



Advanced Computation:
Computational Electromagnetics

Implementation of Rigorous Coupled-Wave Analysis (RCWA)

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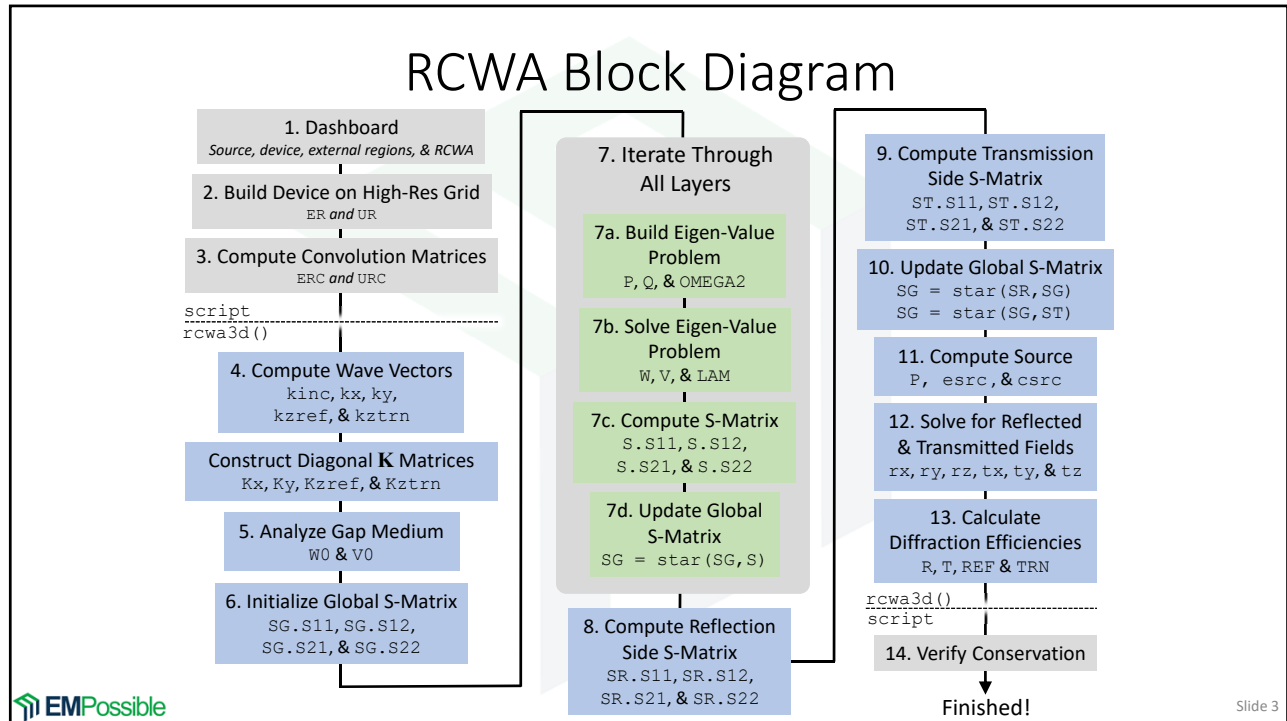
Outline

- Step 0 – Define problem
 - Step 1 – Initialize Program
 - Step 2 – Build device on high resolution grid
 - Step 3 – Compute convolution matrices
 - Step 4 – Compute wave vector expansion
 - Step 5 – Compute eigen-modes of free space
 - Step 6 – Initialize global scattering matrix
 - Step 7 – Main loop through layers
 - Step 8 – Compute reflection side scattering matrix
 - Step 9 – Compute transmission side scattering matrix
 - Step 10 – Update global scattering matrix
 - Step 11 – Compute source terms
 - Step 12 – Compute reflected and transmitted fields
 - Step 13 – Compute diffraction efficiencies
 - Step 14 – Verify conservation of power
- human does this
↓
computer does the rest
- Step 7: Iterate through layers**

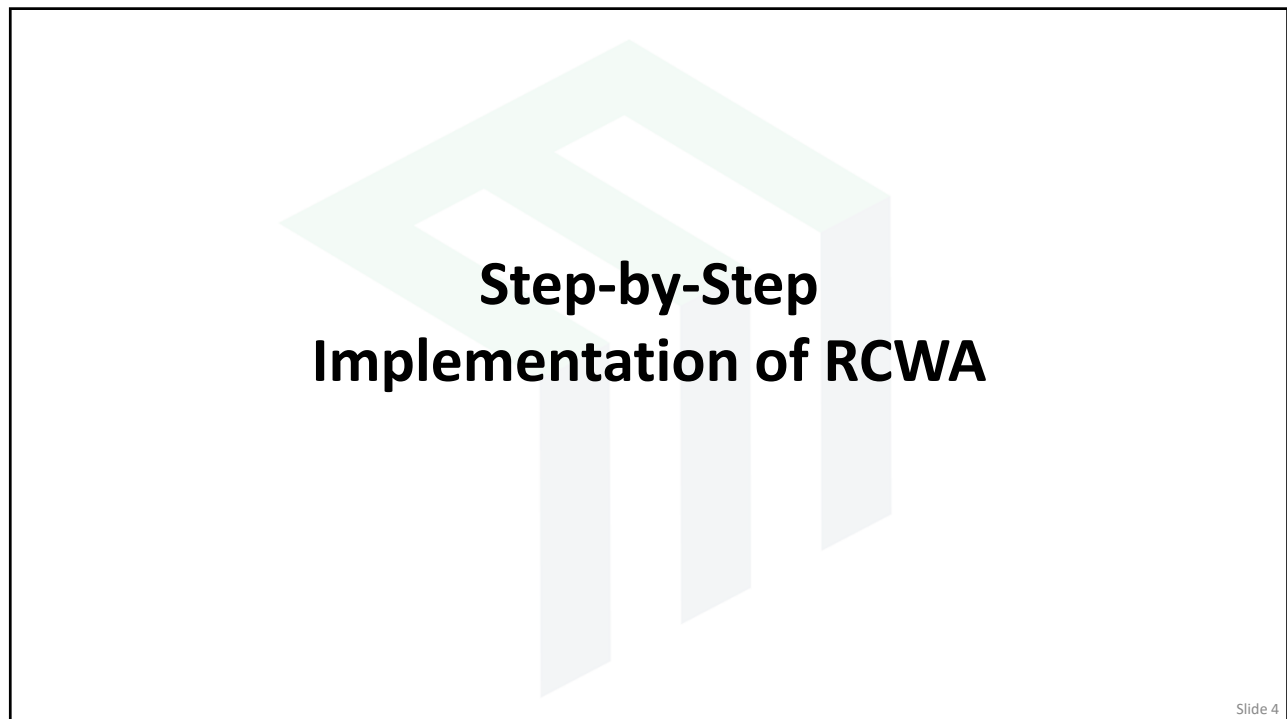
 - Compute **P** and **Q**
 - Compute eigen-modes
 - Compute layer scattering matrix
 - Update global scattering matrix

`rcwa3d()`

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Problem Definition

Use RCWA to simulate transmission and reflection from the following device.

Unit Cell

Reflection Region
Layer 1
Layer 2
Transmission Region

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Step 0: Dimensions and Material Properties

$\mu_{r,ref} = 1.0$
 $\epsilon_{r,ref} = 2.0$
 $\mu_r = 1.0$
 $\epsilon_r = 6.0$
 $\mu_{r,tm} = 1.0$
 $\epsilon_{r,tm} = 9.0$

$\Lambda_x = 1.75$ cm
 $\Lambda_y = 1.50$ cm
 $d_1 = 0.50$ cm
 $d_2 = 0.30$ cm
 $w = 0.8\Lambda_y$

Triangle is centered in unit cell.
Normal incidence.
Field linearly polarized along y axis.
 $\lambda_0 = 2.0$ cm.

$\mu_{r,ref}$
 $\epsilon_{r,ref}$ Region I
Reflection Region

Layer 1
Layer 2

Region II
Transmission Region
 $\mu_{r,tm}$
 $\epsilon_{r,tm}$

μ_r
 ϵ_r

Λ_x Λ_y w $\mu_{r,ref}$ $\epsilon_{r,ref}$ μ_r ϵ_r

Λ_x Λ_y

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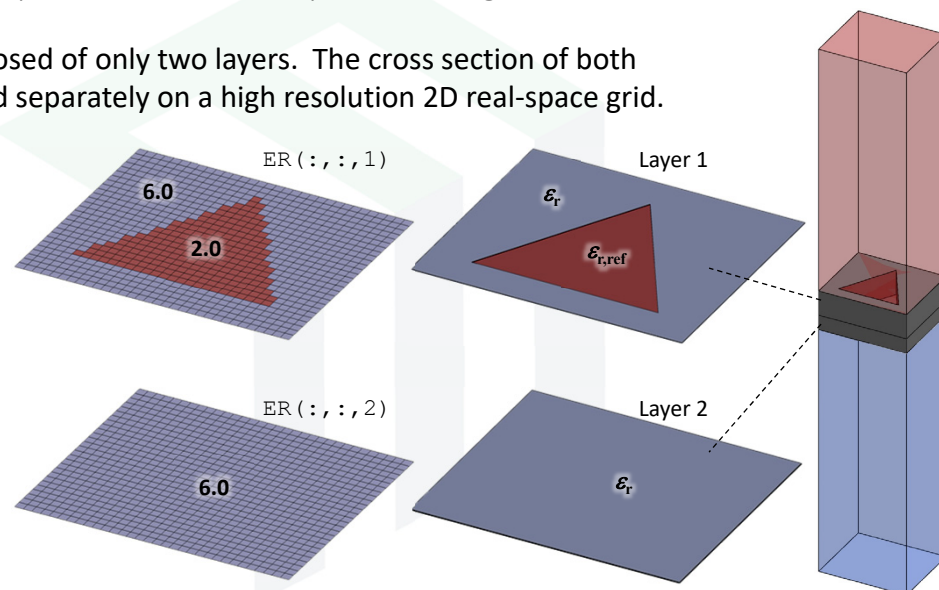
Step 1: Initialize Program

- Initialize MATLAB
- Define units
- Define constants
 - c_0 , μ_0 , ϵ_0 , η_0 , etc.
- Open a figure window if desired
- Define what is to be simulated
 - Source parameters
 - λ_0 , θ , ϕ , , etc. \vec{P}
 - Device parameters
 - Dimensions, material properties, etc.
 - RCWA specific parameters
 - Size of real-space grid, number of harmonics, etc.

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Step 2: Build Device Layers on a High-Resolution Grid

This device is composed of only two layers. The cross section of both must be constructed separately on a high resolution 2D real-space grid.

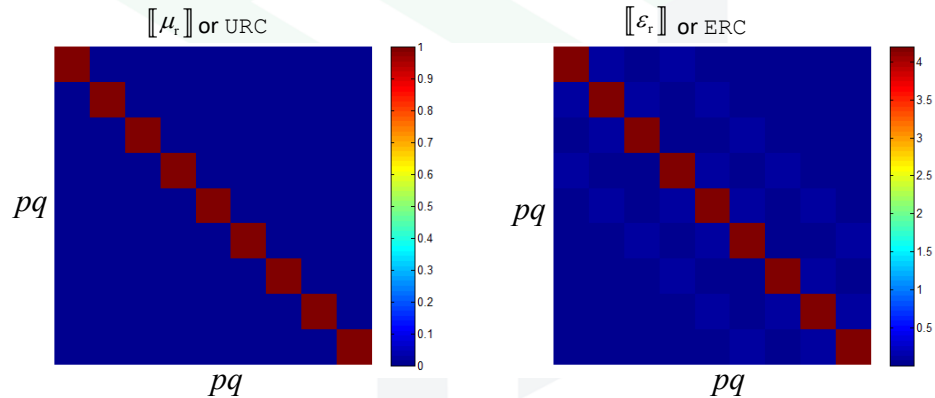


IMPORTANT: Use a very high-resolution grid!

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Step 3: Compute Convolution Matrices

Calculate separate convolution matrices for each layer of the device. Using 3×3 spatial harmonics, the convolution matrices for layer 1 are



Rule of Thumb for # Harmonics: $\# \approx 7 \frac{\Lambda}{\lambda}$

Store the convolution matrices in arrays that are $N \times N \times \text{NLAY}$, where $N = PQ$.

Step 4: Compute Wave Vector Expansion

$$\vec{\tilde{k}}_{\text{inc}} = \vec{k}_{\text{inc}} / k_0 = n_{\text{inc}} (\sin \theta \cos \phi \hat{a}_x + \sin \theta \sin \phi \hat{a}_y + \cos \theta \hat{a}_z)$$

Wave vector components for $\lambda_0 = 2.0$ cm at normal incidence.

$$\tilde{k}_x(m, n) = \tilde{k}_{x,\text{inc}} - mT_{1,x} - nT_{2,x} = \tilde{k}_{x,\text{inc}} - \frac{2\pi m}{k_0 \Lambda_x} \quad m = -M, \dots, -2, -1, 0, 1, 2, \dots, M$$

$$\tilde{k}_y(m, n) = \tilde{k}_{y,\text{inc}} - mT_{1,y} - nT_{2,y} = \tilde{k}_{y,\text{inc}} - \frac{2\pi n}{k_0 \Lambda_y} \quad n = -N, \dots, -2, -1, 0, 1, 2, \dots, N$$

$$\vec{T}_1 = \frac{2\pi}{\Lambda_x} \hat{a}_x \quad \vec{T}_2 = \frac{2\pi}{\Lambda_y} \hat{a}_y$$

Note: k_x and k_y from above will be 2D arrays. Remember to use `meshgrid()` to make k_x and k_y 2D arrays before calculating the k_z terms.

Longitudinal wave vector components in reflection and transmission regions.

$$\tilde{k}_{z,\text{ref}}(m, n) = -\left\{ \sqrt{\mu_{r,\text{ref}}^* \epsilon_{r,\text{ref}}^* - \tilde{k}_x^2(m, n) - \tilde{k}_y^2(m, n)} \right\}^* \quad \tilde{k}_{z,\text{trn}}(m, n) = \left\{ \sqrt{\mu_{r,\text{trn}}^* \epsilon_{r,\text{trn}}^* - \tilde{k}_x^2(m, n) - \tilde{k}_y^2(m, n)} \right\}^*$$

Construct diagonal matrices containing normalized wave vectors.

$$\tilde{\mathbf{K}}_x, \tilde{\mathbf{K}}_y, \tilde{\mathbf{K}}_{z,\text{ref}}, \tilde{\mathbf{K}}_{z,\text{trn}} \quad \mathbf{Kx} = \text{diag}(\text{sparse}(\mathbf{kx}(:)));$$

Step 5: Compute Eigen-Modes of Gap Medium

This is a homogeneous layer so the calculation reduces to

$$\tilde{\mathbf{K}}_z = \left(\sqrt{\mathbf{I} - \tilde{\mathbf{K}}_x^2 - \tilde{\mathbf{K}}_y^2} \right)^*$$

$$\mathbf{Q} = \begin{bmatrix} \tilde{\mathbf{K}}_x \tilde{\mathbf{K}}_y & \mathbf{I} - \tilde{\mathbf{K}}_x^2 \\ \tilde{\mathbf{K}}_y^2 - \mathbf{I} & -\tilde{\mathbf{K}}_x \tilde{\mathbf{K}}_y \end{bmatrix}$$

$$\mathbf{W}_0 = \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix}$$

$$\lambda = \begin{bmatrix} j\tilde{\mathbf{K}}_z & \mathbf{0} \\ \mathbf{0} & j\tilde{\mathbf{K}}_z \end{bmatrix}$$

$$\mathbf{V}_0 = \mathbf{Q}\lambda^{-1}$$

There is no need to construct convolution matrices or to solve an eigen-value problem!

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Step 6: Initialize Device Scattering Matrix

\mathbf{S}_{11} is interpreted as reflection at the first interface so it is initialized as all zeros.

$$\mathbf{S}_{11}^{(\text{device})} = \mathbf{0}$$

$\mathbf{0}$ in this case is a $2PQ \times 2PQ$ matrix of 0's, not a single scalar 0.

\mathbf{S}_{12} is interpreted as transmission in the forward direction so it is initialized as a $2PQ \times 2PQ$ identity matrix.

$$\mathbf{S}_{12}^{(\text{device})} = \mathbf{I}$$

\mathbf{S}_{21} is interpreted as transmission in the backward direction so it is initialized as the identity matrix.

$$\mathbf{S}_{21}^{(\text{device})} = \mathbf{I}$$

\mathbf{S}_{22} is interpreted as reflection at the last interface so it is initialized as all zeros.

$$\mathbf{S}_{22}^{(\text{device})} = \mathbf{0}$$

Not the identity matrix!

$$\mathbf{S}^{(\text{device})} = \begin{bmatrix} \mathbf{0} & \mathbf{I} \\ \mathbf{I} & \mathbf{0} \end{bmatrix}$$

Think of this as a thin slice of "nothing."

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Step 7: Main Loop Iterates Through Layers

a. Build eigen-value problem for the i^{th} layer

$$P_i = \begin{bmatrix} \tilde{\mathbf{K}}_x [\epsilon_{r,i}]^{-1} \tilde{\mathbf{K}}_y & [\mu_{r,i}] - \tilde{\mathbf{K}}_x [\epsilon_{r,i}]^{-1} \tilde{\mathbf{K}}_x \\ \tilde{\mathbf{K}}_y [\epsilon_{r,i}]^{-1} \tilde{\mathbf{K}}_y - [\mu_{r,i}] & -\tilde{\mathbf{K}}_y [\epsilon_{r,i}]^{-1} \tilde{\mathbf{K}}_x \end{bmatrix} \quad Q_i = \begin{bmatrix} \tilde{\mathbf{K}}_x [\mu_{r,i}]^{-1} \tilde{\mathbf{K}}_y & [\epsilon_{r,i}] - \tilde{\mathbf{K}}_x [\mu_{r,i}]^{-1} \tilde{\mathbf{K}}_x \\ \tilde{\mathbf{K}}_y [\mu_{r,i}]^{-1} \tilde{\mathbf{K}}_y - [\epsilon_{r,i}] & -\tilde{\mathbf{K}}_y [\mu_{r,i}]^{-1} \tilde{\mathbf{K}}_x \end{bmatrix} \quad \Omega_i^2 = P_i Q_i$$

b. Compute eigen-modes in the i^{th} layer

$$[W_i, \lambda_i^2] = \text{eig}(\Omega_i^2) \quad V_i = QW_i \lambda_i^{-1}$$

Don't calculate $\sqrt{\Omega_i^2}$!!!

Be sure Ω_i^2 is a full matrix.

```
[W, LAM] = eig(OMEGA2);
LAM = sqrt(LAM);
```

c. Compute layer scattering matrix for the i^{th} layer

$$S_{11}^{(i)} = (\mathbf{A}_{i0} - \mathbf{X}_i \mathbf{B}_{i0} \mathbf{A}_{i0}^{-1} \mathbf{X}_i \mathbf{B}_{i0})^{-1} (\mathbf{X}_i \mathbf{B}_{i0} \mathbf{A}_{i0}^{-1} \mathbf{X}_i \mathbf{A}_{i0} - \mathbf{B}_{i0})$$

$$\mathbf{A}_{i0} = \mathbf{W}_i^{-1} \mathbf{W}_0 + \mathbf{V}_i^{-1} \mathbf{V}_0$$

$$S_{12}^{(i)} = (\mathbf{A}_{i0} - \mathbf{X}_i \mathbf{B}_{i0} \mathbf{A}_{i0}^{-1} \mathbf{X}_i \mathbf{B}_{i0})^{-1} \mathbf{X}_i (\mathbf{A}_{i0} - \mathbf{B}_{i0} \mathbf{A}_{i0}^{-1} \mathbf{B}_{i0})$$

$$\mathbf{B}_{i0} = \mathbf{W}_i^{-1} \mathbf{W}_0 - \mathbf{V}_i^{-1} \mathbf{V}_0$$

$$S_{21}^{(i)} = S_{12}^{(i)}$$

$$\mathbf{X}_i = e^{-\lambda_i k_{z,i} L_i}$$

$$S_{22}^{(i)} = S_{11}^{(i)}$$

$$X = \text{expm}(-LAM * k0 * L(nlay));$$

d. Update device scattering matrix

$$S^{(\text{device})} = S^{(\text{device})} \otimes S^{(i)}$$



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Step 8: Compute Reflection Side Connection S-Matrix

This is a homogeneous layer so the layer parameters can be calculated as

$$Q_{\text{ref}} = \frac{1}{\mu_{r,\text{ref}}} \begin{bmatrix} \tilde{\mathbf{K}}_x \tilde{\mathbf{K}}_y & \mu_{r,\text{ref}} \epsilon_{r,\text{ref}} \mathbf{I} - \tilde{\mathbf{K}}_x^2 \\ \tilde{\mathbf{K}}_y^2 - \mu_{r,\text{ref}} \epsilon_{r,\text{ref}} \mathbf{I} & -\tilde{\mathbf{K}}_y \tilde{\mathbf{K}}_x \end{bmatrix}$$

$$W_{\text{ref}} = \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix} \quad \lambda_{\text{ref}} = \begin{bmatrix} -j\tilde{\mathbf{K}}_{z,\text{ref}} & \mathbf{0} \\ \mathbf{0} & -j\tilde{\mathbf{K}}_{z,\text{ref}} \end{bmatrix}$$

$$V_{\text{ref}} = Q_{\text{ref}} \lambda_{\text{ref}}^{-1}$$

IMPORTANT: DO NOT USE CONVOLUTION MATRICES FOR EXTERNAL REGIONS.

Compute reflection side connection scattering matrix

$$S_{11}^{(\text{ref})} = -\mathbf{A}_{i1}^{-1} \mathbf{B}_{i1}$$

$$\mathbf{A}_{i1} = \mathbf{W}_0^{-1} \mathbf{W}_{\text{ref}} + \mathbf{V}_0^{-1} \mathbf{V}_{\text{ref}}$$

$$A = W0 \backslash W_{\text{ref}} + V0 \backslash V_{\text{ref}};$$

$$B = W0 \backslash W_{\text{ref}} - V0 \backslash V_{\text{ref}};$$

$$S_{12}^{(\text{ref})} = 2\mathbf{A}_{i1}^{-1}$$

$$\mathbf{B}_{i1} = \mathbf{W}_0^{-1} \mathbf{W}_{\text{ref}} - \mathbf{V}_0^{-1} \mathbf{V}_{\text{ref}}$$

$$\text{SR.S11} = -A \backslash B;$$

$$\text{SR.S12} = 2 * \text{inv}(A);$$

$$S_{21}^{(\text{ref})} = 0.5 (\mathbf{A}_{i1} - \mathbf{B}_{i1} \mathbf{A}_{i1}^{-1} \mathbf{B}_{i1})$$

$$\text{SR.S21} = 0.5 * (A - B / A * B);$$

$$S_{22}^{(\text{ref})} = \mathbf{B}_{i1} \mathbf{A}_{i1}^{-1}$$

$$\text{SR.S22} = B / A;$$



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Step 9: Compute Transmission Side Connection S-Matrix

This is a homogeneous layer so the layer parameters can be calculated as

$$\mathbf{Q}_{tm} = \frac{1}{\mu_{tm}} \begin{bmatrix} \tilde{\mathbf{K}}_x \tilde{\mathbf{K}}_y & \mu_{r,tm} \varepsilon_{r,tm} \mathbf{I} - \tilde{\mathbf{K}}_x^2 \\ \tilde{\mathbf{K}}_y^2 - \mu_{r,tm} \varepsilon_{r,tm} \mathbf{I} & -\tilde{\mathbf{K}}_y \tilde{\mathbf{K}}_x \end{bmatrix}$$

$$\mathbf{W}_{tm} = \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix} \quad \lambda_{tm} = \begin{bmatrix} j\tilde{\mathbf{K}}_{z,tm} & \mathbf{0} \\ \mathbf{0} & j\tilde{\mathbf{K}}_{z,tm} \end{bmatrix}$$

$$\mathbf{V}_{tm} = \mathbf{Q}_{tm} \lambda_{tm}^{-1}$$

IMPORTANT: DO NOT USE CONVOLUTION MATRICES FOR EXTERNAL REGIONS.

Compute transmission side connection scattering matrix

$$\mathbf{S}_{11}^{(tm)} = \mathbf{B}_{i2} \mathbf{A}_{i2}^{-1}$$

$$\mathbf{S}_{12}^{(tm)} = 0.5 (\mathbf{A}_{i2} - \mathbf{B}_{i2} \mathbf{A}_{i2}^{-1} \mathbf{B}_{i2})$$

$$\mathbf{S}_{21}^{(tm)} = 2 \mathbf{A}_{i2}^{-1}$$

$$\mathbf{S}_{22}^{(tm)} = -\mathbf{A}_{i2}^{-1} \mathbf{B}_{i2}$$

$$\mathbf{A}_{i2} = \mathbf{W}_0^{-1} \mathbf{W}_{tm} + \mathbf{V}_0^{-1} \mathbf{V}_{tm}$$

$$\mathbf{B}_{i2} = \mathbf{W}_0^{-1} \mathbf{W}_{tm} - \mathbf{V}_0^{-1} \mathbf{V}_{tm}$$

$$\mathbf{A} = \mathbf{W}_0 \backslash \mathbf{W}_{trn} + \mathbf{V}_0 \backslash \mathbf{V}_{trn};$$

$$\mathbf{B} = \mathbf{W}_0 \backslash \mathbf{W}_{trn} - \mathbf{V}_0 \backslash \mathbf{V}_{trn};$$

$$\text{ST.S11} = \mathbf{B} / \mathbf{A};$$

$$\text{ST.S12} = 0.5 * (\mathbf{A} - \mathbf{B} / \mathbf{A} * \mathbf{B});$$

$$\text{ST.S21} = 2 * \text{inv}(\mathbf{A});$$

$$\text{ST.S22} = -\mathbf{A} \backslash \mathbf{B};$$

Step 10: Compute Global Scattering Matrix

Perform a double Redheffer star product to connect the device scattering matrix to the external regions.

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

This is actually performed in two steps.

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

2. $\mathbf{S}^{(\text{global})} = \mathbf{S}^{(\text{global})} \otimes \mathbf{S}^{(\text{tm})}$

Step 11: Compute Source Parameters

Construct Delta Vector

$$\delta_{0,pq} = [0 \ \cdots \ 0 \ 1 \ 0 \ \cdots \ 0]^T$$

'1' at the position that corresponds to the zero-order spatial harmonic to incorporate a unit amplitude source.

Compute Directions of TE and TM Polarization

$$\hat{n} = \hat{a}_z \quad \hat{a}_{TE} = \frac{\hat{n} \times \vec{k}_{inc}}{|\hat{n} \times \vec{k}_{inc}|} \quad \hat{a}_{TM} = \frac{\vec{k}_{inc} \times \hat{a}_{TE}}{|\vec{k}_{inc} \times \hat{a}_{TE}|}$$

For normal incidence, \hat{a}_{TE} can be chosen to be in any direction in the xy plane. An often convenient choice is $\hat{a}_{TE} = \hat{a}_y$.

Compute Polarization Vector

$$\vec{P} = \begin{bmatrix} p_x \\ p_y \\ p_z \end{bmatrix} = p_{TE} \hat{a}_{TE} + p_{TM} \hat{a}_{TM} \quad \text{Note: Best to ensure that } |\vec{P}| = 1$$

Compute Source Field

$$\mathbf{c}_T^{src} = \begin{bmatrix} p_x \delta_{0,pq} \\ p_y \delta_{0,pq} \end{bmatrix} \quad \begin{array}{l} p_x \equiv x \text{ component of electric field polarization vector} \\ p_y \equiv y \text{ component of electric field polarization vector} \end{array}$$



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Step 12: Compute Reflected and Transmitted Fields

Compute mode coefficients of the source

$$\mathbf{c}_{src} = \mathbf{W}_{ref}^{-1} \mathbf{e}_T^{src}$$

Compute transmission and reflection mode coefficients

$$\mathbf{c}_{ref} = \mathbf{S}_{11}^{(global)} \mathbf{c}_{src} \quad \mathbf{c}_{tm} = \mathbf{S}_{21}^{(global)} \mathbf{c}_{src}$$

Compute reflected and transmitted fields

$$\begin{bmatrix} \mathbf{r}_x \\ \mathbf{r}_y \end{bmatrix} = \mathbf{e}_T^{ref} = \mathbf{W}_{ref} \mathbf{c}_{ref} = \mathbf{W}_{ref} \mathbf{S}_{11} \mathbf{c}_{src} \quad \begin{bmatrix} \mathbf{t}_x \\ \mathbf{t}_y \end{bmatrix} = \mathbf{e}_T^{tm} = \mathbf{W}_{tm} \mathbf{c}_{tm} = \mathbf{W}_{tm} \mathbf{S}_{21} \mathbf{c}_{src}$$

Compute longitudinal components

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



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Step 13: Compute Diffraction Efficiencies

Compute Reflected Power

$$|\vec{r}|^2 = |r_x|^2 + |r_y|^2 + |r_z|^2$$

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

$$R_{\text{total}} = \sum_{PQ} R(p, q)$$

Diffraction efficiencies of reflected modes.
This equation assumes unit amplitude source.

```
R2 = abs(rx).^2 + abs(ry).^2 + abs(rz).^2;
R = real(-Kzr/ur1)/real(kinc(3)/ur1)*R2;
R = reshape(R,M,N);
REF = sum(R(:));
```

Compute Transmitted Power

$$|\vec{t}|^2 = |t_x|^2 + |t_y|^2 + |t_z|^2$$

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

$$T_{\text{total}} = \sum_{PQ} T(p, q)$$

Diffraction efficiencies of transmitted modes.
This equation assumes a unit amplitude source.

```
T2 = abs(tx).^2 + abs(ty).^2 + abs(tz).^2;
T = real(Kzt/ur2)/real(kinc(3)/ur1)*T2;
T = reshape(T,M,N);
TRN = sum(T(:));
```

Step 14: Verify Conservation of Power

It is always good practice to check for conservation of power.

$$R_{\text{total}} + T_{\text{total}} \rightarrow \begin{cases} < 1 & \text{loss} \\ = 1 & \text{no loss and no gain} \\ > 1 & \text{gain} \end{cases} \quad \text{General Conservation Equation} \quad R_{\text{total}} + T_{\text{total}} + A_{\text{total}} = 1$$

Even if loss or gain is to be incorporated, turn off the loss or gain at first, test for conservation of power, and then turn it back on.