



Computational Science:  
Introduction to Finite-Difference Time-Domain

## Three-Dimensional FDTD

### Lecture Outline

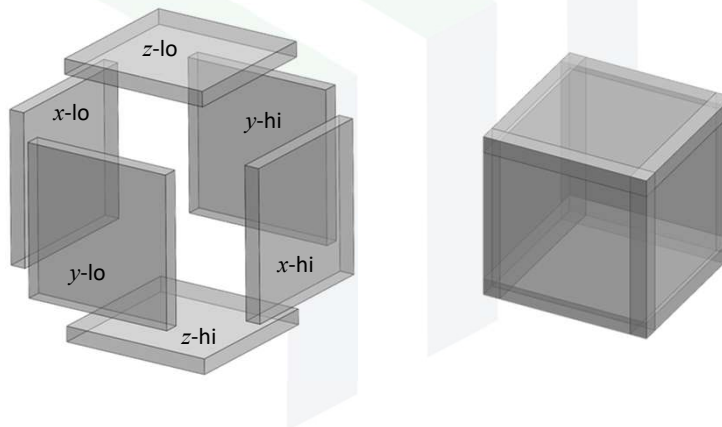
- Two Common Grid Strategies
- Simplifying the update equations for crossed grating devices
- Boundary conditions
- Plane wave source using the total-field/scattered-field technique
- Calculation of transmittance and reflectance
- MATLAB's `slice()` command for 3D visualization

## Two Common Grid Strategies

Slide 3

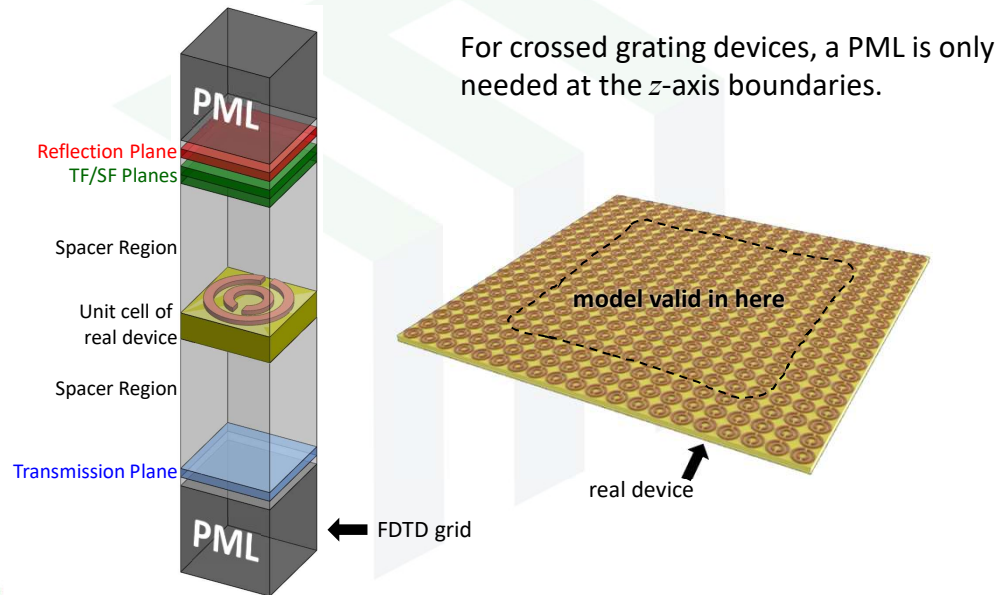
## Grid Scheme for Finite-Size Devices

To simulate scattering from finite-sized devices, a PML is needed at all boundaries.



Slide 4

## Grid Scheme for Crossed Grating Devices



## Simplified Update Equations for Crossed Grating Devices

## Simplify, Simplify, Simplify!

A 3D grid contains many more points than an equivalent 2D grid. For this reason, more attention will be devoted to simplifying and streamlining the update equations.

### 2D Grid

40×200 cells = 8,000 cells

### 3D Grid

40×40×200 = 320,000 cells

There is now...

40× more grid cells

2× more field components

80× more numbers to process

## Important Items to Simplify and Streamline

- We do not need  $x$ -axis or  $y$ -axis PMLs. They should be eliminated from the update equations.
- Integration terms are only needed inside the PML. These should be split into  $z$ -low and  $z$ -high integration terms.

## Simplify Update Equation for $H_x$

The following terms are eliminated from the update coefficients:

$$\begin{aligned}
 m_{Hx0}^{i,j,k} &= \frac{1}{\Delta t} + \left( \frac{\sigma_x^{H^{i,j,k}} + \sigma_z^{H^{i,j,k}}}{2\epsilon_0} \right) + \left( \frac{\sigma_y^{H^{i,j,k}} (\sigma_x^{H^{i,j,k}}) \Delta t}{4\epsilon_0^2} \right) & m_{Hx1}^{i,j,k} &= \frac{1}{m_{Hx0}^{i,j,k}} \left[ \frac{1}{\Delta t} - \left( \frac{\sigma_x^{H^{i,j,k}} + \sigma_z^{H^{i,j,k}}}{2\epsilon_0} \right) - \left( \frac{\sigma_y^{H^{i,j,k}} (\sigma_x^{H^{i,j,k}}) \Delta t}{4\epsilon_0^2} \right) \right] \\
 m_{Hx2}^{i,j,k} &= -\frac{1}{m_{Hx0}^{i,j,k}} \frac{c_0}{\mu_{xx}^{i,j,k}} & m_{Hx3}^{i,j,k} &= -\frac{1}{m_{Hx0}^{i,j,k}} \frac{\epsilon_0 \Delta t \sigma_x^{H^{i,j,k}}}{\epsilon_0 H_{xx}^{i,j,k}} & m_{Hx4}^{i,j,k} &= -\frac{1}{m_{Hx0}^{i,j,k}} \frac{\Delta t}{\epsilon_0} \left( \frac{\sigma_x^{H^{i,j,k}}}{\sigma_y^{H^{i,j,k}}} \right)
 \end{aligned}$$

For  $H_x$ , we no longer need any integration terms!

$$\begin{aligned}
 I_{CE_x}^{i,j,k} &= \sum_{T=0}^t C_x^E |_T^{i,j,k} & I_{H_x}^{i,j,k} &= \sum_{T=0}^{t-\frac{\Delta t}{2}} H_x |_T^{i,j,k} & C_x^E |_t^{i,j,k} &= \frac{\tilde{E}_z |_t^{i,j+1,k} - \tilde{E}_z |_t^{i,j,k}}{\Delta y} - \frac{\tilde{E}_y |_t^{i,j,k+1} - \tilde{E}_y |_t^{i,j,k}}{\Delta z}
 \end{aligned}$$

The third and fourth terms are eliminated from the update equation.

$$H_x |_{t+\Delta t/2}^{i,j,k} = \left( m_{Hx1}^{i,j,k} \right) H_x |_{t-\Delta t/2}^{i,j,k} + \left( m_{Hx2}^{i,j,k} \right) C_x^E |_t^{i,j,k} + \left( m_{Hx3}^{i,j,k} \right) I_{CE_x}^{i,j,k} + \left( m_{Hx4}^{i,j,k} \right) I_{H_x}^{i,j,k}$$

## Final Form of the Update Equation for $H_x$

The update coefficients are computed before the main FDTD loop.

$$\begin{aligned}
 m_{Hx0}^{i,j,k} &= \frac{1}{\Delta t} + \frac{\sigma_z^{H^{i,j,k}}}{2\epsilon_0} & m_{Hx1}^{i,j,k} &= \frac{1}{m_{Hx0}^{i,j,k}} \left[ \frac{1}{\Delta t} - \frac{\sigma_z^{H^{i,j,k}}}{2\epsilon_0} \right] & m_{Hx2}^{i,j,k} &= -\frac{1}{m_{Hx0}^{i,j,k}} \frac{c_0}{\mu_{xx}^{i,j,k}}
 \end{aligned}$$

The curl is computed inside the main FDTD loop, but before the update equation.

$$C_x^E |_t^{i,j,k} = \frac{\tilde{E}_z |_t^{i,j+1,k} - \tilde{E}_z |_t^{i,j,k}}{\Delta y} - \frac{\tilde{E}_y |_t^{i,j,k+1} - \tilde{E}_y |_t^{i,j,k}}{\Delta z}$$

The update equation is computed inside the main FDTD loop immediately after the curl term is calculated.

$$H_x |_{t+\Delta t/2}^{i,j,k} = \left( m_{Hx1}^{i,j,k} \right) H_x |_{t-\Delta t/2}^{i,j,k} + \left( m_{Hx2}^{i,j,k} \right) C_x^E |_t^{i,j,k}$$

## Final Form of the Update Equation for $H_y$

The update coefficients are computed before the main FDTD loop.

$$m_{Hy0}^{i,j,k} = \frac{1}{\Delta t} + \frac{\sigma_z^H |^{i,j,k}}{2\epsilon_0} \quad m_{Hy1}^{i,j,k} = \frac{1}{m_{Hy0}^{i,j,k}} \left[ \frac{1}{\Delta t} - \frac{\sigma_z^H |^{i,j,k}}{2\epsilon_0} \right] \quad m_{Hy2}^{i,j,k} = -\frac{1}{m_{Hy0}^{i,j,k}} \frac{c_0}{\mu_{yy} |^{i,j,k}}$$

The curl term is computed inside the main FDTD loop, but before the update equation.

$$C_y^E |^i_{t,j,k} = \frac{\tilde{E}_x |^i_{t,j,k+1} - \tilde{E}_x |^i_{t,j,k}}{\Delta z} - \frac{\tilde{E}_z |^i_{t,j+1,k} - \tilde{E}_z |^i_{t,j,k}}{\Delta x}$$

The update equation is computed inside the main FDTD loop immediately after the curl term is calculated.

$$H_y |^i_{t+\frac{\Delta t}{2}} = \left( m_{Hy1} |^i_{t,j,k} \right) H_y |^i_{t-\frac{\Delta t}{2}} + \left( m_{Hy2} |^i_{t,j,k} \right) C_y^E |^i_{t,j,k}$$

## Final Form of the Update Equation for $H_z$

The update coefficients are computed before the main FDTD loop.

$$m_{Hz2} |^{i,j,k} = -\frac{c_0 \Delta t}{\mu_z |^{i,j,k}} \quad m_{Hz3} |^{i,j,k} = -\frac{c_0 (\Delta t)^2 \sigma_z^H |^{i,j,k}}{\epsilon_0 \mu_z |^{i,j,k}}$$

The integration term and curl are computed inside the main FDTD loop, but before the update equation.

$$I_{CEz} |^i_{t,j,k} = \sum_{T=0}^t C_z^E |^i_{t,j,k} \quad C_z^E |^i_{t,j,k} = \frac{\tilde{E}_y |^i_{t+1,j,k} - \tilde{E}_y |^i_{t,j,k}}{\Delta x} - \frac{\tilde{E}_x |^i_{t,j+1,k} - \tilde{E}_x |^i_{t,j,k}}{\Delta y}$$

The update equation is computed inside the main FDTD loop immediately after the integration term and curl term are updated.

$$H_z |^i_{t+\frac{\Delta t}{2}} = H_z |^i_{t-\frac{\Delta t}{2}} + \left( m_{Hz2} |^i_{t,j,k} \right) C_z^E |^i_{t,j,k} + \left( m_{Hz3} |^i_{t,j,k} \right) I_{CEz} |^i_{t,j,k}$$

## Final Form of the Update Equation for $D_x$

The update coefficients are computed before the main FDTD loop.

$$m_{Dx0}^{i,j,k} = \frac{1}{\Delta t} + \frac{\sigma_z^D |^{i,j,k}}{2\epsilon_0} \quad m_{Dx1}^{i,j,k} = \frac{1}{m_{Dx0}^{i,j,k}} \left[ \frac{1}{\Delta t} - \frac{\sigma_z^D |^{i,j,k}}{2\epsilon_0} \right] \quad m_{Dx2}^{i,j,k} = \frac{c_0}{m_{Dx0}^{i,j,k}}$$

The curl term is computed inside the main FDTD loop, but before the update equation.

$$C_x^H \Big|_{t+\frac{\Delta t}{2}}^{i,j,k} = \frac{H_z \Big|_{t+\frac{\Delta t}{2}}^{i,j,k} - H_z \Big|_{t+\frac{\Delta t}{2}}^{i,j-1,k}}{\Delta y} - \frac{H_y \Big|_{t+\frac{\Delta t}{2}}^{i,j,k} - H_y \Big|_{t+\frac{\Delta t}{2}}^{i,j,k-1}}{\Delta z}$$

The update equation is computed inside the main FDTD loop immediately after the curl term is calculated.

$$\tilde{D}_x \Big|_{t+\Delta t}^{i,j,k} = \left( m_{Dx1} \Big|_{t+\Delta t}^{i,j,k} \right) \tilde{D}_x \Big|_t^{i,j,k} + \left( m_{Dx2} \Big|_{t+\Delta t}^{i,j,k} \right) C_x^H \Big|_{t+\frac{\Delta t}{2}}^{i,j,k}$$

## Final Form of the Update Equation for $D_y$

The update coefficients are computed before the main FDTD loop.

$$m_{Dy0}^{i,j,k} = \frac{1}{\Delta t} + \frac{\sigma_z^D |^{i,j,k}}{2\epsilon_0} \quad m_{Dy1}^{i,j,k} = \frac{1}{m_{Dy0}^{i,j,k}} \left[ \frac{1}{\Delta t} - \frac{\sigma_z^D |^{i,j,k}}{2\epsilon_0} \right] \quad m_{Dy2}^{i,j,k} = \frac{c_0}{m_{Dy0}^{i,j,k}}$$

The integration terms are computed inside the main FDTD loop, but before the update equation.

$$C_y^H \Big|_{t+\frac{\Delta t}{2}}^{i,j,k} = \frac{H_x \Big|_{t+\frac{\Delta t}{2}}^{i,j,k} - H_x \Big|_{t+\frac{\Delta t}{2}}^{i,j,k-1}}{\Delta z} - \frac{H_z \Big|_{t+\frac{\Delta t}{2}}^{i,j,k} - H_z \Big|_{t+\frac{\Delta t}{2}}^{i-1,j,k}}{\Delta x}$$

The update equation is computed inside the main FDTD loop immediately after the integration terms are updated.

$$\tilde{D}_y \Big|_{t+\Delta t}^{i,j,k} = \left( m_{Dy1} \Big|_{t+\Delta t}^{i,j,k} \right) \tilde{D}_y \Big|_t^{i,j,k} + \left( m_{Dy2} \Big|_{t+\Delta t}^{i,j,k} \right) C_y^H \Big|_{t+\frac{\Delta t}{2}}^{i,j,k}$$

## Final Form of the Update Equation for $D_z$

The update coefficients are computed before the main FDTD loop.

$$m_{Dz2} \Big|_{t+\Delta t}^{i,j,k} = c_0 \Delta t \quad m_{Dz3} \Big|_{t+\Delta t}^{i,j,k} = \frac{c_0 (\Delta t)^2}{\epsilon_0} \sigma_z \Big|_{t+\Delta t}^{i,j,k}$$

The integration term and curl term are computed inside the main FDTD loop, but before the update equation.

$$I_{CHz} \Big|_{t-\frac{\Delta t}{2}}^{i,j,k} = \sum_{T=0}^{t-\frac{\Delta t}{2}} C_z^H \Big|_T^{i,j,k} \quad C_z^H \Big|_{t+\frac{\Delta t}{2}}^{i,j,k} = \frac{H_y \Big|_{t+\frac{\Delta t}{2}}^{i,j,k} - H_y \Big|_{t+\frac{\Delta t}{2}}^{i-1,j,k}}{\Delta x} - \frac{H_x \Big|_{t+\frac{\Delta t}{2}}^{i,j,k} - H_x \Big|_{t+\frac{\Delta t}{2}}^{i,j-1,k}}{\Delta y}$$

The update equation is computed inside the main FDTD loop immediately after the integration and curl terms are updated.

$$\tilde{D}_z \Big|_{t+\Delta t}^{i,j,k} = \tilde{D}_z \Big|_t^{i,j,k} + \left( m_{Dz2} \Big|_{t+\Delta t}^{i,j,k} \right) C_z^H \Big|_{t+\frac{\Delta t}{2}}^{i,j,k} + \left( m_{Dz3} \Big|_{t+\Delta t}^{i,j,k} \right) I_{CHz} \Big|_{t-\frac{\Delta t}{2}}^{i,j,k}$$

## Final Update Equations for $E_x$ , $E_y$ , and $E_z$

The update coefficients are computed before the main FDTD loop.

$$m_{Ex1} \Big|_{t+\Delta t}^{i,j,k} = \frac{1}{\epsilon_{xx} \Big|_{t+\Delta t}^{i,j,k}} \quad m_{Ey1} \Big|_{t+\Delta t}^{i,j,k} = \frac{1}{\epsilon_{yy} \Big|_{t+\Delta t}^{i,j,k}} \quad m_{Ez1} \Big|_{t+\Delta t}^{i,j,k} = \frac{1}{\epsilon_{zz} \Big|_{t+\Delta t}^{i,j,k}}$$

The update equations are computed inside the main FDTD loop.

$$\tilde{E}_x \Big|_{t+\Delta t}^{i,j,k} = \left( m_{Ex1} \Big|_{t+\Delta t}^{i,j,k} \right) \tilde{D}_x \Big|_{t+\Delta t}^{i,j,k}$$

$$\tilde{E}_y \Big|_{t+\Delta t}^{i,j,k} = \left( m_{Ey1} \Big|_{t+\Delta t}^{i,j,k} \right) \tilde{D}_y \Big|_{t+\Delta t}^{i,j,k}$$

$$\tilde{E}_z \Big|_{t+\Delta t}^{i,j,k} = \left( m_{Ez1} \Big|_{t+\Delta t}^{i,j,k} \right) \tilde{D}_z \Big|_{t+\Delta t}^{i,j,k}$$

# Boundary Conditions

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## Periodic Boundary Conditions

All of the spatial derivatives appear in the curl calculations. Therefore, all boundary conditions are implemented in the curl calculations as well.

We will implement periodic boundary conditions all the way around the grid.

Slide 18

## Curl of $\vec{E}$

The curl equations are

$$C_x^E \Big|_t^{i,j,k} = \frac{\tilde{E}_z \Big|_t^{i,j,k+1} - \tilde{E}_z \Big|_t^{i,j,k}}{\Delta y} - \frac{\tilde{E}_y \Big|_t^{i,j,k+1} - \tilde{E}_y \Big|_t^{i,j,k}}{\Delta z}$$

$$C_y^E \Big|_t^{i,j,k} = \frac{\tilde{E}_x \Big|_t^{i,j,k+1} - \tilde{E}_x \Big|_t^{i,j,k}}{\Delta z} - \frac{\tilde{E}_z \Big|_t^{i+1,j,k} - \tilde{E}_z \Big|_t^{i,j,k}}{\Delta x}$$

$$C_z^E \Big|_t^{i,j,k} = \frac{\tilde{E}_y \Big|_t^{i+1,j,k} - \tilde{E}_y \Big|_t^{i,j,k}}{\Delta x} - \frac{\tilde{E}_x \Big|_t^{i,j+1,k} - \tilde{E}_x \Big|_t^{i,j,k}}{\Delta y}$$

Problems arise when calculating these at the  $x$ -high,  $y$ -high, and  $z$ -high boundaries.

## Curl of $\vec{H}$

The curl equations are

$$C_x^H \Big|_{t+\frac{\Delta t}{2}}^{i,j,k} = \frac{H_z \Big|_{t+\frac{\Delta t}{2}}^{i,j,k} - H_z \Big|_{t+\frac{\Delta t}{2}}^{i,j-1,k}}{\Delta y} - \frac{H_y \Big|_{t+\frac{\Delta t}{2}}^{i,j,k} - H_y \Big|_{t+\frac{\Delta t}{2}}^{i,j,k-1}}{\Delta z}$$

$$C_y^H \Big|_{t+\frac{\Delta t}{2}}^{i,j,k} = \frac{H_x \Big|_{t+\frac{\Delta t}{2}}^{i,j,k} - H_x \Big|_{t+\frac{\Delta t}{2}}^{i,j,k-1}}{\Delta z} - \frac{H_z \Big|_{t+\frac{\Delta t}{2}}^{i,j,k} - H_z \Big|_{t+\frac{\Delta t}{2}}^{i-1,j,k}}{\Delta x}$$

$$C_z^H \Big|_{t+\frac{\Delta t}{2}}^{i,j,k} = \frac{H_y \Big|_{t+\frac{\Delta t}{2}}^{i,j,k} - H_y \Big|_{t+\frac{\Delta t}{2}}^{i-1,j,k}}{\Delta x} - \frac{H_x \Big|_{t+\frac{\Delta t}{2}}^{i,j,k} - H_x \Big|_{t+\frac{\Delta t}{2}}^{i,j-1,k}}{\Delta y}$$

Problems arise when calculating these at the  $x$ -low,  $y$ -low, and  $z$ -low boundaries.

## $x$ -Component of Curl of $\vec{E}$ with PBC

There are four cases where the curl must be computed explicitly.

$$C_x^E \Big|_t^{i,j,k} = \begin{cases} \frac{\tilde{E}_z \Big|_t^{i,j+1,k} - \tilde{E}_z \Big|_t^{i,j,k}}{\Delta y} - \frac{\tilde{E}_y \Big|_t^{i,j,k+1} - \tilde{E}_y \Big|_t^{i,j,k}}{\Delta z} & \text{for } j < N_y \text{ and } k < N_z \\ \frac{\tilde{E}_z \Big|_t^{i,1,k} - \tilde{E}_z \Big|_t^{i,N_y,k}}{\Delta y} - \frac{\tilde{E}_y \Big|_t^{i,N_y,k+1} - \tilde{E}_y \Big|_t^{i,N_y,k}}{\Delta z} & \text{for } j = N_y \text{ and } k < N_z \\ \frac{\tilde{E}_z \Big|_t^{i,j+1,N_z} - \tilde{E}_z \Big|_t^{i,j,N_z}}{\Delta y} - \frac{\tilde{E}_y \Big|_t^{i,j,1} - \tilde{E}_y \Big|_t^{i,j,N_z}}{\Delta z} & \text{for } j < N_y \text{ and } k = N_z \\ \frac{\tilde{E}_z \Big|_t^{i,1,N_z} - \tilde{E}_z \Big|_t^{i,N_y,N_z}}{\Delta y} - \frac{\tilde{E}_y \Big|_t^{i,N_y,1} - \tilde{E}_y \Big|_t^{i,N_y,N_z}}{\Delta z} & \text{for } j = N_y \text{ and } k = N_z \end{cases}$$

## MATLAB Code for $x$ -Component of Curl of $\vec{E}$ with PBC

```
% Compute CEx
for nx = 1 : Nx
    for ny = 1 : Ny-1
        for nz = 1 : Nz-1
            CEx(nx,ny,nz) = (Ez(nx,ny+1,nz) - Ez(nx,ny,nz))/dy ...
                - (Ey(nx,ny,nz+1) - Ey(nx,ny,nz))/dz;
        end
        CEx(nx,ny,Nz) = (Ez(nx,ny+1,Nz) - Ez(nx,ny,Nz))/dy ...
            - (Ey(nx,ny,1) - Ey(nx,ny,Nz))/dz;
    end
    for nz = 1 : Nz-1
        CEx(nx,Ny,nz) = (Ez(nx,1,nz) - Ez(nx,Ny,nz))/dy ...
            - (Ey(nx,Ny,nz+1) - Ey(nx,Ny,nz))/dz;
    end
    CEx(nx,Ny,Nz) = (Ez(nx,1,Nz) - Ez(nx,Ny,Nz))/dy ...
        - (Ey(nx,Ny,1) - Ey(nx,Ny,Nz))/dz;
end
```

**Note:** It is important for speed and efficiency that the boundary conditions be incorporated without using `if/then` statements. This should be done explicitly.

## $x$ -Component of Curl of $\vec{H}$ with PBC

There are four cases where the curl must be computed explicitly.

$$C_x^H \Big|_{t+\frac{\Delta t}{2}}^{i,j,k} = \begin{cases} \frac{H_z \Big|_{t+\frac{\Delta t}{2}}^{i,j,k} - H_z \Big|_{t+\frac{\Delta t}{2}}^{i,j-1,k}}{\Delta y} - \frac{H_y \Big|_{t+\frac{\Delta t}{2}}^{i,j,k} - H_y \Big|_{t+\frac{\Delta t}{2}}^{i,j,k-1}}{\Delta z} & \text{for } j > 1 \text{ and } k > 1 \\ \frac{H_z \Big|_{t+\frac{\Delta t}{2}}^{i,1,k} - H_z \Big|_{t+\frac{\Delta t}{2}}^{i,N_y,k}}{\Delta y} - \frac{H_y \Big|_{t+\frac{\Delta t}{2}}^{i,1,k} - H_y \Big|_{t+\frac{\Delta t}{2}}^{i,1,k-1}}{\Delta z} & \text{for } j = 1 \text{ and } k > 1 \\ \frac{H_z \Big|_{t+\frac{\Delta t}{2}}^{i,j,1} - H_z \Big|_{t+\frac{\Delta t}{2}}^{i,j-1,1}}{\Delta y} - \frac{H_y \Big|_{t+\frac{\Delta t}{2}}^{i,j,1} - H_y \Big|_{t+\frac{\Delta t}{2}}^{i,j,N_z}}{\Delta z} & \text{for } j > 1 \text{ and } k = 1 \\ \frac{H_z \Big|_{t+\frac{\Delta t}{2}}^{i,1,1} - H_z \Big|_{t+\frac{\Delta t}{2}}^{i,N_y,1}}{\Delta y} - \frac{H_y \Big|_{t+\frac{\Delta t}{2}}^{i,1,1} - H_y \Big|_{t+\frac{\Delta t}{2}}^{i,1,N_z}}{\Delta z} & \text{for } j = 1 \text{ and } k = 1 \end{cases}$$

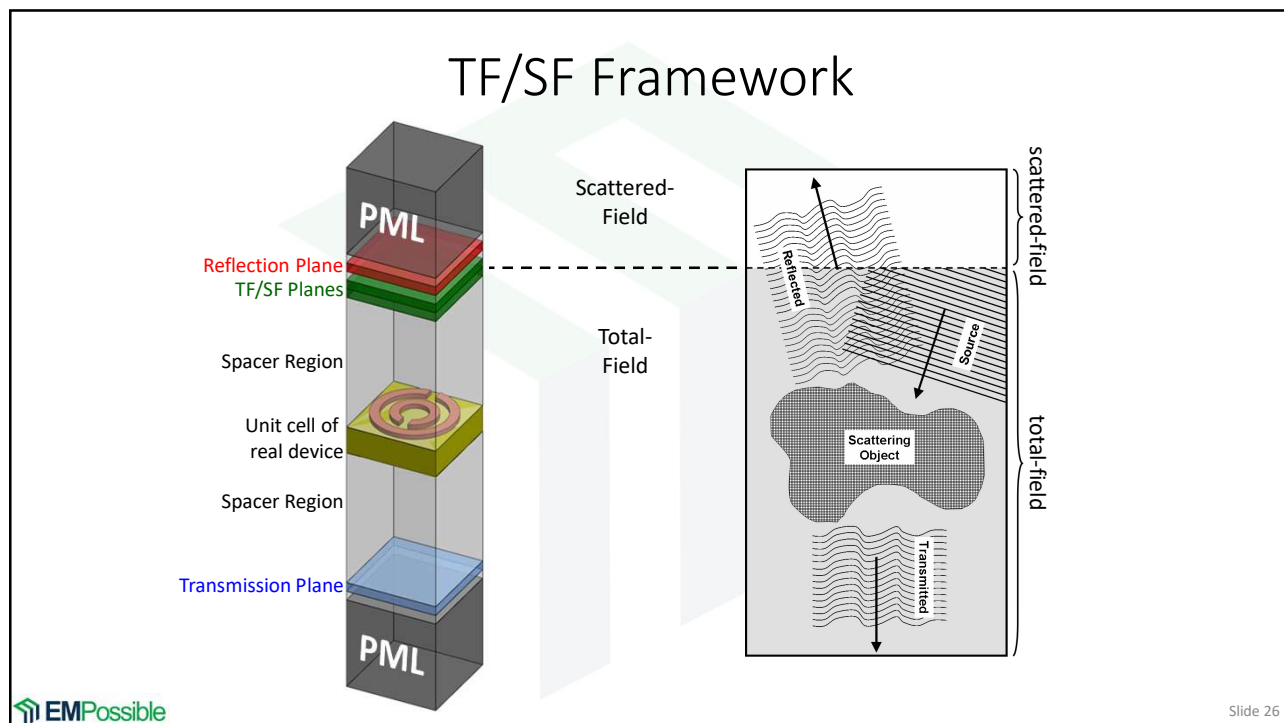
## MATLAB Code for $x$ -Component of Curl of $\vec{H}$ with PBC

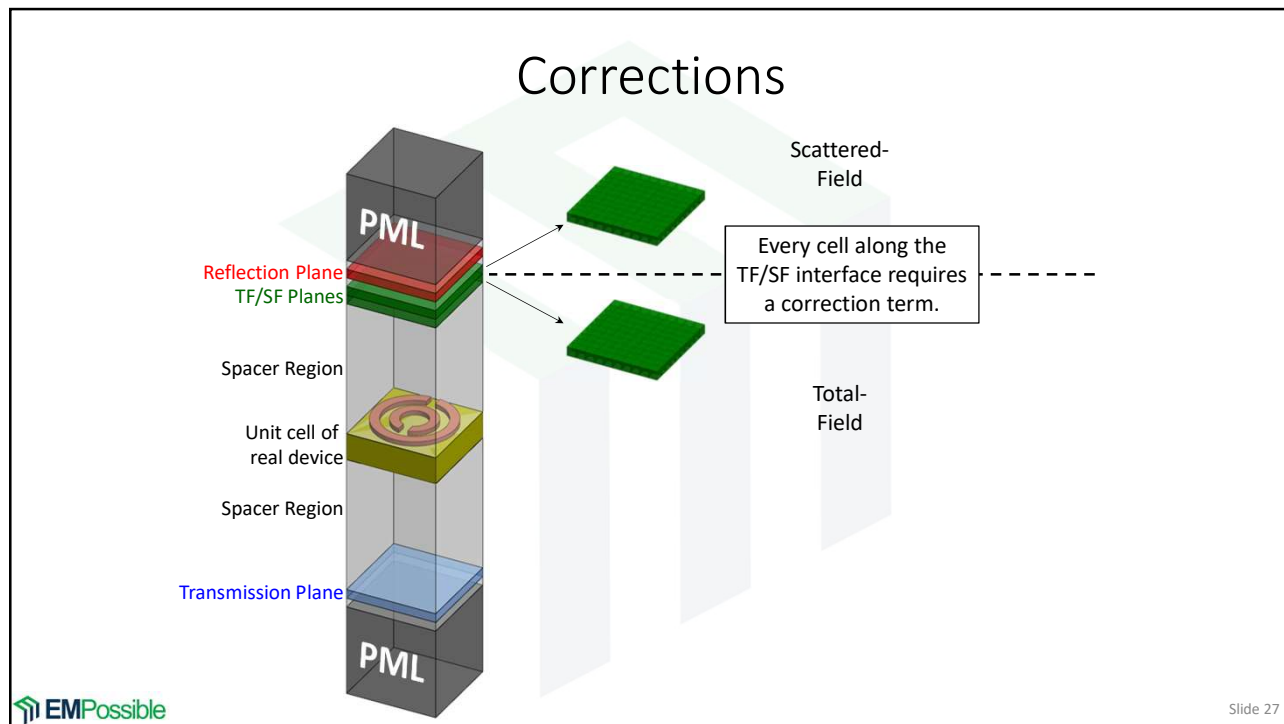
```
% Compute CHx
for nx = 1 : Nx
    CHx(nx,1,1) = (Hz(nx,1,1) - Hz(nx,Ny,1)) / dy ...
                - (Hy(nx,1,1) - Hy(nx,1,Nz)) / dz;
    for nz = 2 : Nz
        CHx(nx,1,nz) = (Hz(nx,1,nz) - Hz(nx,Ny,nz)) / dy ...
                    - (Hy(nx,1,nz) - Hy(nx,1,nz-1)) / dz;
    end
    for ny = 2 : Ny
        CHx(nx,ny,1) = (Hz(nx,ny,1) - Hz(nx,ny-1,1)) / dy ...
                    - (Hy(nx,ny,1) - Hy(nx,ny,Nz)) / dz;
        for nz = 2 : Nz
            CHx(nx,ny,nz) = (Hz(nx,ny,nz) - Hz(nx,ny-1,nz)) / dy ...
                            - (Hy(nx,ny,nz) - Hy(nx,ny,nz-1)) / dz;
        end
    end
end
end
```

**Note:** It is important for speed and efficiency that the boundary conditions be incorporated without using if/then statements. This should be done explicitly.

# Plane Wave Source Using the Total-Field/Scattered-Field Method

Slide 25





## Corrections on Scattered-Field Side (1 of 2)

The diagram shows a unit cell structure similar to the previous slide, but with a focus on the scattered field side. A callout box states: 'It is the curl of  $\vec{E}$  terms that require corrections on the scattered-field side. Here, the source (i.e. corrections) are incorporated through the  $E_x$  and  $E_y$  field components.'

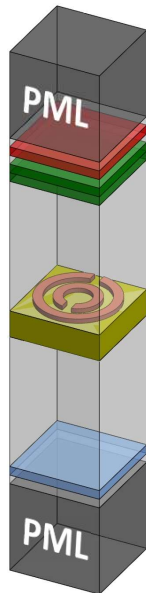
$$C_x^E \Big|_t^{i,j,k} = \frac{\tilde{E}_z \Big|_t^{i,j+1,k} - \tilde{E}_z \Big|_t^{i,j,k}}{\Delta y} - \frac{\tilde{E}_y \Big|_t^{i,j,k+1} - \tilde{E}_y \Big|_t^{i,j,k}}{\Delta z}$$

$$C_y^E \Big|_t^{i,j,k} = \frac{\tilde{E}_x \Big|_t^{i,j,k+1} - \tilde{E}_x \Big|_t^{i,j,k}}{\Delta z} - \frac{\tilde{E}_z \Big|_t^{i+1,j,k} - \tilde{E}_z \Big|_t^{i,j,k}}{\Delta x}$$

$$C_z^E \Big|_t^{i,j,k} = \frac{\tilde{E}_y \Big|_t^{i+1,j,k} - \tilde{E}_y \Big|_t^{i,j,k}}{\Delta x} - \frac{\tilde{E}_x \Big|_t^{i,j+1,k} - \tilde{E}_x \Big|_t^{i,j,k}}{\Delta y}$$

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## Corrections on Scattered-Field Side (2 of 2)



$$C_x^E \Big|_t^{i,j,k} = \frac{\tilde{E}_z \Big|_t^{i,j,k+1} - \tilde{E}_z \Big|_t^{i,j,k}}{\Delta y} - \frac{\tilde{E}_y \Big|_t^{i,j,k+1} - \tilde{E}_y \Big|_t^{i,j,k}}{\Delta z} + \frac{1}{\Delta z} \tilde{E}_y^{\text{src}} \Big|_t^{i,j,k+1}$$

$$C_y^E \Big|_t^{i,j,k} = \frac{\tilde{E}_x \Big|_t^{i,j,k+1} - \tilde{E}_x \Big|_t^{i,j,k}}{\Delta z} - \frac{\tilde{E}_z \Big|_t^{i+1,j,k} - \tilde{E}_z \Big|_t^{i,j,k}}{\Delta x} - \frac{1}{\Delta z} \tilde{E}_x^{\text{src}} \Big|_t^{i,j,k+1}$$

Standard curl equations

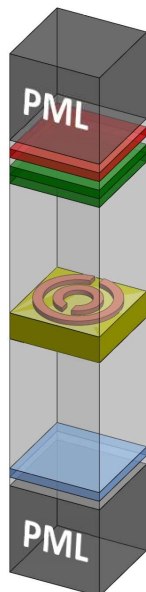
Corrections for TS/SF

⌘ TF/SF Correction

$\text{CEX}(:, :, \text{nz\_src}-1) = \text{CEX}(:, :, \text{nz\_src}-1) + \text{Ey\_src}(T) / \text{dz};$

$\text{CEY}(:, :, \text{nz\_src}-1) = \text{CEY}(:, :, \text{nz\_src}-1) - \text{Ex\_src}(T) / \text{dz};$

## Corrections on Total-Field Side (1 of 2)



It is the curl of  $\vec{H}$  terms that require corrections on the total-field side.

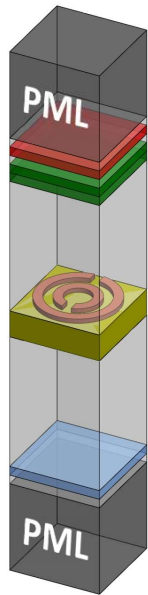
Here, the source (i.e. corrections) are incorporated through the  $H_x$  and  $H_y$  field components.

$$C_x^H \Big|_{t+\frac{\Delta z}{2}}^{i,j,k} = \frac{H_z \Big|_{t+\frac{\Delta z}{2}}^{i,j,k} - H_z \Big|_{t+\frac{\Delta z}{2}}^{i,j-1,k}}{\Delta y} - \frac{H_y \Big|_{t+\frac{\Delta z}{2}}^{i,j,k} - H_y \Big|_{t+\frac{\Delta z}{2}}^{i,j,k-1}}{\Delta z}$$

$$C_y^H \Big|_{t+\frac{\Delta z}{2}}^{i,j,k} = \frac{H_x \Big|_{t+\frac{\Delta z}{2}}^{i,j,k} - H_x \Big|_{t+\frac{\Delta z}{2}}^{i,j,k-1}}{\Delta z} - \frac{H_z \Big|_{t+\frac{\Delta z}{2}}^{i,j,k} - H_z \Big|_{t+\frac{\Delta z}{2}}^{i-1,j,k}}{\Delta x}$$

$$C_z^H \Big|_{t+\frac{\Delta z}{2}}^{i,j,k} = \frac{H_y \Big|_{t+\frac{\Delta z}{2}}^{i,j,k} - H_y \Big|_{t+\frac{\Delta z}{2}}^{i-1,j,k}}{\Delta x} - \frac{H_x \Big|_{t+\frac{\Delta z}{2}}^{i,j,k} - H_x \Big|_{t+\frac{\Delta z}{2}}^{i,j-1,k}}{\Delta y}$$

## Corrections on Total-Field Side (2 of 2)



```
% TF/SF Correction
CHx(:, :, nz_src) = CHx(:, :, nz_src) + Hy_src(T)/dz;
CHy(:, :, nz_src) = CHy(:, :, nz_src) - Hx_src(T)/dz;
```

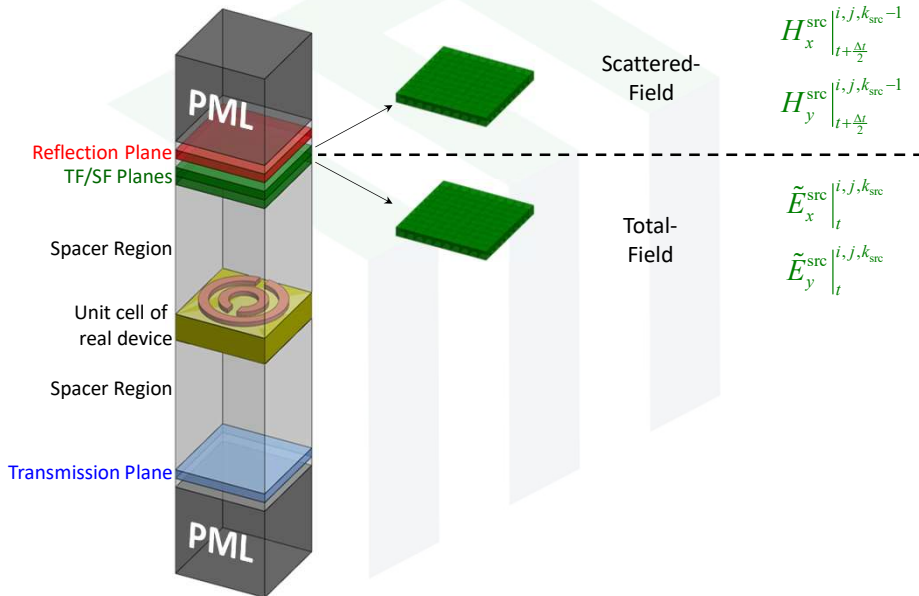
Corrections for TS/SF

Standard curl equations

$$C_x^H \Big|_{t+\frac{\Delta z}{2}}^{i,j,k} = \frac{H_z \Big|_{t+\frac{\Delta z}{2}}^{i,j,k} - H_z \Big|_{t+\frac{\Delta z}{2}}^{i,j-1,k}}{\Delta y} - \frac{H_y \Big|_{t+\frac{\Delta z}{2}}^{i,j,k} - H_y \Big|_{t+\frac{\Delta z}{2}}^{i,j,k-1}}{\Delta z} + \frac{1}{\Delta z} H_y^{\text{src}} \Big|_{t+\frac{\Delta z}{2}}^{i,j,k-1}$$

$$C_y^H \Big|_{t+\frac{\Delta z}{2}}^{i,j,k} = \frac{H_x \Big|_{t+\frac{\Delta z}{2}}^{i,j,k} - H_x \Big|_{t+\frac{\Delta z}{2}}^{i,j,k-1}}{\Delta z} - \frac{H_z \Big|_{t+\frac{\Delta z}{2}}^{i,j,k} - H_z \Big|_{t+\frac{\Delta z}{2}}^{i-1,j,k}}{\Delta x} - \frac{1}{\Delta z} H_x^{\text{src}} \Big|_{t+\frac{\Delta z}{2}}^{i,j,k-1}$$

## Source Functions We Need for TF/SF



$$H_x^{\text{src}} \Big|_{t+\frac{\Delta z}{2}}^{i,j,k_{\text{src}}-1}$$

$$H_y^{\text{src}} \Big|_{t+\frac{\Delta z}{2}}^{i,j,k_{\text{src}}-1}$$

$$\tilde{E}_x^{\text{src}} \Big|_t^{i,j,k_{\text{src}}}$$

$$\tilde{E}_y^{\text{src}} \Big|_t^{i,j,k_{\text{src}}}$$

## Polarization Vector $\vec{P}$

The electric field can be polarized in any direction in the  $x$ - $y$  plane.

Let the incident electric field be expressed as

$$\vec{E}^{\text{src}} = \vec{P} \cos(\omega t - k_0 n_{\text{inc}} z)$$

$$\tilde{E}_x^{\text{src}} \Big|_t^{i,j,k_{\text{src}}} = P_x \cos(\omega t - k_0 n_{\text{inc}} z)$$

$$\tilde{E}_y^{\text{src}} \Big|_t^{i,j,k_{\text{src}}} = P_y \cos(\omega t - k_0 n_{\text{inc}} z)$$

Note:

$$|\vec{P}| = 1$$

Note that the  $P_z$  is not needed in this formulation.

Why isn't this information needed?

## The Magnetic Field

The magnetic field  $\vec{H}$  is related to the electric field  $\vec{E}$  through Maxwell's curl equation.

$$\nabla \times \vec{E}^{\text{src}} = -\frac{\mu_{\text{inc}}}{c_0} \frac{\partial \vec{H}^{\text{src}}}{\partial t}$$

Substituting the plane wave form of the electric field leads to an expression for the magnetic field source.

$$H_x^{\text{src}}(t) = -P_y \sqrt{\frac{\epsilon_{r,\text{src}}}{\mu_{r,\text{src}}}} \cos(\omega t - k_0 n_{\text{inc}} z) \quad H_y^{\text{src}}(t) = P_x \sqrt{\frac{\epsilon_{r,\text{src}}}{\mu_{r,\text{src}}}} \cos(\omega t - k_0 n_{\text{inc}} z)$$

$$H_x^{\text{src}} \Big|_{t+\frac{\Delta t}{2}}^{i,j,k_{\text{src}}-1} = -P_y \sqrt{\frac{\epsilon_{r,\text{src}}}{\mu_{r,\text{src}}}} \cos \left[ \omega \left( t + \frac{\Delta t}{2} \right) - k_0 n_{\text{inc}} (k_{\text{src}} - 1) \Delta z \right]$$

$$H_y^{\text{src}} \Big|_{t+\frac{\Delta t}{2}}^{i,j,k_{\text{src}}-1} = P_x \sqrt{\frac{\epsilon_{r,\text{src}}}{\mu_{r,\text{src}}}} \cos \left[ \omega \left( t + \frac{\Delta t}{2} \right) - k_0 n_{\text{inc}} (k_{\text{src}} - 1) \Delta z \right]$$

## Generalization for a Gaussian Source

A Gaussian source is implemented as

$$\tilde{E}_x^{\text{src}} \Big|_t^{i,j,k_{\text{src}}} = P_x \cdot g(t)$$

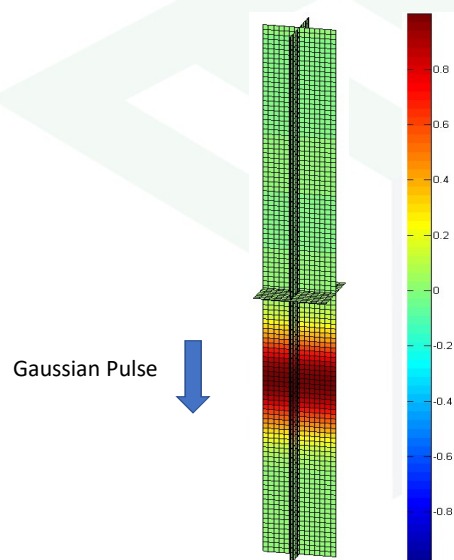
$$\tilde{E}_y^{\text{src}} \Big|_t^{i,j,k_{\text{src}}} = P_y \cdot g(t)$$

$$H_x^{\text{src}} \Big|_{t+\frac{\Delta t}{2}}^{i,j,k_{\text{src}}-1} = -P_y \sqrt{\frac{\epsilon_{r,\text{src}}}{\mu_{r,\text{src}}}} \cdot g(t + \delta t)$$

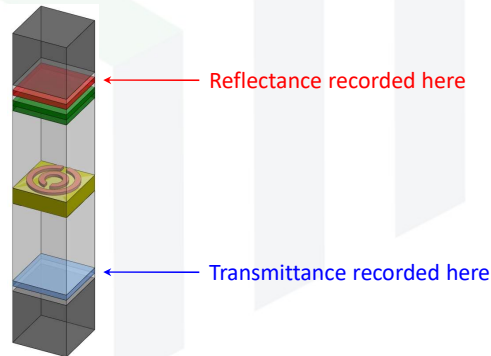
$$H_y^{\text{src}} \Big|_{t+\frac{\Delta t}{2}}^{i,j,k_{\text{src}}-1} = P_x \sqrt{\frac{\epsilon_{r,\text{src}}}{\mu_{r,\text{src}}}} \cdot g(t + \delta t)$$

$$\delta t = -\frac{n_{\text{src}} \Delta z}{2c_0} + \frac{\Delta t}{2}$$

## Typical View of 3D-FDTD with TF/SF

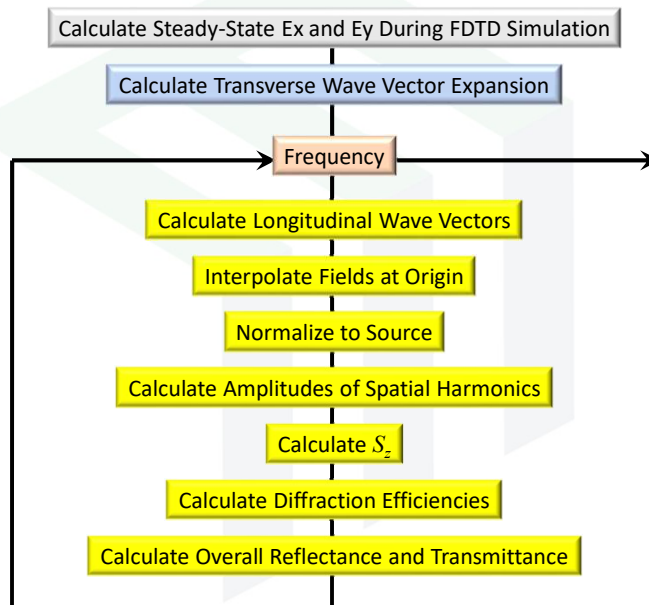


# Calculation of Transmittance and Reflectance



Slide 37

## Block Diagram of Power Calculation



Slide 38

### Calculate of Steady-State Fields During Simulation

Note: We do not calculate  $E_z$ .  
We will do this another way after FDTD.

Slide 39

## Interpolate Field Components

The fields are staggered because they are on a Yee grid. To calculate transmittance and reflectance in 3D, we need to interpolate the fields at a common point in each Yee cell in order to perform calculations with vector quantities.

Here, we will interpolate them at the origin of the Yee cell.

```

% Interpolate Fields at Origin
Exr      = zeros(Nx,Ny);
Exr(1,:) = (Exref(Nx,:,nfreq) + Exref(1,:,nfreq))/2;
Exr(2:Nx,:) = (Exref(1:Nx-1,:,nfreq) + Exref(2:Nx,:,nfreq))/2;
    
```

$$E_{x,ref} \Big|_{\text{origin},k_{ref}} = \frac{E_{x,ref} \Big|^{i,j,k_{ref}} + E_{x,ref} \Big|^{i-1,j,k_{ref}}}{2}$$

$$E_{y,ref} \Big|_{\text{origin},k_{ref}} = \frac{E_{y,ref} \Big|^{i,j,k_{ref}} + E_{y,ref} \Big|^{i,j-1,k_{ref}}}{2}$$

$$E_{x,tm} \Big|_{\text{origin},k_{tm}} = \frac{E_{x,tm} \Big|^{i,j,k_{tm}} + E_{x,tm} \Big|^{i-1,j,k_{tm}}}{2}$$

$$E_{y,tm} \Big|_{\text{origin},k_{tm}} = \frac{E_{y,tm} \Big|^{i,j,k_{tm}} + E_{y,tm} \Big|^{i,j-1,k_{tm}}}{2}$$

Slide 40

## Transverse Wave Vector Expansion (1 of 2)

Crossed grating devices diffraction along two dimensions,  $x$  and  $y$ .

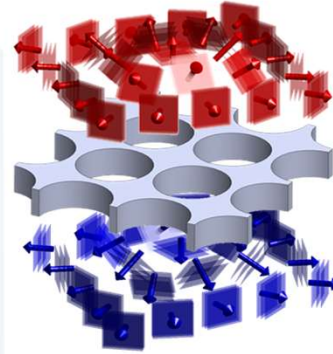
To quantify diffraction for crossed grating structures, we must calculate an expansion for both  $k_x$  and  $k_y$ .

$$k_x(m) = k_{x,\text{inc}} - \frac{2\pi m}{\Lambda_x} \quad m = -\infty, \dots, -2, -1, 0, 1, 2, \dots, \infty$$

$$k_y(n) = k_{y,\text{inc}} - \frac{2\pi n}{\Lambda_y} \quad n = -\infty, \dots, -2, -1, 0, 1, 2, \dots, \infty$$

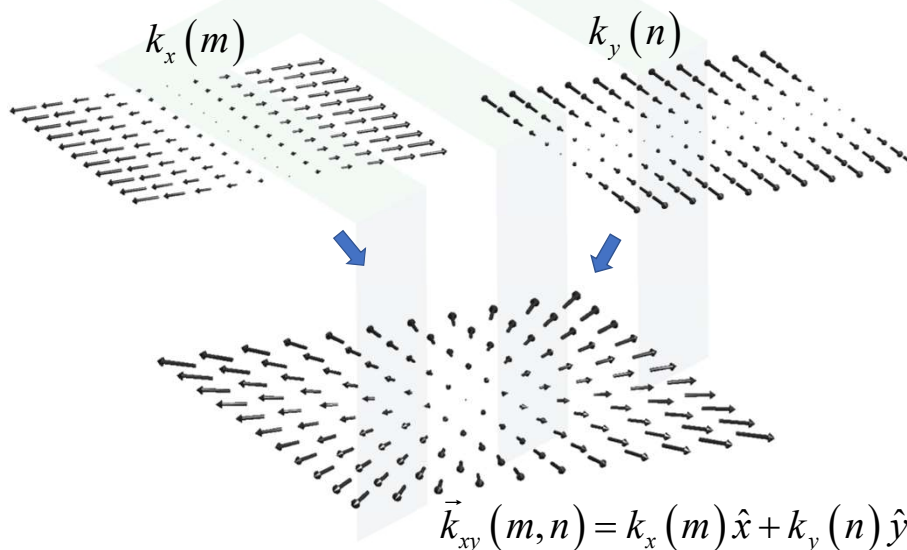
$$\vec{k}_{xy}(m, n) = k_x(m)\hat{x} + k_y(n)\hat{y}$$

```
% TRANSVERSE WAVE VECTOR EXPANSION
M = [-floor(Nx/2):floor(Nx/2)]';
N = [-floor(Ny/2):floor(Ny/2)]';
kx = - 2*pi*M/Sx;
ky = - 2*pi*N/Sy;
[ky, kx] = meshgrid(ky, kx);
```



## Transverse Wave Vector Expansion (2 of 2)

The vector expansions can be visualized this way.



## Longitudinal Wave Vector Expansion (1 of 2)

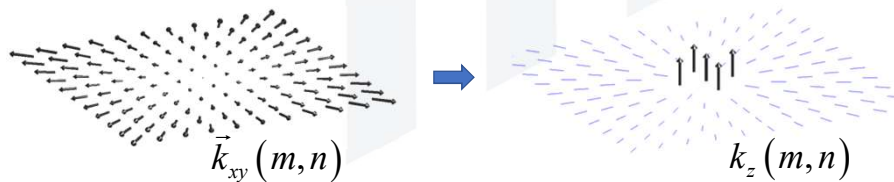
The longitudinal components of the wave vectors are computed as

$$k_{z,\text{ref}}(m,n) = \sqrt{(k_0 n_{\text{ref}})^2 - k_x^2(m) - k_y^2(n)}$$

$$k_{z,\text{tm}}(m,n) = \sqrt{(k_0 n_{\text{tm}})^2 - k_x^2(m) - k_y^2(n)}$$

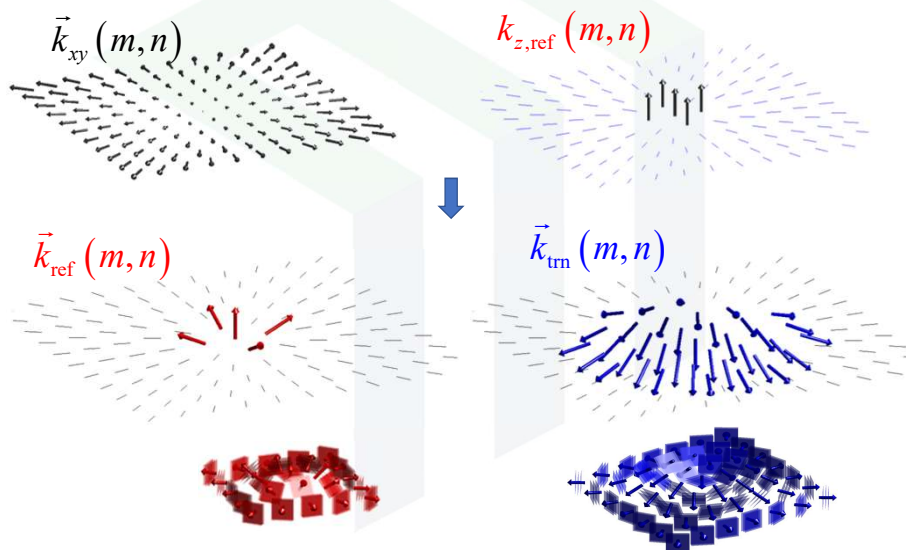
```
% Compute Longitudinal Wave Vector Components
k0 = 2*pi/lam;
kzinc = k0*nref;
kzR = sqrt((k0*nref)^2 - kx.^2 - ky.^2);
kzT = sqrt((k0*ntrn)^2 - kx.^2 - ky.^2);
```

The center few modes will have real  $k_z$ 's. These correspond to propagating waves. The others will have imaginary  $k_z$ 's and correspond to evanescent waves that do not transport energy.



## Longitudinal Wave Vector Expansion (2 of 2)

The overall wave vector expansion can be visualized this way



## Normalize to Source

When a Gaussian source is used, the energy decreases at high frequencies.

If nothing is done, lower energy observed at the high frequencies will be confused with low reflectance or transmittance.

The solution is to normalize the steady-state fields to the source.

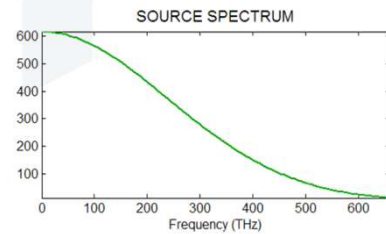
$$E_{x,\text{ref}}(f) = \frac{E_{x,\text{ref}}(f)}{E_{x,\text{src}}(f)}$$

$$E_{y,\text{ref}}(f) = \frac{E_{y,\text{ref}}(f)}{E_{y,\text{src}}(f)}$$

$$E_{x,\text{tm}}(f) = \frac{E_{x,\text{tm}}(f)}{E_{x,\text{src}}(f)}$$

$$E_{y,\text{tm}}(f) = \frac{E_{y,\text{tm}}(f)}{E_{y,\text{src}}(f)}$$

```
% Normalize to Source
Exr = Exr / SRC(nfreq);
Eyr = Eyr / SRC(nfreq);
Ext = Ext / SRC(nfreq);
Eyt = Eyt / SRC(nfreq);
```



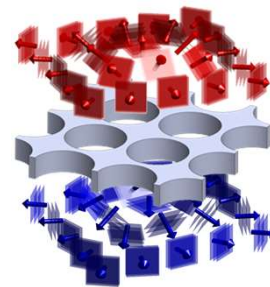
## Calculate Spatial Harmonics

Calculate the  $x$  and  $y$  amplitude coefficients of the spatial harmonics by Fourier transforming the steady-state  $E_x$  and  $E_y$ .

```
% Calculate Amplitude Components of Spatial Harmonics
Sxr = fftshift(fft2(Exr)) / (Nx*Ny);
Syr = fftshift(fft2(Eyr)) / (Nx*Ny);
Sxt = fftshift(fft2(Ext)) / (Nx*Ny);
Syt = fftshift(fft2(Eyt)) / (Nx*Ny);
```

Reflected spatial harmonics →

Transmitted spatial harmonics →



## Calculate $S_z$

It is not necessary to calculate the steady-state field  $E_z$ . Instead, calculate  $S_z$  from  $S_x$  and  $S_y$  using the divergence equation.

$$\nabla \cdot [\varepsilon_r \tilde{\mathbf{E}}(m, n)] = 0$$

$$\nabla \cdot [\tilde{\mathbf{E}}(m, n)] = 0$$

$$\nabla \cdot [\tilde{\mathbf{S}}(m, n) e^{-jk_x(m)x} e^{-jk_y(n)y} e^{-jk_z(m,n)z}] = 0$$

$$\frac{\partial}{\partial x} S_x(m, n) e^{-jk_x(m)x} e^{-jk_y(n)y} e^{-jk_z(m,n)z} + \frac{\partial}{\partial y} S_y(m, n) e^{-jk_x(m)x} e^{-jk_y(n)y} e^{-jk_z(m,n)z} + \frac{\partial}{\partial z} S_z(m, n) e^{-jk_x(m)x} e^{-jk_y(n)y} e^{-jk_z(m,n)z} = 0$$

$$k_x(m) S_x(m, n) + k_y(n) S_y(m, n) + k_z(m, n) S_z(m, n) = 0$$

$$S_z(m, n) = -\frac{k_x(m) S_x(m, n) + k_y(n) S_y(m, n)}{k_z(m, n)}$$

```
% Calculate Longitudinal Components
```

```
Szr = -(kx.*Sxr + ky.*Syr) ./kzR;
```

```
Szt = -(kx.*Sxt + ky.*Syt) ./kzT;
```

## Calculate Diffraction Efficiencies

The diffraction efficiencies are calculated from the wave vector components and the amplitudes of the spatial harmonics.

$$DE_{\text{ref}}(f; m, n) = \left| \tilde{S}_{\text{ref}}(f; m, n) \right|^2 \cdot \text{Re} \left[ \frac{k_{z,\text{ref}}(f; m, n)}{k_{z,\text{inc}}(f)} \right]$$

$$DE_{\text{tm}}(f; m, n) = \left| \tilde{S}_{\text{tm}}(f; m, n) \right|^2 \cdot \text{Re} \left[ \frac{k_{z,\text{tm}}(f; m, n) \mu_{r,\text{ref}}}{k_{z,\text{inc}}(f) \mu_{r,\text{tm}}} \right]$$

```
% Calculate Amplitude of Spatial Harmonics
```

```
Sref = abs(Sxr).^2 + abs(Syr).^2 + abs(Szr).^2;
```

```
Strn = abs(Sxt).^2 + abs(Syt).^2 + abs(Szt).^2;
```

```
% Calculate Diffraction Efficiencies
```

```
ref = real(kzR/kzinc) .* Sref;
```

```
trn = real(kzT*urref/kzinc/urtrn) .* Strn;
```

## Calculate Reflectance and Transmittance

The overall reflectance is the sum of all the diffraction efficiencies of the reflected modes. Similarly, the overall transmittance is the sum of all the diffraction efficiencies of the transmitted modes.

$$R(f) = \sum_n \sum_m DE_{\text{ref}}(f; m, n)$$

$$T(f) = \sum_n \sum_m DE_{\text{trn}}(f; m, n)$$

```
% Compute Reflectance and Transmittance
```

```
REF(nfreq) = sum(ref(:));
```

```
TRN(nfreq) = sum(trn(:));
```

It is always good practice to check for conservation of energy. When no gain or loss is incorporated into the model, the sum of the reflectance and transmittance should be 100%.

$$R(f) + T(f) = 100\%$$

```
% CALCULATE CONSERVATION OF ENERGY
```

```
CON(nfreq) = REF(nfreq) + TRN(nfreq);
```

## MATLAB's `slice()` Command for 3D Visualization

## MATLAB's `slice()` Command

```
slice(X,Y,Z,V,sx,sy,sz)
```

`X`, `Y`, and `Z` are 3D arrays generated using `meshgrid()`.

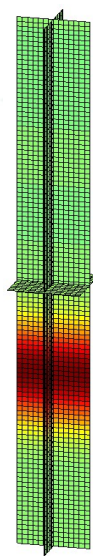
`V` is the 3D array of data to visualize.

`sx` is a 1D array of numbers of where to place slices that are perpendicular to the `x`-axis.

`sy` is a 1D array of numbers of where to place slices that are perpendicular to the `y`-axis.

`sz` is a 1D array of numbers of where to place slices that are perpendicular to the `z`-axis.

## Visualizing a 3D Data Array



```
% Draw Ex Field
slice(Y,X,-Z,Ex,0,0,0);
axis equal tight off;
colorbar;
view(-75,20);
```