



Advanced Computation:
Computational Electromagnetics

The Method of Lines (MoL)

Outline

- Formulation of 3D method of lines
- Formulation of 2D method of lines
- Multilayer devices using scattering matrices
- Comparison to RCWA

Definition of Method of Lines (MoL)

The method of lines was developed by mathematicians to solve partial differential equations (PDEs).

All but one independent variables are discretized.

This leads to a large set of coupled ordinary differential equations (ODEs).

The system of ODEs are solved analytically.

In electromagnetics, the independent variables are usually x , y , and z .

We typically discretize x and y and leave z analytical.

Any method can be used to discretize the independent variables. This includes Fourier transform, finite-differences, finite-elements, etc.

In electromagnetics, the “method of lines” implies that finite-differences are used to discretize x and y .

RCWA is the method of lines, but uses a Fourier transform instead of finite-differences to discretize x and y .

Sign Convention

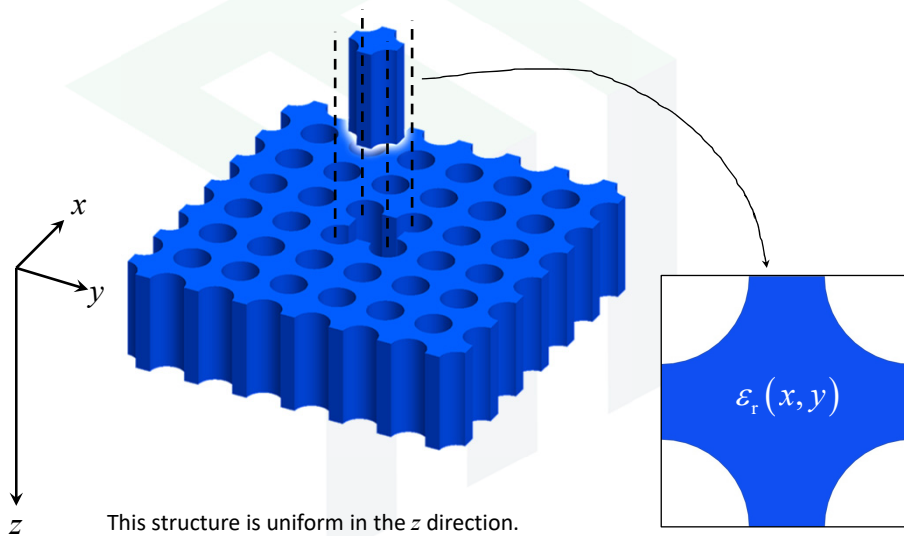
This formulation of the method of lines uses the negative sign convention for waves travelling in the $+z$ direction.

$$e^{-jkz}$$

Formulation of 3D Method of Lines

Slide 5

The 2D Unit Cell



Slide 6

Starting Point for MOL

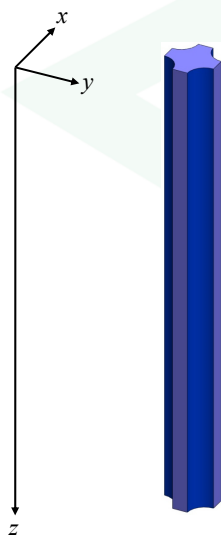
Start with Maxwell's equations in the following form...

$$\begin{aligned} \frac{\partial E_z}{\partial y'} - \frac{\partial E_y}{\partial z'} &= \mu_{xx} \tilde{H}_x & \frac{\partial \tilde{H}_z}{\partial y'} - \frac{\partial \tilde{H}_y}{\partial z'} &= \epsilon_{xx} E_x \\ \frac{\partial E_x}{\partial z'} - \frac{\partial E_z}{\partial x'} &= \mu_{yy} \tilde{H}_y & \frac{\partial \tilde{H}_x}{\partial z'} - \frac{\partial \tilde{H}_z}{\partial x'} &= \epsilon_{yy} E_y \\ \frac{\partial E_y}{\partial x'} - \frac{\partial E_x}{\partial y'} &= \mu_{zz} \tilde{H}_z & \frac{\partial \tilde{H}_y}{\partial x'} - \frac{\partial \tilde{H}_x}{\partial y'} &= \epsilon_{zz} E_z \end{aligned}$$

Recall that we normalized the magnetic field and grid according to

$$\tilde{H} = -j \sqrt{\frac{\mu_0}{\epsilon_0}} \vec{H} \quad x' = k_0 x \quad y' = k_0 y \quad z' = k_0 z$$

z-Uniform Media



Consider Maxwell's equations inside a medium that is uniform in the z direction.

The medium may be inhomogeneous in the x - y plane, but it must be uniform in the z direction.

Semi-Analytical Matrix Form of Maxwell's Equations

We can go straight to matrix form using the concept of matrix derivative operators. We keep the z direction analytical.

$$\begin{aligned}\frac{\partial E_z}{\partial y'} - \frac{\partial E_y}{\partial z'} &= \mu_{xx} \tilde{H}_x \\ \frac{\partial E_x}{\partial z'} - \frac{\partial E_z}{\partial x'} &= \mu_{yy} \tilde{H}_y \\ \frac{\partial E_y}{\partial x'} - \frac{\partial E_x}{\partial y'} &= \mu_{zz} \tilde{H}_z\end{aligned}$$



$$\begin{aligned}\mathbf{D}_{y'}^e \mathbf{e}_z - \frac{d}{dz'} \mathbf{e}_y &= \boldsymbol{\mu}_{xx} \tilde{\mathbf{h}}_x \\ \frac{d}{dz'} \mathbf{e}_x - \mathbf{D}_{x'}^e \mathbf{e}_z &= \boldsymbol{\mu}_{yy} \tilde{\mathbf{h}}_y \\ \mathbf{D}_{x'}^e \mathbf{e}_y - \mathbf{D}_{y'}^e \mathbf{e}_x &= \boldsymbol{\mu}_{zz} \tilde{\mathbf{h}}_z\end{aligned}$$

$$\begin{aligned}\frac{\partial \tilde{H}_z}{\partial y'} - \frac{\partial \tilde{H}_y}{\partial z'} &= \epsilon_{xx} E_x \\ \frac{\partial \tilde{H}_x}{\partial z'} - \frac{\partial \tilde{H}_z}{\partial x'} &= \epsilon_{yy} E_y \\ \frac{\partial \tilde{H}_y}{\partial x'} - \frac{\partial \tilde{H}_x}{\partial y'} &= \epsilon_{zz} E_z\end{aligned}$$



$$\begin{aligned}\mathbf{D}_{y'}^h \tilde{\mathbf{h}}_z - \frac{d}{dz'} \tilde{\mathbf{h}}_y &= \boldsymbol{\epsilon}_{xx} \mathbf{e}_x \\ \frac{d}{dz'} \tilde{\mathbf{h}}_x - \mathbf{D}_{x'}^h \tilde{\mathbf{h}}_z &= \boldsymbol{\epsilon}_{yy} \mathbf{e}_y \\ \mathbf{D}_{x'}^h \tilde{\mathbf{h}}_y - \mathbf{D}_{y'}^h \tilde{\mathbf{h}}_x &= \boldsymbol{\epsilon}_{zz} \mathbf{e}_z\end{aligned}$$

Eliminate Longitudinal Field Components

We solve the third and sixth equation for \mathbf{e}_z and \mathbf{h}_z and substitute these back into the remaining four equations.

$$\begin{aligned}\mathbf{D}_{y'}^e \mathbf{e}_z - \frac{d}{dz'} \mathbf{e}_y &= \boldsymbol{\mu}_{xx} \tilde{\mathbf{h}}_x & \frac{d}{dz'} \mathbf{e}_x &= -\mathbf{D}_{x'}^e \boldsymbol{\epsilon}_{zz}^{-1} \mathbf{D}_{y'}^h \tilde{\mathbf{h}}_x + (\boldsymbol{\mu}_{yy} + \mathbf{D}_{x'}^e \boldsymbol{\epsilon}_{zz}^{-1} \mathbf{D}_{x'}^h) \tilde{\mathbf{h}}_y \\ \frac{d}{dz'} \mathbf{e}_x - \mathbf{D}_{x'}^e \mathbf{e}_z &= \boldsymbol{\mu}_{yy} \tilde{\mathbf{h}}_y & \frac{d}{dz'} \mathbf{e}_y &= -(\boldsymbol{\mu}_{xx} + \mathbf{D}_{y'}^e \boldsymbol{\epsilon}_{zz}^{-1} \mathbf{D}_{y'}^h) \tilde{\mathbf{h}}_x + \mathbf{D}_{y'}^e \boldsymbol{\epsilon}_{zz}^{-1} \mathbf{D}_{x'}^h \tilde{\mathbf{h}}_y \\ \mathbf{D}_{x'}^e \mathbf{e}_y - \mathbf{D}_{y'}^e \mathbf{e}_x &= \boldsymbol{\mu}_{zz} \tilde{\mathbf{h}}_z & \tilde{\mathbf{h}}_z &= \boldsymbol{\mu}_{zz}^{-1} (\mathbf{D}_{x'}^e \mathbf{e}_y - \mathbf{D}_{y'}^e \mathbf{e}_x)\end{aligned}$$

$$\begin{aligned}\mathbf{D}_{y'}^h \tilde{\mathbf{h}}_z - \frac{d}{dz'} \tilde{\mathbf{h}}_y &= \boldsymbol{\epsilon}_{xx} \mathbf{e}_x & \frac{d}{dz'} \tilde{\mathbf{h}}_x &= -\mathbf{D}_{x'}^h \boldsymbol{\mu}_{zz}^{-1} \mathbf{D}_{y'}^e \mathbf{e}_x + (\boldsymbol{\epsilon}_{yy} + \mathbf{D}_{x'}^h \boldsymbol{\mu}_{zz}^{-1} \mathbf{D}_{x'}^e) \mathbf{e}_y \\ \frac{d}{dz'} \tilde{\mathbf{h}}_x - \mathbf{D}_{x'}^h \tilde{\mathbf{h}}_z &= \boldsymbol{\epsilon}_{yy} \mathbf{e}_y & \frac{d}{dz'} \tilde{\mathbf{h}}_y &= -(\boldsymbol{\epsilon}_{xx} + \mathbf{D}_{y'}^h \boldsymbol{\mu}_{zz}^{-1} \mathbf{D}_{y'}^e) \mathbf{e}_x + \mathbf{D}_{y'}^h \boldsymbol{\mu}_{zz}^{-1} \mathbf{D}_{x'}^e \mathbf{e}_y \\ \mathbf{D}_{x'}^h \tilde{\mathbf{h}}_y - \mathbf{D}_{y'}^h \tilde{\mathbf{h}}_x &= \boldsymbol{\epsilon}_{zz} \mathbf{e}_z & \mathbf{e}_z &= \boldsymbol{\epsilon}_{zz}^{-1} (\mathbf{D}_{x'}^h \tilde{\mathbf{h}}_y - \mathbf{D}_{y'}^h \tilde{\mathbf{h}}_x)\end{aligned}$$

Block Matrix Form

We write the remaining four equations in block matrix form as

$$\begin{aligned} \frac{d}{dz'} \mathbf{e}_y &= -(\boldsymbol{\mu}_{xx} + \mathbf{D}_{y'}^e \boldsymbol{\epsilon}_{zz}^{-1} \mathbf{D}_{y'}^h) \tilde{\mathbf{h}}_x + \mathbf{D}_{y'}^e \boldsymbol{\epsilon}_{zz}^{-1} \mathbf{D}_{x'}^h \tilde{\mathbf{h}}_y \\ \frac{d}{dz'} \mathbf{e}_x &= -\mathbf{D}_{y'}^e \boldsymbol{\epsilon}_{zz}^{-1} \mathbf{D}_{y'}^h \tilde{\mathbf{h}}_x + (\boldsymbol{\mu}_{yy} + \mathbf{D}_{x'}^e \boldsymbol{\epsilon}_{zz}^{-1} \mathbf{D}_{x'}^h) \tilde{\mathbf{h}}_y \end{aligned}$$

$$\frac{d}{dz'} \begin{bmatrix} \mathbf{e}_x \\ \mathbf{e}_y \end{bmatrix} = \begin{bmatrix} -\mathbf{D}_{x'}^e \boldsymbol{\epsilon}_{zz}^{-1} \mathbf{D}_{y'}^h & (\boldsymbol{\mu}_{yy} + \mathbf{D}_{x'}^e \boldsymbol{\epsilon}_{zz}^{-1} \mathbf{D}_{x'}^h) \\ -(\boldsymbol{\mu}_{xx} + \mathbf{D}_{y'}^e \boldsymbol{\epsilon}_{zz}^{-1} \mathbf{D}_{y'}^h) & \mathbf{D}_{y'}^e \boldsymbol{\epsilon}_{zz}^{-1} \mathbf{D}_{x'}^h \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{h}}_x \\ \tilde{\mathbf{h}}_y \end{bmatrix}$$

$$\begin{aligned} \frac{d}{dz'} \tilde{\mathbf{h}}_x &= -\mathbf{D}_{x'}^h \boldsymbol{\mu}_{zz}^{-1} \mathbf{D}_{y'}^e \mathbf{e}_x + (\boldsymbol{\epsilon}_{yy} + \mathbf{D}_{x'}^h \boldsymbol{\mu}_{zz}^{-1} \mathbf{D}_{x'}^e) \mathbf{e}_y \\ \frac{d}{dz'} \tilde{\mathbf{h}}_y &= -(\boldsymbol{\epsilon}_{xx} + \mathbf{D}_{y'}^h \boldsymbol{\mu}_{zz}^{-1} \mathbf{D}_{y'}^e) \mathbf{e}_x + \mathbf{D}_{y'}^h \boldsymbol{\mu}_{zz}^{-1} \mathbf{D}_{x'}^e \mathbf{e}_y \end{aligned}$$

$$\frac{d}{dz'} \begin{bmatrix} \tilde{\mathbf{h}}_x \\ \tilde{\mathbf{h}}_y \end{bmatrix} = \begin{bmatrix} -\mathbf{D}_{x'}^h \boldsymbol{\mu}_{zz}^{-1} \mathbf{D}_{y'}^e & (\boldsymbol{\epsilon}_{yy} + \mathbf{D}_{x'}^h \boldsymbol{\mu}_{zz}^{-1} \mathbf{D}_{x'}^e) \\ -(\boldsymbol{\epsilon}_{xx} + \mathbf{D}_{y'}^h \boldsymbol{\mu}_{zz}^{-1} \mathbf{D}_{y'}^e) & \mathbf{D}_{y'}^h \boldsymbol{\mu}_{zz}^{-1} \mathbf{D}_{x'}^e \end{bmatrix} \begin{bmatrix} \mathbf{e}_x \\ \mathbf{e}_y \end{bmatrix}$$

Standard PQ Form

We can now write our two equations in the “standard” **P** and **Q** form.

$$\frac{d}{dz'} \begin{bmatrix} \mathbf{e}_x \\ \mathbf{e}_y \end{bmatrix} = \mathbf{P} \begin{bmatrix} \tilde{\mathbf{h}}_x \\ \tilde{\mathbf{h}}_y \end{bmatrix} \quad \mathbf{P} = \begin{bmatrix} -\mathbf{D}_{x'}^e \boldsymbol{\epsilon}_{zz}^{-1} \mathbf{D}_{y'}^h & (\boldsymbol{\mu}_{yy} + \mathbf{D}_{x'}^e \boldsymbol{\epsilon}_{zz}^{-1} \mathbf{D}_{x'}^h) \\ -(\boldsymbol{\mu}_{xx} + \mathbf{D}_{y'}^e \boldsymbol{\epsilon}_{zz}^{-1} \mathbf{D}_{y'}^h) & \mathbf{D}_{y'}^e \boldsymbol{\epsilon}_{zz}^{-1} \mathbf{D}_{x'}^h \end{bmatrix}$$

$$\frac{d}{dz'} \begin{bmatrix} \tilde{\mathbf{h}}_x \\ \tilde{\mathbf{h}}_y \end{bmatrix} = \mathbf{Q} \begin{bmatrix} \mathbf{e}_x \\ \mathbf{e}_y \end{bmatrix} \quad \mathbf{Q} = \begin{bmatrix} -\mathbf{D}_{x'}^h \boldsymbol{\mu}_{zz}^{-1} \mathbf{D}_{y'}^e & (\boldsymbol{\epsilon}_{yy} + \mathbf{D}_{x'}^h \boldsymbol{\mu}_{zz}^{-1} \mathbf{D}_{x'}^e) \\ -(\boldsymbol{\epsilon}_{xx} + \mathbf{D}_{y'}^h \boldsymbol{\mu}_{zz}^{-1} \mathbf{D}_{y'}^e) & \mathbf{D}_{y'}^h \boldsymbol{\mu}_{zz}^{-1} \mathbf{D}_{x'}^e \end{bmatrix}$$

Matrix Wave Equation

We differentiate the “P” equation with respect to z' and substitute the “Q” equation into the result to derive the matrix wave equation.

$$\begin{aligned} \frac{d}{dz'} \begin{bmatrix} \mathbf{e}_x \\ \mathbf{e}_y \end{bmatrix} &= \mathbf{P} \begin{bmatrix} \tilde{\mathbf{h}}_x \\ \tilde{\mathbf{h}}_y \end{bmatrix} & \frac{d}{dz'} \begin{bmatrix} \tilde{\mathbf{h}}_x \\ \tilde{\mathbf{h}}_y \end{bmatrix} &= \mathbf{Q} \begin{bmatrix} \mathbf{e}_x \\ \mathbf{e}_y \end{bmatrix} \\ \frac{d^2}{dz'^2} \begin{bmatrix} \mathbf{e}_x \\ \mathbf{e}_y \end{bmatrix} &= \mathbf{P} \cdot \frac{d}{dz'} \begin{bmatrix} \tilde{\mathbf{h}}_x \\ \tilde{\mathbf{h}}_y \end{bmatrix} \\ \frac{d^2}{dz'^2} \begin{bmatrix} \mathbf{e}_x \\ \mathbf{e}_y \end{bmatrix} &= \mathbf{PQ} \begin{bmatrix} \mathbf{e}_x \\ \mathbf{e}_y \end{bmatrix} \\ \frac{d^2}{dz'^2} \begin{bmatrix} \mathbf{e}_x \\ \mathbf{e}_y \end{bmatrix} - \mathbf{PQ} \begin{bmatrix} \mathbf{e}_x \\ \mathbf{e}_y \end{bmatrix} &= \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix} \end{aligned} \quad \Rightarrow \quad \begin{aligned} \frac{d^2}{dz'^2} \begin{bmatrix} \mathbf{e}_x \\ \mathbf{e}_y \end{bmatrix} - \mathbf{\Omega}^2 \begin{bmatrix} \mathbf{e}_x \\ \mathbf{e}_y \end{bmatrix} &= \mathbf{0} \\ \mathbf{\Omega}^2 &= \mathbf{PQ} \end{aligned}$$

Solution to the Wave Equation

The solution to the wave equation is written the same as in RCWA and TMM.

$$\begin{bmatrix} \mathbf{e}_x \\ \mathbf{e}_y \end{bmatrix} = \mathbf{W} e^{-\lambda z'} \mathbf{c}^+ + \mathbf{W} e^{\lambda z'} \mathbf{c}^- \quad \text{where } \mathbf{W} \text{ is the eigen-vector matrix and } \lambda^2 \text{ is the eigen-value matrix of } \mathbf{\Omega}^2.$$

The overall solution is then

$$\Psi(\tilde{z}) = \begin{bmatrix} \mathbf{e}_x(\tilde{z}) \\ \mathbf{e}_y(\tilde{z}) \\ \tilde{\mathbf{h}}_x(\tilde{z}) \\ \tilde{\mathbf{h}}_y(\tilde{z}) \end{bmatrix} = \begin{bmatrix} \mathbf{W} & \mathbf{W} \\ -\mathbf{V} & \mathbf{V} \end{bmatrix} \begin{bmatrix} e^{-\lambda z'} & \mathbf{0} \\ \mathbf{0} & e^{\lambda z'} \end{bmatrix} \begin{bmatrix} \mathbf{c}^+ \\ \mathbf{c}^- \end{bmatrix} \quad \mathbf{V} = \mathbf{QW}\lambda^{-1}$$

Based on previous lectures, you know the rest of the story!

Enforcing the Negative Sign Convention

$$e^{-\lambda z'} = e^{-\text{Re}[\lambda]z'} e^{-j\text{Im}[\lambda]z'}$$

Observe that for passive materials

$$\text{Re}[\lambda] \geq 0$$

$$\text{Im}[\lambda] \geq 0$$

To ensure this, recalculate the eigen values as

$$\lambda = |\text{Re}[\lambda]| + j|\text{Im}[\lambda]|$$

Interpretation of the Solution

$$\Psi(\tilde{z}) = \mathbf{W} e^{-\lambda z'} \mathbf{c}$$

$\Psi(z')$ – Overall solution which is the sum of all the modes at plane z' .

\mathbf{W} – Square matrix whose column vectors describe the “modes” that can exist in the material. These are essentially pictures of the modes which quantify the relative amplitudes of $E_x, E_y, H_x,$ and H_y .

\mathbf{c} – Column vector containing the amplitude coefficient of each of the modes. This quantifies how much energy is in each mode.

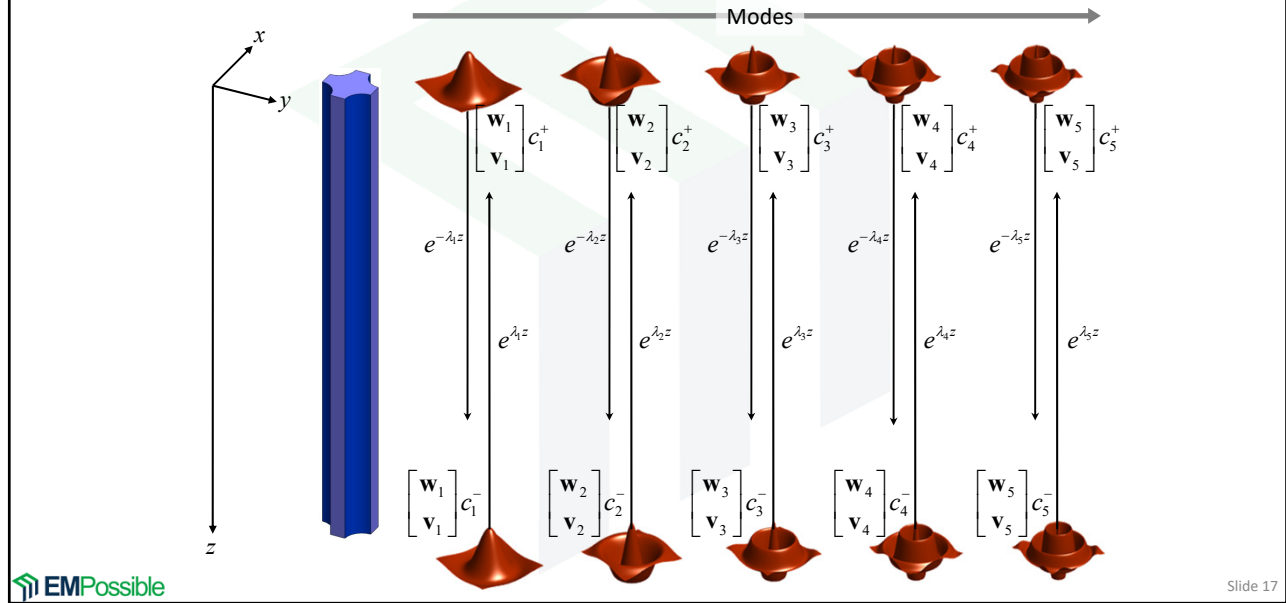
$e^{-\lambda z'}$ Diagonal matrix describing how the modes propagate. This includes accumulation of phase as well as decaying (loss) or growing (gain) amplitude.

Solution in a Homogeneous Layer

In a homogeneous layer, the \mathbf{P} and \mathbf{Q} matrices simplify to

$$\mathbf{P} = \frac{1}{\epsilon_r} \begin{bmatrix} -\mathbf{D}_x^e \mathbf{D}_y^h & (\mu_r \epsilon_r \mathbf{I} + \mathbf{D}_x^e \mathbf{D}_x^h) \\ -(\mu_r \epsilon_r \mathbf{I} + \mathbf{D}_y^e \mathbf{D}_y^h) & \mathbf{D}_y^e \mathbf{D}_x^h \end{bmatrix} \quad \mathbf{Q} = \frac{1}{\mu_r} \begin{bmatrix} -\mathbf{D}_x^h \mathbf{D}_y^e & (\mu_r \epsilon_r \mathbf{I} + \mathbf{D}_x^h \mathbf{D}_x^e) \\ -(\mu_r \epsilon_r \mathbf{I} + \mathbf{D}_y^h \mathbf{D}_y^e) & \mathbf{D}_y^h \mathbf{D}_x^e \end{bmatrix}$$

Visualization of this Solution



Formulation of 2D Method of Lines

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Starting Point

Start with Maxwell's equations in real-space and in matrix form as derived earlier this lecture.

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

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

$$\frac{\partial E_y}{\partial x'} - \frac{\partial E_x}{\partial y'} = \mu_z \tilde{H}_z$$



$$\mathbf{D}_{y'}^e \mathbf{e}_z - \frac{d}{dz'} \mathbf{e}_y = \boldsymbol{\mu}_{xx} \tilde{\mathbf{h}}_x$$

$$\frac{d}{dz'} \mathbf{e}_x - \mathbf{D}_{x'}^e \mathbf{e}_z = \boldsymbol{\mu}_{yy} \tilde{\mathbf{h}}_y$$

$$\mathbf{D}_{x'}^e \mathbf{e}_y - \mathbf{D}_{y'}^e \mathbf{e}_x = \boldsymbol{\mu}_{zz} \tilde{\mathbf{h}}_z$$

$$\frac{\partial \tilde{H}_z}{\partial y'} - \frac{\partial \tilde{H}_y}{\partial z'} = \epsilon_{xx} E_x$$

$$\frac{\partial \tilde{H}_x}{\partial z'} - \frac{\partial \tilde{H}_z}{\partial x'} = \epsilon_{yy} E_y$$

$$\frac{\partial \tilde{H}_y}{\partial x'} - \frac{\partial \tilde{H}_x}{\partial y'} = \epsilon_{zz} E_z$$



$$\mathbf{D}_{y'}^h \tilde{\mathbf{h}}_z - \frac{d}{dz'} \tilde{\mathbf{h}}_y = \boldsymbol{\epsilon}_{xx} \mathbf{e}_x$$

$$\frac{d}{dz'} \tilde{\mathbf{h}}_x - \mathbf{D}_{x'}^h \tilde{\mathbf{h}}_z = \boldsymbol{\epsilon}_{yy} \mathbf{e}_y$$

$$\mathbf{D}_{x'}^h \tilde{\mathbf{h}}_y - \mathbf{D}_{y'}^h \tilde{\mathbf{h}}_x = \boldsymbol{\epsilon}_{zz} \mathbf{e}_z$$

Reduction to Two Dimensions

For diagonally anisotropic devices that are uniform in the y direction and when there is no wave propagation in the y direction, nothing varies in the y direction.

$$\mathbf{D}_{y'}^e = \mathbf{D}_{y'}^h = \mathbf{0}$$

Maxwell's equations reduce to

$$-\frac{d}{dz'} \mathbf{e}_y = \boldsymbol{\mu}_{xx} \tilde{\mathbf{h}}_x$$

$$\frac{d}{dz'} \mathbf{e}_x - \mathbf{D}_{x'}^e \mathbf{e}_z = \boldsymbol{\mu}_{yy} \tilde{\mathbf{h}}_y$$

$$\mathbf{D}_{x'}^e \mathbf{e}_y = \boldsymbol{\mu}_{zz} \tilde{\mathbf{h}}_z$$

$$-\frac{d}{dz'} \tilde{\mathbf{h}}_y = \boldsymbol{\epsilon}_{xx} \mathbf{e}_x$$

$$\frac{d}{dz'} \tilde{\mathbf{h}}_x - \mathbf{D}_{x'}^h \tilde{\mathbf{h}}_z = \boldsymbol{\epsilon}_{yy} \mathbf{e}_y$$

$$\mathbf{D}_{x'}^h \tilde{\mathbf{h}}_y = \boldsymbol{\epsilon}_{zz} \mathbf{e}_z$$

Two Independent Modes

Maxwell's equations have decoupled into two independent modes.

$$-\frac{d}{dz'} \mathbf{e}_y = \mu_{xx} \tilde{\mathbf{h}}_x$$

$$\frac{d}{dz'} \mathbf{e}_x - \mathbf{D}_x^e \mathbf{e}_z = \mu_{yy} \tilde{\mathbf{h}}_y$$

$$\mathbf{D}_x^e \mathbf{e}_y = \mu_{zz} \tilde{\mathbf{h}}_z$$

E Mode

$$\frac{d}{dz'} \tilde{\mathbf{h}}_x - \mathbf{D}_x^h \tilde{\mathbf{h}}_z = \epsilon_{yy} \mathbf{e}_y$$

$$-\frac{d}{dz'} \mathbf{e}_y = \mu_{xx} \tilde{\mathbf{h}}_x$$

$$\mathbf{D}_x^e \mathbf{e}_y = \mu_{zz} \tilde{\mathbf{h}}_z$$

$$-\frac{d}{dz'} \tilde{\mathbf{h}}_y = \epsilon_{xx} \mathbf{e}_x$$

$$\frac{d}{dz'} \tilde{\mathbf{h}}_x - \mathbf{D}_x^h \tilde{\mathbf{h}}_z = \epsilon_{yy} \mathbf{e}_y$$

$$\mathbf{D}_x^h \tilde{\mathbf{h}}_y = \epsilon_{zz} \mathbf{e}_z$$

H Mode

$$\frac{d}{dz'} \mathbf{e}_x - \mathbf{D}_x^e \mathbf{e}_z = \mu_{yy} \tilde{\mathbf{h}}_y$$

$$-\frac{d}{dz'} \tilde{\mathbf{h}}_y = \epsilon_{xx} \mathbf{e}_x$$

$$\mathbf{D}_x^h \tilde{\mathbf{h}}_y = \epsilon_{zz} \mathbf{e}_z$$

Apply Dielectric Smoothing

To improve convergence, dielectric smoothing can be incorporated as follows:

E Mode

$$\frac{d}{dz'} \tilde{\mathbf{h}}_x - \mathbf{D}_x^h \tilde{\mathbf{h}}_z = \langle \epsilon_{yy} \rangle \mathbf{e}_y$$

$$-\frac{d}{dz'} \mathbf{e}_y = \langle \mu_{xx}^{-1} \rangle^{-1} \tilde{\mathbf{h}}_x$$

$$\mathbf{D}_x^e \mathbf{e}_y = \langle \mu_{zz} \rangle \tilde{\mathbf{h}}_z$$

H Mode

$$\frac{d}{dz'} \mathbf{e}_x - \mathbf{D}_x^e \mathbf{e}_z = \langle \mu_{yy} \rangle \tilde{\mathbf{h}}_y$$

$$-\frac{d}{dz'} \tilde{\mathbf{h}}_y = \langle \epsilon_{xx}^{-1} \rangle^{-1} \mathbf{e}_x$$

$$\mathbf{D}_x^h \tilde{\mathbf{h}}_y = \langle \epsilon_{zz} \rangle \mathbf{e}_z$$

Eliminate Longitudinal Components

Solve for the longitudinal components

$$\tilde{\mathbf{h}}_z = \langle \boldsymbol{\mu}_{zz} \rangle^{-1} \mathbf{D}_{x'}^e \mathbf{e}_y$$

$$\mathbf{e}_z = \langle \boldsymbol{\epsilon}_{zz} \rangle^{-1} \mathbf{D}_{x'}^h \tilde{\mathbf{h}}_y$$

and substitute these expressions into the remaining equations.

E Mode

$$\frac{d}{dz'} \tilde{\mathbf{h}}_x = \langle \boldsymbol{\epsilon}_{yy} \rangle \mathbf{e}_y + \mathbf{D}_{x'}^h \langle \boldsymbol{\mu}_{zz} \rangle^{-1} \mathbf{D}_{x'}^e \mathbf{e}_y$$

$$\frac{d}{dz'} \mathbf{e}_y = -\langle \boldsymbol{\mu}_{xx}^{-1} \rangle^{-1} \tilde{\mathbf{h}}_x$$

H Mode

$$\frac{d}{dz'} \mathbf{e}_x = \langle \boldsymbol{\mu}_{yy} \rangle \tilde{\mathbf{h}}_y + \mathbf{D}_{x'}^e \langle \boldsymbol{\epsilon}_{zz} \rangle^{-1} \mathbf{D}_{x'}^h \tilde{\mathbf{h}}_y$$

$$\frac{d}{dz'} \tilde{\mathbf{h}}_y = -\langle \boldsymbol{\epsilon}_{xx}^{-1} \rangle^{-1} \mathbf{e}_x$$

Standard P and Q Form

Write the matrix equations in the standard **PQ** form.

E Mode

$$\frac{d}{dz'} \mathbf{e}_y = \mathbf{P} \tilde{\mathbf{h}}_x$$

$$\frac{d}{dz'} \tilde{\mathbf{h}}_x = \mathbf{Q} \mathbf{e}_y$$

$$\mathbf{P} = -\langle \boldsymbol{\mu}_{xx}^{-1} \rangle^{-1}$$

$$\mathbf{Q} = \langle \boldsymbol{\epsilon}_{yy} \rangle + \mathbf{D}_{x'}^h \langle \boldsymbol{\mu}_{zz} \rangle^{-1} \mathbf{D}_{x'}^e$$

H Mode

$$\frac{d}{dz'} \tilde{\mathbf{h}}_y = \mathbf{P} \mathbf{e}_x$$

$$\frac{d}{dz'} \mathbf{e}_x = \mathbf{Q} \tilde{\mathbf{h}}_y$$

$$\mathbf{P} = -\langle \boldsymbol{\epsilon}_{xx}^{-1} \rangle^{-1}$$

$$\mathbf{Q} = \langle \boldsymbol{\mu}_{yy} \rangle + \mathbf{D}_{x'}^e \langle \boldsymbol{\epsilon}_{zz} \rangle^{-1} \mathbf{D}_{x'}^h$$

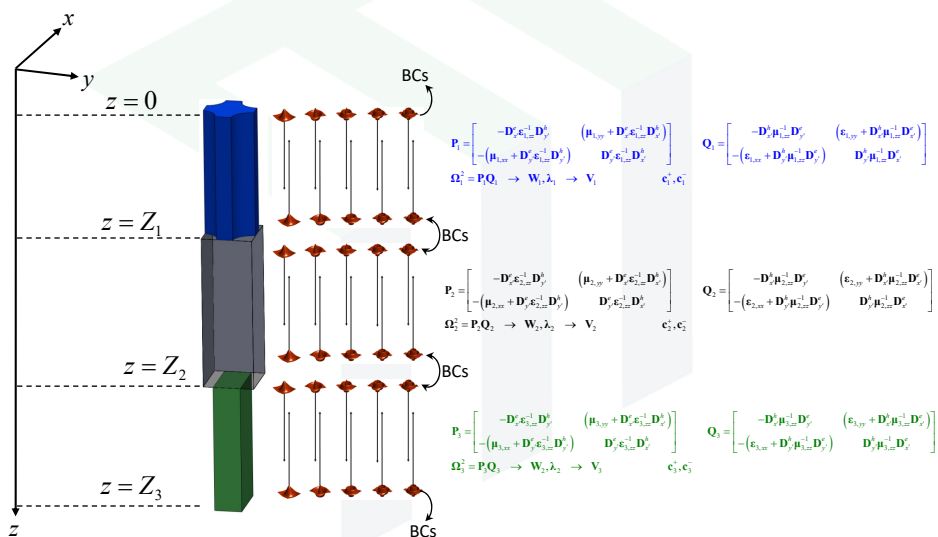
...and now you know the rest of the story.

Multilayer Devices Using Scattering Matrices

R. C. Rumpf, "Improved formulation of scattering matrices for semi-analytical methods that is consistent with convention," PIERS B, Vol. 35, 241-261, 2011.

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Eigen System in Each Layer



Slide 26

Field Relations & Boundary Conditions

Field inside the i^{th} layer:

$$\Psi_i(z') = \begin{bmatrix} \mathbf{e}_x(\tilde{z}) \\ \mathbf{e}_y(\tilde{z}) \\ \tilde{\mathbf{h}}_x(\tilde{z}) \\ \tilde{\mathbf{h}}_y(\tilde{z}) \end{bmatrix} = \begin{bmatrix} \mathbf{W}_i & \mathbf{W}_i \\ -\mathbf{V}_i & \mathbf{V}_i \end{bmatrix} \begin{bmatrix} e^{-\lambda_i z'} & \mathbf{0} \\ \mathbf{0} & e^{\lambda_i z'} \end{bmatrix} \begin{bmatrix} \mathbf{c}_i^+ \\ \mathbf{c}_i^- \end{bmatrix}$$

Boundary conditions at the first interface:

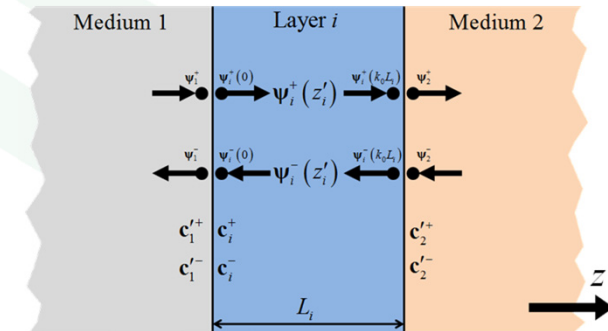
$$\Psi_1 = \Psi_i(0)$$

$$\begin{bmatrix} \mathbf{W}_1 & \mathbf{W}_1 \\ -\mathbf{V}_1 & \mathbf{V}_1 \end{bmatrix} \begin{bmatrix} \mathbf{c}_1^+ \\ \mathbf{c}_1^- \end{bmatrix} = \begin{bmatrix} \mathbf{W}_i & \mathbf{W}_i \\ -\mathbf{V}_i & \mathbf{V}_i \end{bmatrix} \begin{bmatrix} \mathbf{c}_i^+ \\ \mathbf{c}_i^- \end{bmatrix}$$

Boundary conditions at the second interface:

$$\Psi_i(k_0 L_i) = \Psi_2$$

$$\begin{bmatrix} \mathbf{W}_i & \mathbf{W}_i \\ -\mathbf{V}_i & \mathbf{V}_i \end{bmatrix} \begin{bmatrix} e^{-\lambda_i k_0 L_i} & \mathbf{0} \\ \mathbf{0} & e^{\lambda_i k_0 L_i} \end{bmatrix} \begin{bmatrix} \mathbf{c}_i^+ \\ \mathbf{c}_i^- \end{bmatrix} = \begin{bmatrix} \mathbf{W}_2 & \mathbf{W}_2 \\ -\mathbf{V}_2 & \mathbf{V}_2 \end{bmatrix} \begin{bmatrix} \mathbf{c}_2^+ \\ \mathbf{c}_2^- \end{bmatrix}$$



Note: k_0 has been incorporated to normalize L_i .

Adopt the Symmetric S-Matrix Approach

The scattering matrix \mathbf{S}_i of the i^{th} layer is still defined as:

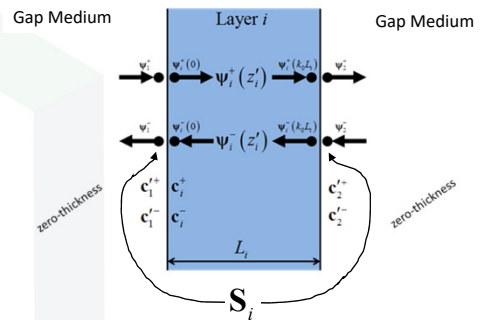
$$\begin{bmatrix} \mathbf{c}_1'^- \\ \mathbf{c}_2'^+ \end{bmatrix} = \mathbf{S}^{(i)} \begin{bmatrix} \mathbf{c}_1'^+ \\ \mathbf{c}_2'^- \end{bmatrix} \quad \mathbf{S}^{(i)} = \begin{bmatrix} \mathbf{S}_{11}^{(i)} & \mathbf{S}_{12}^{(i)} \\ \mathbf{S}_{21}^{(i)} & \mathbf{S}_{22}^{(i)} \end{bmatrix}$$

But the elements are calculated as

$$\mathbf{S}_{11}^{(i)} = (\mathbf{A}_i - \mathbf{X}_i \mathbf{B}_i \mathbf{A}_i^{-1} \mathbf{X}_i \mathbf{B}_i)^{-1} (\mathbf{X}_i \mathbf{B}_i \mathbf{A}_i^{-1} \mathbf{X}_i \mathbf{A}_i - \mathbf{B}_i)$$

$$\mathbf{S}_{12}^{(i)} = (\mathbf{A}_i - \mathbf{X}_i \mathbf{B}_i \mathbf{A}_i^{-1} \mathbf{X}_i \mathbf{B}_i)^{-1} \mathbf{X}_i (\mathbf{A}_i - \mathbf{B}_i \mathbf{A}_i^{-1} \mathbf{B}_i)$$

$$\left. \begin{aligned} \mathbf{S}_{21}^{(i)} &= \mathbf{S}_{12}^{(i)} \\ \mathbf{S}_{22}^{(i)} &= \mathbf{S}_{11}^{(i)} \end{aligned} \right\} \begin{aligned} &\bullet \text{Layers are symmetric so the scattering matrix elements have redundancy.} \\ &\bullet \text{Scattering matrix equations are simplified.} \\ &\bullet \text{Fewer calculations.} \\ &\bullet \text{Less memory storage.} \end{aligned}$$

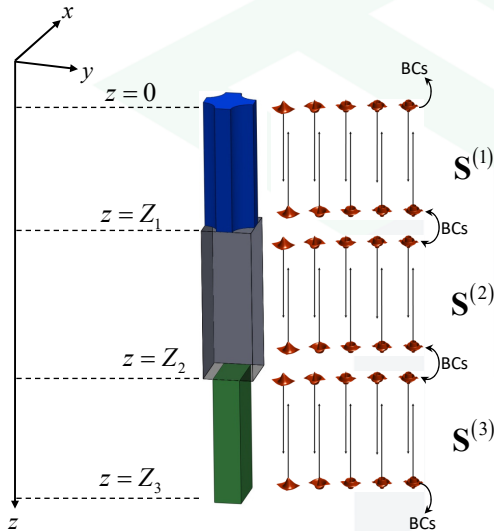


$$\mathbf{A}_i = \mathbf{W}_i^{-1} \mathbf{W}_0 + \mathbf{V}_i^{-1} \mathbf{V}_0$$

$$\mathbf{B}_i = \mathbf{W}_i^{-1} \mathbf{W}_0 - \mathbf{V}_i^{-1} \mathbf{V}_0$$

$$\mathbf{X}_i = e^{-\lambda_i k_0 L_i}$$

Global Scattering Matrix



Scattering matrix for all layers.

$$\mathbf{S}^{(\text{device})} = \mathbf{S}^{(1)} \otimes \mathbf{S}^{(2)} \otimes \mathbf{S}^{(3)}$$

Connection to outside regions

$$\mathbf{S}^{(\text{global})} = \mathbf{S}^{(\text{ref})} \otimes \mathbf{S}^{(\text{device})} \otimes \mathbf{S}^{(\text{tm})}$$

Recall this procedure from TMM.

Reflection/Transmission Side Scattering Matrices

The reflection-side scattering matrix is

$$\mathbf{S}_{11}^{(\text{ref})} = -\mathbf{A}_{\text{ref}}^{-1} \mathbf{B}_{\text{ref}}$$

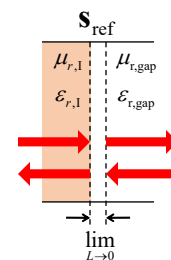
$$\mathbf{S}_{12}^{(\text{ref})} = 2\mathbf{A}_{\text{ref}}^{-1}$$

$$\mathbf{S}_{21}^{(\text{ref})} = 0.5(\mathbf{A}_{\text{ref}} - \mathbf{B}_{\text{ref}} \mathbf{A}_{\text{ref}}^{-1} \mathbf{B}_{\text{ref}})$$

$$\mathbf{S}_{22}^{(\text{ref})} = \mathbf{B}_{\text{ref}} \mathbf{A}_{\text{ref}}^{-1}$$

$$\mathbf{A}_{\text{ref}} = \mathbf{W}_0^{-1} \mathbf{W}_{\text{ref}} + \mathbf{V}_0^{-1} \mathbf{V}_{\text{ref}}$$

$$\mathbf{B}_{\text{ref}} = \mathbf{W}_0^{-1} \mathbf{W}_{\text{ref}} - \mathbf{V}_0^{-1} \mathbf{V}_{\text{ref}}$$



The transmission-side scattering matrix is

$$\mathbf{S}_{11}^{(\text{tm})} = \mathbf{B}_{\text{tm}} \mathbf{A}_{\text{tm}}^{-1}$$

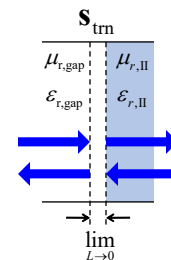
$$\mathbf{S}_{12}^{(\text{tm})} = 0.5(\mathbf{A}_{\text{tm}} - \mathbf{B}_{\text{tm}} \mathbf{A}_{\text{tm}}^{-1} \mathbf{B}_{\text{tm}})$$

$$\mathbf{S}_{21}^{(\text{tm})} = 2\mathbf{A}_{\text{tm}}^{-1}$$

$$\mathbf{S}_{22}^{(\text{tm})} = -\mathbf{A}_{\text{tm}}^{-1} \mathbf{B}_{\text{tm}}$$

$$\mathbf{A}_{\text{tm}} = \mathbf{W}_0^{-1} \mathbf{W}_{\text{tm}} + \mathbf{V}_0^{-1} \mathbf{V}_{\text{tm}}$$

$$\mathbf{B}_{\text{tm}} = \mathbf{W}_0^{-1} \mathbf{W}_{\text{tm}} - \mathbf{V}_0^{-1} \mathbf{V}_{\text{tm}}$$



Calculating the Transmitted and Reflected Fields

The electric field source is calculated as

$$\mathbf{c}_{\text{inc}} = \mathbf{W}_{\text{ref}}^{-1} \bar{\mathbf{e}}_{xy}^{\text{inc}} \quad \bar{\mathbf{e}}_{xy}^{\text{inc}} = \begin{bmatrix} p_x e^{-j(k_{x,\text{inc}}x + k_{y,\text{inc}}y)} \\ p_y e^{-j(k_{x,\text{inc}}x + k_{y,\text{inc}}y)} \end{bmatrix}$$

\mathbf{x} and \mathbf{y} are column vectors containing the coordinates of the points in the cross section.

Recall calculating the polarization components p_x and p_y in TMM.
 $|\bar{\mathbf{p}}| = 1$

Given the global scattering matrix, the coefficients for the reflected and transmitted fields are

$$\mathbf{c}_{\text{ref}} = \mathbf{S}_{11} \mathbf{c}_{\text{inc}} \quad \mathbf{c}_{\text{tm}} = \mathbf{S}_{21} \mathbf{c}_{\text{inc}}$$

The transverse components of the reflected and transmitted fields are then

$$\bar{\mathbf{e}}_{xy}^{\text{ref}} = \mathbf{W}_{\text{ref}} \mathbf{c}_{\text{ref}} = \mathbf{W}_{\text{ref}} \mathbf{S}_{11} \mathbf{c}_{\text{inc}} = \begin{bmatrix} \mathbf{r}_x \\ \mathbf{r}_y \end{bmatrix}$$

$$\bar{\mathbf{e}}_{xy}^{\text{tm}} = \mathbf{W}_{\text{tm}} \mathbf{c}_{\text{tm}} = \mathbf{W}_{\text{tm}} \mathbf{S}_{21} \mathbf{c}_{\text{inc}} = \begin{bmatrix} \mathbf{t}_x \\ \mathbf{t}_y \end{bmatrix}$$

Calculate the Amplitudes of the Spatial Harmonics

Remove the phase tilt

$$A_{x,\text{ref}}(x, y) = r_x(x, y) \div \exp[-j(k_{x,\text{inc}}x + k_{y,\text{inc}}y)]$$

$$A_{y,\text{ref}}(x, y) = r_y(x, y) \div \exp[-j(k_{x,\text{inc}}x + k_{y,\text{inc}}y)]$$

$$A_{x,\text{tm}}(x, y) = t_x(x, y) \div \exp[-j(k_{x,\text{inc}}x + k_{y,\text{inc}}y)]$$

$$A_{y,\text{tm}}(x, y) = t_y(x, y) \div \exp[-j(k_{x,\text{inc}}x + k_{y,\text{inc}}y)]$$

Calculate amplitudes of the spatial harmonics

$$\mathbf{r}_x = \text{FFT}_{2D} \{A_{x,\text{ref}}(x, y)\}$$

$$\mathbf{r}_y = \text{FFT}_{2D} \{A_{y,\text{ref}}(x, y)\}$$

$$\mathbf{t}_x = \text{FFT}_{2D} \{A_{x,\text{tm}}(x, y)\}$$

$$\mathbf{t}_y = \text{FFT}_{2D} \{A_{y,\text{tm}}(x, y)\}$$

Calculating the Longitudinal Components

The longitudinal field components are calculated from the transverse components using the divergence equation.

$$\mathbf{r}_z = -\mathbf{K}_{z,\text{ref}}^{-1} \left(\mathbf{K}_x \mathbf{r}_x + \mathbf{K}_y \mathbf{r}_y \right)$$

$$\mathbf{t}_z = -\mathbf{K}_{z,\text{trn}}^{-1} \left(\mathbf{K}_x \mathbf{t}_x + \mathbf{K}_y \mathbf{t}_y \right)$$

$$\mathbf{K}_{z,\text{ref}} = -\left(\sqrt{\left(k_0 \mu_{r,\text{ref}}^* \epsilon_{r,\text{ref}}^* \right)^2 \mathbf{I} - \mathbf{K}_x^2 - \mathbf{K}_y^2} \right)^*$$

$$\mathbf{K}_{z,\text{trn}} = \left(\sqrt{\left(k_0 \mu_{r,\text{trn}}^* \epsilon_{r,\text{trn}}^* \right)^2 \mathbf{I} - \mathbf{K}_x^2 - \mathbf{K}_y^2} \right)^*$$

The complex conjugates in these equations are to enforce the negative sign convention.

Calculating the Diffraction Efficiencies

The diffraction efficiencies \mathbf{R} and \mathbf{T} are calculated as

$$|\vec{\mathbf{r}}|^2 = |\mathbf{r}_x|^2 + |\mathbf{r}_y|^2 + |\mathbf{r}_z|^2$$

$$|\vec{\mathbf{t}}|^2 = |\mathbf{t}_x|^2 + |\mathbf{t}_y|^2 + |\mathbf{t}_z|^2$$

$$\mathbf{R} = \frac{\text{Re} \left[-\mathbf{K}_{z,\text{ref}} / \mu_{r,\text{inc}} \right]}{\text{Re} \left[k_z^{\text{inc}} / \mu_{r,\text{inc}} \right]} |\vec{\mathbf{r}}|^2$$

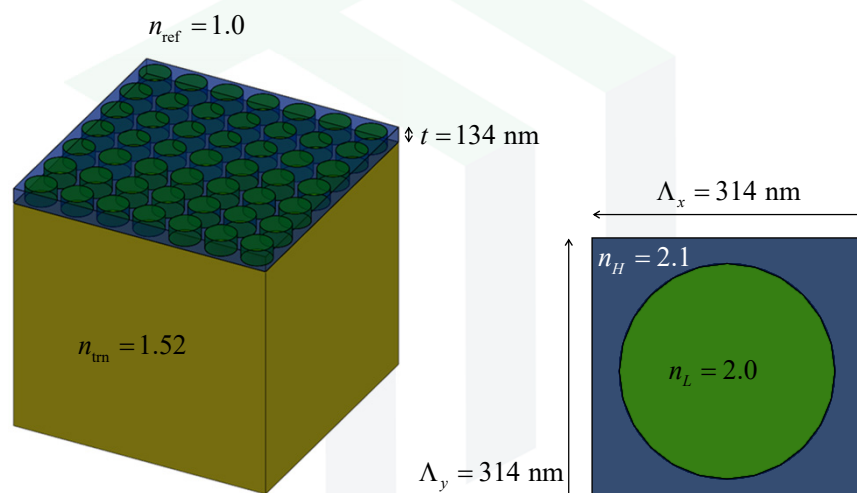
$$\mathbf{T} = \frac{\text{Re} \left[\mathbf{K}_{z,\text{trn}} / \mu_{r,\text{trn}} \right]}{\text{Re} \left[k_z^{\text{inc}} / \mu_{r,\text{inc}} \right]} |\vec{\mathbf{t}}|^2$$

Remember that these equations assume the source was given unit amplitude.

Comparison to RCWA

Slide 35

Dielectric Device Comparison



Slide 36

Comparison of Model Results

