4, Partial Differential Equations

$$A(x,y)\frac{\partial^2 u}{\partial x^2} + B(x,y)\frac{\partial^2 u}{\partial x \partial y} + C(x,y)\frac{\partial^2 u}{\partial y^2} = f(x,y,u,\frac{\partial u}{\partial x},\frac{\partial u}{\partial y}),$$

- Euler method
- Crank-Nicholson method
- Beam Propagation Method
- Slit-Step Fast Fourier Transform
- Finite Difference Time Domain method
- Absorption Boundary Condition
- Periodic Boundary Condition
- Perfect Matching Layers

Maxwell's equations

Faraday's law:

$$\nabla \times E = -\frac{\partial}{\partial t}\mu_0 H - \frac{\partial}{\partial t}\mu_0 M.$$

Ampére's law:

$$\nabla \times H = \frac{\partial}{\partial t}\epsilon_0 E + \frac{\partial}{\partial t}P + J.$$

Gauss's law for the electric field:

$$\nabla \cdot \epsilon_0 E = -\nabla \cdot P + \rho.$$

Gauss's law for the magnetic field:

$$\nabla \cdot \mu_0 H = -\nabla \cdot \mu_0 M.$$

Schrödinger equation

Diffusion equation:

$$\frac{\partial}{\partial t}A(x,t) = \kappa\frac{\partial^2}{\partial x^2}A(x,t)$$

Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + V(x)\Psi(x,t)$$

Nonlinear Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t)+V(x)\Psi(x,t)+\gamma|\Psi(x,t)|^2\Psi(x,t)$$

Forward Time Centered Space

By finite difference,

$$\frac{\partial}{\partial t} A(x,t) = \kappa \frac{\partial}{\partial x} A(x,t)$$

this equation is approximated by

$$\frac{A_j^{n+1} - A_j^n}{\Delta t} + \mathbf{O}(\Delta t) \approx \kappa \frac{A_{j+1}^n - A_{j-1}^n}{2\Delta x} + \mathbf{O}(\Delta x^2).$$

For diffusion equation:

$$\frac{\partial}{\partial t} A(x,t) = \kappa \frac{\partial^2}{\partial x^2} A(x,t)$$

which is approximated by

$$\frac{A_j^{n+1} - A_j^n}{\Delta t} + \mathbf{O}(\Delta t) \approx \kappa \frac{A_{j+1}^n - 2A_j^n + A_{j-1}^n}{\Delta x^2} + \mathbf{O}(\Delta x^2).$$

This is a explicit scheme.

Implicit FTCS scheme

By finite difference,

$$\frac{\partial}{\partial t}A(x,t) = \kappa\frac{\partial}{\partial x}A(x,t)$$

this equation is approximated by

$$\frac{A_j^{n+1} - A_j^n}{\Delta t} + \mathbf{O}(\Delta t) \approx \kappa\frac{A_{j+1}^{n+1} - A_{j-1}^{n+1}}{2\Delta x} + \mathbf{O}(\Delta x^2).$$

For diffusion equation:

$$\frac{\partial}{\partial t}A(x,t) = \kappa\frac{\partial^2}{\partial x^2}A(x,t)$$

which is approximated by

$$\frac{A_j^{n+1} - A_j^n}{\Delta t} + \mathbf{O}(\Delta t) \approx \kappa\frac{A_{j+1}^{n+1} - 2A_j^{n+1} + A_{j-1}^{n+1}}{\Delta x^2} + \mathbf{O}(\Delta x^2).$$

This is a implicit scheme, but also with first-order accuracy.

Implicit Crank-Nicolson scheme

For diffusion equation:

$$\frac{\partial}{\partial t} A(x,t) = \kappa \frac{\partial^2}{\partial x^2} A(x,t)$$

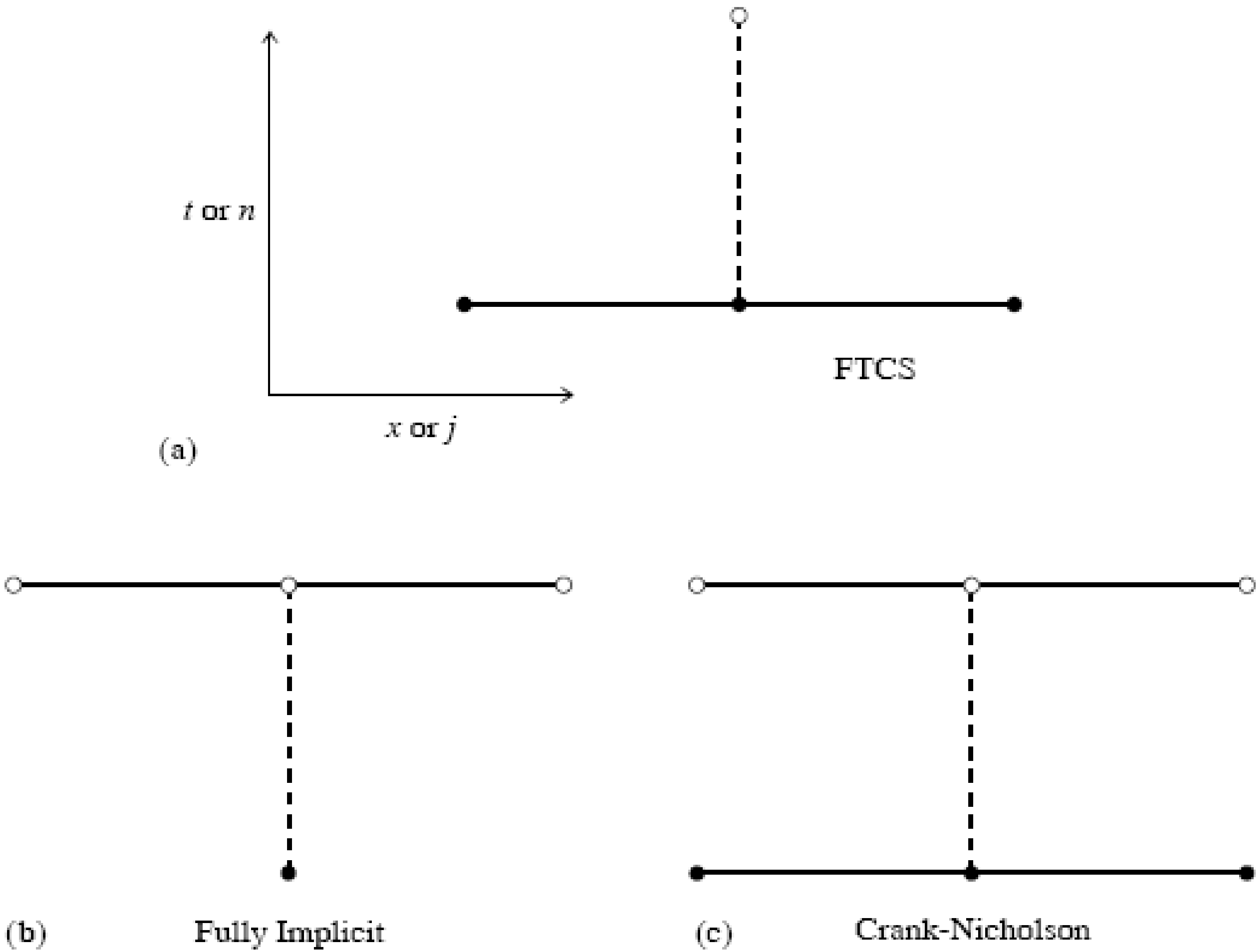
which is approximated by

$$\frac{A_j^{n+1} - A_j^n}{\Delta t} \approx \frac{\kappa}{2}\left(\frac{A_{j+1}^n - 2A_j^n + A_{j-1}^n}{\Delta x^2} + \frac{A_{j+1}^{n+1} - 2A_j^{n+1} + A_{j-1}^{n+1}}{\Delta x^2}\right)$$

This is a implicit scheme, but also with *second-order* accuracy.

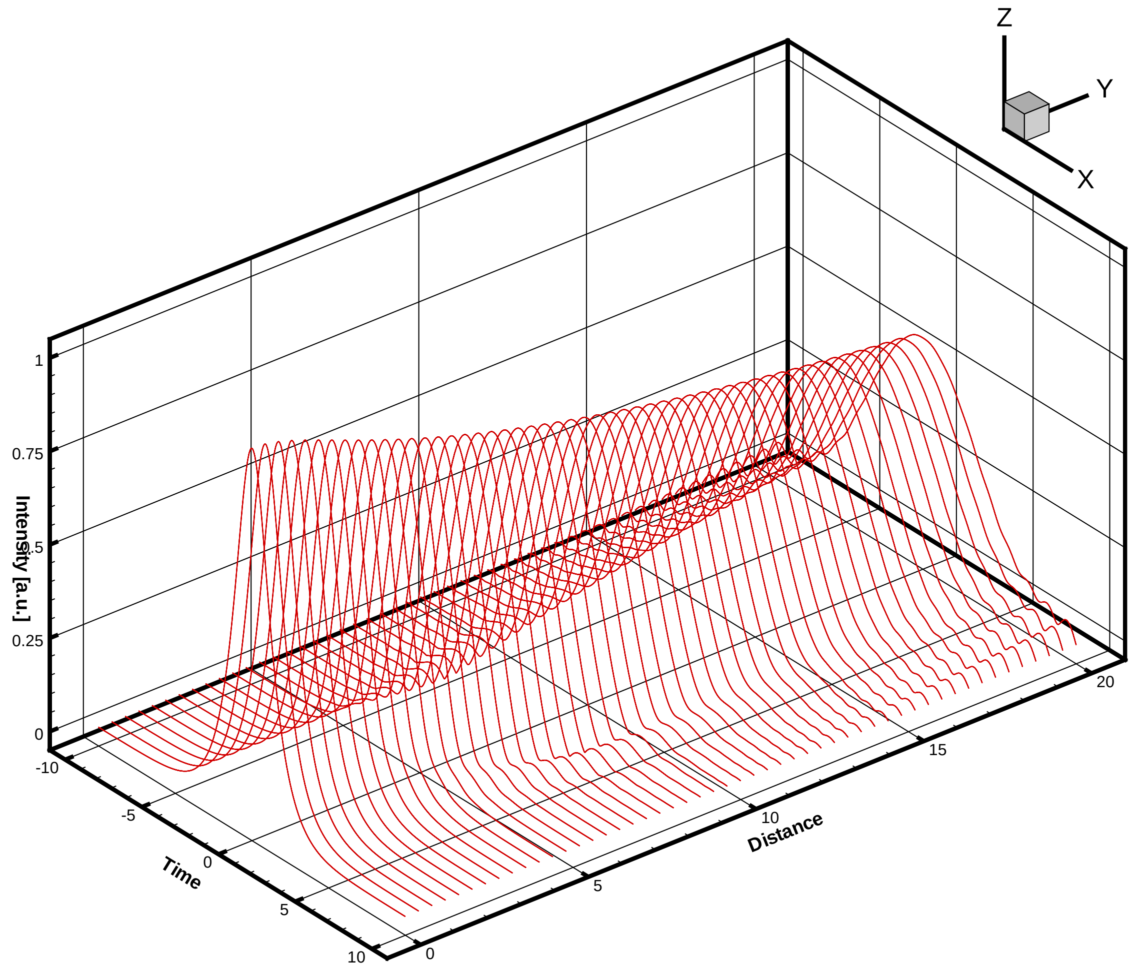
EE.NTHU 國立清華大學 電機工程學系及研究所

Time and Space discretization



Diffusion equation

$$\frac{\partial}{\partial z}U(z,t) = \frac{i}{2}\frac{\partial^2}{\partial t^2}U(z,t)$$



Generalization to fourth-order

For $j = 1, 2, \ldots, N$:

- Let p_j be the unique polynomial of degree ≤ 2 with $p_j(x_{j\pm1}) = u_{j\pm1}$,$p_j(x_j) = u_j$, and $p_j(x_{j\pm2}) = u_{j\pm2}$.
- $u'(x_j) = p'_j(x)$.

$$
\begin{pmatrix} u'_1 \\ \vdots \\ \\ u'_j \\ \vdots \\ \\ u'_N \end{pmatrix}
= h^{-1}
\begin{pmatrix}
 & & \ddots & & \\
 & \ddots & -\frac{1}{12} & \ddots & \\
 & \ddots & \frac{2}{3} & \ddots & \\
\frac{1}{12} & -\frac{2}{3} & 0 & \frac{2}{3} & -\frac{1}{12} \\
 & \ddots & -\frac{2}{3} & \ddots & \\
 & \ddots & \frac{1}{12} & \ddots & \\
 & & \ddots & &
\end{pmatrix}
\begin{pmatrix} u_1 \\ \vdots \\ \\ u_j \\ \vdots \\ \\ u_N \end{pmatrix}
$$

Generalization to Nth-order

$$D_N = \begin{pmatrix} & \vdots & \\ \ddots & \frac{1}{2}\cot\frac{3h}{2} & \\ \ddots & \frac{-1}{2}\cot\frac{2h}{2} & \\ \ddots & \frac{1}{2}\cot\frac{1h}{2} & \\ & 0 & \\ & \frac{-1}{2}\cot\frac{1h}{2} & \ddots \\ & \frac{1}{2}\cot\frac{2h}{2} & \ddots \\ & \frac{-1}{2}\cot\frac{3h}{2} & \ddots \\ & \vdots & \end{pmatrix}$$

Pseudo-spectral (collocation) method

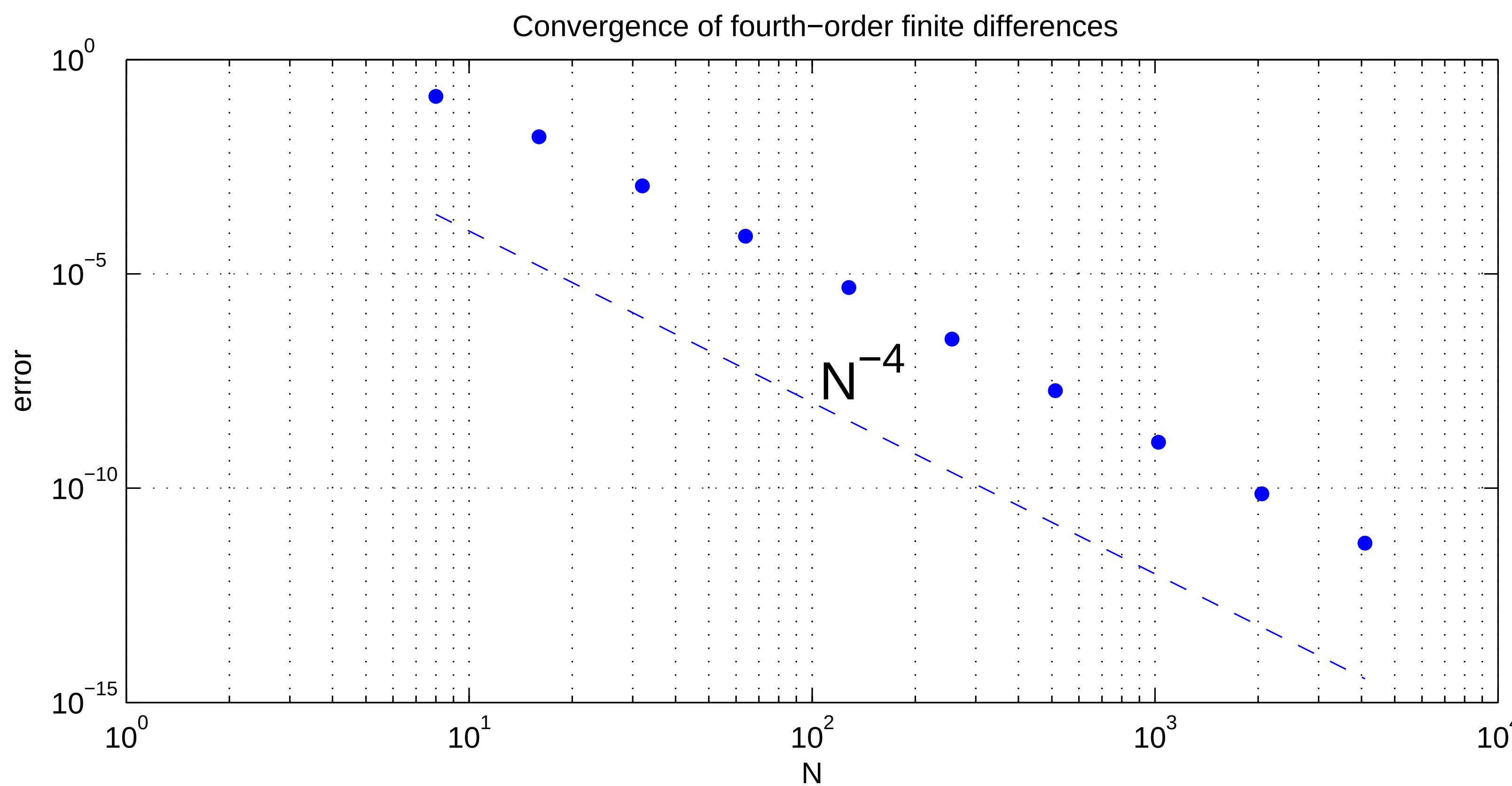
- Given discrete data on a grid,
- Interpolate the data *globally*,
- Evaluate the derivative of the interpolant on the grid,
- Convergence at the rate $O(e^{-cN})$ or $O(e^{-c\sqrt{N}})$, provided the solution is smooth,
- Typical FD or FEM at the rate $O(N^{-2})$ or $O(N^{-4})$.

Some useful references:

1. C. Canuto, *et al.*, "*Spectral methods in fluid dynamics,"* Springer-Verleg (1988).
2. B. Fornberg, *"A practical guide to pseudospectral methods,"* Cambridge Uni. Press (1996).
3. L. N. Trefethen, *"Spectral methods in Matlab,"* SIAM (2000).
4. J. A. C. Weideman and S. C. Reddy, *ACM Tran. on Math. Software* **26**, 465 (2000).
5. J. P. Boyd, *"Chebyshev and Fourier spectral methods,"* Dover Publication (2001).
6. B. Costa and W. S. Don, *PseudoPack*, a software library for numerical differentiation.

Test of the convergence: FD

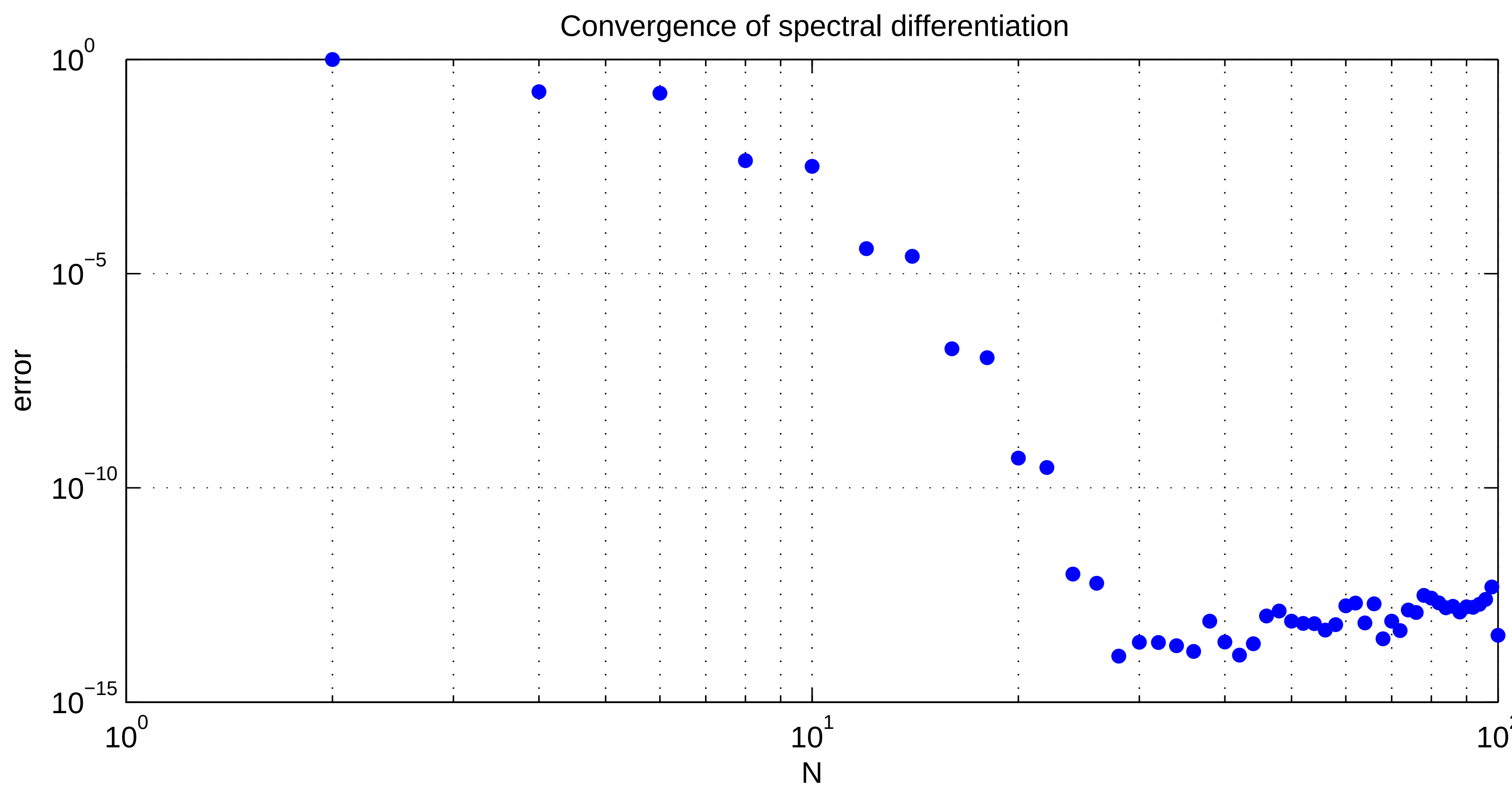
$$u(x) = e^{\sin(x)}, Du(x) = u'(x).$$



L. N. Trefethen, *"Spectral methods in Matlab,"* SIAM (2000).

Test of the convergence: PS

$$u(x) = e^{\sin(x)}, Du(x) = u'(x).$$



L. N. Trefethen, *"Spectral methods in Matlab,"* SIAM (2000).

EE.NTHU 國立清華大學 電機工程學系及研究所

Common adapted basis functions

1. Polynomial based:
   - $[-1, 1]$: Chebyshev polynomials,
   - $(-\infty, \infty)$: Hermite polynomials,
   - $[0, \infty)$: Laguerre polynomials,
2. Nonpolynomial based:
   - $(-\infty, \infty)$: Fourier series,
   - $(-\infty, \infty)$: Sinc series.

J. A. C. Weideman and S. C. Reddy, *ACM Tran. on Math. Software* **26**, 465 (2000).

J. P. Boyd, *"Chebyshev and Fourier spectral methods,"* Dover Publication (2001).

Spectral method

- The unknown functio $\phi(x,t) \equiv \phi(x)$ is expanded in terms of a set of N known interpolating orthogonal function, $\{f_j(x)\}_{j=0}^{N-1}$, as follows,

$$\phi(x) \approx p_{N-1}(x) = \sum_{j=0}^{N-1} \frac{\alpha(x)}{\alpha(x_j)} f_j(x)\phi(x_j),$$

  where $\{x_j\}_{j=0}^{N-1}$ is a set of distinct interpolation nodes, $\alpha(x)$ is a weight function and the funtions $\{f_j(x)\}_{j=0}^{N-1}$ satifsy $f_j(x_k) = \delta_{jk}$.

- The differential matrix can be defined directly, take second-order for example,

$$D^2_{k,j} = \frac{\mathrm{d}^2}{\mathrm{d}\,x^2}[\frac{\alpha(x)}{\alpha(x_j)} f_j(x)]_{x=x_k}.$$

1D scalar wave equation

One-dimensional scalar wave equation:

$$\frac{\partial^2}{\partial t^2} u(x,t) = c^2 \frac{\partial^2}{\partial x^2} u(x,t),$$

has the solution

$$u(x,t) = F(x+ct) + G(x-ct),$$

where F and G are arbitrary function.

Finite-difference approximation:

$$\frac{u_i^{n+1} - 2u_i^n + u_i^{n-1}}{\Delta t^2} + \mathbf{O}(\Delta t^2) = c^2 \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2} + \mathbf{O}(\Delta x^2),$$

for the latest value of u at grid point i,

$$u_i^{n+1} = (c\Delta t)^2 [\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2}] + 2u_i^n - u_i^{n-1} + \mathbf{O}(\Delta t^2) + \mathbf{O}(\Delta x^2).$$

FD-TD solution of the scalar wave equation

- This is a *fully explicit* second-order acuurate expression for u_i^{n+1}.
- All wave quantities on the RHS are known, obtained during the previous time steps, n and $n-1$.
- Upon performing FDTD approximation for all space points, yielding the complete set of u_i^{n+1}.

For the **magic time step**: $c\Delta t/\Delta x = 1$,

$$\begin{aligned} u_i^{n+1} &= (u_{i+1}^n - 2u_i^n + u_{i-1}^n) + 2u_i^n - u_i^{n-1} \\ &= u_{i+1}^n + u_{i-1}^n - u_i^{n-1}, \end{aligned}$$

note that there is *no* remainder (error) term here.

Magic time step

Consider the exact propagating-wave solutions to the 1D scalar wave equation,

$$u_j^n = F(x_i + ct_n) + G(x_i - ct_n),$$

where $x_i = i\Delta x$ and $t_n = n\Delta t$. Then

$$\begin{aligned}
u_i^{n+1} &= u_{i+1}^n + u_{i-1}^n - u_i^{n-1} \\
\begin{bmatrix} F(x_i + ct_{n+1}) \\ +G(x_i - ct_{n+1}) \end{bmatrix} &= \begin{bmatrix} F(x_{i+1} + ct_n) \\ +G(x_{i+1} - ct_n) \end{bmatrix} + \begin{bmatrix} F(x_{i-1} + ct_n) \\ +G(x_{i-1} - ct_n) \end{bmatrix} - \begin{bmatrix} F(x_i + ct_{n-1}) \\ +G(x_i - ct_{n-1}) \end{bmatrix}
\end{aligned}$$

$$\begin{aligned}
\text{RHS} &= \left\{ \begin{matrix} F[(i+1)\Delta x + cn\Delta t] \\ +G[(i+1)\Delta x - cn\Delta t] \end{matrix} \right\} + \left\{ \begin{matrix} F[(i-1)\Delta x + cn\Delta t] \\ +G[(i-1)\Delta x - cn\Delta t] \end{matrix} \right\} \\
&- \left\{ \begin{matrix} F[i\Delta x + c(n-1)\Delta t] \\ +G[i\Delta x - c(n-1)\Delta t] \end{matrix} \right\} \\
&= \left\{ \begin{matrix} F[(i+1+n)\Delta x] \\ +G[(i-1-n)\Delta x] \end{matrix} \right\} = \text{LHS}
\end{aligned}$$

Dispersion relation, phase velocity, and group velocity

For a continuous sinusoidal-travelling-wave solution

$$u(x,t) = e^{j(\omega t - kx)},$$

we have

- dispersion relation:

$$\omega^2 = c^2 k^2,$$

- phase velocity:

$$v_p = \frac{\omega}{k} = \pm c,$$

- group velocity:

$$v_g = \frac{\mathrm{d}\omega}{\mathrm{d}k} = \pm c.$$

Numerical dispersion relation

Finite-difference approximation:

$$u_i^{n+1} \approx (c\Delta t)^2 [\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2}] + 2u_i^n - u_i^{n-1},$$

and at the discrete space-time point (x_i, t_n),

$$u_i^n = u(x_i, t_n) = e^{j(\omega n\Delta t - \bar{k} i \Delta x)},$$

where $\bar{k}$ is the numerical wavenumber.

$$\begin{aligned} e^{j[\omega(n+1)\Delta t - \bar{k} i\Delta x]} &= (\frac{c\Delta t}{\Delta x})^2 \{ e^{j[\omega n\Delta t - \bar{k}(i+1)\Delta x]} - 2e^{j[\omega n \Delta t - \bar{k} i \Delta x]} + e^{j[\omega n\Delta t - \bar{k}(i-1)\Delta} \\ &+ (2e^{j[\omega n\Delta t - \bar{k} i \Delta x]} - e^{j[\omega(n-1)\Delta t - \bar{k} i \Delta x]}) \end{aligned}$$

After factoring out the complex expoential term,

$$\begin{aligned} e^{j\omega\Delta t} &= (\frac{c\Delta t}{\Delta x})^2 \cdot (e^{-j\bar{k}\Delta x} - 2 + e^{j\bar{k}\Delta x}) + (2 - e^{-j\omega\Delta t} \\ \rightarrow \cos(\omega\Delta t) &= (\frac{c\Delta t}{\Delta x})^2 \cdot [\cos(\bar{k}\Delta x) - 1] + 1. \end{aligned}$$

Numerical phase velocity

- Very Fine Mesh: $\Delta t \to 0, \Delta x \to 0$,

$$1 - \frac{(\omega \Delta t)^2}{2} \approx (\frac{c\Delta t}{\Delta x})^2 \cdot [1 - \frac{(\bar{k}\Delta x)^2}{2} - 1] + 1$$

then

$$\omega^2 = c^2 \bar{k}^2.$$

- Magic Time Step: $c\Delta t = \Delta x$,

$$\cos(\omega \Delta t) = 1 \cdot [\cos(\bar{k}\Delta x) - 1] + 1 = \cos(\bar{k}\Delta x),$$

then

$$\bar{k}\Delta x = \pm \omega \Delta t.$$

Dispersive wave

The general solution for FD dispersion relation is

$$\bar{k} = \frac{1}{\Delta x}\cos^{-1}\{1 + (\frac{c\Delta t}{\Delta x})^2 \cdot [\cos(\omega \Delta t) - 1]\}.$$

For example, $c\Delta t = \Delta x/2$, and $\Delta x = \lambda_0/10$, one has

$$\begin{aligned} \bar{k} &= \frac{1}{\Delta x}\cos^{-1}\{1 + 4 \cdot [\cos(\frac{2\pi}{\lambda_0} \cdot \frac{\Delta x}{2}) - 1]\} \\ &= \frac{1}{\Delta x}\cos^{-1}(0.8042) = \frac{0.63642}{\Delta x}, \end{aligned}$$

Then the numerical phase velocity

$$\begin{aligned} \bar{v}_p &= \omega/\bar{k} \\ &= \frac{2\pi(c/\lambda_0)\Delta x}{0.63642} = 0.9873c. \end{aligned}$$

E.NTHU 國立清華大學 電機工程學系及研究所

Maxwell equations

Faraday's law:

$$\nabla \times \mathbf{E} = -\frac{\partial}{\partial t}\mathbf{B} - \mathbf{J}_m$$

Ampére's law:

$$\nabla \times \mathbf{H} = \frac{\partial}{\partial t}\mathbf{D} + \mathbf{J}_e.$$

Gauss's law for the electric field:

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

Gauss's law for the magnetic field:

$$\nabla \cdot \mathbf{B} = 0.$$

Maxwell equations

- For a linear, isotropic nondispersive material,

$$\begin{aligned} \mathbf{B} &= \mu \mathbf{H}, \\ \mathbf{D} &= \epsilon \mathbf{E}. \end{aligned}$$

- magnetic conduction current:

$$\mathbf{J}_m = \rho' \mathbf{H}.$$

- electric conduction current:

$$\mathbf{J}_e = \sigma \mathbf{E}.$$

Then the Maxwell's curl equations becom

$$\begin{aligned} \frac{\partial}{\partial t}\mathbf{H} &= -\frac{1}{\mu}\nabla \times \mathbf{E} - \frac{\rho'}{\mu}\mathbf{H} \\ \frac{\partial}{\partial t}\mathbf{E} &= \frac{1}{\epsilon}\nabla \times \mathbf{H} - \frac{\sigma}{\epsilon}\mathbf{E}. \end{aligned}$$

3D Maxwell equations in rectangular coordinates

$$
\begin{aligned}
\frac{\partial H_x}{\partial t} &= \frac{1}{\mu}\left(\frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial y} - \rho' H_x\right) \\
\frac{\partial H_y}{\partial t} &= \frac{1}{\mu}\left(\frac{\partial E_z}{\partial x} - \frac{\partial E_x}{\partial z} - \rho' H_y\right) \\
\frac{\partial H_z}{\partial t} &= \frac{1}{\mu}\left(\frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} - \rho' H_z\right) \\
\frac{\partial E_x}{\partial t} &= \frac{1}{\epsilon}\left(\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} - \sigma E_x\right) \\
\frac{\partial E_y}{\partial t} &= \frac{1}{\epsilon}\left(\frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} - \sigma E_y\right) \\
\frac{\partial E_z}{\partial t} &= \frac{1}{\epsilon}\left(\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} - \sigma E_z\right)
\end{aligned}
$$

The system of six coupled partial differential equations forms the basis of the FD-TD algorithm for EM wave interactions in 3D. The FD-TD algorithm need not *explcitly* enforce the Guass's Law, however, the FD-TD space grid must be structured so that the Gauss's Law relations are *implicit* in the positions of the electric and magnetic field vector components.

Reduction to 2D

Assume that neigher the EM field excitation nor the modeled geometry has any variation in the z-direction, i.e. $\partial/\partial z = 0$,

- TM mode:

$$
\begin{aligned}
\frac{\partial H_x}{\partial t} &= \frac{1}{\mu}(-\frac{\partial E_z}{\partial y} - \rho' H_x) \\
\frac{\partial H_y}{\partial t} &= \frac{1}{\mu}(\frac{\partial E_z}{\partial x} - \rho' H_y) \\
\frac{\partial E_z}{\partial t} &= \frac{1}{\epsilon}(\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} - \sigma E_z)
\end{aligned}
$$

- TE mode:

$$
\begin{aligned}
\frac{\partial E_x}{\partial t} &= \frac{1}{\epsilon}(\frac{\partial H_z}{\partial y} - \sigma E_x) \\
\frac{\partial E_y}{\partial t} &= \frac{1}{\epsilon}(-\frac{\partial H_z}{\partial x} - \sigma E_y) \\
\frac{\partial H_z}{\partial t} &= \frac{1}{\mu}(\frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} - \rho' H_z)
\end{aligned}
$$

TM and TE modes are decoupled.

Reduction to 1D: TM

Assume further that neigher the EM field excitation nor the modeled geometry has any variation in the y-direction, i.e. $\partial/\partial y = 0$,

- TM mode:

$$
\begin{aligned}
\frac{\partial H_x}{\partial t} &= \frac{1}{\mu}(-\rho' H_x) \\
\frac{\partial H_y}{\partial t} &= \frac{1}{\mu}(\frac{\partial E_z}{\partial x} - \rho' H_y) \\
\frac{\partial E_z}{\partial t} &= \frac{1}{\epsilon}(\frac{\partial H_y}{\partial x} - \sigma E_z)
\end{aligned}
$$

- assuming initial conditions of zero fields, $H_x(t=0) = 0$, then we have only two equations involving H_y and E_x,

$$
\begin{aligned}
\frac{\partial H_y}{\partial t} &= \frac{1}{\mu}(\frac{\partial E_z}{\partial x} - \rho' H_y) \\
\frac{\partial E_z}{\partial t} &= \frac{1}{\epsilon}(\frac{\partial H_y}{\partial x} - \sigma E_z)
\end{aligned}
$$

E.E.NTHU 國立清華大學 電機工程學系及研究所

Equivalence to 1D wave equation

Assume magnetic loss $\rho' = 0$ and electrical loss $\sigma = 0$,

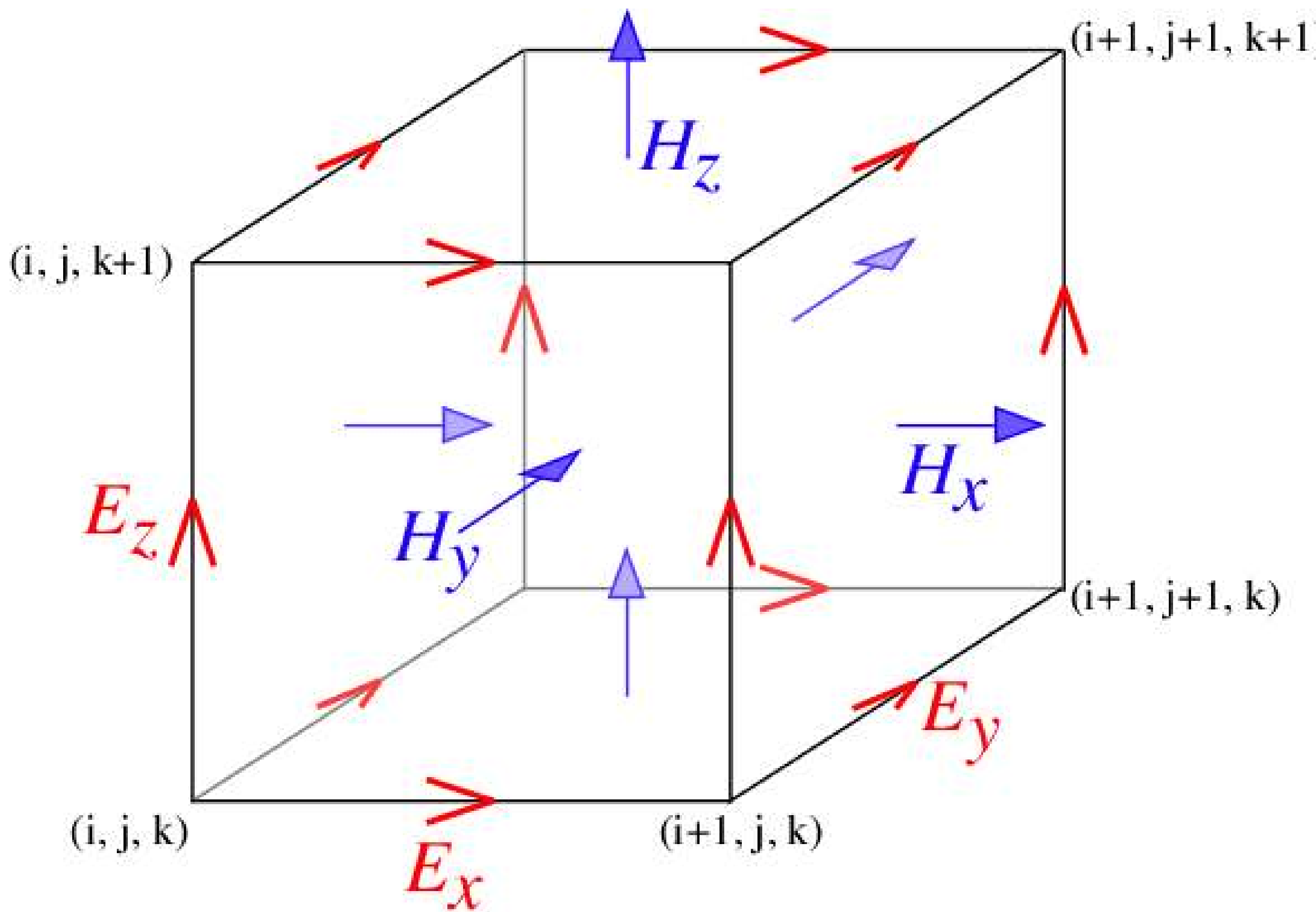
- For H_y:

$$\begin{aligned}\frac{\partial}{\partial t}\left(\frac{\partial H_y}{\partial t}\right) &= \frac{1}{\mu}\frac{\partial^2 E_z}{\partial t \partial x} \\ &= \frac{1}{\mu\epsilon}\frac{\partial^2 H_y}{\partial x^2}\end{aligned}$$

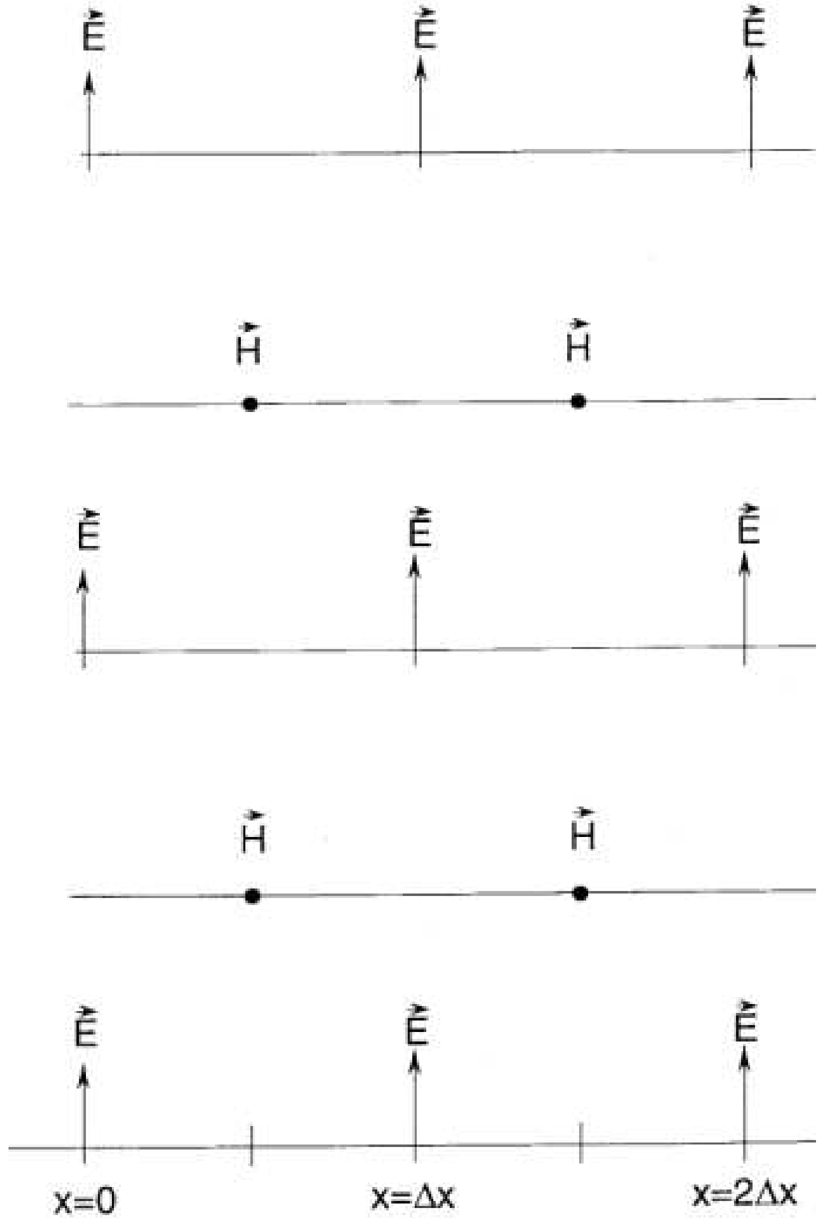
- For E_z:

$$\begin{aligned}\frac{\partial}{\partial t}\left(\frac{\partial E_z}{\partial t}\right) &= \frac{1}{\epsilon}\frac{\partial^2 H_y}{\partial t \partial x} \\ &= \frac{1}{\epsilon\mu}\frac{\partial^2 E_z}{\partial x^2}\end{aligned}$$

Yee's algorithm



Space-Time chart for Yee's algorithm



Finite-difference expression for 3D Maxwell equations

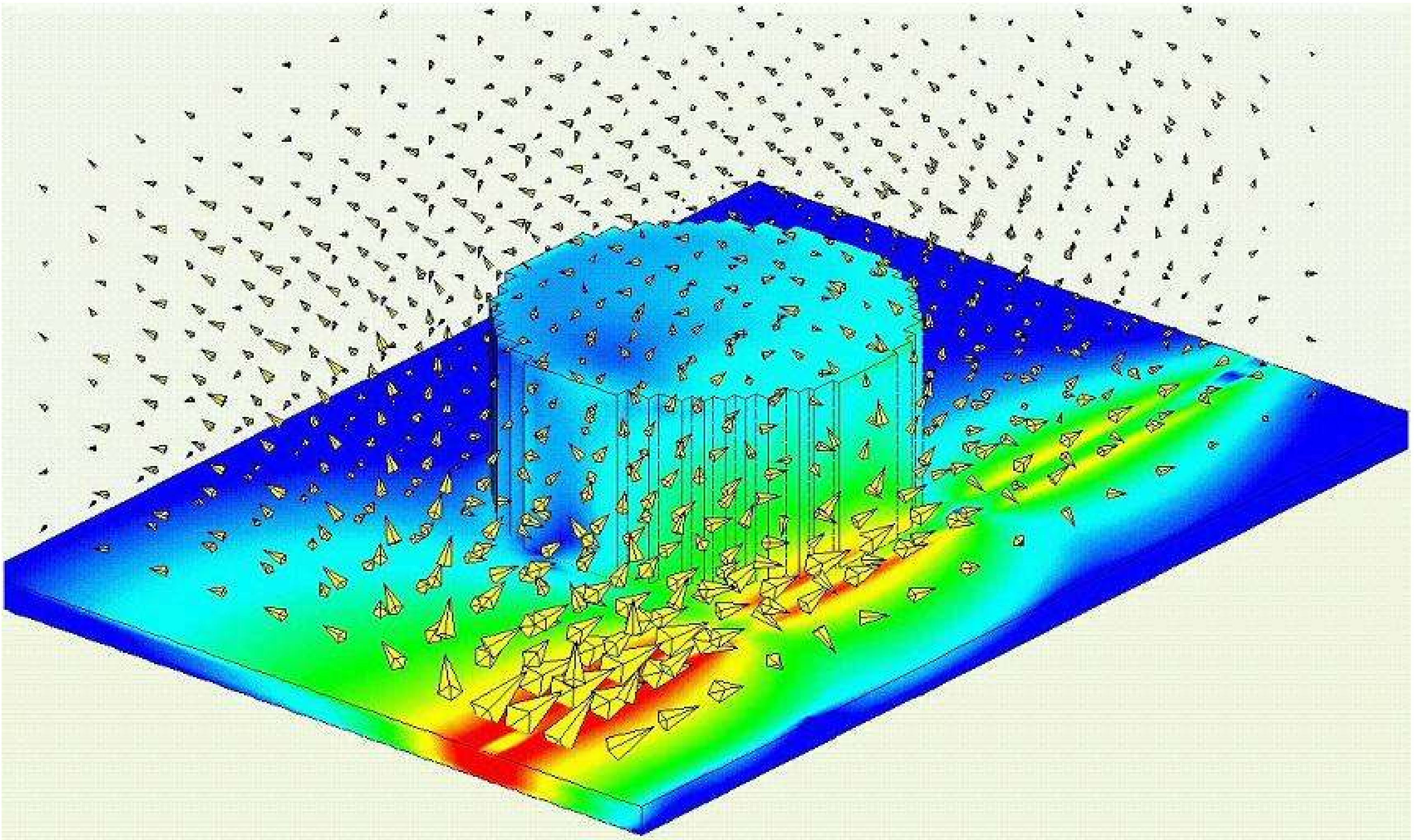
$$\frac{\partial H_x}{\partial t} = \frac{1}{\mu}(\frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial y} - \rho' H_x)$$

discritize at time step n and at space lattice point (i, j, k):

$$\frac{H_x|_{i,j,k}^{n+1/2} - H_x|_{i,j,k}^{n-1/2}}{\Delta t} = \frac{1}{\mu_{i,j,k}} \cdot (\frac{E_y|_{i,j,k+1/2}^{n} - E_y|_{i,j,k-1/2}^{n}}{\Delta z}$$

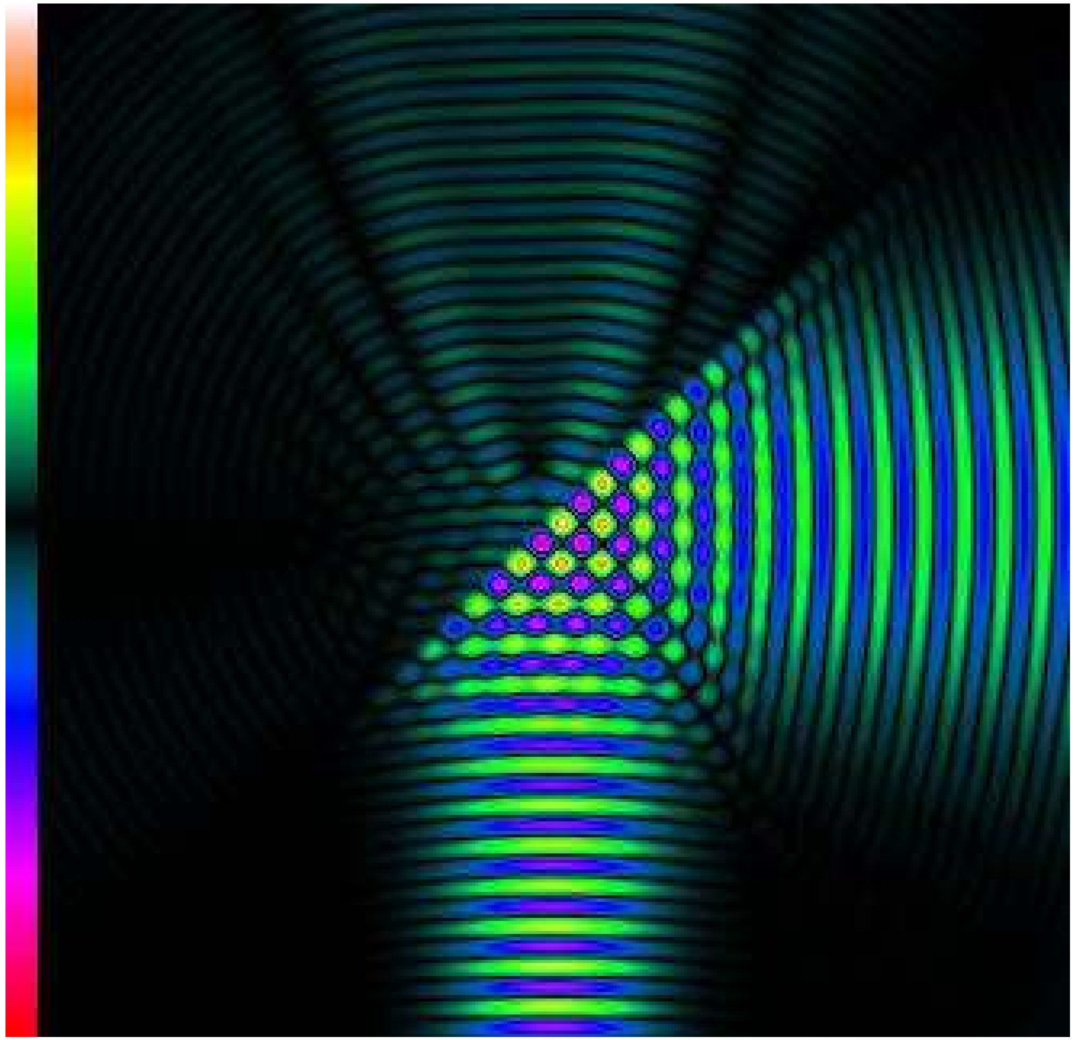
$$- \frac{E_y|_{i,j+1/2,k}^{n} - E_y|_{i,j-1/2,k}^{n}}{\Delta z} - \rho' i, j, k \cdot H_x|_{i,j,k}^{n})$$

FDTD: example



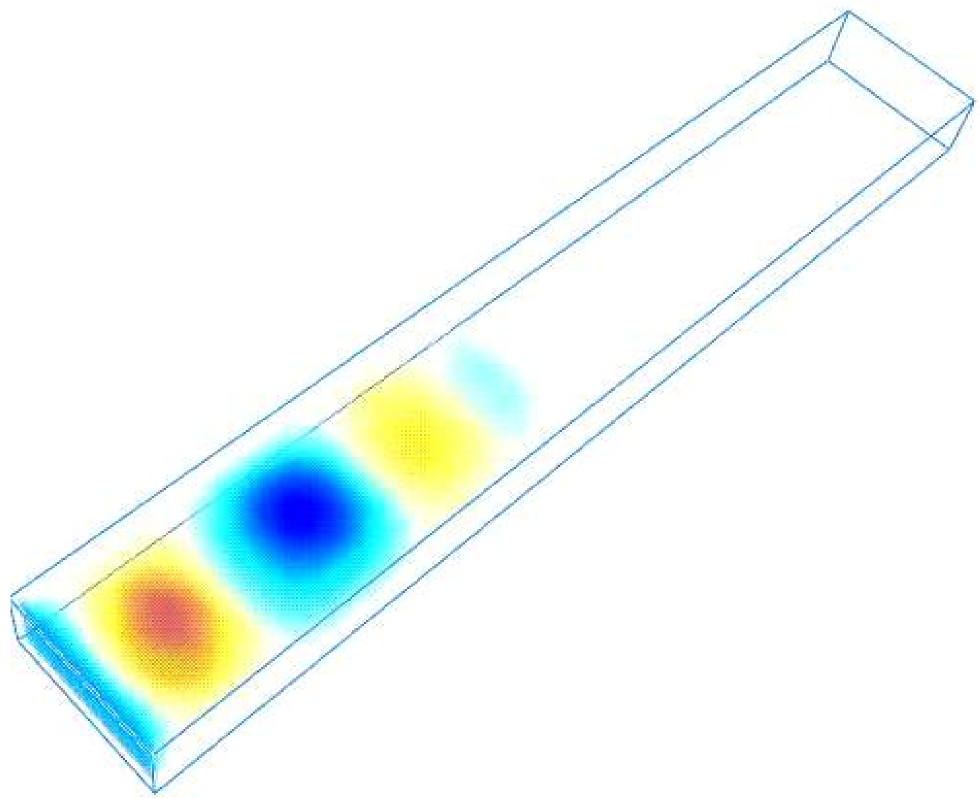
From: http://www.bay-technology.com

FDTD: example



From: http://www.fdtd.org

Metallic Waveguide



by ToyFDTD