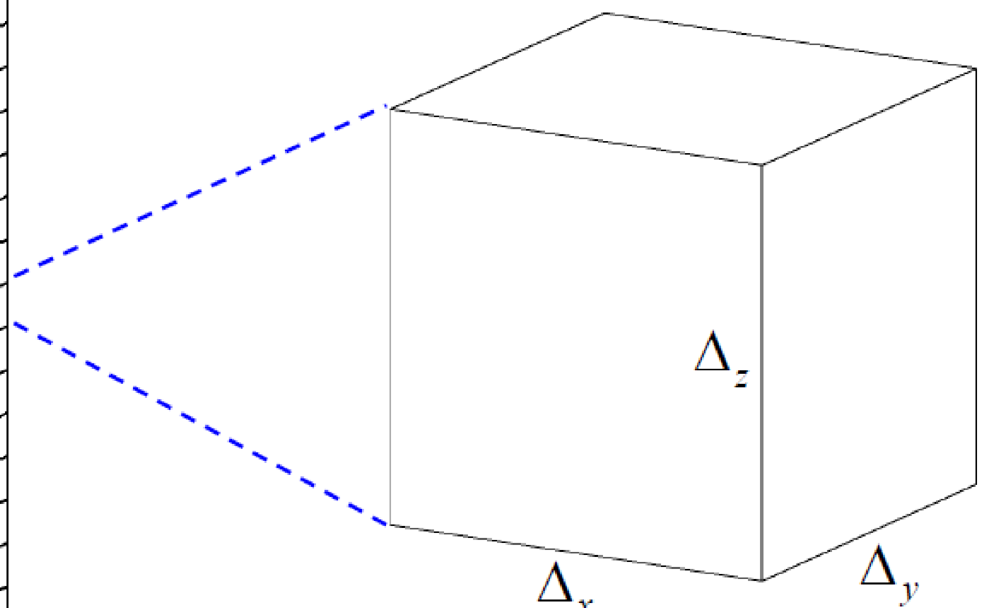
Yee网格—空间离散化

A three-dimensional grid looks like this:



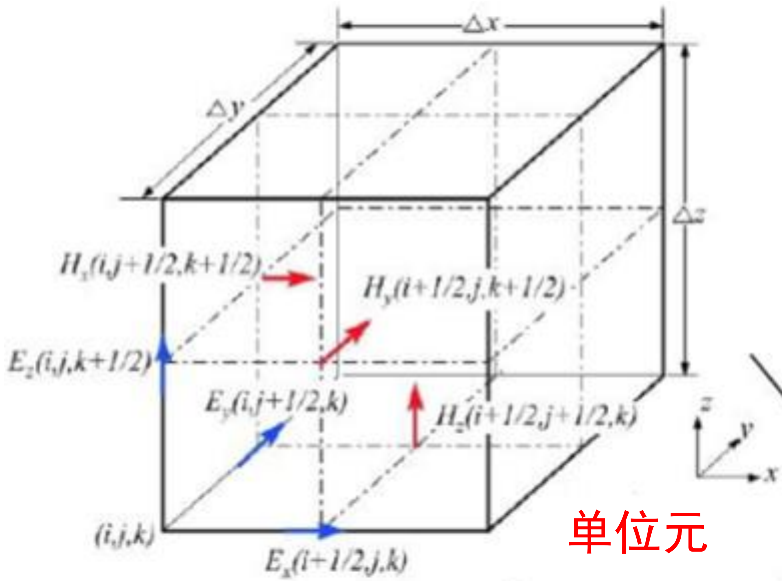
$N_x = 10, N_y = 10, N_z = 15$

A unit cell from the grid looks like this:



$$(\boldsymbol{i}, \boldsymbol{j}, \boldsymbol{k}) = (\boldsymbol{i}\Delta\boldsymbol{x}, \boldsymbol{j}\Delta\boldsymbol{y}, \boldsymbol{k}\Delta\boldsymbol{z})$$

Yee网格—FDTD算法的网络结构

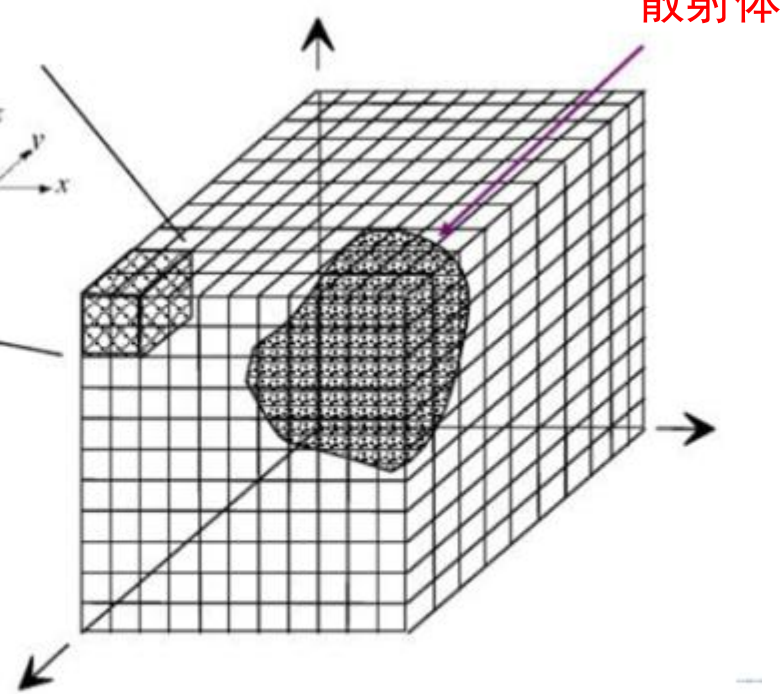


单位元

标准Yee's晶格

整个结构（不只是散射体）网格化！

散射体



$$E(i\Delta x, j\Delta y, k\Delta z) = E_{i,j,k}^{n}$$

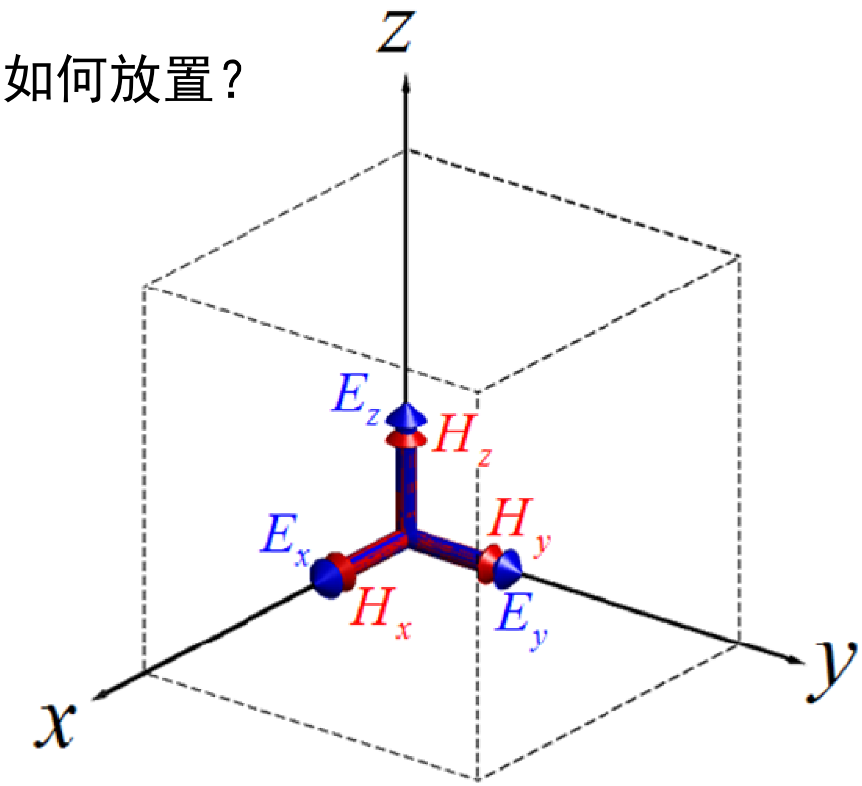
$$H(i\Delta x, j\Delta y, k\Delta z) = H_{i,j,k}^{n}$$

场量既是时间的函数也是空间的函数！

Yee网格—电场磁场分离

Within the unit cell, we need to place the field components E_x, E_y, E_z, H_x, H_y, and H_z.

在一个单元中，场如何放置？

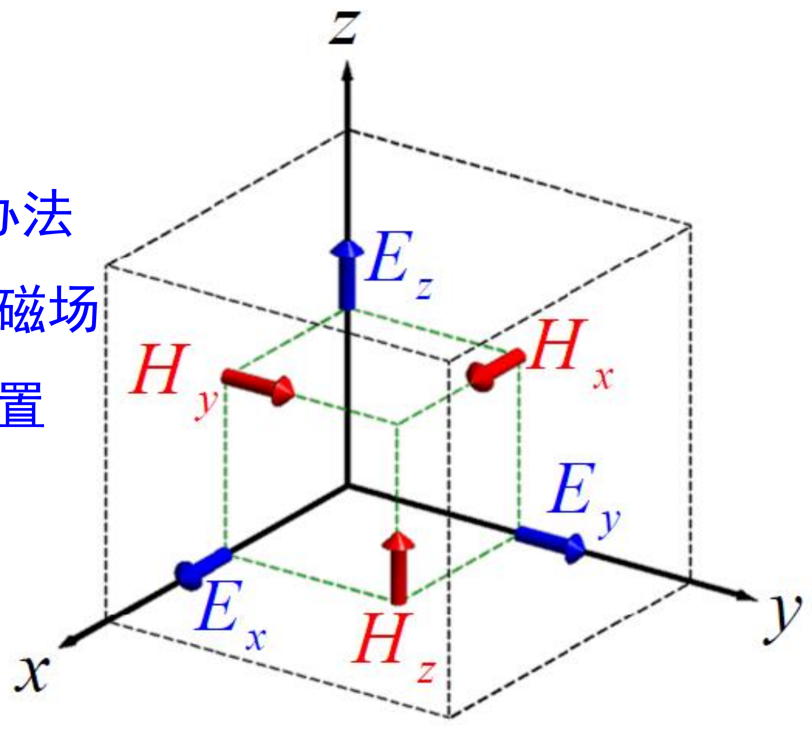


A straightforward approach would be to locate all of the field components within in a grid cell at the origin of the cell.

Yee网格—电场磁场分离/交错

Instead, we are going to stagger the position of each field component within the grid cells.

Yee的办法
电场、磁场
交叠放置



K. S. Yee, "Numerical solution of the initial boundary value problems involving Maxwell's equations in isotropic media," IEEE Trans. Microwave Theory and Techniques, vol. 44, pp. 61–69, 1998.

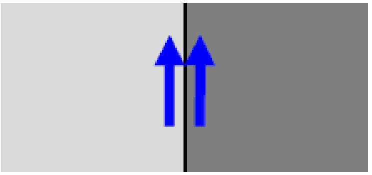
Yee网格—优势

1. Divergence-free

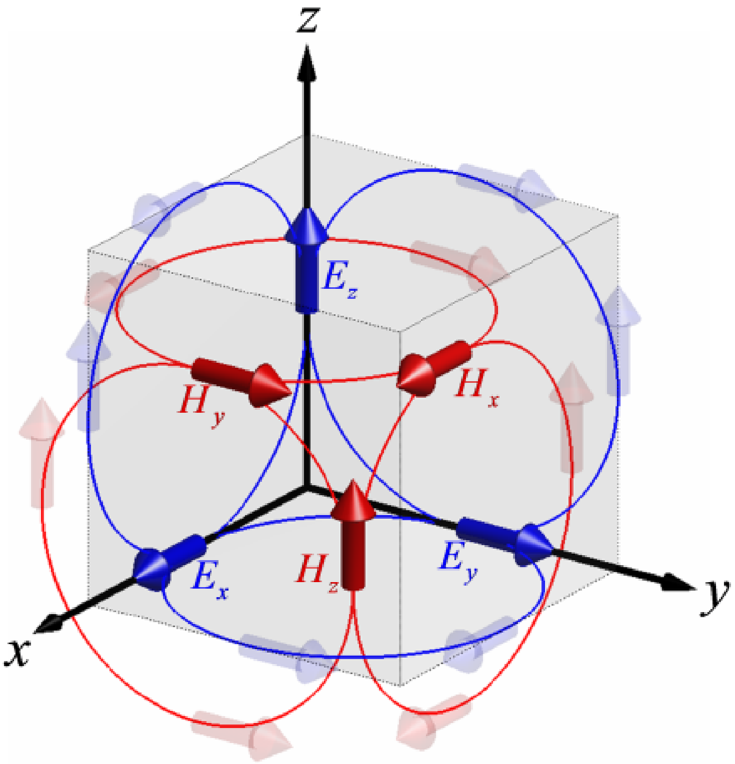
$$\nabla \bullet \left(\varepsilon \vec{E} \right) = 0$$

$$\nabla \bullet \left(\mu \vec{H} \right) = 0$$

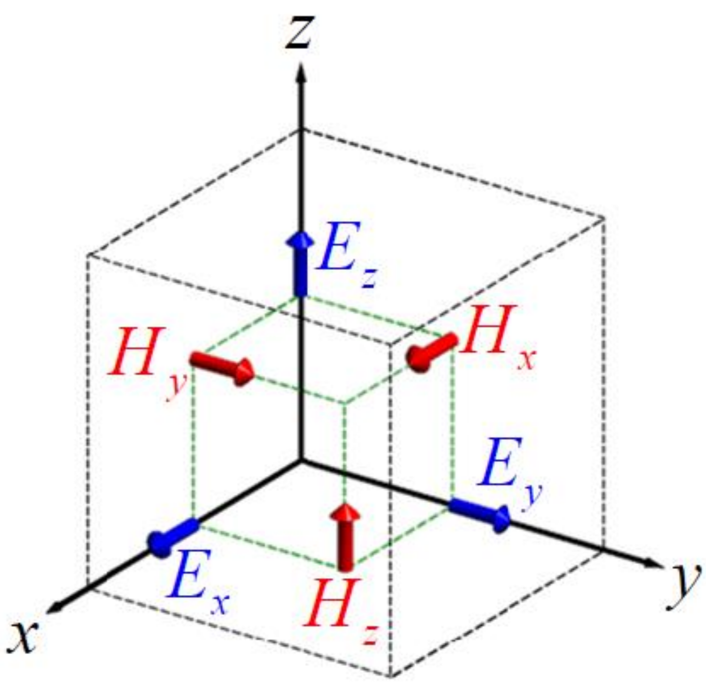
2. Physical boundary conditions are naturally satisfied



3. Elegant arrangement to approximate Maxwell's curl equations



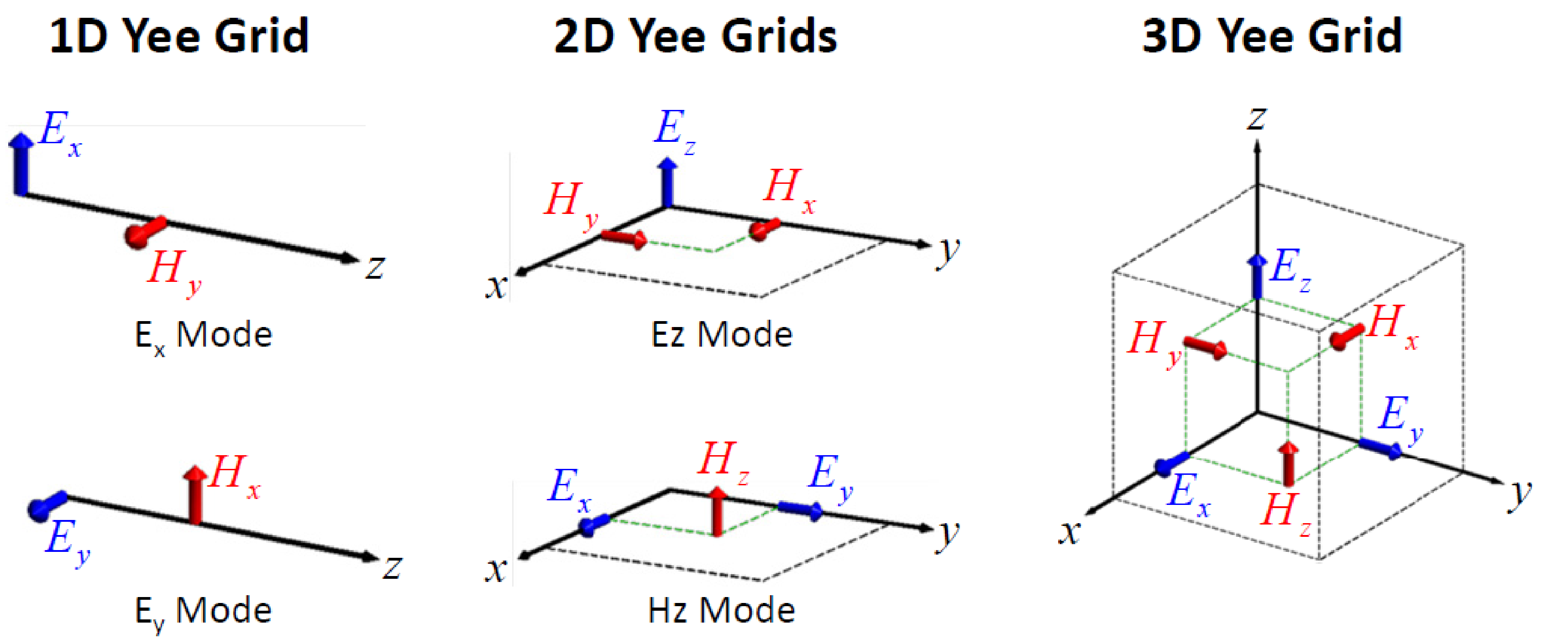
Yee网格—优势



- 场分量物理上位于不同的位置
- 即使场分量位于同一个单元内，场分量也可以在不同的材料中
- 场分量间不同相
- 与时间上的电场、磁场交叠一致

Yee网格—电场磁场分离/交错

不同维度下的Yee网格设置



磁场归一化

真空平面电磁波

$$\frac{E}{H}=\sqrt{\frac{\mu_0}{\varepsilon_0}}=Z_0\approx 377 \qquad \text{真空中的波阻抗}$$

$$\Rightarrow H\approx\frac{1}{377}E=2.65\times 10^{-3}E$$

多次迭代，带来巨大的数值误差！

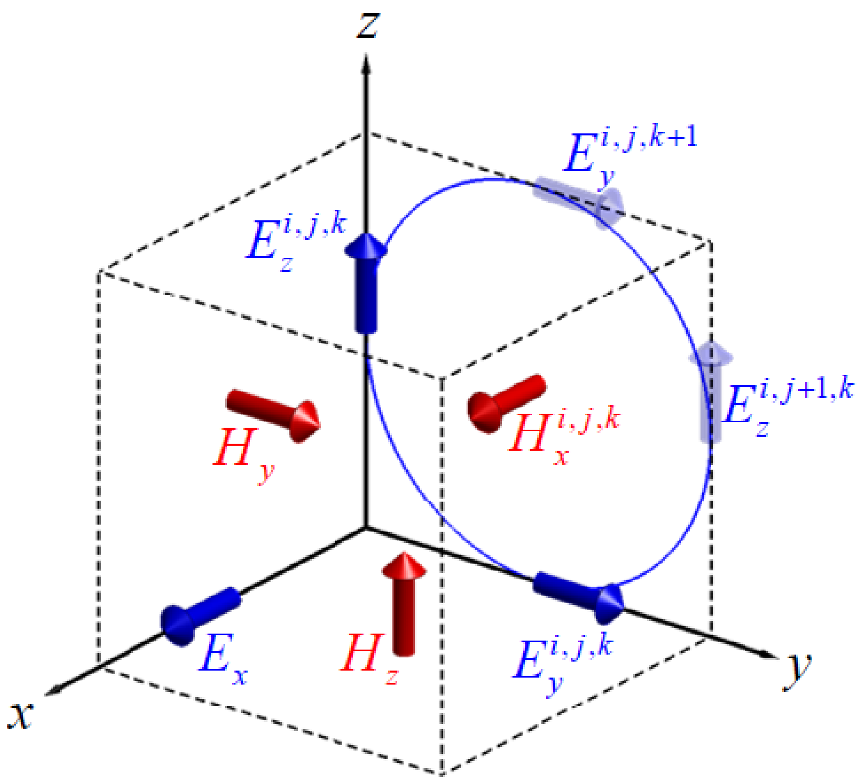
引入归一化磁场： $\tilde{\boldsymbol{H}}=Z_0\boldsymbol{H}$ ➡

$$\begin{cases}\nabla\times\boldsymbol{E}=-\dfrac{\mu_r}{c_0}\dfrac{\partial\tilde{\boldsymbol{H}}}{\partial t}\\[2ex]\nabla\times\tilde{\boldsymbol{H}}=-\dfrac{\varepsilon_r}{c_0}\dfrac{\partial\boldsymbol{E}}{\partial t}\end{cases}$$

其中： c_0 为真空中光速 $c_0=\dfrac{1}{\sqrt{\varepsilon_0\mu_0}}$

Finite-Difference Equation for H_x

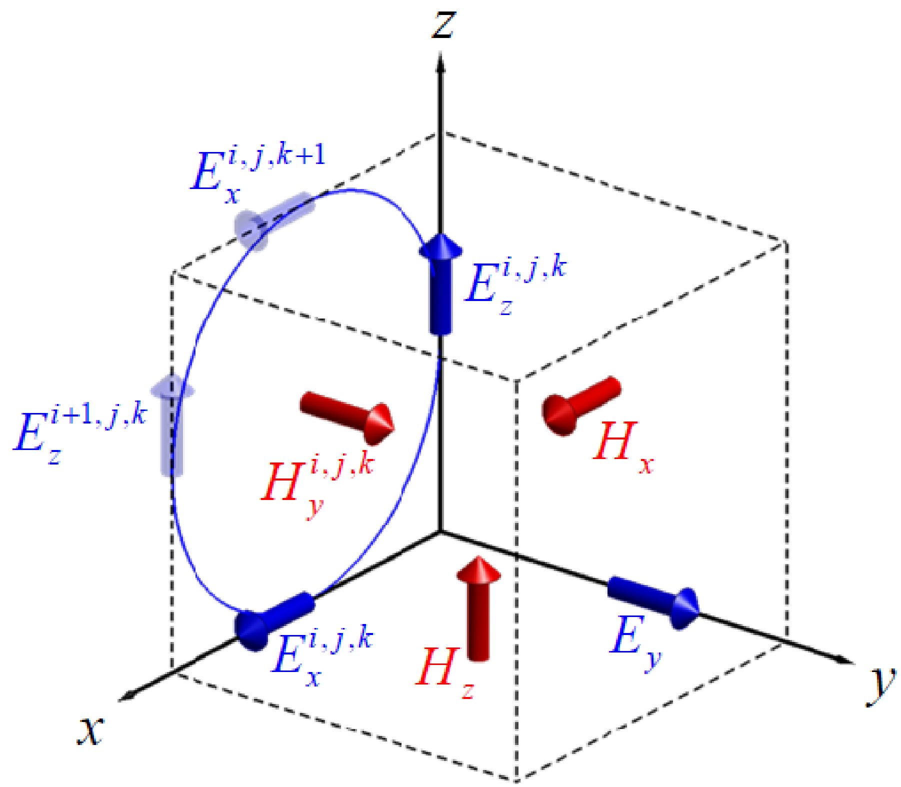
$$\frac{\partial E_z}{\partial y} - \frac{\partial E_y}{\partial z} = -\frac{\mu_{xx}}{c_0}\frac{\partial \tilde{H}_x}{\partial t}$$



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

Finite-Difference Equation for H_y

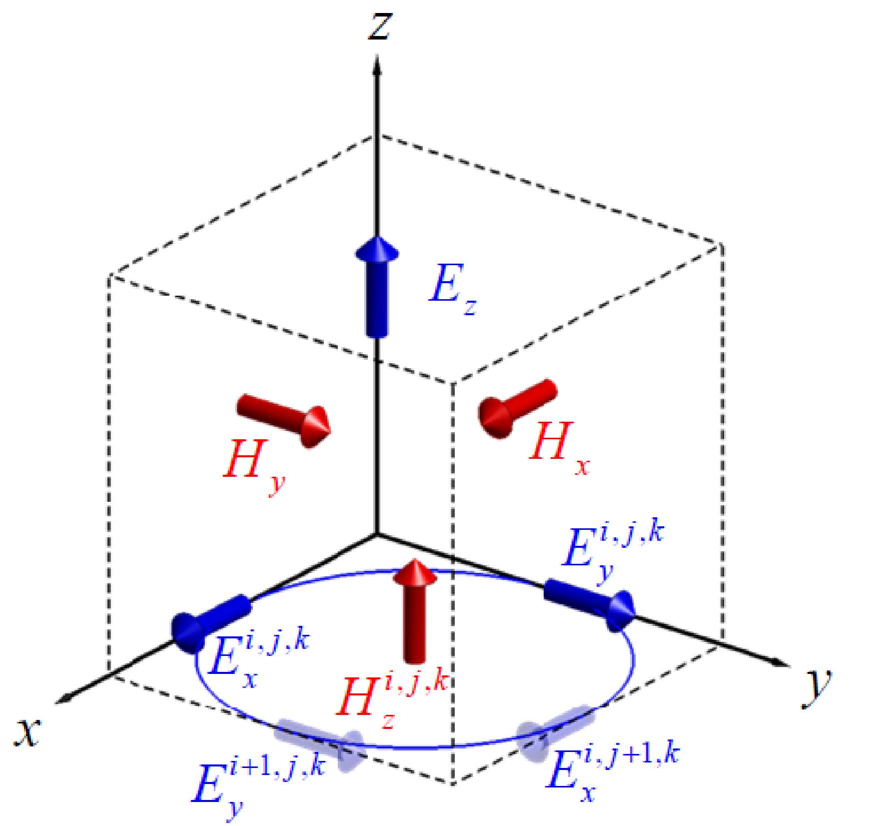
$$\frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x} = -\frac{\mu_{yy}}{c_0}\frac{\partial \tilde{H}_y}{\partial t}$$



$$\frac{E_x^{i,j,k+1}\Big|_t - E_x^{i,j,k}\Big|_t}{\Delta z} - \frac{E_z^{i+1,j,k}\Big|_t - E_z^{i,j,k}\Big|_t}{\Delta x} = -\frac{\mu_{yy}^{i,j,k}}{c_0}\frac{\tilde{H}_y^{i,j,k}\Big|_{t+\frac{\Delta t}{2}} - \tilde{H}_y^{i,j,k}\Big|_{t-\frac{\Delta t}{2}}}{\Delta t}$$

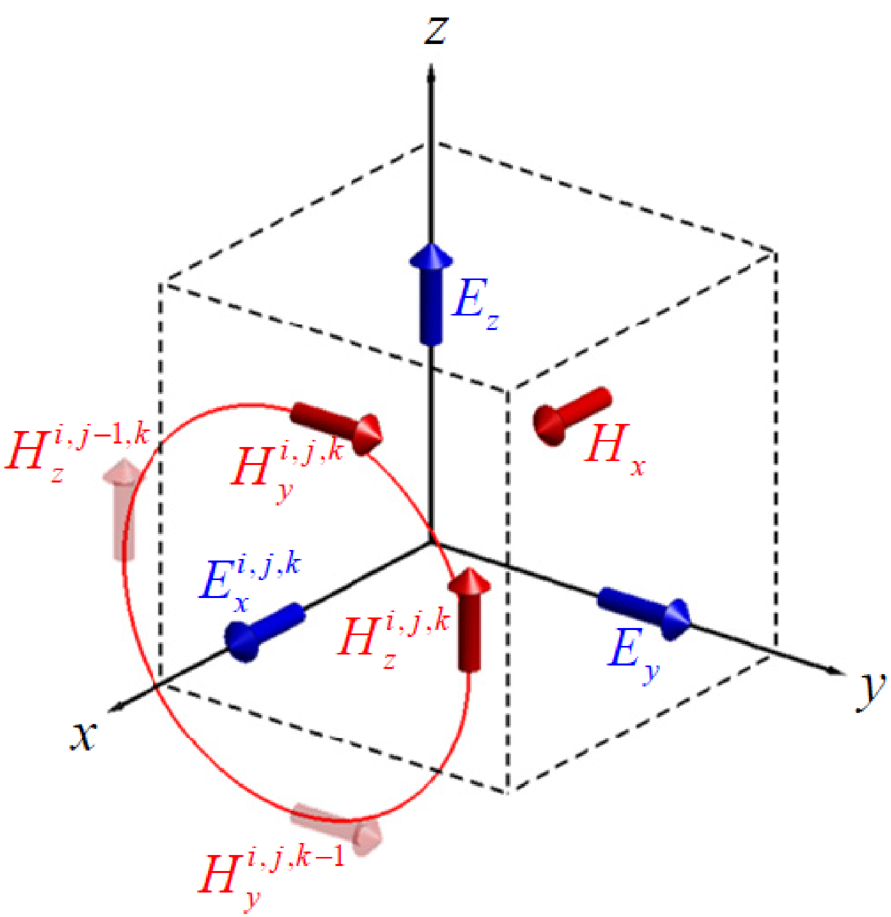
Finite-Difference Equation for H_z

$$\frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} = -\frac{\mu_{zz}}{c_0}\frac{\partial \tilde{H}_z}{\partial t}$$



$$\frac{E_y^{i+1,j,k}\big|_t - E_y^{i,j,k}\big|_t}{\Delta x} - \frac{E_x^{i,j+1,k}\big|_t - E_x^{i,j,k}\big|_t}{\Delta y} = -\frac{\mu_{zz}^{i,j,k}}{c_0}\frac{\tilde{H}_z^{i,j,k}\big|_{t+\frac{\Delta t}{2}} - \tilde{H}_z^{i,j,k}\big|_{t-\frac{\Delta t}{2}}}{\Delta t}$$

Finite-Difference Equation for E_x

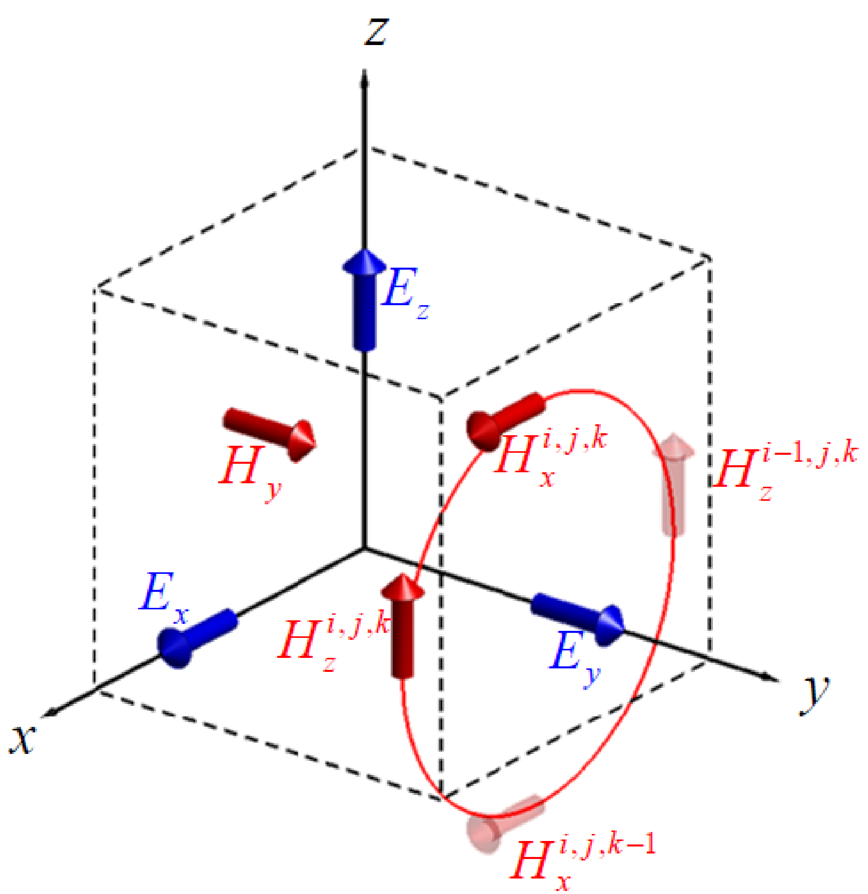


$$\frac{\partial \tilde{H}_z}{\partial y} - \frac{\partial \tilde{H}_y}{\partial z} = \frac{\varepsilon_{xx}}{c_0} \frac{\partial E_x}{\partial t}$$

$$\frac{\left.\tilde{H}_z^{i,j,k}\right|_{t+\frac{\Delta t}{2}} - \left.\tilde{H}_z^{i,j-1,k}\right|_{t+\frac{\Delta t}{2}}}{\Delta y} - \frac{\left.\tilde{H}_y^{i,j,k}\right|_{t+\frac{\Delta t}{2}} - \left.\tilde{H}_y^{i,j,k-1}\right|_{t+\frac{\Delta t}{2}}}{\Delta z} = \frac{\varepsilon_{xx}^{i,j,k}}{c_0} \frac{\left.E_x^{i,j,k}\right|_{t+\Delta t} - \left.E_x^{i,j,k}\right|_{t}}{\Delta t}$$

From Prof. R.C. Rumpf @ utep

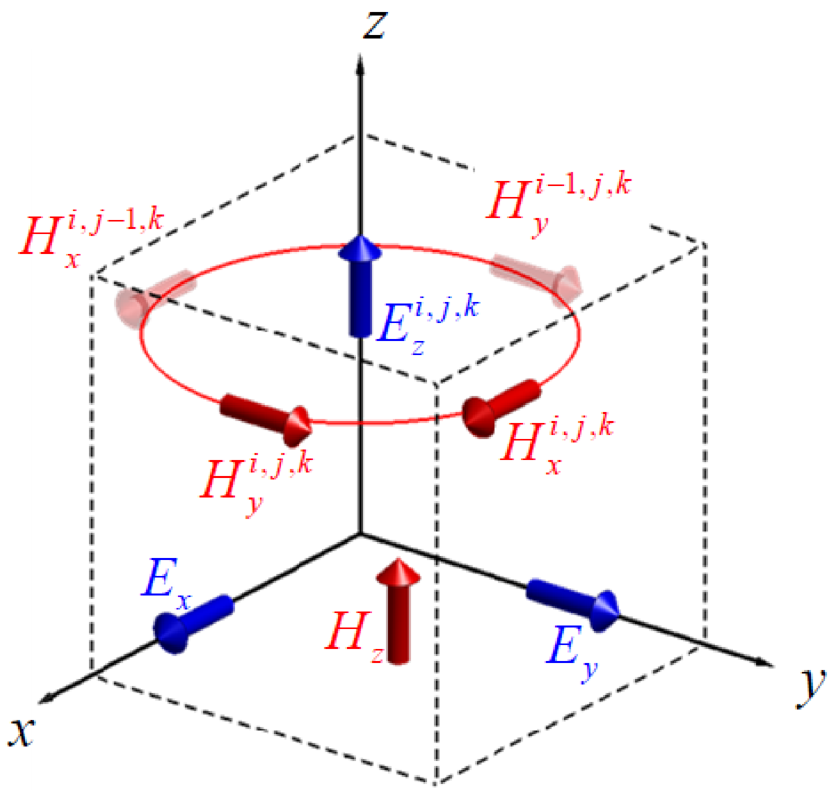
Finite-Difference Equation for E_y



$$\frac{\partial \tilde{H}_x}{\partial z} - \frac{\partial \tilde{H}_z}{\partial x} = \frac{\varepsilon_{yy}}{c_0} \frac{\partial E_y}{\partial t}$$

$$\frac{\tilde{H}_x^{i,j,k}\Big|_{t+\frac{\Delta t}{2}} - \tilde{H}_x^{i,j,k-1}\Big|_{t+\frac{\Delta t}{2}}}{\Delta z} - \frac{\tilde{H}_z^{i,j,k}\Big|_{t+\frac{\Delta t}{2}} - \tilde{H}_z^{i-1,j,k}\Big|_{t+\frac{\Delta t}{2}}}{\Delta x} = \frac{\varepsilon_{yy}^{i,j,k}}{c_0} \frac{E_y^{i,j,k}\Big|_{t+\Delta t} - E_y^{i,j,k}\Big|_{t}}{\Delta t}$$

Finite-Difference Equation for E_z



$$\frac{\partial \tilde{H}_y}{\partial x} - \frac{\partial \tilde{H}_x}{\partial y} = \frac{\varepsilon_{zz}}{c_0} \frac{\partial E_z}{\partial t}$$

$$\frac{\left.\tilde{H}_y^{i,j,k}\right|_{t+\frac{\Delta t}{2}} - \left.\tilde{H}_y^{i-1,j,k}\right|_{t+\frac{\Delta t}{2}}}{\Delta x} - \frac{\left.\tilde{H}_x^{i,j,k}\right|_{t+\frac{\Delta t}{2}} - \left.\tilde{H}_x^{i,j-1,k}\right|_{t+\frac{\Delta t}{2}}}{\Delta y} = \frac{\varepsilon_{zz}^{i,j,k}}{c_0} \frac{\left.E_z^{i,j,k}\right|_{t+\Delta t} - \left.E_z^{i,j,k}\right|_{t}}{\Delta t}$$

Summary of Finite-Difference Equations

$$\frac{\partial E_z}{\partial y}-\frac{\partial E_y}{\partial z}=-\frac{\mu_{xx}}{c_0}\frac{\partial \tilde{H}_x}{\partial t}$$

$$\frac{\partial E_x}{\partial z}-\frac{\partial E_z}{\partial x}=-\frac{\mu_{yy}}{c_0}\frac{\partial \tilde{H}_y}{\partial t}$$

$$\frac{\partial E_y}{\partial x}-\frac{\partial E_x}{\partial y}=-\frac{\mu_{zz}}{c_0}\frac{\partial \tilde{H}_z}{\partial t}$$

$$\Rightarrow$$

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

$$\frac{E_x^{i,j,k+1}\big|_t-E_x^{i,j,k}\big|_t}{\Delta z}-\frac{E_z^{i+1,j,k}\big|_t-E_z^{i,j,k}\big|_t}{\Delta x}=-\frac{\mu_{yy}^{i,j,k}}{c_0}\frac{\tilde{H}_y^{i,j,k}\big|_{t+\frac{\Delta t}{2}}-\tilde{H}_y^{i,j,k}\big|_{t-\frac{\Delta t}{2}}}{\Delta t}$$

$$\frac{E_y^{i+1,j,k}\big|_t-E_y^{i,j,k}\big|_t}{\Delta x}-\frac{E_x^{i,j+1,k}\big|_t-E_x^{i,j,k}\big|_t}{\Delta y}=-\frac{\mu_{zz}^{i,j,k}}{c_0}\frac{\tilde{H}_z^{i,j,k}\big|_{t+\frac{\Delta t}{2}}-\tilde{H}_z^{i,j,k}\big|_{t-\frac{\Delta t}{2}}}{\Delta t}$$

$$\frac{\partial \tilde{H}_z}{\partial y}-\frac{\partial \tilde{H}_y}{\partial z}=\frac{\varepsilon_{xx}}{c_0}\frac{\partial E_x}{\partial t}$$

$$\frac{\partial \tilde{H}_x}{\partial z}-\frac{\partial \tilde{H}_z}{\partial x}=\frac{\varepsilon_{yy}}{c_0}\frac{\partial E_y}{\partial t}$$

$$\frac{\partial \tilde{H}_y}{\partial x}-\frac{\partial \tilde{H}_x}{\partial y}=\frac{\varepsilon_{zz}}{c_0}\frac{\partial E_z}{\partial t}$$

$$\frac{\tilde{H}_z^{i,j,k}\big|_{t+\frac{\Delta t}{2}}-\tilde{H}_z^{i,j-1,k}\big|_{t+\frac{\Delta t}{2}}}{\Delta y}-\frac{\tilde{H}_y^{i,j,k}\big|_{t+\frac{\Delta t}{2}}-\tilde{H}_y^{i,j,k-1}\big|_{t+\frac{\Delta t}{2}}}{\Delta z}=\frac{\varepsilon_{xx}^{i,j,k}}{c_0}\frac{E_x^{i,j,k}\big|_{t+\Delta t}-E_x^{i,j,k}\big|_t}{\Delta t}$$

$$\frac{\tilde{H}_x^{i,j,k}\big|_{t+\frac{\Delta t}{2}}-\tilde{H}_x^{i,j,k-1}\big|_{t+\frac{\Delta t}{2}}}{\Delta z}-\frac{\tilde{H}_z^{i,j,k}\big|_{t+\frac{\Delta t}{2}}-\tilde{H}_z^{i-1,j,k}\big|_{t+\frac{\Delta t}{2}}}{\Delta x}=\frac{\varepsilon_{yy}^{i,j,k}}{c_0}\frac{E_y^{i,j,k}\big|_{t+\Delta t}-E_y^{i,j,k}\big|_t}{\Delta t}$$

$$\frac{\tilde{H}_y^{i,j,k}\big|_{t+\frac{\Delta t}{2}}-\tilde{H}_y^{i-1,j,k}\big|_{t+\frac{\Delta t}{2}}}{\Delta x}-\frac{\tilde{H}_x^{i,j,k}\big|_{t+\frac{\Delta t}{2}}-\tilde{H}_x^{i,j-1,k}\big|_{t+\frac{\Delta t}{2}}}{\Delta y}=\frac{\varepsilon_{zz}^{i,j,k}}{c_0}\frac{E_z^{i,j,k}\big|_{t+\Delta t}-E_z^{i,j,k}\big|_t}{\Delta t}$$

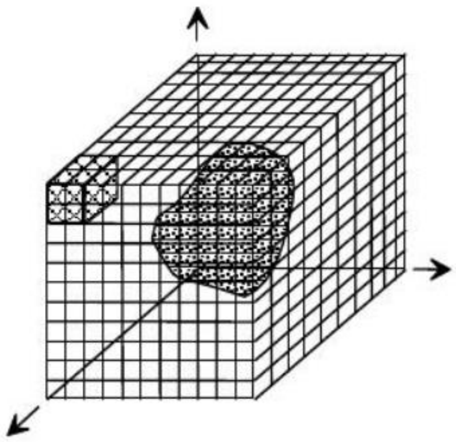
每一个方程对于每一个网格中的单元都独立的执行。每个时间步骤都需要重复计算，直到计算结束。这些方程在整个计算中一直在重复计算。

边界条件

被屏蔽的边界:　　　$\boldsymbol{n}$: 边界法向矢量

■完美电导体(PEC)　　$\boldsymbol{n} \times \boldsymbol{E} = 0$

■完美磁导体(PMC)　　$\boldsymbol{n} \times \boldsymbol{H} = 0$



开放边界:

· 吸收边界条件（ABC）

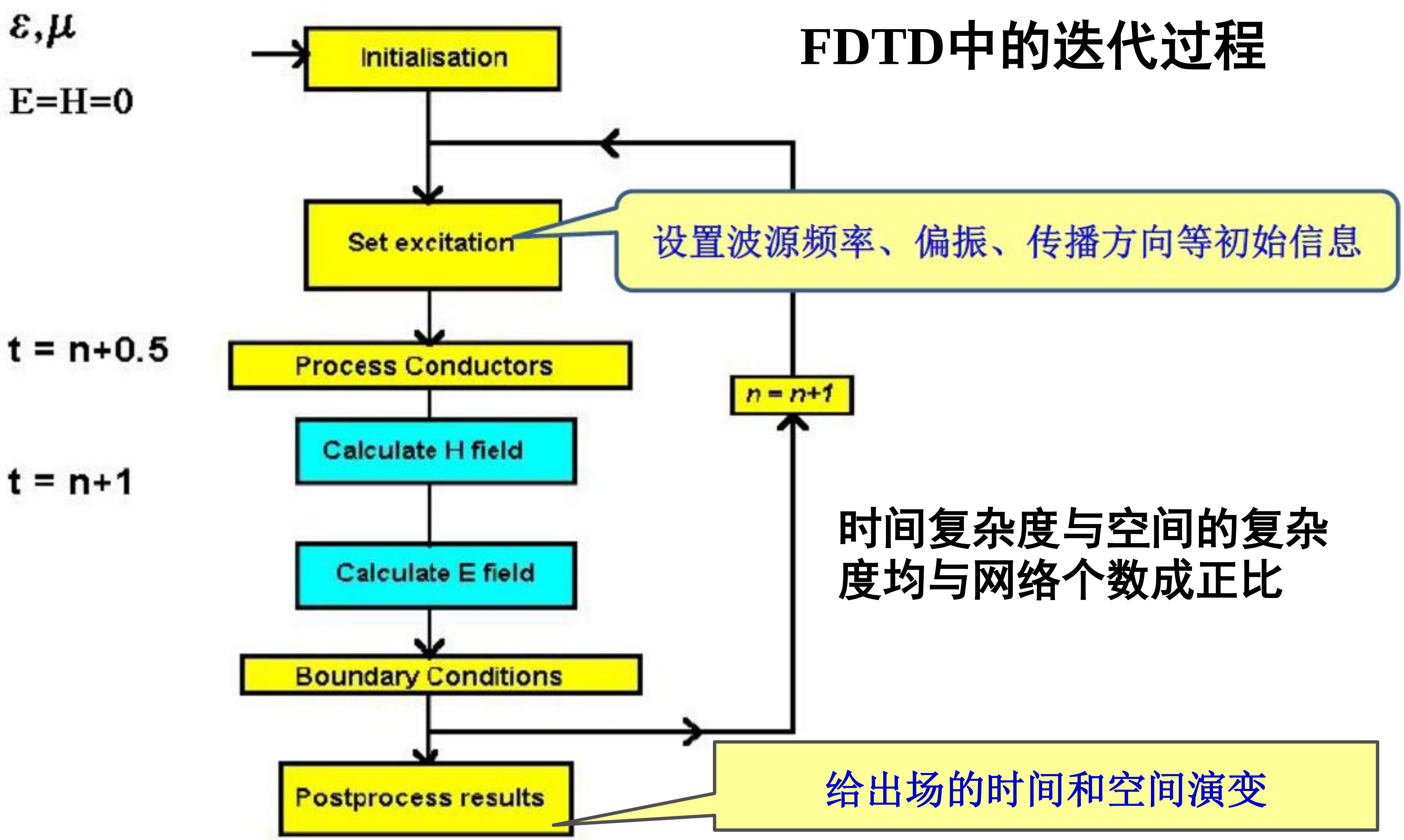
· 完全匹配层（PML）

对电磁波不反射

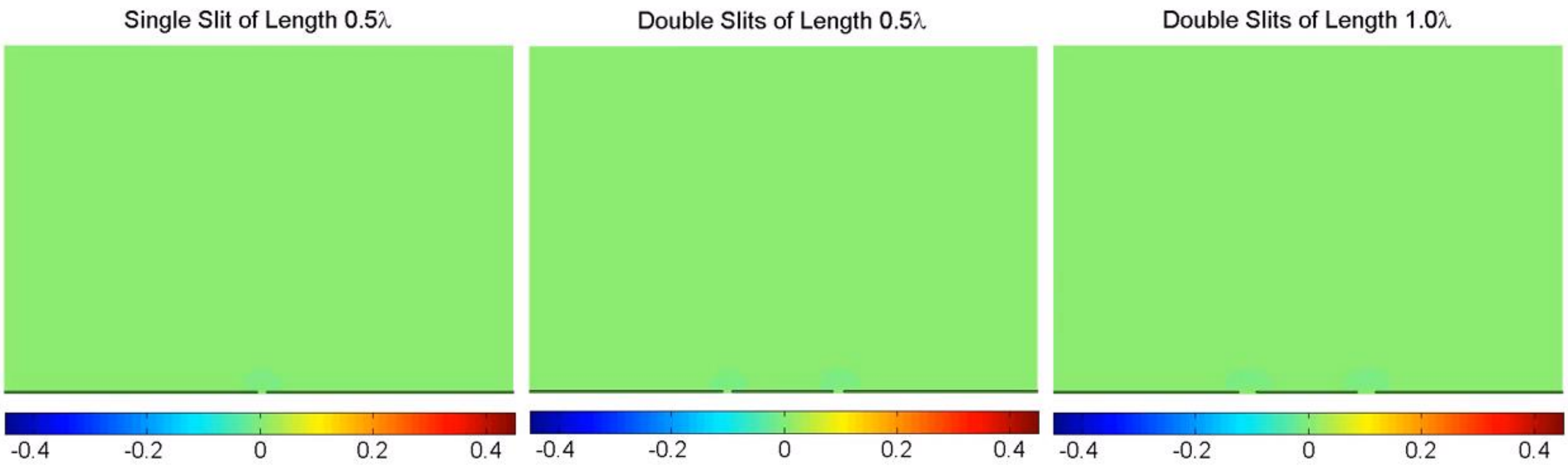
通常在计算域的截断面之外布置完全匹配层，当波进入PML中时，因波阻抗保持不变而无反射发生。理想的吸收边界条件应在截断边界上只有向外传输的波而没有向内的反射波。

求解过程

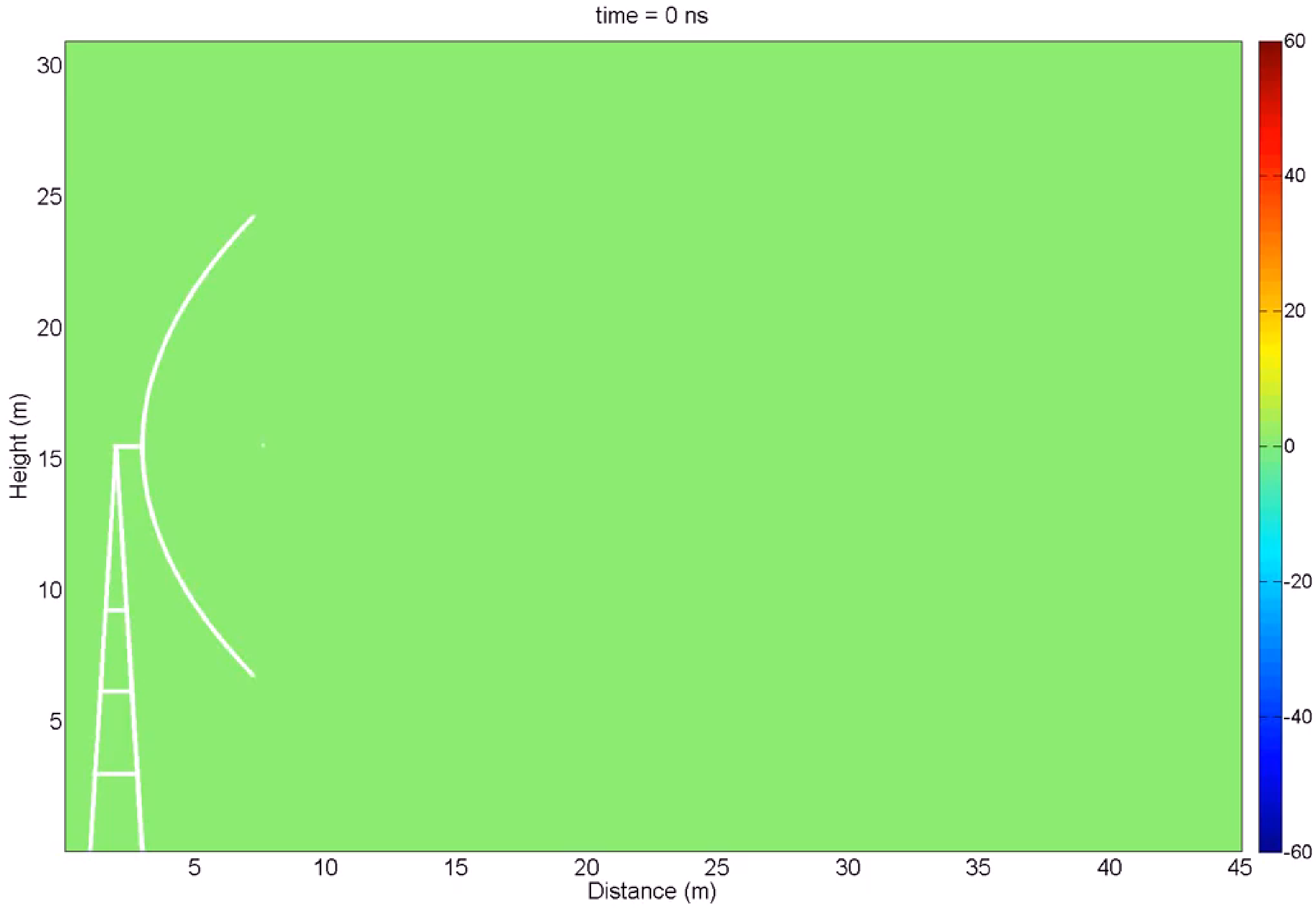
FDTD中的迭代过程



时间复杂度与空间的复杂度均与网络个数成正比

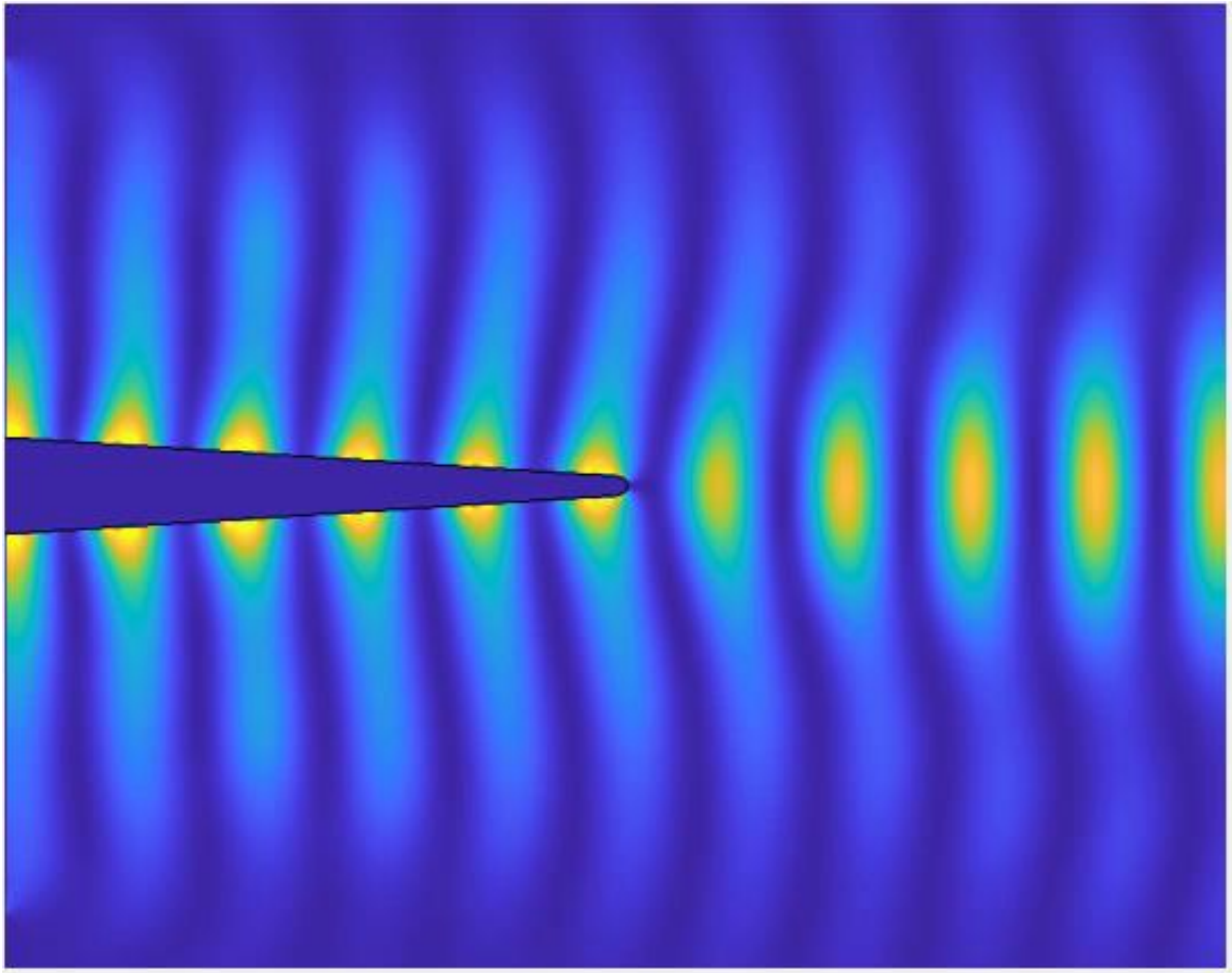

Single Slit of Length 0.5λ
Double Slits of Length 0.5λ
Double Slits of Length 1.0λ
-0.4
-0.2
0
0.2
0.4

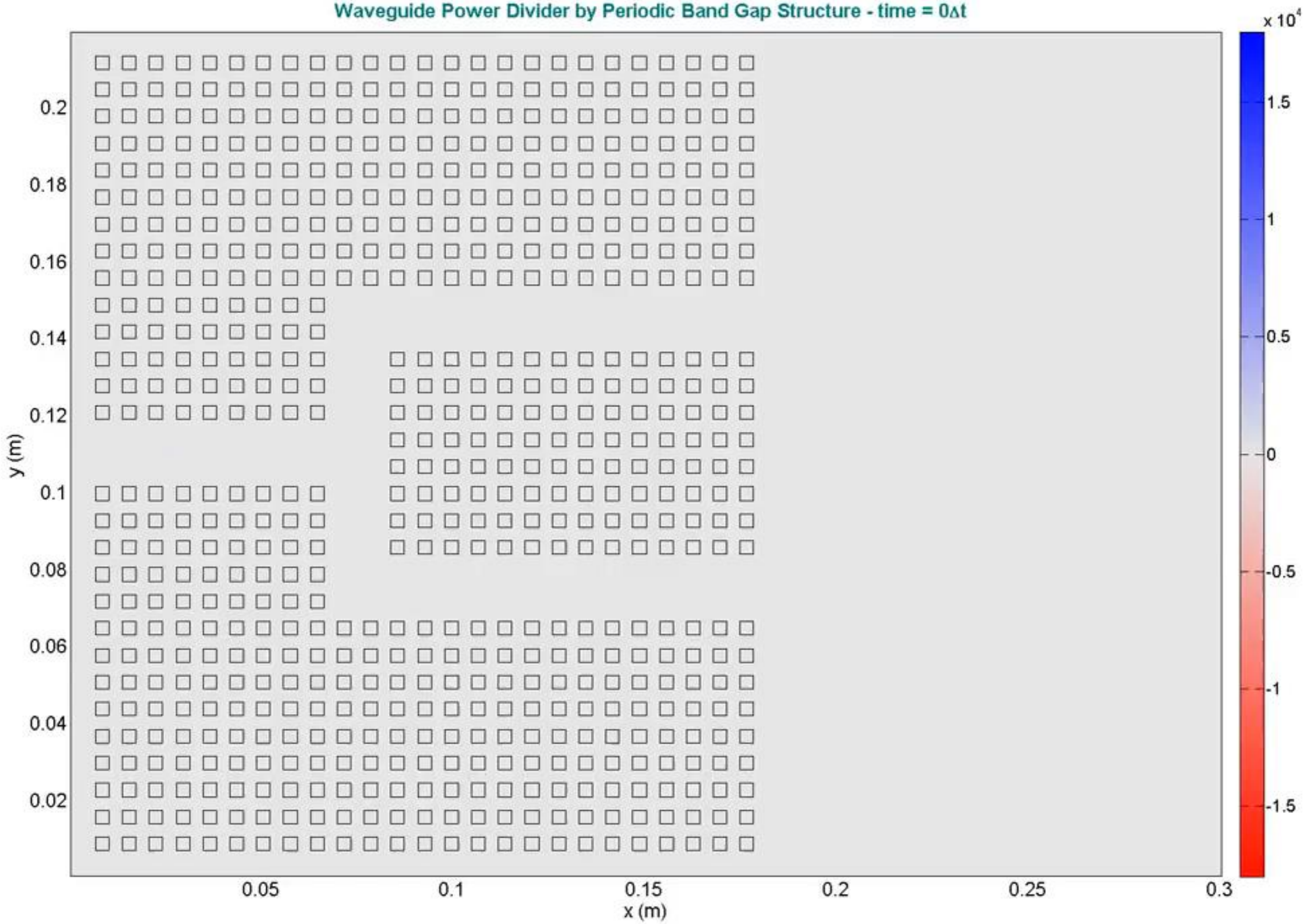
狭缝衍射



天线模拟, two short pulses - first one at central frequency of 100 MHz and the other at 200 MHz are fired from the focal point (VHF regime). f/D (focal length/diameter) ratio is 0.257.

尖端的SPP聚焦





光子晶体 (The frequency of operation is 11.085 GHz. The relative dielectric permittivity of the square blocks are 11.56 and the ambient medium is air. Each block is 3.5 mm x 3.5 mm)

FDTD总结

- ·时域方法，适用于模拟场的空间和时间演化。
- ·明确: E(H)场是从前面计算和存储H(E)场获得的，不再需解联立方程组(矩阵)。
- ·金属的色散不得不通过适当的解析表达式估算，导致在宽频段计算中引入了大量的误差。
- ·通过激发一个宽频段脉冲的一次计算可能获得整个系统的频率响应，并计算出傅立叶变换。
- ·计算负荷∝空间和时间网格点的密度和数量

-细微特征的结构-空间网格必须非常密才能处理精细结构
-远场计算需要大量的网格点
-为了快速准确地得到光与物质相互作用的时间演化过程,需要小时间步长。

$$\Delta t \leqslant \frac{1}{v\sqrt{\frac{1}{(\Delta x_{\min})^2}+\frac{1}{(\Delta y_{\min})^2}+\frac{1}{(\Delta z_{\min})^2}}}, \quad \Delta x,\ \Delta y,\ \Delta z \leqslant \frac{\lambda}{10}$$

一些商业软件:
FDTD Solutions, OptiFDTD, Remcom XFDTD, Zeland Fidelity, APLAC, Empire, Microwave Studio, RM Associate CFDTD

有限元法(FEM)

·FEM:一种求解偏微分方程组的数值方法

·最初应用于结构力学和热力学理论，可以追溯到1950年代

·1960年代末其应用首次出现在电磁学著作中，但1980年代前并未被广泛采用。

·FEM始于麦克斯韦方程组的偏微分形式。

·基本思想:虽然电磁响应在一个大的区域是复杂的，但在小的子区域简单的近似就足够了。

·有限元法的主要原理:将复杂的问题分解成小的、简单的问题来解决，小问题的求解过程是可知和容易的。

有限元

- 基本思想：对偏微分方程的解进行近似
- 加权残差法和变分法均可得到有限元法的公式
- 我们采用加权残差法导出
- 偏微分方程

$$\hat{L}\varphi = f$$

$\hat{L}$ 为微分算子，φ 为待求未知解，f 为源函数。

为了求解 φ ，用一组基函数对 φ 进行线性展开：

$$\varphi = \sum_{j=1}^{N} c_j v_j$$

$v_j,\ j=1,2,\cdots,N$ 为基函数　　$c_j,\ j=1,2,\cdots,N$ 为未知的展开系数

有限元

加权残差法尝试确定 c_j 的方法：

将未知解的线性展开式代入微分方程，等式两边乘以加权函数 w_i，并对整个求解区域 Ω 中积分，即

$$\int_\Omega w_i \hat{L}\left(\sum_{j=1}^{N} c_j v_j\right) \mathrm{d}\Omega = \int_\Omega w_i f \, \mathrm{d}\Omega$$

- 给定一组加权函数，上式就定义了关于 c_j 一组代数方程
- 满足一定的边界条件求解，可以得到 c_j
- 伽辽金法：令加权函数 $w_i = v_i$ 即加权函数和基函数相等

$$\sum_{j=1}^{N} c_j \int_\Omega v_i \left(\hat{L} v_j\right) \mathrm{d}\Omega = \int_\Omega v_i f \, \mathrm{d}\Omega, \quad i = 1, 2, \cdots, N$$

令：

$$S_{ij} = \int_\Omega v_i \left(\hat{L} v_j\right) \mathrm{d}\Omega$$

$$b_i = \int_\Omega v_i f \, \mathrm{d}\Omega$$

有限元

$$\sum_{j=1}^{N} S_{ij} c_j = b_i, \quad i = 1, 2, \cdots, N$$

关于 c_j 的代数线性方程组

对于自共轭问题，有：

$$\int_{\Omega} v_i \left(\hat{L} v_j\right) \mathrm{d}\Omega = \int_{\Omega} v_j \left(\hat{L} v_i\right) \mathrm{d}\Omega$$

即 $S_{ij} = S_{ji}$，即系数矩阵是对称的

有限元法的基本思想：

- 将待求解的区域划分为小的子域，子域称为有限单元（有限元）
- 使用简单的函数，比如线性函数或二次函数来近似每个单元内的未知解，近似函数就是基函数
- 基于边界条件，采用伽辽金或者变分法构建代数方程进行求解

有限元-举例

求解如下一维霍姆霍兹方程的一维边值问题：

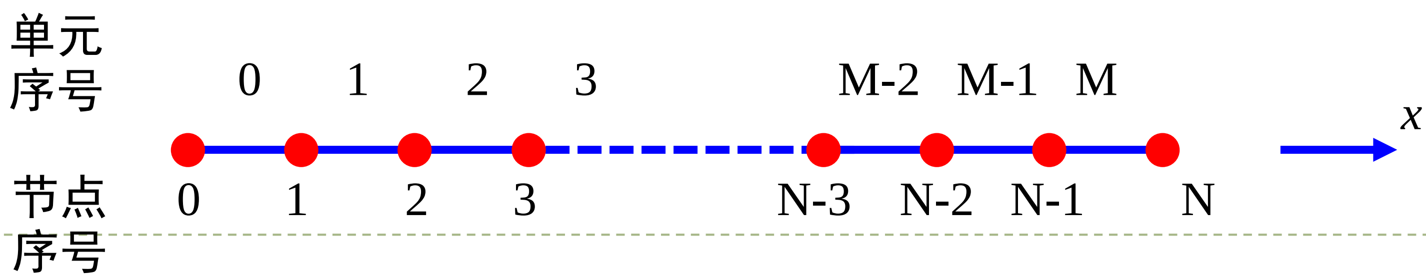
$$\frac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2}+k^2\varphi(x)=f(x),\qquad 0<x<L$$

边界条件：

$$\varphi|_{x=0}=p$$

$$\left[\frac{\mathrm{d}\varphi}{\mathrm{d}x}+\gamma\varphi\right]_{x=L}=q$$

- 有限元法的第一步：将求解区域 $(0, L)$ 划分为多个小的子域
- 一维问题：子域即为短的线段，短线段称为**有限单元**，线段之间的连接处称为**节点**
- 单元足够小，单元上的未知解通过单元两个节点上的 φ 值进行**线性插值得到**

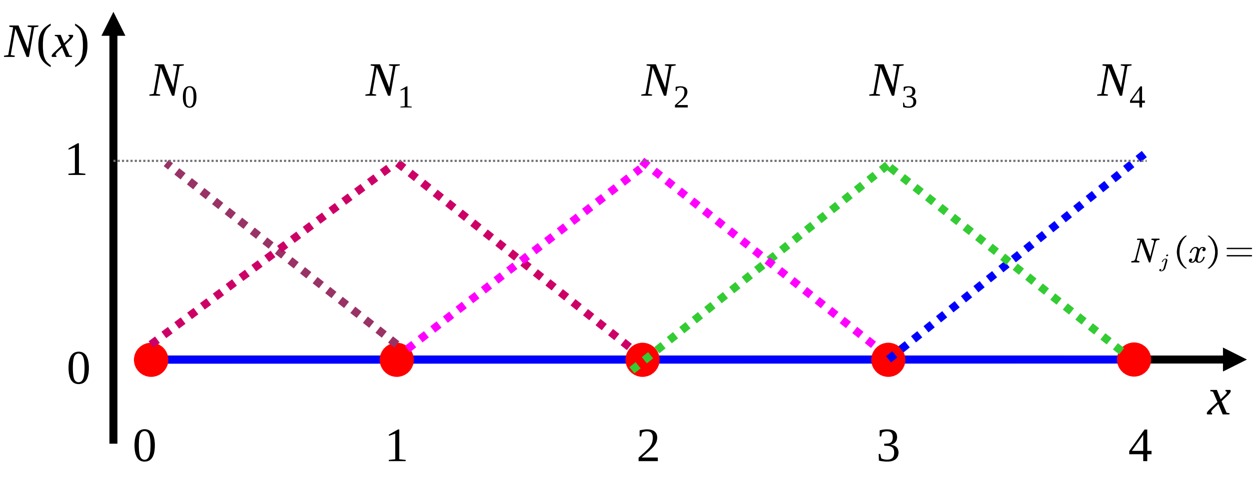


有限元-举例

未知解表示为：

$$\varphi = \sum_{j=0}^{N} \varphi_j N_j(x)$$

- φ_j 为未知函数 φ 在第 j 个单元与第 j+1个单元之间的节点上的值
- $N_j(x)$ 为相应的基函数，除了第一个和最后一个节点， $N_j(x)$ 是一个三角形函数
- 在第 j 和第 j+1 个单元上具有非零值
- 这样设置后： j到 j+1 节点间的函数值就可以用 φ_j 和 φ_{j+1}线性插值得到



$$N_j(x) = \begin{cases} \dfrac{1}{\Delta x}|x - x_j|, & x_{j-1} < x < x_{j+1},\ j \neq 0 \\ -\dfrac{1}{\Delta x}(x - x_1), & x_0 < x < x_1 \\ \dfrac{1}{\Delta x}(x - x_N), & x_{N-1} < x < x_N \\ 0, & \text{others} \end{cases}$$

一维线性基函数示意图

有限元-举例

代入 $x = 0$ 处的初始条件：

$$\varphi(x) = \sum_{j=1}^{N} \varphi_j N_j(x) + pN_0(x)$$

即：$\varphi_0 = p$，其余 φ_j 待求

采用前面所述的伽辽金法：在霍姆霍兹方程两边乘以 $N_i(x)$, i = 1, 2, ..., N, 并在区间 $(0, L)$ 上积分，得到：

$$\int_0^L N_i(x)\left[\frac{\mathrm{d}^2\varphi(x)}{\mathrm{d}x^2} + k^2\varphi(x)\right]\mathrm{d}x = \int_0^L N_i(x) f(x)\,\mathrm{d}x$$

采用分步积分，并利用$N_i(x)$ (i = 1, 2, ..., N)在$x = 0$处为0，得到：

$$\int_0^L \left[\frac{\mathrm{d}N_i(x)}{\mathrm{d}x}\cdot\frac{\mathrm{d}\varphi(x)}{\mathrm{d}x} - k^2 N_i(x)\varphi(x)\right]\mathrm{d}x - \left[N_i(x)\frac{\mathrm{d}\varphi(x)}{\mathrm{d}x}\right]_{x=L} = -\int_0^L N_i(x) f(x)\,\mathrm{d}x$$

由另一边界条件，得到：

$$\int_0^L \left[\frac{\mathrm{d}N_i(x)}{\mathrm{d}x}\cdot\frac{\mathrm{d}\varphi(x)}{\mathrm{d}x} - k^2 N_i(x)\varphi(x)\right]\mathrm{d}x - \left[N_i(x)\left(q - \gamma\varphi\right)\right]_{x=L} = -\int_0^L N_i(x) f(x)\,\mathrm{d}x$$

有限元-举例

把 $\varphi(x)$ 的函数展开式代入上面的方程，得到线性方程组：

$$\sum_{j=1}^{N} K_{ij}\varphi_j = b_i,\ i=1,2,\cdots,N$$

其中：

$$K_{ij} = \int_0^L \left[\frac{\mathrm{d}N_i(x)}{\mathrm{d}x}\cdot\frac{\mathrm{d}N_j(x)}{\mathrm{d}x} - k^2 N_i(x)N_j(x)\right]\mathrm{d}x + \gamma\delta_{iN}\delta_{jN}$$

$$b_i = -\int_0^L N_i(x)f(x)\mathrm{d}x - p\int_0^L \left[\frac{\mathrm{d}N_i(x)}{\mathrm{d}x}\cdot\frac{\mathrm{d}N_0(x)}{\mathrm{d}x} - k^2 N_i(x)N_0(x)\right]\mathrm{d}x + q\delta_{iN}$$

需要注意的是，对于选定的基函数，只有当 $j = i \pm 1$时，$N_i(x)$ 和 $N_j(x)$ 才会有重叠，积分才不为0，即：

$$K_{ii},\ K_{i+1,i},\ \ K_{i,i+1}$$ 非零，其余皆为零

- 每一行最多只有3个非零项
- 大型的对角稀疏矩阵
- 利用计算机，可方便求解待定系数 φ_j
- 增加基函数的阶数可以减小相对误差