Advanced Computation: Computational Electromagnetics

Scattering Matrices for Semi-Analytical Methods

Outline

• Preliminary topics
• Formulation of the general scattering matrix
• Formulation of the improved scattering matrix
• Notes about scattering matrices
• Multilayer structures
Preliminary Topics

Definition of a Scattering Matrix

\[
\begin{bmatrix}
  c_1'^{-} \\
  c_2'^{+}
\end{bmatrix} =
\begin{bmatrix}
  S_{11} & S_{12} \\
  S_{21} & S_{22}
\end{bmatrix}
\begin{bmatrix}
  c_1'^{+} \\
  c_2'^{-}
\end{bmatrix}
\]

This is consistent with network theory and experimental convention.

\( S_{11} \equiv \text{reflection} \)
\( S_{21} \equiv \text{transmission} \)
Motivation for Scattering Matrices

Scattering matrices offer several important features and benefits:

• Unconditionally stable method.
• Parameters have physical meaning.
• Parameters correspond to those measured in the lab.
• Can be used to extract dispersion.
• Very memory efficient.
• Can be used to exploit longitudinal periodicity.
• Mature and proven approach.
• Much greater wealth of literature available.

However, excellent alternatives to S-matrices do exist!

WARNING: Scattering Matrices in the Literature

For some reason, the computational electromagnetics community has: (1) deviated from network theory convention, and (2) formulated inefficient scattering matrices.

\[
\begin{bmatrix}
    \mathbf{c}_{i-1}^- \\
    \mathbf{c}_i^+
\end{bmatrix} =
\begin{bmatrix}
    S_{11} & S_{12} \\
    S_{21} & S_{22}
\end{bmatrix}
\begin{bmatrix}
    \mathbf{c}_i^- \\
    \mathbf{c}_{i-1}^+
\end{bmatrix}
\]

• Here $S_{11}$ is not reflection. Instead, it is backward transmission!
• Here $S_{22}$ is not transmission. Instead, it is a reflection parameter!
• Scattering matrices can not be interchanged.
• Scattering matrices are not symmetric so they take twice the memory to store and are more time-consuming to calculate.
Formulation of the General Scattering Matrix


Geometry of a Single Layer

- Indicates a point that lies on an interface, but associated with a particular side.

$\psi^+_{i-1} \left( z_{i-1} \right) \quad \psi^+_{i} \left( z_{i} \right) \quad \psi^+_{i+1} \left( z_{i+1} \right)$

$\psi^-_{i-1} \left( z_{i-1} \right) \quad \psi^-_{i} \left( z_{i} \right) \quad \psi^-_{i+1} \left( z_{i+1} \right)$

$\mathbf{c}^+_{i-1} \quad \mathbf{c}^+_{i} \quad \mathbf{c}^+_{i+1}$

$\mathbf{c}^-_{i-1} \quad \mathbf{c}^-_{i} \quad \mathbf{c}^-_{i+1}$

Medium 1 | Layer $i$ | Medium 2

$\psi^+_{i-1} \left( z_{i-1} \right) = \text{field within } i^{th} \text{ layer}$

$\mathbf{c}^+_{i} = \text{mode coefficients inside } i^{th} \text{ layer}$

$\mathbf{c}^-_{i} = \text{mode coefficients outside } i^{th} \text{ layer}$

$\psi^-_{i} \left( z_{i} \right)$

Infinite Half-space (not a layer)

Medium 1

Medium 2

$Z$
### Enforce the Boundary Conditions

Field inside the \(i^{th}\) layer:

\[
\psi_i(z_i) = \frac{E_{r,i}(z'_i)}{H_{r,i}(z'_i)} = \begin{bmatrix} W_i & W_i \\ V_i & V_i \end{bmatrix} e^{j\lambda z_i} \begin{bmatrix} c_i^+ \\ 0 \end{bmatrix} + \begin{bmatrix} 0 & c_i^- \\ e^{-j\lambda z_i} & 0 \end{bmatrix} \begin{bmatrix} c_i^- \\ 0 \end{bmatrix} + \begin{bmatrix} e^{j\lambda z_i} & 0 \\ 0 & e^{-j\lambda z_i} \end{bmatrix} \begin{bmatrix} c_i^+ \\ c_i^- \end{bmatrix}
\]

#### Boundary conditions at the first interface:

\[
\psi_1(z_1) = \psi_i(0) = \begin{bmatrix} W_1 & W_1 \\ V_1 & V_1 \end{bmatrix} c_i^+ = \begin{bmatrix} c_i^+ \\ c_i^- \end{bmatrix} = \begin{bmatrix} W_2 & W_2 \\ V_2 & V_2 \end{bmatrix} c_i^-
\]

#### Boundary conditions at the second interface:

\[
\psi_2(z_2) = \psi_i(k_0 L_i) = \psi_i(z_2) = \begin{bmatrix} W_1 & W_1 \\ V_1 & V_1 \end{bmatrix} e^{j\lambda L_i} c_i^+ + \begin{bmatrix} 0 & c_i^- \\ e^{-j\lambda L_i} & 0 \end{bmatrix} c_i^- = \begin{bmatrix} W_2 & W_2 \\ V_2 & V_2 \end{bmatrix} c_i^-
\]

Note: \(k_0\) has been incorporated to normalize \(L_i\).

### Derivation of the Scattering Matrix

Solve both boundary condition equations for the intermediate mode coefficients \(c_i^+\) and \(c_i^-\).

\[
\begin{align*}
\begin{bmatrix} c_i^+ \\ c_i^- \end{bmatrix} &= \begin{bmatrix} W_1 & W_1 & c_i^+ \\ V_1 & V_1 & c_i^- \end{bmatrix} = \begin{bmatrix} c_i^+ \\ c_i^- \end{bmatrix} = \begin{bmatrix} W_2 & W_2 & c_i^+ \\ V_2 & V_2 & c_i^- \end{bmatrix} \\
\end{align*}
\]

Both of these equations have a common term that can be simplified.

\[
\begin{align*}
\begin{bmatrix} W_1 & W_1 \\ V_1 & V_1 \end{bmatrix} &= \begin{bmatrix} A_{11} & B_{11} \\ A_{12} & B_{12} \end{bmatrix} \\
\begin{bmatrix} W_2 & W_2 \\ V_2 & V_2 \end{bmatrix} &= \begin{bmatrix} A_{21} & B_{21} \\ A_{22} & B_{22} \end{bmatrix} \\
\end{align*}
\]

Substitute this result into the first two equations and then set them equal to eliminate the intermediate mode coefficients \(c_i^+\) and \(c_i^-\).

\[
\begin{align*}
\frac{1}{2} \begin{bmatrix} A_{11} & B_{11} \\ A_{12} & B_{12} \end{bmatrix} \begin{bmatrix} c_i^+ \\ c_i^- \end{bmatrix} &= \frac{1}{2} \begin{bmatrix} e^{j\lambda L_i} & 0 \\ 0 & e^{-j\lambda L_i} \end{bmatrix} \begin{bmatrix} A_{11} & B_{11} \\ A_{12} & B_{12} \end{bmatrix} \begin{bmatrix} c_i^- \\ c_i^+ \end{bmatrix} \\
\end{align*}
\]

Write this as two matrix equations and rearrange the terms until they have the form of a scattering matrix.

\[
\begin{align*}
\begin{bmatrix} c_i^+ \\ c_i^- \end{bmatrix} &= \begin{bmatrix} ? & ? \\ ? & ? \end{bmatrix} \begin{bmatrix} c_i^+ \\ c_i^- \end{bmatrix} \\
\end{align*}
\]
The Scattering Matrix

The scattering matrix $S_i$ of the $i^{th}$ layer is defined as:

$$
\begin{bmatrix}
  c_1^- \\
  c_2^+
\end{bmatrix} = S^{(i)}
\begin{bmatrix}
  c_1^+ \\
  c_2^-
\end{bmatrix}
$$

$$
S^{(i)} = \begin{bmatrix}
  S_{11}^{(i)} & S_{12}^{(i)} \\
  S_{21}^{(i)} & S_{22}^{(i)}
\end{bmatrix}
$$

After some algebra, the components of the scattering matrix are calculating using

$$
S_{11}^{(i)} = \left( A_{i1} - X_{i1}A_{i2}X_{i2}B_{i2} \right)^{-1} \left( X_{i1}B_{i2}A_{i2}X_{i2}A_{i1} - B_{i1} \right)
$$

$$
S_{12}^{(i)} = \left( A_{i1} - X_{i1}A_{i2}X_{i2}B_{i2} \right)^{-1} X_{i2} \left( A_{i2} - B_{i2}A_{i1}B_{i1} \right)
$$

$$
S_{21}^{(i)} = \left( A_{i2} - X_{i2}A_{i1}X_{i1}B_{i1} \right)^{-1} X_{i1} \left( A_{i1} - B_{i1}A_{i2}B_{i2} \right)
$$

$$
S_{22}^{(i)} = \left( A_{i2} - X_{i2}A_{i1}X_{i1}B_{i1} \right)^{-1} \left( X_{i2}B_{i1}A_{i1}X_{i1}A_{i2} - B_{i2} \right)
$$

$i$ is the layer number.

$j$ is either 1 or 2 depending on which external medium is being referenced.

Limitation of General S-Matrix Formulation

Note that the elements of a scattering matrix are a function of materials outside of the layer.

This makes it difficult to interchange scattering matrices arbitrarily.

For example, there are only three unique layers in the multilayer structure below, yet 20 separate computations of scattering matrices are needed.
Formulation of the Improved Scattering Matrix


Introduction of a Gap Medium

Recall the problem with a 20-layer stack.

Three unique layers
Introduction of a Gap Medium

Recall the problem with a 20-layer stack.

The solution is to separate each of the layers with a gap medium of zero thickness.

Scattering matrices for just the three unique layers can be used for all 20 layers because all layers are surrounded by the same medium.

Faster! Simpler! More memory efficient!

Recall General Geometry of a Single Layer

- Indicates a point that lies on an interface, but associated with a particular side.

$\psi^i(z) =$ field within $i^{th}$ layer

$c^+_i =$ mode coefficients inside $i^{th}$ layer

$c^-_i =$ mode coefficients outside $i^{th}$ layer
Recall General Geometry of a Single Layer

- Indicates a point that lies on an interface, but associated with a particular side.

\[
\psi_i^+ (z) = \text{field within } i^{th} \text{ layer}
\]

\[c_i^+ = \text{mode coefficients inside } i^{th} \text{ layer}\]

\[c_i^- = \text{mode coefficients outside } i^{th} \text{ layer}\]

Calculating Revised Scattering Matrices

The scattering matrix \(S_i\) of the \(i^{th}\) layer is still defined as:

\[
\begin{bmatrix}
  c_i^- \\
  c_i^+ \\
\end{bmatrix} = S^{(i)}
\begin{bmatrix}
  c_i^- \\
  c_i^+ \\
\end{bmatrix}
\]

But the equations to calculate the elements reduce to

\[
S_{11}^{(i)} = (A_i - X_i B_i A_i^{-1} X_i B_i)^{-1} (X_i B_i A_i^{-1} X_i A_i - B_i)
\]

\[
S_{12}^{(i)} = (A_i - X_i B_i A_i^{-1} X_i B_i)^{-1} X_i (A_i - B_i A_i^{-1} B_i)
\]

\[
S_{21}^{(i)} = S_{12}^{(i)}
\]

\[
S_{22}^{(i)} = S_{11}^{(i)}
\]

- Layers are symmetric so the scattering matrix elements have redundancy.
- Scattering matrix equations are simplified.
- Fewer calculations.
- Less memory storage.

\[
X_i = e^{i k L_i}
\]

\[
A_i = W_i^{-1} W_g + V_i^{-1} V_g
\]

\[
B_i = W_i^{-1} W_g - V_i^{-1} V_g
\]
Notes About Scattering Matrices

These S-Matrices are Actually 4-Port Networks

The scattering matrices have been written as 2×2 block matrices.

\[
\begin{bmatrix}
S_{11} & S_{12} \\
S_{21} & S_{22}
\end{bmatrix}
\]

For TMM, this actually expands to a 4×4 element scattering matrix.

\[
\begin{bmatrix}
S_{11} & S_{12} \\
S_{21} & S_{22}
\end{bmatrix} = \begin{bmatrix}
S_{11} & S_{12} & S_{13} & S_{14} \\
S_{21} & S_{22} & S_{23} & S_{24}
\end{bmatrix}
\]

\[
S_{11} = \begin{bmatrix}
S_{11} & S_{12} \\
S_{21} & S_{22}
\end{bmatrix}
\]

\[
S_{12} = \begin{bmatrix}
S_{13} & S_{14} \\
S_{23} & S_{24}
\end{bmatrix}
\]

Each mode provides an I/O mechanism and there are two modes on each side of the layer in each direction.
Scattering Matrices in Lossless Media are Unitary

If a scattering matrix is composed of materials that have no loss and no gain, the scattering matrix must conserve power. That is, all incident power must either reflect or transmit.

This implies that the scattering matrix is unitary.

If the scattering matrix is unitary, it must obey the following rules:

\[
S^H = S^{-1} \\
S^H S = SS^H = S^{-1} S = SS^{-1} = I
\]

Note: If the regions external to the layer are different from each other, the scattering matrices will not be unitary. This is because the field amplitudes will be different even though the field carries the same amount of power.

Hints About Stability in These Formulations

• Diagonal elements \( S_{11} \) and \( S_{22} \) tend to be the largest. Divide by these instead of any off-diagonal elements for best numerical stability.

\[
S = \begin{bmatrix}
S_{11} & S_{12} \\
S_{21} & S_{22}
\end{bmatrix}
\]

• \( X \) describes propagation through an entire layer. Don’t divide by \( X \) or the algorithm can become unstable.
Multilayer Structures


Solution Using Scattering Matrices

Using scattering matrices consists of working through the device one layer at a time and calculating an overall scattering matrix.

\[ S^{\text{device}} = S^{(1)} \odot S^{(2)} \odot S^{(3)} \odot S^{(4)} \odot S^{(5)} \]

Redheffer star product. NOT matrix multiplication!
Derivation of the Redheffer Star Product

Start with the equations for the two adjacent scattering matrices.

\[
\begin{bmatrix}
    c_{1}^- \\
    c_{1}^+
\end{bmatrix} = \begin{bmatrix}
    S_{11}^{(A)} & S_{12}^{(A)} \\
    S_{21}^{(A)} & S_{22}^{(A)}
\end{bmatrix} \begin{bmatrix}
    c_{1}^- \\
    c_{1}^+
\end{bmatrix}
\]

\[
\begin{bmatrix}
    c_{2}^- \\
    c_{2}^+
\end{bmatrix} = \begin{bmatrix}
    S_{11}^{(B)} & S_{12}^{(B)} \\
    S_{21}^{(B)} & S_{22}^{(B)}
\end{bmatrix} \begin{bmatrix}
    c_{2}^- \\
    c_{2}^+
\end{bmatrix}
\]

Expand these into four matrix equations.

\[
c_{1}^- = S_{11}^{(A)}c_{1}^+ + S_{12}^{(A)}c_{2}^- \quad \text{Eq. (1)}
\]

\[
c_{1}^+ = S_{21}^{(A)}c_{1}^+ + S_{22}^{(A)}c_{2}^- \quad \text{Eq. (2)}
\]

\[
c_{2}^- = S_{11}^{(B)}c_{2}^+ + S_{12}^{(B)}c_{2}^- \quad \text{Eq. (3)}
\]

\[
c_{2}^+ = S_{21}^{(B)}c_{2}^+ + S_{22}^{(B)}c_{2}^- \quad \text{Eq. (4)}
\]

Substitute Eq. (2) into Eq. (3) to get an equation with only \( c_{2}^+ \).

Substitute Eq. (3) into Eq. (2) to get an equation with only \( c_{2}^- \).

\[
(I - S_{11}^{(B)}S_{11}^{(A)})c_{2}^+ = S_{11}^{(B)}c_{1}^+ + S_{12}^{(B)}c_{2}^- \quad \text{Eq. (5)}
\]

\[
(I - S_{21}^{(B)}S_{11}^{(A)})c_{2}^+ = S_{21}^{(B)}c_{1}^+ + S_{22}^{(B)}c_{2}^- \quad \text{Eq. (6)}
\]

Eliminate \( c_{2}^- \) and \( c_{2}^+ \) by substituting these equations into Eq. (1) and (4). Then rearrange terms into the form of a scattering matrix.

\[
\begin{bmatrix}
    c_{1}^- \\
    c_{1}^+
\end{bmatrix} = \begin{bmatrix}
    ? & ? \\
    ? & ?
\end{bmatrix}
\]

Overall, this is just algebra. Start with 4 equations and 6 unknowns and reduce it to 2 equations with 4 unknowns.

Redheffer Star Product

Two scattering matrices may be combined into a single scattering matrix using Redheffer’s star product.

\[
S^{(AB)} = S^{(A)} \otimes S^{(B)}
\]

\[
S^{(A)} = \begin{bmatrix}
    S_{11}^{(A)} & S_{12}^{(A)} \\
    S_{21}^{(A)} & S_{22}^{(A)}
\end{bmatrix}
\]

\[
S^{(B)} = \begin{bmatrix}
    S_{11}^{(B)} & S_{12}^{(B)} \\
    S_{21}^{(B)} & S_{22}^{(B)}
\end{bmatrix}
\]

The combined scattering matrix is calculated according to

\[
S^{(AB)} = \begin{bmatrix}
    S_{11}^{(AB)} & S_{12}^{(AB)} \\
    S_{21}^{(AB)} & S_{22}^{(AB)}
\end{bmatrix}
\]

\[
S_{11}^{(AB)} = S_{11}^{(A)} + S_{12}^{(A)}(I - S_{11}^{(B)}S_{22}^{(A)})^{-1} S_{11}^{(B)}S_{21}^{(A)}
\]

\[
S_{12}^{(AB)} = S_{12}^{(A)}(I - S_{11}^{(B)}S_{22}^{(A)})^{-1} S_{12}^{(B)}
\]

\[
S_{21}^{(AB)} = S_{21}^{(B)}(I - S_{11}^{(A)}S_{11}^{(B)})^{-1} S_{21}^{(A)}
\]

\[
S_{22}^{(AB)} = S_{22}^{(B)} + S_{21}^{(B)}(I - S_{11}^{(A)}S_{11}^{(B)})^{-1} S_{22}^{(A)}
\]

Putting it All Together (1 of 2)

First, calculate the device scattering matrix by iterating through each layer of the device and combining the individual scattering matrices using the Redheffer star product.

\[
S_{\text{device}}^{(1)} \otimes S_{\text{device}}^{(2)} \otimes S_{\text{device}}^{(3)} \otimes \cdots \otimes S_{\text{device}}^{(N)}
\]

Putting it All Together (2 of 2)

Second, connect the device scattering matrix to the external regions to get the global scattering matrix. Use connection scattering matrices to do this.

\[
S_{\text{global}} = S_{\text{ref}} \otimes S_{\text{device}}^{(1)} \otimes S_{\text{device}}^{(2)} \otimes S_{\text{device}}^{(3)} \otimes \cdots \otimes S_{\text{device}}^{(N)} \otimes S_{\text{tm}}
\]
Reflection/Transmission Side Scattering Matrices

The reflection-side scattering matrix is

\[ S_{11}^{\text{ref}} = -A_{\text{ref}}^{-1} B_{\text{ref}} \]
\[ S_{12}^{\text{ref}} = 2A_{\text{ref}}^{-1} \]
\[ S_{21}^{\text{ref}} = 0.5 \left( A_{\text{ref}} - B_{\text{ref}} A_{\text{ref}}^{-1} B_{\text{ref}} \right) \]
\[ S_{22}^{\text{ref}} = B_{\text{ref}} A_{\text{ref}}^{-1} \]

The transmission-side scattering matrix is

\[ S_{11}^{\text{tm}} = B_{\text{mn}} A_{\text{tm}}^{-1} \]
\[ S_{12}^{\text{tm}} = 0.5 \left( A_{\text{tm}} - B_{\text{mn}} A_{\text{tm}}^{-1} B_{\text{mn}} \right) \]
\[ S_{21}^{\text{tm}} = 2A_{\text{tm}}^{-1} \]
\[ S_{22}^{\text{tm}} = -A_{\text{tm}}^{-1} B_{\text{mn}} \]

Summary of Using Scattering Matrices

\[ S^{(\text{global})} = S^{(\text{ref})} \otimes \left[ S^{(1)} \otimes S^{(2)} \otimes \cdots \otimes S^{(N)} \right] \otimes S^{(\text{tm})} \]