How to Simulate and Optimize Microwave, THz and Optical Metamaterials

Lumerical Solutions, Inc.
Outline

- Introduction
  - About Lumerical
  - Metamaterials and their applications
  - Challenges in simulation

- Simulation methodology
  - Groups, parameterization
  - Sweep and optimization
  - Material fitting and MCM
  - Source and boundary conditions

- Examples and demos

- Simulation tips

- Questions and Answers
About Lumerical

Our Technology

MODE Solutions

FDTD Solutions

INTERCONNECT

DEVICE
About Lumerical

Dedicated to providing leading edge nanophotonics design software

- Our customers have published thousands of papers in leading journals and magazines
- There are more than 100 metamaterial publications

FEATURED PUBLICATION COUNT

<table>
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<tbody>
<tr>
<td>2008</td>
<td>68</td>
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<td>2009</td>
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<td>2010</td>
<td>161</td>
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<td>2011</td>
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Introduction

What is a metamaterial?

- Natural materials exhibit only a small part of electromagnetic properties available in theory
- Electromagnetic metamaterials are artificially structured materials that are designed to interact with and control electromagnetic waves (D.R. Smith)
  - Gain their properties from an artificial “unit cell” or “atom” to create effective macroscopic behaviors
    - Sub-wavelength and periodic structure
  - Can be constructed to have a user-designed EM response
    - Can achieve negative or unnaturally-high index of refraction, etc
  - Are typically designed for applications in microwave (MHz~GHz), THz (0.1-30 THz), or optical ranges (UV to IR)
Introduction

Potential applications

- Sensing
- Imaging
- Communications
- Cloaking
- and more…
Simulations are essential to predict the performance of such devices because we cannot obtain accurate results using analytic methods.

Simulations give the opportunity to cheaply and quickly test ideas, optimize designs and solve problems:

- Expensive and time-consuming to build prototypes.
- Design optimization is challenging and results are not always intuitive.

Why simulate metamaterials?
Simulation Challenges

- Complicated simulation methodology
  - Complex device geometry with many sub-wavelength features
    - The devices can have features sizes that are orders of magnitude smaller than the wavelength
  - Source modeling
    - Broadband
    - Circular polarization
  - Material dispersion
    - Usually metals are involved
  - Challenging post processing to extract key parameters
    - S parameters
    - Effective bulk properties
Introduction

What do we want to calculate?

- S parameters
- Effective material parameters
  - Refractive index
  - Permittivity
  - Permeability
- Transmission and reflections
- Scattering and absorption cross sections
- Polarization effects such as circular dichroism
- Bandstructure
- ...

...
Introduction

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

- Few inherent approximations = **accurate**
- A very general technique that can deal with many types of problems
- Arbitrarily complex geometries
- One simulation gives broadband results

We will show how FDTD Solutions can be used to simulate metamaterials in different frequency ranges
Simulation methodology

- Parameterization and groups
- Material properties
- Unit cell simulations with proper BCs
- Source setup for different (circular) polarizations
- Parameter extraction
- Parameter sweeps and optimization
Simulation methodology

Design parameterization

- Essential for
  - Reproducibility
  - Easy parameter sweeps
  - Optimization

- Lumerical’s hierarchical group layout and script based parameterization makes almost anything possible

- It is worth the initial investment!
Simulation methodology

Grouping allows for parameterization of the simulation.
Simulation methodology

Structure groups

```
# choose the parameters that define the structure
# Other parameters from the Chen paper
L = 3e-6;
S = 2e-6;
D = 10e-6;
W = 4e-6;

# choose the number of periods to layout (should be odd
Nz = 3;
Nx = 3;

for (j=1:Nz) {
    ox = x*(i-(Nz+1)/2);
    oy = y*(j-(Nz+1)/2);
    address;
    set("name","substrate");
    set("material","dielectric");
    set("x",ox);
    set("y",oy);
    set("w",S);
    set("h",W);
    set("xmin",-L/2);
}
```
Parameter extraction

S parameter analysis group

- Insert from our object library
  - Automatically calculates S parameters and effective bulk properties
Simulation methodology

Analysis groups

Obtain the desired results
Material properties

How we model materials depends on the frequency range

- In the MHz/THz range we can use simple material models
  - Metals are ideal
    - The skin depth is effectively 0 and can be ignored
    - We can use a Perfect Electrical Conductors (PEC) approximation

- In the optical range, material dispersion is critical
  - Mesh size smaller than the skin depth
  - Use **Multi-Coefficient Model** MCM
Material properties – dispersive materials

- For dispersive materials
  - Well-known frequency domain relationship
    \[ \vec{D}(\omega) = \varepsilon(\omega)\vec{E}(\omega) \]
  - Users can define their own model, or import from experimental data (real and imaginary \( \varepsilon(\omega) \))
  - FDTD is a time domain technique: relationship?
    \[ \vec{D}(t) = \varepsilon(t) * \vec{E}(t) = \int_{0}^{t} \vec{E}(t')\varepsilon(t - t')dt' \]
  - Need analytical model to present dispersive properties
Material properties – dispersive materials

- Common solutions are Lorentzian or Drude models
  - Often insufficient for real materials
- Lumerical’s **Multi-Coefficient Model** (MCM) can solve for materials with arbitrary dispersion such as GaAs, Au, Al, etc.
Simulation methodology

- Metamaterials are periodic: use a unit cell with periodic boundary conditions

Boundary conditions

- For normal incidence, periodic BCs are used.
- For angled incidence, Bloch BCs must be used.
  - Note about wavelength dependent angle of injection.
- To increase simulation efficiency, using symmetric/anti-symmetric BCs by taking source polarization into consideration.
Sources

- Plane wave source is inherently linearly polarized in FDTD
- To create a circularly polarized source:
  - Using two orthogonal linearly polarized sources with 90 degree phase difference in one simulation file: circular polarization, or
  - Using two orthogonal linearly polarized sources in two separated simulation files: any elliptical polarization can be analyzed

Parameter extraction

S parameters

- Scatter parameters describe a 2X2 transmission line or network behaviors:

\[
\begin{pmatrix}
    b_1 \\
    b_2
\end{pmatrix} =
\begin{pmatrix}
    S_{11} & S_{12} \\
    S_{21} & S_{22}
\end{pmatrix}
\begin{pmatrix}
    a_1 \\
    a_2
\end{pmatrix}
\]

a: input signals
b: output signals
Parameter extraction

- **S parameters**

- S parameters are the complex amplitude reflection and transmission coefficients

  - $S_{21} = \frac{E_{\text{transmitted}}}{E_{\text{incident1}}}$
  - $S_{11} = \frac{E_{\text{reflected}}}{E_{\text{incident2}}}$

  - If there is diffraction to more than 1 order, more advanced analysis is necessary

- The S-parameters are directly proportional to the electric fields
  - $S_{21} = \frac{E_{\text{transmitted}}}{E_{\text{incident1}}}$
  - $S_{11} = \frac{E_{\text{reflected}}}{E_{\text{incident2}}}$
  - If there is diffraction to more than 1 order, more advanced analysis is necessary
Parameter extraction

- Ideally, the fields would be recorded on the edge of the unit cell.
- In practice, measurements must be done some distance from the metamaterial. We must compensate for phase accumulated between the metamaterial and measurement points.
  - Phase accumulated from S to R: \( k(r_s + r_r) \)
  - Phase accumulated from S to T: \( k(r_s + r_t) \)
Parameter extraction is difficult because the functions are complex and multi-valued. Selecting the correct root and branch is difficult.

The S-parameter extraction analysis object in our Object library uses the extraction technique for a homogeneous system described in


Homogeneous system

\[ n = \frac{1}{kd} \cos^{-1} \left[ \frac{1}{2S_{21}} (1 - S_{11}^2 + S_{21}^2) \right], \]  \hspace{1cm} (9)

\[ z = \sqrt{\frac{(1 + S_{11})^2 - S_{21}^2}{(1 - S_{11})^2 - S_{21}^2}}, \]  \hspace{1cm} (10)

Parameter extraction is still an area of active research:

Fitting: Y. Hollander and R. Shavit, Constitutive parameter extraction and experimental validation of single and double negative metamaterials IET Microw. Antennas Propag. -- 12 January 2011 -- Volume 5, Issue 1, p.84–94

Examples

- Wavelength 15~60mm
- Simulation time set 5ns
- Use PEC approximation

Examples

GHz negative refractive index

Negative effective refractive index
Examples

THz metamaterials

- PEC on GaAs substrate, simulation time 50ps

Examples

**THz metamaterials**

- To reduce simulation time, we use a coarse mesh. Use a finer mesh for your final results.
Examples

Optical chiral metamaterials

- Gammadion shaped periodic structure
- Silver sandwiched aluminum on dielectric substrate
  - At optical frequencies, we can’t use the PEC approximation. We use the MCM to accurately model the dispersion of Silver.

Examples

Optical chiral metamaterials

- **Circular dichroism**
  \[ CD = |T_R - T_L| \]
  - \( T_R \) and \( T_L \) are transmittance for right- and left- circularly polarized plane wave

- **Typically, two simulations would be required.**
  - For this structure, with 90° rotational symmetry, we can calculate the left and right handed response from a single simulation

\[
F_R(x, y, z) = F_x(x, y, z) + F_y(x, y, z)e^{\pi/2}
\]
\[
F_L(x, y, z) = F_y(x, y, z) + F_y(x, y, z)e^{-\pi/2}
\]

Examples

Optical chiral metamaterials

Figure 2:
Transmittance \( T_R \) and \( T_L \) against Wavelength [nm].

Figure 5:
CR against Wavelength [nm].
Optimization demo

Optical chiral metamaterials

- Parameterized the design
  - 7 parameters

- Define a figure of merit (fom)
  - fom = \text{max}(|T_R - T_L|)
  - Other figures of merit could easily be used
Optimized parameters are \( P=700\text{nm}, l=554\text{nm}, w=135\text{nm}, r=28\text{ nm}, s=105\text{nm}, d=20\text{nm}, \text{ and } t=50\text{nm} \)

Optimization demo: optimized result

- Circular dichroism is improved from \( \sim 0.25 \) to \( \sim 0.7 \)
  
  Note that the resonant wavelength shifts because the fom did not constrain the resonant wavelength
Concurrent computing

- Optimization and parameter sweep require 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 optimization or parameter sweep results N times faster!
Simulation tips: How to set the simulation time

- Simulation time must be set to let the pulse interact with the structure and decay to zero.
  - The default simulation time is appropriate for optical frequencies. For Microwave frequencies, the simulation time must be increased.
  - Check if the source pulse is long enough

Correct

Wrong
Simulation tips: periodic structures

- Use only ONE unit cell: equivalent to 2X2 periods, but 4 times faster.

- Two simulations are required to obtain all polarization effects
  - Use simple script to get final result
  - If the unit cell has the appropriate symmetry, one simulation may be sufficient.
**Simulation tips: Boundary conditions**

- **Boundary conditions**
  - Periodic for normal incidence
  - Bloch for angled incidence
    - Be aware that the angle of incidence changes with wavelength
  - Use unit cell symmetry to further reduce simulation volume
    - Be cautious about the source polarization
  - PML absorbing boundaries in direction of propagation
Simulation tips: use coarse mesh

- Use a coarse mesh for initial simulations
  - Memory scales as $d x^3$
  - Simulation time scales as $d x^4$
Simulation tips: extremely thin layers

- Often we have extremely thin metal layers
  - Thickness $<< \lambda$

- The mesh size must be smaller than the layer thickness.
  - Very thin layers force a very small mesh, leading to long simulation times.

- In many microwave & THz devices, we can use a much thicker layer in the simulation
  - The exact thickness of these layers has very little impact on the device performance as long as thickness $<< \lambda$
Simulation tips: extremely thin layers

- Minimum wavelength: 15mm
- Actual physical thickness 17\(\mu\)m

<table>
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<tr>
<th>thickness</th>
<th>17(\mu)m</th>
<th>75(\mu)m</th>
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<tbody>
<tr>
<td>Override dz</td>
<td>1(\mu)m</td>
<td>5(\mu)m</td>
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<tr>
<td>Time used</td>
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<td>6.5 min</td>
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![Permittivity and Permeability](image.png)
### Challenges and solutions

<table>
<thead>
<tr>
<th>Challenge</th>
<th>Solutions and best practices</th>
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<tbody>
<tr>
<td>Sub-wavelength scale patterning</td>
<td>Full vectorial 3D Maxwell solver can capture all physical effects</td>
</tr>
<tr>
<td>Complex 3D geometries</td>
<td>• Parameterize designs</td>
</tr>
</tbody>
</table>
| Simulation methodology             | • Simulate only 1 unit cell  
• Take advantage symmetry in the simulation  
• Use PEC approximation if applicable  
• Use thicker layer in simulation for extremely thin layers  
• Extract S parameters from complex reflected and transmitted fields  
• Effective properties can be calculated from S parameters  
• Post processing can be simplified and automated with scripts and analysis objects                                                                   |
| Simulation setup                   | • Ensure simulation time is sufficient (longer for low frequencies)  
• Store only necessary field data  
• Use coarse mesh size where possible  
  • Always for initial simulations  
  • Do convergence testing of mesh size last!  
• Use distributed parallelism to run each simulation as fast as possible                                                                                   |
| Broadband simulation               | • Time domain gives broadband results  
• Highly dispersive materials may require multi-pole material models  
  • Check the material fit before running the simulation                                                                                                  |
| Parameter sweeps and optimization  | • Use concurrent computing to use all your available computer resources optimally                                                                        |
# Question and Answer

<table>
<thead>
<tr>
<th>Dr. James Pond</th>
<th>Dr. Guilin Sun</th>
</tr>
</thead>
<tbody>
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<th>Dr. Mitsunori Kawano</th>
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<td>Director of Technical Services</td>
<td>Technical Sales Engineer</td>
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http://www.lumerical.com/company/representatives.html

Free, 30 day trial at www.lumerical.com
Question and Answer

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