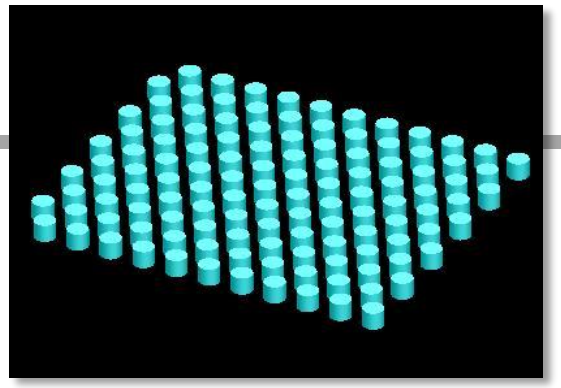


Bandstructure Calculations in FDTD Solutions

LUMERICAL SOLUTIONS INC.

Outline

Introduction

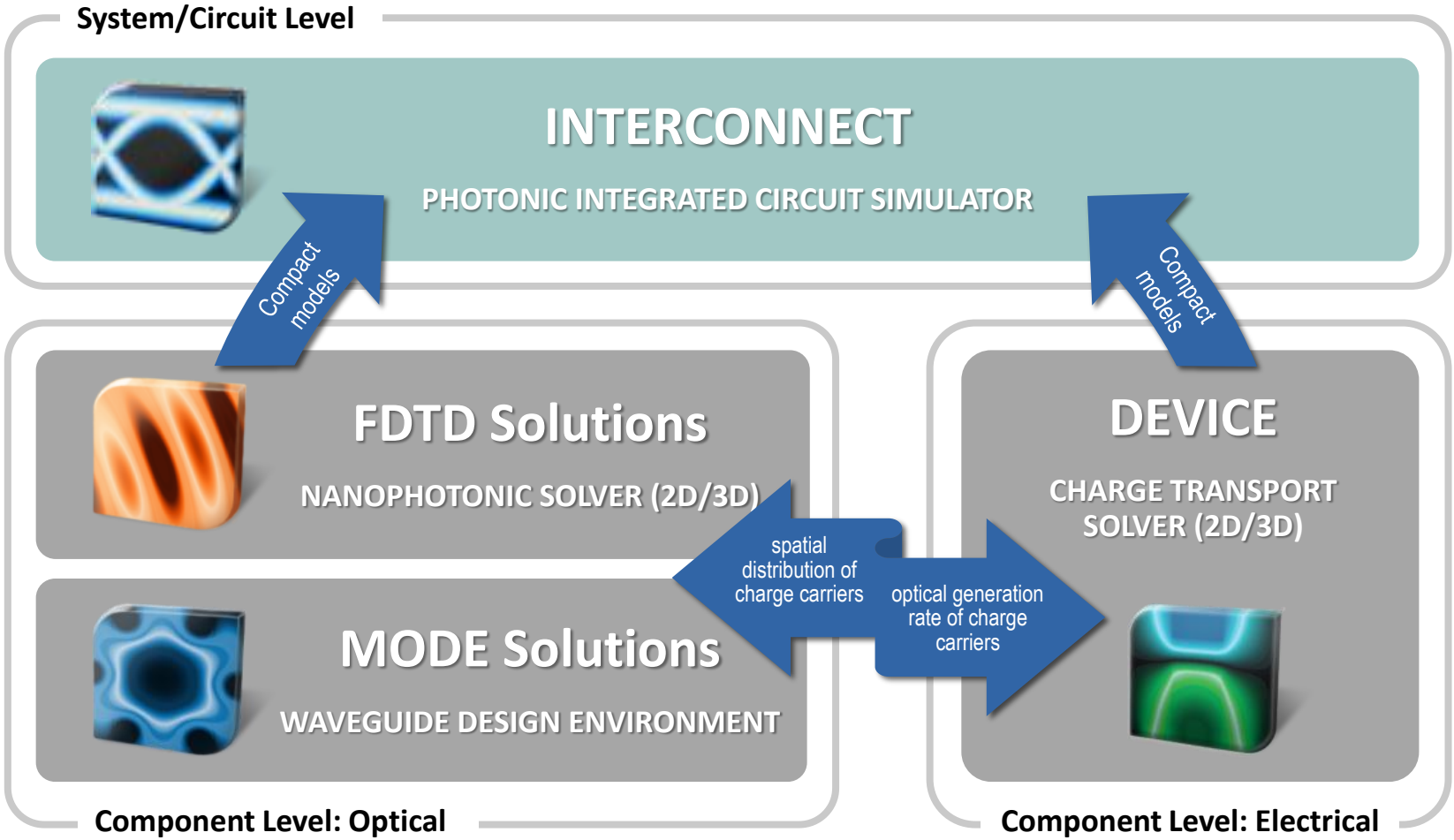
Simulation methodology
- Simulation setup
- Analysis

Demonstration (2D triangular lattice)

Simulations with loss
- Problems associated with loss
- Tips
- Example (1D chain of metallic spheres)

Q&A

Our Products



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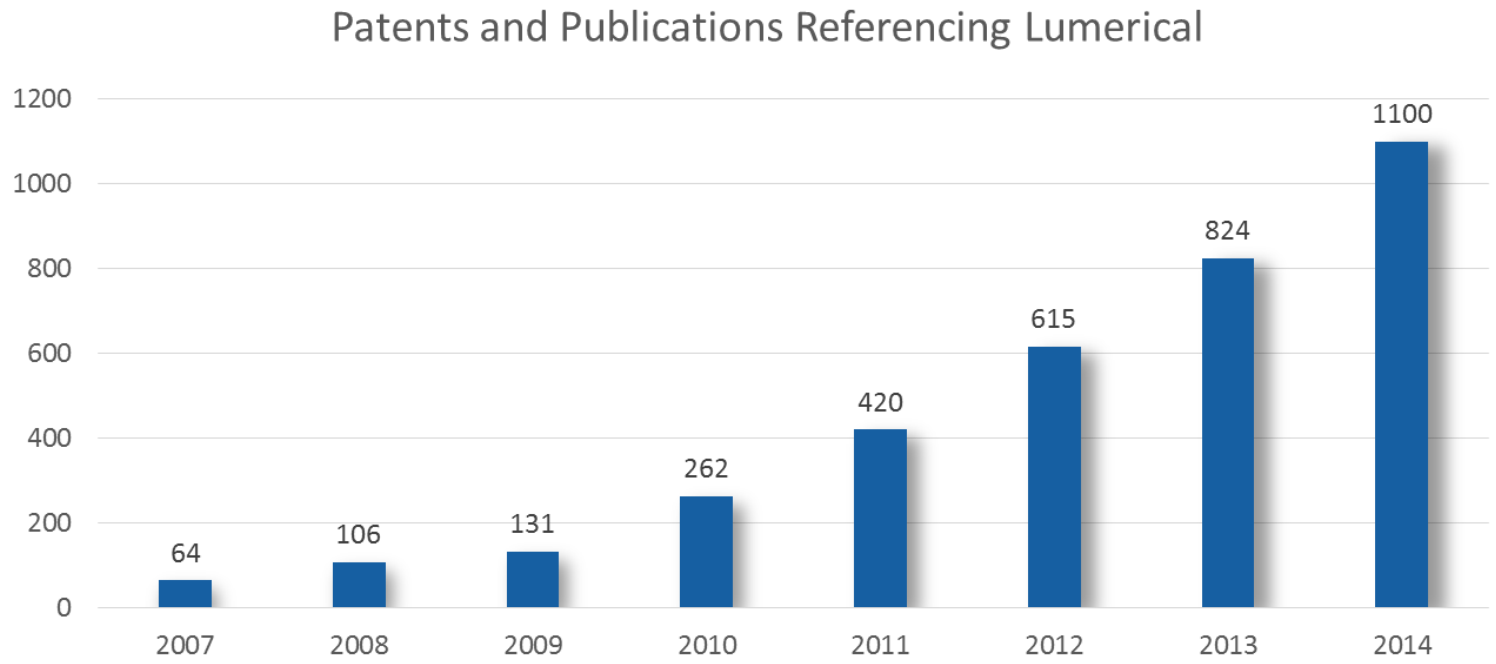
Lumerical empowers R&D professionals with best-in-class design tools and services to support the creation of better photonic technologies



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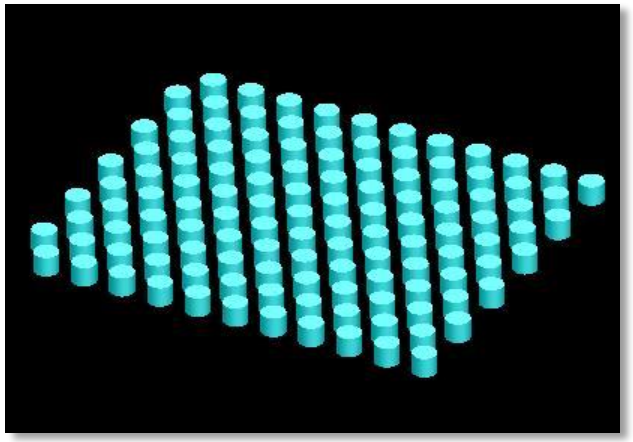
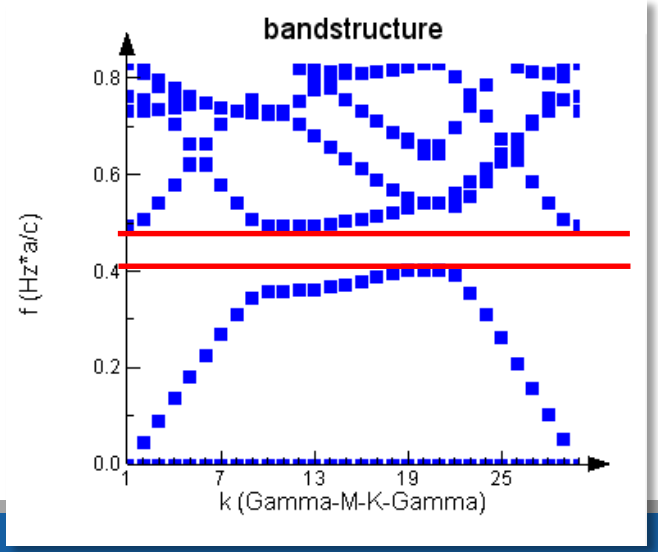
Introduction

Bandstructure (dispersion) plots can be calculated for structures which have periodicity in at least one dimension

Use this information to

- Find photonic band gaps (frequency ranges where light cannot propagate through the crystal in any direction)
- Plot Bloch mode profiles
- Determine loss and group velocity of a photonic crystal waveguide mode



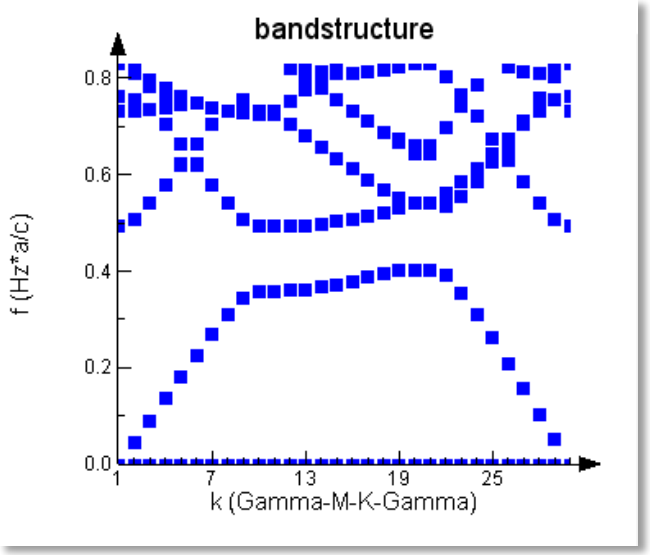


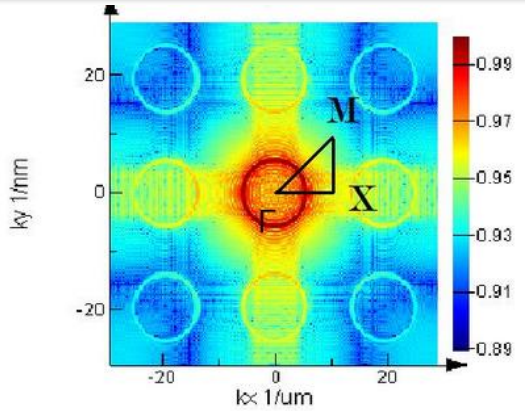
band gap

Introduction > Background

Bloch vectors, k

- Represent angles of light propagation within the structure
- All distinct modes of the structure occur for Bloch vectors within the first Brillouin zone of the reciprocal lattice of the structure
- Brillouin zone points that we sweep depend on the type of lattice
  - For more information about determining the Brillouin zone points see the text “Photonic Crystals: Molding the Flow of Light” by Joannopolous et al.





Simulated Brillouin zones

Introduction > General Method

Use dipoles to inject energy into the simulation region

Restrict the angle of propagation by using the boundary conditions

Light at frequencies that are not supported by the structure in the propagation direction will decay quickly while light that gets coupled into a mode of the structure will continue to propagate for a longer time

Use time monitors to record the fields over time

Bandstructure analysis group performs a Fourier transform analysis to determine frequencies of modes that are supported by the structure for a certain angle of propagation

Use the parameter sweep tool to modify the boundary conditions and sweep over range of propagation angles to get the final plot of band frequencies versus propagation direction

Introduction > FDTD

Finite Difference Time Domain (FDTD) is a state-of-the-art method for solving Maxwell's equations for complex geometries

- Few inherent approximations
- General technique that can deal with many types of problems
- Arbitrary complex geometries
- One simulation gives broadband results
- Not just for bandstructure calculation, but can also simulate other devices such as waveguides, photonic crystal cavities, etc.

Simulation Methodology > Overview

Simulation setup

- Parameterization
- Structure
- Simulation region
- Sources and monitors

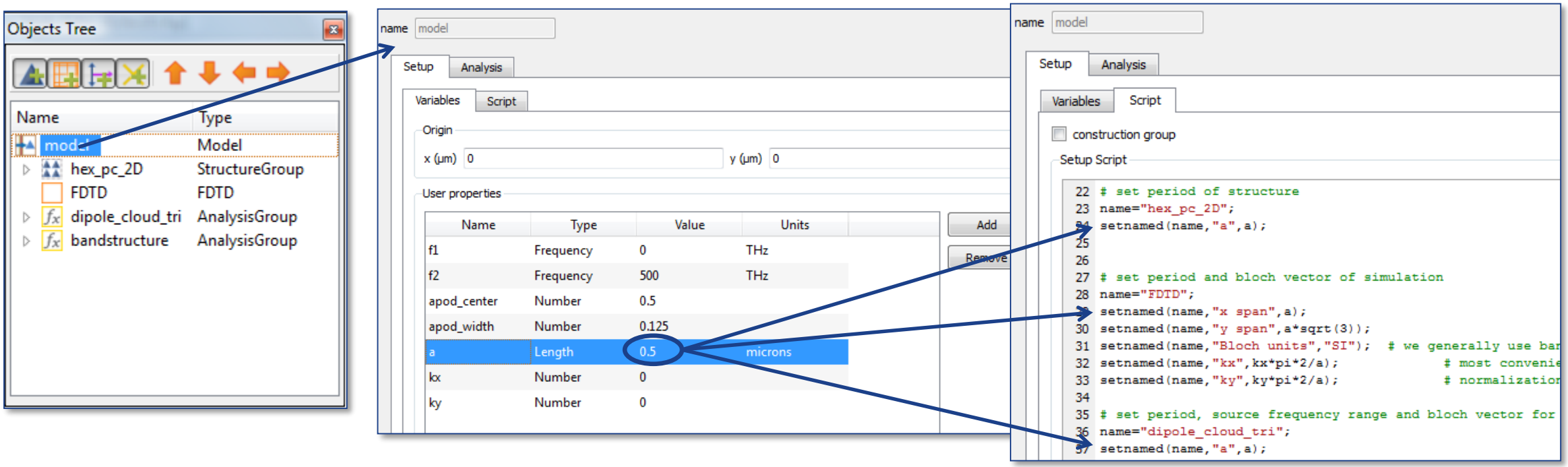
Calculations

- Fourier transform
- Summation of FFTs
- Sweep over k
- Collecting results

Simulation Methodology > Setup

Design parameterization

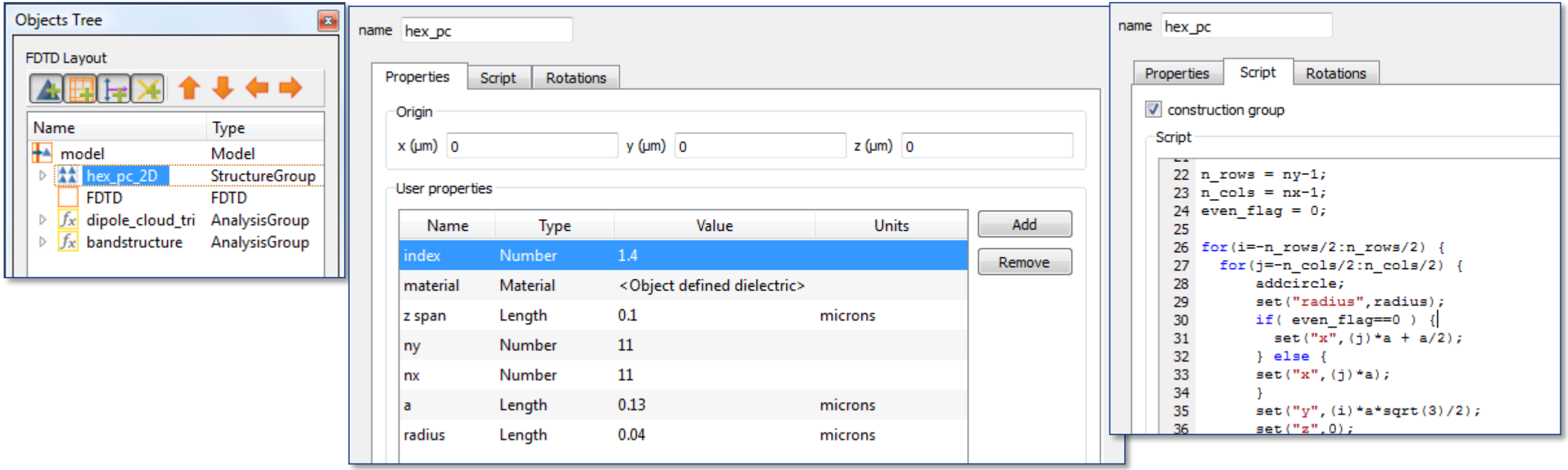
- Model analysis group



Simulation Methodology > Setup

Design parameterization

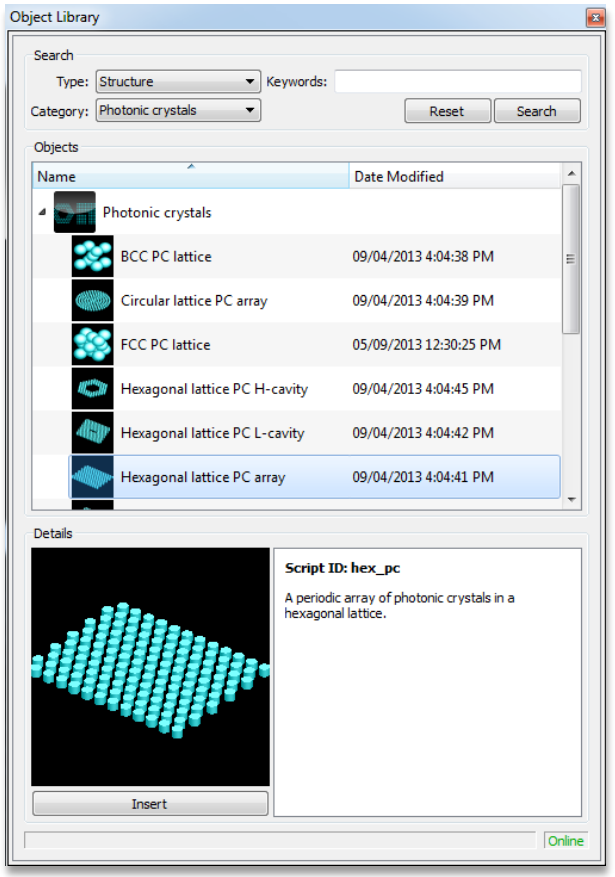
- Structure group

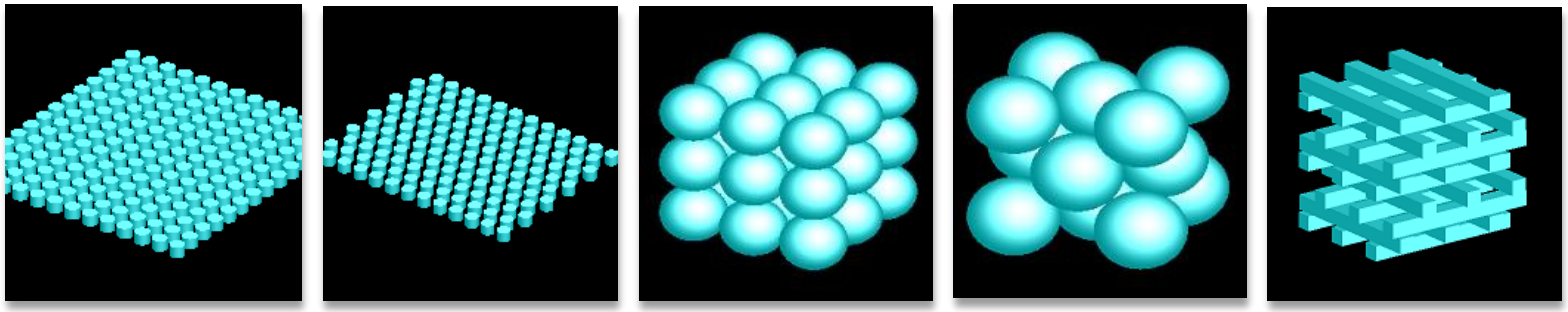


Simulation Methodology > Setup

Structure

- Only necessary to include one unit cell in the simulation for square, rectangular, body-centered cubic (BCC) lattices
- Simulate multiple unit cells for non-rectangular lattices eg. Triangular (hexagonal), face-centered cubic (FCC)
- Pre-made photonic crystal lattice structures can be inserted from the Object Library

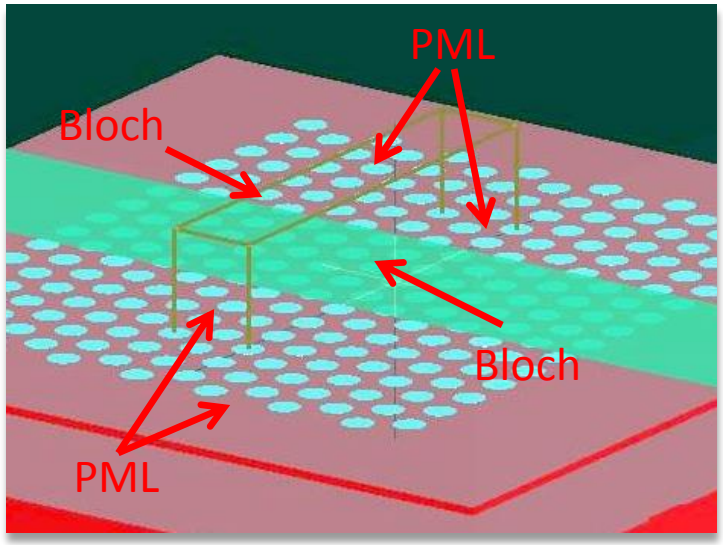


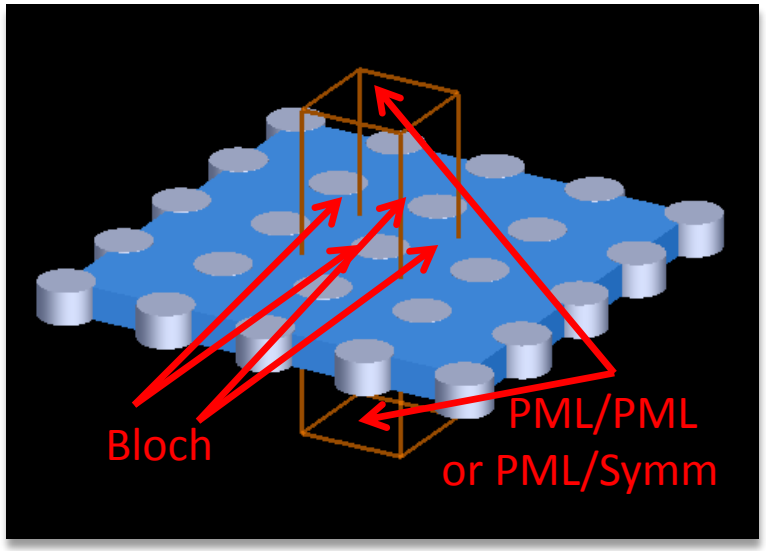


Simulation Methodology > Setup

Simulation region

- Bloch boundary conditions in directions where structure is periodic
- Band frequencies are determined by setting the Bloch vector, k
- PML boundary conditions in non-periodic directions with symmetry to isolate TE/TM modes

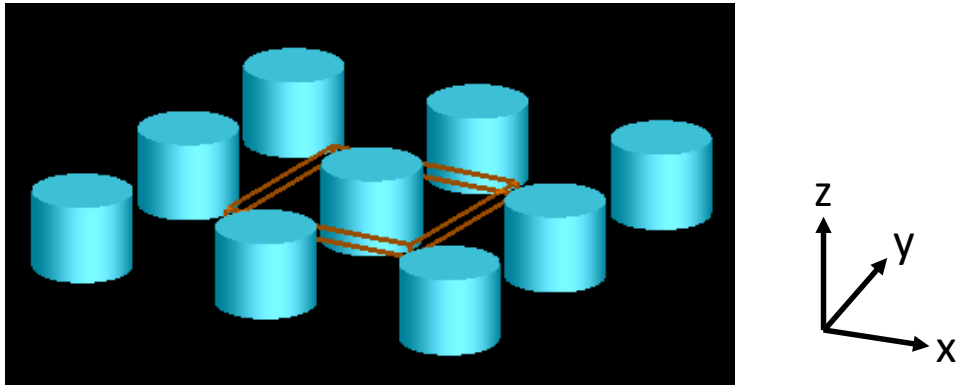




Simulation Methodology > Setup

Simulation region for out-of-plane bandstructure

- Bloch boundary conditions in the out-of-plane direction



- 2D periodic square lattice shown above
  - 3D simulation region one mesh cell thick in the out-of-plane direction (z-direction)
  - Bloch boundaries in z-direction allows us to set Bloch vector in out-of-plane direction
  - Periodic boundaries in periodic (x and y) directions

Simulation Methodology > Setup

Simulation region for non-rectangular lattices

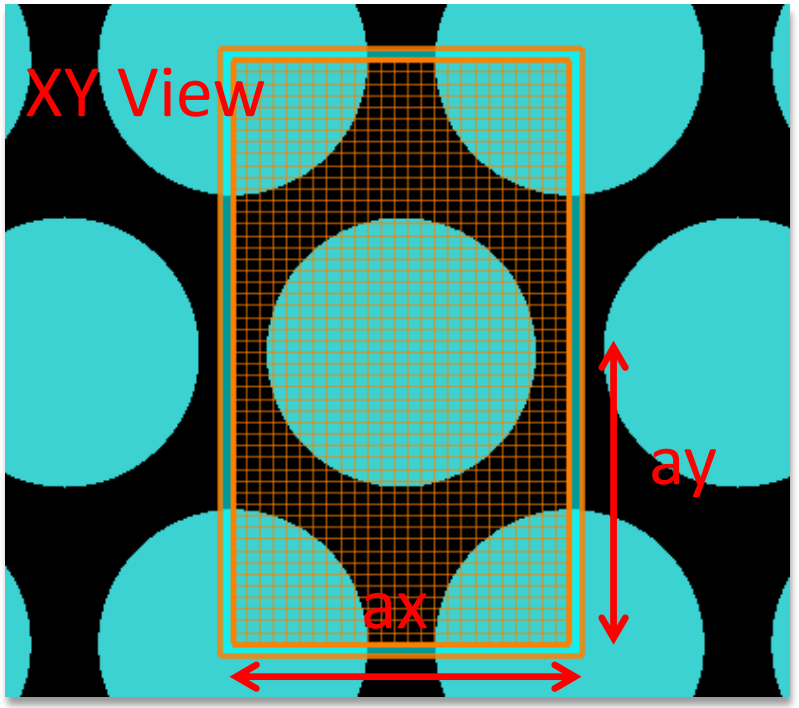
- FDTD simulation region is rectangular so for non-rectangular lattices, multiple unit cells can be included in the simulation to form a rectangular unit cell
- If multiple unit cells of the structure are included in the simulation region, mesh step size needs to be adjusted to include an integer number of mesh cells in each unit cell
  - Ensures that each unit cell is meshed the same way

Simulation Methodology > Setup

Simulation region for non-rectangular lattices

- Example: 2D hexagonal lattice
  - The smallest rectangular unit cell includes 2 unit cells of the hexagonal lattice
  - Lattice constant a
  - ax=a
  - ay=a*sqrt(3)/2
  - Set mesh step size in y-direction
    - Dx=ax/n
    - Dy=ay/m

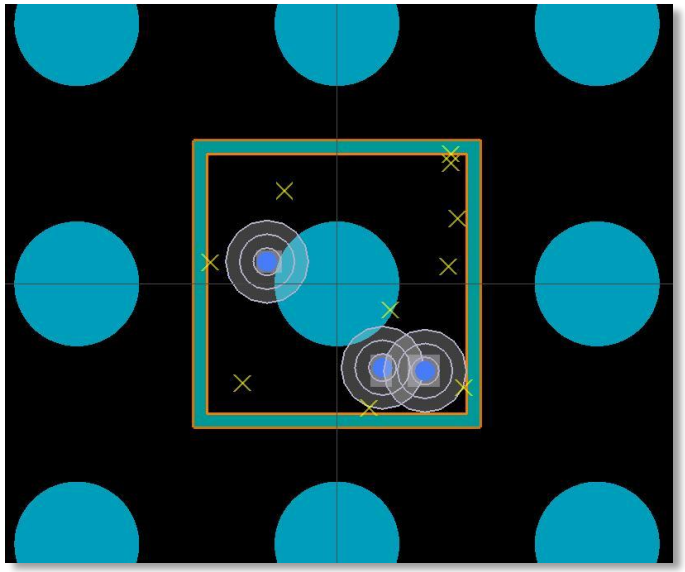
    where n,m are integers



Simulation Methodology > Setup

Sources and monitors

- Randomly positioned cloud of dipoles to excite all modes
  - 1 dipole at a single position and orientation may not excite all of the modes of the device since it may be located at a node position where energy will not couple into the mode
- Several randomly positioned time monitors collect fields over time



Simulation Methodology > Setup

Sources for non-rectangular lattices

- Matched dipoles in each unit cell of the structure inside simulation region (for non-rectangular lattices)
  - Phase matching condition

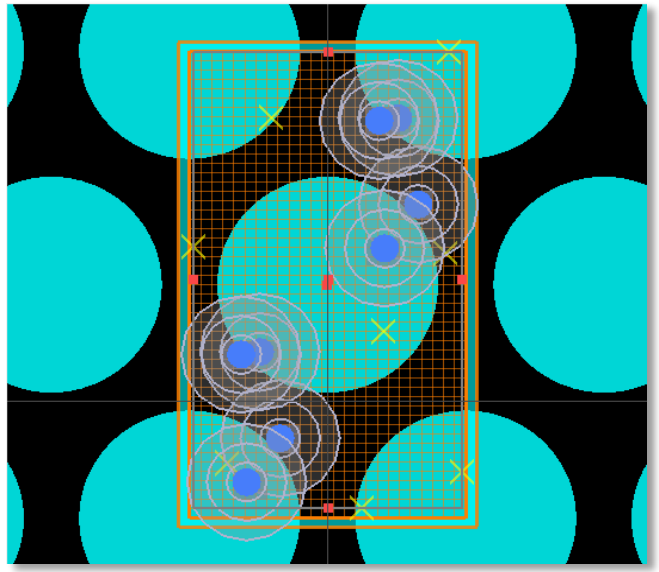
$$\Delta\theta = -\frac{180}{\pi}\vec{k}\cdot\Delta\vec{r}$$

where

$\Delta\theta$ = phase offset from reference dipole

$\vec{k}$ = simulation wave vector

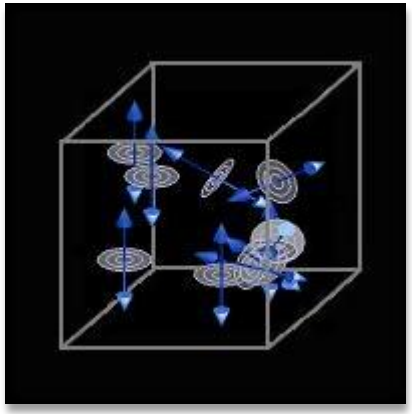
$\Delta\vec{r}$ = position offset from reference dipole



Simulation Methodology > Setup

Dipole cloud analysis group

- Insert from Object Library
- Specify lattice type and period as an input variables
- Setup script automatically sets up randomly positioned and oriented dipoles
- Matching dipoles are set up automatically for non-rectangular lattice types



Simulation Methodology > Setup

Summary of setup method

- Parameterize using Model analysis group and structure groups
- Use Bloch boundaries in periodic directions
- Random cloud of dipoles and monitors
- Rectangular lattices
  - Only need to include 1 unit cell in the simulation region
- Non-rectangular lattices
  - Include multiple unit cells that form the smallest rectangular unit cell
  - Each unit cell should be meshed the same way
  - Matching dipole positions in each unit cell with phase matching

Simulation Methodology > Calculations

Overview of calculation:

Step 1 – Fourier transform to get spectrum

Step 2 – Summation of spectra

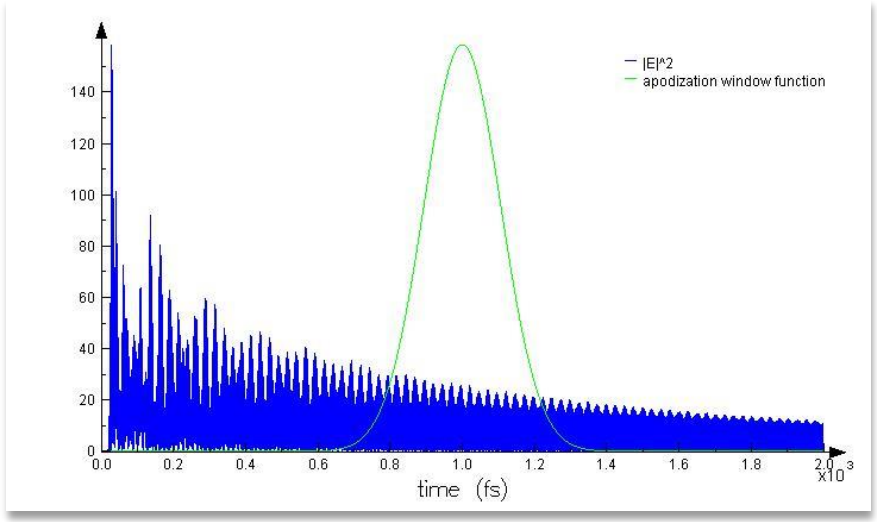
Step 3 – Repeat for all k

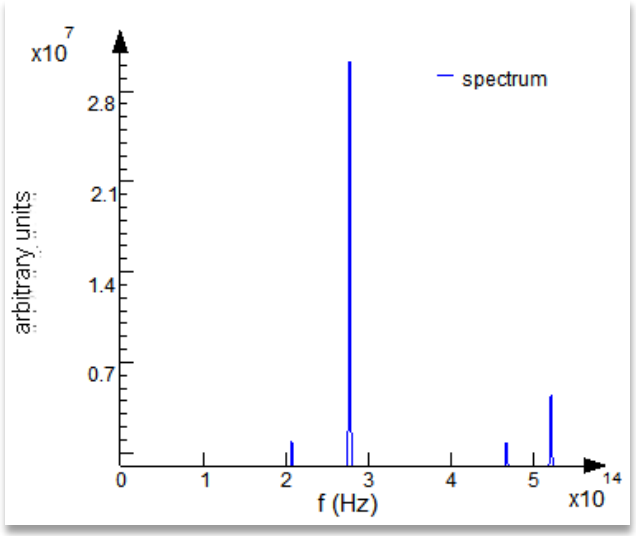
Step 4 – Collect sweep results, find resonances

Simulation Methodology > Calculations

Fourier transform

- Apply apodization to filter out start and end effects
  - Applies Gaussian windowing function to the time domain fields to exclude transient fields
  - Apodization parameters are set in the bandstructure analysis group
- Apply Fast Fourier transform (FFT) to apodized time signal to get the spectrum





Simulation Methodology > Calculations

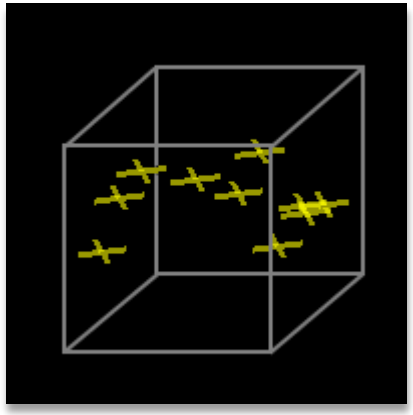
Summation of spectra

- Sum the Fourier transformed time signals from each field component of each time monitor
- Summing over several monitors ensures that all resonant frequencies are found even if one monitors is located in a node of a particular mode

Fourier transform and summation are done using the banstructure analysis group which can be inserted from the Object Library

Simulation Methodology > Calculations

Bandstructure analysis group

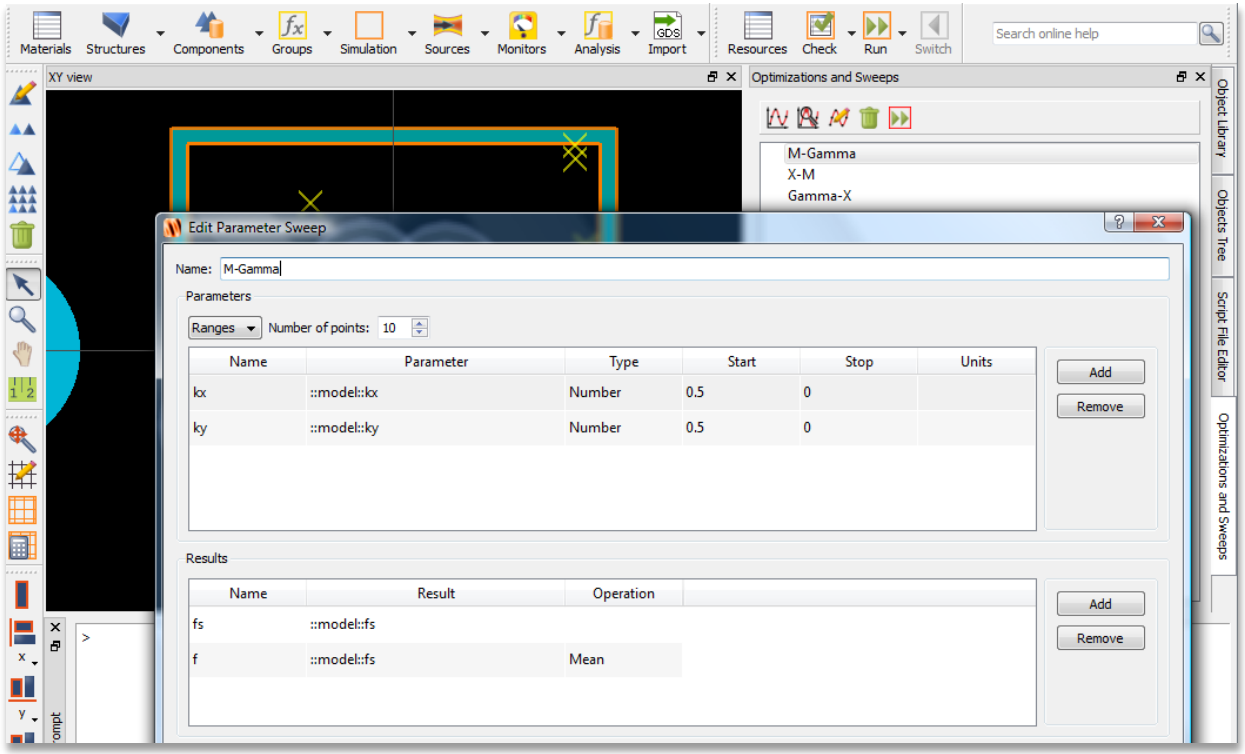


- Insert from Object Library
- Contains cloud of time monitors
- Set apodizations parameters
- Calculation spectrum
  - Gets field component from each time monitor
  - Applies apodization to the time signal based on input parameters
  - Takes Fourier transform
  - Sums results from each monitor
- Returns a dataset called “spectrum” which includes the spectrum data and corresponding vector of frequencies

Simulation Methodology > Calculations

Repeat for all k

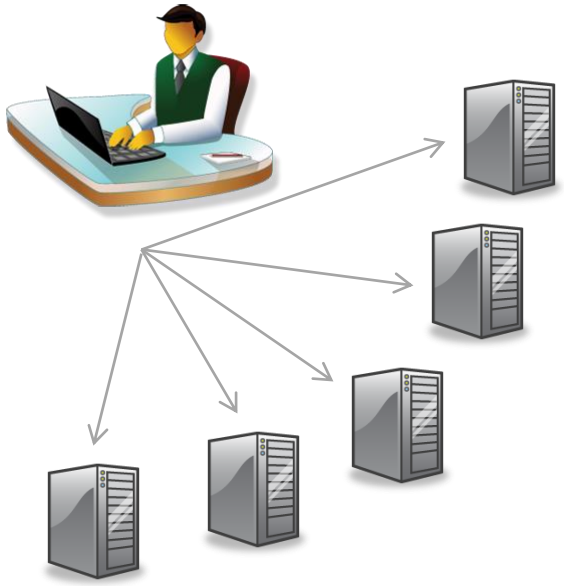
- One simulation provides the spectrum for a single Bloch vector
- Use the parameter sweep tool to run simulations over a range of Bloch vectors and collect the spectrum result for each simulation



Simulation Methodology > Calculations

Concurrent computing

- Parameter sweeps require running many simulations
- Send them to many different workstations
  - Each workstation can run in distributed computing mode using all cores

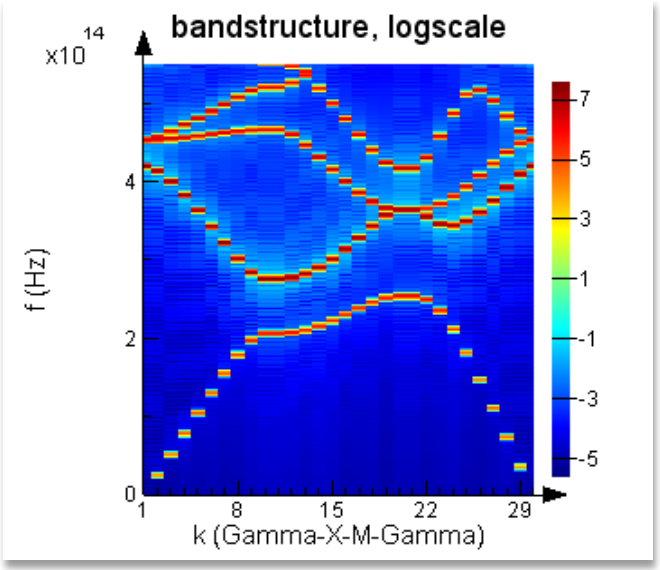


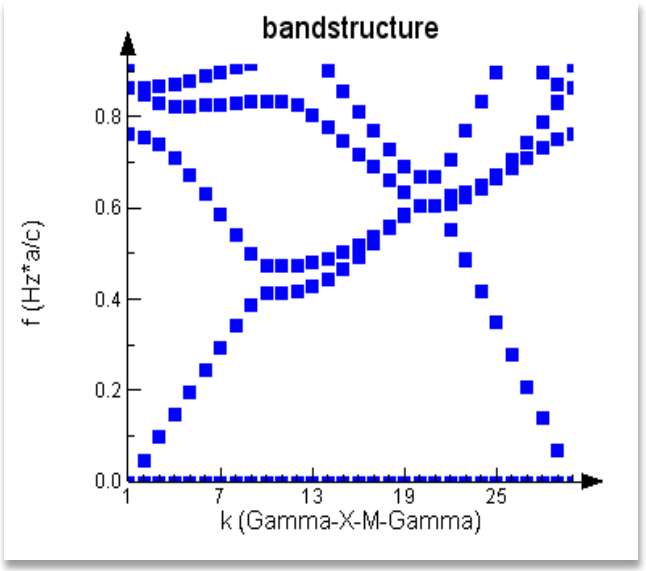
N computers means you can get your parameter sweep results N times faster!

Simulation Methodology > Calculations

Collect sweep results, find resonances

- Using a script file, collect the spectrum results from the parameter sweep
  - http://docs.lumerical.com/en/index.html?diffractive_optics_pc_bandstructure.html
- Directly plot the spectrum for all k
- Find locations of resonant peaks to plot band diagram
  - Set number of bands to look for and the tolerance in the script file settings





Simulation Methodology > Calculations

```
# User defined settings:
tolerance = 1e-4;
num_band = 10;

ay = getnamed("::model","ay");

# simple imaging
sweepname="ky";
spectrum=getsweepresult(sweepname,"spectrum");
f=c/spectrum.lambda;
fs=spectrum.fs;
ky=spectrum.ky_simulation;
image(ky,f,transpose(fs),"ky","f (Hz)","bandstructure, linearscale");
image(ky,f,transpose(fs),"ky","f (Hz)","bandstructure, logscale", "logplot");

# plot bandstructure
bandstructure=matrix(num_band,length(ky));
f_band = matrix(num_band);
for(i=1:length(ky)) {
  #use findpeaks to find the maximum peaks
  temp = findpeaks(fs(1:length(f),i),num_band);

  #collect data for any peaks that are more than 'tolerance' of the maximum peak
  minvalue = fs(temp(1),i)*tolerance;
  for(bandcount = 1:num_band) {
    if( fs(temp(bandcount),i) > minvalue) {
      f_band(bandcount) = f(temp(bandcount));
    }
  }
f_band_norm = f_band*ay/c;  # normalize the frequency vector
bandstructure(1:num_band,i)=f_band_norm;
}

# plot bandstructure
plot(ky,transpose(bandstructure),"k","f(Hz*a/c)","bandstructure","plot points");
```

Set number bands to look for and tolerance

Collect sweep results

Plot spectrum versus Bloch vector

Loop over each Bloch vector and look for peaks in the spectrum

Plot extracted bandstructure result

Simulation Methodology > Calculations

Summary of calculation methodology:

- Apply apodization to time signals
- Fourier transform apodized time signal to get spectrum
- Sum spectra from each monitor

} Performed by bandstructure analysis group

- Run parameter sweep over a range of Bloch vectors
- Collect spectrum result from each point in the sweep
- Find peaks in the spectrum at each k to get bandstructure diagram

Example > 2D Hexagonal Lattice

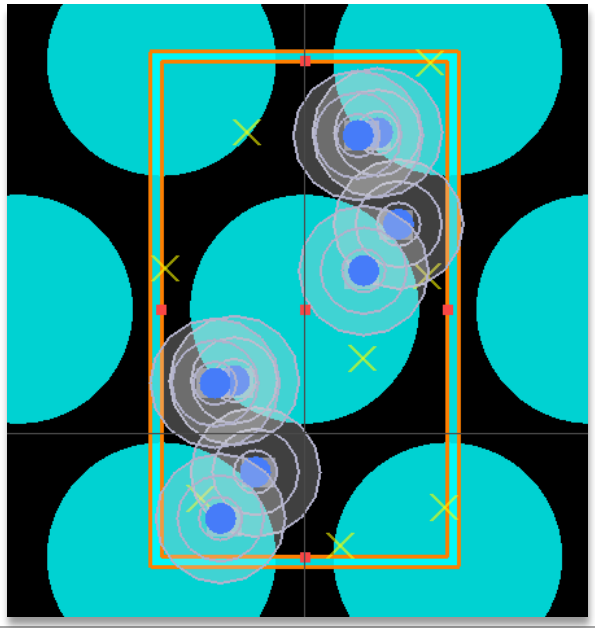
Hexagonal (triangular) lattice of index n=1 circles with background index n=2

Simulation region covers 2 unit cells

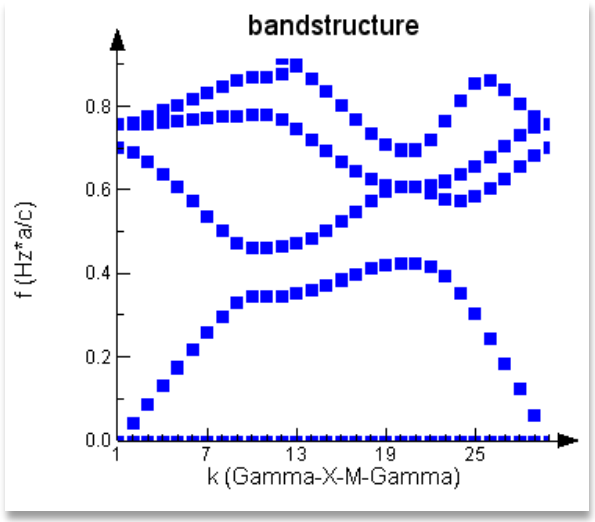
Matching dipoles in each unit cell with phase offset

TE or TM modes excited based on dipole orientation

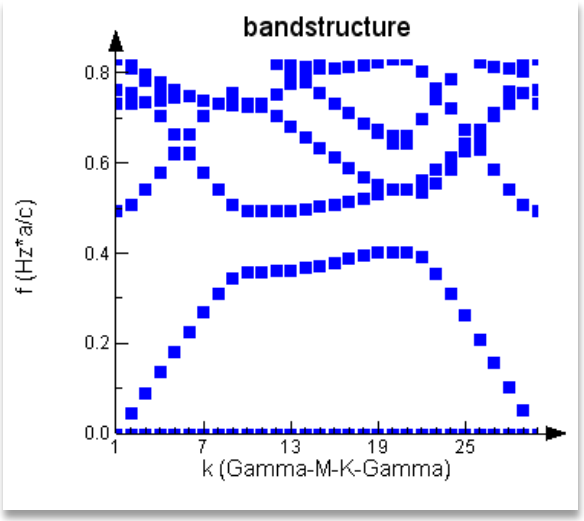
Script file collects sweep results, extracts and plots bandstructure



TM case



TE case



Simulations With Loss

Problems associated with loss

Tips for lossy simulations

- Source and monitor placement
- Apodization settings
- Symmetry boundary conditions
- Source spectrum
- Tolerance

Particle chain example

Simulations With Loss > Problems Associated

Sources of loss

- Absorbing materials
- Radiation

Problems associated with loss

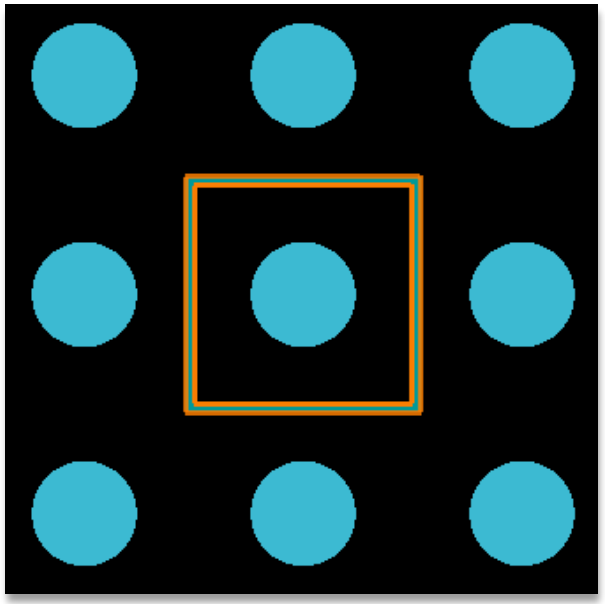
- Resonant fields decay quickly
  - Useful part of the time signal is shortened
- Fourier transform of time signal is noisy
  - Difficult to extract resonant peaks

With more deliberate setup, we can increase the strength of the signal from modes that we are interested in and decrease the signal from other modes and noise so we can more easily extract a clear bandstructure diagram

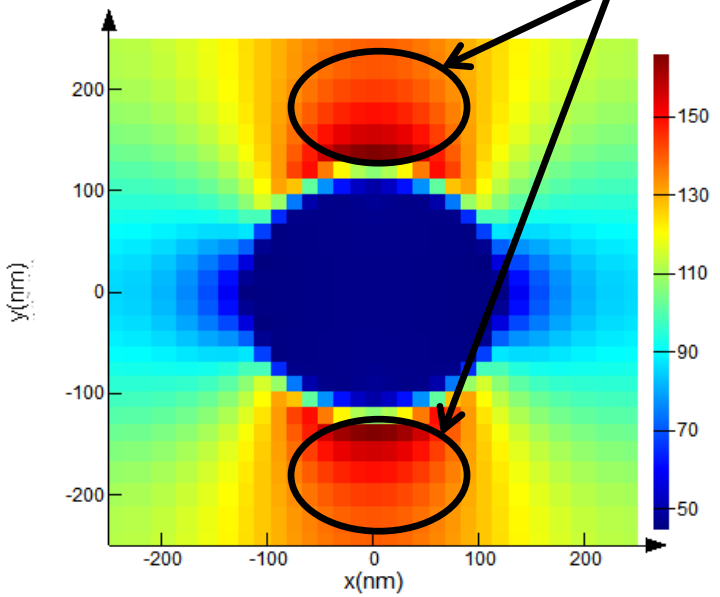
Simulations With Loss > Tips

Source and monitor placement

- Place source in an area where you expect fields to be strong for the mode or modes you are interested in
- Similar placement of monitors



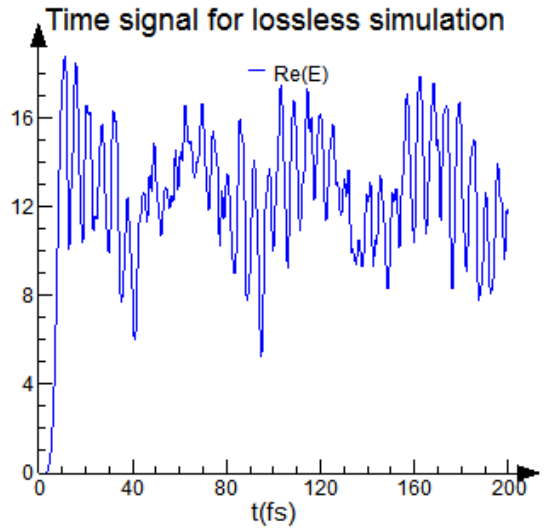
Place sources and monitors in strong modal field regions



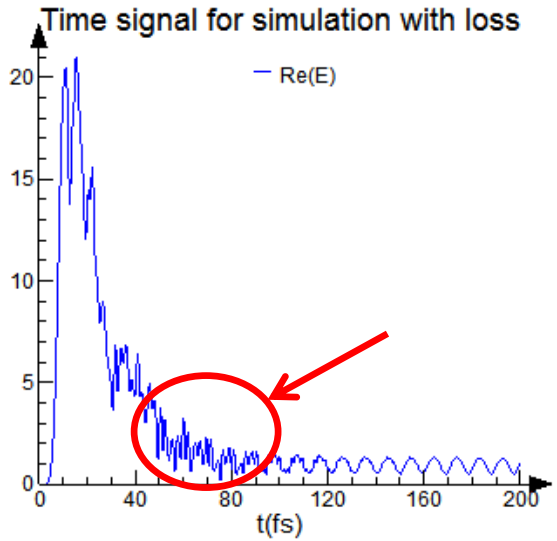
Simulations With Loss > Tips

Apodization settings

- Modify the center and width of the apodization window
  - These settings can be found in the bandstructure analysis group
- Use a movie monitor to help determine the time and duration of the resonance



Signal does not decay by the end of the simulation so any portion of signal is okay

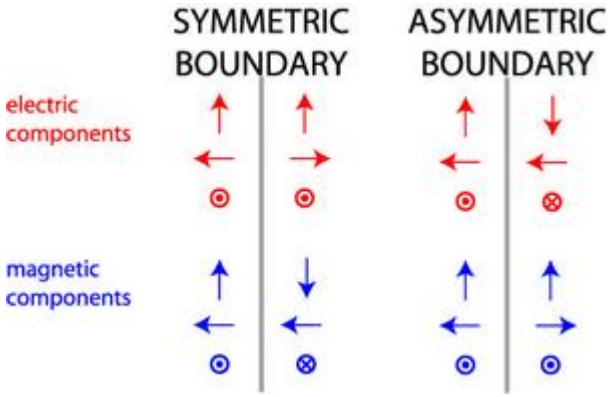


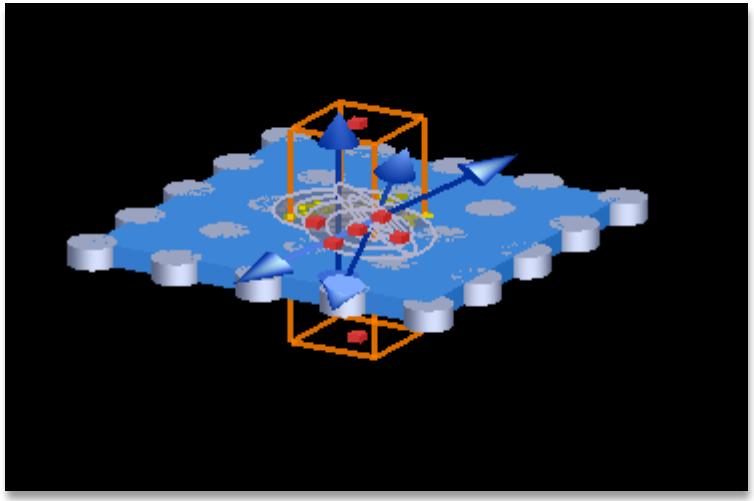
Strength of signal from mode of interest may be strongest in this particular stretch of time

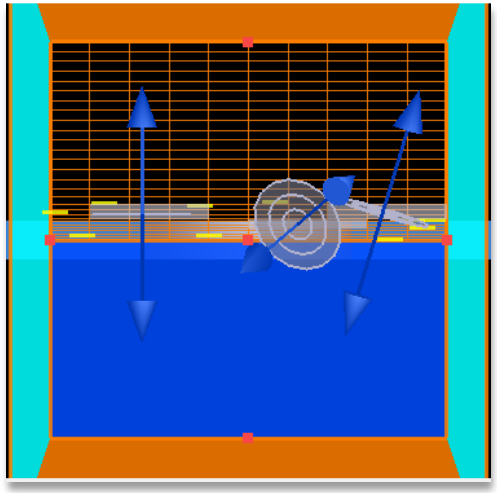
Simulations With Loss > Tips

Symmetry

- Use symmetric/anti-symmetry boundary conditions to isolate modes of interest



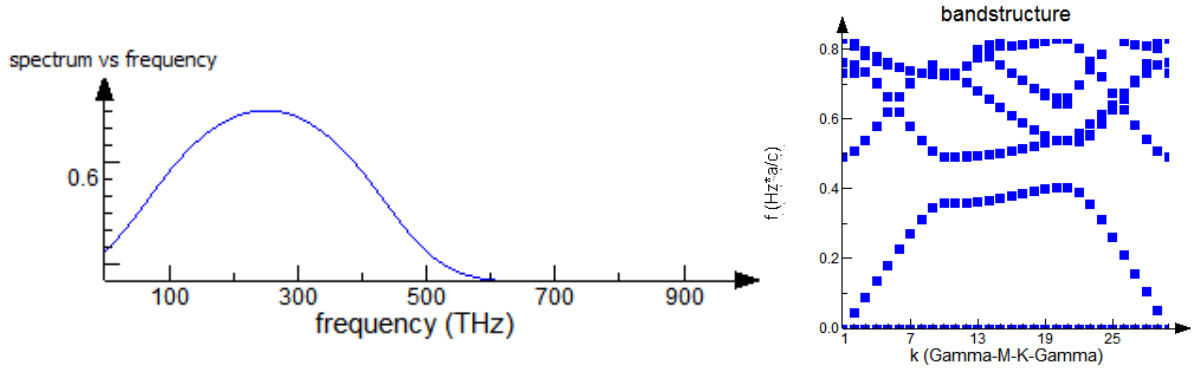


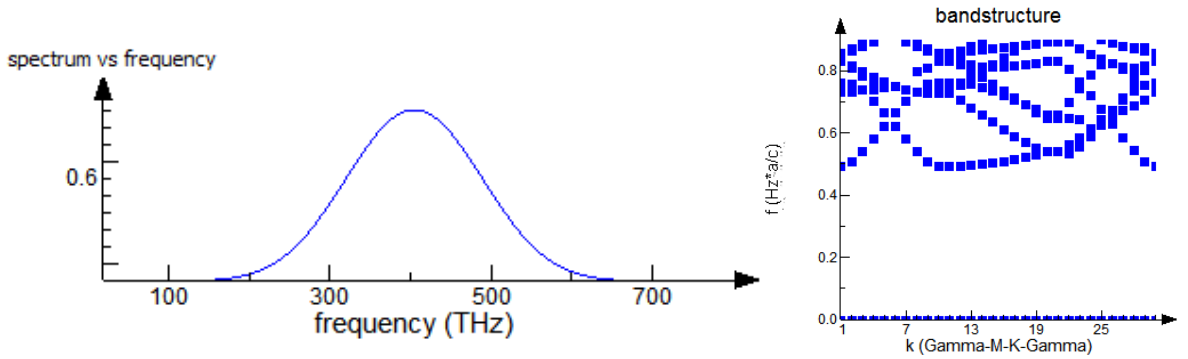


Simulations With Loss > Tips

Source spectrum

- A broadband source pulse is used by default
- Modify the source center frequency and bandwidth to overlap with the expected frequency of the bands so more energy is coupled into the modes of interest

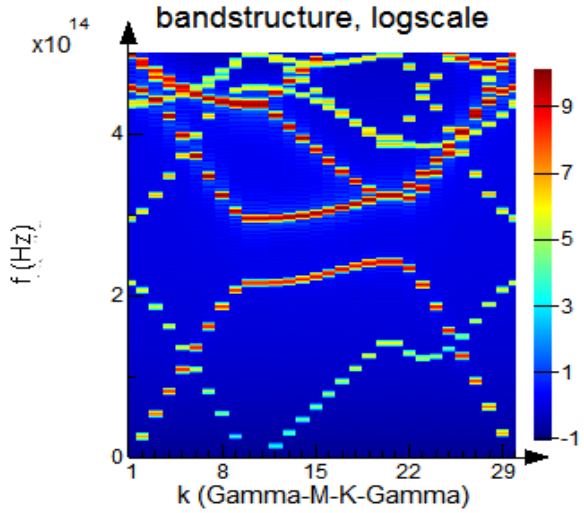


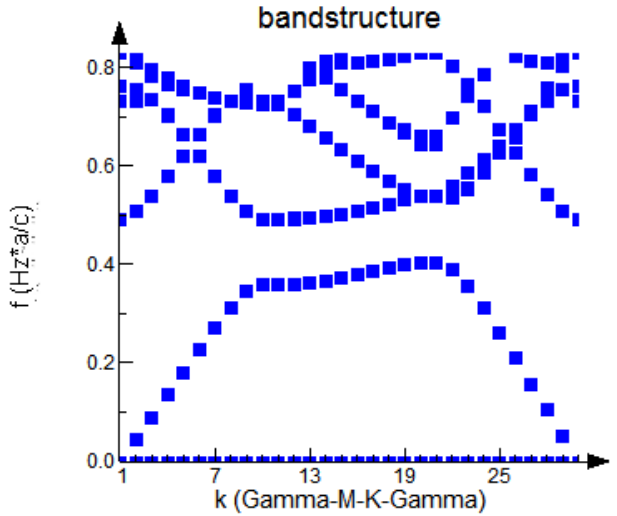


Simulations With Loss > Tips

Tolerance

- Peaks in spectrum with heights below tolerance are not included in the extracted bandstructure plot
- In other words, peak height must be larger than
  tolerance*(max peak height)
- Lower value of tolerance if bands can be seen clearly in the plot of fs vs k before the bandstructure plot is extracted

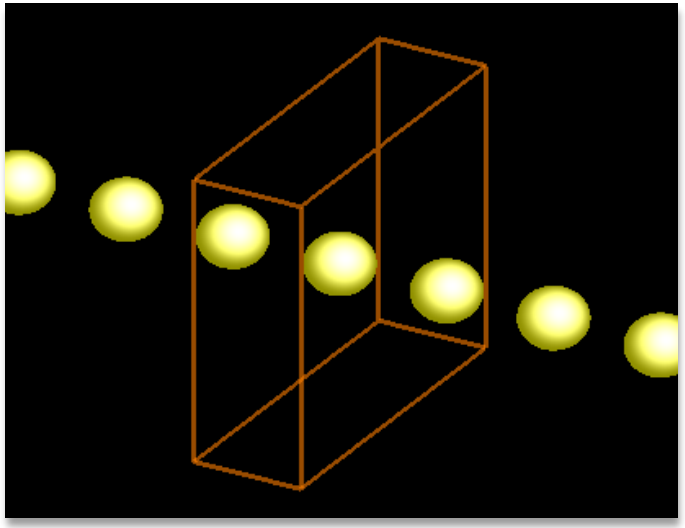




Example > Particle Chain

1D chain of gold spheres periodic along x-axis

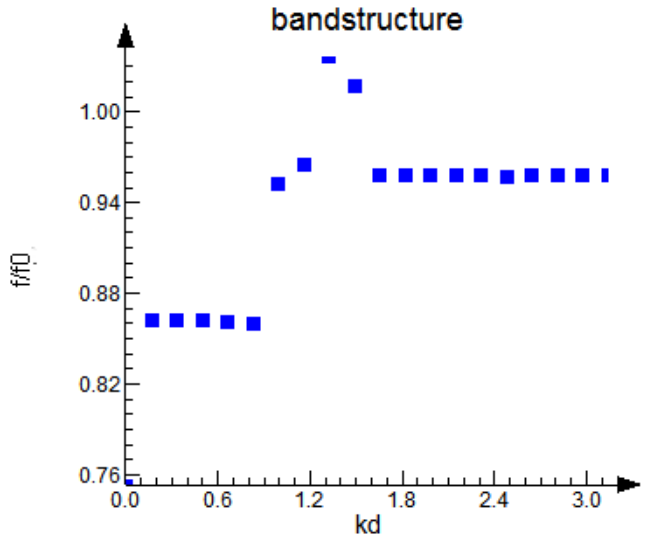
Goal is to plot the band corresponding to the longitudinal mode of the structure which has strong fields in the region between the spheres



Example > Particle Chain

With the typical method of using random cloud of dipoles we are not able to clearly extract the band of interest

- Transverse modes of the chain are also excited
- Not enough energy is coupled into the longitudinal mode to extract a clear resonance peak

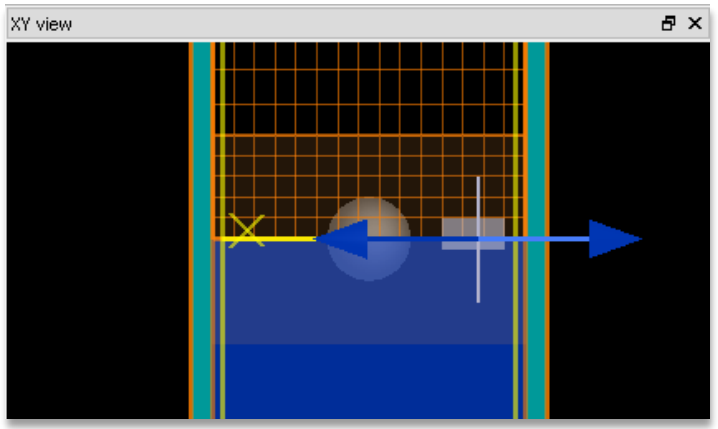


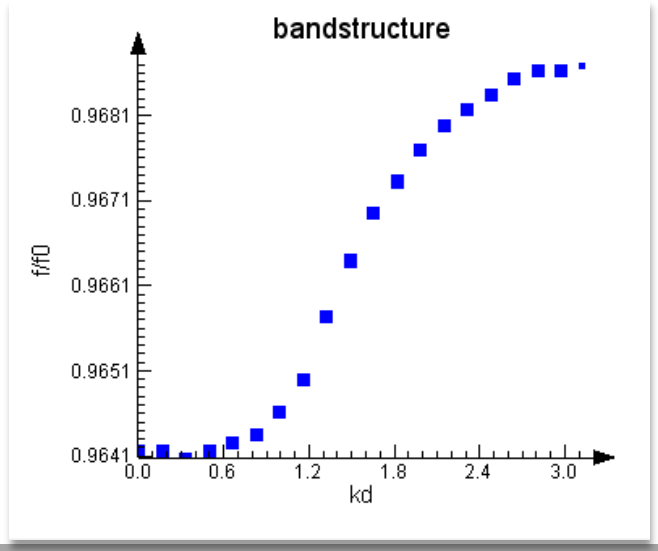
Example > Particle Chain

Setup strategy

- Single dipole and time monitor placed along the x-axis in the region between spheres
- Mode of interest has symmetry across y=0 and z=0 planes so use symmetry boundary conditions in y and z directions

More energy couples into the longitudinal mode resulting in stronger peaks compared to other modes





Summary

Challenge	Solutions and best practices
Accuracy	Full vectorial 3D Maxwell solver can capture all physical effects
Complicated simulation methodology	Bandstructure and dipole cloud analysis groups from Object Library include setup and analysis scripts to carry out much of the analysis automatically
Complex 3D geometries	Parameterize designs Use pre-made structure groups from Object Library
Simulation time	Take advantage of periodicity to reduce size of simulations Use distributed parallel computation to take advantage of modern hardware
Broadband simulations	Time domain simulation gives broadband results
Parameter sweeps	Use concurrent computing to use all your available computer resources optimally

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