Electromagnetic scattering 1: Finite-difference time-domain method (FDTD)

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Finite-difference time-domain (FDTD)

- Numerical technique for solving Maxwell's equations in time domain
- Maxwell's equations are directly discretized by finite-differences
- Central difference approximations to the space and time derivatives
- The space is approximated by cubical cells

Finite-difference time-domain (Yee-algorithm)

Strengths:

- Universal applicability
- Broadband response obtained with one simulation
- Inhomegeneous, anisotropic, non-linear materials are easily modelled
- Matrix inversion is not needed (recursive update scheme)
- Simple implementation
- Evolution of fields can be studied in time

Weaknesses:

- Accuracy -Error is dispersive and accumulates as waves propagate through the grid
- Staircase approximation
- Time-step is a function of grid size
- PML is needed for open region problems

FDTD literature

Introduction to FDTD, FEM, IEM

- Sheng Xin-Qing, Song Wei, Essentials of computational electromagnetics, IEEE,Wiley, 2012.

Some FDTD books

- Allen Taflove and Susan C. Hagness, Computational Electrodynamics: The Finite-Difference Time-Domain Method, Artech House Publishers, 2005.
- Wenhua Yu, Raj Mittra, Tao Su, Yongjun Liu, and Xiaoling Yang, Parallel Finite-Difference Time-Domain Method, Artech House Publishers, 2006.

Maxwell's equation

Faraday's law

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \tag{1}$$

Ampères law

$$\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \sigma \mathbf{E} + \mathbf{J} \tag{2}$$

Gauss's law for elecric field

$$\nabla \cdot \mathbf{D} = \rho \tag{3}$$

Gauss's law for magnetic field

$$\nabla \cdot \mathbf{B} = 0 \tag{4}$$

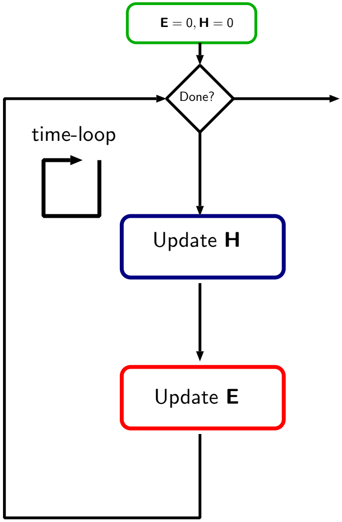
Constitutive relations:

$$\mathbf{D} = \epsilon * \mathbf{E} \tag{5}$$

$$\mathbf{B} = \mu * \mathbf{H} \tag{6}$$

ϵ electric permittivity
μ magnetic permeability

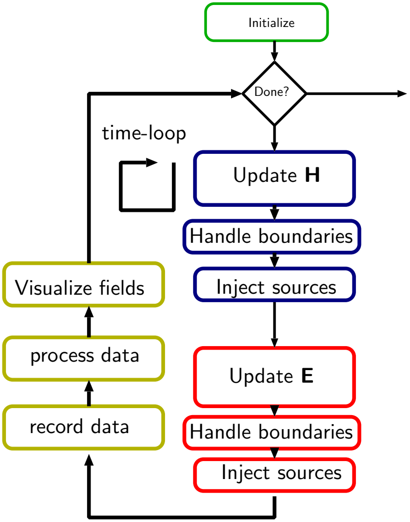
FDTD engine (empty space)



Set $\mathbf{E} = 0$ and $\mathbf{H} = 0$
Marching-in-time procedure:

- Update $\mathbf{H}$:
  $\nabla \times \mathbf{E} = -\mu_0 \frac{\partial \mathbf{H}}{\partial t}$
- Update $\mathbf{E}$:
  $\nabla \times \mathbf{H} = \epsilon_0 \frac{\partial \mathbf{E}}{\partial t}$

FDTD engine (more realistic case)



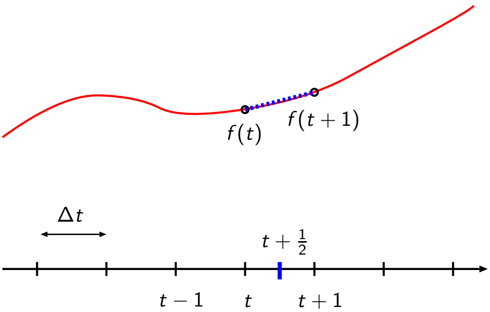
Initialize everything
Marching-in-time procedure:

- Update **H**:
- PML
- Gaussin pulse
- Update **E**:
- PML
- Gaussin pulse
- Fourier transform, etc.

Update equations

Finite-difference formula (central difference)

$$\frac{\partial f(t+\frac{\Delta t}{2})}{\partial t} \approx \frac{f(t+\Delta t)-f(t)}{\Delta t} \tag{7}$$



Difference is defined at “half integer point” in discrete time-domain

Update equations

Faraday's law

$$\nabla \times \mathbf{E} = -\mu \frac{\partial \mathbf{H}}{\partial t} => \frac{\partial \mathbf{H}}{\partial t} = -\mu^{-1} \nabla \times \mathbf{E} \tag{8}$$

Apply finite-difference formula for $\frac{\partial \mathbf{H}}{\partial t}$

$$\frac{\mathbf{H}|^{t+\frac{1}{2}} - \mathbf{H}|^{t-\frac{1}{2}}}{\Delta t} = -\mu^{-1} \nabla \times \mathbf{E}|^{t} \tag{9}$$

The update equation for **H** read as

$$\mathbf{H}|^{t+\frac{1}{2}} = \mathbf{H}|^{t-\frac{1}{2}} - \Delta t \, \mu^{-1} \nabla \times \mathbf{E}|^{t} \tag{10}$$

Update equations

Ampère's law

$$\nabla \times \mathbf{H} = \epsilon \frac{\partial \mathbf{E}}{\partial t} => \frac{\partial \mathbf{E}}{\partial t} = \epsilon^{-1} \nabla \times \mathbf{H} \tag{11}$$

Apply finite-difference formula for $\frac{\partial \mathbf{E}}{\partial t}$

$$\frac{\mathbf{E}|^{t+1} - \mathbf{E}|^{t}}{\Delta t} = \epsilon^{-1} \nabla \times \mathbf{H}|^{t+\frac{1}{2}} \tag{12}$$

The update equation for **E** read as

$$\mathbf{E}|^{t+1} = \mathbf{E}|^{t} + \Delta t \, \epsilon^{-1} \nabla \times \mathbf{H}|^{t+\frac{1}{2}} \tag{13}$$

Update equations for components of $\mathbf{H}$

Assume μ is diagonal

$$\mathbf{H}\big|^{t+\frac{1}{2}} = \mathbf{H}\big|^{t-\frac{1}{2}} - \Delta t\, \mu^{-1} \nabla \times \mathbf{E}\big|^{t} \tag{14}$$

$$\nabla \times \mathbf{E} = \hat{\mathbf{x}} \left(\frac{\partial E_z}{\partial y} - \frac{\partial E_y}{\partial z} \right) + \hat{\mathbf{y}} \left(\frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x} \right) + \hat{\mathbf{z}} \left(\frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} \right) \tag{15}$$

x-component:

$$H_x\big|^{t+\frac{1}{2}} = H_x\big|^{t-\frac{1}{2}} - \Delta t\, \mu_{xx}^{-1} \left(\frac{\partial E_z}{\partial y} - \frac{\partial E_y}{\partial z} \right)\Bigg|^{t} \tag{16}$$

y-component:

$$H_y\big|^{t+\frac{1}{2}} = H_y\big|^{t-\frac{1}{2}} - \Delta t\, \mu_{yy}^{-1} \left(\frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x} \right)\Bigg|^{t} \tag{17}$$

z-component:

$$H_z\big|^{t+\frac{1}{2}} = H_z\big|^{t-\frac{1}{2}} - \Delta t\, \mu_{zz}^{-1} \left(\frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} \right)\Bigg|^{t} \tag{18}$$

Update equations for components of E

Assume ϵ is diagonal

$$\mathbf{E}\big|^{t+1} = \mathbf{E}\big|^{t} + \Delta t\, \epsilon^{-1} \nabla \times \mathbf{H}\big|^{t+\frac{1}{2}} \tag{19}$$

x-component:

$$E_x\big|^{t+1} = E_x\big|^{t} + \Delta t\, \epsilon_{xx}^{-1} \left(\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} \right)\Bigg|^{t+\frac{1}{2}} \tag{20}$$

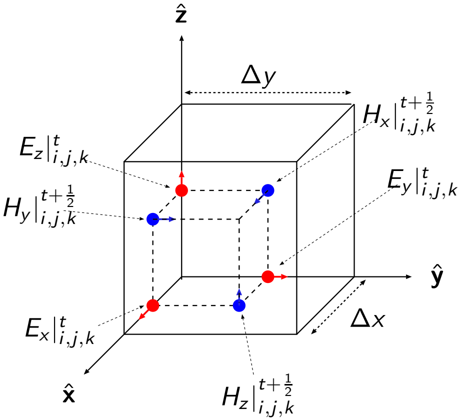
y-component:

$$E_y\big|^{t+1} = E_y\big|^{t} + \Delta t\, \epsilon_{yy}^{-1} \left(\frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} \right)\Bigg|^{t+\frac{1}{2}} \tag{21}$$

z-component:

$$E_z\big|^{t+1} = E_z\big|^{t} + \Delta t\, \epsilon_{zz}^{-1} \left(\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} \right)\Bigg|^{t+\frac{1}{2}} \tag{22}$$

Yee's unit cell



Components of vectors in each cell (i, j, k) are located at different points in space!

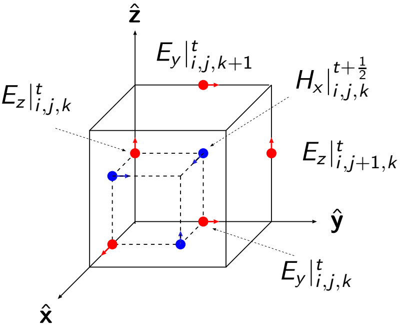
- Automatically satisfies divergence conditions
- Automatically satisfies interface conditions
- Simplifies the FDTD-algorithm

(K. Yee, "Numerical solution of initial boundary value problems involving maxwell's equations in isotropic media," *IEEE Trans. Antennas and Propagation*, vol.14, no.3, pp.302–307, May 1966)

Update equation for x-component of H-field

$$H_x\big|_{i,j,k}^{t+\frac{1}{2}} = H_x\big|_{i,j,k}^{t-\frac{1}{2}} - \Delta t\, \mu_{xx}^{-1} \left(\frac{\partial E_z}{\partial y} - \frac{\partial E_y}{\partial z} \right)\Bigg|^{t} \qquad (23)$$

$$\left(\frac{\partial E_z}{\partial y} - \frac{\partial E_y}{\partial z} \right) = \frac{E_z\big|_{i,j+1,k}^{t} - E_z\big|_{i,j,k}^{t}}{\Delta y} - \frac{E_y\big|_{i,j,k+1}^{t} - E_y\big|_{i,j,k}^{t}}{\Delta z} \qquad (24)$$



Update equations for H-field

y-component:

$$H_y\Big|_{i,j,k}^{t+\frac{1}{2}} = H_y\Big|_{i,j,k}^{t-\frac{1}{2}} - \Delta t\, \mu_{yy}^{-1} \left(\frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x} \right)\Bigg|^{t} \tag{25}$$

$$\left(\frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x} \right) = \frac{E_x|_{i,j,k+1}^{t} - E_x|_{i,j,k}^{t}}{\Delta z} - \frac{E_z|_{i+1,j,k}^{t} - E_z|_{i,j,k}^{t}}{\Delta x} \tag{26}$$

z-component:

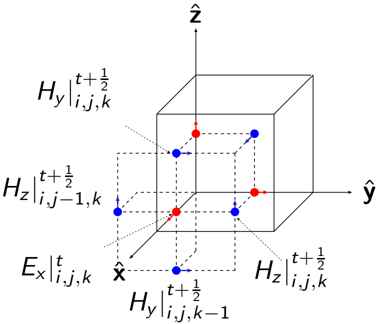
$$H_z\Big|_{i,j,k}^{t+\frac{1}{2}} = H_z\Big|_{i,j,k}^{t-\frac{1}{2}} - \Delta t\, \mu_{zz}^{-1} \left(\frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} \right)\Bigg|^{t} \tag{27}$$

$$\left(\frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} \right) = \frac{E_y|_{i+1,j,k}^{t} - E_y|_{i,j,k}^{t}}{\Delta x} - \frac{E_x|_{i,j+1,k}^{t} - E_x|_{i,j,k}^{t}}{\Delta y} \tag{28}$$

Update equation for the x-component of E-field

$$E_x\big|_{i,j,k}^{t+1} = E_x\big|_{i,j,k}^{t} + \Delta t\, \epsilon_{xx}^{-1} \left(\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} \right) \Bigg|^{t+\frac{1}{2}} \quad (29)$$

$$\left(\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} \right) = \frac{H_z\big|_{i,j,k}^{t+\frac{1}{2}} - H_z\big|_{i,j-1,k}^{t+\frac{1}{2}}}{\Delta y} - \frac{H_y\big|_{i,j,k}^{t+\frac{1}{2}} - H_y\big|_{i,j,k-1}^{t+\frac{1}{2}}}{\Delta z} \quad (30)$$



Update equations for E-field

y-component:

$$E_y\big|_{i,j,k}^{t+1} = E_y\big|_{i,j,k}^{t} + \Delta t\, \epsilon_{yy}^{-1} \left(\frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} \right)\Bigg|^{t+\frac{1}{2}} \tag{31}$$

$$\left(\frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} \right) = \frac{H_x\big|_{i,j,k}^{t+\frac{1}{2}} - H_x\big|_{i,j,k-1}^{t+\frac{1}{2}}}{\Delta z} - \frac{H_z\big|_{i,j,k}^{t+\frac{1}{2}} - H_z\big|_{i-1,j,k}^{t+\frac{1}{2}}}{\Delta x} \tag{32}$$

z-component:

$$E_z\big|_{i,j,k}^{t+1} = E_z\big|_{i,j,k}^{t} + \Delta t\, \epsilon_{zz}^{-1} \left(\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} \right)\Bigg|^{t+\frac{1}{2}} \tag{33}$$

$$\left(\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} \right) = \frac{H_y\big|_{i,j,k}^{t+\frac{1}{2}} - H_y\big|_{i-1,j,k}^{t+\frac{1}{2}}}{\Delta x} - \frac{H_x\big|_{i,j,k}^{t+\frac{1}{2}} - H_x\big|_{i,j-1,k}^{t+\frac{1}{2}}}{\Delta y} \tag{34}$$

Boundary conditions

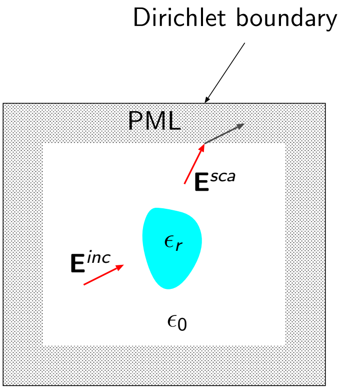
- In differential equation methods the unknowns are generally global i.e. they $\mathbf{E}, \mathbf{H} \in \mathbb{R}^3$
- We have to terminate the region of interest somehow
- We can use boundary conditions such as Dirichlet, Neumann, periodic, boundary, absorbing conditions
- Perfectly match layer (PML) for mimicking free space

Boundary conditions

- Consider FDTD-grid of size $1 : N_x, 1 : N_y, 1 : N_z$
- To calculate $\nabla \times \mathbf{H}$, we need to know values of terms $H_{i-1,j,k}$, $H_{i,j-1,k}$, and $H_{i,j,k-1}$. These, however, are not defined when i=1, j = 1, k=1, respectively, since they are out of the computational domain.
- Similarly, $\nabla \times \mathbf{E}$ contain terms $E_{i+1,j,k}$, $E_{i,j+1,k}$, and $E_{i,j,k+1}$ which not defined when $i = N_x$, $j = N_y$, $k = N_z$.
- Force these values to be something (physically reasonable) by a boundary condition

Perfectly match layer (PML)

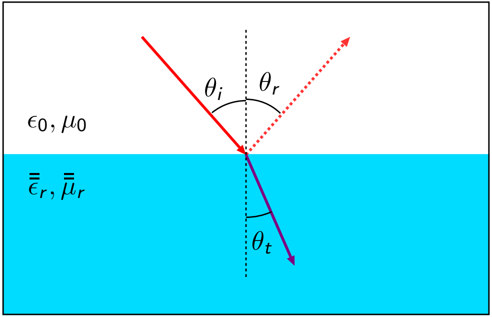
- In unbounded problems, e.g. scattering problems, we want to eliminate reflections from computational boundaries
- We introduce loss to absorb outgoing waves in the PML, and at the same time match the impedance to prevent reflections
- This has to be done for all incident angels and polarizations



Uniaxial perfectly match layer (UPML)

Consider a planewave reflection from a diagonally anisotropic interface with

$$\bar{\bar{\epsilon}}_r = \bar{\bar{\mu}}_r = \begin{pmatrix} a_2 & 0 & 0 \\ 0 & b_2 & 0 \\ 0 & 0 & c_2 \end{pmatrix} \quad (35)$$



Uniaxial perfectly match layer (UPML)

Refraction into a diagonally anisotropic material

$$\sin\theta_i = \sqrt{b_2 c_2}\sin\theta_t \tag{36}$$

Reflection coefficients (z-axis normal to the interface)

$$R^{TE} = \frac{\cos\theta_i - \sqrt{b_2/a_2}\cos\theta_t}{\cos\theta_i + \sqrt{b_2/a_2}\cos\theta_t} \tag{37}$$

$$R^{TM} = \frac{\sqrt{b_2/a_2}\cos\theta_t - \cos\theta_i}{\cos\theta_i + \sqrt{b_2/a_2}\cos\theta_t} \tag{38}$$

By choosing $\sqrt{b_2 c_2} = 1 \rightarrow \theta_i = \theta_t$ and $\sqrt{b_2/a_2} = 1$ we can see that $R^{TE} = 0$ and $R^{TM} = 0$,i.e., no reflection

We choose $b_2 = a_2$ and $c_2 = 1/b_2$

Uniaxial perfectly match layer (UPML)

By introducing losses a uniaxial material does the trick (for propagating waves, evanecent waves are more complicated but we can place the PML far enough from the scatterer)

$$\bar{\bar{\epsilon}}_r = \bar{\bar{\mu}}_r = \begin{bmatrix} S_y S_z / S_x & 0 & 0 \\ 0 & S_x S_z / S_y & 0 \\ 0 & 0 & S_x S_y / S_z \end{bmatrix} \tag{39}$$

Parameter can be chosen e.g.

$$S_x = 1 - \frac{\sigma_x(x)}{i\omega\epsilon_0}, \quad \sigma_x(x) = \frac{\epsilon_0}{2\Delta}(\frac{x}{L_x})^3 \tag{40}$$

$$S_y = 1 - \frac{\sigma_y(y)}{i\omega\epsilon_0}, \quad \sigma_y(y) = \frac{\epsilon_0}{2\Delta}(\frac{y}{L_y})^3 \tag{41}$$

$$S_z = 1 - \frac{\sigma_z(z)}{i\omega\epsilon_0}, \quad \sigma_z(z) = \frac{\epsilon_0}{2\Delta}(\frac{z}{L_z})^3 \tag{42}$$

Uniaxial perfectly match layer (UPML)

UPML is a frequency domain concept hence we need convert it back to the time domain by Fourier transform

Some Fourier transform properties:

$$F(\omega) \leftrightarrow \partial f(t) \tag{43}$$

$$i\omega F(\omega) \leftrightarrow \frac{\partial f(t)}{\partial t} \tag{44}$$

$$\frac{1}{i\omega} F(\omega) \leftrightarrow \int_{-\infty}^{t} f(\tau)\,\mathrm{d}\tau \tag{45}$$

Leads to more complicated update equations containing e.g. convolutions!

Stability of the FDTD algorithm

Maximum cell size:

$$\Delta_{max} < \frac{1}{10}\frac{\lambda}{\sqrt{\epsilon_r \mu_r}}, \quad \Delta_x, \Delta_y, \Delta_z < \Delta_{max} \tag{46}$$

and cells should be able to model geometrical details
Numerical velocity should not exceed c_0
$->$Courant stability condition:

$$\Delta t < \frac{\sqrt{\epsilon_r \mu_r}}{c_0\sqrt{\frac{1}{(\Delta x)^2}+\frac{1}{(\Delta y)^2}+\frac{1}{(\Delta z)^2}}} \tag{47}$$

Dispersion relation

Consider a plane electromagnetic wave propagating along z-axis

$$\mathbf{E} = \mathbf{E}_0 e^{i(\omega t - kz)} \tag{48}$$

How fast a constant phase “point” propagates?

$$\frac{d}{dt}(\omega t - kz) = \frac{d}{dt}(\text{constant}) \tag{49}$$

Phase velocity

$$c_p = \frac{dz}{dt} = \frac{\omega}{k} \tag{50}$$

Unfortunately, the dispersion is not the same in the FDTD-grid

Numerical dispersion 1D

Planewave propagating z-direction

$$E_x|_q^t = E_0 e^{-i(\omega n\Delta t - \tilde{k}_z q\Delta z)} \tag{51}$$

$$H_y|_q^t = H_0 e^{-i(\omega n\Delta t - \tilde{k}_z q\Delta z)} \tag{52}$$

Faraday's law in free-space

$$\nabla \times \mathbf{E} = -\mu_0 \frac{\partial \mathbf{H}}{\partial t} \tag{53}$$

Faraday's law for the above planewave (y-component)

$$\frac{\partial E_x}{\partial z} = -\mu \frac{\partial H_y}{\partial t} \tag{54}$$

Spatial finite-difference for the planewave

$$\frac{\partial E_x}{\partial z} = \frac{\left(e^{i\tilde{k}_z \frac{\Delta z}{2}} - e^{-i\tilde{k}_z \frac{\Delta z}{2}}\right)}{\Delta z} E_x|_q^t \tag{55}$$

Numerical dispersion 1D

Temporal finite-difference for the planewave

$$\frac{\partial H_y}{\partial t} = \frac{(e^{-i\omega\frac{\Delta t}{2}} - e^{i\omega\frac{\Delta t}{2}})}{\Delta t} H_y|_q^t \tag{56}$$

FD-Faraday law read as

$$\frac{(e^{i\tilde{k}_z\frac{\Delta z}{2}} - e^{-i\tilde{k}_z\frac{\Delta z}{2}})}{\Delta z} E_x|_q^t = -\mu_0 \frac{(e^{-i\omega\frac{\Delta t}{2}} - e^{i\omega\frac{\Delta t}{2}})}{\Delta t} H_y|_q^t \tag{57}$$

Since

$$\frac{E_x}{H_y} = \sqrt{\frac{\mu_0}{\epsilon_0}} \tag{58}$$

we can write the numerical dispersion relation as

$$\frac{1}{\Delta z} \sin\left(\frac{\tilde{k}_z \Delta z}{2}\right) = \frac{1}{c_p \Delta t} \sin\left(\frac{\omega \Delta t}{2}\right) \tag{59}$$

Numerical dispersion 1D

Numerical dispersion relation

$$\frac{1}{\Delta z}\sin\left(\frac{\tilde{k}_z \Delta z}{2}\right) = \frac{1}{c\Delta t}\sin\left(\frac{\omega \Delta t}{2}\right) \tag{60}$$

Case 1: $\Delta t, \Delta z \to 0$, for small x

$$\sin x = x - \frac{x^3}{3!} + \frac{5^3}{5!} + \mathcal{O}(x^7) \tag{61}$$

$$k_z = \frac{\omega}{c_p} \tag{62}$$

Case 2: set $\Delta t = \Delta z / c$

$$\frac{1}{\Delta z}\sin\left(\frac{\tilde{k}_z \Delta z}{2}\right) = \frac{1}{\Delta z}\sin\left(\frac{\omega \Delta z}{2c}\right) \to \tilde{k}_z = \frac{\omega}{c} \tag{63}$$

Magic time-step!

Numerical dispersion 3D

Three-dimensional case

$$\left[\frac{1}{c_p\Delta t}\sin\left(\frac{\omega\Delta t}{2}\right)\right]^2 = \left[\frac{1}{\Delta x}\sin\left(\frac{\tilde{k}_x\Delta x}{2}\right)\right]^2 + \left[\frac{1}{\Delta y}\sin\left(\frac{\tilde{k}_y\Delta y}{2}\right)\right]^2 + \left[\frac{1}{\Delta z}\sin\left(\frac{\tilde{k}_z\Delta z}{2}\right)\right]^2 \tag{64}$$

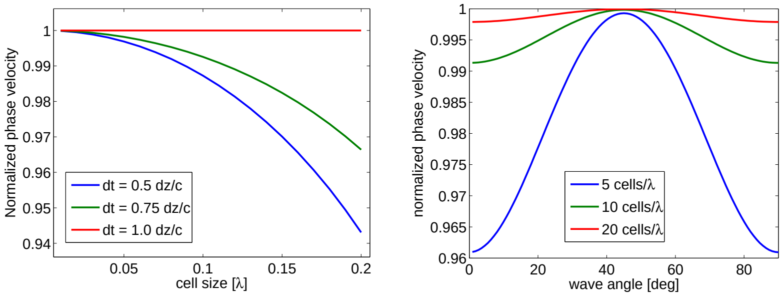
Depends on the time ans spatial resolution, and propagation direction! Numerical dispersion is anisotropic.

Approaches the continuous dispersion relation

$$\left(\frac{\omega}{c_p}\right)^2 = \tilde{k}_x^2 + \tilde{k}_y^2 + \tilde{k}_z^2 \tag{65}$$

when $\Delta t, \Delta x, \Delta y, \Delta z \to 0$, however a magic time-step does not exist!

Numerical dispersion



Numerical dispersion can be reduced by decreasing cell size

Recall: Courant stability condition $->$ smaller time-step

Implementation of 1-D FDTD

1D problem

Consider uniform problem in the x and y-directions

$$\frac{\partial}{\partial x} = \frac{\partial}{\partial y} = 0 \tag{66}$$

System decouples into two independent modes
E_x/H_y mode:

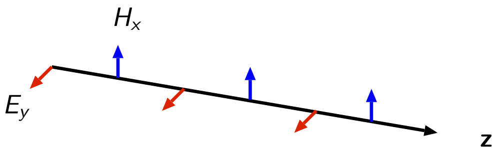
$$\frac{\partial E_x}{\partial z} = -\mu_{yy}\frac{\partial H_y}{\partial t}, \quad -\frac{\partial H_y}{\partial z} = -\epsilon_{xx}\frac{\partial E_x}{\partial t} \tag{67}$$

E_y/H_x mode:

$$\frac{\partial E_y}{\partial z} = \mu_{xx}\frac{\partial H_x}{\partial t}, \quad \frac{\partial H_x}{\partial z} = \epsilon_{yy}\frac{\partial E_y}{\partial t} \tag{68}$$

1D update equation

We consider E_y/H_x-mode



$$H_x\big|_k^{t+\frac{1}{2}} = H_x\big|_k^{t-\frac{1}{2}} + m_{Hx}^k\left(\frac{E_y\big|_{k+1}^t - E_y\big|_k^t}{\Delta z}\right) \tag{69}$$

$$E_y\big|_k^{t+1} = E_y\big|_k^t + m_{Ey}^k\left(\frac{H_x\big|_k^{t+\frac{1}{2}} - H_x\big|_{k-1}^{t+\frac{1}{2}}}{\Delta z}\right) \tag{70}$$

where the update coefficients are defined as $m_{Hx}^k = \frac{\Delta t}{\mu_{xx}^k}$ and $m_{Ey}^k = \frac{\Delta t}{\epsilon_{yy}^k}$

PEC and PMC boundary conditions

Consider 1D-FDTD grid where $k = 1 : N_k$
When $k = N_k$, the update equation for H_x read as

$$H_x|_{N_k}^{t+\frac{1}{2}} = H_x|_{N_k}^{t-\frac{1}{2}} + m_{Hx}^{N_k} \left(\frac{E_y|_{N_k+1}^{t} - E_y|_{N_k}^{t}}{\Delta z} \right) \tag{71}$$

and $E_y|_{N_k+1}^{t}$ exists outside the computational domain. Setting $E_y|_{N_k+1}^{t} = 0$ enforces the PEC boundary condition $\mathbf{n} \times \mathbf{E} = 0$

When $k = 1$, the update equation for E_y read as

$$E_y|_1^{t+1} = E_y|_1^{t} + m_{Ey}^{k} \left(\frac{H_x|_1^{t+\frac{1}{2}} - H_x|_0^{t+\frac{1}{2}}}{\Delta z} \right) \tag{72}$$

and $H_x|_0^{t+\frac{1}{2}}$ exists outside the computational domain. Setting $H_x|_0^{t+\frac{1}{2}} = 0$ enforces the PMC boundary condition $\mathbf{n} \times \mathbf{H} = 0$

Basic 1D FDTD engine

Algorithm 1 1D-fdtd engine with PEC and PMC

Initialize grid
for $t = 1$ to N_t **do**
    for $k = 1$ to $N_k - 1$ **do**
        Update H_x
    end for
    Compute $H_x(N_k)$ with BC
    for $k = 2$ to N_k **do**
        Update E_y
    end for
    Compute $E_y(1)$ with BC
end for

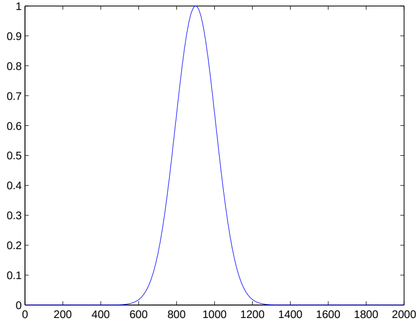
When we run this algorithm everything should stay zeros (no source included)

The Gaussian source for 1D-FDTD

The Gaussian pulse is a typical source in FDTD-simulations since it excites a broad range of frequencies.

$$g(t) = \exp\left[-\left(\frac{t - t_0}{\tau}\right)^2\right] \tag{73}$$

t_0 is the delay and τ is the width of the pulse. Note, from the Fourier transform we can see that the bandwidth is about $B = \frac{1}{\pi\tau}$



Simple soft-source

Simple transparent Gaussian source. Add the source function to some field component at one point on the grid e.g.

$$E_y|_k^{t+1} = E_y|_k^{t+1} + g|_k \tag{74}$$

Algorithm 2 1D-fdtd engine with PEC/PMC and soft source

```
Compute source
Initialize grid
for t = 1 to N_t do
    for k = 1 to N_k - 1 do
        Update H_x
    end for
    Compute H_x(N_k) with BC
    for k = 2 to N_k do
        Update E_y
    end for
    Compute E_y(1) with BC
    Inject Source E_y|_s = E_y|_s + g|_s
end for
```

"two-way source" useful for testing boundary conditions

Ideal absorbing boundary condition

In 1D , it is possible find a perfectly absorbing boundary condition if

- Waves travelling only outward at the boundary
- Materials at both boundaries are linear, isotropic homogeneous and non-dispersive (same material for both boundaries)
- $\Delta t = \sqrt{\epsilon_r \mu_r} \Delta z/(2c)$

Waves propagate exactly one cell in two time-steps

$$E_y|_{N_k+1}^{t} = E_y|_{N_k}^{t-2} \tag{75}$$

$$H_x|_0^{t+\frac{1}{2}} = H_x|_1^{t-\frac{3}{2}} \tag{76}$$

Record field values at the boundaries and use recorded values as boundary conditions

Ideal absorbing boundary condition

At $k = 1$ record H-field values and modify the E-field update equation

$$\begin{aligned} h_3 &= h_2 \\ h_2 &= h_1 \\ h_1 &= H_x\big|_1^{t+\frac{1}{2}} \\ E_y\big|_1^{t+1} &= E_y\big|_1^{t} + m_{Ey}^1 \frac{H_x\big|_1^{t+\frac{1}{2}} - h_3}{\Delta z} \end{aligned} \tag{77}$$

At $k = N_k$ record E-field values and modify the H-field update equation

$$\begin{aligned} e_3 &= e_2 \\ e_2 &= e_1 \\ e_1 &= E_y\big|_{N_k}^{t} \\ H_x\big|_{N_k}^{t+\frac{1}{2}} &= H_x\big|_{N_k}^{t-\frac{1}{2}} + m_{Hx}^{N_k} \frac{E_y\big|_{N_k}^{t} - e_3}{\Delta z} \end{aligned} \tag{78}$$

Simple but works only in a special case

Ideal absorbing boundary condition

Algorithm 3 1D-fdtd engine with the ABC and soft source

Compute time-step
Compute source
Initialize grid

for $t = 1$ to N_t **do**

  for $k = 1$ to $N_k - 1$ **do**
    Update H_x
  end for
  Compute $H_x(N_k)$ with e_3 BC
  Record H-field $h_3 = h_2, h_2 = h_1, h_1 = H_x|_1$

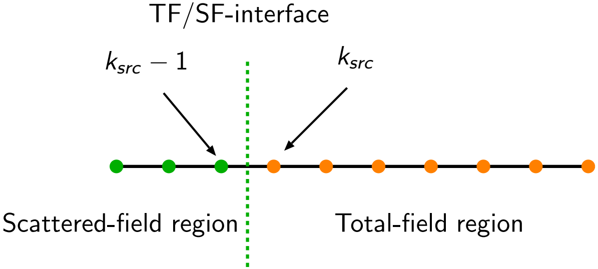
  for $k = 2$ to N_k **do**
    Update E_y
  end for
  Compute $E_y(1)$ with h_3 BC
  Record E-field $e_3 = e_2, e_2 = e_1, e_1 = E_y|_{N_k}$

  Inject Source $E_y|_s = E_y|_s + g|_s$
end for

Total-field/scattered-field (TF/SF) source

Eliminates backward propagating waves“One way source”

Divide the grid into total-field region and scattered-field region



Total-field/scattered-field (TF/SF) source

Consider update equation for H_x at $k_{src} - 1$ (Scattered-field side)

$$H_x\Big|_{k_{src}-1}^{t+\frac{1}{2}} = H_x\Big|_{k_{src}-1}^{t-\frac{1}{2}} + m_{Hx}^{k_{src}-1}\left(\frac{E_y\big|_{k_{src}}^{t} - E_y\big|_{k_{src-1}}^{t}}{\Delta z}\right) \tag{79}$$

$E_y\big|_{k_{src}}^{t}$ exists at the total-field side.

Since $\mathbf{E}^{tot} = \mathbf{E}^{src} + \mathbf{E}^{sca}$, we need to subtract the source-field from the total-field to obtain the scattered-field

$$H_x\Big|_{k_{src}-1}^{t+\frac{1}{2}} = H_x\Big|_{k_{src}-1}^{t-\frac{1}{2}} + m_{Hx}^{k_{src}-1}\left(\frac{(E_y\big|_{k_{src}}^{t} - E_y^{src}\big|_{k_{src}}^{t}) - E_y\big|_{k_{src-1}}^{t}}{\Delta z}\right) \tag{80}$$

This can be written as

$$H_x\Big|_{k_{src}-1}^{t+\frac{1}{2}} = H_x\Big|_{k_{src}-1}^{t-\frac{1}{2}} + m_{Hx}^{k_{src}-1}\left(\frac{E_y\big|_{k_{src}}^{t} - E_y\big|_{k_{src-1}}^{t}}{\Delta z}\right) - \frac{m_{Hx}^{k_{src}-1}}{\Delta z}E_y^{src}\big|_{k_{src}}^{t} \tag{81}$$

i.e. the standard update equation + a correction term

Total-field/scattered-field (TF/SF) source

Consider update equation for E_y at k_{src} (Total-field side)

$$E_y\Big|_{k_{src}}^{t+1} = E_y\Big|_{k_{src}}^{t} + m_{Ey}^{k_{src}} \left(\frac{H_x\Big|_{k_{src}}^{t+\frac{1}{2}} - H_x\Big|_{k_{src}-1}^{t+\frac{1}{2}}}{\Delta z} \right) \quad (82)$$

$H_x\Big|_{k_{src}-1}^{t+\frac{1}{2}}$ exists at the scattered-field side. We must add the source to it

$$E_y\Big|_{k_{src}}^{t+1} = E_y\Big|_{k_{src}}^{t} + m_{Ey}^{k_{src}} \left(\frac{H_x\Big|_{k_{src}}^{t+\frac{1}{2}} - \left(H_x\Big|_{k_{src}-1}^{t+\frac{1}{2}} + H_x^{src}\Big|_{k_{src}-1}^{t+\frac{1}{2}}\right)}{\Delta z} \right) \quad (83)$$

and this can be expressed as

$$E_y\Big|_{k_{src}}^{t+1} = E_y\Big|_{k_{src}}^{t} + m_{Ey}^{k_{src}} \left(\frac{H_x\Big|_{k_{src}}^{t+\frac{1}{2}} - H_x\Big|_{k_{src}-1}^{t+\frac{1}{2}}}{\Delta z} \right) - \frac{m_{Ey}^{k_{src}}}{\Delta z} H_x^{src}\Big|_{k_{src}-1}^{t+\frac{1}{2}} \quad (84)$$

Total-field/scattered-field (TF/SF) source

Two source functions are needed:

$$E_y^{src}\Big|_{k_{src}}^{t} \text{ and } H_x^{src}\Big|_{k_{src}-1}^{t+\frac{1}{2}} \tag{85}$$

Note, these function exist at different locations in space and time $\rightarrow$ time-delay

$$E_y^{src}\Big|_{k_{src}}^{t} = g(t) \tag{86}$$

$$H_x^{src}\Big|_{k_{src}-1}^{t+\frac{1}{2}} = -\sqrt{\frac{\epsilon_{k_{src}}}{\mu_{k_{src}}}} g\left(t + \frac{\sqrt{\epsilon_r \mu_r}\Delta z}{2c} + \frac{\Delta t}{2}\right) \tag{87}$$

half grid delay

half time-step delay

Ideal absorbing boundary condition

Algorithm 4 1D-fdtd engine with the ABC and TF/SF source

Compute time-step
Compute sources
Initialize grid
for $t = 1$ to N_t **do**
    for $k = 1$ to $N_k - 1$ **do**
        Update H_x
    end for
    Compute $H_x(N_k)$ with e_3 BC
    Record H-field $h_3 = h_2, h_2 = h_1, h_1 = H_x|_1$
    Inject H-field source $H_x|_{s-1}^{t+1/2} = H_x|_{s-1}^{t+1/2} + \dots$
    for $k = 2$ to N_k **do**
        Update E_y
    end for
    Compute $E_y(1)$ with h_3 BC
    Record E-field $e_3 = e_2, e_2 = e_1, e_1 = E_y|_{N_k}$
    Inject E-field source $E_y|_s^{t+1} = E_y|_s^{t+1} + \dots$
end for

Fourier transforms

In many cases, we want to study scattering properties in frequency domain.

Fourier transform: conversion between time and frequency domains

$$G(f) = \int_{-\infty}^{\infty} g(t)\exp(-i2\pi ft)\,\mathrm{d}t \tag{88}$$

Inverse transform

$$g(t) = \int_{-\infty}^{\infty} G(f)\exp(i2\pi tf)\,\mathrm{d}x \tag{89}$$

Discrete transform:

$$G(f) = \sum_{n=1}^{N_t} g(n\Delta t)\exp(-i2\pi fn\Delta t)\Delta t \tag{90}$$

Calculation of reflectance and transmittance

Normalize the spectra by dividing the relection and transmission spectrum by the source spectrum Reflectance:

$$R(f) = \left(\frac{DFT[E_{ref}(t)]}{DFT[E_{src}(t)]} \right)^2 \tag{91}$$

Transmittance:

$$R(f) = \left(\frac{DFT[E_{trn}(t)]}{DFT[E_{src}(t)]} \right)^2 \tag{92}$$

Note: Nyquist theorem $\rightarrow$ maximum frequency

$$f_{max} = \frac{1}{2\Delta t} \tag{93}$$

$$\Delta f \cong \frac{1}{N_{steps} \Delta t} \tag{94}$$

Last FDTD example

Algorithm 5 1D-fdtd engine with the ABC, TF/SF source and DFT

for $t = 1$ to N_t **do**

    for $k = 1$ to $N_k - 1$ **do**

        Update H_x

    end for

    Compute $H_x(N_k)$ with e_3 BC

    Record H-field $h_3 = h_2, h_2 = h_1, h_1 = H_x|_1$

    Inject H-field source $H_x|_{s-1}^{t+1/2} = H_x|_{s-1}^{t+1/2} + \dots$

    for $k = 2$ to N_k **do**

        Update E_y

    end for

    Compute $E_y(1)$ with h_3 BC

    Record E-field $e_3 = e_2, e_2 = e_1, e_1 = E_y|_{N_k}$

    Inject E-field source $E_y|_s^{t+1} = E_y|_s^{t+1} + \dots$

    for $q = 1$ to N_q **do**

        Compute DFT $E_{ref}(q) = E_{ref}(q) + \Delta t exp(-i2\pi f_q t\Delta t))E_y|_2$

        Compute DFT $E_{trn}(q) = E_{trn}(q) + \Delta t exp(-i2\pi f_q t\Delta t))E_y|_{N_k-2}$

    end for

end for