Computational Science:
Introduction to Finite-Difference Time-Domain

Waveguide Circuit Analysis
Using FDTD

Lecture Outline

• Slab Waveguides
• Frequency-Domain Analysis of Slab Waveguides
• Waveguide Sources in FDTD
• Reflection and Transmission in Waveguides
2D Approximation of Optical Integrated Circuits

It is possible to very accurately simulate an optical integrated circuit in two dimensions using the effective index method.

Effective indices are best computed by modeling the vertical cross section as a slab waveguide.

A simple average index can also produce good results.
The Critical Angle and Total Internal Reflection

When an electromagnetic wave is incident on a material with a lower refractive index, it is totally reflected when the angle of incidence is greater than the critical angle.

\[ \theta_c = \sin^{-1}\left(\frac{n_2}{n_1}\right) \]

Example

What is the critical angle for fused silica (glass).

The refractive index at optical frequencies is around 1.5.

\[ \theta_c = \sin^{-1}\left(\frac{1.0}{1.5}\right) = 41.81^\circ \]

The Slab Waveguide

If a slab of material is placed between two materials with lower refractive index, a slab waveguide is formed.

Conditions

\[ n_2 > n_1 \]

and

\[ n_2 > n_3 \]
The round trip phase of a ray must be an integer multiple of $2\pi$. Because of this, only certain angles are allowed to propagate in the waveguide. Only discrete directions are possible.

$$\beta = k_0 n_{\text{eff}} = k_0 n \sin \theta$$

**Slide 7**

**Ray Tracing Analysis**

**Slide 8**

**Frequency-Domain Analysis of Slab Waveguides**
Maxwell’s Equations

In a previous lecture, the electric field quantities were normalized and Maxwell’s
equations were expressed in terms of the normalized parameters as follows:
\[
\nabla \times \vec{H} = \frac{1}{c_0} \frac{\partial \vec{D}}{\partial t} \\
\nabla \times \vec{E} = \left[ \mu_0 \right] \frac{\partial \vec{H}}{\partial t}
\]

\[
\vec{D} = [\varepsilon_i] \vec{E}
\]

For this slab waveguide analysis in the frequency domain, the \( \vec{D} \) field is eliminated.

\[
\nabla \times \vec{H} = j \omega \left[ \frac{\varepsilon_i}{c_0} \right] \vec{E} \\
\nabla \times \vec{E} = -j \omega \left[ \frac{\mu_0}{c_0} \right] \vec{H} 
\]

Waveguide Modes

Assume a Solution

Modes in a waveguide have the following form:
\[
\vec{E}(x,y,z) = \vec{A}(x,z) e^{j\beta y} \\
\vec{H}(x,y,z) = \vec{B}(x,z) e^{j\beta y}
\]

The \( y \)-Derivative
\[
\frac{\partial \vec{E}}{\partial y} = \vec{A}(x,z) \frac{\partial}{\partial y} e^{j\beta y} + e^{j\beta y} \frac{\partial \vec{A}(x,z)}{\partial y} = j \beta \vec{A}(x,z) e^{j\beta y} = j \beta \vec{E} 
\]
\[
\frac{\partial \vec{H}}{\partial y} = \vec{B}(x,z) \frac{\partial}{\partial y} e^{j\beta y} + e^{j\beta y} \frac{\partial \vec{B}(x,y)}{\partial y} = j \beta \vec{B}(x,y) e^{j\beta y} = j \beta \vec{H}
\]

Conclusion \( \Rightarrow \frac{\partial}{\partial y} = j \beta \)
Reduction of Dimensions

Slab Waveguides are Uniform Along $y$ and $z$

$$\frac{\partial}{\partial z} = 0 \quad \frac{\partial}{\partial y} = j\beta$$

Maxwell’s Equations Reduce to

$$\begin{align*}
  j\beta B_z &= j\omega \frac{\varepsilon_y}{c_0} A_y \\
  -\frac{\partial B_y}{\partial x} &= j\omega \frac{\varepsilon_y}{c_0} A_y \\
  \frac{\partial B_y}{\partial x} - j\beta B_y &= j\omega \frac{\varepsilon_x}{c_0} A_x \\
  \frac{\partial A_y}{\partial x} - j\beta A_x &= -j\omega \frac{\mu_y}{c_0} B_y \\
  \frac{\partial A_x}{\partial x} - j\beta A_x &= -j\omega \frac{\mu_x}{c_0} B_z
\end{align*}$$

Two Distinct Modes

Maxwell’s equations have decoupled into two sets of three equations.

**Ez Mode**

$$\begin{align*}
  A_x &= A_y = B_z = 0 \\
  \frac{\partial B_y}{\partial x} - j\beta B_y &= j\omega \frac{\varepsilon_y}{c_0} A_y \\
  j\beta A_y &= -j\omega \frac{\mu_y}{c_0} B_y \\
  \frac{\partial A_x}{\partial x} &= -j\omega \frac{\mu_y}{c_0} B_y
\end{align*}$$

**Hz Mode**

$$\begin{align*}
  B_z &= B_y = A_y = 0 \\
  \frac{\partial A_y}{\partial x} - j\beta A_y &= -j\omega \frac{\mu_y}{c_0} B_y \\
  j\beta B_y &= j\omega \frac{\varepsilon_x}{c_0} A_x \\
  \frac{\partial B_z}{\partial x} &= j\omega \frac{\varepsilon_x}{c_0} A_x
\end{align*}$$
Normalize the Grid

The grid coordinate are normalized as follows:

\[ x' = k_0 x \]

Also, observe that

\[ \beta = k_0 n_{eff} = \frac{\omega}{c_0} n_{eff} \]

Under these conditions, Maxwell’s equations for the two modes become

**Ez Mode**

\[ \frac{\partial B_y}{\partial x} - j n_{eff} B_z = j \varepsilon_{xx} A_z \]

\[ n_{eff} A_z = -\mu_{xx} B_z \]

\[ \frac{\partial A_x}{\partial x} = j \mu_{yy} B_y \]

**Hz Mode**

\[ \frac{\partial A_x}{\partial x} - j n_{eff} A_z = -j \mu_{yy} B_z \]

\[ n_{eff} B_z = \varepsilon_{xx} A_z \]

\[ -\frac{\partial B_y}{\partial x'} = j \varepsilon_{yy} A_z \]

Matrix Representation of Fields on a Grid

1-D Systems

2-D Systems
Maxwell’s Equations in Matrix Form

The equations for the $E_z$ mode can be written in matrix form as

$$
\frac{\partial B_y}{\partial x} - j n_{\text{eff}} B_z = j \varepsilon_{\text{eff}} A_z
$$

$$
\frac{\partial A_x}{\partial x} = j \mu_{\text{eff}} B_y
$$

$$
\begin{bmatrix}
\varepsilon_{\text{eff}}(1) & 0 \\
0 & \varepsilon_{\text{eff}}(N_y)
\end{bmatrix}
\begin{bmatrix}
\mathbf{a}_x
\end{bmatrix}
= \begin{bmatrix}
-1 & 1 & 0 \\
-1 & 1 & 0
\end{bmatrix}
\begin{bmatrix}
\mathbf{b}_x
\end{bmatrix}
$$

$$
\begin{bmatrix}
\mu_{\text{eff}}(1) & 0 \\
0 & \mu_{\text{eff}}(N_y)
\end{bmatrix}
\begin{bmatrix}
\mathbf{a}_y
\end{bmatrix}
= \begin{bmatrix}
1 & 0 \\
-1 & 1
\end{bmatrix}
\begin{bmatrix}
\mathbf{b}_y
\end{bmatrix}
$$

Matrix Wave Equation

Start with Maxwell’s equations in matrix form.

$$
\begin{bmatrix}
\mathbf{D}' & -j n_{\text{eff}} \mathbf{b}_z = j \varepsilon_{\text{eff}} \mathbf{a}_z \\
n_{\text{eff}} \mathbf{a}_z = -\mu_{\text{eff}} \mathbf{b}_y \\
\mathbf{D}' \mathbf{a}_z = j \mu_{\text{eff}} \mathbf{b}_y
\end{bmatrix}
\begin{bmatrix}
\mathbf{b}_x
\end{bmatrix}
= \begin{bmatrix}
\lambda \mathbf{b}_z
\end{bmatrix}
$$

Solve the second two equations for the magnetic field quantities.

$$
\mathbf{b}_x = -n_{\text{eff}} \mu_{\text{eff}}^{-1} \mathbf{a}_x
$$

$$
\mathbf{b}_y = -j \mu_{\text{eff}}^{-1} \mathbf{D}' \mathbf{a}_z
$$

Substitute these into the first equation to get the matrix wave equation.

$$
\begin{bmatrix}
\mathbf{D}' & -j n_{\text{eff}} \mathbf{b}_z = j \varepsilon_{\text{eff}} \mathbf{a}_z \\
n_{\text{eff}} \mathbf{a}_z = -\mu_{\text{eff}} \mathbf{b}_y \\
\mathbf{D}' \mathbf{a}_z = j \mu_{\text{eff}} \mathbf{b}_y
\end{bmatrix}
\begin{bmatrix}
\mathbf{b}_x
\end{bmatrix}
= \begin{bmatrix}
\lambda \mathbf{b}_z
\end{bmatrix}
$$

This equation will be used again later. Remember it!

This is a generalized eigen-value problem

$$
\mathbf{A} \mathbf{x} = \lambda \mathbf{B} \mathbf{x}
$$

$$
\mathbf{A} = \mathbf{D}' \mu_{\text{eff}} \mathbf{D}' + \varepsilon_{\text{eff}}
$$

$$
\mathbf{B} = \mu_{\text{eff}}^{-1} \mathbf{x} = \mathbf{a}_x
$$

$$
\lambda = n_{\text{eff}}^2
$$
Solving the Eigen-Value Problem

Use MATLAB's built-in `eig()` function to solve this eigen-value problem.

```matlab
[V,D] = eig(A,B);
```

The solution can be interpreted as

$$V = \begin{bmatrix}
A_0^{(1)} & A_0^{(2)} & \cdots & A_0^{(N_x)} \\
A_1^{(1)} & A_1^{(2)} & \cdots & A_1^{(N_x)} \\
\vdots & \vdots & \ddots & \vdots \\
A_{N_y}^{(1)} & A_{N_y}^{(2)} & \cdots & A_{N_y}^{(N_x)}
\end{bmatrix}
$$

The eigen-vectors describe the amplitude profile of the modes.

$$A_{n} (x) \cdot e^{jk_0 n_{eff} y}$$

The eigen-values describe the accumulation of phase.

Concept of the Eigen-Vector Matrix

The columns of the eigen-vector matrix are the “modes” of the waveguide.
MATLAB Code for Slab Waveguide Analysis

```matlab
function [Ez_src,Hx_src,neff,AZ,ind] = ezmode(URxx,URyy,ERzz,dxp)
% EZMODE Calculate the Fundamental Mode of a Slab Waveguide
% for the Ez Mode
%
% [Ez_src,Hx_src,neff,AZ,ind] = fmode(URxx,URyy,ERzz,dxp)
%
% dxp is the normalized grid resolution
% dxp = k0*dx
%
% DETERMINE NUMBER OF POINTS ON GRID
Nx = length(ERzz);
%
% CONSTRUCT DIAGONAL MATERIAL MATRICES
URxx = diag(sparse(URxx(:)));
URyy = diag(sparse(URyy(:)));
ERzz = diag(sparse(ERzz(:)));
%
% BUILD DERIVATIVE OPERATORS
DHX = spdiags(-ones(Nx,1)/dxp,-1,sparse(Nx,Nx));
DHX = spdiags(ones(Nx,1)/dxp,0,DHX);
DEX = spdiags(-ones(Nx,1)/dxp,0,sparse(Nx,Nx));
DEX = spdiags(ones(Nx,1)/dxp,1,DEX);
%
% SOLVE EIGEN-VALUE PROBLEM
A = full(ERzz + DHX/URyy*DEX);
B = full(inv(URxx));
[AZ,NEFF] = eig(A,B);
NEFF = sqrt(diag(NEFF));
%
% FIND FUNDAMENTAL MODE
[neff,ind] = max(real(NEFF));
Ez_src = AZ(:,ind);
%
% COMPUTE Hx_src
Hx_src = -neff*(URxx 来自原始文本)
```

We identify the fundamental mode as the mode with the largest real value.

Typical Modes in a Slab Waveguide ($E_z$ Mode)

Typical Modes in a Slab Waveguide ($E_z$ Mode)

```

Typical Modes in a Slab Waveguide ($E_z$ Mode)

- $n_1 = 1.0$
- $n_2 = 2.0$
- $n_3 = 1.0$
```

See Slide 16
Waveguide Sources in FDTD

Recall Total-Field/Scattered-Field
Recall Injecting a Plane Wave ($E_z$ Mode)

Calculate the electric field as

$$E_z^{\text{sec}}|_{t+\Delta t} = g(t)$$

Calculate the magnetic field as

$$\tilde{H}_x^{\text{sec}}|_{t+\frac{\Delta t}{2}} = \sqrt{\frac{\varepsilon_{t,\text{sec}}}{\mu_{t,\text{sec}}}} g\left(t + \frac{n \Delta y}{2 c_0} + \frac{\Delta t}{2}\right)$$

- Amplitude due to Maxwell’s equations
- Delay through one half of a grid cell
- Half time step difference

Modification for Waveguide Sources

Plane Wave Source

$$E_z^{\text{sec}}|_{t+\Delta t} = g(t)$$

$$\tilde{H}_x^{\text{sec}}|_{t+\frac{\Delta t}{2}} = \sqrt{\frac{\varepsilon_{t,\text{sec}}}{\mu_{t,\text{sec}}}} g(t + \delta t)$$

Waveguide Source

$$E_z^{\text{sec}}|_{t+\Delta t} = r(t) \cdot \text{Re}\left\{v_e(x) \exp[-j2\pi ft]\right\}$$

$$\tilde{H}_x^{\text{sec}}|_{t+\frac{\Delta t}{2}} = r(t) \cdot \text{Re}\left\{v_p(x) \exp[-j2\pi f(t + \delta t)]\right\}$$

- Ramp function
- Complex mode amplitudes from $ezmode()$
- Harmonic oscillation (pure frequency)

Note: These sources are at a single frequency $f$. 
Extracting the Slab Waveguide(s) from FDTD

A “window” just outside the top PML is used for the source and to analyze reflected waves.

Another “window” just outside the side PML is used for analyzing transmitted waves.

Animation of a Waveguide Simulation

Source Profile

Waves exiting transmission plane

Waves scattered from waveguide
Reflection From and Transmission Through Waveguides

Modify the Fourier Transform

For waveguide circuits, the typical source operates at a single frequency (i.e. pure frequency source). To calculate a Fourier transform from a sinusoidal source, the simulation is run until steady-state has been reached, then integrate over a single period. This is not necessary, but is faster.

Start with the standard Fourier transform, but it is only necessary to integrate over one period because the function will just keep repeating as long as it is at steady-state.

\[
F(f_0) = 2f_0 \int_{t_0}^{t_0 + 1/f_0} f(t) e^{-j2\pi f_0 t} dt
\]

This is implemented in FDTD as

\[
F(f_0) \approx 2\Delta t \cdot f_0 \cdot \sum_{m} (e^{-j2\pi f_0 \Delta t})^m \cdot f(m)
\]
MATLAB Code for Revised Fourier Transform

We must ensure that one wave cycle is resolved with an integer number of time steps.

```matlab
% SNAP TIME STEP SO WAVE PERIOD IS AN INTEGER NUMBER OF STEPS
period = 1/f0;
Nt = ceil(period/dt);
dt = period/Nt;

The Fourier transform is computed during the last wave cycle of the simulation.

```matlab
% Update Fourier Transform
if T>(STEPS-Nt)
    Eref = Eref + (K^(T-STEPS+Nt))*Ez(:,nyref);
    Etrn = Etrn + (K^(T-STEPS+Nt))*Ez(nxtrn,:);
end
```

After the main loop, we finish the transform as

```matlab
% FINISH TRANSFORMS
Eref = Eref * (2*dt/period);  % Note: A pure sinusoid source is used so there is no need to
Etrn = Etrn * (2*dt/period);  % Fourier transform the source or divide by its amplitude.
```

Field Across a Waveguide

During the FDTD simulation, use the revised Fourier transform procedure to calculate the steady-state field across the waveguide.
Field In Terms of Eigen-Modes

The field across the waveguide is a linear sum of the eigen-modes.

\[ \mathbf{e}_z = \left[ \begin{array}{c} \mathbf{a}_1 \\ \mathbf{a}_2 \\ \mathbf{a}_3 \\ \mathbf{a}_4 \\ \mathbf{a}_5 \end{array} \right] = a_1 \mathbf{v}_1 + a_2 \mathbf{v}_2 + a_3 \mathbf{v}_3 + a_4 \mathbf{v}_4 + a_5 \mathbf{v}_5 = \mathbf{Va} \]

Calculating the Energy in Each Mode

The steady-state field \( \mathbf{e}_z \) is calculated around the input and output(s) of the waveguide circuit using FDTD. From this, the complex amplitudes of all the modes can be calculated.

\[ \mathbf{e}_z^{\text{ref}} = \mathbf{V}_{\text{ref}} \mathbf{a}_{\text{ref}} \quad \rightarrow \quad \mathbf{a}_{\text{ref}} = \mathbf{V}_{\text{ref}}^{-1} \mathbf{e}_z^{\text{ref}} \]
\[ \mathbf{e}_z^{\text{tm}} = \mathbf{V}_{\text{tm}} \mathbf{a}_{\text{tm}} \quad \rightarrow \quad \mathbf{a}_{\text{tm}} = \mathbf{V}_{\text{tm}}^{-1} \mathbf{e}_z^{\text{tm}} \]

Now the fraction of power in all of the modes can be calculated.

\[ P_{\text{ref}} = \left| \frac{1}{a_{\text{inc}}^{\text{ref}}} \mathbf{a}_{\text{ref}} \right|^2 \]
\[ P_{\text{tm}} = \left| \frac{1}{a_{\text{inc}}^{\text{tm}}} \mathbf{a}_{\text{tm}} \right|^2 \]

Most of the time we only care about the fraction of power in the fundamental mode.
MATLAB Code for Power Calculation

First calculate the complex amplitudes of the eigen-modes.

```matlab
% CALCULATE MODE AMPLITUDES
aref = EZR
deg(NPML(1)+1:Nx-NPML(2));
atrn = ETX

deg(NPML(3)+1:Ny-NPML(4))';
```

Second, calculate reflectance and transmittance.

```matlab
% CALCULATE TRANSMITTANCE AND REFLECTANCE OF FUNDAMENTAL MODE
REF = abs(aref(ind_ref)) ^ 2;
TRN = abs(atrn(ind_trn)) ^ 2;
```

Example Transmission Calculation

Assuming the waveguide was sourced with only the fundamental mode with unit amplitude...

\[
\begin{bmatrix}
1.0 \\
0 \\
0 \\
0 \\
0
\end{bmatrix} \Rightarrow \begin{bmatrix}
0.87 \\
0.02 \\
0.06 \\
0.15 \\
0.05
\end{bmatrix}
\]

\[R \approx 0\%\]

\[T \approx \left( \frac{0.87^2}{1} \right) \approx 76\%\]
Benchmark Simulations

The waveguide parameters are...

- $\lambda_0 = 1.55 \, \mu\text{m}$
- $n_{\text{clad}} = 1.5$
- $n_{\text{core}} = 2.0$
- $a = 0.5 \, \mu\text{m}$