



Advanced Computation:
Computational Electromagnetics

RCWA Extras

1

Outline

- Calculating internal fields
- One spatial harmonic: $P=Q=1$
- Simulation of 1D Gratings with 3D-RCWA
- Formulation of 2D-RCWA with fast Fourier factorization
- Danger of RCWA and convergence
- RCWA and curved structures
- Strategically truncating the set of spatial harmonics
- RCWA for generalized symmetries
- Modeling hexagonal gratings with rectangular RCWA
- Enhanced transmittance matrix approach

2

Calculating Internal Fields

Slide 3

3

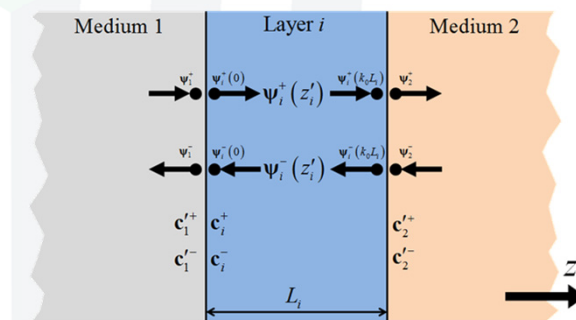
Information Needed

The field inside the i^{th} layer is calculated as:

$$\Psi_i(z'_i) = \begin{bmatrix} s_x(z'_i) \\ s_y(z'_i) \\ u_x(z'_i) \\ u_y(z'_i) \end{bmatrix} = \begin{bmatrix} \mathbf{W}_i & \mathbf{W}_i \\ -\mathbf{V}_i & \mathbf{V}_i \end{bmatrix} \begin{bmatrix} e^{-\lambda_i z'_i} & \mathbf{0} \\ \mathbf{0} & e^{\lambda_i z'_i} \end{bmatrix} \begin{bmatrix} \mathbf{c}_i^+ \\ \mathbf{c}_i^- \end{bmatrix}$$

To do this, the parameters \mathbf{W}_i , \mathbf{V}_i and λ_i must be recorded when analyzing the i^{th} layer.

But how are \mathbf{c}_i^+ and \mathbf{c}_i^- calculated?



Slide 4

4

Calculating the Internal Mode Coefficients

The scattering matrices calculate mode coefficients, \mathbf{c}_{i1}^{\pm} and \mathbf{c}_{i2}^{\pm} , that are external of the i th layer. However, it is the internal mode coefficients \mathbf{c}_i^{\pm} that are needed.

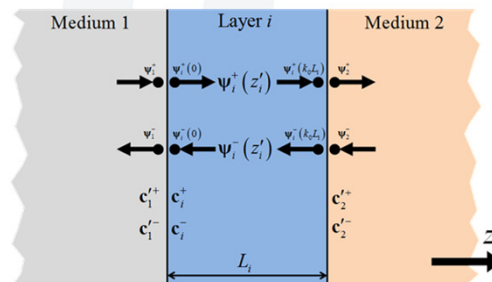
Boundary conditions require the fields to be continuous across an interface. Recall the boundary condition for the first interface is

$$\psi_{i1} = \psi_i(0)$$

$$\begin{bmatrix} \mathbf{W}_{i1} & \mathbf{W}_{i1} \\ -\mathbf{V}_{i1} & \mathbf{V}_{i1} \end{bmatrix} \begin{bmatrix} \mathbf{c}_{i1}^+ \\ \mathbf{c}_{i1}^- \end{bmatrix} = \begin{bmatrix} \mathbf{W}_i & \mathbf{W}_i \\ -\mathbf{V}_i & \mathbf{V}_i \end{bmatrix} \begin{bmatrix} \mathbf{c}_i^+ \\ \mathbf{c}_i^- \end{bmatrix}$$

Solving for the internal mode coefficients gives

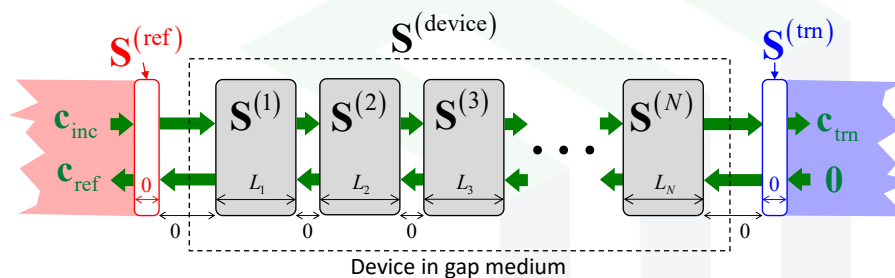
$$\begin{bmatrix} \mathbf{c}_i^+ \\ \mathbf{c}_i^- \end{bmatrix} = \begin{bmatrix} \mathbf{W}_i & \mathbf{W}_i \\ -\mathbf{V}_i & \mathbf{V}_i \end{bmatrix}^{-1} \begin{bmatrix} \mathbf{W}_{i1} & \mathbf{W}_{i1} \\ -\mathbf{V}_{i1} & \mathbf{V}_{i1} \end{bmatrix} \begin{bmatrix} \mathbf{c}_{i1}^+ \\ \mathbf{c}_{i1}^- \end{bmatrix}$$



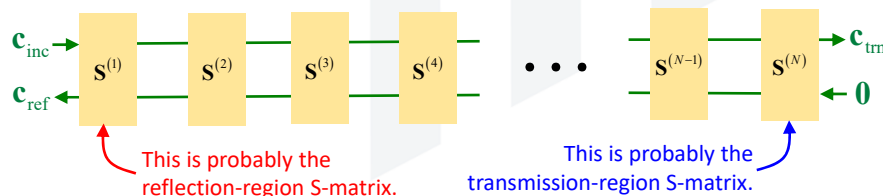
5

General Scattering Matrix Framework

The simulation is really just a series of scattering matrices.



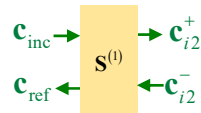
Consider this in a simplified framework as



6

Algorithm: Forward Pass

Progressing from left to right, the global scattering matrix is built one layer at a time.



Record:

$$\mathbf{W}_1$$

$$\mathbf{V}_1$$

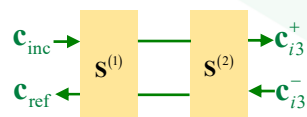
$$\lambda_1$$

$$\mathbf{S}^{(G1)} = \mathbf{S}^{(1)}$$

Note, it is only necessary to store these intermediate parameters if the fields inside of this layer are to be calculated.

Algorithm: Forward Pass

Progressing from left to right, the global scattering matrix is built one layer at a time.



Record:

$$\mathbf{W}_2$$

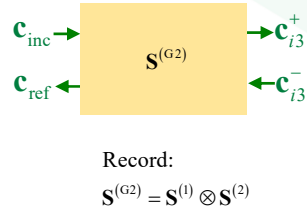
$$\mathbf{V}_2$$

$$\lambda_2$$

Note, it is only necessary to store these intermediate parameters if the fields inside of this layer are to be calculated.

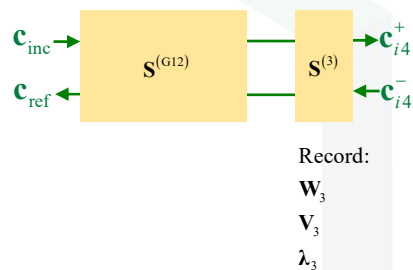
Algorithm: Forward Pass

Progressing from left to right, the global scattering matrix is built one layer at a time.



Algorithm: Forward Pass

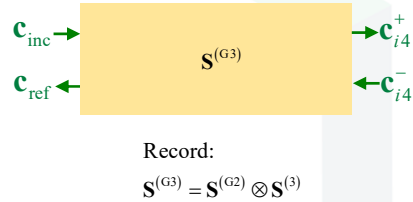
Progressing from left to right, the global scattering matrix is built one layer at a time.



Note, it is only necessary to store these intermediate parameters if the fields inside of this layer are to be calculated.

Algorithm: Forward Pass

Progressing from left to right, the global scattering matrix is built one layer at a time.

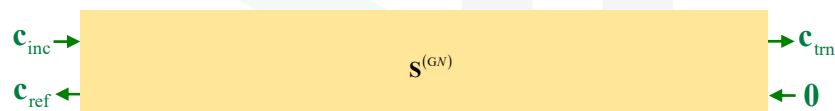


11

Algorithm: Forward Pass

The final global scattering matrix is

$$\begin{bmatrix} \mathbf{c}_{\text{ref}} \\ \mathbf{c}_{\text{trn}} \end{bmatrix} = \underbrace{\left(\begin{bmatrix} \mathbf{S}_{11}^{(1)} & \mathbf{S}_{12}^{(1)} \\ \mathbf{S}_{21}^{(1)} & \mathbf{S}_{22}^{(1)} \end{bmatrix} \otimes \begin{bmatrix} \mathbf{S}_{11}^{(2)} & \mathbf{S}_{12}^{(2)} \\ \mathbf{S}_{21}^{(2)} & \mathbf{S}_{22}^{(2)} \end{bmatrix} \otimes \dots \otimes \begin{bmatrix} \mathbf{S}_{11}^{(N-1)} & \mathbf{S}_{12}^{(N-1)} \\ \mathbf{S}_{21}^{(N-1)} & \mathbf{S}_{22}^{(N-1)} \end{bmatrix} \otimes \begin{bmatrix} \mathbf{S}_{11}^{(N)} & \mathbf{S}_{12}^{(N)} \\ \mathbf{S}_{21}^{(N)} & \mathbf{S}_{22}^{(N)} \end{bmatrix} \right)}_{\mathbf{S}^{(GN)}} \begin{bmatrix} \mathbf{c}_{\text{inc}} \\ \mathbf{0} \end{bmatrix}$$



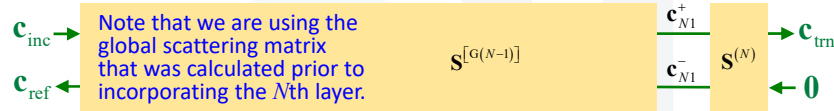
Record:
 $\mathbf{S}^{(GN)} = \mathbf{S}^{[G(N-1)]} \otimes \mathbf{S}^{(N)}$

12

Algorithm: Backward Pass

Now the external mode coefficients, \mathbf{c}_{N1}^+ and \mathbf{c}_{N1}^- can be calculated on the left side of layer N .

$$\begin{bmatrix} \mathbf{c}_{\text{ref}} \\ \mathbf{c}_{N1}^+ \end{bmatrix} = \mathbf{S}^{[G(N-1)]} \begin{bmatrix} \mathbf{c}_{\text{inc}} \\ \mathbf{c}_{N1}^- \end{bmatrix} \rightarrow \begin{aligned} \mathbf{c}_{N1}^- &= \left(\mathbf{S}_{12}^{[G(N-1)]} \right)^{-1} \left(\mathbf{c}_{\text{ref}} - \mathbf{S}_{11}^{[G(N-1)]} \mathbf{c}_{\text{inc}} \right) \\ \mathbf{c}_{N1}^+ &= \mathbf{S}_{21}^{[G(N-1)]} \mathbf{c}_{\text{inc}} + \mathbf{S}_{22}^{[G(N-1)]} \mathbf{c}_{N1}^- \end{aligned}$$



The internal mode coefficients \mathbf{c}_N^+ and \mathbf{c}_N^- of the N th layer are then

$$\begin{bmatrix} \mathbf{c}_N^+ \\ \mathbf{c}_N^- \end{bmatrix} = \begin{bmatrix} \mathbf{W}_N & \mathbf{W}_N \\ -\mathbf{V}_N & \mathbf{V}_N \end{bmatrix}^{-1} \begin{bmatrix} \mathbf{W}_{N1} & \mathbf{W}_{N1} \\ -\mathbf{V}_{N1} & \mathbf{V}_{N1} \end{bmatrix} \begin{bmatrix} \mathbf{c}_{N1}^+ \\ \mathbf{c}_{N1}^- \end{bmatrix}$$

Note: for isotropic TMM

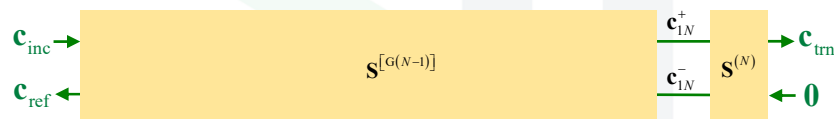
$\mathbf{W}_N = \mathbf{W}_{N1} = \mathbf{I}$

$\mathbf{V}_{N1} = \mathbf{V}_g$ for internal layers

Algorithm: Backward Pass

The internal fields of the N th layer can now be calculated at any position z'_N .

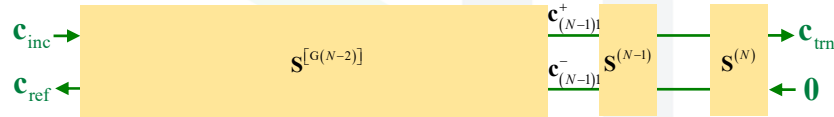
$$\Psi_N(z'_N) = \begin{bmatrix} \mathbf{s}_{x,N}(z'_N) \\ \mathbf{s}_{y,N}(z'_N) \\ \mathbf{u}_{x,N}(z'_N) \\ \mathbf{u}_{y,N}(z'_N) \end{bmatrix} = \begin{bmatrix} \mathbf{W}_N & \mathbf{W}_N \\ -\mathbf{V}_N & \mathbf{V}_N \end{bmatrix} \begin{bmatrix} e^{-\lambda_N z'_N} & \mathbf{0} \\ \mathbf{0} & e^{\lambda_N z'_N} \end{bmatrix} \begin{bmatrix} \mathbf{c}_N^+ \\ \mathbf{c}_N^- \end{bmatrix}$$



Algorithm: Backward Pass

It is now possible to calculate the mode coefficients inside layer $N-1$.

$$\begin{bmatrix} \mathbf{c}_{\text{ref}} \\ \mathbf{c}_{(N-1)l}^+ \end{bmatrix} = \mathbf{S}^{[G(N-2)]} \begin{bmatrix} \mathbf{c}_{\text{inc}} \\ \mathbf{c}_{(N-1)l}^- \end{bmatrix} \rightarrow \begin{aligned} \mathbf{c}_{(N-1)l}^- &= \left(\mathbf{S}_{12}^{[G(N-2)]} \right)^{-1} \left(\mathbf{c}_{\text{ref}} - \mathbf{S}_{11}^{[G(N-2)]} \mathbf{c}_{\text{inc}} \right) \\ \mathbf{c}_{(N-1)l}^+ &= \mathbf{S}_{21}^{[G(N-2)]} \mathbf{c}_{\text{inc}} + \mathbf{S}_{22}^{[G(N-2)]} \mathbf{c}_{(N-1)l}^- \end{aligned}$$



The internal mode coefficients \mathbf{c}_{N-1}^+ and \mathbf{c}_{N-1}^- of the N th layer are

$$\begin{bmatrix} \mathbf{c}_{N-1}^+ \\ \mathbf{c}_{N-1}^- \end{bmatrix} = \begin{bmatrix} \mathbf{W}_{N-1} & \mathbf{W}_{N-1} \\ -\mathbf{V}_{N-1} & \mathbf{V}_{N-1} \end{bmatrix}^{-1} \begin{bmatrix} \mathbf{W}_{(N-1)l} & \mathbf{W}_{(N-1)l} \\ -\mathbf{V}_{(N-1)l} & \mathbf{V}_{(N-1)l} \end{bmatrix} \begin{bmatrix} \mathbf{c}_{(N-1)l}^+ \\ \mathbf{c}_{(N-1)l}^- \end{bmatrix}$$

Note: for isotropic TMM

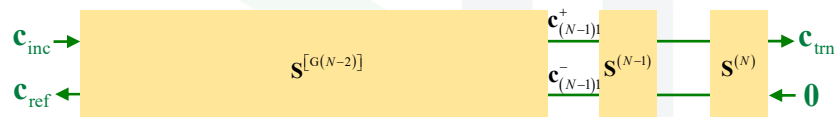
$$\mathbf{W}_{N-1} = \mathbf{W}_{(N-1)l} = \mathbf{I}$$

$$\mathbf{V}_{(N-1)l} = \mathbf{V}_g \text{ for internal layers}$$

Algorithm: Backward Pass

The internal fields can now be calculated inside of the $(N-1)$ th layer.

$$\Psi_{N-1}(z'_{N-1}) = \begin{bmatrix} \mathbf{s}_{x,N-1}(z'_{N-1}) \\ \mathbf{s}_{y,N-1}(z'_{N-1}) \\ \mathbf{u}_{x,N-1}(z'_{N-1}) \\ \mathbf{u}_{y,N-1}(z'_{N-1}) \end{bmatrix} = \begin{bmatrix} \mathbf{W}_{N-1} & \mathbf{W}_{N-1} \\ -\mathbf{V}_{N-1} & \mathbf{V}_{N-1} \end{bmatrix} \begin{bmatrix} e^{-\lambda_{N-1} z'_{N-1}} & \mathbf{0} \\ \mathbf{0} & e^{\lambda_{N-1} z'_{N-1}} \end{bmatrix} \begin{bmatrix} \mathbf{c}_{N-1}^+ \\ \mathbf{c}_{N-1}^- \end{bmatrix}$$



Summary of the Algorithm

Forward Pass:

Perform simulation as usual, building the global scattering matrix from left to right.

During this forward pass, record \mathbf{W}_i , \mathbf{V}_i , λ_i and $\mathbf{S}^{(Gi)}$ calculated for each layer where the internal field is to be calculated.

Backward Pass:

For each layer of interest, calculate the external mode coefficients.

$$\mathbf{c}_{il}^- = \left(\mathbf{S}_{12}^{[G(i-1)]} \right)^{-1} \left(\mathbf{c}_{\text{ref}} - \mathbf{S}_{11}^{[G(i-1)]} \mathbf{c}_{\text{inc}} \right)$$

$$\mathbf{c}_{il}^+ = \mathbf{S}_{21}^{[G(i-1)]} \mathbf{c}_{\text{inc}} + \mathbf{S}_{22}^{[G(i-1)]} \mathbf{c}_{il}^-$$

...and then the internal mode coefficients

$$\begin{bmatrix} \mathbf{c}_i^+ \\ \mathbf{c}_i^- \end{bmatrix} = \begin{bmatrix} \mathbf{W}_i & \mathbf{W}_i \\ -\mathbf{V}_i & \mathbf{V}_i \end{bmatrix}^{-1} \begin{bmatrix} \mathbf{W}_{il} & \mathbf{W}_{il} \\ -\mathbf{V}_{il} & \mathbf{V}_{il} \end{bmatrix} \begin{bmatrix} \mathbf{c}_{il}^+ \\ \mathbf{c}_{il}^- \end{bmatrix}$$

...and finally the internal fields

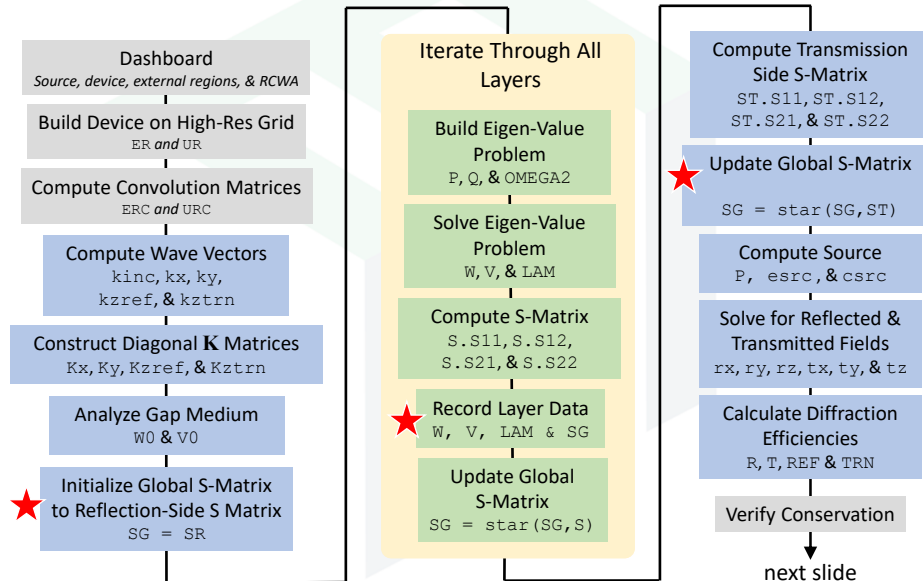
$$\Psi_i(z_i) = \begin{bmatrix} s_{x,i}(z_i) \\ s_{y,i}(z_i) \\ u_{x,i}(z_i) \\ u_{y,i}(z_i) \end{bmatrix} = \begin{bmatrix} \mathbf{W}_i & \mathbf{W}_i \\ -\mathbf{V}_i & \mathbf{V}_i \end{bmatrix} \begin{bmatrix} e^{-k_0 \lambda_i z_i} & \mathbf{0} \\ \mathbf{0} & e^{k_0 \lambda_i z_i} \end{bmatrix} \begin{bmatrix} \mathbf{c}_i^+ \\ \mathbf{c}_i^- \end{bmatrix}$$



Slide 17

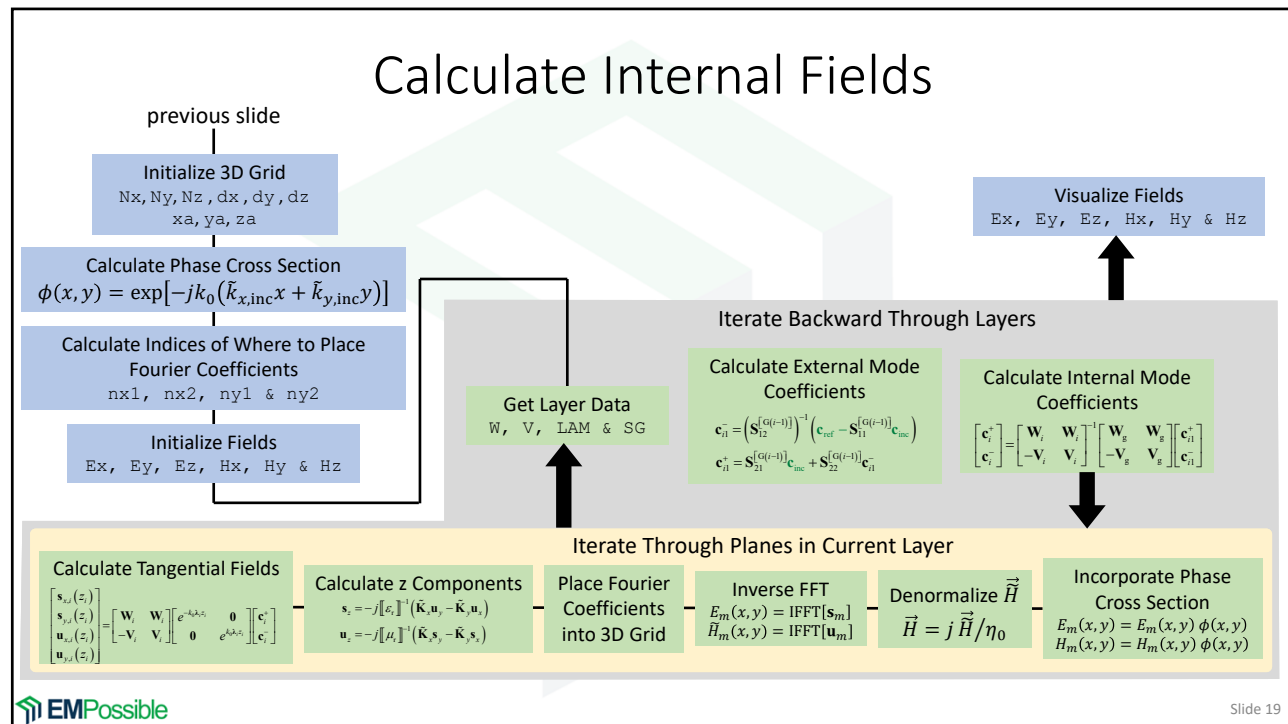
17

Modifications to RCWA Algorithm

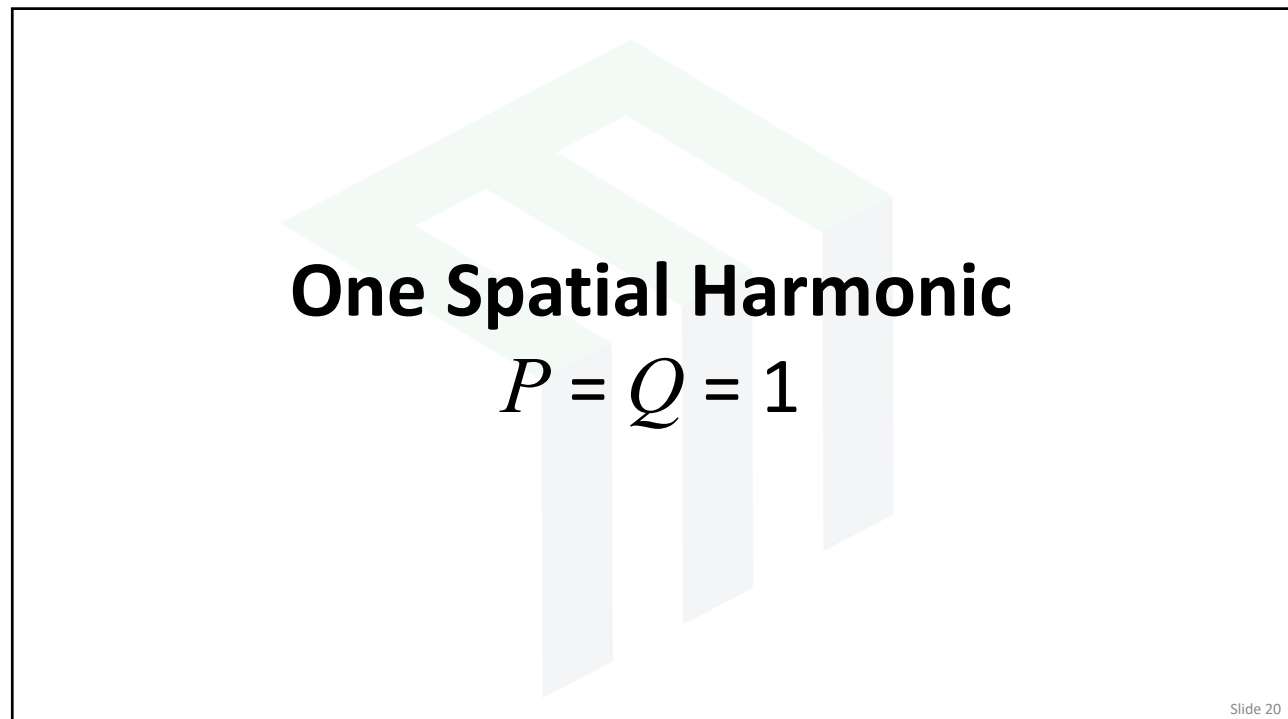


Slide 18

18

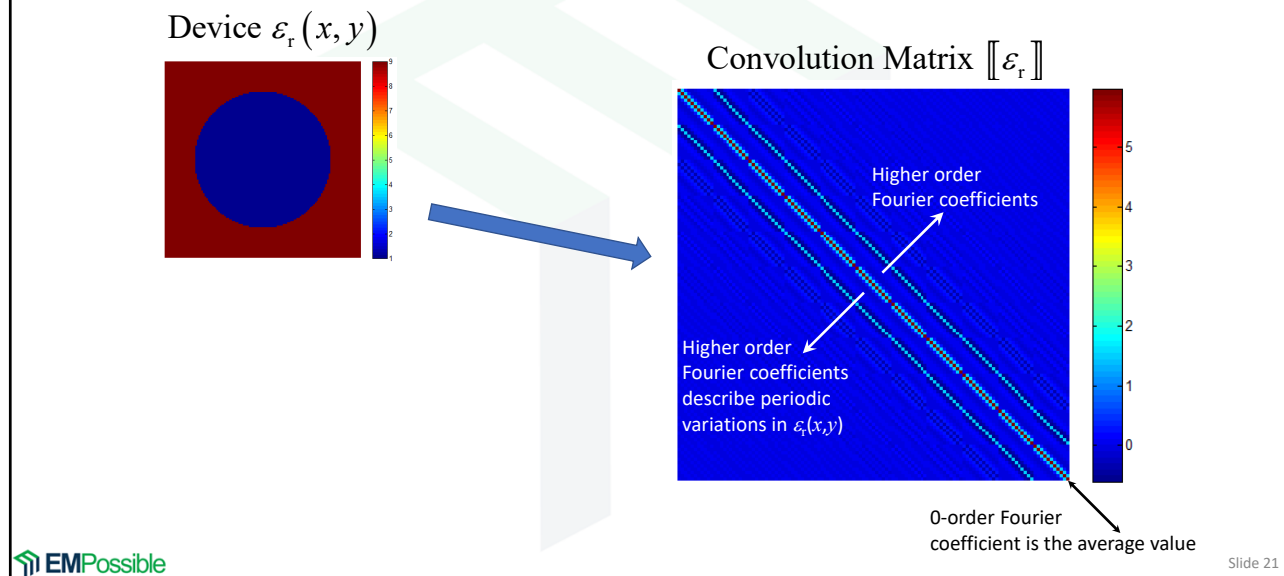


19



20

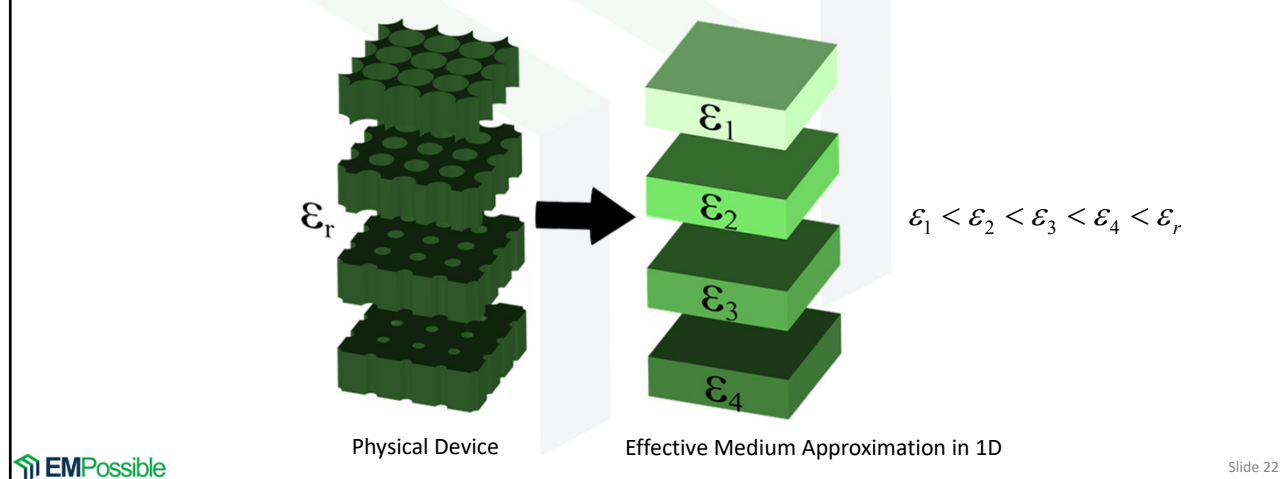
Anatomy of the Convolution Matrix



21

One Spatial Harmonic ($P=Q=1$)

When only one spatial harmonic is used, RCWA reduces to the 1D transfer matrix method, but uses the average value for the material properties in each layer. This is first-order “effective medium theory” and can make use of fast Fourier factorization so it is more sophisticated than the standard TMM.



22

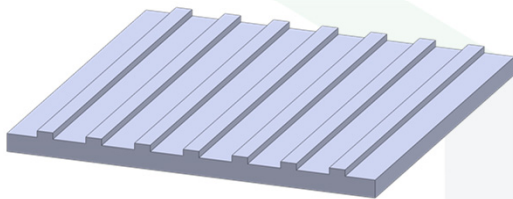
Simulation of 1D Gratings with 3D-RCWA

Slide 23

23

Grating Terminology

1D grating
Ruled grating



Requires a 2D simulation

2D grating
Crossed grating



Requires a 3D simulation

Slide 24

24

3D-RCWA for 1D Gratings

Three-dimensional RCWA simulates all polarizations at the same time.

For 1D Gratings, Maxwell's equations decouple into the E mode and the H mode.

It is possible to reformulate RCWA specifically for 1D Gratings so that it will only simulate either the E mode or H mode, but not both. This approach will be several times faster due to smaller matrices.

It is my experience that 3D-RCWA is fast enough that few applications warrant formulating a 2D-RCWA code. Exceptions include when fast Fourier factorization is important or for running optimizations that require many thousands of simulations to be iterated.

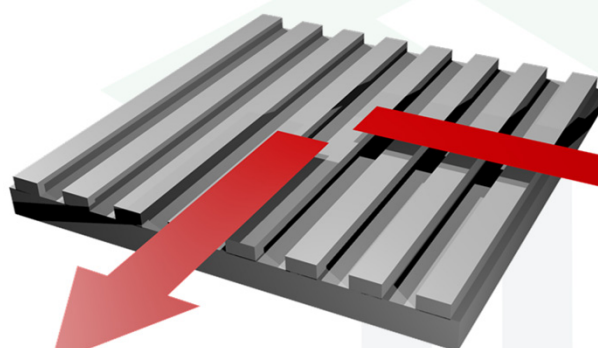
There are some tricks that can be used when using RCWA to model 1D gratings to maximize the speed and efficiency.



Slide 25

25

Number of Spatial Harmonics



There is no contrast in this direction. Only one spatial harmonic is needed.

$$Q = 1$$

$$N_y = 1$$

You must use some number of spatial harmonics in this direction.

$$P \sim 7 \frac{\Lambda}{\lambda}$$

$$N_x > 500$$

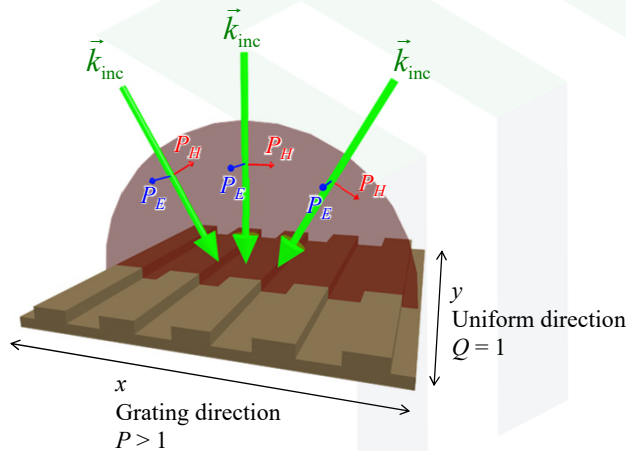


Slide 26

26

E and H Modes with 3D-RCWA

The field for both E and H modes are thought of completely in terms of the polarization vector for the electric field. If you have implemented your codes following these lectures, no changes to your code are needed outside of the dashboard.



Source Wave Vector

$$\vec{k}_{inc} = k_0 n_{inc} \begin{bmatrix} \sin \theta \\ 0 \\ \cos \theta \end{bmatrix}$$

Source Polarization Vector

$$\vec{P}_E = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \quad \text{E Mode}$$

$$\vec{P}_H = \begin{bmatrix} \cos \theta \\ 0 \\ \sin \theta \end{bmatrix} \quad \text{H Mode}$$

The concept of E and H modes only apply when: (1) LHI or diagonally anisotropic materials, (2) device is uniform in y direction, and (3) propagation is restricted to x - z plane.



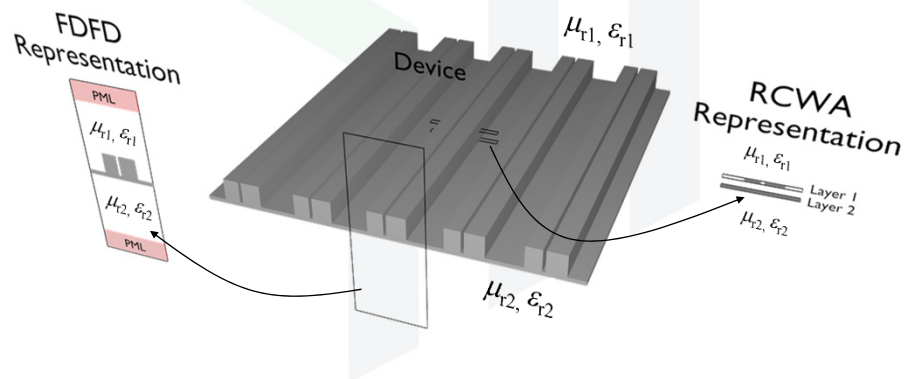
Slide 27

27

FDFD Vs. RCWA Representations

FDFD represents a device as the side view of a single unit cell.

In contrast, RCWA represents a device as a top view of each layer of a single unit cell.



Slide 28

28

Formulation of 2D RCWA with FFF (1D Gratings)

Slide 29

29

Starting Point for Derivation

We will start with the semi-analytical matrix form of Maxwell's equations in Fourier-space. These are rigorous and valid even for 3D devices.

$$-j\tilde{\mathbf{K}}_y \mathbf{u}_z - \frac{d}{d\tilde{z}} \mathbf{u}_y = [\![\varepsilon_r]\!] \mathbf{s}_x$$

$$\frac{d}{d\tilde{z}} \mathbf{u}_x + j\tilde{\mathbf{K}}_x \mathbf{u}_z = [\![\varepsilon_r]\!] \mathbf{s}_y$$

$$\tilde{\mathbf{K}}_x \mathbf{u}_y - \tilde{\mathbf{K}}_y \mathbf{u}_x = j[\![\varepsilon_r]\!] \mathbf{s}_z$$

$$-j\tilde{\mathbf{K}}_y \mathbf{s}_z - \frac{d}{d\tilde{z}} \mathbf{s}_y = [\![\mu_r]\!] \mathbf{u}_x$$

$$\frac{d}{d\tilde{z}} \mathbf{s}_x + j\tilde{\mathbf{K}}_x \mathbf{s}_z = [\![\mu_r]\!] \mathbf{u}_y$$

$$\tilde{\mathbf{K}}_x \mathbf{s}_y - \tilde{\mathbf{K}}_y \mathbf{s}_x = j[\![\mu_r]\!] \mathbf{u}_z$$

Slide 30

30

Reduction to Two Dimensions

When devices are uniform in the y -direction and no wave propagation occurs in this direction, we have

$$\tilde{\mathbf{K}}_y = \mathbf{0}$$

Our matrix equations reduce to

$$\begin{aligned} -\frac{d}{d\tilde{z}} \mathbf{u}_y &= [\epsilon_r] \mathbf{s}_x & -\frac{d}{d\tilde{z}} \mathbf{s}_y &= [\mu_r] \mathbf{u}_x \\ \frac{d}{d\tilde{z}} \mathbf{u}_x + j\tilde{\mathbf{K}}_x \mathbf{u}_z &= [\epsilon_r] \mathbf{s}_y & \frac{d}{d\tilde{z}} \mathbf{s}_x + j\tilde{\mathbf{K}}_x \mathbf{s}_z &= [\mu_r] \mathbf{u}_y \\ \tilde{\mathbf{K}}_x \mathbf{u}_y &= j[\epsilon_r] \mathbf{s}_z & \tilde{\mathbf{K}}_x \mathbf{s}_y &= j[\mu_r] \mathbf{u}_z \end{aligned}$$

Two Independent Modes

We see that Maxwell's equations have decoupled into two independent modes.

$$\begin{aligned} -\frac{d}{d\tilde{z}} \mathbf{u}_y &= [\epsilon_r] \mathbf{s}_x & -\frac{d}{d\tilde{z}} \mathbf{s}_y &= [\mu_r] \mathbf{u}_x \\ \frac{d}{d\tilde{z}} \mathbf{u}_x + j\tilde{\mathbf{K}}_x \mathbf{u}_z &= [\epsilon_r] \mathbf{s}_y & \frac{d}{d\tilde{z}} \mathbf{s}_x + j\tilde{\mathbf{K}}_x \mathbf{s}_z &= [\mu_r] \mathbf{u}_y \\ \tilde{\mathbf{K}}_x \mathbf{u}_y &= j[\epsilon_r] \mathbf{s}_z & \tilde{\mathbf{K}}_x \mathbf{s}_y &= j[\mu_r] \mathbf{u}_z \end{aligned}$$

E Mode

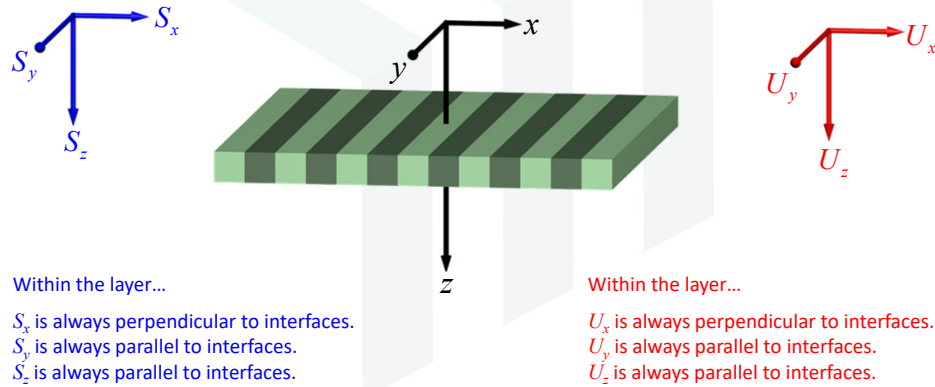
$$\begin{aligned} \frac{d}{d\tilde{z}} \mathbf{u}_x + j\tilde{\mathbf{K}}_x \mathbf{u}_z &= [\epsilon_r] \mathbf{s}_y \\ -\frac{d}{d\tilde{z}} \mathbf{s}_y &= [\mu_r] \mathbf{u}_x \\ \tilde{\mathbf{K}}_x \mathbf{s}_y &= j[\mu_r] \mathbf{u}_z \end{aligned}$$

H Mode

$$\begin{aligned} \frac{d}{d\tilde{z}} \mathbf{s}_x + j\tilde{\mathbf{K}}_x \mathbf{s}_z &= [\mu_r] \mathbf{u}_y \\ -\frac{d}{d\tilde{z}} \mathbf{u}_y &= [\epsilon_r] \mathbf{s}_x \\ \tilde{\mathbf{K}}_x \mathbf{u}_y &= j[\epsilon_r] \mathbf{s}_z \end{aligned}$$

Orientation of the Field Components

For 1D gratings, the orientation of the field components relative to the interfaces is fixed. In this case, it is straightforward to incorporate fast Fourier factorization into the formulation.



Incorporating Fast Fourier Factorization

For 1D gratings, it is very straightforward to incorporate fast Fourier factorization rules. This will improve convergence rates.

E Mode

$$\begin{aligned}\frac{d}{d\tilde{z}} \mathbf{u}_x + j\tilde{\mathbf{K}}_x \mathbf{u}_z &= [\boldsymbol{\varepsilon}_r] \mathbf{s}_y \\ -\frac{d}{d\tilde{z}} \mathbf{s}_y &= [1/\mu_r]^{-1} \mathbf{u}_x \\ \tilde{\mathbf{K}}_x \mathbf{s}_y &= j[\mu_r] \mathbf{u}_z\end{aligned}$$

\mathbf{s}_y is always parallel to interfaces so $[\boldsymbol{\varepsilon}_r]$ is the standard convolution matrix.

\mathbf{u}_x is always perpendicular so FFF rules are used to construct $[1/\mu_r]^{-1}$.

\mathbf{u}_z is always parallel to interfaces so $[\mu_r]$ is the standard convolution matrix.

H Mode

$$\begin{aligned}\frac{d}{d\tilde{z}} \mathbf{s}_x + j\tilde{\mathbf{K}}_x \mathbf{s}_z &= [\mu_r] \mathbf{u}_y \\ -\frac{d}{d\tilde{z}} \mathbf{u}_y &= [1/\varepsilon_r]^{-1} \mathbf{s}_x \\ \tilde{\mathbf{K}}_x \mathbf{u}_y &= j[\boldsymbol{\varepsilon}_r] \mathbf{s}_z\end{aligned}$$

\mathbf{u}_y is always parallel to interfaces so $[\mu_r]$ is the standard convolution matrix.

\mathbf{s}_x is always perpendicular so FFF rules are used to construct $[1/\varepsilon_r]^{-1}$.

\mathbf{s}_z is always parallel to interfaces so $[\boldsymbol{\varepsilon}_r]$ is the standard convolution matrix.

Eliminate Longitudinal Components

We solve the third equation for \mathbf{u}_z and the sixth equation for \mathbf{s}_z to obtain

$$\mathbf{u}_z = -j[\mu_r]^{-1} \tilde{\mathbf{K}}_x \mathbf{s}_y$$

$$\mathbf{s}_z = -j[\varepsilon_r]^{-1} \tilde{\mathbf{K}}_x \mathbf{u}_y$$

We substitute these expressions into the remaining Maxwell's equations.

E Mode

$$\begin{aligned} \frac{d}{d\tilde{z}} \mathbf{u}_x &= [\varepsilon_r] \mathbf{s}_y - \tilde{\mathbf{K}}_x [\mu_r]^{-1} \tilde{\mathbf{K}}_x \mathbf{s}_y \\ \frac{d}{d\tilde{z}} \mathbf{s}_y &= -[1/\mu_r]^{-1} \mathbf{u}_x \end{aligned}$$

H Mode

$$\begin{aligned} \frac{d}{d\tilde{z}} \mathbf{s}_x &= [\mu_r] \mathbf{u}_y - \tilde{\mathbf{K}}_x [\varepsilon_r]^{-1} \tilde{\mathbf{K}}_x \mathbf{u}_y \\ \frac{d}{d\tilde{z}} \mathbf{u}_y &= -[1/\varepsilon_r]^{-1} \mathbf{s}_x \end{aligned}$$

Standard P and Q Form

E Mode

$$\begin{aligned} \frac{d}{d\tilde{z}} \mathbf{s}_y &= \mathbf{P} \mathbf{u}_x \\ \frac{d}{d\tilde{z}} \mathbf{u}_x &= \mathbf{Q} \mathbf{s}_y \end{aligned}$$

$$\mathbf{P} = -[1/\mu_r]^{-1}$$

$$\mathbf{Q} = [\varepsilon_r] - \tilde{\mathbf{K}}_x [\mu_r]^{-1} \tilde{\mathbf{K}}_x$$

H Mode

$$\begin{aligned} \frac{d}{d\tilde{z}} \mathbf{u}_y &= \mathbf{P} \mathbf{s}_x \\ \frac{d}{d\tilde{z}} \mathbf{s}_x &= \mathbf{Q} \mathbf{u}_y \end{aligned}$$

$$\mathbf{P} = -[1/\varepsilon_r]^{-1}$$

$$\mathbf{Q} = [\mu_r] - \tilde{\mathbf{K}}_x [\varepsilon_r]^{-1} \tilde{\mathbf{K}}_x$$

We see that FFF is incorporated solely into the matrix \mathbf{P} .

Matrix Wave Equations

Now that we have our equations in standard **P** and **Q** form, we derive the wave equations in the same manner as before.

E Mode

$$\frac{d^2}{d\tilde{z}^2} \mathbf{s}_y - \mathbf{\Omega}^2 \mathbf{s}_y = \mathbf{0}$$

$$\mathbf{\Omega}^2 = \mathbf{PQ}$$

H Mode

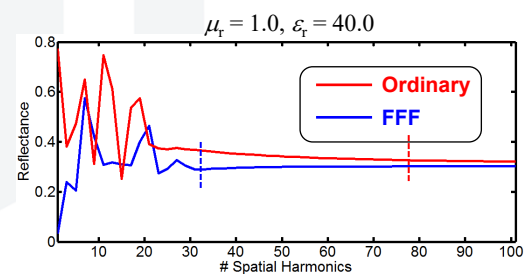
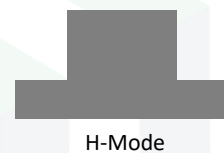
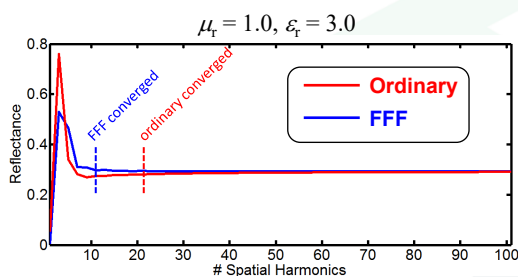
$$\frac{d^2}{d\tilde{z}^2} \mathbf{u}_y - \mathbf{\Omega}^2 \mathbf{u}_y = \mathbf{0}$$

$$\mathbf{\Omega}^2 = \mathbf{PQ}$$

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

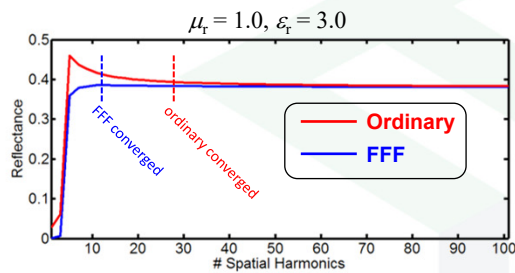
37

Convergence Study for 1D Gratings

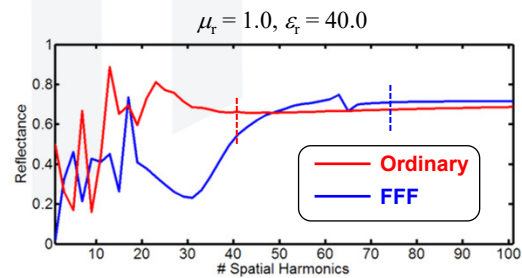


38

Convergence Study for 1D Curved Structures



H-Mode



Danger of RCWA and Convergence

Danger of RCWA

In real-space, poor grid resolution led to fluctuations in conservation of power and other very recognizable signs that things are wrong.

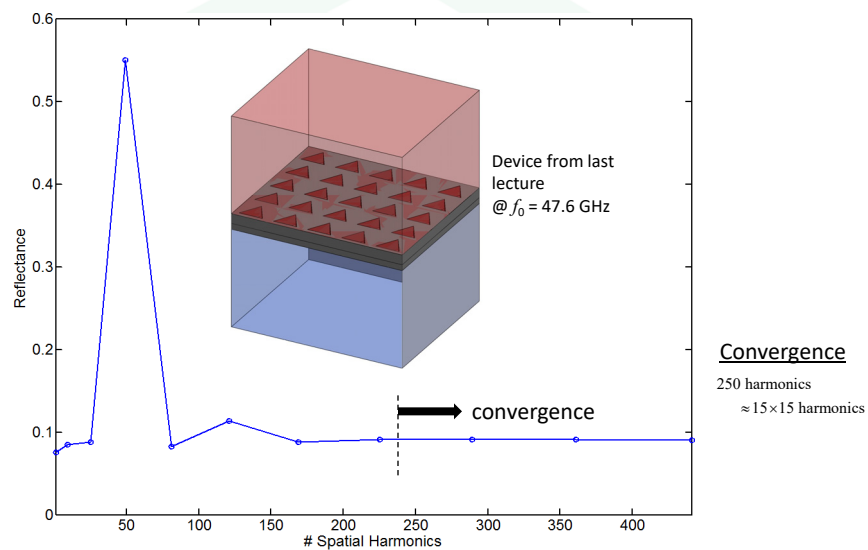
The danger of RCWA is that results can “look” correct even with very few spatial harmonics.

Conservation of power will always be obeyed in RCWA even using just one spatial harmonic.

It must become habit to look for convergence, as there are few other signs that more spatial harmonics are needed.



Typical Convergence Plot

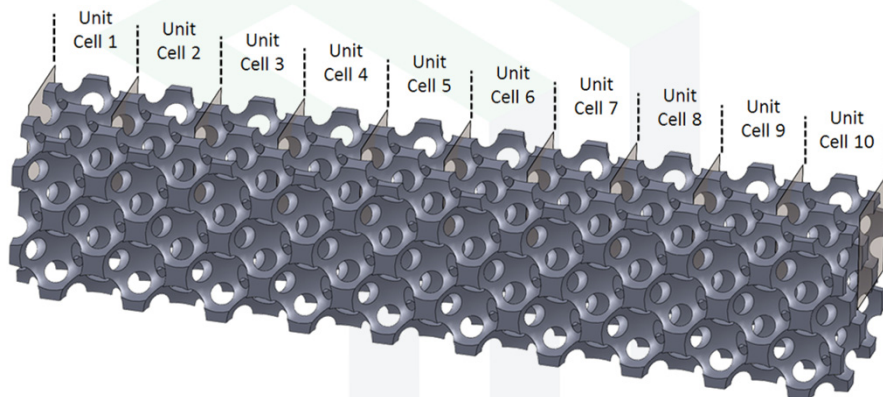


RCWA and Curved Structures

Slide 43

43

EBG Material

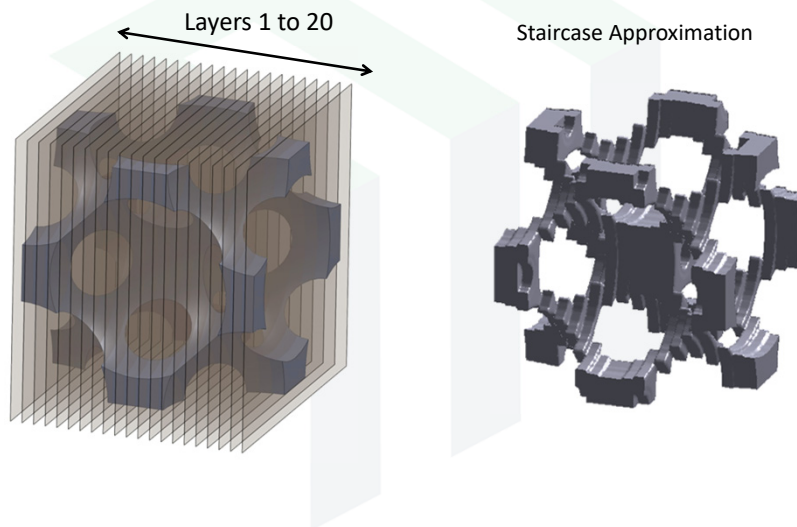


EMPossible

Slide 44

44

Divide into Thin Layers



Strategically Truncating the Set of Spatial Harmonics

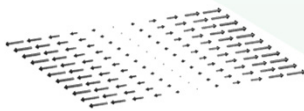
Notes on Truncating the Set of Spatial Harmonics

- The choice of which spatial harmonics to include in the expansion is arbitrary.
- Improper choice can lead to slow convergence and inaccurate results.
- We chose directions consistent with the physics of diffraction and a rectangular Fourier-space grid for simplicity.
- The number of harmonics retained in a particular direction determines the spatial resolution of structures with contrast in that direction.
- It seems optimal to keep the number of spatial harmonics uniform in all directions.

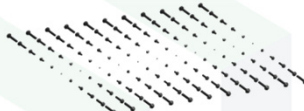
Fourier-Space Grid Notation

The components of the wave vector expansion look like:

$$\tilde{k}_x(m)$$



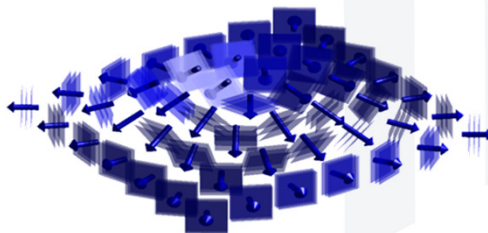
$$\tilde{k}_y(n)$$



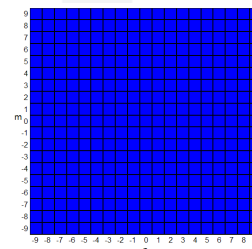
$$\tilde{k}_z(m,n) = \left(\sqrt{\mu_r^* \epsilon_r^* - \tilde{k}_x^2(m) - \tilde{k}_y^2(n)} \right)^*$$



We visualized it this way:



A simpler view of our 2D Fourier-space grid is

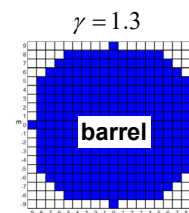
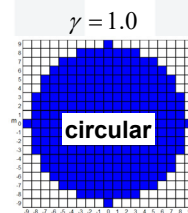
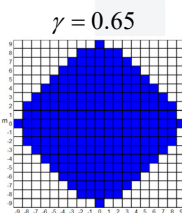
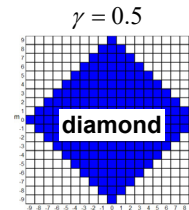
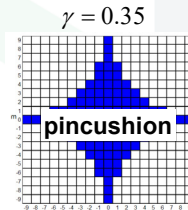
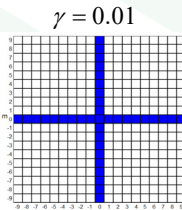
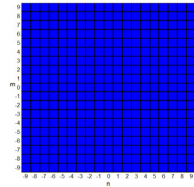


Simple Grid Truncation Scheme

We will retain all spatial harmonics with indices that satisfy the following equation:

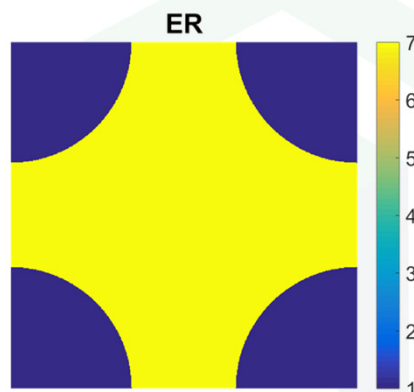
$$\left| \frac{m}{M} \right|^{2\gamma} + \left| \frac{n}{N} \right|^{2\gamma} \leq 1$$

Conventional
 $|n| \leq N$ and $|m| \leq M$



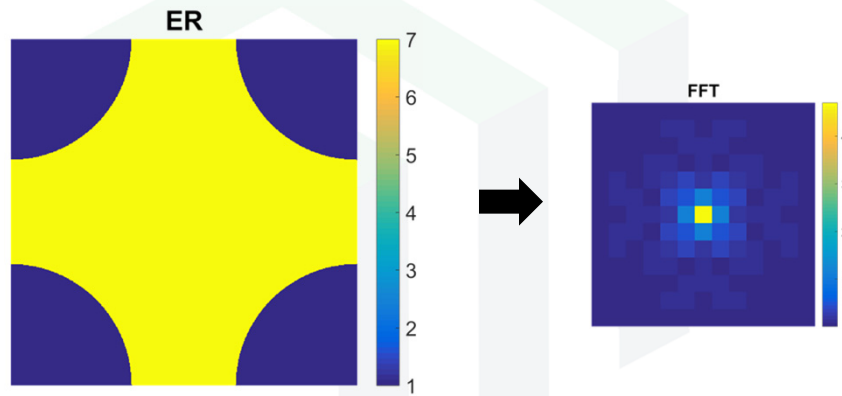
Implementation

Step 1 – Build Unit Cell on High-Resolution Grid



Implementation

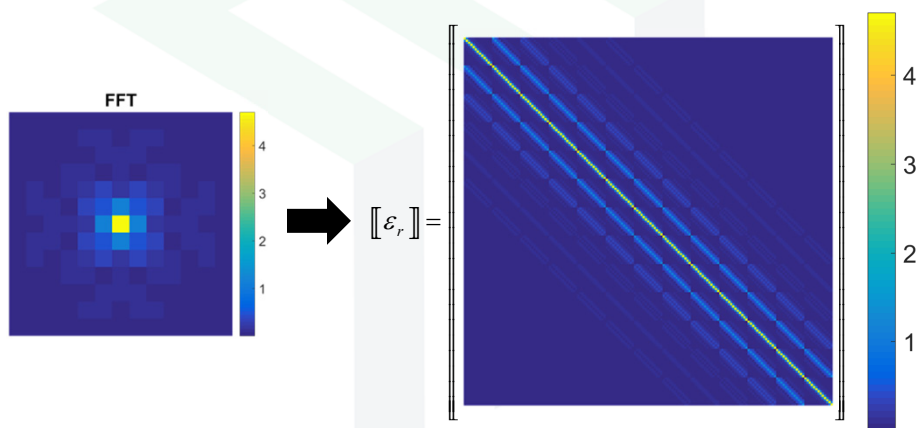
Step 2 – Calculate Fourier Coefficients Using FFT Technique



51

Implementation

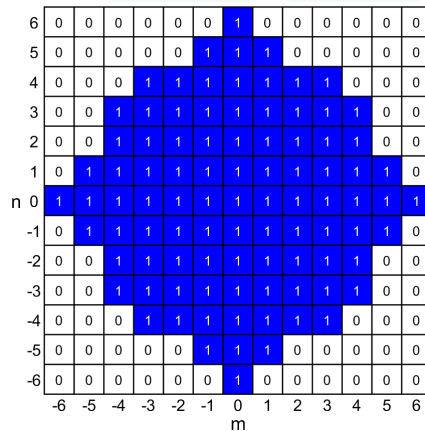
Step 3 – Assemble Standard Convolution Matrix From Fourier Coefficients



52

Implementation

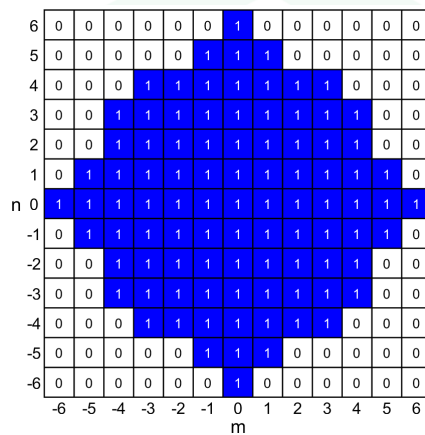
Step 4 – Build Truncation Map



```
% Construct Truncation Map
TMAP = abs(m/M).^(2*p) ...
      + abs(n/N).^(2*p);
TMAP = (TMAP <= 1);
```

Implementation

Step 5 – Extract Indices of Spatial Harmonics to Retain

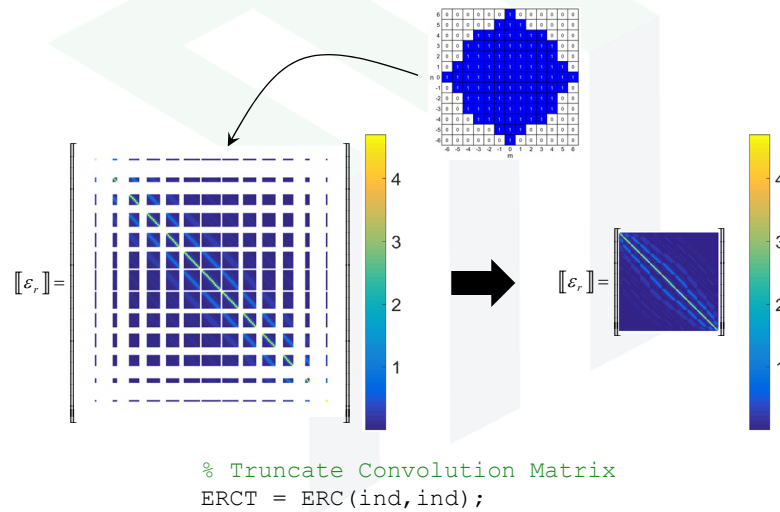


```
% Construct Truncation Map
TMAP = abs(m/M).^(2*p) ...
      + abs(n/N).^(2*p);
TMAP = (TMAP <= 1);
```

```
% Extract Array Indices
ind = find(TMAP(:));
```

Implementation

Step 6 – Truncate Convolution Matrix



Implementation

Step 7 – Perform RCWA

The rest of the RCWA algorithm remains virtually unchanged.

You will need to consider your truncation again:

1. When you calculate the source.
2. If you calculate the fields from the eigen-modes.

RCWA for Generalized Symmetries

Slide 57

57

Revised Fourier Transforms

The materials...

$$\varepsilon_r(\vec{r}) = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} a_{m,n} e^{j(m\vec{T}_1 + n\vec{T}_2) \cdot \vec{r}}$$

$$a_{m,n} = \frac{1}{A} \iint_{\text{unit cell}} \varepsilon_r(\vec{r}) e^{-j(m\vec{T}_1 + n\vec{T}_2) \cdot \vec{r}} dA$$

$$\mu_r(\vec{r}) = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} a_{m,n} e^{j(m\vec{T}_1 + n\vec{T}_2) \cdot \vec{r}}$$

$$b_{m,n} = \frac{1}{A} \iint_{\text{unit cell}} \mu_r(\vec{r}) e^{-j(m\vec{T}_1 + n\vec{T}_2) \cdot \vec{r}} dA$$

The fields...

$$E_x(\vec{r}, z) = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} S_x(m, n; z) \cdot e^{-jk_z(m,n) \cdot \vec{r}}$$

$$E_y(\vec{r}, z) = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} S_y(m, n; z) \cdot e^{-jk_z(m,n) \cdot \vec{r}}$$

$$E_z(\vec{r}, z) = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} S_z(m, n; z) \cdot e^{-jk_z(m,n) \cdot \vec{r}}$$

$$\tilde{H}_x(\vec{r}, z) = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} U_x(m, n; z) \cdot e^{-jk_z(m,n) \cdot \vec{r}}$$

$$\tilde{H}_y(\vec{r}, z) = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} U_y(m, n; z) \cdot e^{-jk_z(m,n) \cdot \vec{r}}$$

$$\tilde{H}_z(\vec{r}, z) = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} U_z(m, n; z) \cdot e^{-jk_z(m,n) \cdot \vec{r}}$$

Wave vector expansion...

$$\vec{k}_i(m, n) = \vec{k}_{\text{inc}} - m\vec{T}_1 - n\vec{T}_2$$

$$k_z(m, n) = \left(\sqrt{k_0^2 \mu_r \varepsilon_r - \left| \vec{k}_i(m, n) \right|^2} \right)^*$$

$$m = -\infty, \dots, -2, -1, 0, 1, 2, \dots, \infty$$

$$n = -\infty, \dots, -2, -1, 0, 1, 2, \dots, \infty$$

$$\vec{T}_1, \vec{T}_2 \equiv \text{reciprocal lattice vectors of the unit cell}$$

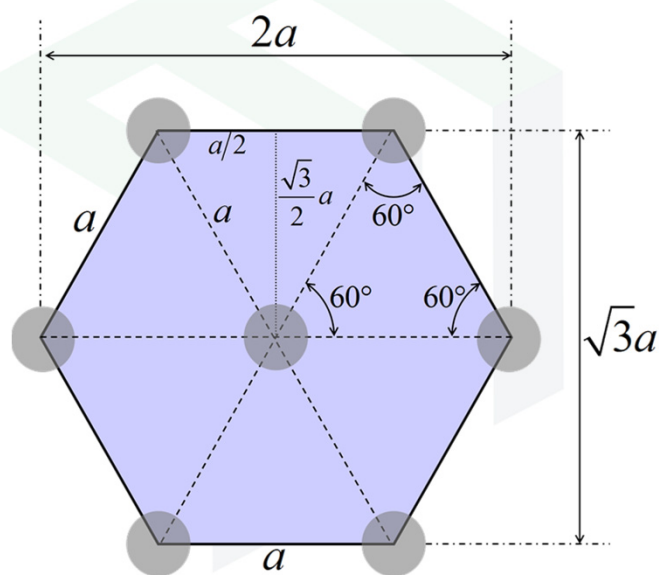
Slide 58

58

Modeling Hexagonal Gratings with Rectangular RCWA

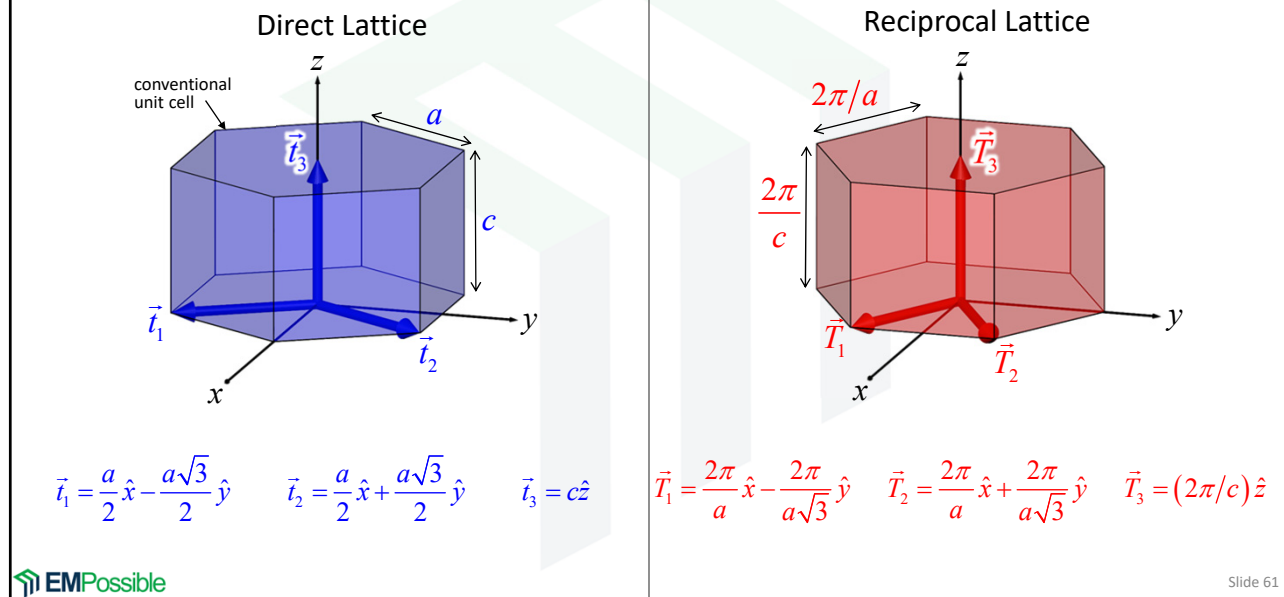
59

Geometry of a Hexagon



60

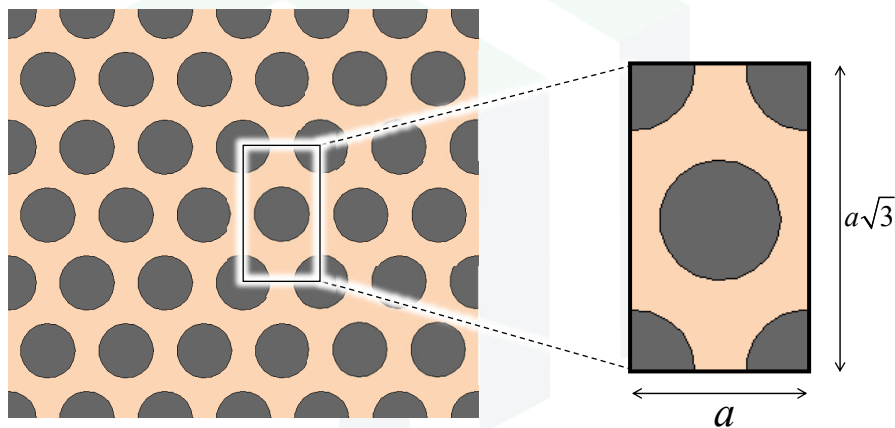
Grating Vectors of Hexagonal Structures



61

Rectangular Unit Cell in Hexagonal Array

We must identify a rectangular unit cell that reconstructs a hexagonal array.



This implies that we will need more spatial harmonics along the y direction than x .

$$Q = \text{round}(P \cdot S_y / S_x);$$

EMPossible

Slide 62

62

Enhanced Transmittance Matrix Approach

M. G. Moharam, Drew A. Pommet, Eric B. Grann, "Stable implementation of the rigorous coupled-wave analysis for surface-relief gratings: enhanced transmittance matrix approach," J. Opt. Soc. Am. A, Vol. 12, No. 5, pp. 1077-1086, May 1995.

Slide 63

63

Motivation

The enhanced transmittance matrix (ETM) method involves less matrix manipulations so it is much faster than using scattering matrices. Maybe $\sim 10\times$. It also provides easier computation of internal fields.

ETM works by first stepping backward through each layer (backward analysis) and then stepping forward (forward analysis). Intermediate parameters must be stored for each layer during the backward analysis that are recalled during the forward analysis. This leads to severe memory limitations when many layers are used.

Conclusion → Unless the device is composed of prohibitively large number of layers or if other features of scattering matrices are not needed, use ETM.

Slide 64

64

The Problem

The source of the instability is the following matrix.

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

$$\mathbf{X}_i^- = e^{\Omega_i k_0 L_i} \quad \leftarrow \text{Growing exponentials!!!} \quad \text{😞}$$

The enhanced transmittance matrix (ETM) method was the first technique applied to RCWA that fixed the instability.

ETM is much faster than scattering matrices, but is much less memory efficient because it requires parameters to be stored for all layers at the same time. Scattering matrices can proceed one layer at a time, forgetting everything about previous layers.

Boundary Conditions

First interface:

$$\mathbf{s} + \mathbf{A}\mathbf{r} = \mathbf{F}_1 \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{X}_1 \end{bmatrix} \mathbf{c}_1$$

unknown

Intermediate interfaces:

$$\mathbf{F}_i \begin{bmatrix} \mathbf{X}_i & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix} \mathbf{c}_i = \mathbf{F}_{i+1} \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{X}_{i+1} \end{bmatrix} \mathbf{c}_{i+1}$$

Last interface:

$$\mathbf{F}_N \begin{bmatrix} \mathbf{X}_N & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix} \mathbf{c}_N = \mathbf{B}\mathbf{t}$$

unknown

$$\mathbf{A} = \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \\ -\frac{j}{\mu_1} \frac{\tilde{\mathbf{K}}_x \tilde{\mathbf{K}}_y}{\tilde{\mathbf{K}}_{z,1}} & -\frac{j}{\mu_1} \frac{\tilde{\mathbf{K}}_y^2 + \tilde{\mathbf{K}}_{z,1}^2}{\tilde{\mathbf{K}}_{z,1}} \\ \frac{j}{\mu_1} \frac{\tilde{\mathbf{K}}_x^2 + \tilde{\mathbf{K}}_{z,1}^2}{\tilde{\mathbf{K}}_{z,1}} & \frac{j}{\mu_1} \frac{\tilde{\mathbf{K}}_x \tilde{\mathbf{K}}_y}{\tilde{\mathbf{K}}_{z,1}} \end{bmatrix}$$

$$\mathbf{B} = \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \\ \frac{j}{\mu_{II}} \frac{\tilde{\mathbf{K}}_x \tilde{\mathbf{K}}_y}{\tilde{\mathbf{K}}_{z,II}} & \frac{j}{\mu_{II}} \frac{\tilde{\mathbf{K}}_y^2 + \tilde{\mathbf{K}}_{z,II}^2}{\tilde{\mathbf{K}}_{z,II}} \\ -\frac{j}{\mu_{II}} \frac{\tilde{\mathbf{K}}_x^2 + \tilde{\mathbf{K}}_{z,II}^2}{\tilde{\mathbf{K}}_{z,II}} & -\frac{j}{\mu_{II}} \frac{\tilde{\mathbf{K}}_x \tilde{\mathbf{K}}_y}{\tilde{\mathbf{K}}_{z,II}} \end{bmatrix}$$

$$\mathbf{s} = \begin{bmatrix} p_x \delta_{0,pq} \\ p_y \delta_{0,pq} \\ \frac{j}{\mu_1} (k_{z,inc} p_y - k_{y,inc} p_z) \delta_{0,pq} \\ \frac{j}{\mu_1} (k_{x,inc} p_z - k_{z,inc} p_x) \delta_{0,pq} \end{bmatrix}$$

$$\mathbf{F}_i = \begin{bmatrix} \mathbf{W}_i & \mathbf{W}_i \\ -\mathbf{V}_i & \mathbf{V}_i \end{bmatrix}$$

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

Work Backward Through Layers (1 of 4)

The goal is to solve for \mathbf{r} and \mathbf{t} without using \mathbf{X}^{-1} .

We start by solving the equation at the last interface for \mathbf{c}_N .

$$\mathbf{F}_N \begin{bmatrix} \mathbf{X}_N & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix} \mathbf{c}_N = \mathbf{B}\mathbf{t} \rightarrow \mathbf{c}_N = \begin{bmatrix} \mathbf{X}_N^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix} \mathbf{F}_N^{-1} \mathbf{B}\mathbf{t}$$

We write this as

$$\mathbf{c}_N = \begin{bmatrix} \mathbf{X}_N^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{a}_N \\ \mathbf{b}_N \end{bmatrix} \mathbf{t}_N \quad \begin{bmatrix} \mathbf{a}_N \\ \mathbf{b}_N \end{bmatrix} = \mathbf{F}_N^{-1} \mathbf{B}$$

Work Backward Through Layers (2 of 4)

To eliminate the potentially ill conditioned matrix \mathbf{X}_N^{-1} , we introduce an intermediate transmittance matrix parameter \mathbf{t}_N defined as

$$\mathbf{t} = \mathbf{a}_N^{-1} \mathbf{X}_N \mathbf{t}_N \quad \leftarrow \mathbf{t} \text{ and } \mathbf{t}_N \text{ remain unknown.}$$

Our equation for \mathbf{c}_N becomes

$$\mathbf{c}_N = \begin{bmatrix} \mathbf{X}_N^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{a}_N \\ \mathbf{b}_N \end{bmatrix} \mathbf{t}_N \rightarrow \mathbf{c}_N = \begin{bmatrix} \mathbf{I} \\ \mathbf{b}_N \mathbf{a}_N^{-1} \mathbf{X}_N \end{bmatrix} \mathbf{t}_N$$

Work Backward Through Layers (3 of 4)

The boundary condition equation at the second-to-last interface is

$$\mathbf{F}_{N-1} \begin{bmatrix} \mathbf{X}_{N-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix} \mathbf{c}_{N-1} = \mathbf{F}_N \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{X}_N \end{bmatrix} \mathbf{c}_N$$

Substituting our expression for \mathbf{c}_N into the equation yields

$$\mathbf{F}_{N-1} \begin{bmatrix} \mathbf{X}_{N-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix} \mathbf{c}_{N-1} = \mathbf{F}_N \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{X}_N \end{bmatrix} \begin{bmatrix} \mathbf{I} \\ \mathbf{b}_N \mathbf{a}_N^{-1} \mathbf{X}_N \end{bmatrix} \mathbf{t}_N$$

Solving this for \mathbf{c}_{N-1} leads to

$$\mathbf{c}_{N-1} = \begin{bmatrix} \mathbf{X}_{N-1}^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix} \mathbf{F}_{N-1}^{-1} \mathbf{F}_N \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{X}_N \end{bmatrix} \begin{bmatrix} \mathbf{I} \\ \mathbf{b}_N \mathbf{a}_N^{-1} \mathbf{X}_N \end{bmatrix} \mathbf{t}_N$$

We have now worked backward by one layer while avoiding \mathbf{X}_N^{-1} .

Work Backward Through Layers (4 of 4)

This process continues through all the layers.

$$\mathbf{c}_{N-1} = \begin{bmatrix} \mathbf{X}_{N-1}^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix} \mathbf{F}_{N-1}^{-1} \mathbf{F}_N \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{X}_N \end{bmatrix} \begin{bmatrix} \mathbf{I} \\ \mathbf{b}_N \mathbf{a}_N^{-1} \mathbf{X}_N \end{bmatrix} \mathbf{t}_N$$

$$\mathbf{c}_{N-1} = \begin{bmatrix} \mathbf{X}_{N-1}^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{a}_{N-1} \\ \mathbf{b}_{N-1} \end{bmatrix} \mathbf{t}_N \quad \begin{bmatrix} \mathbf{a}_{N-1} \\ \mathbf{b}_{N-1} \end{bmatrix} = \mathbf{F}_{N-1}^{-1} \mathbf{F}_N \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{X}_N \end{bmatrix} \begin{bmatrix} \mathbf{I} \\ \mathbf{b}_N \mathbf{a}_N^{-1} \mathbf{X}_N \end{bmatrix}$$

$$\mathbf{c}_{N-1} = \begin{bmatrix} \mathbf{I} \\ \mathbf{b}_{N-1} \mathbf{a}_{N-1}^{-1} \mathbf{X}_{N-1} \end{bmatrix} \mathbf{t}_{N-1}$$

$$\mathbf{t}_N = \mathbf{a}_{N-1}^{-1} \mathbf{X}_{N-1} \mathbf{t}_{N-1} \quad \leftarrow \mathbf{T}_{N-1} \text{ and } \mathbf{T}_N \text{ remain unknown.}$$

\vdots

Solve for Reflected and Transmitted Fields

After working through all interfaces, we are left with

$$\mathbf{s} + \mathbf{A}\mathbf{r} = \mathbf{F}_1 \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{X}_1 \end{bmatrix} \begin{bmatrix} \mathbf{I} \\ \mathbf{b}_1 \mathbf{a}_1^{-1} \mathbf{X}_1 \end{bmatrix} \mathbf{t}_1$$

We solve this matrix equation for \mathbf{r} and \mathbf{t}_1 .

$$\begin{bmatrix} \mathbf{r} \\ \mathbf{t}_1 \end{bmatrix} = [-\mathbf{A} \quad \mathbf{B}']^{-1} \mathbf{S} \quad \mathbf{B}' = \mathbf{F}_1 \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{X}_1 \end{bmatrix} \begin{bmatrix} \mathbf{I} \\ \mathbf{b}_1 \mathbf{a}_1^{-1} \mathbf{X}_1 \end{bmatrix} \mathbf{t}_1$$

Now that we know \mathbf{t}_1 , we can work forward through the layers to solve for \mathbf{t} .

$$\mathbf{t}_2 = \mathbf{a}_1^{-1} \mathbf{X}_1 \mathbf{t}_1$$

$$\mathbf{t}_3 = \mathbf{a}_2^{-1} \mathbf{X}_2 \mathbf{t}_2$$

$$\vdots$$

$$\mathbf{t}_N = \mathbf{a}_{N-1}^{-1} \mathbf{X}_{N-1} \mathbf{t}_{N-1}$$

$$\mathbf{t} = \mathbf{a}_N^{-1} \mathbf{X}_N \mathbf{t}_N$$

Note: we must store \mathbf{a} and \mathbf{X} for each layer.
This leads to poor memory efficiency.

Calculating the Diffraction Efficiencies

First, we calculate the longitudinal field components.

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

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

Second, we calculate the diffraction efficiencies.

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

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

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

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

Block Diagram of ETM

