Computational Science:
Introduction to Finite-Difference Time-Domain

Review & Walkthrough of One-Dimensional FDTD

Lecture #8 – Outline

- Formulation
  - Prepare Maxwell's equations
  - Finite-difference approximations
  - Reduction to one dimension
  - Derivation of Update Equations
  - Bells and whistles
    - Grid resolution, time step, sources, boundary conditions, Fourier transforms, transmittance and reflectance
- Implementation
- Sequence for Code Development
- Walkthrough

Formulation of 1D FDTD

Prepare Maxwell's Equations

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Normalize the Magnetic Field $\vec{H}$

The divergence equations were satisfied by adopting the Yee grid scheme. Only the curl equations remain to deal with.

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

The $\vec{E}$ and $\vec{H}$ fields are two to three orders of magnitude different. This may cause rounding errors in a simulation and it is always good practice to normalize parameters so they are all the same order of magnitude. Here the magnetic field is the one normalized.

$$\vec{\tilde{H}} = \sqrt{\frac{\mu_0}{\varepsilon_0}}\vec{H} \quad \Rightarrow \quad \nabla \times \vec{E} = -\frac{[\mu_r]}{c_0}\frac{\partial \vec{\tilde{H}}}{\partial t} \qquad \nabla \times \vec{\tilde{H}} = \frac{[\varepsilon_r]}{c_0}\frac{\partial \vec{E}}{\partial t}$$

Note: $c_0 = \dfrac{1}{\sqrt{\mu_0 \varepsilon_0}}$

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Expand the Curl Equations

$$\nabla \times \vec{E} = -\frac{[\mu_r]}{c_0}\frac{\partial \vec{\tilde{H}}}{\partial t} \quad \Rightarrow \quad \begin{aligned} \frac{\partial E_z}{\partial y} - \frac{\partial E_y}{\partial z} &= -\frac{\mu_{xx}}{c_0}\frac{\partial \tilde{H}_x}{\partial t} \\ \frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x} &= -\frac{\mu_{yy}}{c_0}\frac{\partial \tilde{H}_y}{\partial t} \\ \frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} &= -\frac{\mu_{zz}}{c_0}\frac{\partial \tilde{H}_z}{\partial t} \end{aligned}$$

$$\nabla \times \vec{\tilde{H}} = \frac{[\varepsilon_r]}{c_0}\frac{\partial \vec{E}}{\partial t} \quad \Rightarrow \quad \begin{aligned} \frac{\partial \tilde{H}_z}{\partial y} - \frac{\partial \tilde{H}_y}{\partial z} &= \frac{\varepsilon_{xx}}{c_0}\frac{\partial E_x}{\partial t} \\ \frac{\partial \tilde{H}_x}{\partial z} - \frac{\partial \tilde{H}_z}{\partial x} &= \frac{\varepsilon_{yy}}{c_0}\frac{\partial E_y}{\partial t} \\ \frac{\partial \tilde{H}_y}{\partial x} - \frac{\partial \tilde{H}_x}{\partial y} &= \frac{\varepsilon_{zz}}{c_0}\frac{\partial E_z}{\partial t} \end{aligned}$$

Here it is assumed linear and non-dispersive materials with diagonal tensors.

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Formulation of 1D FDTD

Finite-Difference Approximations

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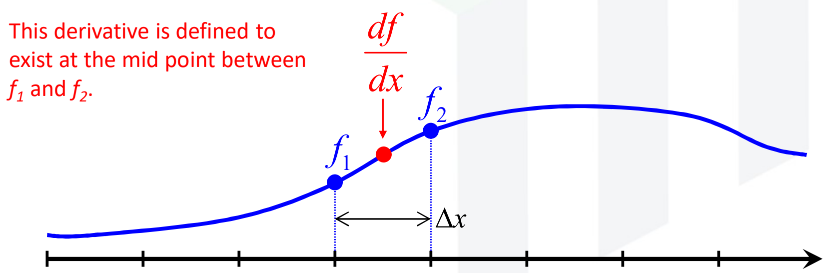
Finite-Difference Approximations

$$\frac{df_{1.5}}{dx} \approx \frac{f_2 - f_1}{\Delta x}$$

second-order accurate first-order derivative



Finite-Difference Approximation of Time Derivatives

All of the derivatives in Maxwell's equations are approximated with finite-differences.

$$\nabla \times \vec{E} = -\frac{[\mu_r]}{c_0}\frac{\partial \vec{\tilde{H}}}{\partial t} \quad \Rightarrow \quad \nabla \times \vec{E}\Big|_t \cong -\frac{[\mu_r]}{c_0}\frac{\vec{\tilde{H}}\Big|_{t+\Delta t/2} - \vec{\tilde{H}}\Big|_{t-\Delta t/2}}{\Delta t}$$

$$\nabla \times \vec{\tilde{H}} = \frac{[\varepsilon_r]}{c_0}\frac{\partial \vec{E}}{\partial t} \quad \Rightarrow \quad \nabla \times \vec{\tilde{H}}\Big|_{t+\Delta t/2} \cong \frac{[\varepsilon_r]}{c_0}\frac{\vec{E}\Big|_{t+\Delta t} - \vec{E}\Big|_t}{\Delta t}$$

The electric and magnetic fields are staggered in time by $\Delta t/2$ so that every term in the finite-difference equations exists at the same instant in time.

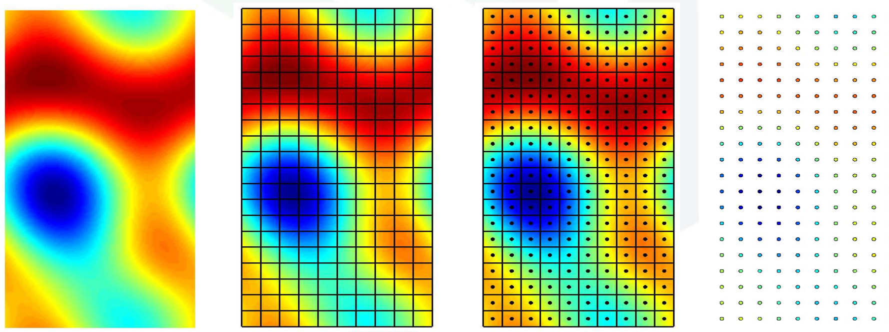
Representing Functions on a Grid

Example physical (continuous) 2D function

A grid is constructed by dividing space into discrete cells

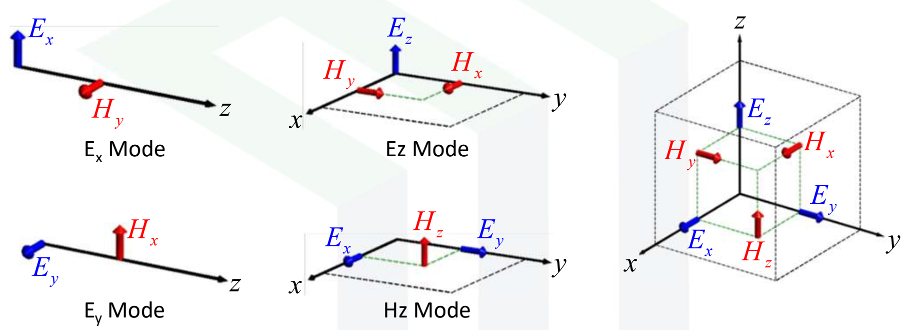
Function is known only at discrete points

Representation of what is actually stored in memory



Yee Cell for 1D, 2D, and 3D Grids

1D Yee Grid **2D Yee Grids** **3D Yee Grid**



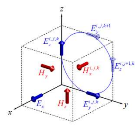
<u>Benefits</u>
- Implicitly satisfies divergence equations
- Naturally handles physical boundary conditions
- Elegant approximation of the curl equations using finite-differences

<u>Consequences</u>
- Field components are in physically different locations
- Field components may reside in different materials even if they are in the same unit cell
- Field components will be out of phase

Finite-Difference Approximations on a Yee Grid

Finite-Difference Equation for H_x

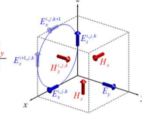
$$\frac{\partial E_z}{\partial y} - \frac{\partial E_y}{\partial z} = -\frac{\mu_{xx}}{c_0}\frac{\partial \tilde{H}_x}{\partial t}$$



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

Finite-Difference Equation for H_y

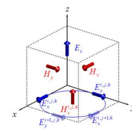
$$\frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x} = -\frac{\mu_{yy}}{c_0}\frac{\partial \tilde{H}_y}{\partial t}$$



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

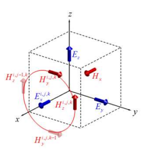
Finite-Difference Equation for H_z

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



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

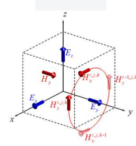
Finite-Difference Equation for E_x



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

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

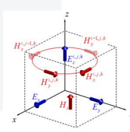
Finite-Difference Equation for E_y



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

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

Finite-Difference Equation for E_z



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

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

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Formulation of 1D FDTD

Reduction to One Dimension

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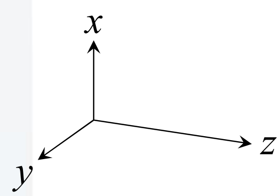
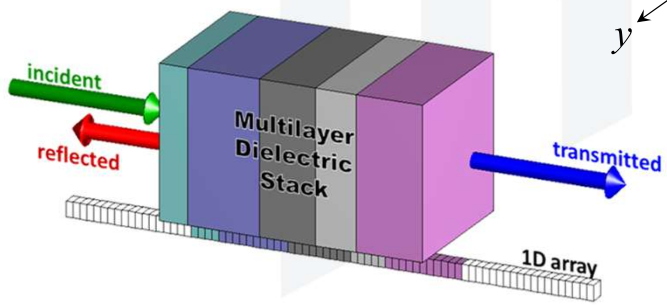
Reduction to One Dimension

It was observed in previous lectures that some problems composed of dielectric slabs can be described in just one dimension. In this case, the materials and the fields are uniform in two directions. Derivatives in these uniform directions will be zero. We will define the uniform directions to be the x and y axes.

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





x and y Derivatives are Zero

The spatial derivatives were approximated with finite-differences on a Yee grid.

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

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

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

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

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

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

$\Rightarrow$

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

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

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

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

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

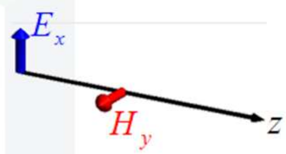
$$\cancel{\frac{\tilde{H}_y\big|_{t+\frac{\Delta t}{2}}^{i,j,k} - \tilde{H}_y\big|_{t+\frac{\Delta t}{2}}^{i-1,j,k}}{\Delta x}} - \cancel{\frac{\tilde{H}_x\big|_{t+\frac{\Delta t}{2}}^{i,j,k} - \tilde{H}_x\big|_{t+\frac{\Delta t}{2}}^{i,j-1,k}}{\Delta y}} = \frac{\varepsilon_{zz}\big|^{i,j,k}}{c_0}\frac{E_z\big|_{t+\Delta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

Summary of 1D FDTD Modes

E_x/H_y Mode

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

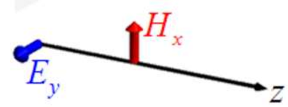
$$-\frac{\tilde{H}_y\big|_{t+\frac{\Delta t}{2}}^{k} - \tilde{H}_y\big|_{t+\frac{\Delta t}{2}}^{k-1}}{\Delta z} = \frac{\varepsilon_{xx}\big|^k}{c_0}\frac{E_x\big|_{t+\Delta t}^{k} - E_x\big|_t^{k}}{\Delta t}$$



E_y/H_x Mode

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

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



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Formulation of 1D FDTD

Derivation of Update Equations

E_y/H_x Mode: Update Equation for E_y

Start with the finite-difference equation which has E_y in the time-derivative:

$$\frac{\left.\tilde{H}_x\right|_{t+\frac{\Delta t}{2}}^{k}-\left.\tilde{H}_x\right|_{t+\frac{\Delta t}{2}}^{k-1}}{\Delta z}=\frac{\left.\varepsilon_{yy}\right|^{k}}{c_0}\frac{\left.E_y\right|_{t+\Delta t}^{k}-\left.E_y\right|_{t}^{k}}{\Delta t}$$

Solve this for the field at the future time value.

$$\frac{\left.\varepsilon_{yy}\right|^{k}}{c_0}\frac{\left.E_y\right|_{t+\Delta t}^{k}-\left.E_y\right|_{t}^{k}}{\Delta t}=\frac{\left.\tilde{H}_x\right|_{t+\frac{\Delta t}{2}}^{k}-\left.\tilde{H}_x\right|_{t+\frac{\Delta t}{2}}^{k-1}}{\Delta z}$$

$$\left.E_y\right|_{t+\Delta t}^{k}-\left.E_y\right|_{t}^{k}=\frac{c_0\Delta t}{\left.\varepsilon_{yy}\right|^{k}}\left(\frac{\left.\tilde{H}_x\right|_{t+\frac{\Delta t}{2}}^{k}-\left.\tilde{H}_x\right|_{t+\frac{\Delta t}{2}}^{k-1}}{\Delta z}\right)$$

$$\left.E_y\right|_{t+\Delta t}^{k}=\left.E_y\right|_{t}^{k}+\left(\frac{c_0\Delta t}{\left.\varepsilon_{yy}\right|^{k}}\right)\left(\frac{\left.\tilde{H}_x\right|_{t+\frac{\Delta t}{2}}^{k}-\left.\tilde{H}_x\right|_{t+\frac{\Delta t}{2}}^{k-1}}{\Delta z}\right)$$

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E_y/H_x Mode: Update Equation for H_x

Start with the finite-difference equation which has H_x in the time-derivative:

$$-\frac{\left.E_y\right|_{t}^{k+1}-\left.E_y\right|_{t}^{k}}{\Delta z}=-\frac{\left.\mu_{xx}\right|^{k}}{c_0}\frac{\left.\tilde{H}_x\right|_{t+\frac{\Delta t}{2}}^{k}-\left.\tilde{H}_x\right|_{t-\frac{\Delta t}{2}}^{k}}{\Delta t}$$

Solve this for the field at the future time value.

$$-\frac{\left.\mu_{xx}\right|^{k}}{c_0}\frac{\left.\tilde{H}_x\right|_{t+\frac{\Delta t}{2}}^{k}-\left.\tilde{H}_x\right|_{t-\frac{\Delta t}{2}}^{k}}{\Delta t}=-\frac{\left.E_y\right|_{t}^{k+1}-\left.E_y\right|_{t}^{k}}{\Delta z}$$

$$\left.\tilde{H}_x\right|_{t+\frac{\Delta t}{2}}^{k}-\left.\tilde{H}_x\right|_{t-\frac{\Delta t}{2}}^{k}=\frac{c_0\Delta t}{\left.\mu_{xx}\right|^{k}}\left(\frac{\left.E_y\right|_{t}^{k+1}-\left.E_y\right|_{t}^{k}}{\Delta z}\right)$$

$$\left.\tilde{H}_x\right|_{t+\frac{\Delta t}{2}}^{k}=\left.\tilde{H}_x\right|_{t-\frac{\Delta t}{2}}^{k}+\left(\frac{c_0\Delta t}{\left.\mu_{xx}\right|^{k}}\right)\left(\frac{\left.E_y\right|_{t}^{k+1}-\left.E_y\right|_{t}^{k}}{\Delta z}\right)$$

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Update Equations and Update Coefficients

The update coefficients do not change their value during the simulation. They should be computed only once before the main FDTD loop and not at each iteration inside the loop.

The finite-difference equations in terms of the update coefficients are:

$$\tilde{H}_x\Big|_{t+\frac{\Delta t}{2}}^{k} = \tilde{H}_x\Big|_{t-\frac{\Delta t}{2}}^{k} + \left(m_{Hx}\Big|^{k}\right)\left(\frac{E_y\Big|_t^{k+1} - E_y\Big|_t^{k}}{\Delta z}\right)$$

$$E_y\Big|_{t+\Delta t}^{k} = E_y\Big|_t^{k} + \left(m_{Ey}\Big|^{k}\right)\left(\frac{\tilde{H}_x\Big|_{t+\frac{\Delta t}{2}}^{k} - \tilde{H}_x\Big|_{t+\frac{\Delta t}{2}}^{k-1}}{\Delta z}\right)$$

$$m_{Ey}\Big|^{k} = \frac{c_0 \Delta t}{\varepsilon_{yy}\Big|^{k}} \qquad m_{Hx}\Big|^{k} = \frac{c_0 \Delta t}{\mu_{xx}\Big|^{k}}$$

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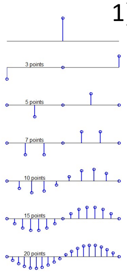
Formulation of 1D FDTD

Bells and Whistles

Computing Grid Resolution

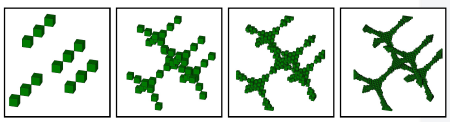
1) Resolve Wavelength



$$\lambda_{\min} = \frac{c_0}{f_{\max} n_{\max}}$$

$$\Delta_\lambda \approx \frac{\lambda_{\min}}{N_\lambda} \qquad N_\lambda \geq 10$$

2) Resolve Features



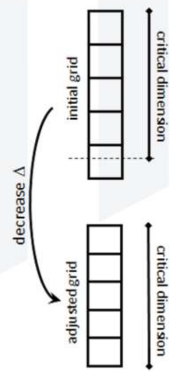
$N_d << 1$ $\quad N_d < 1$ $\quad N_d = 1$ $\quad N_d = 4$

$$\Delta_d \approx \frac{d_{\min}}{N_d} \qquad N_d \geq 1$$

3) Initial Resolution

$$\Delta' = \min\left[\Delta_\lambda, \Delta_d\right]$$

4) "Snap" Grid to Critical Dimensions



$$N = \text{ceil}\left(d_c / \Delta'\right)$$

$$\Delta = d_c / N$$

Computing the Time Step Δt

Generalized Courant Stability Condition

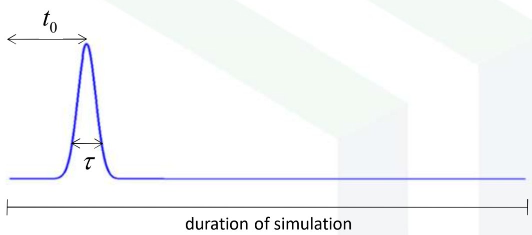
$$\Delta t < \frac{n_{\min}}{c_0 \sqrt{\frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2} + \frac{1}{(\Delta z)^2}}}$$

For 1D Grids with Perfectly Absorbing Boundary Condition

$$\Delta t = \frac{n_{\text{bc}} \Delta z}{2 c_0} \qquad n_{\text{bc}} \equiv \text{refractive index at boundaries}$$

The Gaussian Source

The Gaussian source approximates an impulse so that a structure can be characterized over an enormous range of frequencies in a single simulation.



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

$$\tau \cong \frac{0.5}{f_{\max}} \qquad t_0 \approx 6\tau$$

Estimating Total Number of Iterations

Total Simulation Time

$$T = 12\tau + 5t_{\text{prop}}$$

$$t_{\text{prop}} = \frac{n_{\max} N_z \Delta z}{c_0} \equiv$$ time it takes for a wave to propagate across the grid one time.

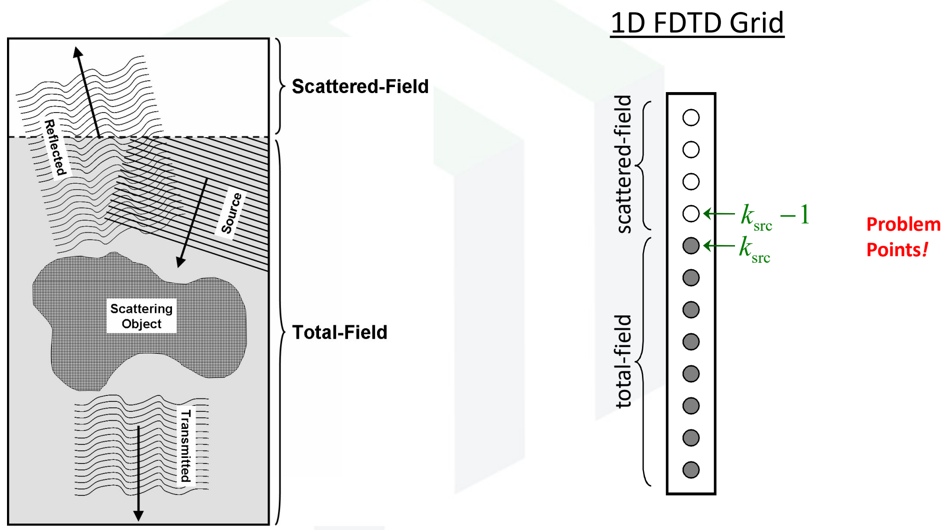
- $5t_{\text{prop}}$: Allow for 5 bounces. Highly resonant devices will need much more.
- 12τ: Allow for the entire pulse without cutting it off.

Total Number of Iterations

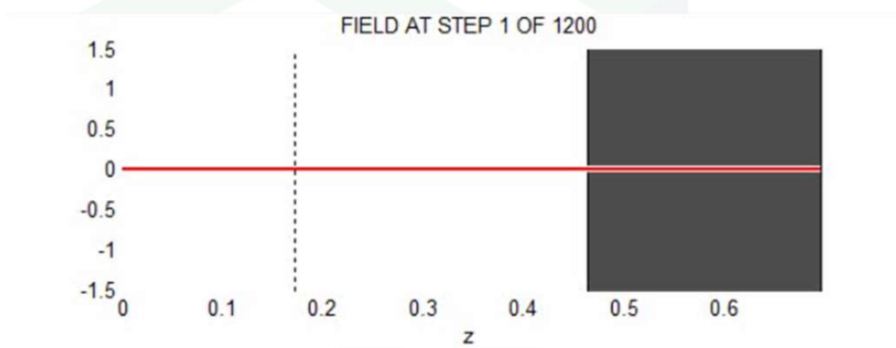
$$\text{STEPS} = \text{round}\uparrow\left[\frac{T}{\Delta t}\right]$$

This must be an integer quantity.

The Total-Field/Scattered-Field Framework



Animation of TF/SF in 1D-FDTD



Correction to Finite-Difference Equations at the Problem Cells (1 of 2)

On the scattered-field side of the TF/SF interface, the finite-difference equation contains a term from the total-field side. Due to the staggered nature of the Yee grid, this only occurs in the update equation for a magnetic field.

$$\tilde{H}_x\Big|_{t+\frac{\Delta t}{2}}^{k_{src}-1} = \tilde{H}_x\Big|_{t-\frac{\Delta t}{2}}^{k_{src}-1} + \left(m_{Hx}\Big|^{k_{src}-1}\right)\left[\frac{E_y\Big|_t^{k_{src}} - E_y\Big|_t^{k_{src}-1}}{\Delta z}\right]$$

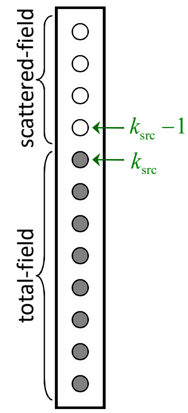
This is an equation in the scattered-field, but $E_y^{k_{src}}$ is a total-field quantity.

Subtract the source from $E_y^{k_{src}}$ to make it look like a scattered-field quantity.

$$\tilde{H}_x\Big|_{t+\frac{\Delta t}{2}}^{k_{src}-1} = \tilde{H}_x\Big|_{t-\frac{\Delta t}{2}}^{k_{src}-1} + \left(m_{Hx}\Big|^{k_{src}-1}\right)\left[\frac{\left(E_y\Big|_t^{k_{src}} - E_y^{src}\Big|_t^{k_{src}}\right) - E_y\Big|_t^{k_{src}-1}}{\Delta z}\right]$$

$$\underbrace{\tilde{H}_x\Big|_{t+\frac{\Delta t}{2}}^{k_{src}-1} = \tilde{H}_x\Big|_{t-\frac{\Delta t}{2}}^{k_{src}-1} + \left(m_{Hx}\Big|^{k_{src}-1}\right)\left[\frac{E_y\Big|_t^{k_{src}} - E_y\Big|_t^{k_{src}-1}}{\Delta z}\right]}_{\text{standard update equation}} - \frac{\left(m_{Hx}\Big|^{k_{src}-1}\right)}{\Delta z} E_y^{src}\Big|_t^{k_{src}}$$

This is a correction term that can be implemented after the standard update equation to inject a source.



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Correction to Finite-Difference Equations at the Problem Cells (2 of 2)

On the total-field side of the TF/SF interface, the finite-difference equation contains a term from the scattered-field side. Due to the staggered nature of the Yee grid, this only occurs in the update equation for an electric field.

$$E_y\Big|_{t+\Delta t}^{k_{src}} = E_y\Big|_t^{k_{src}} + \left(m_{Ey}\Big|^{k_{src}}\right)\left[\frac{\tilde{H}_x\Big|_{t+\frac{\Delta t}{2}}^{k_{src}} - \tilde{H}_x\Big|_{t+\frac{\Delta t}{2}}^{k_{src}-1}}{\Delta z}\right]$$

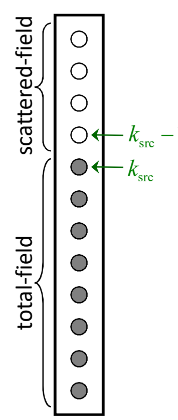
This is an equation in the scattered-field, but $\tilde{H}_x^{k_{src}-1}$ is a total-field quantity.

Add the source to $\tilde{H}_x^{k_{src}-1}$ to make it look like a total-field quantity.

$$E_y\Big|_{t+\Delta t}^{k_{src}} = E_y\Big|_t^{k_{src}} + \left(m_{Ey}\Big|^{k_{src}}\right)\left[\frac{\tilde{H}_x\Big|_{t+\frac{\Delta t}{2}}^{k_{src}} - \left(\tilde{H}_x\Big|_{t+\frac{\Delta t}{2}}^{k_{src}-1} + \tilde{H}_x^{src}\Big|_{t+\frac{\Delta t}{2}}^{k_{src}-1}\right)}{\Delta z}\right]$$

$$\underbrace{E_y\Big|_{t+\Delta t}^{k_{src}} = E_y\Big|_t^{k_{src}} + \left(m_{Ey}\Big|^{k_{src}}\right)\left[\frac{\tilde{H}_x\Big|_{t+\frac{\Delta t}{2}}^{k_{src}} - \tilde{H}_x\Big|_{t+\frac{\Delta t}{2}}^{k_{src}-1}}{\Delta z}\right]}_{\text{standard update equation}} - \frac{\left(m_{Ey}\Big|^{k_{src}}\right)}{\Delta z} \tilde{H}_x^{src}\Big|_{t+\frac{\Delta t}{2}}^{k_{src}-1}$$

This is a correction term that can be implemented after the standard update equation to inject a source.



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The Two Source Terms

From the previous slides, it is known that to calculate two source functions before the main FDTD loop. These are:

$$\tilde{H}_x^{\text{src}}\Big|_{t+\frac{\Delta t}{2}}^{k_{\text{src}}-1} \qquad E_y^{\text{src}}\Big|_{t}^{k_{\text{src}}}$$

A few observations must be accounted for before these source functions can be calculated correctly.

1. The amplitude of these functions can be different as $\vec{E}$ and $\vec{H}$ are related through the material impedance.
2. These functions are a half grid cell apart and have a small time delay between them
3. These functions exist at different time steps.

Calculation of the Source Functions

E_x/H_y Mode

We calculate the electric field as

$$E_x^{\text{src}}\Big|_{t}^{k_{\text{src}}} = g(t)$$

We calculate the magnetic field as

$$\tilde{H}_y^{\text{src}}\Big|_{t+\frac{\Delta t}{2}}^{k_{\text{src}}-1} = \sqrt{\frac{\varepsilon_r^{(k_{\text{src}})}}{\mu_r^{(k_{\text{src}})}}}\, g\left(t + \frac{n_{\text{src}}\Delta z}{2c_0} - \frac{\Delta t}{2}\right)$$

Amplitude due to Maxwell's equations

Delay through one half of a grid cell

Half time step difference

E_y/H_x Mode

We calculate the electric field as

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

We calculate the magnetic field as

$$\tilde{H}_x^{\text{src}}\Big|_{t+\frac{\Delta t}{2}}^{k_{\text{src}}-1} = -\sqrt{\frac{\varepsilon_r^{(k_{\text{src}})}}{\mu_r^{(k_{\text{src}})}}}\, g\left(t + \frac{n_{\text{src}}\Delta z}{2c_0} + \frac{\Delta t}{2}\right)$$

Amplitude due to Maxwell's equations

Delay through one half of a grid cell

Half time step difference

$\mu_{\text{r,src}},\ \varepsilon_{\text{r,src}},\ n_{\text{src}} \equiv$ material properties where source is injected

Dirichlet Boundary Condition

Dirichlet boundary conditions assume that all field quantities outside of the grid are zero.

The update equations are modified as follows.

$$\tilde{H}_x^k\Big|_{t+\frac{\Delta t}{2}} = \tilde{H}_x^k\Big|_{t-\frac{\Delta t}{2}} + m_{Hx}^k\left(\frac{E_y^{k+1}\big|_t - E_y^k\big|_t}{\Delta z}\right) \qquad k < N_z$$

$$\tilde{H}_x^{N_z}\Big|_{t+\frac{\Delta t}{2}} = \tilde{H}_x^{N_z}\Big|_{t-\frac{\Delta t}{2}} + m_{Hx}^{N_z}\left(\frac{0 - E_y^{N_z}\big|_t}{\Delta z}\right) \qquad k = N_z$$

$$E_y^k\Big|_{t+\Delta t} = E_y^k\Big|_t + m_{Ey}^k\left(\frac{\tilde{H}_x^k\big|_{t+\frac{\Delta t}{2}} - \tilde{H}_x^{k-1}\big|_{t+\frac{\Delta t}{2}}}{\Delta z}\right) \qquad k > 1$$

$$E_y^1\Big|_{t+\Delta t} = E_y^1\Big|_t + m_{Ey}^1\left(\frac{\tilde{H}_x^1\big|_{t+\frac{\Delta t}{2}} - 0}{\Delta z}\right) \qquad k = 1$$

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Perfectly Absorbing Boundary Condition

Conditions

- Waves at the boundaries are only travelling outward.
- Materials at the boundaries are linear, homogeneous, isotropic and non-dispersive.
- Time step is chosen so physical waves travel 1 cell in two time steps.
  $\Delta t = n\Delta z/(2c_0)$

Implementation at z-Low Boundary

At the z-low boundary, only the E-field update equation is modified.

$$h_2 = h_1 \qquad h_1 = \tilde{H}_x\Big|_{t+\frac{\Delta t}{2}}^1 \qquad E_y\Big|_{t+\Delta t}^1 = E_y\Big|_t^1 + m_{Ey}^k\left(\frac{\tilde{H}_x\big|_{t+\frac{\Delta t}{2}}^1 - h_2}{\Delta z}\right)$$

Implementation at z-High Boundary

At the z-high boundary, only the H-field update equation is modified.

$$e_2 = e_1 \qquad e_1 = E_y\Big|_t^{N_z} \qquad \tilde{H}_x^{N_z}\Big|_{t+\frac{\Delta t}{2}} = \tilde{H}_x^{N_z}\Big|_{t-\frac{\Delta t}{2}} + m_{Hx}^k\left(\frac{e_2 - E_y\big|_t^{N_z}}{\Delta z}\right)$$

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Efficient Fourier Transform (1 of 2)

The standard Fourier transform is defined as

$$F(f) = \int_{-\infty}^{\infty} f(t) e^{-j2\pi ft} dt$$

If the function $f(t)$ is only known at discrete points, the Fourier transform can be approximated numerically as

$$F(f) \cong \sum_{m=1}^{M} f(m\Delta t) e^{-j2\pi fm\Delta t} \Delta t$$

$M \equiv$ Total number of time steps

$m \equiv$ time step

This can be written in a slightly different form.

$$F(f) \cong \Delta t \sum_{m=1}^{M} \left(e^{-j2\pi f \Delta t} \right)^m \cdot f(m\Delta t)$$

Example

$\Delta t = 33.3564$ ps

$f = 1.0000$ GHz

$K = 0.9781 - i0.2081$

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Efficient Fourier Transform (2 of 2)

The final form on the previous slide suggests an efficient implementation. The Fourier transform is updated every iteration so by the end of the main loop:

$$F(f) \cong \Delta t \sum_{m=1}^{M} \left(e^{-j2\pi f \Delta t} \right)^m \cdot f(m)$$

This multiplication can be done after the main FDTD loop in a post-processing step.

This is simply the field value of interest at the current time step.

$e^{-j2\pi f \Delta t}$

This "kernel" can be computed prior to the main FDTD loop for each frequency of interest. The kernels can be stored in a 1D array.

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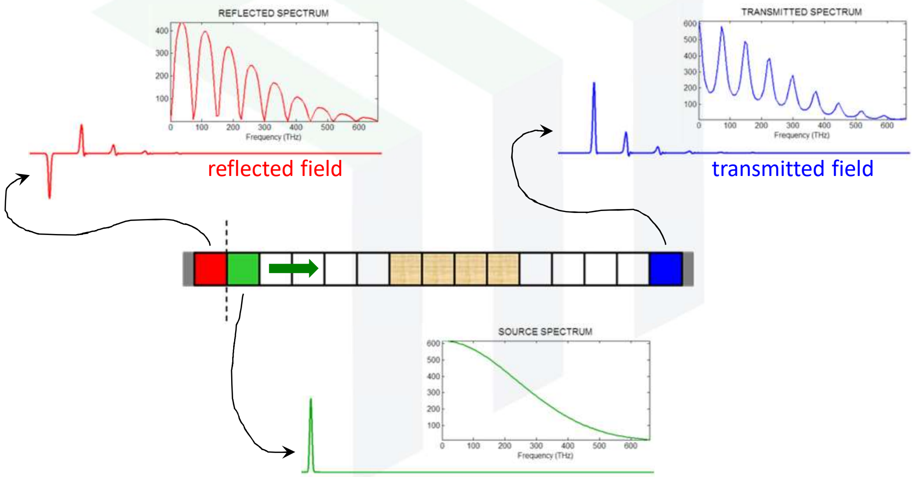
Fourier Transforms in FDTD

The easiest, but least memory efficient, method to compute a Fourier transform is to perform a simulation and record the desired field as a function of time. After the simulation is finished, these functions can be Fourier transformed using an FFT.



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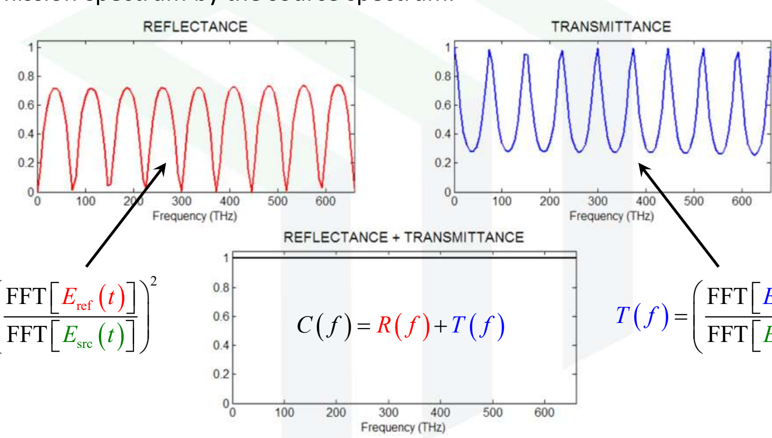
Post-Processing the Fourier Transforms

The spectra must be normalized to calculate transmittance and reflectance. This is done by dividing the reflection and transmission spectrum by the source spectrum.



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

$$C(f)=R(f)+T(f)$$

$$T(f)=\left(\frac{\mathrm{FFT}\left[E_{\mathrm{trn}}(t)\right]}{\mathrm{FFT}\left[E_{\mathrm{src}}(t)\right]}\right)^2$$

It is ALWAYS good practice to check for energy conservation by adding the reflectance and transmittance and ensuring the sum equals 100% (assuming no loss or gain in your device).

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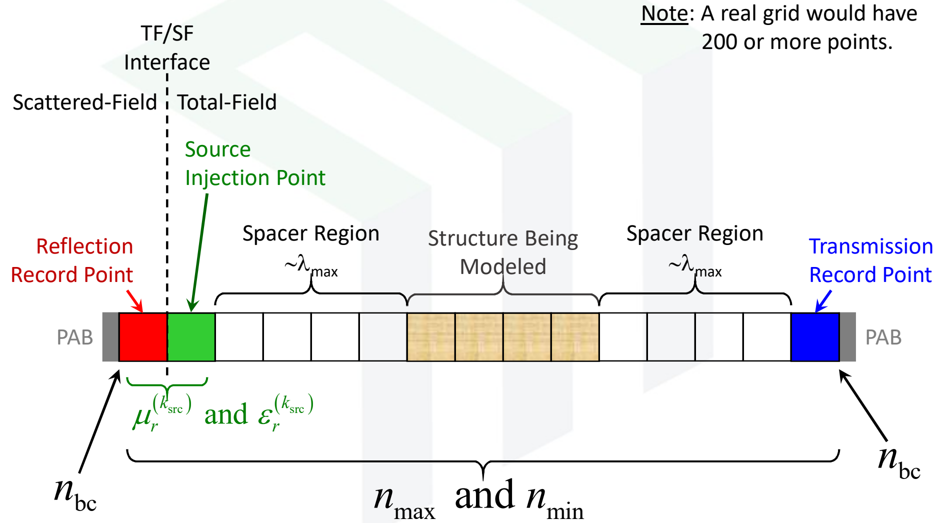
Implementation of 1D FDTD

1D-FDTD Grid

Note: A real grid would have 200 or more points.



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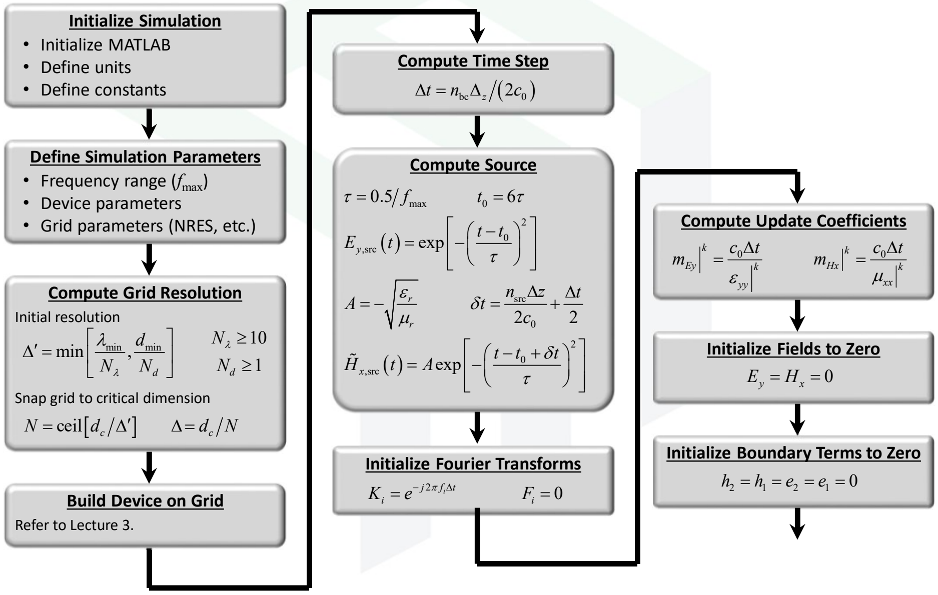
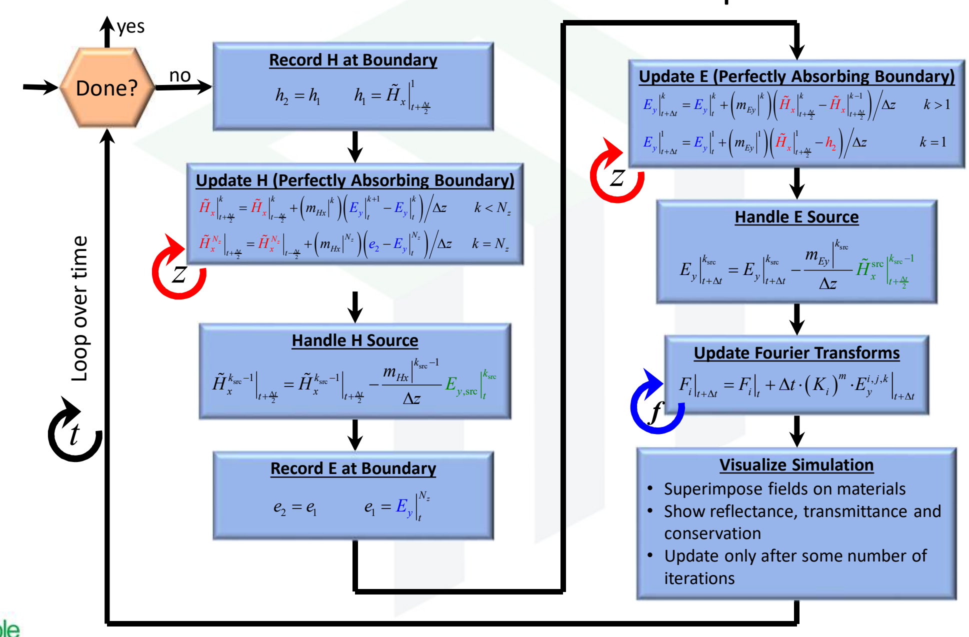
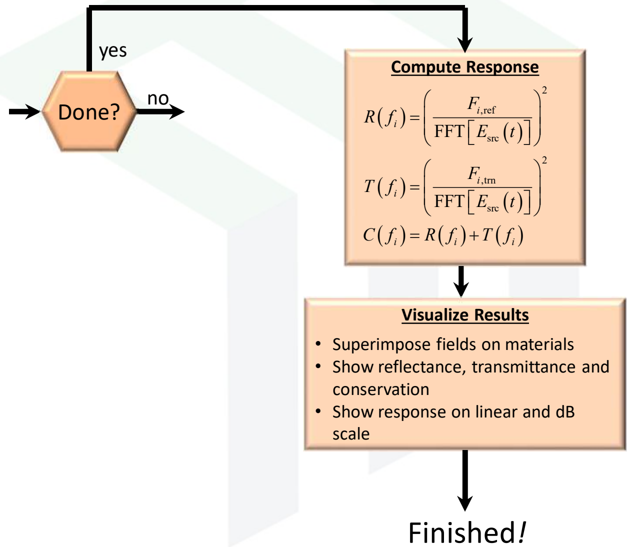
Initializing the FDTD Simulation



The Main FDTD Loop



Post Processing



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Sequence for Code Development

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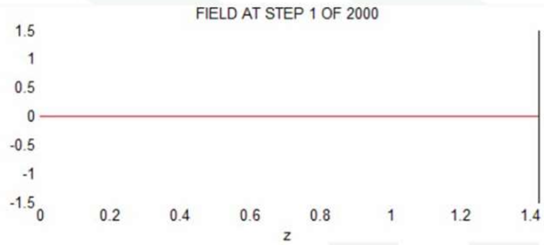
Step 1 – Basic FDTD Algorithm

- Basic update equations



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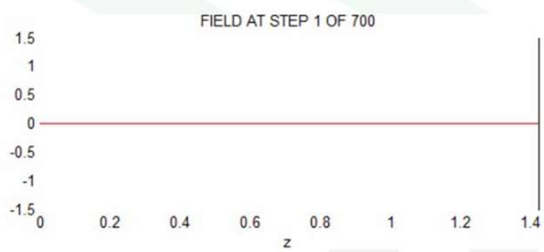
Step 2 – Add Soft Source

- Basic update equations
- Add a soft source



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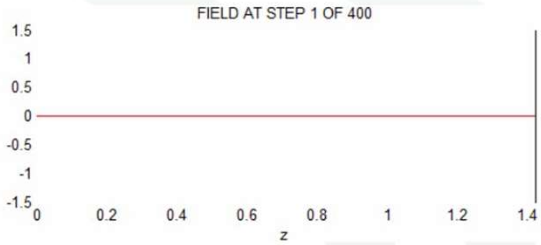
Step 3 – Add Absorbing Boundary



- Basic update equations
- Add a soft source
- Add perfect boundary condition

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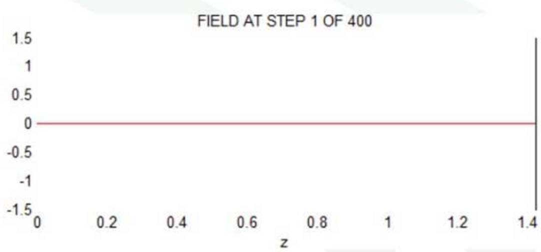
Step 4 – Add TF/SF



- Basic update equations
- Add a soft source
- Add perfect boundary condition
- Incorporate TF/SF “one-way” source

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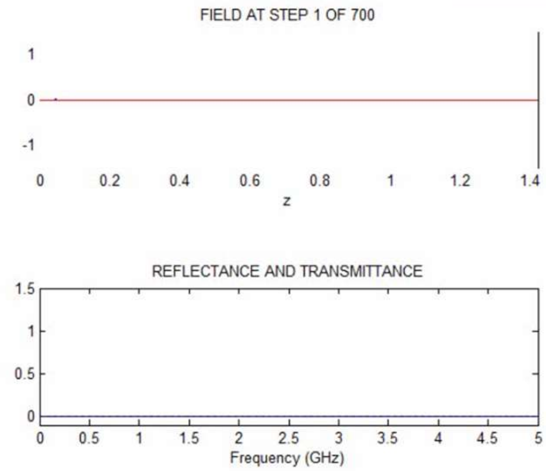
Step 5 – Move Source & Add T/R



- Basic update equations
- Add a soft source
- Add perfect boundary condition
- Incorporate TF/SF "one-way" source
- Move position of source
- Calculate transmittance and reflectance

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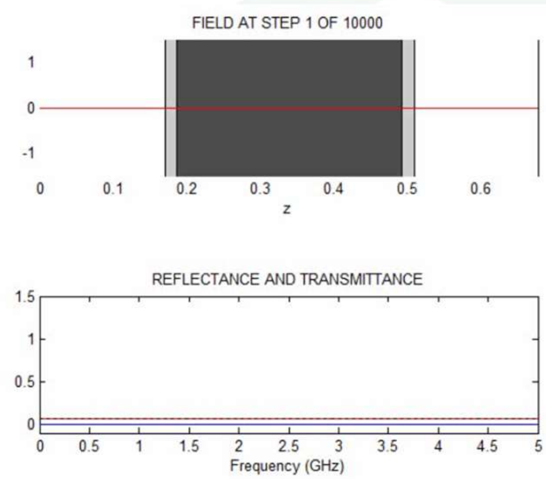
Step 6 – Add Device (Complete Algorithm)



- Basic update equations
- Add a soft source
- Add perfect boundary condition
- Incorporate TF/SF "one-way" source
- Move position of source
- Calculate transmittance and reflectance
- Add a real device

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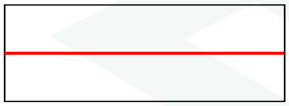
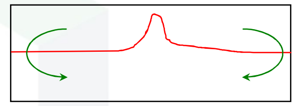
Summary of Code Development Sequence

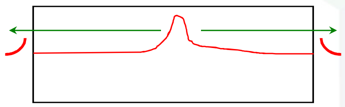
Step 1 – Implement basic FDTD algorithm



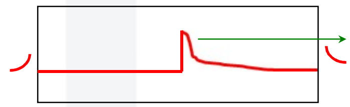
Step 2 – Add the source



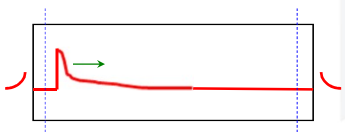
Step 3 – Add absorbing boundary



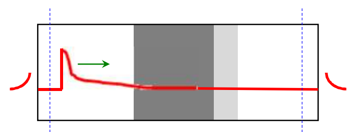
Step 4 – Add "one-way" source



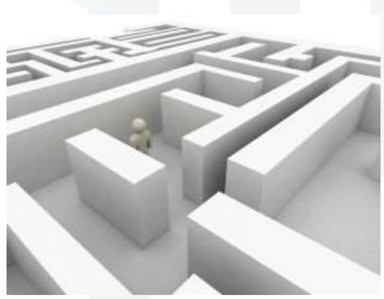
Step 5 – Calculate transmittance and reflectance



Step 6 – Add a device



FDTD Analysis Walkthrough



Outline of Steps for FDTD Analysis

- Step 1: Define problem
  - What device are you modeling?
  - What is its geometry?
  - What materials is it made of?
  - What do you want to learn about the device?
- Step 2: Initialize FDTD
  - Compute grid resolution
  - Assign materials values to points on the grid
  - Compute time step
  - Initialize Fourier transforms
- Step 3: Run FDTD
- Step 4: Post-process the data

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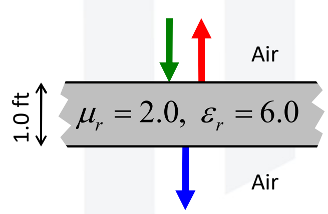
Step 1: Define the Problem

What device are you modeling? –A dielectric slab
What is its geometry? –1 foot thick slab
What materials it is made from? –μ_r=2.0, ε_r=6.0 (outside is air)
What do you want to learn? –reflectance and transmittance from 0 to 1 GHz



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Step 2: Compute Grid (1 of 2)

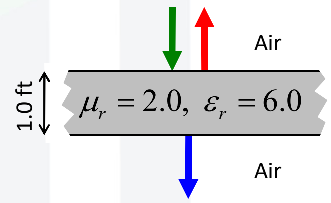
Initial Grid Resolution (Wavelength)

$$N_\lambda = 20$$

$$n_{max} = \sqrt{\mu_r \varepsilon_r} = \sqrt{(2.0)(6.0)} = 3.46$$

$$\lambda_{min} = \frac{c_0}{f_{max} n_{max}} = \frac{299792458 \ \frac{m}{s}}{(1.0 \text{ GHz})(3.46)} = 8.6543 \text{ cm}$$

$$\Delta_\lambda = \frac{\lambda_{min}}{N_\lambda} = \frac{8.6543 \text{ cm}}{20} = 0.4327 \text{ cm}$$



Initial Grid Resolution (Structure)

$$N_d = 4$$

$$\Delta_d = \frac{d}{N_d} = \frac{30.48 \text{ cm}}{4} = 7.6200 \text{ cm}$$

Initial Grid Resolution (Overall)

$$\Delta z' = \min[\Delta_\lambda, \Delta_d] = 0.4327 \text{ cm}$$

Step 2: Compute Grid (2 of 2)

Snap Grid to Critical Dimension(s)

The number of grid cells representing the thickness of the dielectric slab is

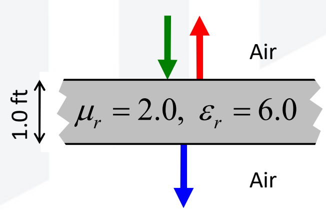
$$N' = \frac{d_c}{\Delta z'} = \frac{30.48 \text{ cm}}{0.4327 \text{ cm}} = 70.44 \text{ cells}$$

It is impossible to represent the thickness of the slab exactly with this grid resolution.

To represent the thickness of the slab exactly, we round *N'* up to the nearest integer and then calculate the grid resolution based on this quantity.

$$N = \text{round}\uparrow[N'] = 71 \text{ cells}$$

$$\Delta z = \frac{d_c}{N} = \frac{30.48 \text{ cm}}{71} = 0.4293 \text{ cm}$$



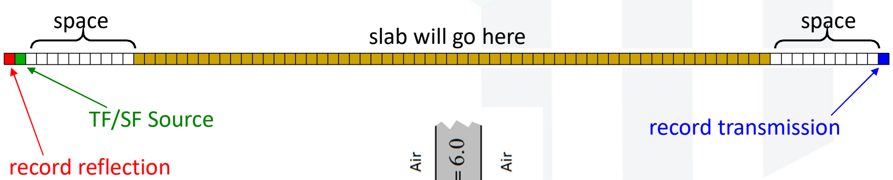
Step 2: Build Device on the Grid (1 of 2)

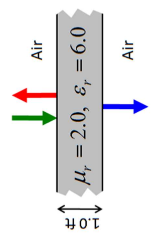
Determine Size of Grid

We need to have enough grid cells to fit the device being modeled, some space on either side of the device (10 cells for now), and cells for injecting the source and recording transmitted and reflected fields.

$$N_z = 71 + 2(10 \text{ cells}) + 3 = 94 \text{ cells}$$

- TRN/REF/SRC cells
- spacer regions
- cells for device





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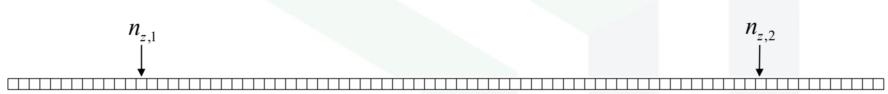
Step 2: Build Device on the Grid (2 of 2)

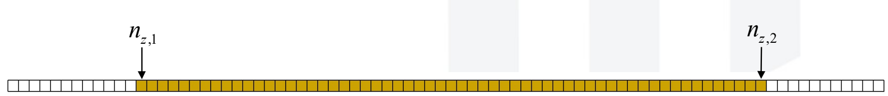
Compute Position of Materials on Grid

$$n_{z,1} = 2 + 10 + 1 = 13$$

$$n_{z,2} = n_{z,1} + \text{round}[d/\Delta z] - 1 = 13 + 71 - 1 = 83$$



Add Materials to Grid




```
UR(nz1:nz2) = ur;
ER(nz1:nz2) = er;
```

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Step 2: Initialize FDTD (1 of 2)

Compute the Time Step Δt

$$\Delta t = \frac{n_{bc}\Delta z}{2c_0} = \frac{(1.0)(0.4293\text{ cm})}{2(299792458\ \frac{m}{s})} = 7.1599\times10^{-12}\text{ sec}$$

Compute Source Parameters t_0 and τ

$$\tau = \frac{1}{2f_{max}} = \frac{1}{2(1\text{ GHz})} = 5.00\times10^{-10}\text{ sec}$$

$$t_0 = 6\tau = 3.00\times10^{-9}\text{ sec}$$

$\boxed{t_0 = 6\tau}$ Rule of thumb

Compute Number of Time Steps, STEPS

$$t_{prop} = \frac{n_{max}N_z\Delta z}{c_0} = \frac{(3.46)(94)(0.4293\text{ cm})}{(299792458\ \frac{m}{s})} = 4.6629\times10^{-9}\text{ sec}$$

Time it takes a wave to propagate across the grid.

$$T = 12\tau + 5t_{prop} = 12(5\times10^{-10}\text{ s}) + 5(4.6597\times10^{-9}\text{ s}) = 2.9314\times10^{-8}\text{ sec}$$

$$\text{STEPS} = \text{round}\uparrow\left[\frac{T}{\Delta t}\right] = 4095$$

$\boxed{T = 12\tau + 5t_{prop}}$ Rule of thumb

STEPS must be an integer

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Step 2: Initialize FDTD (2 of 2)

Compute the Source Functions for E_y/H_x Mode

$$\delta t = \frac{n_{src}\Delta z}{2c_0} + \frac{\Delta t}{2} = \frac{3\Delta t}{2} = 1.0740\times10^{-11}\text{ sec}$$

$$A = -\sqrt{\frac{\varepsilon_r^{(k_{src})}}{\mu_r^{(k_{src})}}} = -\sqrt{\frac{1.0}{1.0}} = -1$$

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

$$\tilde{H}_x(t) = A\exp\left[-\left(\frac{t-t_0+\delta t}{\tau}\right)^2\right]$$

```
% COMPUTE GAUSSIAN SOURCE FUNCTIONS
t       = [0:STEPS-1]*dt;                     %time axis
delt    = nsrc*dz/(2*c0) + dt/2;              %total delay between E and H
A       = - sqrt(ersrc/ursrc);                %amplitude of H field
Esrc    = exp(-((t-t0)/tau).^2);              %E field source
Hsrc    = A*exp(-((t-t0+delt)/tau).^2);       %H field source
```

Initialize the Fourier Transforms

```
% INITIALIZE FOURIER TRANSFORMS
NFREQ = 100;
FREQ  = linspace(0,1*gigahertz,NFREQ);
K     = exp(-i*2*pi*dt.*FREQ);
REF   = zeros(1,NFREQ);
TRN   = zeros(1,NFREQ);
SRC   = zeros(1,NFREQ);
```

Frequency, f	Kernel, K
0.0 MHz	1.0
50.5 MHz	1.0 - i0.0023
202.0 MHz	1.0 - i0.0091
747.5 MHz	0.9994 - i0.0336
1.0 GHz	0.9990 - i0.0450

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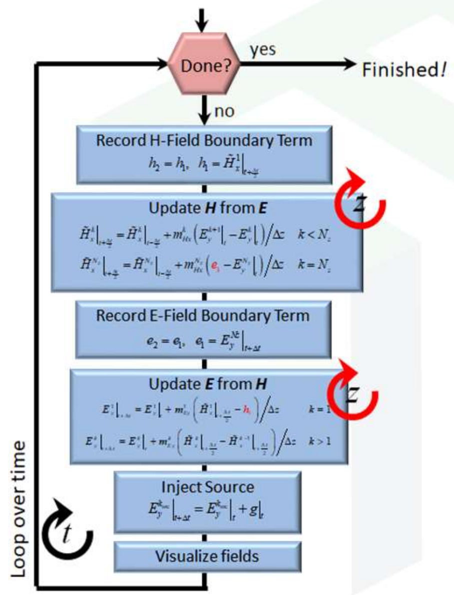
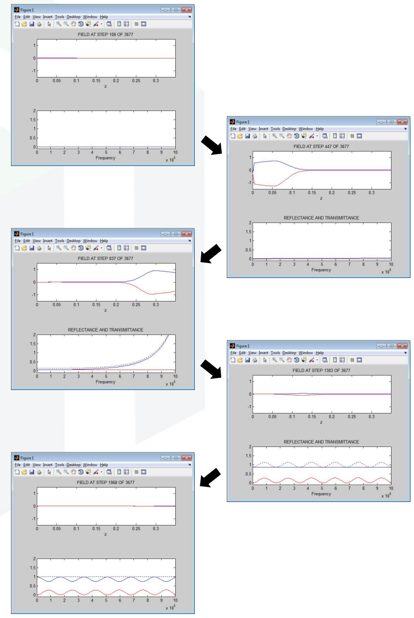
Step 3: Run FDTD (3 of 3)





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Step 4: Post-Process the Data

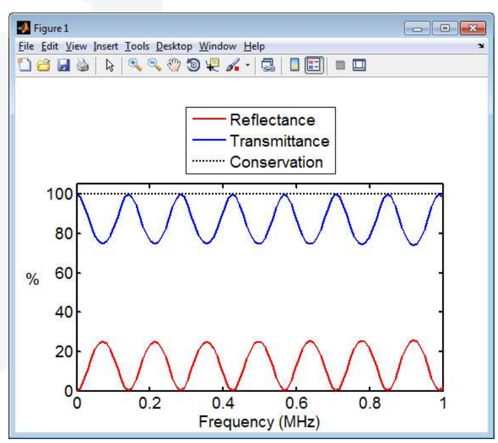
Normalize the Data to the Source Spectrum

$$R(f)=\left(\frac{F_{\text{ref}}(f)}{\text{FFT}\left[E_{\text{src}}(t)\right]}\right)^2$$

$$T(f)=\left(\frac{F_{\text{trn}}(f)}{\text{FFT}\left[E_{\text{src}}(t)\right]}\right)^2$$

$$C(f)=R(f)+T(f)$$

```
% COMPUTE REFLECTANCE
% AND TRANSMITTANCE
REF = abs(REF./SRC).^2;
TRN = abs(TRN./SRC).^2;
CON = REF + TRN;
```



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