Computational Science:
Introduction to Finite-Difference Time-Domain

Power Flow & PML Placement

Lecture Outline

- Review
- Total Power by Integrating the Poynting Vector
- Total Power by Plane Wave Spectrum
- Example of Grating Diffraction
- PML Placement

Review

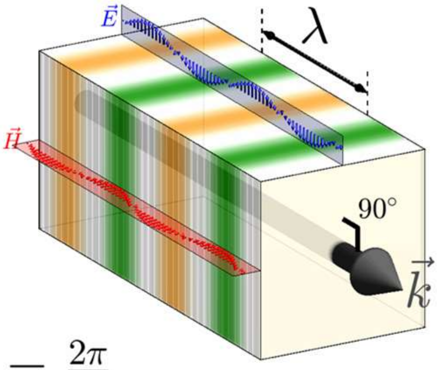
Wave Vector $\vec{k}$

The wave vector $\vec{k}$ conveys two pieces of information: (1) Magnitude conveys the wavelength λ inside the medium, and (2) direction conveys the direction of the wave and is perpendicular to the wave fronts.

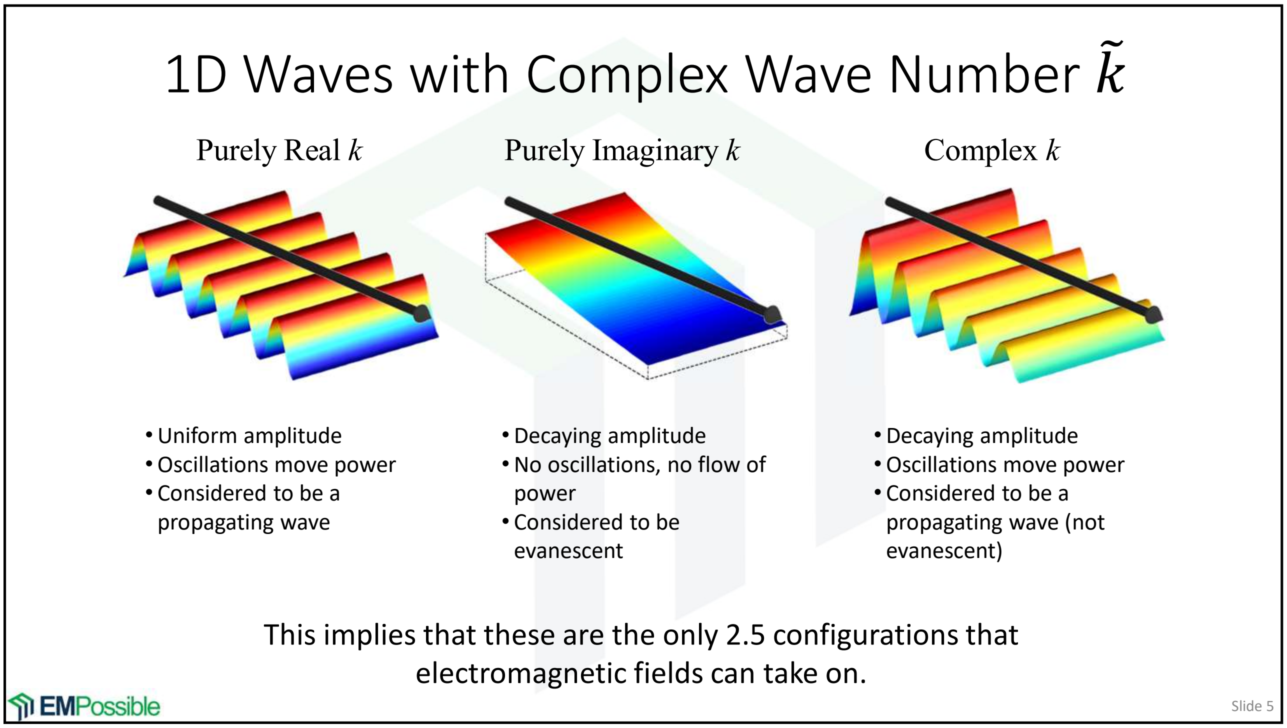
$$E(\vec{r}) = E_0 \exp\left(-j\vec{k} \bullet \vec{r}\right)$$

$$\vec{k} = k_x \hat{a}_x + k_y \hat{a}_y + k_z \hat{a}_z$$

$$\vec{r} = x\hat{x} + y\hat{y} + z\hat{z}$$ position vector



$$|\vec{k}| = \frac{2\pi}{\lambda}$$



1D Waves with Complex Wave Number $\tilde{k}$

Purely Real k

- Uniform amplitude
- Oscillations move power
- Considered to be a propagating wave

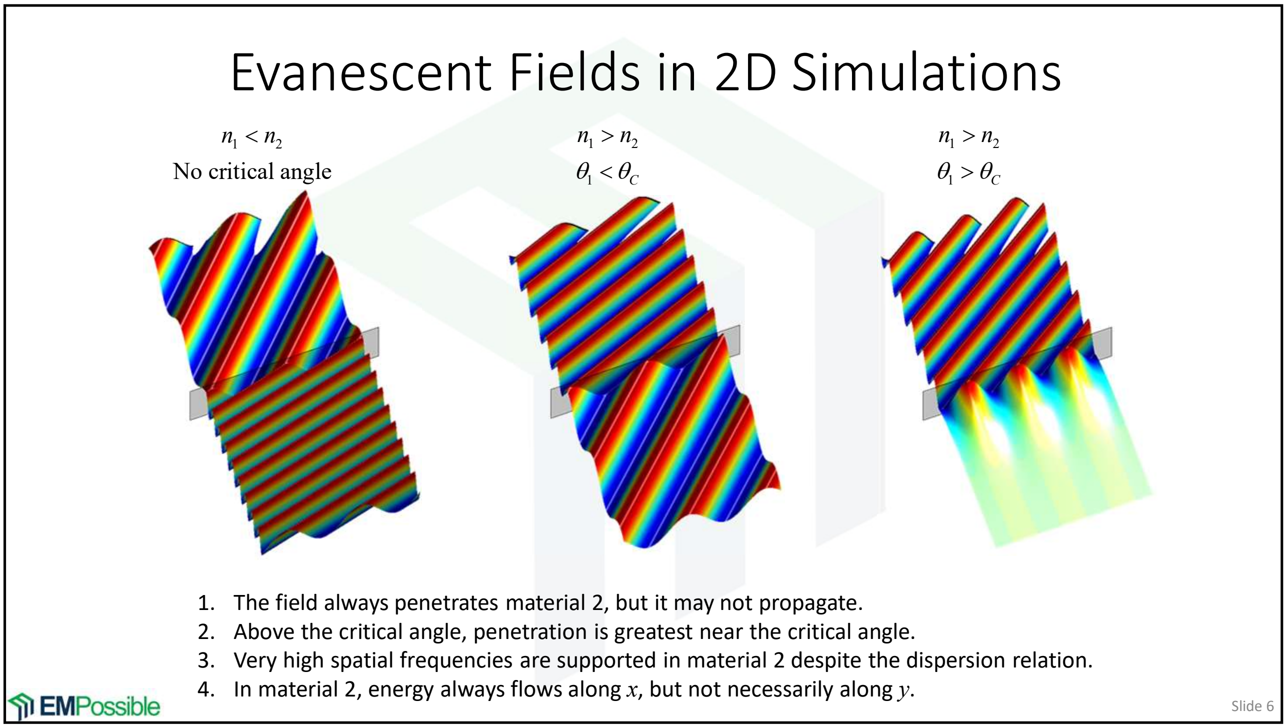
Purely Imaginary k

- Decaying amplitude
- No oscillations, no flow of power
- Considered to be evanescent

Complex k

- Decaying amplitude
- Oscillations move power
- Considered to be a propagating wave (not evanescent)

This implies that these are the only 2.5 configurations that electromagnetic fields can take on.



Evanescent Fields in 2D Simulations

$n_1 < n_2$
No critical angle

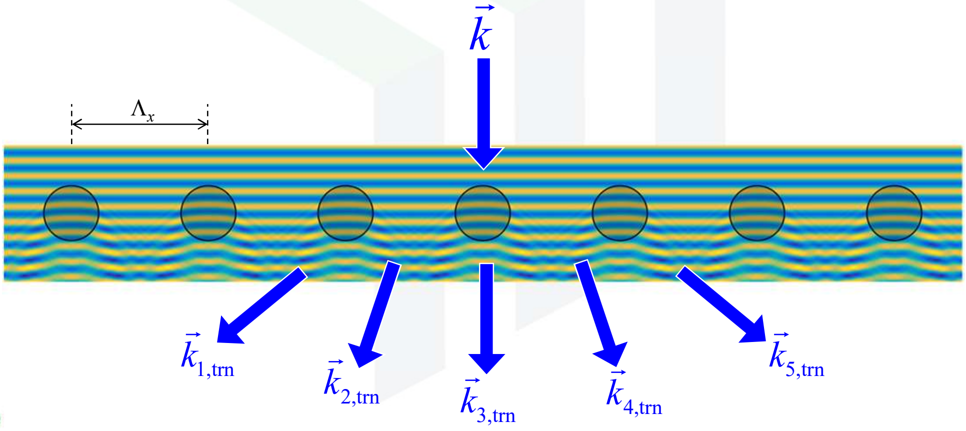
$n_1 > n_2$
$\theta_1 < \theta_C$

$n_1 > n_2$
$\theta_1 > \theta_C$

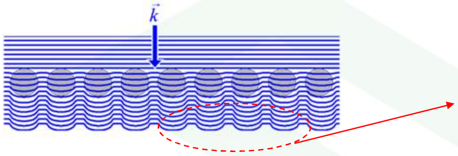
1. The field always penetrates material 2, but it may not propagate.
2. Above the critical angle, penetration is greatest near the critical angle.
3. Very high spatial frequencies are supported in material 2 despite the dispersion relation.
4. In material 2, energy always flows along x, but not necessarily along y.

Fields in Periodic Structures

Waves in periodic structures take on the same periodicity as their host.

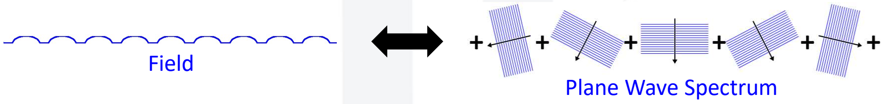


The Plane Wave Spectrum

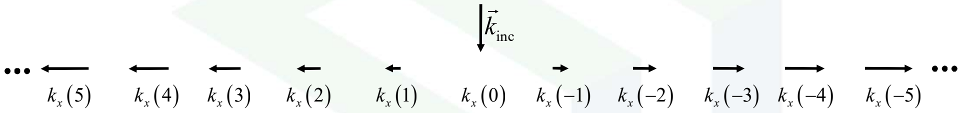


$$E(x,y)=\sum_{m=-\infty}^{\infty} S(m)\,e^{j\vec{k}(m)\bullet\vec{r}}$$

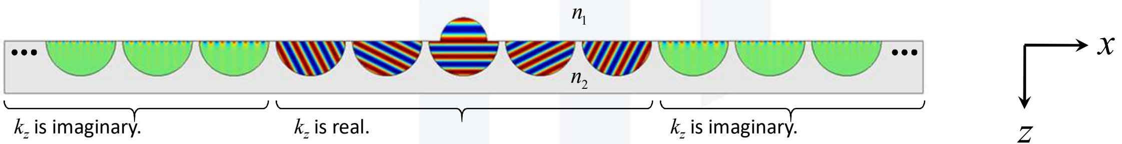
Terms were rearranged to show that a periodic field can also be thought of as an infinite sum of plane waves at different angles. This is the "plane wave spectrum" of a periodic field.



Visualizing Phase Matching into the Grating



Each of these is phase matched into material 2. The longitudinal component of the wave vector is calculated using the dispersion relation in material 2.



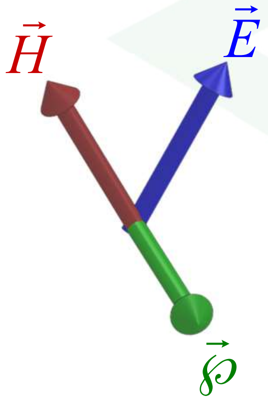
k_z is imaginary.
The field in material 2
is evanescent.

k_z is real.
A wave propagates into material 2.

k_z is imaginary.
The field in material 2
is evanescent.

Total Power by Integrating Poynting Vector

Concept of Integrating the Poynting Vector



The Poynting vector is the instantaneous flow of power.

$$\vec{\wp}(t)=\vec{E}(t)\times\vec{H}(t)$$

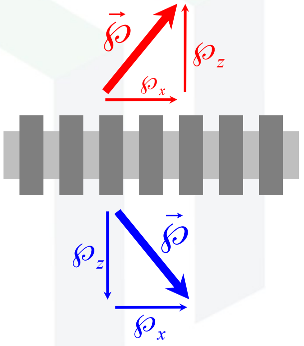
Integrate the Poynting vector to calculate total power flowing out of the grid at any instant.

$$P=\iint_S \vec{\wp}\bullet d\vec{s}$$

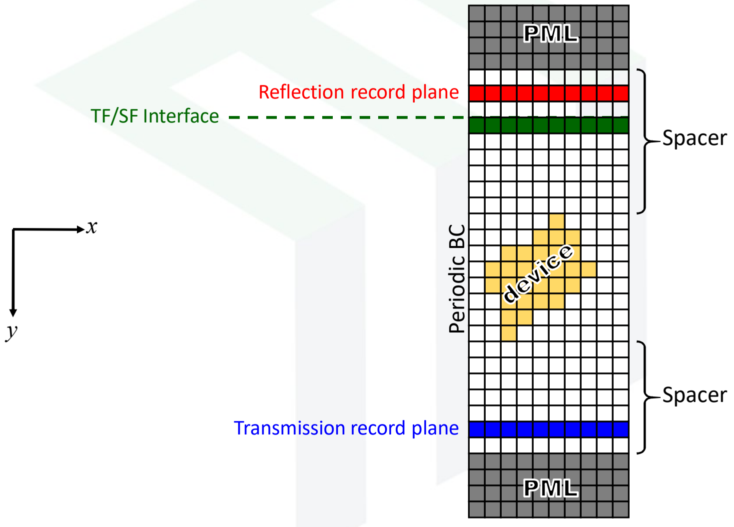
S is the cross section of the grid.

Power Flow Out of Devices

To calculate the power flow away from a device, we are only interested in the normal component of the Poynting vector $\wp_z$. For the diagram below, it is the z-component.



Grid Strategy



Power Flow in Electromagnetics

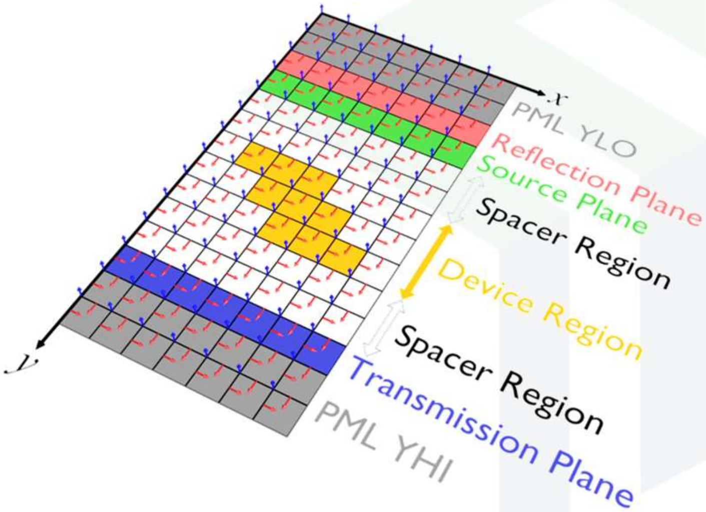
The power density of an electromagnetic wave is quantified by the Poynting vector $\vec{\wp}$.

$$\vec{\wp}_{\text{rms}} = \frac{1}{2}\text{Re}\left[\vec{E}\times\vec{H}^*\right] = -\frac{1}{2\eta_0}\text{Re}\left[j\vec{E}\times\vec{\tilde{H}}^*\right]$$

Total power flow through an area A is calculated by integrating the Poynting vector over that area.

$$P = \iint_A \vec{\wp}_{\text{rms}}\,dA$$

Power Flow on 2D Yee Grid



Only power flowing the y direction is of interest.

$$\wp_y^{i,j} = \frac{1}{2\eta_0}\text{Re}\left[jE_z^{i,j}\left(\tilde{H}_x^{i,j}\right)^*\right]$$

PROBLEM!!

E_z and H_x are at physically different locations in each cell.

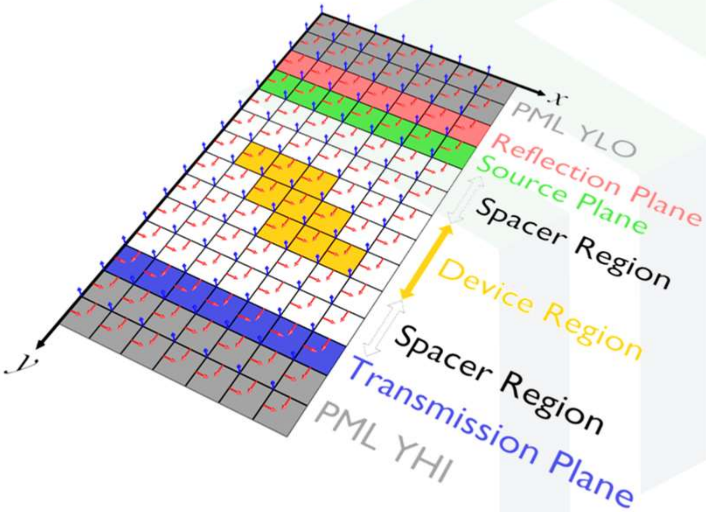
Must interpolate H_x to exist at same points at E_z .

$$\left\langle \tilde{H}_x^{i,j} \right\rangle = \frac{\tilde{H}_x^{i,j-1} + \tilde{H}_x^{i,j}}{2}$$

Power flow is then

$$\wp_y^{i,j} = \frac{1}{2\eta_0}\text{Re}\left[jE_z^{i,j}\left(\frac{\tilde{H}_x^{i,j-1} + \tilde{H}_x^{i,j}}{2}\right)^*\right]$$

Reflectance & Transmittance



Total Power Flow

$$P_{\text{inc}} \propto \cos\left(\theta_{\text{inc}}\right) N_x / n_{\text{inc}}$$

$$P_{\text{ref}} \propto \sum_{i=1}^{N_x} \wp_y^{i,j_{\text{ref}}}$$

$$P_{\text{trn}} \propto \sum_{i=1}^{N_x} \wp_y^{i,j_{\text{trn}}}$$

Reflectance & Transmittance

$$R = \frac{P_{\text{ref}}}{P_{\text{inc}}} \equiv \text{Reflectance}$$

$$T = \frac{P_{\text{trn}}}{P_{\text{inc}}} \equiv \text{Transmittance}$$

Total Power by Plane Wave Spectrum

Electromagnetic Power Flow

The instantaneous direction and intensity of power flow at any point in space is given by the Poynting vector.

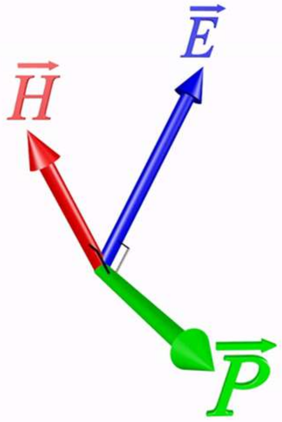
$$\vec{\wp}(\vec{r},t)=\vec{E}(\vec{r},t)\times\vec{H}(\vec{r},t)$$

The RMS power flow is then

$$\vec{\wp}(\vec{r},\omega)=\frac{1}{2}\text{Re}\left[\vec{E}(\vec{r},\omega)\times\vec{H}^{*}(\vec{r},\omega)\right]$$

This is typically just written in the frequency-domain as

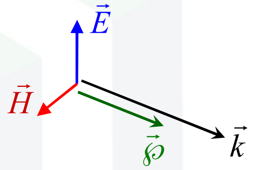
$$\vec{\wp}=\frac{1}{2}\text{Re}\left[\vec{E}\times\vec{H}^{*}\right] \qquad * \equiv \text{complex conjugate}$$



Power Flow in LHI Materials

The regions outside a grating are almost always linear, homogeneous, and isotropic (LHI). In this case $\vec{E}$, $\vec{H}$, and $\vec{k}$ are all perpendicular. In addition, power flows in the same direction as $\vec{k}$.

$$\vec{E}\perp\vec{H}\perp\vec{k} \qquad \frac{\vec{\wp}}{|\vec{\wp}|}=\frac{\vec{k}}{|\vec{k}|}$$



Under these conditions, the expression for RMS power flow becomes

$$\begin{aligned}\vec{\wp}&=\frac{1}{2}\mathrm{Re}\left[\vec{E}\times\vec{H}^*\right]\\&=\frac{1}{2}\mathrm{Re}\left[\frac{\vec{k}}{|\vec{k}|}\cdot|\vec{E}|\cdot|\vec{H}|\right]\end{aligned}$$

$|\vec{E}|\cdot|\vec{H}|$ is the magnitude of the cross product

$\frac{\vec{k}}{|\vec{k}|}$ is the direction of the cross product

Eliminate the Magnetic Field

The field magnitudes in LHI materials are related through the material impedance η.

$$\frac{|\vec{E}|}{|\vec{H}|}=\eta$$

This is sort of like Ohm's law from circuit theory.

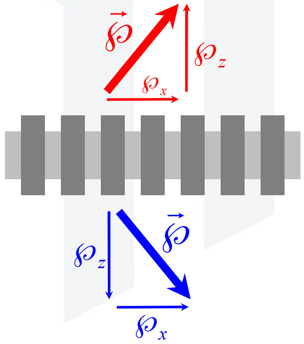
Given this relation, we can eliminate $\vec{H}$ from the expression for RMS power flow.

$$\vec{\wp}=\frac{1}{2}\mathrm{Re}\left[\frac{\vec{k}}{|\vec{k}|}\cdot|\vec{E}|\cdot|\vec{H}|\right]=\frac{1}{2}\mathrm{Re}\left[\frac{\vec{k}}{|\vec{k}|}\frac{|\vec{E}|^2}{\eta}\right]$$

Power Flow Away From Grating

To calculate the power flowing away from the grating, only the z-component of the Poynting vector is of interest.

$$\vec{\wp} = \frac{1}{2}\mathrm{Re}\left[\frac{\vec{k}}{\left|\vec{k}\right|}\frac{\left|\vec{E}\right|^2}{\eta}\right] \rightarrow \wp_z = \frac{1}{2}\mathrm{Re}\left[\frac{k_z}{\left|\vec{k}\right|}\frac{\left|\vec{E}\right|^2}{\eta}\right]$$



RMS Power of the Diffracted Modes

Recall that the field scattered from a periodic structure can be decomposed into a Fourier series.

$$\vec{E}(x,z) = \sum_{m=-\infty}^{\infty} \vec{S}(m)\, e^{-jk_x(m)x} e^{-jk_z(m)z}$$

$$k_x(m) = k_{x,\mathrm{inc}} - \frac{2\pi m}{\Lambda_x}$$

$$k_z(m) = \sqrt{(k_0 n)^2 - k_x^2(m)}$$

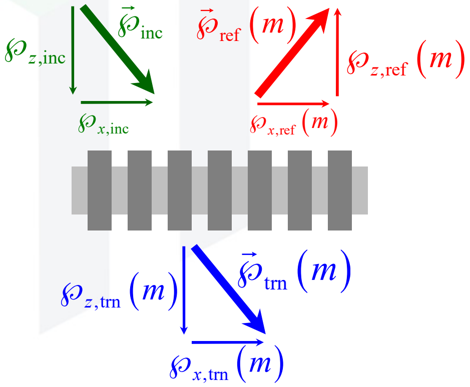
The term $S(m)$ is the amplitude and polarization of the m^{th} diffracted harmonic. Therefore, power flow away from the grating due to the m^{th} diffracted order is

$$\wp_z = \frac{1}{2}\mathrm{Re}\left[\frac{k_z}{\left|\vec{k}\right|}\frac{\left|\vec{E}\right|^2}{\eta}\right] \rightarrow \wp_z(m) = \frac{1}{2}\mathrm{Re}\left[\frac{k_z(m)}{\left|\vec{k}(m)\right|}\frac{\left|\vec{S}(m)\right|^2}{\eta}\right]$$

Power of the Incident Wave

From the previous equation, the power flow of the incident wave into the grating is

$$\wp_{z,\text{inc}} = \frac{1}{2}\text{Re}\left[\frac{k_{z,\text{inc}}}{\left|\vec{k}_{\text{inc}}\right|}\frac{\left|\vec{S}_{\text{inc}}\right|^2}{\eta_{\text{inc}}}\right]$$



Diffraction Efficiency

Diffraction efficiency is defined as the power in a specific diffraction order divided by the applied incident power.

$$\text{DE}(m) = \frac{\wp_z(m)}{\wp_{z,\text{inc}}}$$

Despite the title "efficiency," we don't always want this number to be large. We often want to control how much power gets diffracted into each mode. So it is not good or bad to have high or low diffraction efficiency.

Assuming the materials have no loss or gain, conservation of energy requires that

$$1 = \sum_{m=-\infty}^{\infty}\text{DE}_{\text{ref}}(m) + \sum_{m=-\infty}^{\infty}\text{DE}_{\text{trn}}(m)$$

General Case

$$\left(\sum_{m=-\infty}^{\infty}\text{DE}_{\text{ref}}(m) + \sum_{m=-\infty}^{\infty}\text{DE}_{\text{trn}}(m)\right) \begin{array}{ll} <1 & \text{materials have loss} \\ =1 & \text{materials have no loss} \\ >1 & \text{materials have gain} \end{array}$$

Conservation of Power

The power injected into a device by the source wave must go somewhere. It can only be reflected, transmitted, or absorbed.

This leads to the conservation equation:

$$\begin{pmatrix}\text{Source}\\\text{Power}\end{pmatrix}=\begin{pmatrix}\text{Absorbed}\\\text{Power}\end{pmatrix}+\begin{pmatrix}\text{Reflected}\\\text{Power}\end{pmatrix}+\begin{pmatrix}\text{Transmitted}\\\text{Power}\end{pmatrix}$$

$$P_{\text{src}} = P_{\Omega} + P_{\text{ref}} + P_{\text{trn}}$$

Typically, we normalize this equation by dividing by P_{src}.
This normalizes the parameters to the power of the source.

$$\boxed{1 = A + R + T}$$

Absorbance Reflectance Transmittance

Putting it All Together

So far, expressions have been derived for the incident power and power in the spatial harmonics.

$$\wp_{z,\text{inc}} = \frac{1}{2}\text{Re}\left[\frac{k_{z,\text{inc}}}{\left|\vec{k}_{\text{inc}}\right|}\frac{\left|\vec{S}_{\text{inc}}\right|^2}{\eta_{\text{inc}}}\right] \qquad \wp_{z,\text{ref}}(m) = \frac{1}{2}\text{Re}\left[\frac{k_{z,\text{ref}}(m)}{\left|\vec{k}_{\text{ref}}(m)\right|}\frac{\left|\vec{S}_{\text{ref}}(m)\right|^2}{\eta_{\text{ref}}}\right] \qquad \wp_{z,\text{trn}}(m) = \frac{1}{2}\text{Re}\left[\frac{k_{z,\text{trn}}(m)}{\left|\vec{k}_{\text{trn}}(m)\right|}\frac{\left|\vec{S}_{\text{trn}}(m)\right|^2}{\eta_{\text{trn}}}\right]$$

The diffraction efficiency of the m^{th} harmonic was also defined.

$$\text{DE}(m) = \frac{\wp_z(m)}{\wp_{z,\text{inc}}}$$

Now, expressions for the diffraction efficiencies of the spatial harmonics can be derived by combining the above expressions.

$$\text{DE}_{\text{ref}}(m) = \frac{\wp_{z,\text{ref}}(m)}{\wp_{z,\text{inc}}} = \frac{\left|\vec{S}_{\text{ref}}(m)\right|^2}{\left|\vec{S}_{\text{inc}}\right|^2}\text{Re}\left[\frac{k_{z,\text{ref}}(m)}{k_{z,\text{inc}}}\right] \qquad \text{DE}_{\text{trn}}(m) = \frac{\wp_{z,\text{trn}}(m)}{\wp_{z,\text{inc}}} = \frac{\left|\vec{S}_{\text{trn}}(m)\right|^2}{\left|\vec{S}_{\text{inc}}\right|^2}\text{Re}\left[\frac{k_{z,\text{trn}}(m)}{k_{z,\text{inc}}}\frac{\mu_{r,\text{ref}}}{\mu_{r,\text{trn}}}\right]$$

Note that:

$$\left|\vec{k}_{\text{inc}}\right| = \left|\vec{k}_{\text{ref}}(m)\right|$$

$$\eta_{\text{inc}} = \eta_{\text{ref}}$$

Diffraction Efficiency for Magnetic Fields

Diffraction efficiency equations were just derived that are based on having calculated the electric fields only.

$$\vec{S}_m \equiv \text{Electric field amplitude of the } m^{\text{th}} \text{ spatial harmonic}$$

$$\text{DE}_{\text{ref}}(m) = \frac{\wp_{z,\text{ref}}(m)}{\wp_{z,\text{inc}}} = \frac{\left|\vec{S}_{\text{ref}}(m)\right|^2}{\left|\vec{S}_{\text{inc}}\right|^2}\text{Re}\left[\frac{k_{z,\text{ref}}(m)}{k_{z,\text{inc}}}\right] \qquad \text{DE}_{\text{trn}}(m) = \frac{\wp_{z,\text{trn}}(m)}{\wp_{z,\text{inc}}} = \frac{\left|\vec{S}_{\text{trn}}(m)\right|^2}{\left|\vec{S}_{\text{inc}}\right|^2}\text{Re}\left[\frac{k_{z,\text{trn}}(m)}{k_{z,\text{inc}}}\frac{\mu_{r,\text{ref}}}{\mu_{r,\text{trn}}}\right]$$

Sometimes Maxwell's equations are solved for the magnetic fields (i.e. Hz mode) In this case, the diffraction efficiency equations are

$$\vec{U}_m \equiv \text{Magnetic field amplitude of the } m^{\text{th}} \text{ spatial harmonic}$$

$$\text{DE}_{\text{ref}}(m) = \frac{\wp_{z,\text{ref}}(m)}{\wp_{z,\text{inc}}} = \frac{\left|\vec{U}_{\text{ref}}(m)\right|^2}{\left|\vec{U}_{\text{inc}}\right|^2}\text{Re}\left[\frac{k_{z,\text{ref}}(m)}{k_{z,\text{inc}}}\right] \qquad \text{DE}_{\text{trn}}(m) = \frac{\wp_{z,\text{trn}}(m)}{\wp_{z,\text{inc}}} = \frac{\left|\vec{U}_{\text{trn}}(m)\right|^2}{\left|\vec{U}_{\text{inc}}\right|^2}\text{Re}\left[\frac{k_{z,\text{trn}}(m)}{k_{z,\text{inc}}}\frac{\varepsilon_{r,\text{ref}}}{\varepsilon_{r,\text{trn}}}\right]$$

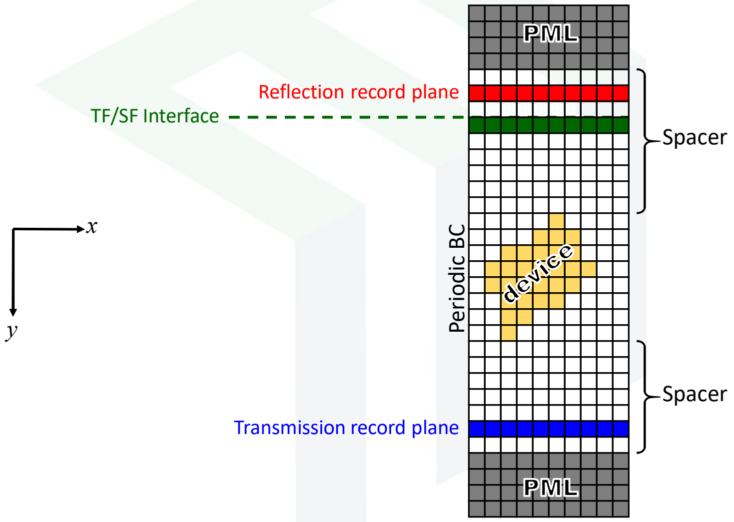
Calculating Power Flow in FDTD

Process of Calculating Transmittance and Reflectance

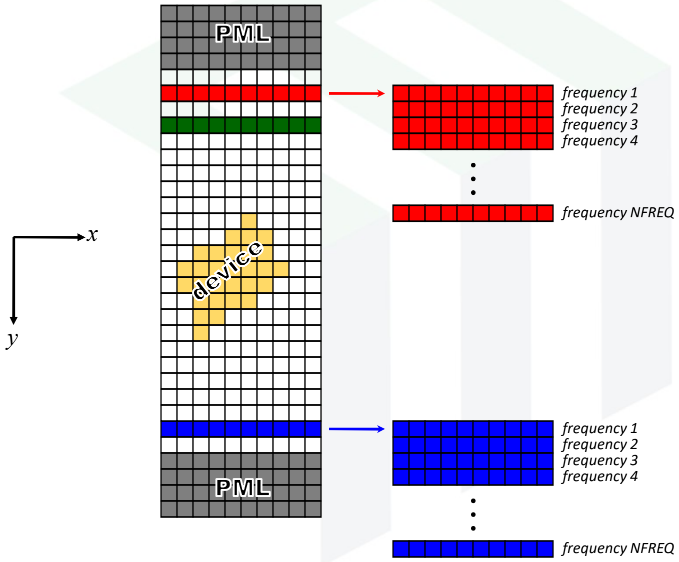
1. Perform FDTD simulation
   a) Calculate the steady-state field in the reflected and transmitted record planes.

2. For each frequency of interest…
   a) Calculate the wave vector components of the spatial harmonics
   b) Calculate the complex amplitude of the spatial harmonics
   c) Calculate the diffraction efficiency of the spatial harmonics
   d) Calculate over all reflectance and transmittance
   e) Calculate energy conservation.

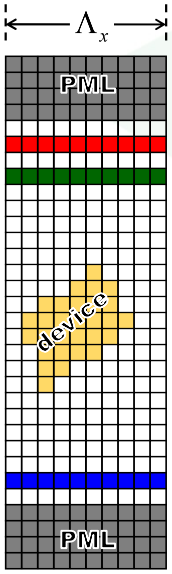
Step 1: Perform FDTD Simulation



Step 2: Calculate Steady-State Fields



Step 3: Calculate Wave Vector Components



`Nx` points across

Note: This calculation is performed separately for every frequency of interest.

Transverse Components

$$k_x(m) = -\frac{2\pi m}{\Lambda_x}$$

$$m = -\operatorname{floor}\left(\frac{N_x}{2}\right), \cdots, -2, -1, 0, 1, 2, \cdots, \operatorname{floor}\left(\frac{N_x}{2}\right)$$

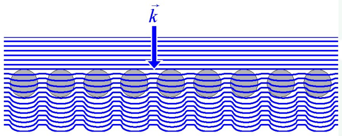
Longitudinal Components

$$k_{y,\text{ref}}(m) = \sqrt{\left(k_0 n_{\text{ref}}\right)^2 - k_x^2(m)}$$

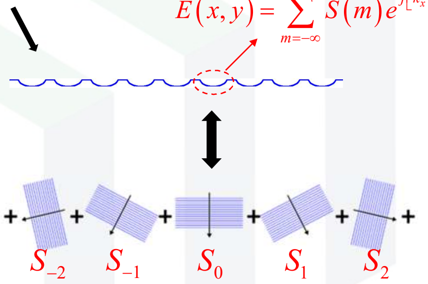
$$k_{y,\text{trn}}(m) = \sqrt{\left(k_0 n_{\text{trn}}\right)^2 - k_x^2(m)}$$

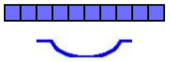
Step 4: Calculate the Amplitudes of the Spatial Harmonics

Note: This calculation is performed separately for every frequency of interest.



$$E(x,y)=\sum_{m=-\infty}^{\infty} S(m)e^{j\left[k_x(m)x+k_y(m)y\right]}$$





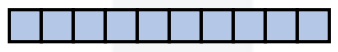
$$\text{FFT}\left[\quad\right]=\left[S_{-M}\ \cdots\ S_{-2}\ S_{-1}\ S_0\ S_1\ S_2\ \cdots\ S_M\right]$$

Step 5: Calculate Diffraction Efficiencies

Note: This calculation is performed separately for every frequency of interest.

$$\text{DE}_{\text{ref}}(m)=\frac{\left|\vec{S}_{\text{ref}}(m)\right|^2}{\left|\vec{S}_{\text{inc}}\right|^2}\text{Re}\left[\frac{k_{z,\text{ref}}(m)}{k_{z,\text{inc}}}\right]$$

$$\text{DE}_{\text{trn}}(m)=\frac{\left|\vec{S}_{\text{trn}}(m)\right|^2}{\left|\vec{S}_{\text{inc}}\right|^2}\text{Re}\left[\frac{k_{z,\text{trn}}(m)}{k_{z,\text{inc}}}\frac{\mu_{r,\text{ref}}}{\mu_{r,\text{trn}}}\right]$$



Note 1: $\left|\vec{S}_{\text{inc}}\right|$ is the amplitude of the source obtained by Fourier transforming the source function.

Note 2: This operation is performed for every frequency of interest.

Step 6: Reflectance and Transmittance

Reflectance is the total fraction of power reflected from a device. Therefore, it is equal to the sum of all the reflected modes.

$$R\left(f\right)=\sum_{N_x}\mathrm{DE}_{\mathrm{ref}}\left(m,f\right)$$ 🟧

Note: This calculation is performed separately for every frequency of interest.

Transmittance is the total fraction of power transmitted through a device. Therefore, it is equal to the sum of all the transmitted modes.

$$T\left(f\right)=\sum_{N_x}\mathrm{DE}_{\mathrm{trn}}\left(m,f\right)$$ 🟦

Step 7: Calculate Power Conservation

Assuming you have not included loss or gain into your simulation, the reflectance plus transmittance should equal 100%.

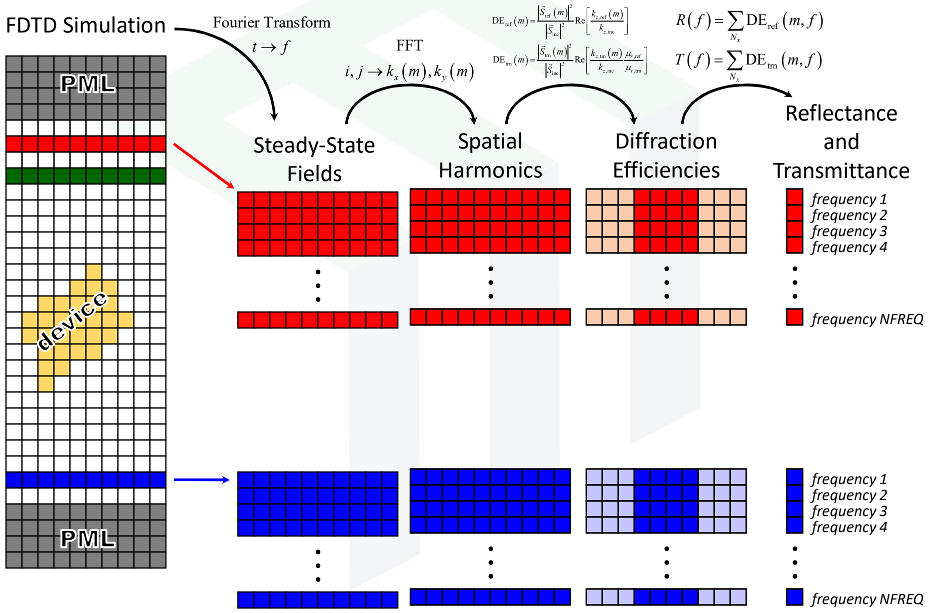
$$R\left(f\right)+T\left(f\right)=100\%$$ ⬛

Note: This calculation is performed separately for every frequency of interest.

It is ALWAYS good practice to calculate this total to check for conservation of energy. This may deviate from 100% when:

- Energy still remains on the grid and more iterations are needed.
- The boundary conditions are not working properly and need to be corrected.
- Rounding errors are two severe and greater grid resolution is needed.
- You have included loss or gain into you materials.

Visualizing All of the Data Arrays



$$\mathrm{DE}_{\mathrm{ref}}(m) = \frac{\left|\vec{S}_{\mathrm{ref}}(m)\right|^2}{\left|\vec{S}_{\mathrm{inc}}\right|^2}\mathrm{Re}\left[\frac{k_{z,\mathrm{ref}}(m)}{k_{z,\mathrm{inc}}}\right]$$

$$\mathrm{DE}_{\mathrm{trn}}(m) = \frac{\left|\vec{S}_{\mathrm{trn}}(m)\right|^2}{\left|\vec{S}_{\mathrm{inc}}\right|^2}\mathrm{Re}\left[\frac{k_{z,\mathrm{trn}}(m)}{k_{z,\mathrm{inc}}}\frac{\mu_{r,\mathrm{ref}}}{\mu_{r,\mathrm{trn}}}\right]$$

$$R(f) = \sum_{N_x}\mathrm{DE}_{\mathrm{ref}}(m,f)$$

$$T(f) = \sum_{N_x}\mathrm{DE}_{\mathrm{trn}}(m,f)$$

Procedure for FDTD

1. Simulate the device using FDTD and calculate the steady-state field at the reflection and transmission record planes.
   $E_{\mathrm{ref}}(x,f), E_{\mathrm{trn}}(x,f)$ and $E_{\mathrm{src}}(f)$
2. Calculate the incident wave vector: $k_{y,\mathrm{inc}} = k_0 n_{\mathrm{inc}}$
3. Calculate periodic expansion of the transverse wave vector
   $k_x(m) = -2\pi m / L_x \qquad m = -\mathrm{floor}[N_x/2], \cdots, -1, 0, 1, \cdots \mathrm{floor}[N_x/2]$
4. Calculate longitudinal wave vector components in the reflected and transmitted regions.
   $k_{y,\mathrm{ref}}(m) = \sqrt{(k_0 n_{\mathrm{ref}})^2 - k_x^2(m)} \qquad k_{y,\mathrm{trn}}(m) = \sqrt{(k_0 n_{\mathrm{trn}})^2 - k_x^2(m)}$
5. Normalize the steady-state fields to the source
   $\hat{E}_{\mathrm{ref}}(x,f) = E_{\mathrm{ref}}(x,f) \div E_{\mathrm{src}}(f) \qquad \hat{E}_{\mathrm{trn}}(x,f) = E_{\mathrm{trn}}(x,f) \div E_{\mathrm{src}}(f)$
6. Calculate the complex amplitudes of the spatial harmonics
   $S_{\mathrm{ref}}(m,f) = \mathrm{FFT}\left\{\hat{E}_{\mathrm{ref}}(x,f)\right\} \qquad S_{\mathrm{trn}}(m,f) = \mathrm{FFT}\left\{\hat{E}_{\mathrm{trn}}(x,f)\right\}$
7. Calculate the diffraction efficiencies of the spatial harmonics
   $\mathrm{DE}_{\mathrm{ref}}(m,f) = \left|S_{\mathrm{ref}}(m,f)\right|^2 \cdot \mathrm{Re}\left[\frac{k_{y,\mathrm{ref}}(m)}{k_{y,\mathrm{inc}}}\right] \qquad \mathrm{DE}_{\mathrm{trn}}(m,f) = \left|S_{\mathrm{trn}}(m,f)\right|^2 \cdot \mathrm{Re}\left[\frac{k_{y,\mathrm{trn}}(m)}{k_{y,\mathrm{inc}}}\frac{\mu_{\mathrm{ref}}}{\mu_{\mathrm{trn}}}\right]$
8. Calculate reflectance, transmittance, and conservation of energy.
   $R(f) = \sum_m \mathrm{DE}_{\mathrm{ref}}(m,f) \qquad T(f) = \sum_m \mathrm{DE}_{\mathrm{trn}}(m,f) \qquad C(f) = R(f) + T(f)$

frequency

MATLAB Code for Calculating Power

```
% INITIALIZE REFLECTANCE AND TRANSMITTANCE
REF = zeros(1,NFREQ);
TRN = zeros(1,NFREQ);

% LOOP OVER FREQUENCY
for nfreq = 1 : NFREQ
    % Compute Wave Vector Components
    lam0  = c0/FREQ(nfreq);                 %free space wavelength
    k0    = 2*pi/lam0;                      %free space wave number
    kyinc = k0*nref;                        %incident wave vector
    m     = [-floor(Nx/2):floor(Nx/2)]';    %spatial harmonic orders
    kx    =  - 2*pi*m/Sx;                   %wave vector expansion
    kyR   = sqrt((k0*nref)^2 - kx.^2);      %ky in reflection region
    kyT   = sqrt((k0*ntrn)^2 - kx.^2);      %ky in transmission region

    % Compute Reflectance
    ref = Eref(:,nfreq)/SRC(nfreq);         %normalize to source
    ref = fftshift(fft(ref))/Nx;            %compute spatial harmonics
    ref = real(kyR/kyinc) .* abs(ref).^2;   %compute diffraction eff.
    REF(nfreq) = sum(ref);                  %compute reflectance

    % Compute Transmittance
    trn = Etrn(:,nfreq)/SRC(nfreq);         %normalize to source
    trn = fftshift(fft(trn))/Nx;            %compute spatial harmonics
    trn = real(kyT/kyinc) .* abs(trn).^2;   %compute diffraction eff.
    TRN(nfreq) = sum(trn);                  %compute transmittance
end

% CALCULATE CONSERVATION OF ENERGY
CON = REF + TRN;
```

EMPossible

Example of Grating Diffraction

Binary Grating (Use as a Benchmark)

$\Lambda = 1.5\text{ cm}$

$d = 0.75\text{ cm}$

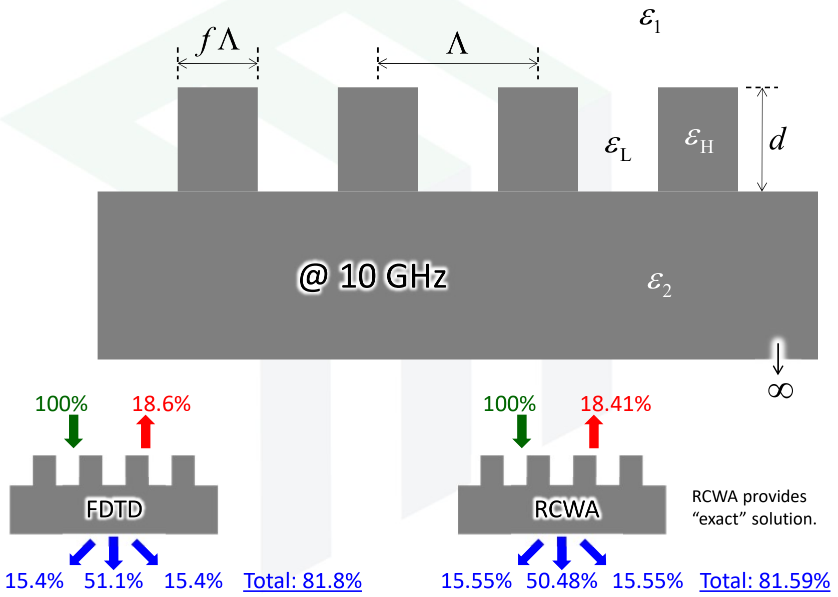
$f = 50\%$

$\varepsilon_1 = 1.0$

$\varepsilon_2 = 9.0$

$\varepsilon_L = 1.0$

$\varepsilon_H = 9.0$



RCWA provides "exact" solution.

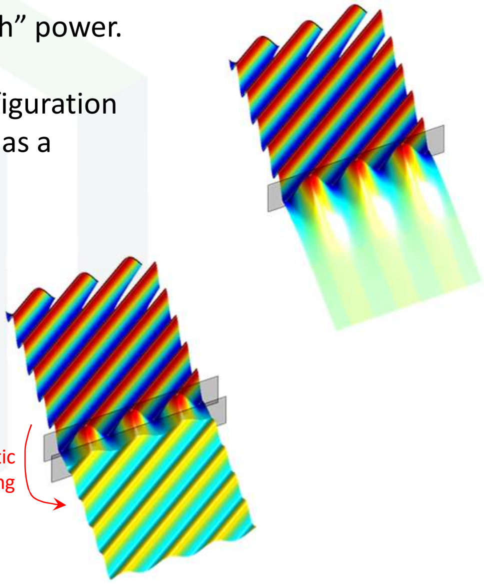
PML Placement

Electromagnetic Tunneling

Evanescent fields do not oscillate so they cannot “push” power.

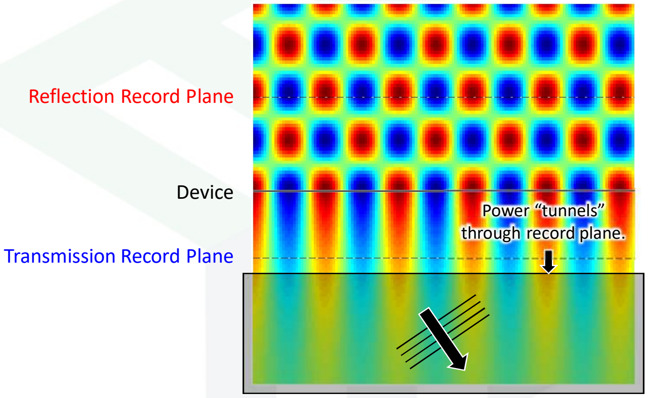
Usually, an evanescent field is just a “temporary” configuration field power is stored. Eventually, the power leaks out as a propagating wave.

There exists one exception (maybe more) where evanescent fields contribute to power transport. This happens when a high refractive index material cuts through the evanescent field. The field may then become propagating in the high-index material. This is analogous to electron tunneling in semiconductors.



Electromagnetic Tunneling

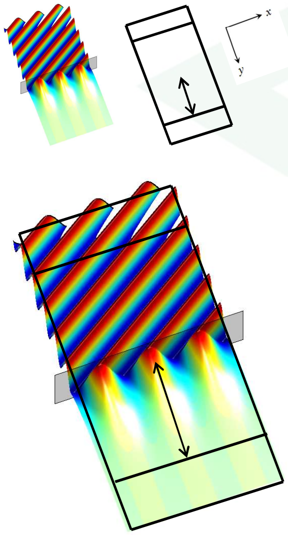
PMLs Should Not Touch Evanescent Fields



Power “tunnels” through record plane.

- Fields that are evanescent at the record plane will not be counted as transmitted power.
- Evanescent fields can become propagating waves inside the PML and tunnel power out of the model.
- This provides an unaccounted for escape path for power.

Evanescent Fields in 2D Simulations



When a model incorporates waves at angles, fields can become evanescent.

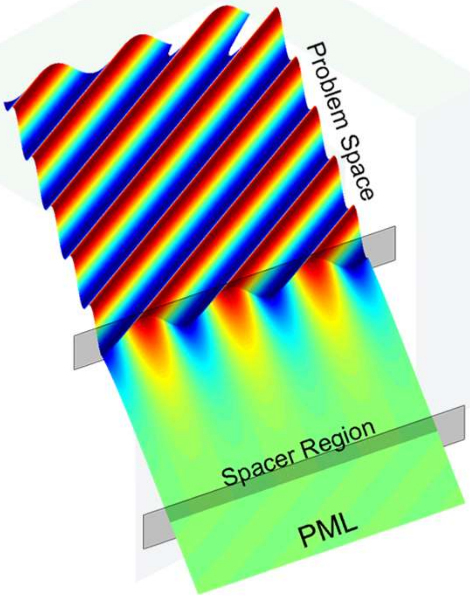
It is good practice to place the PML well outside of the evanescent field.

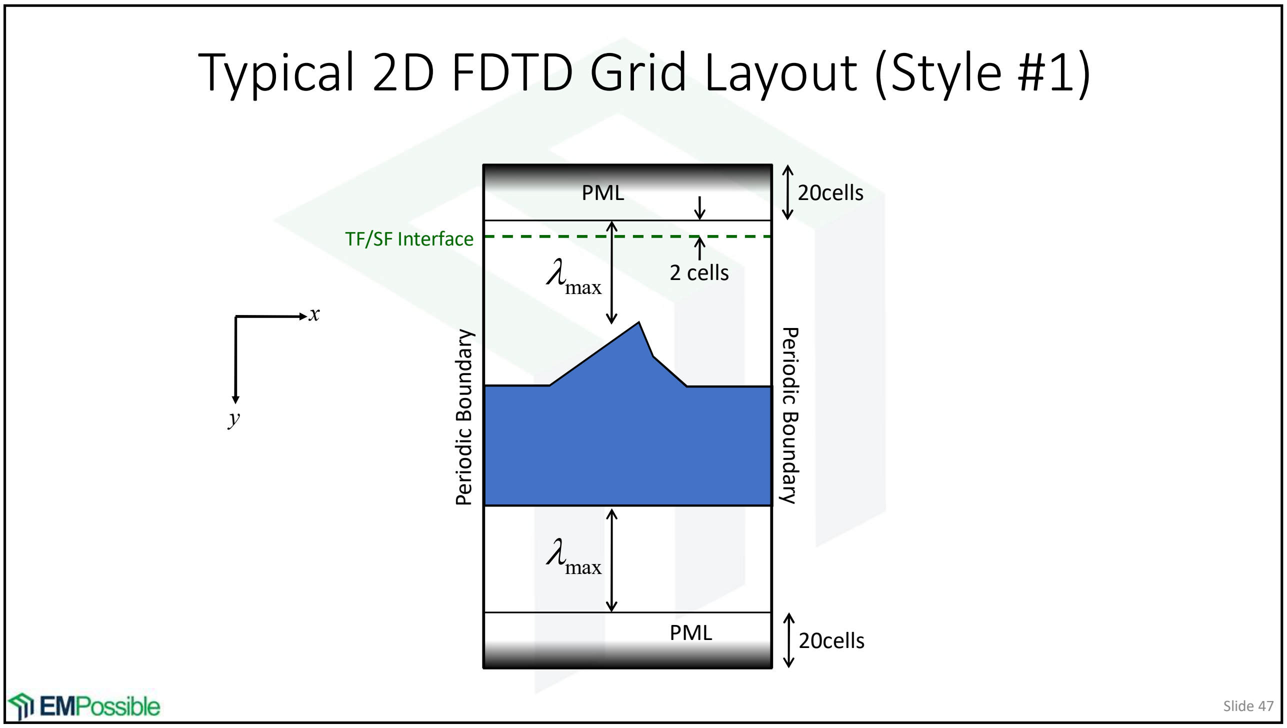
For non-resonant devices, the space between the device and PML is typically $\lambda/4$. For resonant devices, this is more commonly λ.

Some structures have evanescent fields that extend many wavelengths. You can identify this situation by visualizing your fields during the simulation.

To be sure, run a simulation and visualize the field.

Animation of Impact of Spacer Region





Typical 2D FDTD Grid Layout (Style #1)

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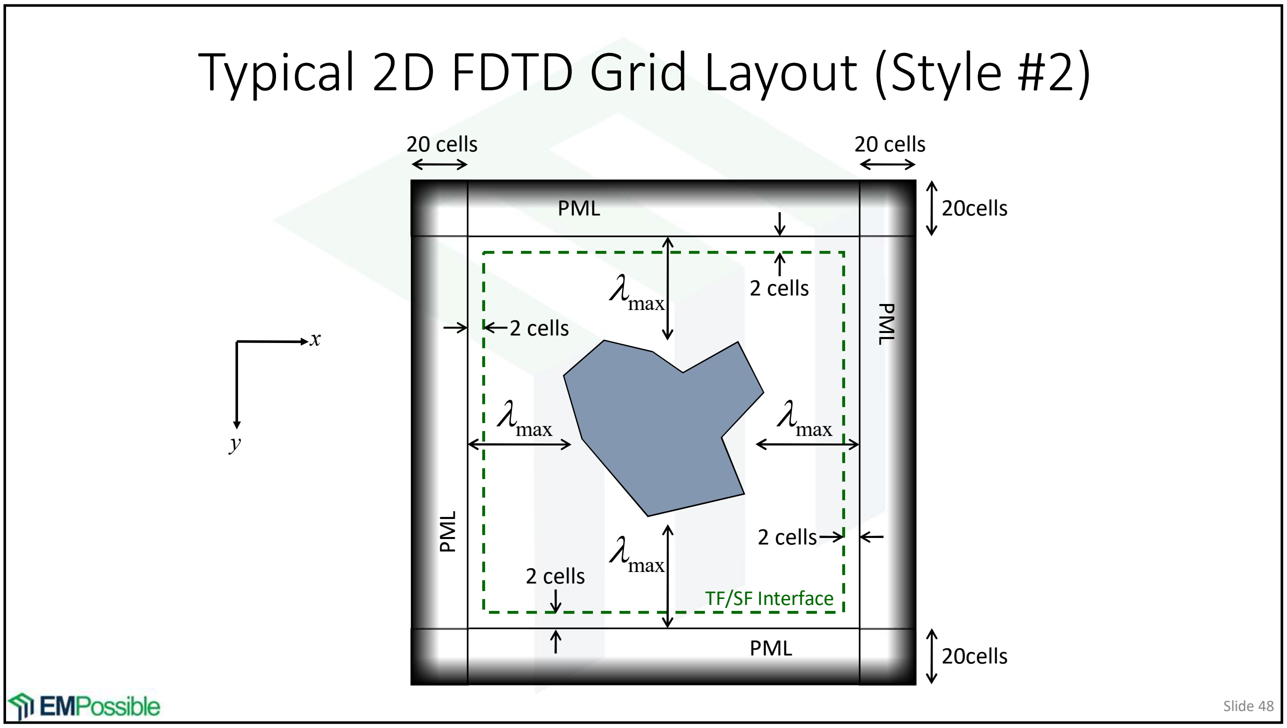

Typical 2D FDTD Grid Layout (Style #2)

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