Computational Science:
Introduction to Finite-Difference Time-Domain

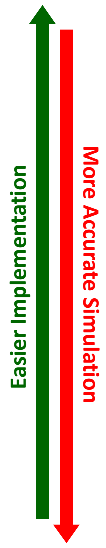
Periodic Structures in FDTD

Lecture Outline

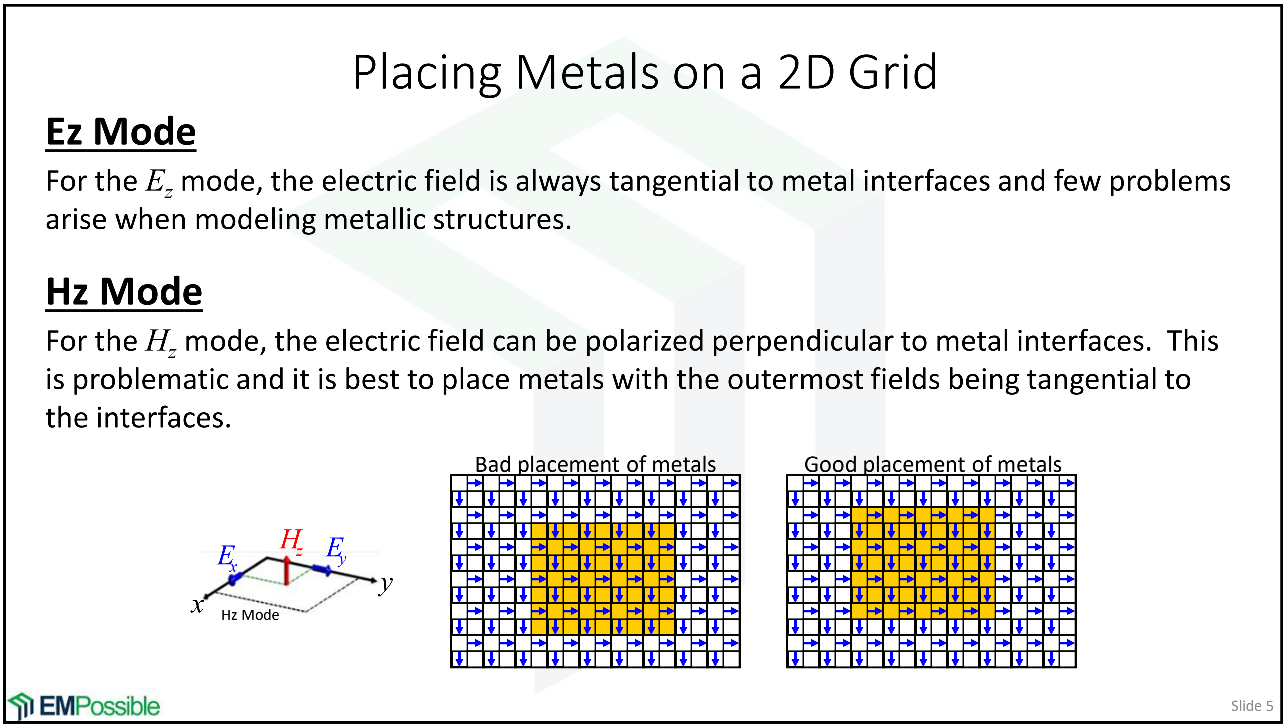
- Review
- Periodic Structures
- Periodic Boundary Conditions in FDTD
- Electromagnetic Band Calculation using FDTD

Review

Methods for Incorporating Metals



- Extreme Dielectric Constant
  - Easiest because no modification to the code is necessary, but it does not account for loss.
- Perfect Electric Conductor
  - Requires minimal modification to the code, but does not account for loss.
- σ
  - Requires greater modification to the formulation of the update equations. It can account for loss, but cannot account for frequency dependence.
- Lorentz-Drude Model
  - Requires a much more complicated formulation and implementation, but it can account for loss and frequency dependence.



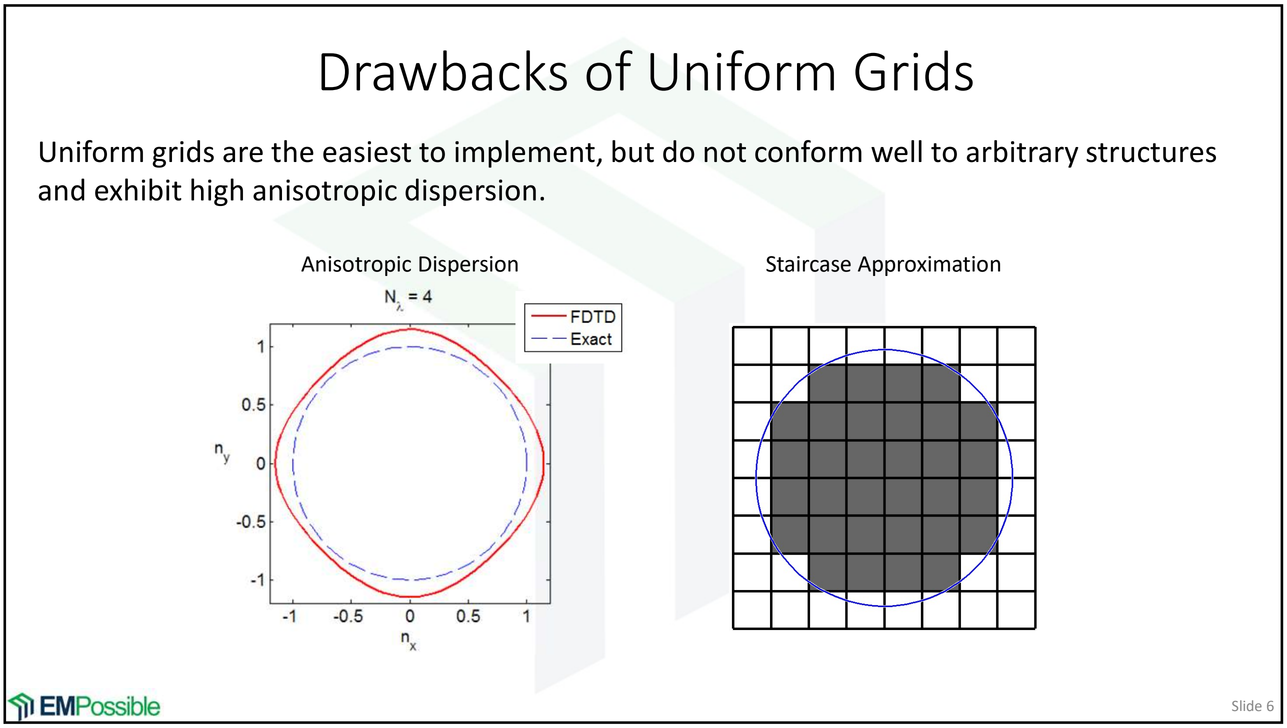
Placing Metals on a 2D Grid

Ez Mode

For the E_z mode, the electric field is always tangential to metal interfaces and few problems arise when modeling metallic structures.

Hz Mode

For the H_z mode, the electric field can be polarized perpendicular to metal interfaces. This is problematic and it is best to place metals with the outermost fields being tangential to the interfaces.



Drawbacks of Uniform Grids

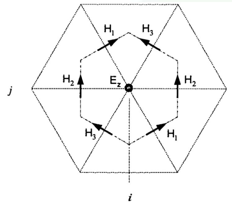
Uniform grids are the easiest to implement, but do not conform well to arbitrary structures and exhibit high anisotropic dispersion.

Anisotropic Dispersion

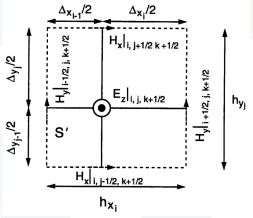
Staircase Approximation

Alternative Grid Schemes

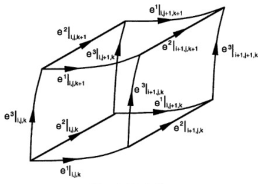
Hexagonal Grids



Nonuniform Grids

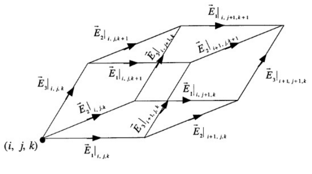


Curvilinear Grids



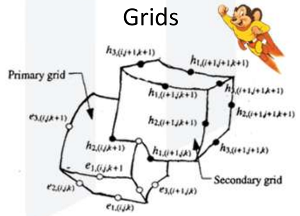
(a) ~ electric field

Nonorthogonal Grids

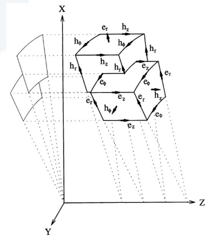


(a) Covariant electric fields.

Irregular Unstructured Grids



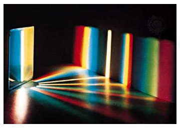
Bodies of Revolution



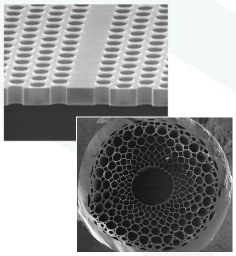
Periodic Structures

Examples of Periodic Electromagnetic Devices

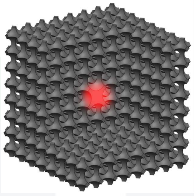
Diffraction Gratings



Waveguides

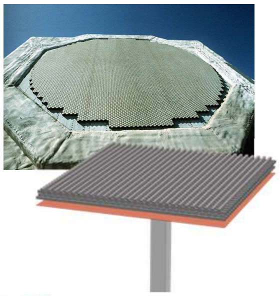


Band Gap Materials

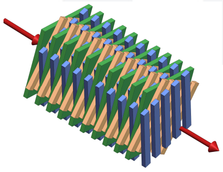


Metamaterials

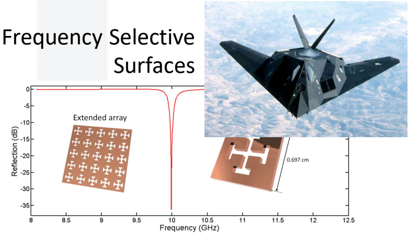
Antennas



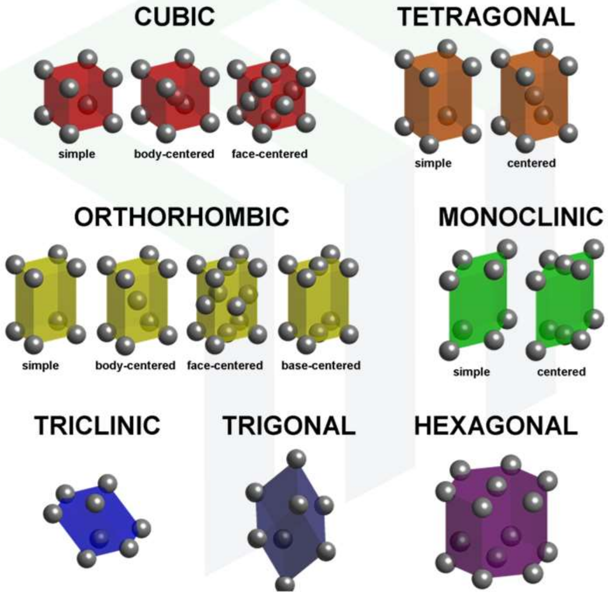
Slow Wave Devices



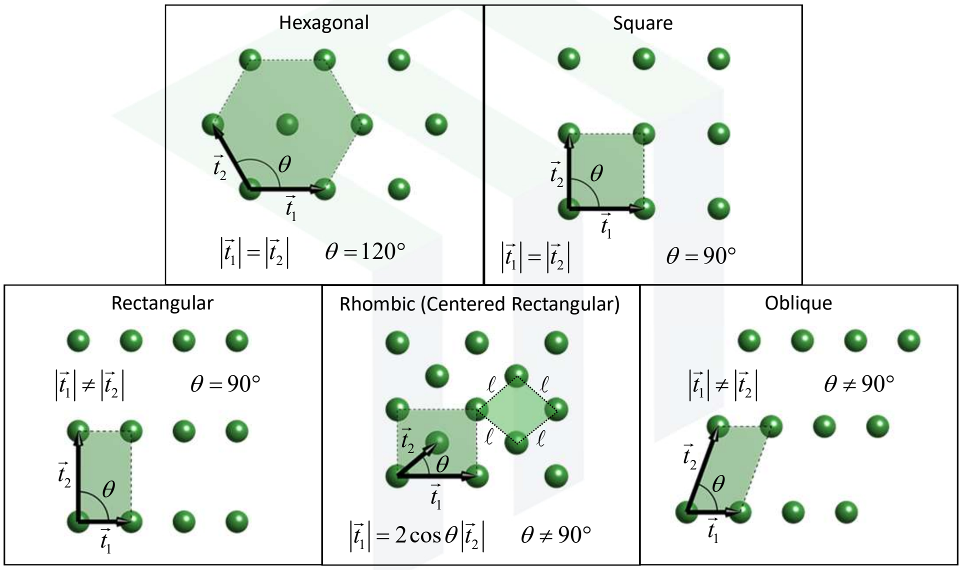
Frequency Selective Surfaces



The Bravais Lattices and Seven Crystal Systems

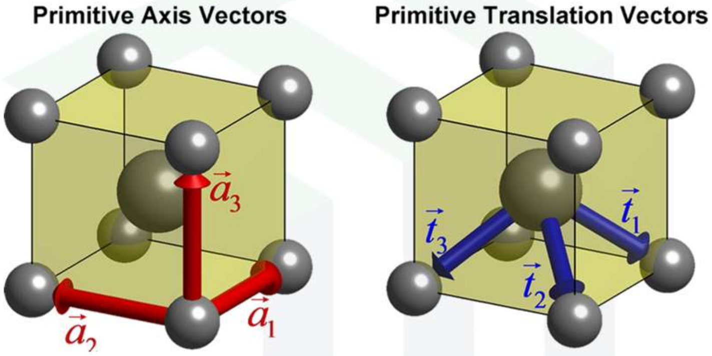


Two-Dimensional Bravais Lattices



Axis vectors = translation vectors for 2D lattices

Primitive Lattice Vectors



Axis vectors most intuitively define the shape and orientation of the unit cell. They cannot uniquely describe all 14 Bravais lattices.

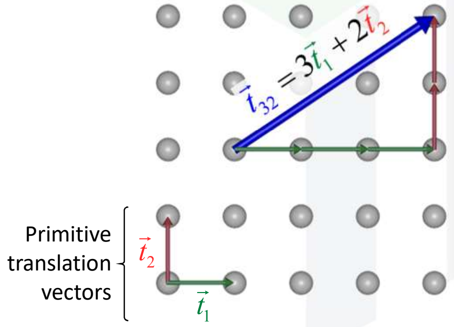
Translation vectors connect adjacent points in the lattice and can uniquely describe all 14 Bravais lattices. They are less intuitive to interpret.

Primitive lattice vectors are the smallest possible vectors that still describe the unit cell.

Non-Primitive Lattice Vectors

Almost always, the label “lattice vector” refers to the translation vectors, not the axis vectors.

A translation vector is any vector that connects two points in a lattice. They must be an integer combination of the primitive translation vectors.

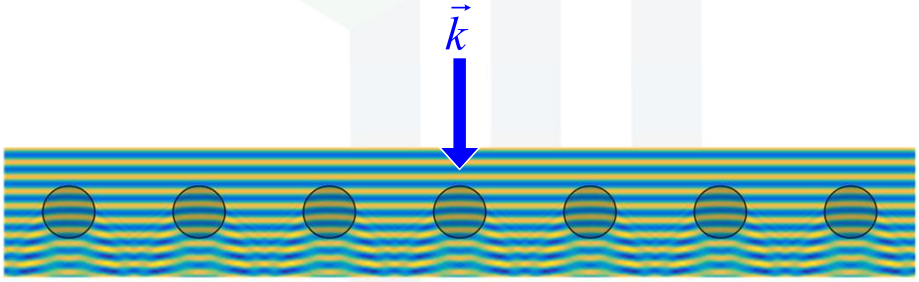


$$\vec{t}_{pqr} = p\vec{t}_1 + q\vec{t}_2 + r\vec{t}_3$$

$$p = \cdots,-2,-1,0,1,2,\cdots$$
$$q = \cdots,-2,-1,0,1,2,\cdots$$
$$r = \cdots,-2,-1,0,1,2,\cdots$$

Fields in Periodic Structures

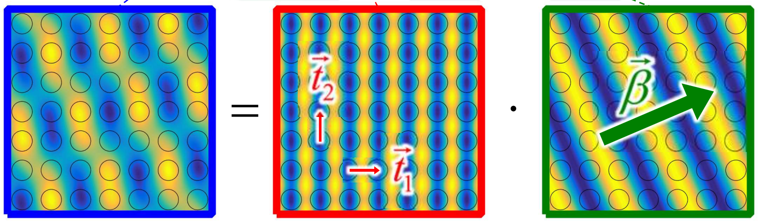
Waves in periodic structures take on the same periodicity as their host.



The Bloch Theorem

Waves inside of a periodic structure are like plane waves, but they are modulated by an envelope function. It is the envelope function that takes on the same symmetry and periodicity as the structure.

$$\vec{E}(\vec{r}) = \vec{A}(\vec{r})\, e^{j\vec{\beta}\bullet\vec{r}}$$



Overall field is the combination of the envelope and plane wave term.

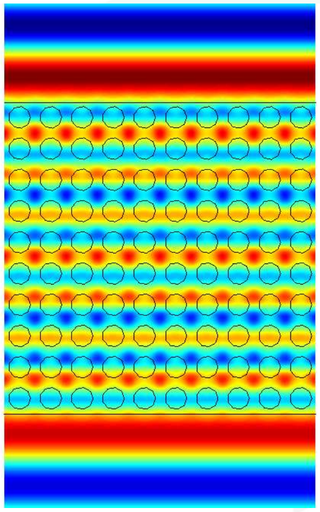
Envelope function has the same symmetry and periodicity as the periodic structure.

Plane-wave like phase "tilt" term.

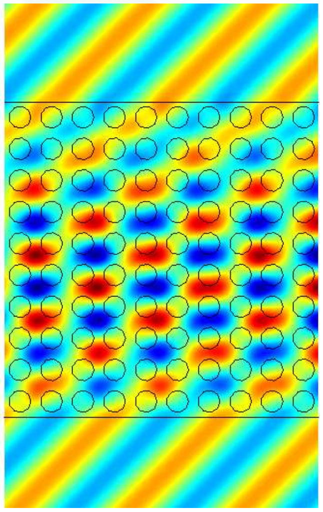
$\vec{\beta} \equiv$ Bloch wave vector

Bloch Waves

Wave normally incident on a periodic structure.



Wave incident at 45° on the same periodic structure.



Mathematical Description of Periodicity

A structure is periodic if its material properties repeat. Given the lattice vectors, the periodicity is expressed as

$$\varepsilon\left(\vec{r}+\vec{t}_{pqr}\right)=\varepsilon\left(\vec{r}\right) \qquad \vec{t}_{pqr}=p\vec{t}_1+q\vec{t}_2+r\vec{t}_3$$

Recall that it is the amplitude of the Bloch wave that has the same periodicity as the structure the wave is in. Therefore,

$$A\left(\vec{r}+\vec{t}_{pqr}\right)=A\left(\vec{r}\right) \qquad \vec{t}_{pqr}=p\vec{t}_1+q\vec{t}_2+r\vec{t}_3$$

For a device that is periodic only along one direction, these relations reduce to

$$\begin{array}{c} \varepsilon\left(x+p\Lambda_x,y,z\right)=\varepsilon\left(x,y,z\right) \\ A\left(x+p\Lambda_x,y,z\right)=A\left(x,y,z\right) \end{array} \xrightarrow{\text{more compact notation}} \begin{array}{c} \varepsilon\left(x+p\Lambda_x\right)=\varepsilon\left(x\right) \\ A\left(x+p\Lambda_x\right)=A\left(x\right) \end{array}$$

Periodic Boundary Conditions in FDTD

Generalized Periodic Boundary Condition

For a device that is periodic along x with period Λ_x, Bloch's theorem can be written as

$$\vec{E}(\vec{r}) = \vec{A}(\vec{r}) \cdot e^{j\beta_x x} e^{j\beta_y y}$$

Periodicity requires that the amplitude also have period Λ_x.

$$\vec{A}(x) = \vec{A}(x + m\Lambda_x) \qquad m = -\infty, \cdots, -2, -1, 0, 1, 2, \cdots, \infty$$

The phase tilt term, however, can have any period along the x axis.

An equation can be derived that describes the periodic boundary condition (PBC) from the Bloch theorem.

$$\vec{E}(x \pm \Lambda_x) = \vec{A}(x \pm \Lambda_x) \cdot e^{j\beta_x (x \pm \Lambda_x)} e^{j\beta_y y}$$
$$\vec{E}(x \pm \Lambda_x) = \left[\vec{A}(x) \cdot e^{j\beta_x x} e^{j\beta_y y}\right] e^{\pm j\beta_x \Lambda_x}$$
$$\vec{E}(x \pm \Lambda_x) = \vec{E}(x) \cdot e^{\pm j\beta_x \Lambda_x}$$

$$\boxed{\vec{E}(x \pm \Lambda_x) = \vec{E}(x) \cdot e^{\pm j\beta_x \Lambda_x}}$$

Periodic Boundary Condition in the Time-Domain

The generalized PBC in the frequency-domain was derived from the Bloch theorem to be

$$\vec{E}(x \pm \Lambda_x, \omega) = \vec{E}(x, \omega) \cdot e^{\pm j\beta_x \Lambda_x}$$

Recall the following property of the Fourier transform

$$\Im\left[g(x, t - t_0)\right] = G(x, \omega) \cdot e^{-j\omega t_0}$$

It follows that the generalized PBC in the time-domain is

$$\vec{E}(x \pm \Lambda_x, t) = \vec{E}(x, t \mp \tau)$$

$$\tau = \frac{\beta_x \Lambda_x}{\omega} = \frac{\Lambda_x}{c_0} \sin\theta$$

$\tau > 0$ value from the future

$\tau < 0$ value from the past

Generalized PBC At Normal Incidence

At normal incidence, β_x=0.

The generalized PBC reduces to

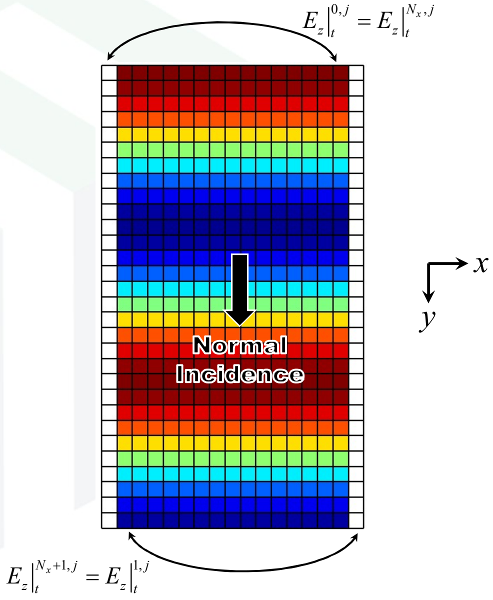
$$\vec{E}\left(x \pm \Lambda_x, t\right) = \vec{E}\left(x, t\right)$$

At the x-low boundary, this is

$$E_z\big|_t^{0,j} = E_z\big|_t^{N_x,j}$$

At the x-high boundary, this is

$$E_z\big|_t^{N_x+1,j} = E_z\big|_t^{1,j}$$



Generalized PBC At Oblique Incidence

At oblique incidence, $\beta_x \neq 0$.

The generalized PBC becomes

$$\vec{E}\left(x \pm \Lambda_x, t\right) = \vec{E}\left(x, t \mp \tau\right)$$

At the x-low boundary, this is

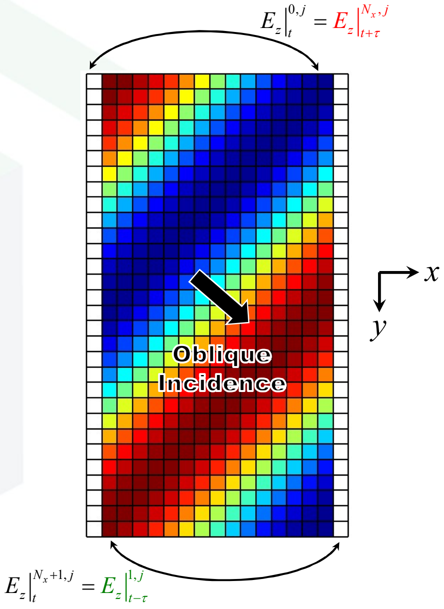
$$E_z\big|_t^{0,j} = E_z\big|_{t+\tau}^{N_x,j}$$

☹ How is the $\vec{E}$ field calculated at a future time?

At the x-high boundary, this is

$$E_z\big|_t^{N_x+1,j} = E_z\big|_{t-\tau}^{1,j}$$

☺ The electric field can always be computed at the past time of $t-\tau$ by storing a record of the fields at the boundary and interpolating.

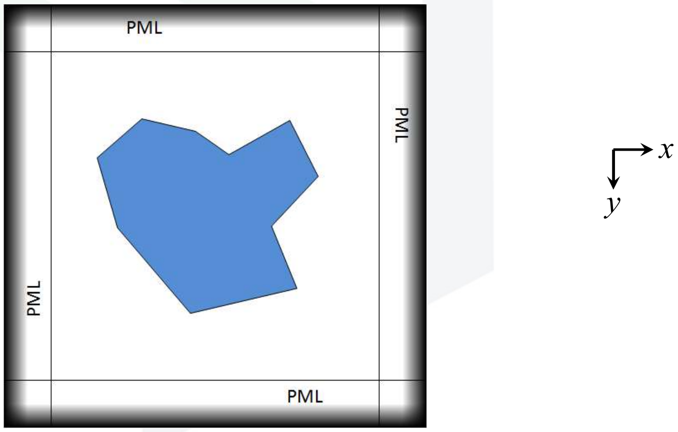


Conclusions

- Time-domain methods have serious problems when the following conditions exist simultaneously
  - Periodic boundary condition
  - Oblique incidence
  - Pulsed source
- Good solutions exist when any one of these conditions can be removed.
- One limited solution exists when all of these conditions exist at the same time.
  - Angled-update method

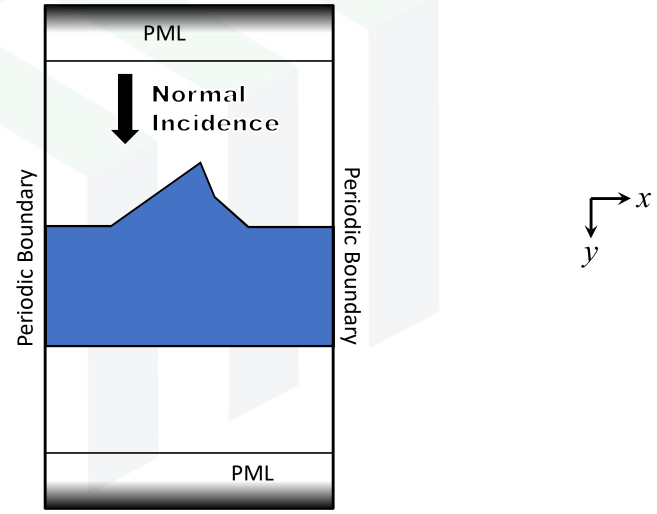
Case #1: No Periodic Boundary

In this case, scattering from a finite size device is being simulated so only PMLs are needed and not a periodic boundary condition.



Case #2: No Oblique Incidence

In this case, the standard PBC we already discussed can be used.

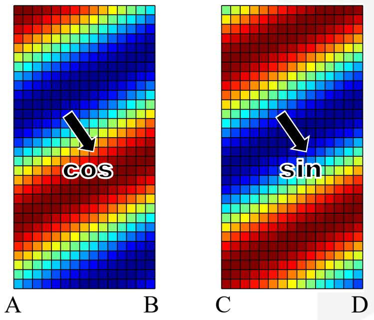


Case #3: Pure Frequency Source

When a device can be modeled with a single frequency, it becomes possible to incorporate a generalized periodic boundary condition.

We lose the wideband capability of FDTD, but retain all other benefits.

Sine-Cosine Method



$$e^{j\psi} = \cos\psi + j\sin\psi$$

$$E_z(A) = \mathrm{Re}\left\{\left[E_z(B) + jE_z(D)\right]e^{jk_x\Lambda_x}\right\}$$

$$E_z(C) = \mathrm{Im}\left\{\left[E_z(B) + jE_z(D)\right]e^{jk_x\Lambda_x}\right\}$$

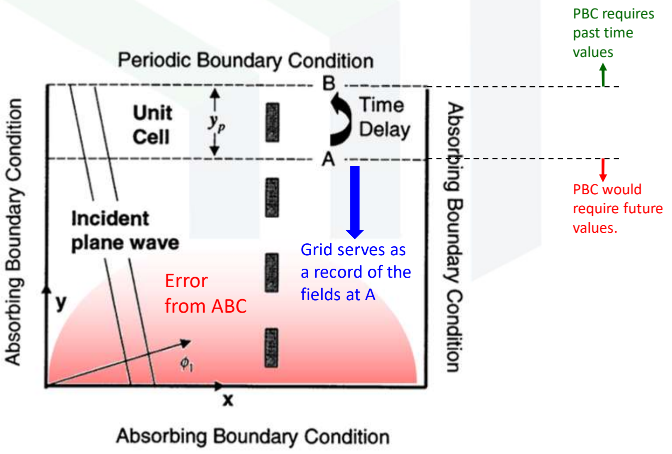
$$H_x(B) = \mathrm{Re}\left\{\left[H_x(A) + jH_x(C)\right]e^{-jk_x\Lambda_x}\right\}$$

$$H_x(D) = \mathrm{Im}\left\{\left[H_x(A) + jH_x(C)\right]e^{-jk_x\Lambda_x}\right\}$$

Case #4: All Conditions (1 of 4)

There is no known general solution.
There does exist several limited solutions.

Method #1: Multiple Unit Cell Method



PBC requires past time values

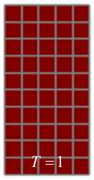
PBC would require future values.

Grid serves as a record of the fields at A

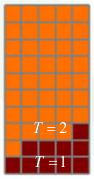
Error from ABC

Case #4: All Conditions (2 of 4)

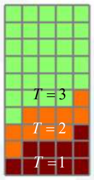
Method #2: Angled-Update Method (1 of 2)



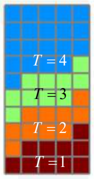
Envision a grid where all the field components exist at T=1.



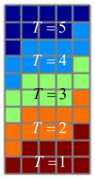
We could then update all the field components up to some slanted boundary.



Again, we could update all the field components up to some slanted boundary that is away from the first slanted boundary.



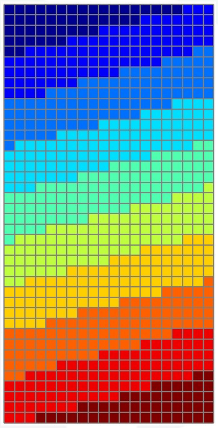
And again…



We have now built a time gradient into the grid.

Case #4: All Conditions (3 of 4)

Method #2: Angled-Update Method (2 of 2)



This boundary requires fields from future time values.

The right side of grid contains field values at future time steps.

☺

This boundary requires fields from past time values.

The left side of the grid contains field values at previous time steps.

☺

From here, we iterate over the whole grid very much like the standard FDTD algorithm. The difference is that we store the boundary fields for a few iterations from which we interpolate the field at whatever time value is needed.

$\theta_{\max} < 45°$ for 2D

$\theta_{\max} < 35°$ for 3D

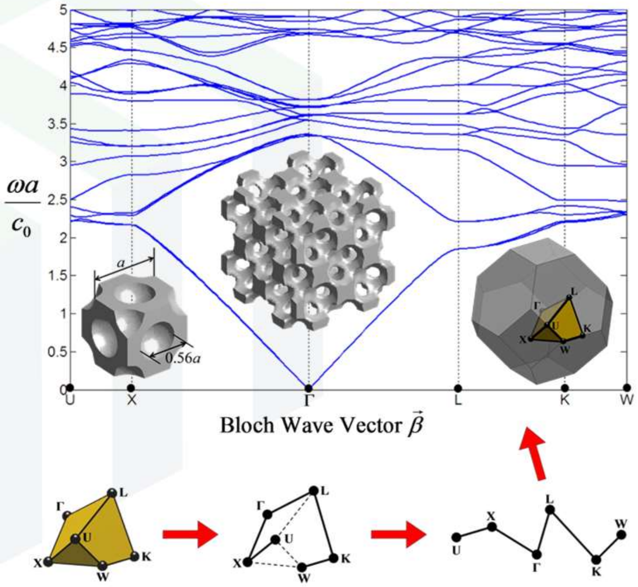
Case #4: All Conditions (4 of 4)

- Field-Transformation Technique
  - Larger angles possible than for angled-update method
  - Difficult to implement
  - Stability is an issue
  - See Text, pp. 567-583
- Split-Field Method
  - Difficult to implement
  - Stability is an issue
  - See Text, pp. 583-594

Electromagnetic Band Calculation using FDTD

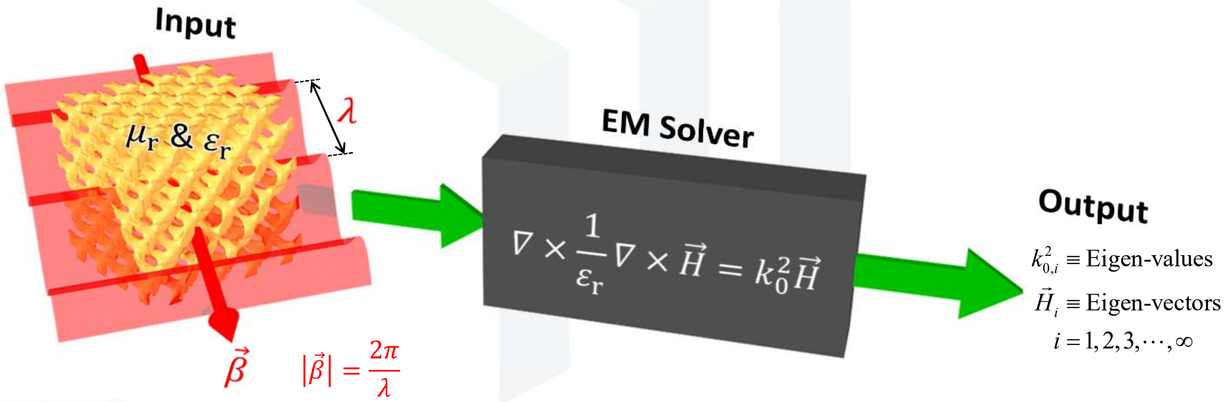
Band Diagrams

Band diagrams relate frequency to the direction and period of a Bloch wave propagating inside a periodic structure. They indicate which frequencies support waves with a given direction and wavelength in that periodic structure.

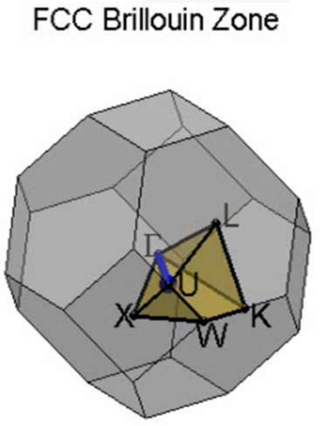


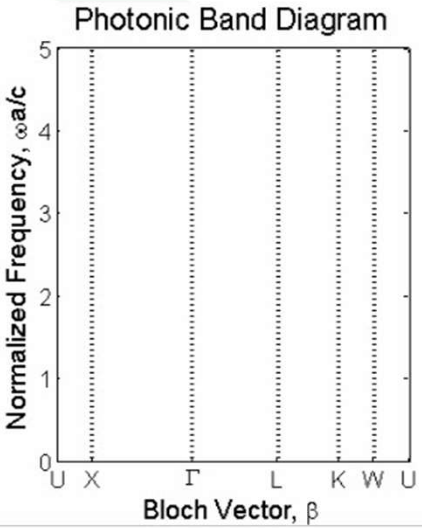
Computation of Band Diagrams

Band diagrams are a compact, but incomplete, means of characterizing the electromagnetic properties of a periodic structure. It is essentially a map of the frequencies of the eigen-modes as a function of the Bloch wave vector $\vec{\beta}$.



Animation of Construction of a Band Diagram





Benefits and Drawbacks of FDTD for Band Calculations

- Benefits
  - Wideband
  - Can account for dispersion (very unique)
  - Excellent for large unit cells
  - Excellent for structures with metals or high dielectric contrast
- Drawbacks
  - A large number of iterations is needed to accurately identify bands
  - Difficult to distinguish bands when they are in close proximity (degenerate modes)
  - No guarantee that all modes are excited and/or detected

Revised PBC for Band Calculations

The generalized periodic boundary condition for a 3D periodic structure is

$$\vec{E}\left(\vec{r}+\vec{t}_{pqr}\right)=\vec{E}\left(\vec{r}\right)\cdot e^{j\vec{\beta}\bullet\vec{t}_{pqr}}$$

Recall that periodic boundary conditions are incorporated into the curl equations. For band calculations, this is

$$C_{Ex}^{i,N_y,k}=\frac{\phi_y\tilde{E}_{i,1,k}^z-\tilde{E}_{i,j,k}^z}{\Delta y}-\frac{\tilde{E}_{i,j,k+1}^y-\tilde{E}_{i,j,k}^y}{\Delta z} \qquad C_{Ex}^{i,j,N_z}=\frac{\tilde{E}_{i,j+1,k}^z-\tilde{E}_{i,j,k}^z}{\Delta y}-\frac{\phi_z\tilde{E}_{i,j,1}^y-\tilde{E}_{i,j,k}^y}{\Delta z} \qquad \phi_x=e^{-j\beta_x\Lambda_x}$$

$$C_{Ey}^{i,j,N_z}=\frac{\phi_z\tilde{E}_{i,j,1}^x-\tilde{E}_{i,j,k}^x}{\Delta z}-\frac{\tilde{E}_{i+1,j,k}^z-\tilde{E}_{i,j,k}^z}{\Delta x} \qquad C_{Ey}^{N_x,j,k}=\frac{\tilde{E}_{i,j,k+1}^x-\tilde{E}_{i,j,k}^x}{\Delta z}-\frac{\phi_x\tilde{E}_{1,j,k}^z-\tilde{E}_{i,j,k}^z}{\Delta x} \qquad \phi_y=e^{-j\beta_y\Lambda_y}$$

$$C_{Ez}^{N_x,j,k}=\frac{\phi_x\tilde{E}_{1,j,k}^y-\tilde{E}_{i,j,k}^y}{\Delta x}-\frac{\tilde{E}_{i,j+1,k}^x-\tilde{E}_{i,j,k}^x}{\Delta y} \qquad C_{Ez}^{i,N_y,k}=\frac{\tilde{E}_{i+1,j,k}^y-\tilde{E}_{i,j,k}^y}{\Delta x}-\frac{\phi_y\tilde{E}_{i,1,k}^x-\tilde{E}_{i,j,k}^x}{\Delta y} \qquad \phi_z=e^{-j\beta_z\Lambda_z}$$

$$C_{Hx}^{i,1,k}=\frac{H_{i,j,k}^z-\phi_y^*H_{i,N_y,k}^z}{\Delta y}-\frac{H_{i,j,k}^y-H_{i,j,k-1}^y}{\Delta z} \qquad C_{Hx}^{i,j,1}=\frac{H_{i,j,k}^z-H_{i,j-1,k}^z}{\Delta y}-\frac{H_{i,j,k}^y-\phi_z^*H_{i,j,N_z}^y}{\Delta z} \qquad \phi_x^*=e^{j\beta_x\Lambda_x}$$

$$C_{Hy}^{i,j,1}=\frac{H_{i,j,k}^x-\phi_z^*H_{i,j,N_z}^x}{\Delta z}-\frac{H_{i,j,k}^z-H_{i-1,j,k}^z}{\Delta x} \qquad C_{Hy}^{1,j,k}=\frac{H_{i,j,k}^x-H_{i,j,k-1}^x}{\Delta z}-\frac{H_{i,j,k}^z-\phi_x^*H_{N_x,j,k}^z}{\Delta x} \qquad \phi_y^*=e^{j\beta_y\Lambda_y}$$

$$C_{Hz}^{1,j,k}=\frac{H_{i,j,k}^y-\phi_x^*H_{N_x,j,k}^y}{\Delta x}-\frac{H_{i,j,k}^x-H_{i,j-1,k}^x}{\Delta y} \qquad C_{Hz}^{i,1,k}=\frac{H_{i,j,k}^y-H_{i-1,j,k}^y}{\Delta x}-\frac{H_{i,j,k}^x-\phi_y^*H_{i,N_y,k}^x}{\Delta y} \qquad \phi_z^*=e^{j\beta_z\Lambda_z}$$

Implementation of PBC in MATLAB

```
% Calculate Phase Across Grid
phix = exp(-1i*bx*Sx);
phiy = exp(-1i*by*Sy);
```

$$\phi_x = e^{-j\beta_x\Lambda_x}$$

$$\phi_y = e^{-j\beta_y\Lambda_y}$$

$$C_{Hz}^{1,j,k} = \frac{H_{i,j,k}^{y} - \phi_x^{*}H_{N_x,j,k}^{y}}{\Delta x} - \frac{H_{i,j,k}^{x} - H_{i,j-1,k}^{x}}{\Delta y}$$

$$C_{Hz}^{i,1,k} = \frac{H_{i,j,k}^{y} - H_{i-1,j,k}^{y}}{\Delta x} - \frac{H_{i,j,k}^{x} - \phi_y^{*}H_{i,N_y,k}^{x}}{\Delta y}$$

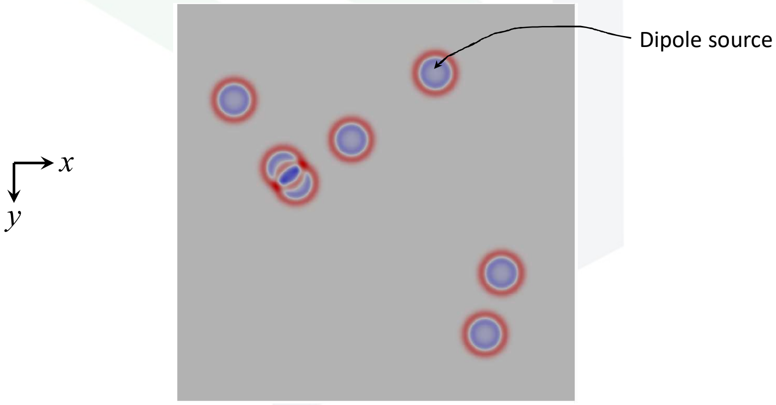
```
% Compute CHz
CHz(1,1) = (Hy(1,1) - conj(phix)*Hy(Nx,1))/dx ...
         - (Hx(1,1) - conj(phiy)*Hx(1,Ny))/dy;
for nx = 2 : Nx
    CHz(nx,1) = (Hy(nx,1) - Hy(nx-1,1))/dx ...
              - (Hx(nx,1) - conj(phiy)*Hx(nx,Ny))/dy;
end
for ny = 2 : Ny
    CHz(1,ny) = (Hy(1,ny) - conj(phix)*Hy(Nx,ny))/dx ...
              - (Hx(1,ny) - Hx(1,ny-1))/dy;
    for nx = 2 : Nx
        CHz(nx,ny) = (Hy(nx,ny) - Hy(nx-1,ny))/dx ...
                   - (Hx(nx,ny) - Hx(nx,ny-1))/dy;
    end
end
```

Implications of Revised PBC

- FDTD for band calculations is very much like the sin-cosine method
- Field values in the grid will be complex.
  - This is not a problem for MATLAB and FORTRAN
  - Other languages require separate grids for real and imaginary components (i.e. sin-cosine method)
- While FDTD for band calculations is wideband, the PBCs are possible because the field is periodic and the spatial period of the wave is fixed.

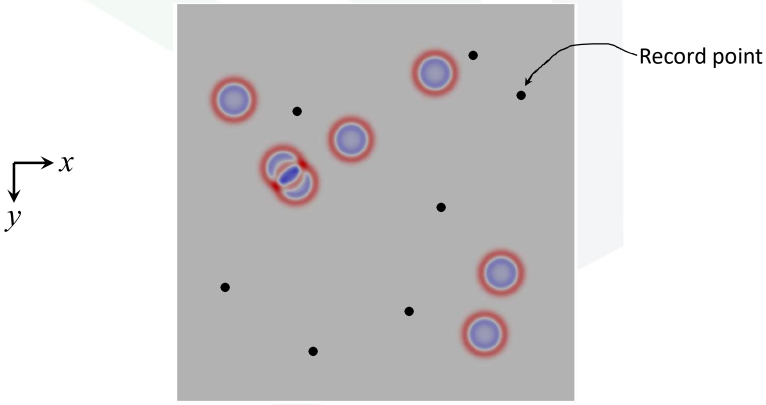
The Source

For band calculations in FDTD, we use simple dipole sources that are randomly polarized and randomly distributed throughout the unit cell. It is best to avoid locations that are obvious symmetry points. This is done to ensure that all possible modes are excited.



Record Points

Similarly, we record the response at multiple record points that are distributed randomly throughout the lattice like the source points.



Identifying the Bloch Mode Frequencies

First, we FFT the record arrays to calculate the power spectral density recorded at each record point.

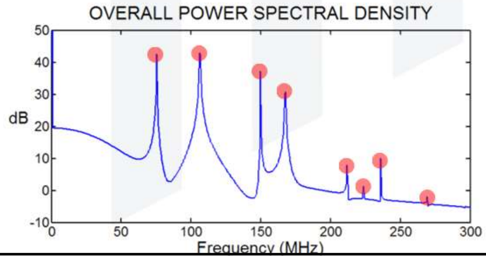
$$\mathrm{PSD}_p(\omega) = \left|\mathrm{FFT}\left\{E_z(t)\big|^p\right\}\right|^2 \qquad p \equiv \text{source }\#$$

Second, we add the power spectral densities from all the recorded points.

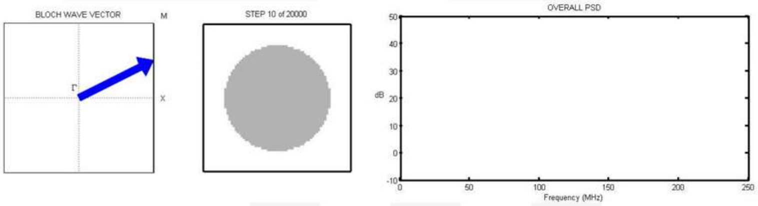
$$\mathrm{PSD}(\omega) = \sum_p \mathrm{PSD}_p(\omega)$$

Third, frequencies corresponding to Bloch modes are identified as sharp peaks in the overall PSD.

● indicates an eigen-frequency



Animation of Calculating Eigen-Frequencies

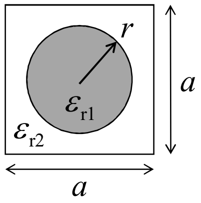


- An arbitrary Bloch wave vector was chosen for this simulation.
- Peaks are identified in the PSD by the red circles.
- A larger number of iterations is needed before the peaks can be identified accurately.
- Poor, or unlucky, selection of source and record points can fail to excite or detect certain bands.

$r = 0.35a$

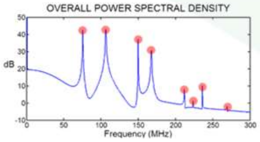
$\varepsilon_{\mathrm{r}1} = 6.0$

$\varepsilon_{\mathrm{r}2} = 1.0$

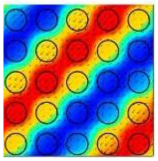


Calculating the Fields of the Bloch Modes

Step 1: Run a simulation and identify the eigen-frequencies of the modes you are interested in.



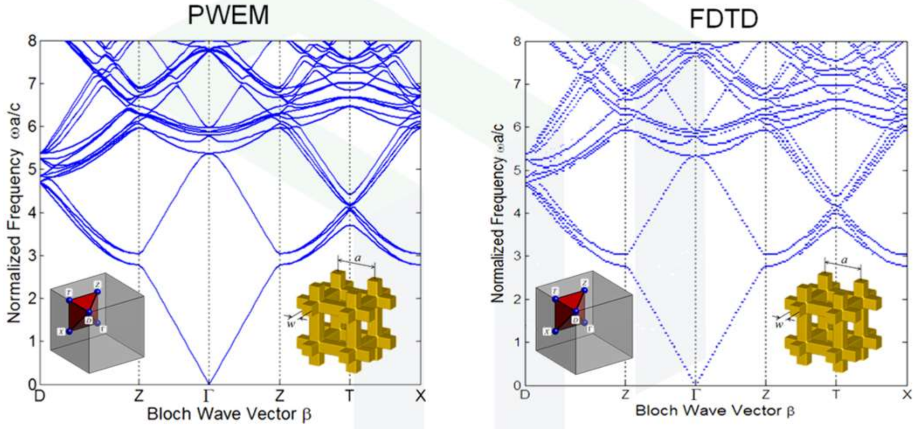
Step 2: Run a second simulation and calculate the steady-state field at each eigen-frequency of interest at each point throughout the grid.



Procedure for Calculating Band Diagrams

- Build unit cell on a grid
- Iterate over a list of Bloch wave vectors
  - Initialize random sources and record points
  - Run FDTD and record fields at record points
  - Compute overall PSD
  - Identify eigen-frequencies
- Plot the eigen-frequencies as a function of the Bloch wave vector
- You have now produced an electromagnetic band diagram using FDTD*!*

Example 3D Simulation

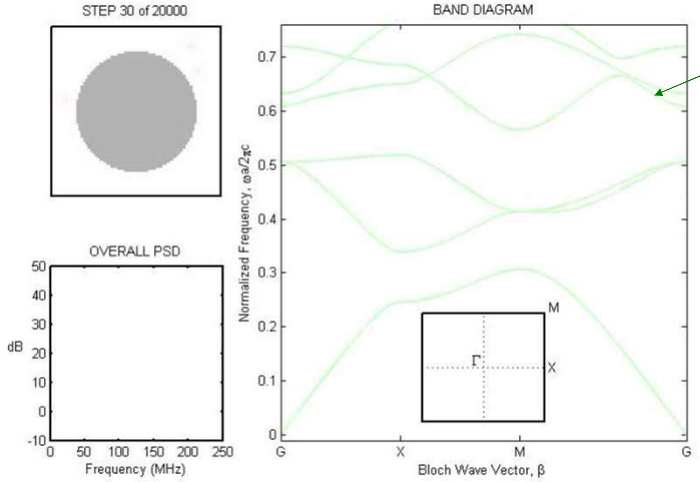


$$w = 0.1a$$

$$\varepsilon_r = 2.34$$

EMPossible

Animation of Band Diagram Construction Using FDTD



"Exact" bands calculated using the plane wave expansion method.

○ Eigen-Frequencies

EMPossible