



Computational Science:
Introduction to Finite-Difference Time-Domain

Learning From One-Dimensional FDTD

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Lecture Outline

- Review of Lecture 6
- Total-Field/Scattered-Field Soft Source
- Fourier Transform
- Reflectance and Transmittance
- Displaying the Results

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Review

Slide 3

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Dirichlet Boundary Condition

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

The update equations are modified as follows.

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

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

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

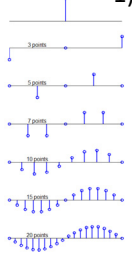
$$E_y^k \Big|_{t+\Delta t} = E_y^k \Big|_t + m_{Ey}^k \left(\frac{\tilde{H}_x^1 \Big|_{t+\frac{\Delta z}{2}} - 0}{\Delta z} \right) \quad k = 1$$

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Computing Grid Resolution

1) Resolve Wavelength



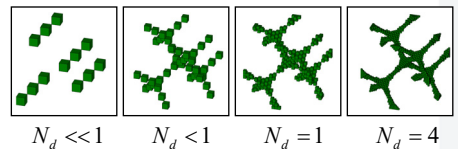
$$\lambda_{\min} = \frac{c_0}{f_{\max} n_{\max}}$$

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

3) Initial Resolution

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

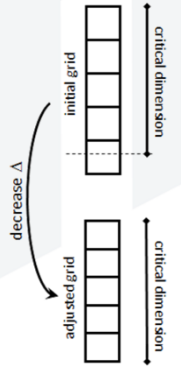
2) Resolve Features



$N_d \ll 1$ $N_d < 1$ $N_d = 1$ $N_d = 4$


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

4) "Snap" Grid to Critical Dimensions



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

$$\Delta = d_c / N$$

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Courant Stability Condition

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

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

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Perfectly Absorbing Boundary Condition

Necessary Conditions

- Waves at the boundaries are only travelling outward.
- Materials at the boundaries are linear, homogeneous, isotropic and non-dispersive.
- Refractive index must be the same about both boundaries.
- 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, we need only modify the E-field update equation.

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

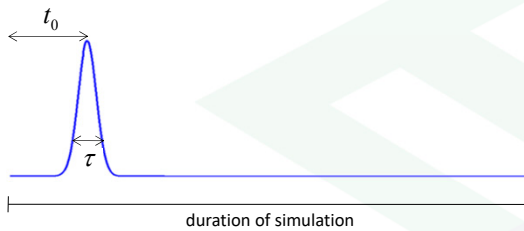
Implementation at z-High Boundary

At the z-high boundary, we need only modify the H-field update equation.

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

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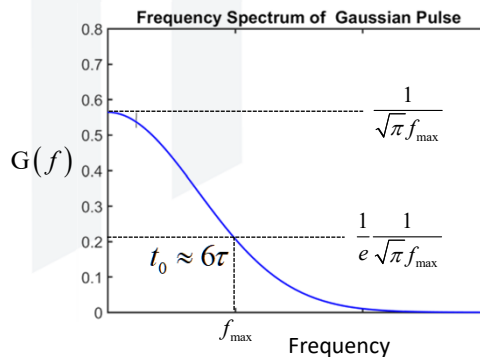
The Gaussian Source



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

$$\tau \cong \frac{0.5}{f_{\max}}$$

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



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Estimating Total Number of Iterations

Total Simulation Time

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

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

Allow for 3-5 bounces.
Highly resonant devices will need much more.

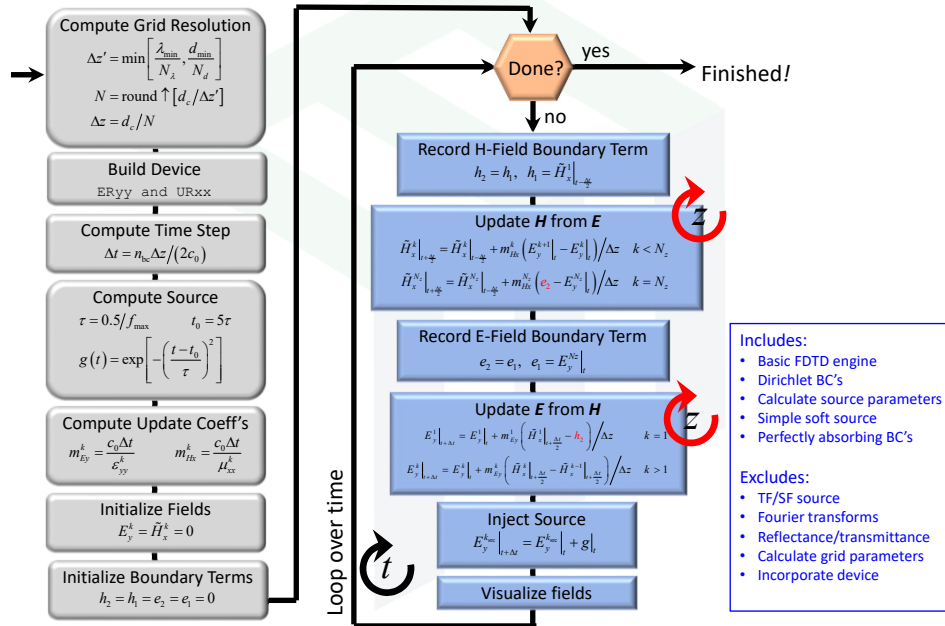
Allow for the entire pulse without cutting it off.

Total Number of Iterations

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

This must be an integer quantity.

Revised FDTD Algorithm



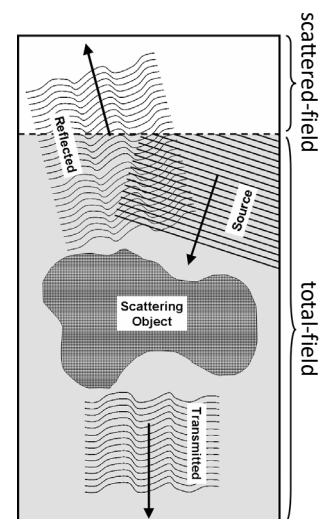
Total-Field/Scattered-Field Field Soft Source

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Total-Field / Scattered-Field

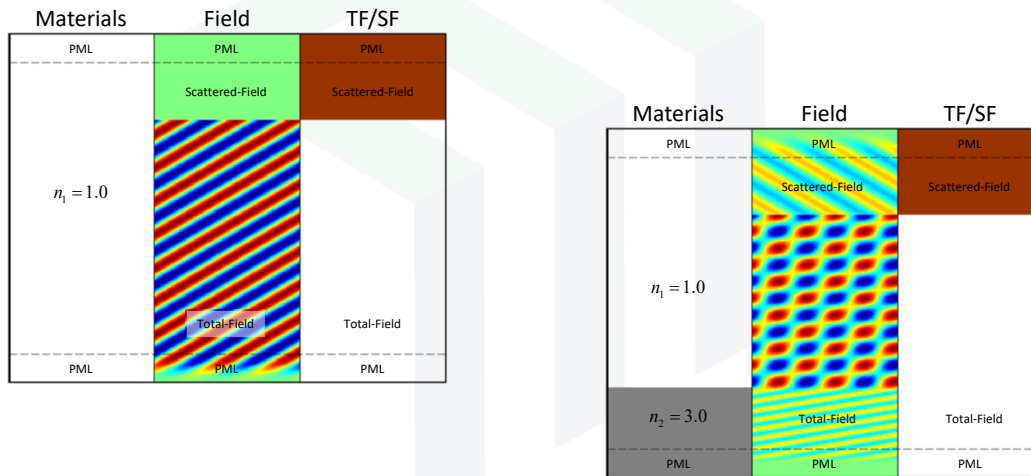
- The total-field/scattered-field (TF/SF) is a technique to inject a “one-way” source.
- Benefits
 - Eliminates backward propagating waves
 - Ensures waves at the boundaries are only travelling outward
 - 100% of power injected by the source is incident on the device being simulated.



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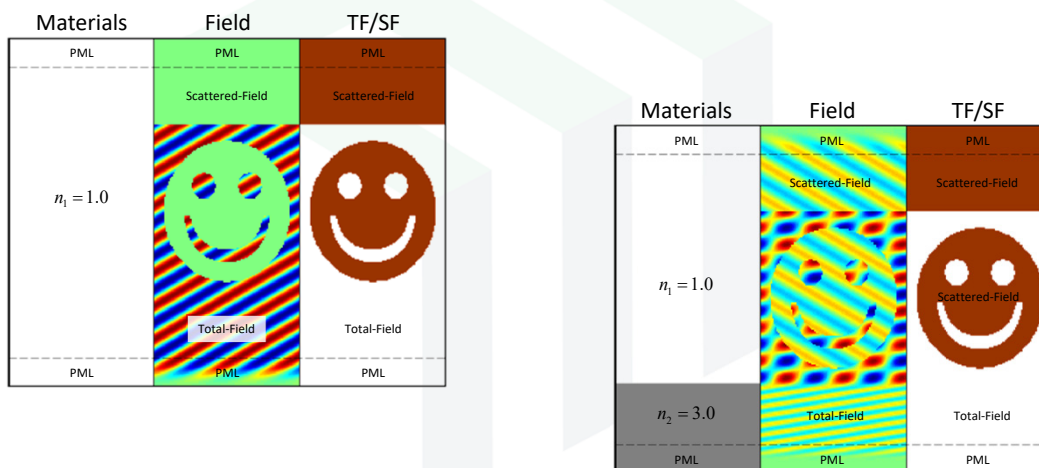
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Example Simulation #1



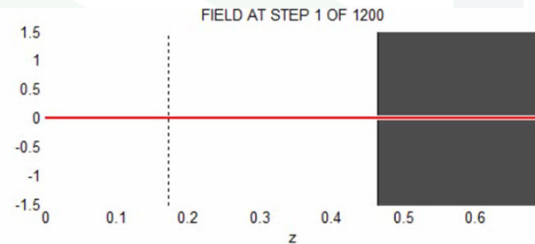
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Example Simulation #2



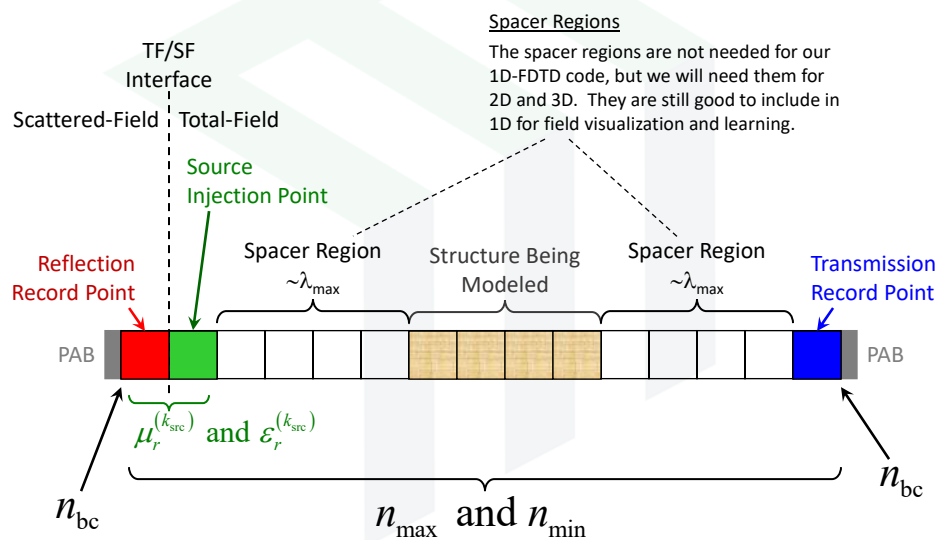
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Animation of TF/SF in 1D-FDTD



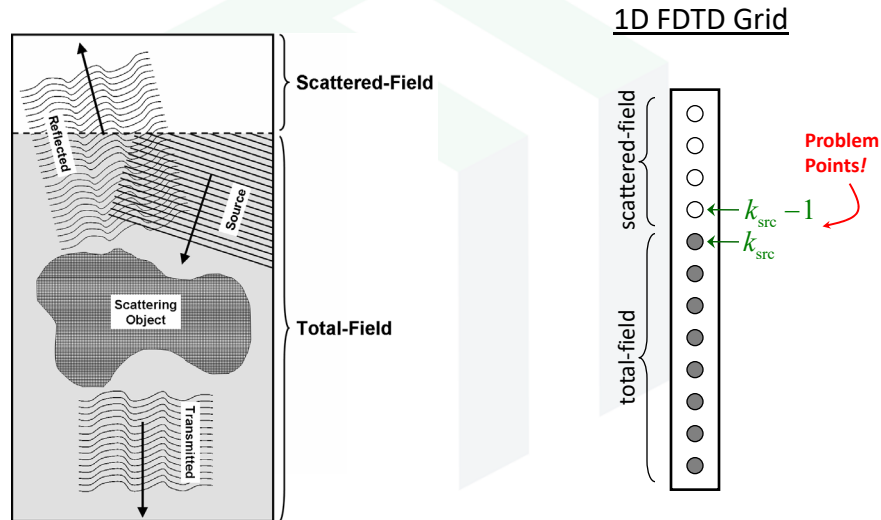
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1D-FDTD Grid Strategy



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The Total-Field/Scattered-Field Framework



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.

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

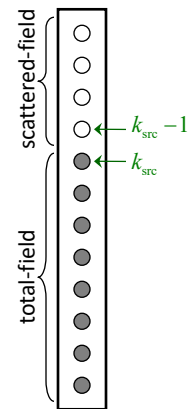
This is an equation in the scattered-field, but $E_y^{k_{src}}$ is a total-field quantity.

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

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

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

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



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.

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

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

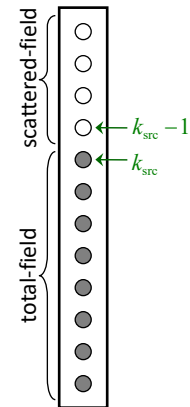
Add the source to $\tilde{H}_x^{k_{\text{src}}-1}$ to make it look like a total-field quantity.

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

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

standard update equation

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



The Two Source Terms

From the previous slides, two source functions must be calculated before entering the main FDTD loop. These are:

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

A few observations must be accounted for before we can calculate these source functions 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.

Amplitude of the \vec{H} Field (1 of 3)

Assuming the source is injected inside a homogeneous material, the fields must be plane waves. The electric field has the form:

$$E_y(t) = \sin(\omega t - \beta z)$$

We must find the amplitude A and phase ϕ of the magnetic field relative to the electric field. In general, the magnetic field can be written as

$$\tilde{H}_x(t) = A \sin(\omega t - \beta z - \phi)$$

Amplitude of the \vec{H} Field (2 of 3)

Substitute the sine wave expressions into Maxwell's equations...

$$\frac{\partial \tilde{H}_x(t)}{\partial z} = \frac{\epsilon_r}{c_0} \frac{\partial E_y(t)}{\partial t}$$

$$\frac{\partial}{\partial z} A \sin(\omega t - \beta z - \phi) = \frac{\epsilon_r}{c_0} \frac{\partial}{\partial t} \sin(\omega t - \beta z)$$

$$-\beta A \cos(\omega t - \beta z - \phi) = \frac{\omega \epsilon_r}{c_0} \cos(\omega t - \beta z)$$

In order for this equation to be true, the follow two equations must be satisfied. Recall that $\beta = \omega \sqrt{\mu \epsilon}$ and $c_0 = 1/\sqrt{\mu_0 \epsilon_0}$.

$$-\beta A = \frac{\omega \epsilon_r}{c_0} \quad A = -\frac{\omega \epsilon_r}{\beta c_0} = -\sqrt{\frac{\epsilon_r}{\mu_r}} \quad \phi = 0$$

Amplitude of the \vec{H} Field (3 of 3)

The answer for the E_y/H_x mode is

$$A_{EyHx} = -\sqrt{\frac{\epsilon_{r,src}}{\mu_{r,src}}} \quad \phi_{EyHx} = 0$$

We could similarly show for the E_x/H_y mode that

$$A_{ExHy} = \sqrt{\frac{\epsilon_{r,src}}{\mu_{r,src}}} \quad \phi_{ExHy} = 0$$

IMPORTANT:

The permittivity $\epsilon_{r,src}$ and permeability $\mu_{r,src}$ in these equations are the material properties where the source is to be injected.

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Calculation of the Source Functions

E_x/H_y Mode

We calculate the electric field as

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

We calculate the magnetic field as

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

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

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

We calculate the magnetic field as

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

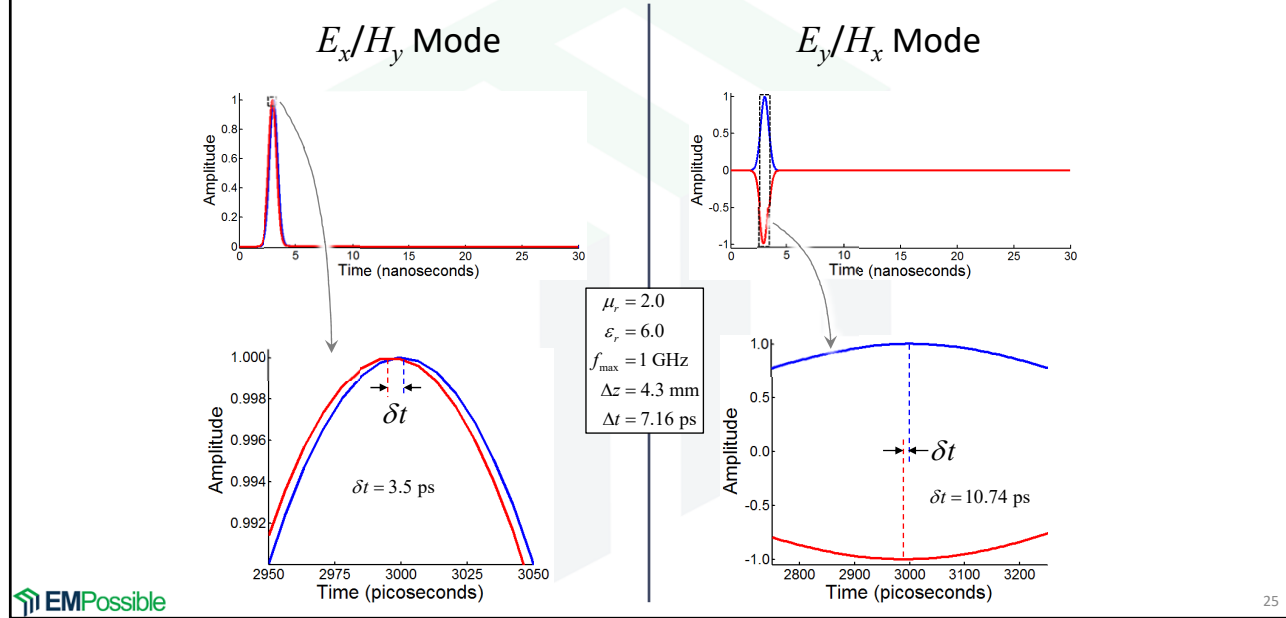
Amplitude due to
Maxwell's equations

Delay through one
half of a grid cell

Half time step
difference

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Visualizing the Source Functions



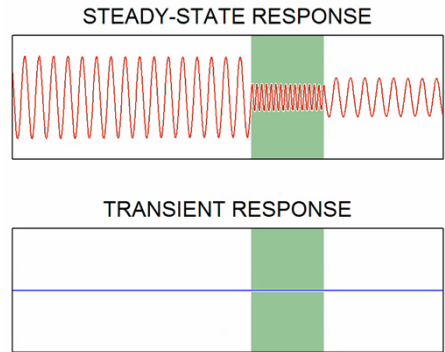
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Fourier Transforms

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Recall Transient Vs. Steady-State



The steady-state response is the Fourier transform of the transient response.

Steady-State Response

$$H(\omega) = \text{FFT} \{h(t)\}$$

What is being plotted?

$$\text{Re}[H(\omega)e^{j\omega t}]$$

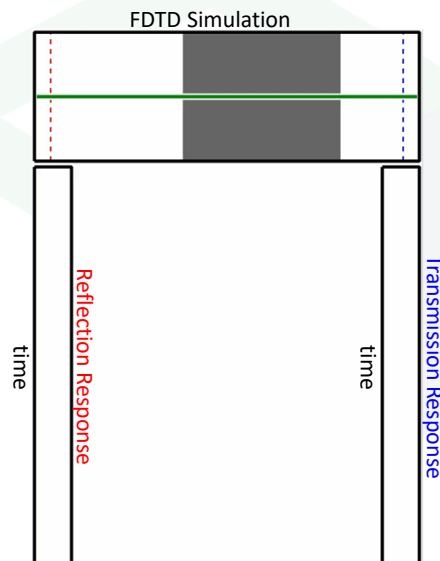
Transient Response

$$h(t) = \text{FFT}^{-1} \{H(\omega)\}$$

What is being plotted?

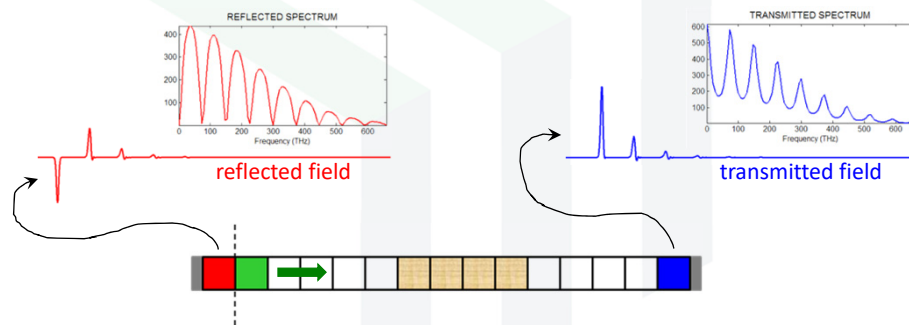
$$h(t)$$

Recording the Reflection and Transmission Responses



Brute Force Fourier Transforms

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.



Storing the response functions is seldom done because it can require a lot of memory, especially when the response is recorded at many points on the grid.

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

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

$M \equiv$ total number of time steps

$m \equiv$ integer time step

This can be written in a slightly different form.

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

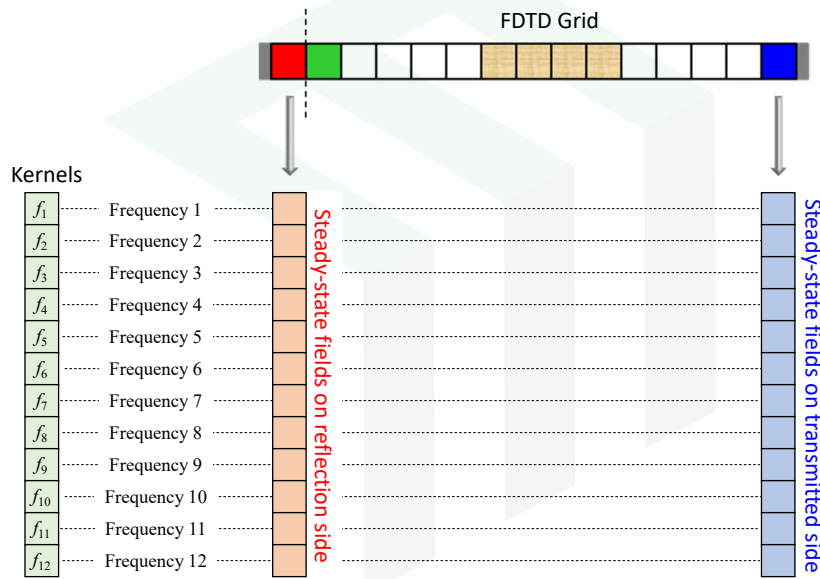
Example

$\Delta t = 33.3564$ ps

$f = 1.0000$ GHz

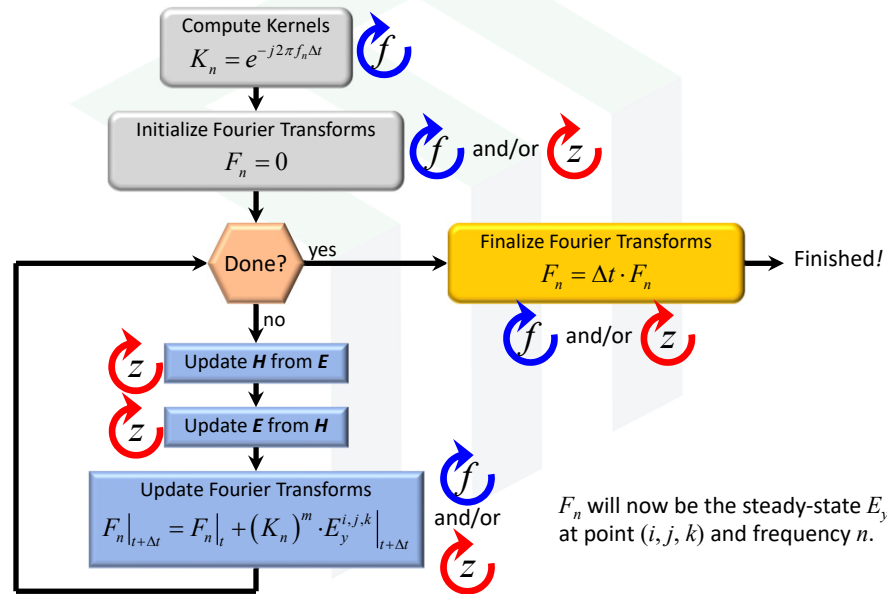
$K = 0.9781 - i0.2081$

Visualizing the Data Structures for Calculating Transmittance and Reflectance



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Efficient Fourier Transform Algorithm



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MATLAB Code for Fourier Transforms

```

% SOURCE PARAMETERS
f2 = 5.0 * gigahertz;
NFREQ = 1000;
FREQ = linspace(0, f2, NFREQ);

% INITIALIZE FOURIER TRANSFORMS
K = exp(-1i*2*pi*dt*FREQ);
EyR = zeros(1, NFREQ);
EyT = zeros(1, NFREQ);

% MAIN FDTD LOOP
for T = 1 : STEPS
    % Perform FDTD Functions

    % Update Fourier Transforms
    for nf = 1 : NFREQ
        EyR(nf) = EyR(nf) + (K(nf)^T)*Ey(1);
        EyT(nf) = EyT(nf) + (K(nf)^T)*Ey(Nz);
    end

    % Visualize
end

% FINISH FOURIER TRANSFORMS
EyR = EyR*dt;
EyT = EyT*dt;

```

REMEMBER! We are not finished the Fourier transforms until we multiply by Δt .

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Calculating Reflectance and Transmittance

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Absorptance, Reflectance and Transmittance

When simulating passive devices, the most common output is a plot of the absorptance, reflectance and/or transmittance as a function of frequency.

Absorptance, A : fraction of power absorbed by a device.

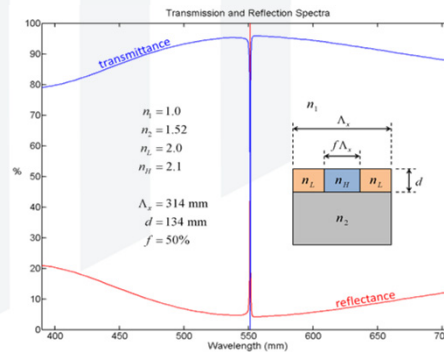
Reflectance, R : fraction of power reflected from a device.

Transmittance, T : fraction of power transmitted through a device.

Conservation of Power

$$A + R + T = 1$$

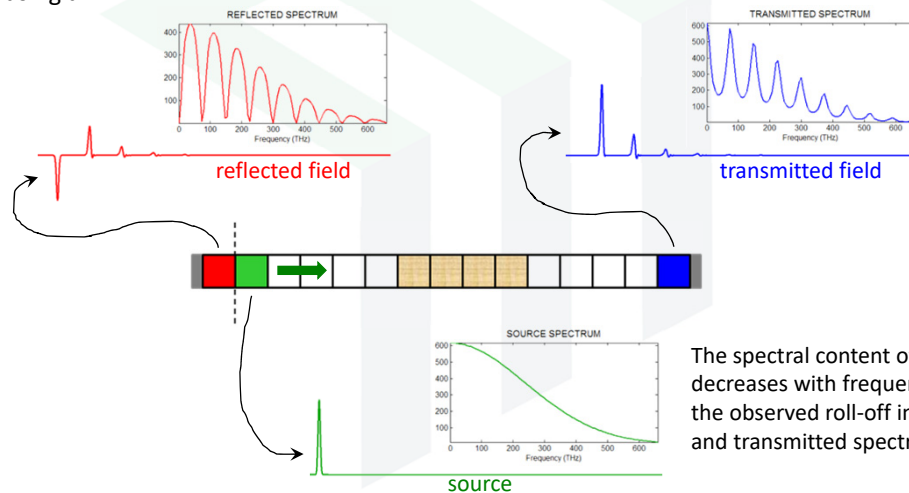
In this course, we will mostly ignore losses and assume $A = 0$.



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The Response of a Device in FDTD

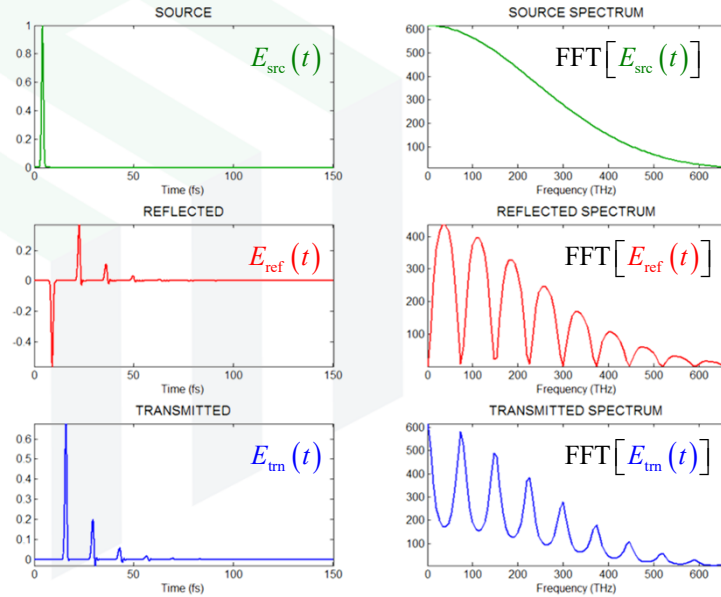
The easiest, but least memory efficient, method to compute a Fourier transform is to perform a simulation and record the desired field as a function of time. After the simulation is finished, these functions can be Fourier transformed using an FFT.



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The Fourier Transforms

It is typical to start the computation of power by Fourier transforming the reflected and transmitted field using one of the methods described previously. Typical FDTD simulation results look like this

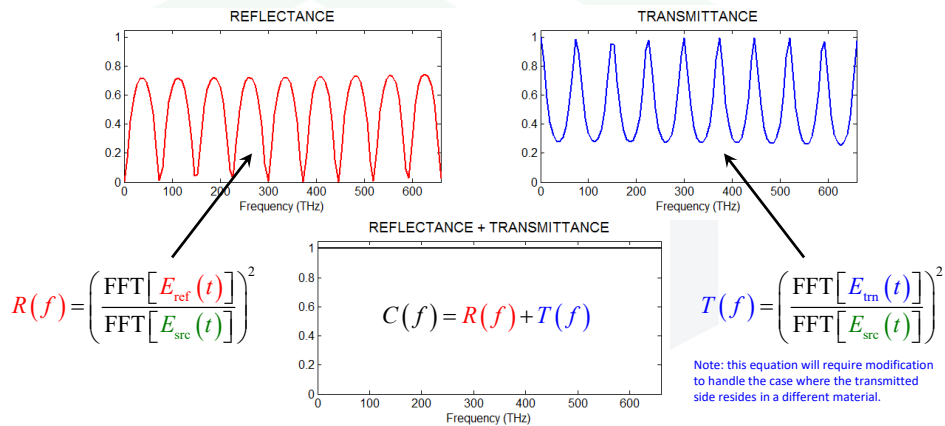


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Normalizing the Fourier Transforms

It is necessary to normalize the spectra to calculate transmittance and reflectance. This is one by dividing the reflection and transmission spectrum by the source spectrum.



Note: this equation will require modification to handle the case where the transmitted side resides in a different material.

It is ALWAYS good practice to check for power 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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MATLAB Code for Reflectance and Transmittance

```

% SOURCE PARAMETERS
f2 = 5.0 * gigahertz;
NFREQ = 1000;
FREQ = linspace(0, f2, NFREQ);

% INITIALIZE FOURIER TRANSFORMS
K = exp(-1i*2*pi*dt*FREQ);
EyR = zeros(1, NFREQ);
EyT = zeros(1, NFREQ);
SRC = zeros(1, NFREQ);

% MAIN FDTD LOOP
for T = 1 : STEPS
    % Perform FDTD Functions

    % Update Fourier Transforms
    for nf = 1 : NFREQ
        EyR(nf) = EyR(nf) + (K(nf)^T)*Ey(1);
        EyT(nf) = EyT(nf) + (K(nf)^T)*Ey(Nz);
        SRC(nf) = SRC(nf) + (K(nf)^T)*Esrc(T);
    end

    % Visualize
end

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

```

No need to multiply by Δt here because that term would cancel after performing the divisions.

The Time & Frequency Axes

Time Axis

The time axis is calculated according to

$$T = [0 : STEPS - 1] * dt;$$

Frequency Axis

The FDTD algorithm is performed in small time increments Δt .

The Nyquist theorem tells us that the upper frequency we can resolve with this time step is

$$f_{\max} = \frac{0.5}{\Delta t}$$

Staying consistent with this notation, our frequency axis after an `fftshift(fft())` is computed as:

```
fmax = 0.5/dt;
freq = linspace(-fmax, +fmax, STEPS);
```

STEPS should be an odd number here.

Frequency Resolution Vs. Upper Frequency

Upper Frequency Limit

The time step Δt determines the upper frequency that can be resolved by your FDTD model.

$$f_{\max} = \frac{0.5}{\Delta t}$$

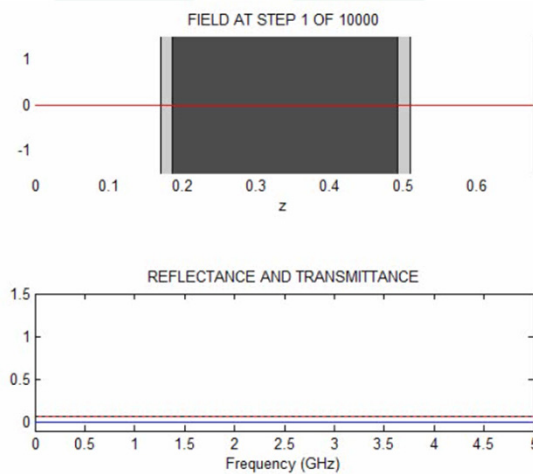
Frequency Resolution

The number of time iterations (STEPS) determines how finely the frequencies can be resolved.

$$\Delta f \cong \frac{1}{\Delta t \cdot \text{STEPS}}$$

[Note](#): the frequency spacing between your kernels only controls your graphical frequency resolution, not the actual frequency resolution.

Movie of Real-Time Fourier Transforms

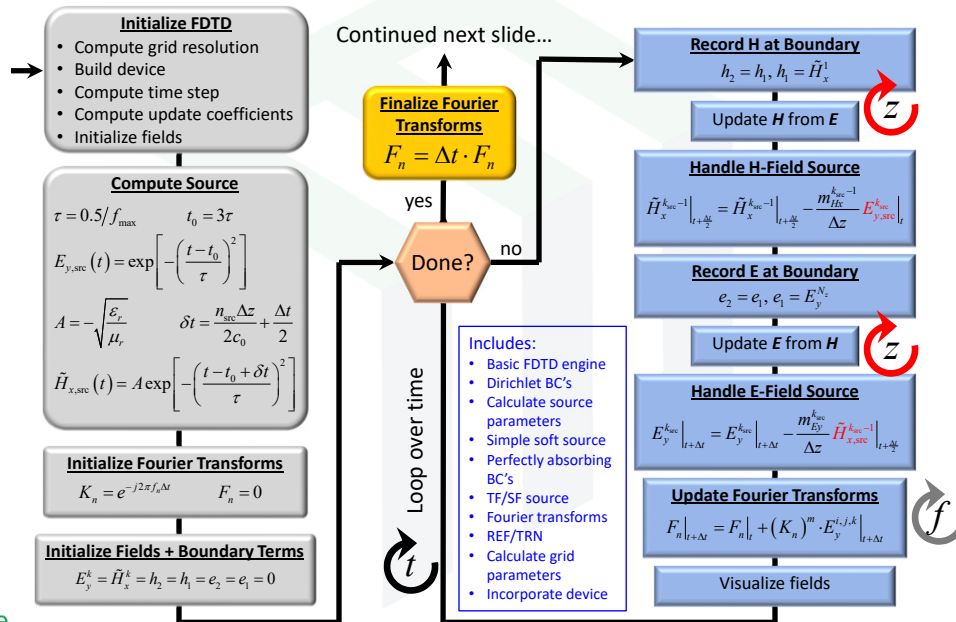


Revised FDTD Algorithm

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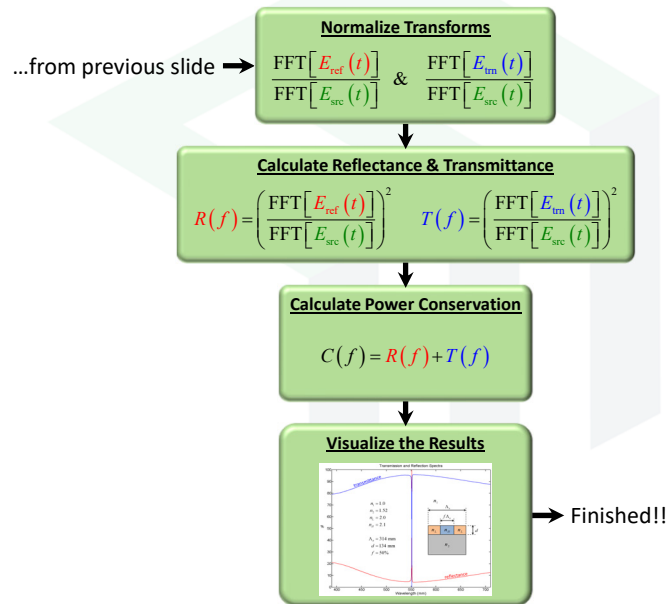
Revised FDTD Algorithm (1 of 2)



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Revised FDTD Algorithm (2 of 2)



Tips for Visualization in FDTD

- Always show the materials **and** fields during the simulation. Superimposed is best.
- Try to show all the field components in the model. If your code is unstable, this may help point to the reason.
- Graphics commands slow the simulation dramatically. Update graphics after some duration of time, after some number of iterations, and limit any fancy formatting.
- Try to display transmittance, reflectance, and power conservation during the simulation. Often, you can identify problems during the simulation and not have to wait until it finishes.