Finite Difference Gridding

MRI data of a human head

Allocation of field components

Digitizing

Each “brick“ with different material properties

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Taylor expansions about $x_i$

$$u(x_i + \Delta x)|_{t_n} = u|_{x_i,t_n} + \Delta x \cdot \left. \frac{\partial u}{\partial x} \right|_{x_i,t_n} + \frac{(\Delta x)^2}{2} \cdot \left. \frac{\partial^2 u}{\partial x^2} \right|_{x_i,t_n}$$

$$+ \frac{(\Delta x)^3}{6} \cdot \left. \frac{\partial^3 u}{\partial x^3} \right|_{x_i,t_n} + \frac{(\Delta x)^4}{24} \cdot \left. \frac{\partial^4 u}{\partial x^4} \right|_{\xi_1,t_n}$$

$$u(x_i - \Delta x)|_{t_n} = u|_{x_i,t_n} - \Delta x \cdot \left. \frac{\partial u}{\partial x} \right|_{x_i,t_n} + \frac{(\Delta x)^2}{2} \cdot \left. \frac{\partial^2 u}{\partial x^2} \right|_{x_i,t_n}$$

$$- \frac{(\Delta x)^3}{6} \cdot \left. \frac{\partial^3 u}{\partial x^3} \right|_{x_i,t_n} + \frac{(\Delta x)^4}{24} \cdot \left. \frac{\partial^4 u}{\partial x^4} \right|_{\xi_2,t_n}$$
Central-difference approximation

\[ u(x_i + \Delta x)_{t_n} + u(x_i - \Delta x)_{t_n} = 2 \cdot u_{x_i,t_n} + (\Delta x)^2 \frac{\partial^2 u}{\partial x^2}_{x_i,t_n} + \frac{(\Delta x)^4}{12} \frac{\partial^4 u}{\partial x^4}_{\xi_3,t_n} \]

2nd derivative of \( u \) at spatial location \( x_i \) and time \( t_n \)

\[ \frac{\partial^2 u}{\partial x^2}_{x_i,t_n} = \left[ \frac{u(x_i + \Delta x) - 2 \cdot u(x_i) + u(x_i - \Delta x)}{(\Delta x)^2} \right]_{t_n} + O[(\Delta x)^2] \]

Shorthand notation

\[ \frac{\partial^2 u}{\partial x^2}_{x_i,t_n} = \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2} + O[(\Delta x)^2] \]

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Finite Difference: Scalar Wave Equation

\[
\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}
\]

Scalar wave equation

\[
u^{n+1}_i - 2u^n_i + u^{n-1}_i \quad \frac{\Delta t^2}{(\Delta t)^2} + O[(\Delta t)^2] = c^2 \left\{ \frac{u^n_{i+1} - 2u^n_i + u^n_{i-1}}{(\Delta x)^2} + O[(\Delta x)^2] \right\}
\]

FD update equation for \( u_i \)

\[
u^{n+1}_i \approx (c\Delta t)^2 \left[ \frac{u^n_{i+1} - 2u^n_i + u^n_{i-1}}{(\Delta x)^2} \right] + 2u^n_i - u^{n-1}_i
\]
Maxwell’s Equations

- **Faraday’s law:**
  \[
  \frac{\partial B}{\partial t} = -\nabla \times E - M
  \]
  \[
  \frac{\partial}{\partial t} \iiint_A B \cdot dA = -\oint_L E \cdot dL - \iiint_A M \cdot dA
  \]

- **Ampere’s law:**
  \[
  \frac{\partial D}{\partial t} = \nabla \times H - J
  \]
  \[
  \frac{\partial}{\partial t} \iiint_A D \cdot dA = \oint_L H \cdot dL - \iiint_A J \cdot dA
  \]

- **Gauss’ law for electric field:**
  \[
  \nabla \cdot D = 0
  \]
  \[
  \oiint_A D \cdot dA = 0
  \]

- **Gauss’ law for magnetic field:**
  \[
  \nabla \cdot B = 0
  \]
  \[
  \oiint_A B \cdot dA = 0
  \]

Electric and Magnetic fields
coupled in Maxwell’s equations

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Vector Components of Faraday’s and Ampere’s Law

\[
\frac{\partial H_x}{\partial t} = \frac{1}{\mu} \left[ \frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial y} - \left( M_{\text{source}_x} + \sigma^* H_x \right) \right]
\]

\[
\frac{\partial H_y}{\partial t} = \frac{1}{\mu} \left[ \frac{\partial E_z}{\partial x} - \frac{\partial E_x}{\partial z} - \left( M_{\text{source}_y} + \sigma^* H_y \right) \right]
\]

\[
\frac{\partial H_z}{\partial t} = \frac{1}{\mu} \left[ \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} - \left( M_{\text{source}_z} + \sigma^* H_z \right) \right]
\]

\[
\frac{\partial E_x}{\partial t} = \frac{1}{\varepsilon} \left[ \frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} - \left( J_{\text{source}_x} + \sigma E_x \right) \right]
\]

\[
\frac{\partial E_y}{\partial t} = \frac{1}{\varepsilon} \left[ \frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} - \left( J_{\text{source}_y} + \sigma E_y \right) \right]
\]

\[
\frac{\partial E_z}{\partial t} = \frac{1}{\varepsilon} \left[ \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} - \left( J_{\text{source}_z} + \sigma E_z \right) \right]
\]
Finite Difference Time Domain 3-D Yee-Cell

Dual spatial grid is commonly used for coupled electric and magnetic fields

H components surrounded by four circulating E fields and vice versa

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1-D Time-Step Leapfrog Method

H is updated half a time step after E

H is located half a spatial step from E

Update E at t=0.0*dt

Update H at t=0.5*dt

Update E at t=1.0*dt

Update H at t=1.5*dt

Update E at t=2.0*dt

X-direction

Time

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E-field Update Equations

\[ \frac{\partial u}{\partial t}(i\Delta x, j\Delta y, k\Delta z, n\Delta t) = \frac{u_{i,j,k}^{n+1/2} - u_{i,j,k}^{n-1/2}}{\Delta t} + O[(\Delta t)^2] \]

Partial derivative of the electric field via Maxwell's equations

\[ \frac{\partial E_x}{\partial t} = \frac{1}{\varepsilon} \left[ \frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} - \left(J_{\text{source}} + \sigma E_x \right) \right] \]

FDTD approximation of the partial derivative of E w.r.t. time

\[ E_x |_{i,j+1/2,k+1/2}^{n+1/2} - E_x |_{i,j+1/2,k+1/2}^{n-1/2} = \frac{\Delta t}{\varepsilon_{i,j+1/2,k+1/2}} \left( \frac{H_z |_{i,j,k+1/2}^{n} - H_z |_{i,j,k+1/2}^{n}}{\Delta y} - \frac{H_y |_{i,j,k+1/2}^{n} - H_y |_{i,j,k+1/2}^{n}}{\Delta z} - J_{\text{source}} |_{i,j+1/2,k+1/2}^{n} - \sigma E_x |_{i,j+1/2,k+1/2}^{n} \right) \]

Leapfrog time-stepping

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2-D FDTD Update

TE sub Z-mode

2-D FDTD grid cells

FDTD is divergence-free

\[ E_{2Y}^{n+\frac{1}{2}} = C_1 E_{2Y}^{n-\frac{1}{2}} + \frac{\Delta t \Delta x}{C_2 \varepsilon A} (H_1^n - H_2^n) \]

\[ H_1^{n+1} = H_1^n + \frac{\Delta t \Delta x}{\mu A} \left( E_{1Y}^{n+\frac{1}{2}} - E_{2Y}^{n+\frac{1}{2}} + E_{1X}^{n+\frac{1}{2}} - E_{2X}^{n+\frac{1}{2}} \right) \]

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2-D TM\(_z\) Mode

\[ \frac{\partial H_x}{\partial t} = \frac{1}{\mu} \left[ -\frac{\partial E_z}{\partial y} - \left(M_{\text{source}_x} + \sigma^* H_x \right) \right] \]

\[ \frac{\partial H_y}{\partial t} = \frac{1}{\mu} \left[ \frac{\partial E_z}{\partial x} - \left(M_{\text{source}_y} + \sigma^* H_y \right) \right] \]

\[ \frac{\partial E_z}{\partial t} = \frac{1}{\varepsilon} \left[ \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} - \left(J_{\text{source}_z} + \sigma E_z \right) \right] \]
2-D FDTD Update for TM\(_z\) Mode

\[
H_{x}^{n+1}_{i-1/2, j+1} = D_{a}(m) \left( H_{x}^{n}_{i-1/2, j+1} \right) + D_{b}(m) \cdot \left( E_{z}^{n+1/2}_{i-1/2, j+1/2} - E_{z}^{n+1/2}_{i-1/2, j+3/2} - M_{\text{source}_{x}}^{n+1/2} \Delta \right)
\]

\[
H_{y}^{n+1}_{i, j+1/2} = D_{a}(m) \left( H_{y}^{n}_{i, j+1/2} \right) + D_{b}(m) \cdot \left( E_{z}^{n+1/2}_{i+1/2, j+1/2} - E_{z}^{n+1/2}_{i-1/2, j+1/2} - M_{\text{source}_{y}}^{n+1/2} \Delta \right)
\]

\[
E_{z}^{n+1/2}_{i-1/2, j+1/2} = C_{a}(m) \left( E_{z}^{n-1/2}_{i-1/2, j+1/2} \right) + C_{b}(m) \cdot \left( H_{y}^{n}_{i, j+1/2} \right) - \left( H_{y}^{n}_{i-1, j+1/2} + H_{x}^{n}_{i-1/2, j} - H_{x}^{n}_{i-1/2, j+1} - J_{\text{source}_{z}}^{n} \Delta \right)
\]

\[
D_{a} \mid i, j, k = \left( 1 - \frac{\sigma_{i, j, k} \Delta t}{2 \mu_{i, j, k}} \right) / \left( 1 + \frac{\sigma_{i, j, k} \Delta t}{2 \mu_{i, j, k}} \right)
\]

\[
D_{b} \mid i, j, k = \left( \frac{\Delta t}{\mu_{i, j, k} \Delta_{1}} \right) / \left( 1 + \frac{\sigma_{i, j, k} \Delta t}{2 \mu_{i, j, k}} \right)
\]

\[
C_{a} \mid i, j, k = \left( 1 - \frac{\sigma_{i, j, k} \Delta t}{2 \varepsilon_{i, j, k}} \right) / \left( 1 + \frac{\sigma_{i, j, k} \Delta t}{2 \varepsilon_{i, j, k}} \right)
\]

\[
C_{b} \mid i, j, k = \left( \frac{\Delta t}{\varepsilon_{i, j, k} \Delta_{1}} \right) / \left( 1 + \frac{\sigma_{i, j, k} \Delta t}{2 \varepsilon_{i, j, k}} \right)
\]
FDTD Considerations

- Grid resolution affects …
  - Geometry discretization
  - Frequency resolution
  - Numerical phase velocity
  - Accuracy
  - Simulation speed

- Time step affects …
  - Numerical stability
  - Simulation speed

- Absorbing boundary conditions affects …
  - Non-physical reflections from computational domain
  - Accuracy
  - Simulation speed and computer memory requirements

- Meshing algorithm (staircased/conformal/nonorthogonal) affects …
  - Numerical stability
  - Complexity of programming
  - Accuracy
  - Simulation speed and computer memory requirements

Numerical phase velocity is anisotropic
Grid resolution affects numerical phase velocity

Variation of the normalized numerical phase velocity and attenuation per grid cell as a function of the grid sampling density ($1 \leq N \leq 10$) for a Courant stability factor $S = 0.5$
Numerical Phase Velocity Anisotropy

Variation of the numerical phase velocity with wave-propagation angle in a 2-D FDTD grid for three sampling densities of the square unit cells. $S = c \Delta t = 0.5$ for all cases.

Phase Velocity is lowest along horizontal and vertical directions.
Numerical Stability

- Complex issue based on boundary conditions, (un)structured meshing, lossy/dispersive materials.
- Courant condition must be satisfied in all cases that we will consider

1-d interpretation: Field energy may not transit through more than one complete mesh cell in a single time-step

\[
\begin{align*}
\Delta t &= \frac{\Delta x}{c} \\
\Delta t &= \frac{\Delta x}{c\sqrt{2}} \\
\Delta t &= \frac{\Delta x}{c\sqrt{3}}
\end{align*}
\]

\( \Delta x \) is the smallest mesh cell in the FDTD grid
Perfectly Matched Layer (PML)

PML($\sigma_{x1}, \sigma_{x1}^*, \sigma_{y2}, \sigma_{y2}^*$)

PML($0, 0, \sigma_{y2}, \sigma_{y2}^*$)

PML($\sigma_{x2}, \sigma_{x2}^*, \sigma_{y2}, \sigma_{y2}^*$)

PML($\sigma_{x1}, \sigma_{x1}^*, 0, 0$)

PML($\sigma_{x1}, \sigma_{x1}^*, \sigma_{y1}, \sigma_{y1}^*$)

PML($0, 0, \sigma_{y1}, \sigma_{y1}^*$)

PML($\sigma_{x2}, \sigma_{x2}^*, \sigma_{y1}, \sigma_{y1}^*$)

PEC

Wave source in vacuum

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PML: Wave Incidence Angle

Computational Domain

PML region

Source

Relative error vs. time (ns)

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PML Thickness

PML with various thicknesses surround antenna

Source

Probe point

$E_y$

$J_z$

100 mm

25 mm

Relative error

$10^{-2}$

$10^{-3}$

$10^{-4}$

$10^{-5}$

$10^{-6}$

$10^{-7}$

$10^{-8}$

$t$ (ns)

0

1

2

3

4

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FDTD Geometry Staircasing

- Significant deformations of the original geometry
- Inflexible meshing capabilities
- Standard FDTD edge is a single material
- FDTD grid cell is entirely inside or outside material

O(n^2) accuracy does not include meshing inaccuracies

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Non-Orthogonal Mesh

- Irregular, non-orthogonal grids offer the greatest geometric flexibility
- Finite element meshing algorithm
- Pre-existing reliable mesh generators from CFM solvers
- Maps boundaries much more precisely without requiring dense mesh
- Permits modeling of arbitrary objects with fine spatial features
- Reduces solution time due to fewer mesh cells
- No regular meshing structure necessitates complex methodology
Non-Orthogonal Algorithm

- B is orthogonal to cell face and is calculated from Maxwell’s equations
- H is collinear with cell edge and requires a projection operation
- Vector sum of B fields is calculated and averaged on the corners
- Resultant B field is projected onto non-orthogonal cell edge
- Unstable algorithm stabilized by creating a symmetric matrix update
- Non-physical term added to update eqns. degrades accuracy

Irregular mesh degrades solution accuracy

Non-orthogonal mesh dual grid
Locally Conformal Method

- Locally conformal meshes are the most reliable and proven methods
- Alters existing orthogonal FDTD grid
- Modifies edge lengths and areas only at intersection points
- Remainder of FDTD grid undisturbed
- Easy to implement with current FDTD electromagnetic solvers
- Difficult mesh generation
CP-FDTD Update Equations

- Typical update

\[ H_1^{n+1} = H_1^n + \frac{\Delta t}{\mu A_1} \left( \frac{E_{1Y}^{\frac{1}{2}} l_{1Y} - E_{2Y}^{\frac{1}{2}} l_{2Y}}{2} + E_{1X}^{\frac{1}{2}} l_{1X} - E_{2X}^{\frac{1}{2}} l_{2X} \right) \]

- Cell expansion

\[ H_1^{n+1} = H_1^n + \frac{\Delta t}{\mu (A_1 + A_2)} \left( E_{1Y}^{\frac{1}{2}} l_{1Y} - E_{2X}^{\frac{1}{2}} l_{2X} + E_{1X}^{\frac{1}{2}} (l_{1X} + l_{3X}) \right) \]

\[ E_{3X} = E_{1X} \]

- Instability issues resolved, but somewhat difficult to implement – simpler solutions exist.

Contour-Path Method, Jurgens and Taflove

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D-FDTD Update Equations

• **Typical update**

\[
H_1^{n+1} = H_1^n + \frac{\Delta t}{\mu A_1} \left( \frac{n+1}{2} E_{1Y}^2 l_{1Y} - \frac{n+1}{2} E_{2Y}^2 l_{2Y} \\
+ \frac{n+1}{2} E_{1X}^2 l_{1X} - \frac{n+1}{2} E_{2X}^2 l_{2X} \right)
\]

• **Stability criterion violated**

\[
\frac{n+1}{2} E_{1Y}^2 = \frac{n+1}{2} E_{1X}^2 = \frac{n+1}{2} E_{2Y}^2 = \frac{n+1}{2} E_{2X}^2 = 0
\]

Stability criterion restricts minimum cell area and maximum ratio of edge length to area.

D-FDTD reduces the number of mesh cells and does not severely effect the minimum time step.

Dey-Mitra FDTD (D-FDTD) method for PEC (IEEE MGW Letters September, 1997)

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Field Leakage

- Special consideration must be made to account for field leakage since grid edges do not lie along surface of geometry as in a non-orthogonal grid.

- D-FDTD update equation for $H_2$

$$H_2^{n+1} = H_2^n - \frac{\Delta t}{\mu A_1} \left( \frac{E_{2Y}^{n+1}}{2} * I_{2Y} + E_{2X}^{n+1} * I_{2X} \right)$$

- D-FDTD update for $E_{1Y}$ in the PEC

$$E_{1Y}^{n+\frac{1}{2}} = E_{1Y}^{n-\frac{1}{2}} + \frac{\Delta t}{\varepsilon \Delta x} \left( H_1^n - H_2^n \right)$$

Partial edge lengths allow fields to pass through boundary of geometry into PEC
D-FDTD Results

• 3-D cylindrical resonator tilted at angles ranging from 0 to 45 degrees in the FDTD grid is compared with simple staircased mesh.

Error of the dominant mode resonant frequency

Electric wall

Locally conformal mesh

(IEEE MTT Railton C., Schneider J., Jan., 1999)

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Slow-wave Structures: Twisted Resonators

- Slow-wave structure can be designed by twisting waveguide.
- Phase velocity can be controlled by pitch of the twist.

Floquet’s theorem explicitly shows the relationship with the fields at a given location in a periodic structure to the fields a period away.

\[ \overline{E}(r, z, t) = \sum_{n=-\infty}^{\infty} a_n(r)e^{j{\beta_o + \frac{2\pi n}{L}}z}e^{j\omega t} \]

\[ \overline{E_z}(r, z, t) = \sum_{n=-\infty}^{\infty} E_nJ_0(K_n r)e^{j(\omega t - \beta_n z)} \]
Twisted Resonator: Rectangular

Fundamental and higher order mode resonant frequency errors at $\lambda/20$ resolution

Twisted rectangular resonator

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Twisted Resonator: Elliptical

- Elliptical cross-section not easily meshed with cubical FDTD grid
- Conformal algorithms well suited to geometry

Fundamental mode resonant frequency error with grid resolutions from $\lambda/8$ to $\lambda/32$
MAFIA™ does not use conformal meshing algorithm.

Smoothly twisted waveguide can not be modeled by staircasing.

Stacked disk, twisted waveguide approximates actual design.

Stacked notch resonator

Fundamental and higher order mode resonant frequency errors

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Twisted Resonator: Smooth Notch

- Requires a conformal algorithm to model accurately.
- FEA and locally conformal meshes can be used to evaluate actual waveguide geometry.
- Typical mesh in D-FDTD for a four-period twisted notched waveguide included 50,000 modified FDTD grid edges.
- Mesh created in 5 minutes.
- Efficient and accurate results.

FEA solver HFSS™ v. 8.0 required 500 MB of memory and 4 hours for the solution of a 3-period twisted waveguide to retrieve 20 modes.

D-FDTD requires 20 MB of memory and 30 minutes for the same solution and retrieved frequency data across 5 GHz bandwidth.

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• Write a Matlab or C-program that models 1-D x-directed plane-wave propagation in a uniform FDTD Yee grid using the necessary 2-D equations described for the TMz mode (assume Hx=0).
  – Assume material with sigma=1e-3, and use the time step dt=dx/c.
  – Terminate the grid in Ez components at its far-left and far-right boundaries.
  – Source the grid with an Ez field at the far-left boundary with a 1GHz sinusoid to create a rightward-propagating wave.
  – Set Ez=0 at the far-right boundary to simulate PEC. Perform visualizations of the field components within the grid at a number of time snapshots before and after the propagating wave reaches the far-right grid boundary.
  – Set the time step to dt=1.01*dx/c. Compare results.
  – Repeat the previous experiment using H=0 at the right boundary and note the differences.