

OptiFDTD

Technical Background

Finite-Difference Time-Domain

OptiFDTD Version 16.0.1 for Microsoft Windows® 10 64-bit



Table of Contents

1 FDTD Basics	5
1.1 2D FDTD Equations	5
1.2 3D FDTD Equations	9
1.3 Discretization of space and time	11
1.4 OptiFDTD Simulation Procedures	13
1.5 Output data	13
1.6 References	15
2 Material Models	16
2.1 Constant Dielectrics (Including Loss).....	16
2.2 2D Dispersive Materials.....	18
2.3 3D Dispersive Materials (Lorentz-Drude)	20
2.4 Nonlinear Materials Models.....	25
3 OptiFDTD Boundary Conditions.....	29
3.1 PML Boundary Conditions	29
3.2 PMC / PEC boundary conditions and plane wave simulations	30
3.3 PBC Boundary Conditions	34
4 Light Sources.....	36
4.1 Input planes.....	36
4.2 Point Sources	41
5 S-Parameters.....	44
5.1 Technical Background on the Eigenmode Expansion of an Electromagnetic Field.....	44
5.2 Calculate and Export S-Parameters with OptiFDTD.....	47
6 Plane Wave Expansion (PWE) method	48
6.1 References:.....	49
7 Post-simulation Data Analysis.....	50

7.1 Spectral response (Fourier transforms)	50
7.2 Power calculation	51
7.3 Far Field Transform.....	53
7.4 Heat Absorption	56

Copyright © 2022 Optiwave, All rights reserved.

All OptiFDTD documents, including this one, and the information contained therein, are copyright material. No part of this document may be reproduced, stored in a retrieval system, or transmitted in any form or by any means whatsoever, including recording, photocopying, or faxing without prior written approval of Optiwave.

Disclaimer

Optiwave makes no representation or warranty with respect to the adequacy of this documentation or the programs which it describes for any particular purpose or with respect to its adequacy to produce any particular result. In no event shall Optiwave, its employees, its contractors or the authors of this documentation, be liable for special, direct, indirect, or consequential damages, losses, costs, charges, claims, demands, or claim for lost profits, fees, or expenses of any nature or kind.

1 FDTD Basics

OptiFDTD is a powerful, highly integrated, user-friendly software that allows computer aided design and simulation of advanced passive photonic components.

The OptiFDTD software package is based on the finite-difference time-domain (FDTD) method, which has been established as a powerful engineering tool for integrated and diffractive optics device simulations. This is due to its ability to simultaneously model light propagation, scattering, diffraction, reflection, and polarization effects. It can also model material anisotropy and dispersion without any assumptions of field behavior such as the slowly varying envelope approximation. The method allows for the effective and powerful simulation and analysis of sub-micron devices with very fine structural details. A sub-micron scale implies a high degree of light confinement and correspondingly, the large refractive index difference of the materials (mostly semiconductors) to be used in a typical device design.

1.1 2D FDTD Equations

The FDTD approach is based on a direct numerical solution of the time-dependent Maxwell's curl equations. The lossless and source free expressions are

$$\begin{aligned}\frac{\partial H_x}{\partial t} &= \frac{1}{\mu_0} \left[\frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial y} \right] \\ \frac{\partial H_y}{\partial t} &= \frac{1}{\mu_0} \left[\frac{\partial E_z}{\partial x} - \frac{\partial E_x}{\partial z} \right] \\ \frac{\partial H_z}{\partial t} &= \frac{1}{\mu_0} \left[\frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} \right] \\ \frac{\partial E_x}{\partial t} &= -\frac{1}{\epsilon} \left[\frac{\partial H_y}{\partial z} - \frac{\partial H_z}{\partial y} \right] \\ \frac{\partial E_y}{\partial t} &= -\frac{1}{\epsilon} \left[\frac{\partial H_z}{\partial x} - \frac{\partial H_x}{\partial z} \right] \\ \frac{\partial E_z}{\partial t} &= -\frac{1}{\epsilon} \left[\frac{\partial H_x}{\partial y} - \frac{\partial H_y}{\partial x} \right]\end{aligned}$$

When using OptiFDTD in 2D, the photonic device is laid out in the **xz** plane, the propagation is along the Z axis while the structure is taken to be infinite along the Y. The structure being infinite along Y removes any term containing a spatial derivative in Y from Maxwell's equations. This allows the six equations become partially uncoupled and can be placed in two groups: (E_y , H_x , and H_z) and (H_y , E_x , and E_z). These two groups are designated **TE** and **TM**; however, there are different conventions regarding which group gets which designation. OptiFDTD follows conventional standards based on waveguiding which looks at the solutions to the field components

that will result in a wave equation, E_y and H_y . The Transverse Electric (**TE**) designation goes to the group that has a electric wave equation along the axis perpendicular to the direction of propagation: (E_y , H_x , and H_z). The Transverse Magnetic (**TM**) designation goes to the group that has the magnetic wave equation along y: (H_y , E_x , and E_z). This is different than conventions such as that used by Taflove so readers must keep this in mind when comparing multiple references.

1.1.1 TE waves

As discussed the 2D TE case solve the expressions for E_y , H_x , and H_z while setting the other components to zero:

$$\begin{aligned}\frac{\partial E_y}{\partial t} &= \frac{1}{\epsilon} \left(\frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} \right) \\ \frac{\partial H_x}{\partial t} &= \frac{1}{\mu_0} \frac{\partial E_y}{\partial z} \\ \frac{\partial H_z}{\partial t} &= -\frac{1}{\mu_0} \frac{\partial E_y}{\partial x}\end{aligned}$$

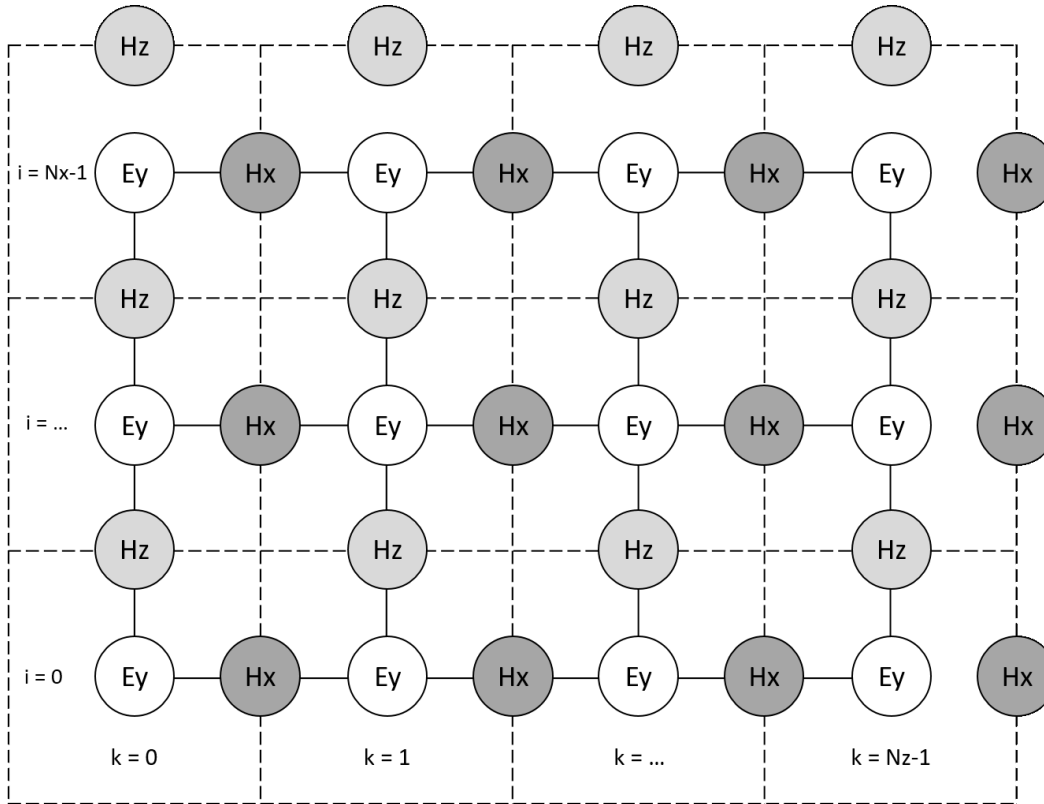
where

$\epsilon = \epsilon_0 \epsilon_r$, is the dielectric permittivity of the material
 μ_0 , is the magnetic permeability of free-space.

The refractive index of the material is defined by:

$$n = \sqrt{\epsilon_r}.$$

Each field is represented by a 2D array: $E_y(i, k)$, $H_x(i, k)$, and $H_z(i, k)$. The indices, i and k account for the number of space steps in the X and Z direction, respectively. In the case of TE, the location of the fields in the mesh is shown below.



1 Location of the TE fields components in the computational domain

The separation of the TE fields is based upon the 2D Yee Cell. The E_y field is considered to be the center of the FDTD spatial cell which is defined by the dashed lines. The magnetic fields, H_x and H_z , are associated with cell edges. The reason for the offset fields is that the derivatives within Maxwell's equations will be discretized and expressed using central finite differences ensuring second-order accuracy in both space and time. .

- The E_y field is associated with integer values of the indices i and k .
- The H_x field is associated with integer i and $(k + 0.5)$ indices.
- The H_z field is associated with $(i + 0.5)$ and integer k indices.

The discretization of Maxwell's equations along the grid are

$$E_y^n(i, k) = E_y^{n-1}(i, k) + \frac{\Delta t}{\epsilon \Delta z} \left[H_x^{n-\frac{1}{2}}(i, k + \frac{1}{2}) - H_x^{n-\frac{1}{2}}(i, k - \frac{1}{2}) \right] - \frac{\Delta t}{\epsilon \Delta x} \left[H_z^{n-\frac{1}{2}}(i + \frac{1}{2}, k) - H_z^{n-\frac{1}{2}}(i - \frac{1}{2}, k) \right]$$

$$H_x^{n+\frac{1}{2}}(i, k + \frac{1}{2}) = H_x^{n-\frac{1}{2}}(i, k + \frac{1}{2}) + \frac{\Delta t}{\mu_0 \Delta z} [E_y^n(i, k + 1) - E_y^n(i, k)]$$

$$H_z^{n+\frac{1}{2}}(i + \frac{1}{2}, k) = H_z^{n-\frac{1}{2}}(i + \frac{1}{2}, k) - \frac{\Delta t}{\mu_0 \Delta x} [E_y^n(i + 1, k) - E_y^n(i, k)]$$

where

n discretized time step

Δx is the size in real units of a space step along the X direction

Δz is the size in real units of a space step along the Z direction

Δt is the size in real units of a time step

There are two considerations when selecting the space and time step sizes. To ensure that the source is properly represented the spatial step size is typically set to 10 to 20 steps per wavelength. This is a basic starting point as complex materials or designs with feature sizes smaller than the source wavelength will require higher resolutions. Scanning the mesh size and performing convergence testing should always be considered. The sampling in time is chosen to ensure numerical stability of the algorithm and is specified by the . The time step is determined by the **Courant** or **Courant-Friedrichs-Levy (CFL) condition**:

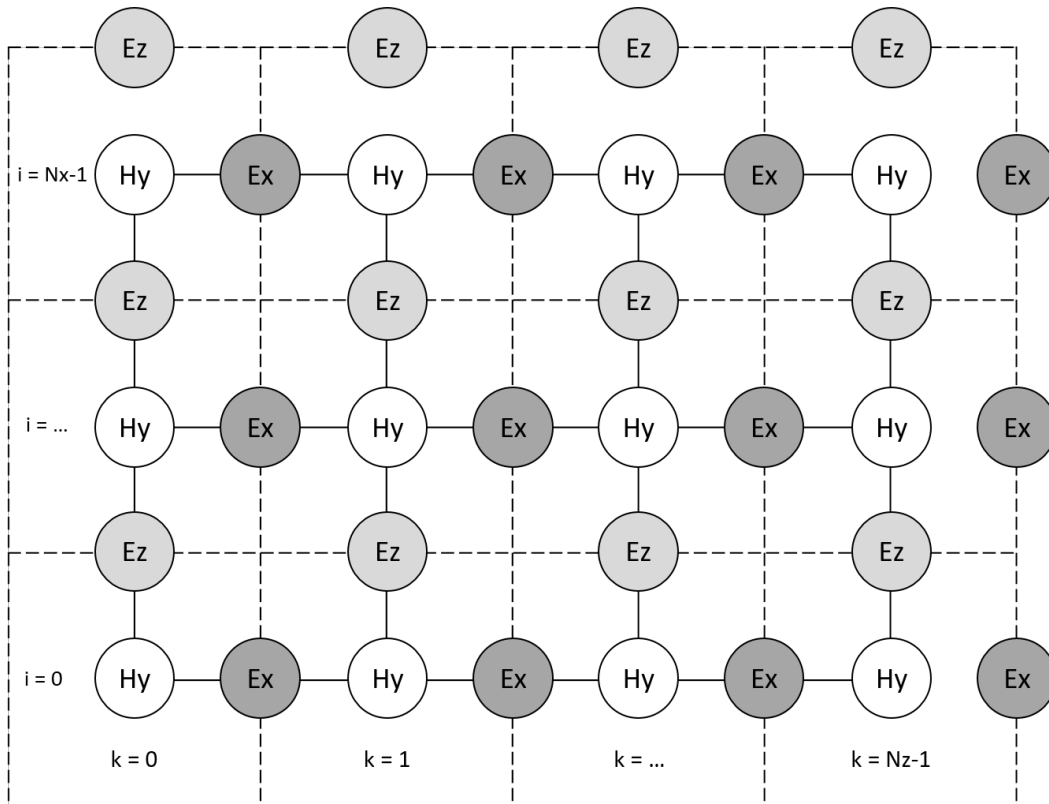
$$\Delta t \leq \frac{1}{c \sqrt{\frac{1}{(\Delta x)^2} + \frac{1}{(\Delta z)^2}}}$$

1.1.2 TM waves

In the 2D TM case it is the H_y , E_x , and E_z field components that are solved for. Maxwell's equations take the following form:

$$\begin{aligned} \frac{\partial H_y}{\partial t} &= -\frac{1}{\mu_0} \left(\frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x} \right) \\ \frac{\partial E_x}{\partial t} &= -\frac{1}{\epsilon} \frac{\partial H_y}{\partial z} \\ \frac{\partial E_z}{\partial t} &= \frac{1}{\epsilon} \frac{\partial H_y}{\partial x} \end{aligned}$$

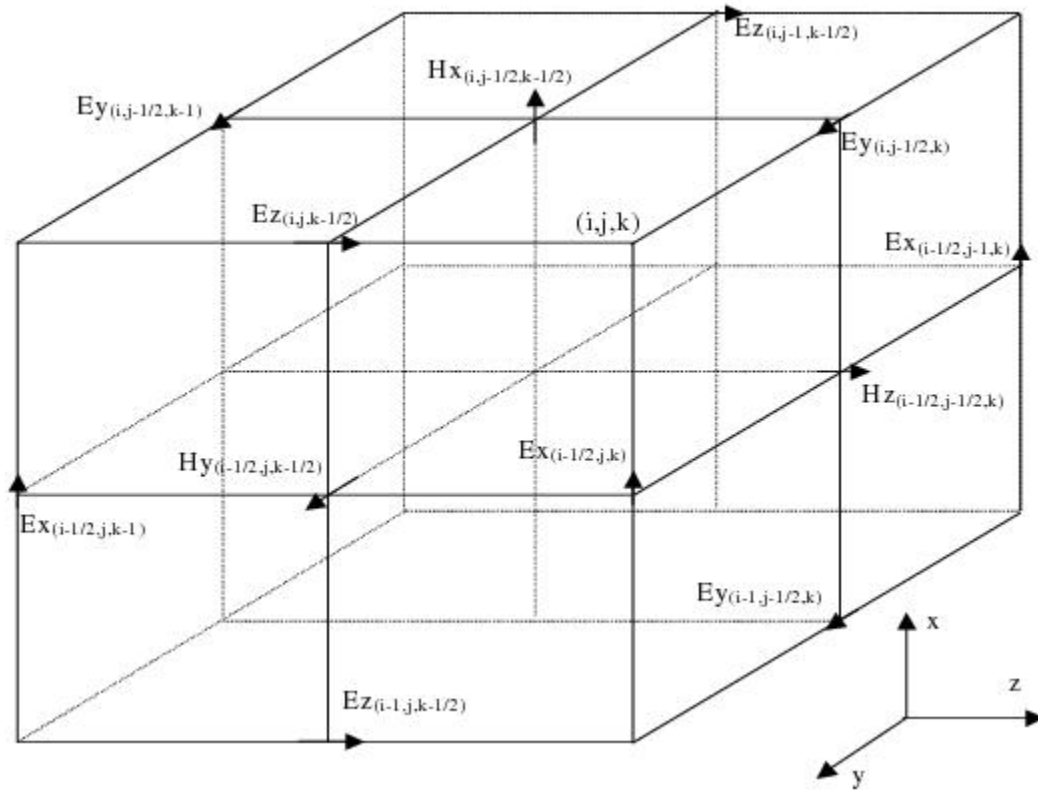
The location of the TM fields in the computational domain within the 2D Yee cell can be seen below. In the TM case the H_y fields are defined at the center of the cell while the E_x and E_z fields are defined along the cell edges.



2 Location of the TM fields components in the computational domain

1.2 3D FDTD Equations

In 3D simulations each field components is represented by a 3D array: $E_x(i,j,k)$, $E_y(i,j,k)$, $E_z(i,j,k)$, $H_x(i,j,k)$, $H_y(i,j,k)$, $H_z(i,j,k)$. These fields are defined in space according to the complete **Yee Cell** where E and H fields are spaced $1/2$ step in both space and time and interleaved such that central difference expressions for components have the required information. In this algorithm the E and H fields are solved in a leapfrog fashion where E fields are calculated using H from the previous half time step and then vice versa.



3 A 3D Yee cell showing the E and H field components

The source free time domain vectorial Maxwell's equations are given in differential form by:

$$\begin{aligned}\mu \frac{\partial \mathbf{H}}{\partial t} &= -\nabla \times \mathbf{E} \\ \epsilon \frac{\partial \mathbf{E}}{\partial t} + \sigma \mathbf{E} &= \nabla \times \mathbf{H}\end{aligned}$$

The ability to use these expressions on a grid with discretized space and time requires the use of central finite difference expressions which provides second-order accuracy. The 3D-FDTD formulas can be written, using Allen Taflove's notation, as:

E components

$$\begin{aligned}
E_x \Big|_{i-1/2, j, k}^{n+1} &= \frac{2\epsilon - \sigma\Delta t}{2\epsilon + \sigma\Delta t} E_x \Big|_{i-1/2, j, k}^n \\
&+ \frac{2\Delta t}{(2\epsilon + \sigma\Delta t)} \left[\frac{H_z \Big|_{i-1/2, j+1/2, k}^{n+1/2} - H_z \Big|_{i-1/2, j-1/2, k}^{n+1/2}}{\Delta y} - \frac{H_y \Big|_{i-1/2, j, k+1/2}^{n+1/2} - H_y \Big|_{i-1/2, j, k-1/2}^{n+1/2}}{\Delta z} \right] \\
E_y \Big|_{i, j-1/2, k}^{n+1} &= \frac{2\epsilon - \sigma\Delta t}{2\epsilon + \sigma\Delta t} E_y \Big|_{i, j-1/2, k}^n \\
&+ \frac{2\Delta t}{(2\epsilon + \sigma\Delta t)} \left[\frac{H_x \Big|_{i, j-1/2, k+1/2}^{n+1/2} - H_x \Big|_{i, j-1/2, k-1/2}^{n+1/2}}{\Delta z} - \frac{H_z \Big|_{i+1/2, j-1/2, k}^{n+1/2} - H_z \Big|_{i-1/2, j-1/2, k}^{n+1/2}}{\Delta x} \right] \\
E_z \Big|_{i, j, k-1/2}^{n+1} &= \frac{2\epsilon - \sigma\Delta t}{2\epsilon + \sigma\Delta t} E_z \Big|_{i, j, k-1/2}^n \\
&+ \frac{2\Delta t}{(2\epsilon + \sigma\Delta t)} \left[\frac{H_y \Big|_{i+1/2, j, k-1/2}^{n+1/2} - H_y \Big|_{i-1/2, j, k-1/2}^{n+1/2}}{\Delta x} - \frac{H_x \Big|_{i, j+1/2, k-1/2}^{n+1/2} - H_x \Big|_{i, j-1/2, k-1/2}^{n+1/2}}{\Delta y} \right]
\end{aligned}$$

H components

$$\begin{aligned}
H_x \Big|_{i, j-1/2, k-1/2}^{n+1/2} &= H_x \Big|_{i, j-1/2, k-1/2}^{n-1/2} \\
&+ \frac{\Delta t}{\mu_0} \left[\frac{E_y \Big|_{i, j-1/2, k}^n - E_y \Big|_{i, j-1/2, k-1}^n}{\Delta z} - \frac{E_z \Big|_{i, j, k-1/2}^n - E_z \Big|_{i, j-1, k-1/2}^n}{\Delta y} \right] \\
H_y \Big|_{i-1/2, j, k-1/2}^{n+1/2} &= H_y \Big|_{i-1/2, j, k-1/2}^{n-1/2} \\
&+ \frac{\Delta t}{\mu_0} \left[\frac{E_z \Big|_{i, j, k-1/2}^n - E_z \Big|_{i-1, j, k-1/2}^n}{\Delta x} - \frac{E_x \Big|_{i-1/2, j, k}^n - E_x \Big|_{i-1/2, j, k-1}^n}{\Delta z} \right] \\
H_z \Big|_{i-1/2, j-1/2, k}^{n+1/2} &= H_z \Big|_{i-1/2, j-1/2, k}^{n-1/2} \\
&+ \frac{\Delta t}{\mu_0} \left[\frac{E_x \Big|_{i-1/2, j, k}^n - E_x \Big|_{i-1/2, j-1, k}^n}{\Delta y} - \frac{E_y \Big|_{i, j-1/2, k}^n - E_y \Big|_{i-1, j-1/2, k}^n}{\Delta x} \right]
\end{aligned}$$

1.3 Discretization of space and time

There are 2 fundamental constraints to the FDTD method when it comes to the discretization of the simulation space. These are the size of the spatial steps and its impact on accuracy and the step size for the time steps and its impact on the stability of the simulation. This section will discuss the constraints and general rules for setting the discretization parameters of a simulation.

1.3.1 Spatial step size

The spatial step size affects the simulation results in two ways:

1. The resolution is not sufficiently fine enough to properly characterize either the source or the structure under test.
2. If the step size is too large numerical dispersion can be introduced that results from the discretization of the derivatives.

A well known general rule for spatial discretizations in FDTD simulations is that the spatial step size should correspond to 1/10th of a wavelength, or "**10 points per wavelength**". Understandable this is referring to the wavelength of the source in the highest refractive index material in the simulation. This is the criteria used in the *Auto* setting in OptiFDTD.

$$\max(\Delta x, \Delta y, \Delta z) \leq \frac{\lambda_{min}}{10n_{max}}$$

where n_{max} is the maximum refractive index value in the computational domain.

It should be noted that this is merely a good starting point. For example if the design includes features that are less than or on the same order as the wavelength then this rule may not provide sufficient resolution to properly characterize these features, one suggestion would be to set the resolution to be 1/10 of the smallest feature size. It is for this reason, and to verify that numerical dispersion is at a minimum that convergence testing is always highly recommended. Convergence testing is done by repeatedly running simulations with increasingly smaller spatial step sizes and comparing the results to ensure that they sufficiently converged relative to the discretization.

1.3.2 Time step size

The second major constraint on the discretization of an FDTD simulation is the size of the time step Δt . In order to ensure stability in the numerical solution it is necessary that the time step size satisfies the **Courant-Friedrichs-Levy (CFL) condition**. This is the condition that is used in the *Auto* setting for an OptiFDTD simulation.

For a 3D FDTD simulation, the CFL condition is [1, §4.7] :

$$\Delta t \leq \frac{1}{v \sqrt{\left(\frac{1}{\Delta x}\right)^2 + \left(\frac{1}{\Delta y}\right)^2 + \left(\frac{1}{\Delta z}\right)^2}}$$

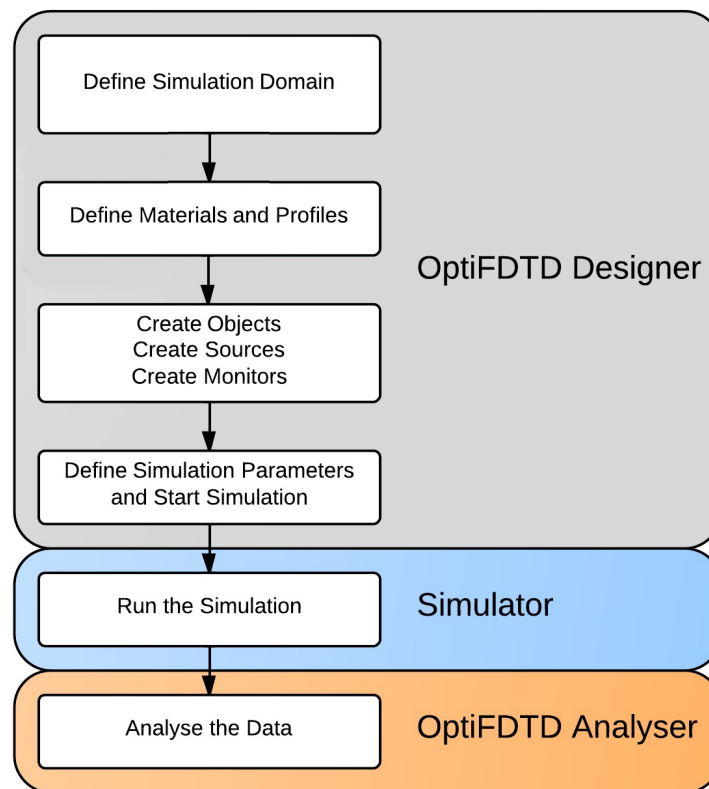
where v is the speed of the light in the medium.

1.3.3 References

1. Allen Taflove and Susan Hagness, *Computational Electrodynamics: The Finite-Difference Time-Domain Method*, third edition, Norwood MA: Artech House, 2005.

1.4 OptiFDTD Simulation Procedures

The following is the workflow chart for project design, simulation and analysis in OptiFDTD.



4 FDTD Simulation Flow Chart in OptiFDTD

1.5 Output data

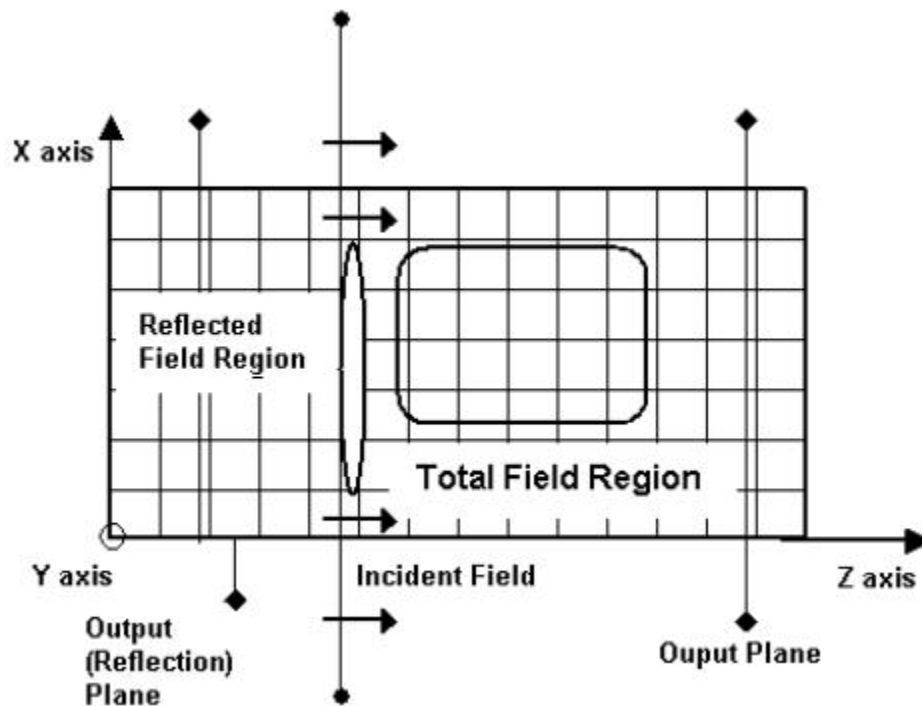
The FDTD algorithm, as described in the 2D and 3D sections calculates the fields and their propagation within the time domain. At each location of the computational domain for a given time t they have are of the form

$$E(x, y, z) = A \cdot G(x, y, z) \sin(\omega t + \phi_i)$$

where A is the amplitude of the field at the given location, G is the wave profile or the envelope, and ϕ_i is the corresponding phase. It should be noted that the phase information cannot be directly taken from a time domain simulation. If the source has multiple frequencies it is also not possible to determine what portion of the $A \cdot G$ is due to any given frequency component.

In order to get the full amplitude/phase wave information as a function of the frequencies present in the simulation, it is necessary to obtain the stationary complex fields that correspond to the waveform of the above equation. These complex fields are calculated by performing a Discrete Fourier transform on the time domain results of an FDTD simulation. The final complex fields can be solved at specific output Planes and visualized.

The information being sought plays a vital role in the placement of the output planes.



5 Output Planes

OptiFDTD uses **the TF/SF** (total field/scattering field) technique for the incident plane. The region behind the incident plane, only contains field contributions that are scattered from the simulation space, these can also be called the reflections allowing the reflection coefficient or reflectance to be calculated. The region in the propagation or transmission region for the plane contain the total field region and information recorded here contains the transmission characteristics of the space being modelled. When the Observation detectors are placed in the field transmission region, the transmission coefficient or transmittance can be calculated.

1.6 References

1. Yee, K. S., "Numerical solution of initial boundary value problems involving Maxwell's equations in isotropic media," IEEE Transactions on Antennas and Propagation, 302-307, (1966).
2. Chu, S. T., Chaudhuri, S.K., "A finite-difference time-domain method for the design and analysis of guided-wave optical structures," Journal of Lightwave Technology, 2033-2038, (1989).
3. Taflove, A., Hagness, S., "Computational Electrodynamics: The Finite-Difference Time-Domain Method," Second edition, Artech House, Boston, (2000).

2 Material Models

One of the main advantages of the FDTD approach is the lack of approximations for the propagating field—light is modeled in its full richness and complexity. The other significant advantage is the great variety of materials that can be consistently modeled within the FDTD context. In this sub-section we make a brief review of some of the main material properties that can be handled.

2.1 Constant Dielectrics (Including Loss)

2.1.1 Complex refractive index

Constant dielectric materials are expressed by a complex refractive index value (\tilde{n}) or relative permittivity value (ϵ_r).

$$\begin{aligned}\tilde{n} &= n - j\kappa \\ \epsilon_r &= \epsilon_r' - j\epsilon_r''\end{aligned}$$

where, n is the refractive index indicating the phase velocity information in the medium, κ is the extinction coefficient that indicates the amount of absorption loss when the electromagnetic wave propagates through the material.



- In OptiFDTD, the engineering convention ($\mathbf{E} \propto e^{j\omega t}$) is used which drives the use of the negative imaginary component for \tilde{n} (the physics convention will use a positive). With both conventions a negative imaginary part, positive κ , will express a loss.
- This convention carries over to the definition of the permittivity.
- For the constant dielectric model the user specifies the real and imaginary parts so the user is defining n and $-\kappa$.

The expressions for the refractive index and permittivity are linked through the following relationship

$$\begin{aligned}\epsilon_r &= \tilde{n}^2 \\ \epsilon_r' &= n^2 - \kappa^2 \\ \epsilon_r'' &= 2n\kappa\end{aligned}$$

The propagation constant is given by

$$\begin{aligned}\gamma &= \alpha + j\beta \\ \alpha &= \frac{2\pi\kappa}{\lambda_0} \\ \beta &= \frac{2\pi n}{\lambda_0}\end{aligned}$$

where α is the attenuation constant, β is the phase constant, and λ_0 is the wavelength in vacuum.

⚠ With a constant dielectric (i.e. frequency-independent permittivity) and $\epsilon'_r < 0$ or equivalently $n < \kappa$, the solution to Maxwell's equations grows exponentially with time. Simulations with these materials are therefore unstable. If one wants to model a material with $\epsilon'_r < 0$, dispersive materials (e.g. Lorentz-Drude) should be used instead.

2.1.2 Loss through conductivity

The material losses can also be expressed as a function of the material conductivity. In the derivation it should be emphasized that in the time domain all the \mathbf{H} and \mathbf{E} fields are real quantities. Therefore, accounting for loss requires a non-zero conductivity of the medium:

$$\begin{aligned}\nabla \times \mathbf{H} &= \epsilon_0 \epsilon_r \frac{\partial \mathbf{E}}{\partial t} + \sigma \mathbf{E} \\ &= j\omega \epsilon_0 \left(\epsilon_r - j \frac{\sigma}{\omega \epsilon_0} \right) \mathbf{E} \\ &= j\omega \epsilon_0 \epsilon_{eff} \mathbf{E}\end{aligned}$$

where

$$\begin{aligned}\epsilon_{eff} &= \epsilon_r - j \frac{\sigma}{\omega \epsilon_0} \\ &= \epsilon'_r - j \epsilon''_r \\ &= (n - j\kappa)^2\end{aligned}$$

Relating the real and imaginary part of the permittivity in both approaches yields the requirement that

$$\kappa = \frac{\sigma}{2\epsilon_0 \omega n}$$

Provided that the above relation is held both the refractive index and conductivity methods of incorporating loss are equivalent.

Therefore if a user wishes to define a constant dielectric where they know the conductivity it can be defined by setting the imaginary part of the refractive index to

$$im(\tilde{n}) = -\frac{\sigma}{2\epsilon_0\omega n}$$

2.1.3 Sellmeier

If the user would prefer to define the constant dielectric through the Sellmeier equation for a specific reference wavelength (λ). This can be done by selecting the Sellmeier check box, entering the reference wavelength and in the Sellmeier tab specifying the coefficients for the desired material. The Sellmeier relation to permittivity as used in OptiFDTD is

$$\epsilon_r = \epsilon_{r0} + \sum_{i=1}^M \frac{A_i \lambda^2}{\lambda^2 + j\Gamma_i \lambda - \lambda_i^2}$$

Where A_i is the Strength, Γ_i is the damping factor or collision wavelength, and λ_i is the oscillating wavelength.

⚠ It is important that users note the constant nature of the dielectric defined by the Sellmeier expression in OptiFDTD. The refractive index of the material will be constant throughout a simulation regardless of the wavelength of the source (either CW or pulsed). While the refractive index is dependent on wavelength in OptiFDTD it is the reference wavelength within the definition of the material that is used not the source. If the user requires a material that includes dispersive effects they should use the Lorentz-Drude dispersive material functionality

2.2 2D Dispersive Materials

2.2.1 Lorentz dispersive materials

Lorentz dispersion materials are materials for which the frequency dependence of the dielectric permittivity can be described as the sum of multiple resonant Lorentzian functions:

$$\epsilon_r(\omega) = \epsilon_\infty + \sum_{m=1}^N \frac{\chi_0 G_m \omega_{0m}^2}{\omega_{0m}^2 + j\Gamma_m \omega - \omega^2}$$

where

- ω_{0m} are the resonant frequencies
- G_m is the Oscillator strength coefficients
- Γ_m are the damping coefficients
- ϵ_∞ is the permittivity at infinite frequency
- χ_0 is the permittivity at $\omega = 0$

In the lossless case, the above equation is directly related to the Sellmeier equation, which in the case of three resonances can be presented as:

$$n^2 = \epsilon_\infty + \frac{\chi_0 G_1 \lambda^2}{\lambda^2 - \lambda_1^2} + \frac{\chi_0 G_2 \lambda^2}{\lambda^2 - \lambda_2^2} + \frac{\chi_0 G_3 \lambda^2}{\lambda^2 - \lambda_3^2}$$

In the lossy case, the Sellmeier equation can be written in a generalized form, accounting for a non-zero damping coefficient Γ_m as well as for anisotropy in the dispersion properties:

$$n^2(\omega) = \epsilon_\infty + \frac{\chi_0 G_1 \lambda^2}{\lambda^2 + j\Gamma_1 \lambda - \lambda_1^2} + \frac{\chi_0 G_2 \lambda^2}{\lambda^2 + j\Gamma_2 \lambda - \lambda_2^2} + \frac{\chi_0 G_3 \lambda^2}{\lambda^2 + j\Gamma_3 \lambda - \lambda_3^2}$$

There are different ways to implement the Lorentz model into the FDTD formalism. OptiFDTD considers the polarization equation approach in the single resonance case where an auxiliary differential equation can be derived that will work in conjunction with the Maxwell's equations. It uses the dielectric susceptibility function:

$$\chi(\omega) = \frac{\chi_0 \omega_0^2}{\omega_0^2 + j\Gamma\omega - \omega^2}$$

and the relation between the polarization and the electric field:

$$\mathbf{P} = \epsilon_0 \chi(\omega) \mathbf{E}$$

If the susceptibility function and the relationship between the polarization and electric field are combined and the inverse Fourier transform of the result is taken (frequency to time domain) then the following differential equation is obtained,

$$\frac{\partial^2 \mathbf{P}}{\partial t^2} + \Gamma \frac{\partial \mathbf{P}}{\partial t} + \omega_0^2 \mathbf{P} = \epsilon_0 \chi_0 \omega_0^2 \mathbf{E}$$

If a change of coordinates is used relating the polarization to the current density,

$$\frac{\partial \mathbf{P}}{\partial t} = \mathbf{J}$$

then, the differential equation becomes:

$$\frac{\partial \mathbf{J}}{\partial t} + \Gamma \mathbf{J} + \omega_0^2 \mathbf{P} = \epsilon_0 \chi_0 \omega_0^2 \mathbf{E}$$

This can be combined into the H term in the differential form of the 3D maxwell's equations, taking the form:

$$\nabla \times \mathbf{H} = \epsilon \frac{\partial \mathbf{E}}{\partial t} + \mathbf{P} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J}$$

This can be solved using the FDTD method as described in [3D FDTD Equations](#).

⚠ The Lorentz model is only supported in 2D simulations. Lorentz-Drude materials, that are a generalization of the Lorentz model, are supported for both 2D and 3D simulations.

2.2.2 Drude materials

Drude dispersive materials in OptiFDTD are characterized by the following dielectric function:

$$\epsilon_r(\omega) = \epsilon_{r\infty} + \frac{\omega_p^2}{j\Gamma\omega - \omega^2}$$

Where $\epsilon_{r\infty}$ is the permittivity for infinity frequency, ω_p is the plasma frequency, and Γ is the collision frequency or damping factor. This can be incorporated into the FDTD field equations in a similar fashion to the Lorentz model.

⚠ The Drude model is only supported in 2D simulations. Lorentz-Drude materials, that are a generalization of the Drude model, are supported for both 2D and 3D simulations.

2.3 3D Dispersive Materials (Lorentz-Drude)

2.3.1 Lorentz-Drude Model in Frequency Domain

The Lorent-Drude model [1] is a general model that defines a complex dielectric function capable of modelling conductivity, and dispersion that is of the following form:

$$\epsilon_r(\omega) = \epsilon_r^f(\omega) + \epsilon_r^b(\omega)$$

This form separates explicitly the intraband effects ($\epsilon_r^f(\omega)$ - usually referred to as free electron effects) from interband effect ($\epsilon_r^b(\omega)$ - usually referred to as bound-electron effects).

The intraband contribution of the dielectric function is described by the well known free-electron or Drude model [2,3]:

$$\epsilon_r^f(\omega) = 1 + \frac{\Omega_p^2}{j\omega\Gamma_0 - \omega^2}$$

The plasma frequency associated with intraband transitions can be written as:

$$\Omega_p = \sqrt{G_0\omega_p}$$

where G_0 is the oscillator strength.

The interband part of the dielectric function is described by the following simple semi-quantum model resembling the Lorentz results for dielectrics:

$$\epsilon_r^b(\omega) = \sum_{m=1}^M \frac{\Omega_p^2}{\omega_m^2 - \omega^2 + j\omega\Gamma_m}$$

Where:

- Ω_p is the plasma frequency
- M is the number of oscillators
- ω_m is the m-th oscillator frequency
- Γ_m is the m-th oscillator damping coefficient

The separate effects can be brought together as the Lorentz-Drude Model in a general equation

$$\epsilon_r(\omega) = \epsilon_{r\infty} + \sum_{m=0}^{M-1} \frac{G_m\Omega_m^2}{\omega_m^2 - \omega^2 + j\omega\Gamma_m}$$

where:

- M is the number of oscillators
- $\epsilon_{r\infty}$ is the relative permittivity at infinity
- Ω_m is the m-th plasma frequency
- ω_m is the m-th oscillator frequency
- Γ_m is the m-th oscillator damping coefficient
- G_m is the m-th oscillator strength coefficient

If only the Drude model is required the user can set $M = 1$ (only $m = 0$ term) and $\omega_0 = 0$.

If only the Lorentz model is required then set $m = 1..M$ and $\Omega_1 = \Omega_2 = \Omega_p$.

Reference [1] gives the Lorentz-Drude parameters for 11 noble metals and the "OptiFDTD Material Library" manual contains parameters compiled by Optiwave that describe noble metals and other dispersive materials.

2.3.2 Lorentz-Drude Model in Time Domain

The direct use of the Lorentz-Drude model within an FDTD simulation presents complications as it is a frequency domain model while FDTD is a time domain method. It is necessary to incorporate the inverse transform of Lorentz-Drude model with the Polarization term in Maxwell's equations in order for OptiFDTD to capture the dispersive characteristics. Including the Polarization term, Maxwell's equations are

$$\begin{aligned}\nabla \times \mathbf{E} &= -\mu_0 \frac{\partial \mathbf{H}}{\partial t} \\ \nabla \times \mathbf{H} &= \epsilon_0 \frac{\partial \mathbf{E}}{\partial t} + \frac{\partial \mathbf{P}}{\partial t}\end{aligned}$$

where we have used the relationship $\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P}$ and set $\epsilon_{r\infty} = 1$. If we treat each resonance in the Lorentz-Drude model as a contribution to the Polarization ($\mathbf{P} = \sum_{m=0}^{M-1} \mathbf{P}_m$) we can express the equations that need to be discretized in the Yee cell as

$$\begin{aligned}\nabla \times \mathbf{E} &= -\mu_0 \frac{\partial \mathbf{H}}{\partial t} \\ \nabla \times \mathbf{H} &= \epsilon_0 \frac{\partial \mathbf{E}}{\partial t} + \sum_{m=0}^{M-1} \frac{\partial \mathbf{P}_m}{\partial t}\end{aligned}$$

It is now necessary to work with the Lorentz-Drude model and express it in such a way that we can create an auxiliary differential equation that will allow the calculation of each \mathbf{P}_m by using the relationship between the polarization and electric field.

$$\mathbf{P}_m = \epsilon_0 G_m \omega_m^2 \mathbf{E}$$

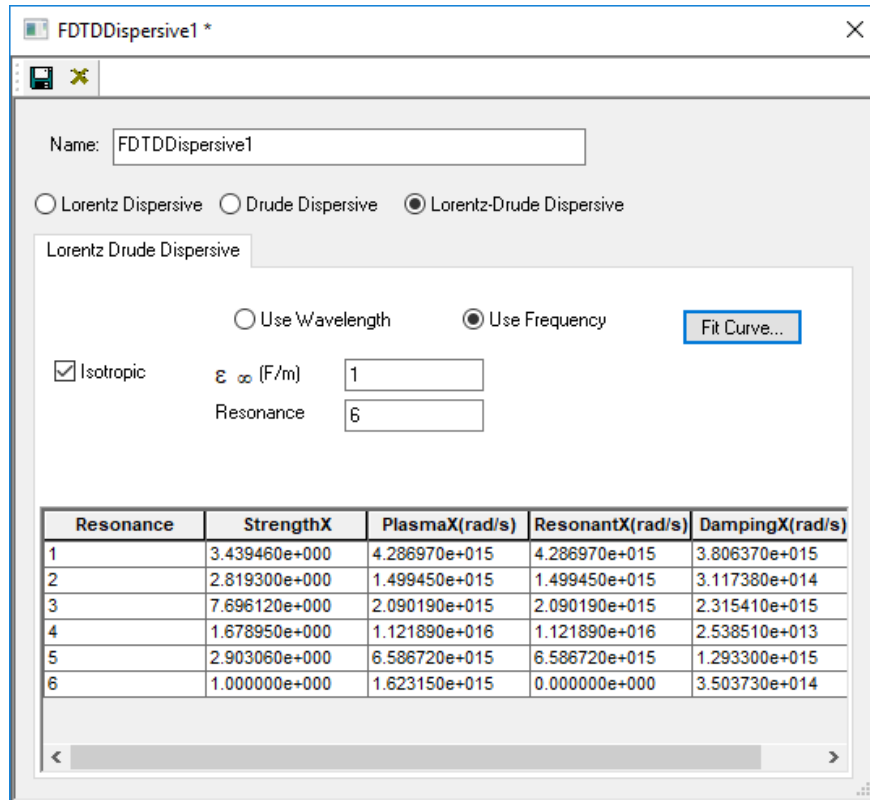
Taking the Fourier transform of the last equation leads to the following differential equation:

$$\frac{\partial^2 \mathbf{P}_m}{\partial t^2} + \Gamma_m \frac{\partial \mathbf{P}_m}{\partial t} + \omega_m^2 \mathbf{P}_m = \epsilon_0 G_m \Omega_m^2 \mathbf{E}$$

This differential equation can be solved for each of the resonances with each time step for each position as the system updates the electric and magnetic fields within the FDTD update algorithm.

2.3.3 Lorentz-Drude model user interface in OptiFDTD

The Lorentz-Drude model user interface is shown below.



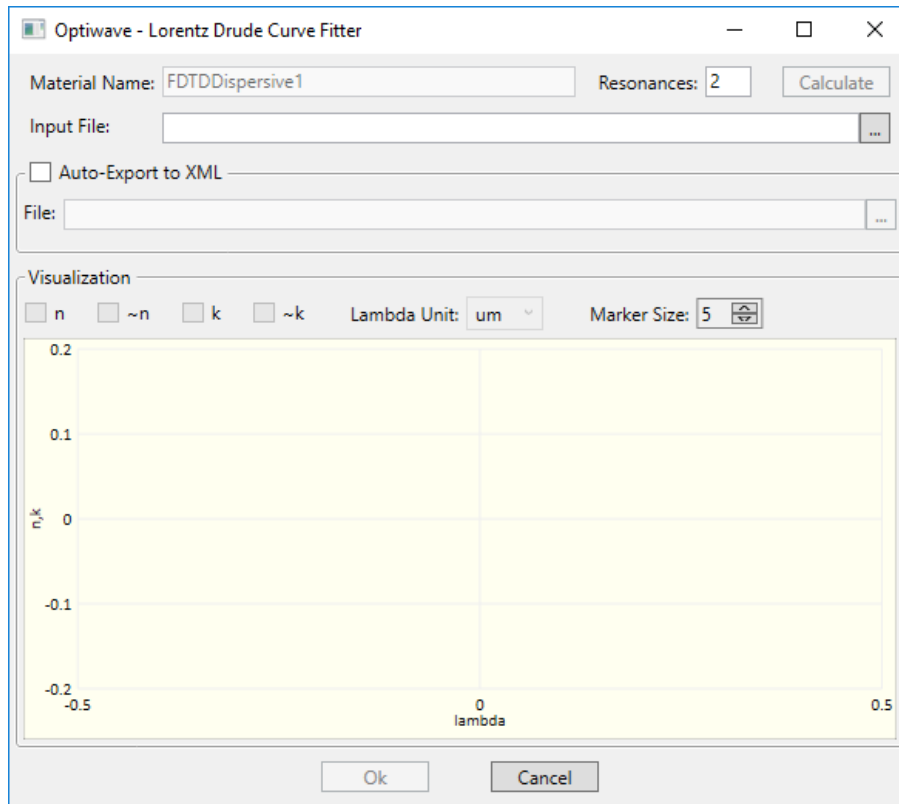
6 Dispersive Material Form

In this dialog, the user has 2 options for setting a Lorentz-Drude model, either they can enter the required coefficients for each resonant term as defined in the previous equations or the user can use the fit functionality to have the software calculate the required coefficients from a refractive index file. The following notation is used for the coefficients:

- **resonance**: number of resonance terms (This will be # Lorentz terms + 1 Drude term, in this example 5 Lorentz terms and 1 Drude)
- **Strength**: Strength of the corresponding resonance term
- **Plasma (rad/s)**: Plasma frequency
- **Resonant (rad/s)**: Resonant frequency
- **Damping (rad/s)**: Collision frequency (or damping factor)

2.3.3.1 Lorentz-Drude fitting functionality

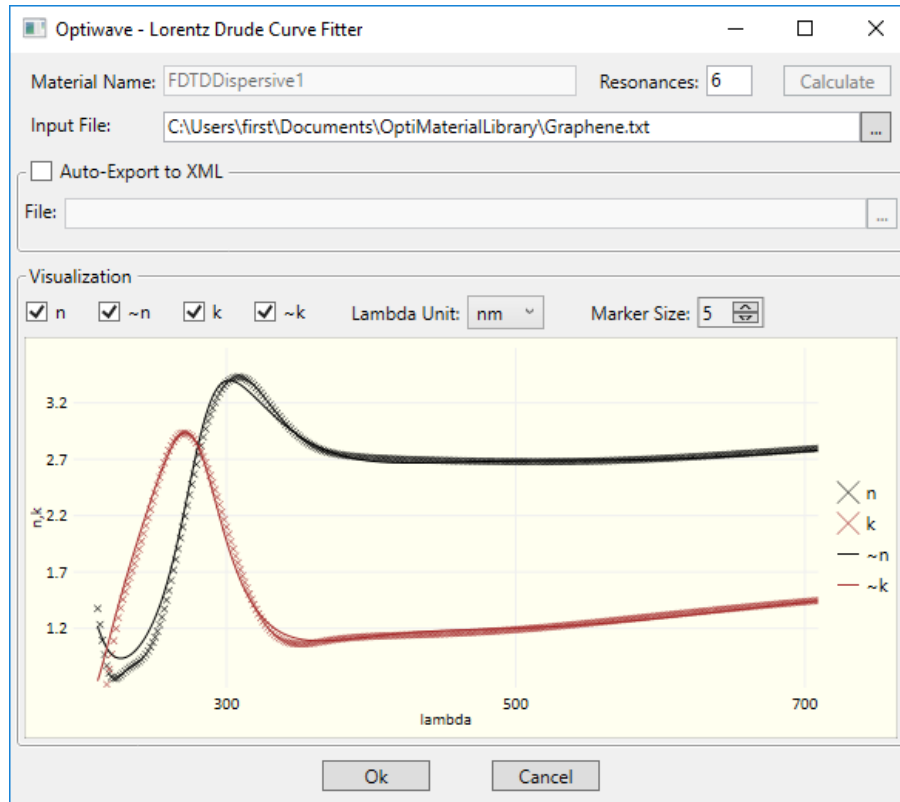
Within the main Lorentz-Drude dialog the user can have the software perform the Lorentz-Drude fit to a complex refractive index spectrum ($\kappa > 0$ is absorption) and give4n the number of resonances, provide the coefficients. This functionality is accessed through the **Fit Curve...** button which launches the *Lorentz-Drude Curve Fitter*.



7 Lorentz-Drude Curve Fitter

The dialog controls are:

- *Resonances* - the number of resonances to use in the fit this will include the number of Lorentz terms and one Drude term, in this example 1 Lorentz terms and 1 Drude.
- *Calculate* - activates the fitting functionality, will only be enabled once an input file has been provided.
- *Input File* - the input file needs to be 3 columns: lambda, n , and κ . The file can be accessed through the ... button on the right of the field.
- *Auto-Export to XML* - If the check box is selected the material fit can will automatically be saved to the location specified in the file which is selected using the ... button. The default location will be the users material library. The save is triggered by the *Calculate* or *Ok* buttons
- n , $\sim n$, κ , $\sim \kappa$ - check boxes that enable or disable the visualization of the graphs of the data from the file and the fit results (indicated by \sim).
- *Lambda Unit* - allows the user to indicate the units used in the input file.
- *Marker Size* - allows the user to control the size of the markers used in the graph.
- *Ok* - save the material to file (if Auto-Export is enabled) and transfer the fit coefficients to the main Lorentz-Drude form.
- *Cancel* - exit form without transferring results to main form.



8 Lorentz-Drude Curve Fitter - Example Graphene Fit

2.3.4 References

1. Aleksandar D. Rakic, Aleksandra B. Djuricic, et. al., "Optical Properties of Metallic Films for Vertical - Cavity Optoelectronic Devices". 1998 Optical Society of America, August, Vol. 37, No. 22, Applied Optics, pp. 5271-5283.
2. M. I. Markovic and A. D. Rakic, " Determination of reflection coefficients of laser light of wavelength (0.22 um, 200um) from the surface of aluminum using the Lorentz-Drude model", Appl. Opt. 29, 3479-3483 (1990).
3. M. I. Markovic and A. D. Rakic, " Determination of optical properties of aluminum including electron reradiation in the Lorentz-Drude Model", Opt. Laser technol. 22, 394-398, (1990).
4. Ziolkowski, R. W., "Incorporation of microscopic material models into FDTD approach for ultrafast optical propagation," IEEE Transactions on Antennas and Propagation, 375-391, (1997).
5. Liang, T., Ziolkowski, R. W., "Dispersion effects on grating-assisted output couplers under ultra-fast pulse excitations", Microwave and Opt. Tech. Lett., **17**, 17-23, (1998).

2.4 Nonlinear Materials Models

Nonlinear optical behavior can be typically attributed to the dependence of the polarization $P(t)$

on the applied electric field, $\mathbf{E}(t)$. Assuming an isotropic dispersive material, Maxwell's equations are:

$$\begin{aligned}\mu_0 \frac{\partial \mathbf{H}}{\partial t} &= -\nabla \times \mathbf{E} \\ \frac{\partial \mathbf{D}}{\partial t} &= \nabla \times \mathbf{H}\end{aligned}$$

where \mathbf{D} is expressed as linear (L) and nonlinear (NL) contributions

$$\mathbf{D} = \mathbf{P}^L + \mathbf{P}^{NL}$$

2.4.1 Linear Polarization

The linear polarization term, \mathbf{P}^L , can be written as a Lorentz oscillator differential equation:

$$\frac{\partial^2 \mathbf{P}_m^L}{\partial t^2} + \Gamma_m \frac{\partial \mathbf{P}_m^L}{\partial t} + \omega_m^2 \mathbf{P}_m^L = \epsilon_0 \chi_0 G_m \omega_m^2 \mathbf{E}$$

where \mathbf{P}^L is generally referred to as:

$$\mathbf{P}^L = \epsilon_0 \epsilon_L \mathbf{E}$$

where ϵ_L is the linear relative permittivity.

2.4.2 Nonlinear Polarization

The nonlinear polarization \mathbf{P}^{NL} may come from various models. Currently OptiFDTD can handle four kinds of nonlinearity:

- Dispersive second-order nonlinear materials
- Dispersive third-order nonlinear materials
- Dispersive Kerr effect
- Dispersive Raman effect

For all four possible nonlinear models, the 2D Lorentz model can be included by selecting the labelled check mark and entering the required coefficients in the Lorentz tab within the dialog.

2.4.2.1 Dispersive 2nd order nonlinear materials

In this model, the nonlinear polarization is expressed as

$$\mathbf{P}^{NL}(t) = \epsilon_0 \chi^{(2)} * \mathbf{E}^2(t)$$

where $\chi^{(2)}$ is the second order isotropic susceptibility. In order to simulate second order nonlinear effects, two parameters are required: the linear relative permittivity, ϵ_L , and the second order isotropic susceptibility, $\chi^{(2)}$.

2.4.2.2 Dispersive 3rd order (Kerr) nonlinear materials

Like the second-order nonlinearity, OptiFDTD can model third-order nonlinearity with the nonlinear polarization

$$\mathbf{P}^{NL}(t) = \epsilon_0 \chi^{(3)} * \mathbf{E}^3(t)$$

where $\chi^{(3)}$ is the third order isotropic susceptibility. Again the only two parameters required are the linear relative permittivity, ϵ_L , and the second order isotropic susceptibility, $\chi^{(3)}$.

2.4.2.3 Dispersive 3rd order (Kerr - Response Time) materials

If the time scale over which the medium changed is greater than the pulse width, we should take into account the effects of the finite response time of the medium. The theory for this model is well documented in the work of Prof. Richard W. Ziolkowski 's work [1-4], OptiFDTD treats the nonlinear effect with a finite response time as well as an instantaneous manner by solving the phenomenological susceptibility equation simultaneously with Maxwell's equation:

$$\begin{aligned} \mathbf{P}^{NL}(t) &= \epsilon_0 \chi^{NL} \mathbf{E}(t) \\ \frac{\partial \chi^{NL}}{\partial t} + \frac{1}{\tau} \chi^{NL} &= \frac{1}{\tau} \epsilon_2 |E|^2 \end{aligned}$$

where

- χ^{NL} is the nonlinear susceptibility
- τ is the response time of the material
- ϵ_2 is the Kerr permittivity

are the three parameters that are required when configuring a 3rd order material with the response time included.

2.4.2.4 Dispersive Raman effect

The Raman model allows another way to simulate the nonlinear phenomenon where the nonlinear susceptibility is modeled by a second-order derivative equation which is related to the resonant wavelength and the response time

$$\begin{aligned} \mathbf{P}^{NL}(t) &= \epsilon_0 \chi^{NL} \mathbf{E}(t) \\ \frac{\partial^2 \chi^{NL}}{\partial t^2} + \omega_R^2 \tau_R \frac{\partial \chi^{NL}}{\partial t} + \omega_R \chi^{NL} &= \epsilon_R \omega_R^2 |E|^2 \end{aligned}$$

where

- χ^{NL} is the nonlinear susceptibility
- τ is the response time of the material
- ϵ_R is the Raman permittivity
- ω_R is the Raman resonant frequency

are the four parameters required when configuring a Raman material.

2.4.2.5 Nonlinear effects simulation

To observe nonlinear effects in commonly used materials, a high-intensity light source is required. When creating a design, the user should pay special attention to the input wave amplitude and/or the power level. Each nonlinear effect has a different threshold which is controlled by the parameters and as such varying the input may be required in order to observe the desired nonlinear phenomenon.

2.4.2.6 References

1. Ziolkowski, Richard W., Judkins, Justin B., "Full-wave vector Maxwell equation modeling of the self-focusing of ultrashort optical pulses in a nonlinear Kerr medium exhibiting a finite response time", J. Opt. Soc. Am. B, **2**, 186-198 (1993).
2. Ziolkowski, Richard W., Judkins, Justin B., "Nonlinear finite-difference time-domain modeling of linear and nonlinear corrugate waveguides", J. Opt. Soc. Am. B, **9**, 1565-1575, (1994).
3. Ziolkowski, Richard W., Judkins, Justin B., "Applications of the nonlinear finite-difference time-domain (NL-FDTD) method to pulse propagation in nonlinear media: self-focusing and linear-nonlinear interfaces", Radio Science, 901-911, (1993).
4. Ziolkowski, Richard W., "The incorporation of microscopic material models into the FDTD approach for ultrafast optical pulse simulations", IEEE Trans. On Antenna and Propagation, **3**, 375-391, (1997).
5. Joseph, Rose M., Taflove, Allen, "FDTD Maxwell's equations models for nonlinear electrodynamics and optic", IEEE Trans. On Antenna and Propagation, **3**, 364-374, (1997).
6. Goorjian, Peter M., Taflove, Allen, Joseph, Rose M., "Computational modeling of Femtosecond optical soliton from Maxwell's equation", IEEE Journal of Quantum electronics, **10**, 2416-2422, (1992).
7. Joseph, Rose M., Taflove, Allen, " Spatial soliton deflection mechanism indicated by FD-TD Maxwell's equations modeling", IEEE Photonics Technology Letters, **10**, 1251-1254, (1994).

3 OptiFDTD Boundary Conditions

While modelling the propagation of light an FDTD simulation must address how to calculate the field at boundaries as information required by the updating equation would not be present. The basic FDTD algorithm must be modified at the boundaries of the computational window. The boundary conditions that can be used can vary from absorbing boundary conditions (ABC) or perfect conductor to periodic conditions. There are 4 boundary conditions available within OptiFDTD:

- Perfectly Matched Layers (**PML**)
- Perfect Electric Conductor (**PEC**)
- Perfect Magnetic Conductor (**PMC**)
- Periodic Boundary Condition (**PBC**)

This section will explore the details of each of the boundary conditions.

3.1 PML Boundary Conditions

A PML or perfectly matched layer boundary condition is one in which the refractive index within the simulation domain is match, therefore reducing reflections, but a loss is introduced through the layer such that there is no field to return to the simulation domain when it is reflected. OptiFDTD uses the Anisotropic PML, or so-called Un-split PML (UPML) implementation. The theory of the UPML is very well explained in the provided references [1-3]. The UPML boundary conditions are physical rather than numerical because their implementation is based on a Maxwellian formulation rather than on a mathematical model. Their absorbing properties are physically equivalent to the properties of an absorbing uni-axial anisotropic medium with the following permittivity and permeability tensors:

$$\begin{aligned}\hat{\epsilon} &= \epsilon \hat{S} \\ \hat{\mu} &= \mu \hat{S}\end{aligned}$$

Where:

$$\begin{aligned}\hat{S} &= \begin{pmatrix} s^{-1} & 0 & 0 \\ 0 & s & 0 \\ 0 & 0 & s \end{pmatrix} \\ s &= \kappa - j \frac{\sigma}{\epsilon_0 \omega}\end{aligned}$$

A plane wave incident on a half space composed of the above uni-axial medium with an interface in the $x = \text{a constant}$ plane is purely transmitted into it, it has match the material on the simulation side of the boundary. This reflection/transmission property is completely independent of the angle of incidence, polarization or frequency of the incident wave.

The numerical implementation of the UPML in a 2D (X-Z) computational window requires the introduction of such perfectly matched absorbing layers on all four sides of the simulation domain. The corners, where a vertical layer overlaps a horizontal layer, require special attention. In these regions the permittivity and permeability tensors must be modified to:

$$\hat{S} = \begin{pmatrix} s_x^{-1} & 0 & 0 \\ 0 & s_x & 0 \\ 0 & 0 & s_x \end{pmatrix} \begin{pmatrix} s_z & 0 & 0 \\ 0 & s_z & 0 \\ 0 & 0 & s_z^{-1} \end{pmatrix}$$

$$s_x = \kappa_x - j \frac{\sigma_x}{\epsilon_0 \omega}$$

$$s_z = \kappa_z - j \frac{\sigma_z}{\epsilon_0 \omega}$$

The minimization of the numerical reflectance of the Anisotropic PML layers requires spatial scaling of the conductivity profile, the source of the required losses, from zero (at the interface of the PML) to a maximum value (the end of the computational window):

$$\sigma(x) = \sigma_{max} \left(\frac{x}{L} \right)^m$$

$$\kappa(x) = 1 + (\kappa_{max} - 1) \left(\frac{x}{L} \right)^m$$

where L is the thickness of the Anisotropic PML. Typical values for the parameter m are between 2 and 4.

3.1.1 References

1. Bérenger, J. P., "A perfectly matched layer for the absorption of electromagnetic waves," *Journal of Computational Physics*, **114**, 185-200, (1994).
2. Gedney, S. D., "An anisotropic perfectly matched layer absorbing media for the truncation of FDTD lattices," *IEEE Transactions on Antennas and Propagation*, 1630-1639, (1996).
3. Taflov, A., "Advances in Computational Electrodynamics—The Finite-Difference Time-Domain Method", Artech House, Boston, Ch. 5, (1998).

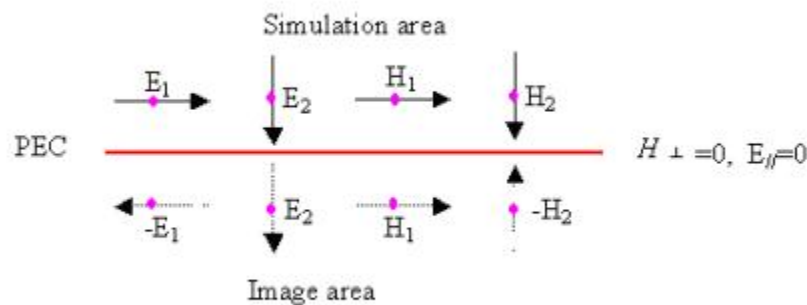
3.2 PMC / PEC boundary conditions and plane wave simulations

Perfect Magnetic Conductor (**PMC**) and Perfect Electric Conductor (**PEC**) boundary conditions can be used as "mirrors" for specific field components. These boundary conditions, along with symmetry within a given design can be used to reduce the computational domain size. They are mainly used in the following types of simulations:

- Plane wave simulation
- Domain reduced simulation for symmetric, periodic, or photonic band gap structures

3.2.1 Perfect Electric Conductor

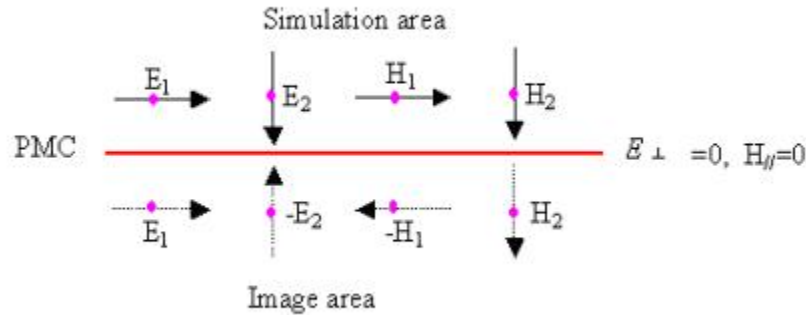
The following figure shows the field components (perpendicular, \perp , and parallel, \parallel) across a PEC wall (zero thickness) along with their image values. Along the perfect electric conductor the parallel E field (E_{\parallel}) and total perpendicular H field (H_{\perp}) must be zero. Therefore from opposing sides of the boundary these components are equal magnitude and opposite sign. The other field components are mirrored across the boundary.



9 Field across a PEC and image area

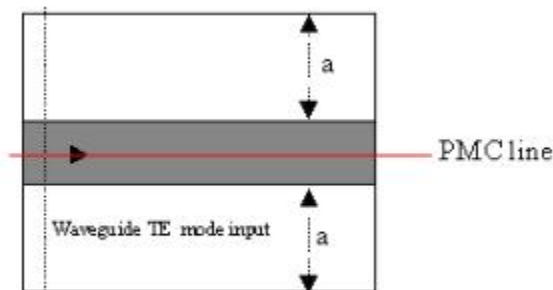
3.2.2 Perfect Magnetic Conductor

The perfect magnetic conductor, as shown below, is a layer that enforces that the parallel H components and perpendicular E components are zero along the boundary while all other components are mirrored across the boundary.



10 Field across a PMC and image area

When determining the use of symmetry it is useful to identify the fields that should be mirrored over the symmetry and identify the required conductor according to the descriptions above. In the structure seen below the E field (TE and therefore E_y) must be mirrored. As the E_y component with a waveguide solution is parallel to the symmetry axes it is necessary for a PMC boundary (Parallel E fields are copied) to be used to act as the symmetry axis for a structure such as depicted below. this would allow only the top half of the simulation to be calculated yet yield the same results (for the half-space) as it would have if the entire simulation was run. :

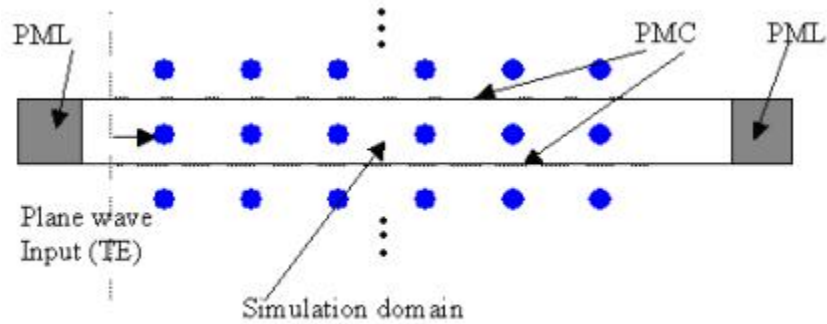


11 PMC wall in a symmetric waveguide excited by symmetric TE waveguide mode

3.2.3 Plane waves in symmetric and periodic structures

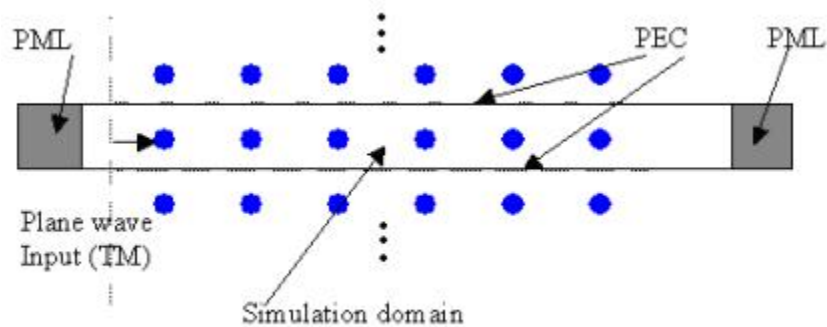
A plane wave within OptiFDTD can be created using the rectangular wave parameters in the **Input Wave Properties** dialog box and using appropriate boundary conditions. The graph below shows how a simulation with a plane wave source can be realized within a symmetric structure. For a 2D TE simulation (E_y, H_x, H_z), the boundaries parallel to the propagation direction are along the z axis, within the YZ plane. As the E field (E_y) is expected to be symmetric, this is the waveguide

solution for this polarization, about these boundaries and it is parallel to the plane containing the boundary the condition placed on this boundary should be that of a PMC in order to obtain a plane wave.



12 Plane wave in TE simulation

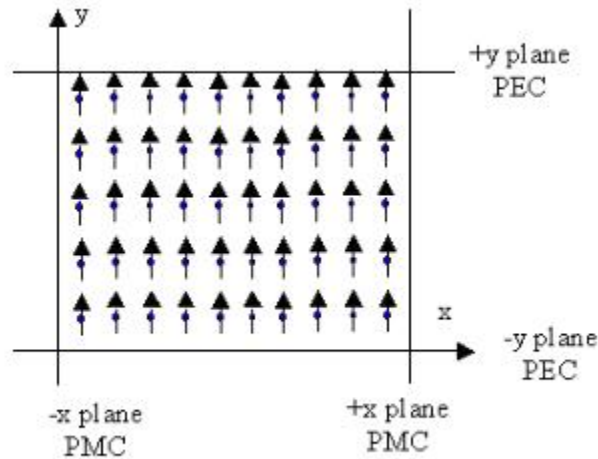
For a 2D TM simulation (H_y , E_x , E_z), it is the the H_y component with the waveguide solution that is parallel to the plane containing the boundaries. As such it is PEC conditions that are required.



13 Plane wave in TM simulation

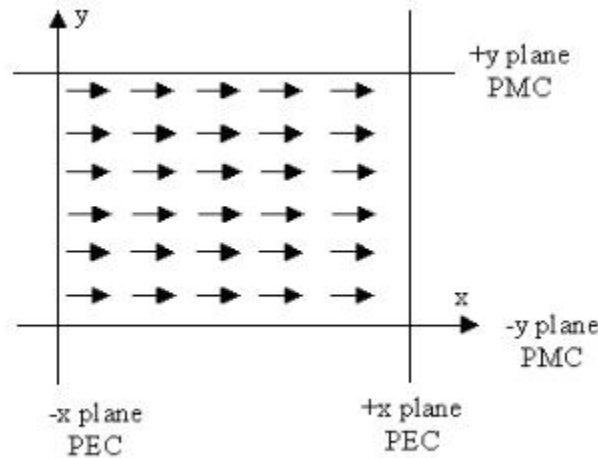
For a 3D simulation, a correct plane wave realization depends on the wave polarization (dominant field component) and the boundary condition setup at different edges of the propagation plane.

With Z-directed propagation and a polarization along Y, the dominant field component is E_y . This component is parallel to the YZ plane, requires a PMC, and perpendicular to the XZ plane, requires a PEC.



14 Y-polarized plane wave propagating along Z with boundary conditions

If the wave propagating in the Z-direction is polarized along X, then the dominant field component, E_x , is parallel to the XZ plane, and perpendicular to the YZ plane, requires a PMC, and perpendicular to the YZ plane, requires a PEC.



15 X-polarized plane wave propagating along Z with boundary conditions

3.3 PBC Boundary Conditions

OptiFDTD provides the option to use simplified **Periodic Boundary Conditions (PBC)**. PBCs can work with other boundary conditions such as Anisotropic PML, PMC, and PEC. When creating simulations that are periodic or require plane wave sources a PBC can be used in place of determining the nature of the boundary condition and using the required PMC or PEC.

The simplified PBC is based on Bloch's Theorem:

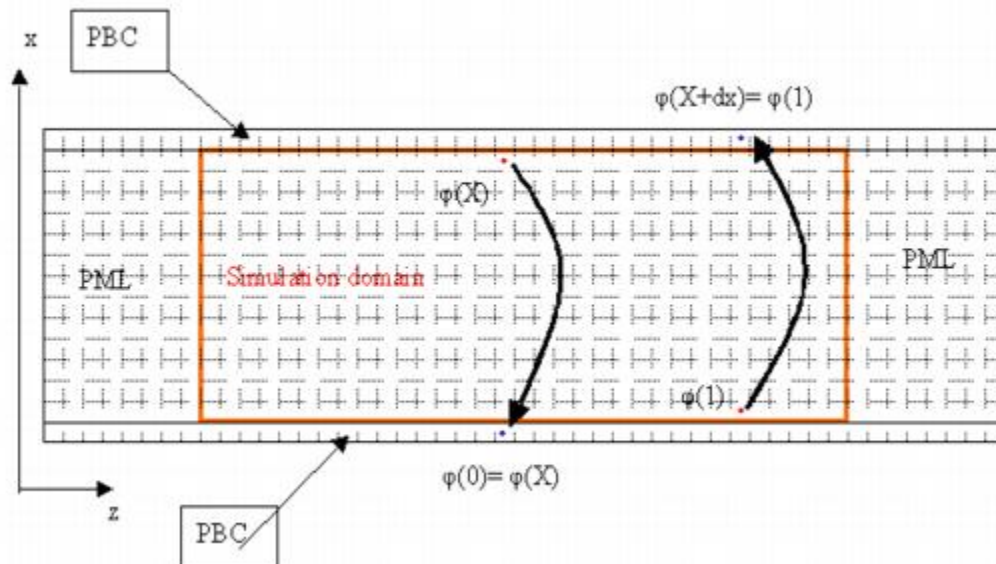
For a periodic layout with a period of $\Delta\gamma$, the wave function, ψ , is written as the combination of a cell periodic component and a wave-like component:

$$\psi(\gamma + \Delta\gamma) = \psi(\gamma)e^{jk\Delta\gamma}$$

The equation above needs to have a predefined value for the k vector, k , for the wave-like component; a quantity not feasible for a time domain simulation such as FDTD, particularly in the case of pulsed input (broadband). Therefore, the the problem is simplified by setting the k -vector in one specific direction as zero, which then leads to the input wave being the axis-propagated wave, and then the equation becomes:

$$\psi(\gamma + \Delta\gamma) = \phi(\gamma)$$

With this simplification $\psi(\gamma)$ is the field component at one edge of the simulation domain, and $\psi(\gamma + \Delta\gamma)$ is the corresponding field value at the boundary of the opposite edge. The figure below shows the relationship between these values:



16 PBC applied to a 2D periodic mesh

4 Light Sources

Light sources are the means through which energy is injected into an FDTD simulation. There are 2 light sources available to the user within OptiFDTD.

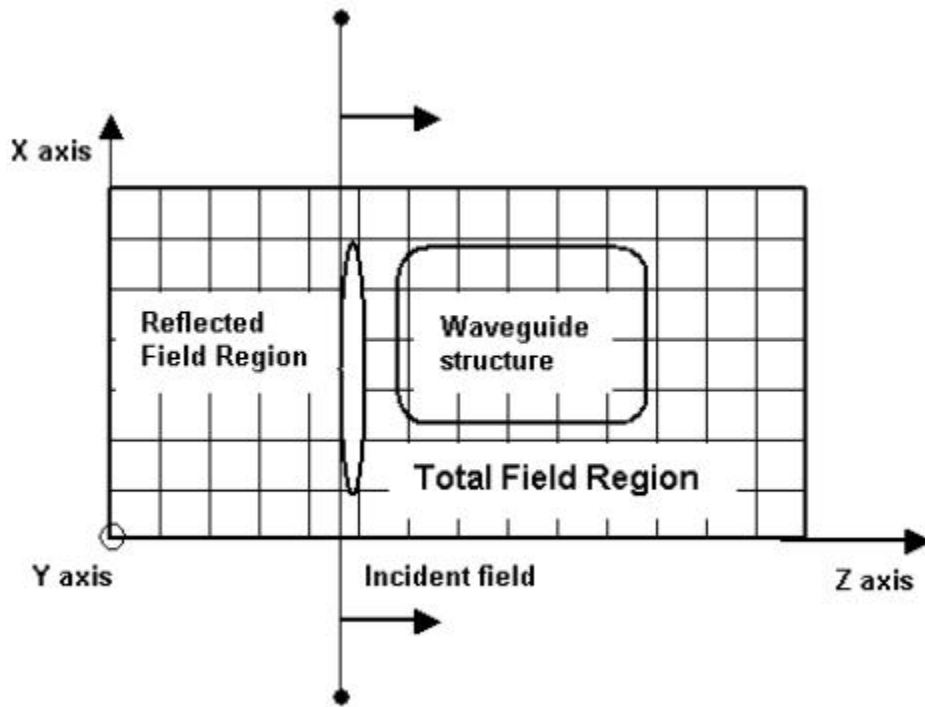
- Input planes
- Point sources

Input planes are used when light can be injected through a plane in the simulation domain. It propagates in a particular direction and has an intensity distribution across the incidence plane. Point sources can be used to simulate point emitters, for example quantum wells or quantum dots, or dipole sources.

4.1 Input planes

The FDTD numerical method yields the solution of an initial value problem where on the first time step of the simulation all fields are set to zero. The algorithm then requires the initial field excitation that will be propagated through the computational domain. The FDTD Total/Reflected Field formulation is used in defining a propagating incident field. 2D simulations support propagation in X and Z while 3D simulations support propagation in X, Y, and Z.

The OptiFDTD input plane is implemented through a Total/Reflected field formulation where the computational domain is separated into two sub-regions as shown in the figure below. The two regions, the *total field region* and the *reflected field region*, are separated by the plane called the *incident field* where the incident wave can be generated by specifying the exact field distribution on the incident plane at each time interval..



17 Total/Reflected field formulation

The Total Field Region contains information for both the incident and scattered (reflected) waves. As such this is the region where any structures under test ideally should be created. The Reflected Field will only contain propagating waves that are fields reflected from the Total Field Region. A simple explanation would be to consider the incident field as being generated by a flashlight located on the incidence plane facing the assigned direction. Before starting the simulation the flashlight is turned off and the field values in the whole computational domain are equal to zero. The flashlight is switched on at $t = 0$ and illuminates only the Total Field Region. Provided that the excitation scheme is perfect, there should not be any light detected by an observer located in the Reflected Field Region, unless there are some obstacles within the total field region which would generate the reflections.

Either the continuous wave (CW, single wavelength) or pulsed (broadband) excitations can be used.

4.1.1 Continuous Wave (CW) excitation

In CW excitation, the time dependence of the incident field is a single frequency sinusoidal function which modifies the field amplitude. For example, an incident E_y field from a Z direction input plane in a 2D TE simulation would have the following form:

$$E_y^{inc}(x, z_{inc}) = A \cdot F(x, z_{inc}) \cdot \left[1 - e^{-t/t_r} \right] \cdot \sin(\omega t + \theta_i)$$

where

- A is the field amplitude
- $A \cdot F(x, z_{inc})$ is the transverse field profile at the incident plane location z_{inc}
- θ_i is the initial phase (i.e. at $t = 0$) of the field at the center of the source.
- ω is the angular frequency of the input wave.
- t_r is a constant (equal to λ/c) which defines the rise time coefficient of the exponential function used to ramp the CW signal to full amplitude. In the CW case the optical wave propagates until it reaches the stationary state everywhere in the computational window.

4.1.2 Pulsed excitation

Pulsed excitations within OptiFDTD are created with a Gaussian pulse envelope function in time and has the form:

$$E_y^{inc}(x, z_{inc}) = A \cdot T(t) \cdot F(x, z_{inc}) \cdot \sin(\omega(t - t_{delay}) + \theta_i)$$

where

$$T(t) = \exp \left[-\frac{1}{2} \left(\frac{t - t_{delay}}{\sigma} \right)^2 \right]$$

is the pulse envelope function, t_{delay} is the time delay and σ is the standard deviation of the Gaussian function.

⚠ Please note that in OptiFDTD the definition of σ is linked to the the full width at half maximum (FWHM) as $FWHM = 2(\sqrt{2\ln 2})\sigma$

For pulsed excitation, the time stepping continues until the desired time pulse response is observed at the field points of interest. It is good practice to include observation points to monitor this response on top of any detectors required for the simulation.

4.1.3 Transverse profiles

There are four profile types available: Gaussian, rectangular, modal, and user-defined. The notation used here assumes a Z direction input plane. Also, in these equations, $k = -j\gamma$, where γ is the propagation constant. If the refractive index is real then $k = 2\pi n/\lambda$. See the page [Constant Dielectrics \(Including Loss\)](#) for more details.

4.1.3.1 Gaussian

For 3D simulations, the Gaussian profile of the source is calculated using the scalar elliptical Gaussian beam equation [1]. The coordinate system (x, y, z) is that of the Gaussian beam, with $(0, 0, 0)$ being at the center of the beam waist and z being the propagation axis. The magnitude of the electric field on the input plane is given by

$$E(x, y, z) = E_0 \sqrt{\frac{w_{0x} w_{0y}}{w_x(z) w_y(z)}} e^{-x^2/w_x(z)^2 - y^2/w_y(z)^2} e^{-j(kz + kx^2/2R_x(z) + ky^2/2R_y(z) - \Phi_x(z)/2 - \Phi_y(z)/2)}$$

where E_0 is the amplitude (a real constant). w_{0x} and w_{0y} are the beam waist radii, measured along the X and Y axes. This is the distance between the center of the source, where $|E| = E_0$, and where the electric field drops to $|E| = E_0/e$. $w_x(z)$ and $w_y(z)$ are the beam radii a distance z from the beam waist, $R_x(z)$ and $R_y(z)$ are the radii of curvature, and $\Phi_x(z)$ and $\Phi_y(z)$ are the x and y contributions to the Gouy phase. These quantities are computed with the following equations.

$$\begin{aligned} w_x(z) &= w_{0x} \sqrt{1 + (z/z_{rx})^2}, & w_y(z) &= w_{0y} \sqrt{1 + (z/z_{ry})^2}, \\ R_x(z) &= z(1 + (z_{rx}/z)), & R_y(z) &= z(1 + (z_{ry}/z)), \\ \Phi_x(z) &= \arctan(z/z_{rx}), & \Phi_y(z) &= \arctan(z/z_{ry}). \end{aligned}$$

In the above, $z_{rx} = w_{0x}^2 k/2$ and $z_{ry} = w_{0y}^2 k/2$ are the Rayleigh lengths, and $k = -j\gamma$, where γ is the propagation constant.

When $w_{0x} = w_{0y} = w_0$, the field has no azimuthal dependence and the Gaussian beam equation reduces to

$$E(r, z) = E_0 \frac{w_0}{w(z)} e^{-r^2/w(z)^2} e^{-j(kz + kr^2/2R(z) - \Phi(z))}$$

where $r = \sqrt{x^2 + y^2}$, $w(z) = w_0 \sqrt{1 + (z/z_r)^2}$, $R(z) = z(1 + z_r/z)$, $\Phi(z) = \arctan(z/z_r)$, and $z_r = w_0^2 k/2$. This is also the equation used to compute the fields on the input plane for 2D simulations.

In OptiFDTD Designer, the user can set the "Full Width at $1/e^2$ " of the Gaussian profile. This is equal to twice the beam waist radius of the intensity of the source. Note that the full width at $1/e^2$ of the intensity is equal to the full width at $1/e$ of the electric field.

4.1.3.2 Rectangular

The rectangular profile is modeled as a plane wave with a finite width. The equation used is, in the coordinate system of the plane wave,

$$E(x, y, z) = \begin{cases} E_0 e^{-jkz}, & \text{if } |x| < w_{0x} \text{ and } |y| < w_{0y} \\ 0, & \text{otherwise} \end{cases}$$

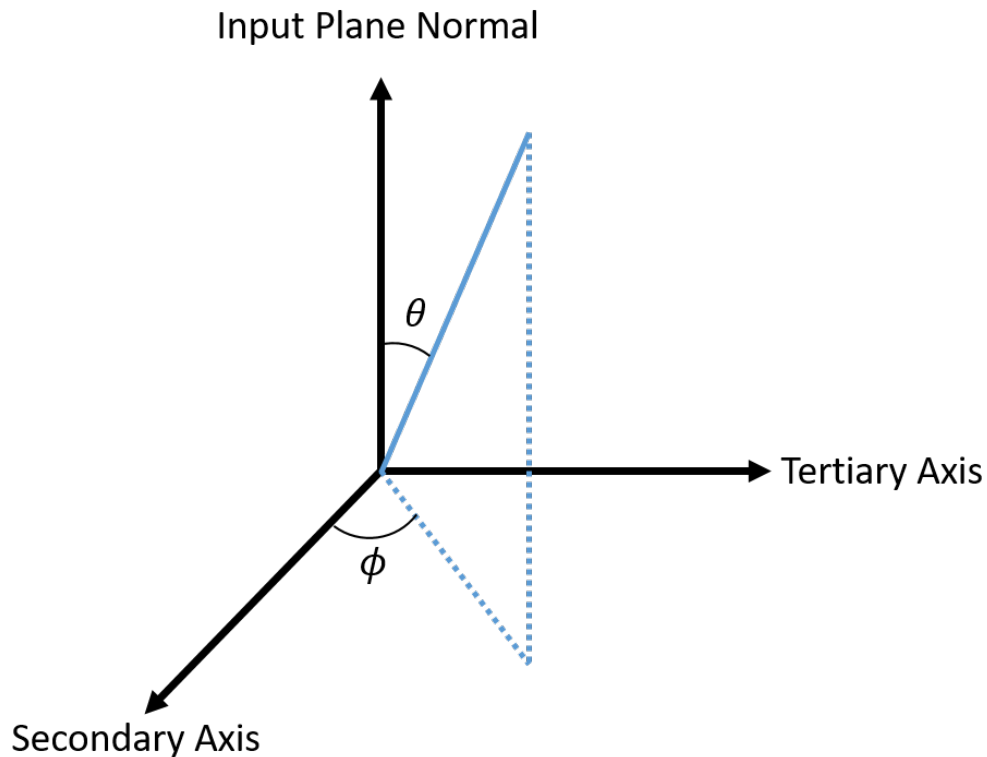
4.1.4 Tilted source

The propagation axis of the Gaussian, rectangular, and modal profiles can be angled with respect to the input plane normal.

4.1.4.1 Gaussian and rectangular

In a 2D simulation, the tilting angle is measured with respect to the input plane normal, anticlockwise around the Y axis, regardless of input plane direction.

In a 3D simulation, a spherical coordinate system is used to define the tilting angle. θ is the inclination angle, measured with respect to the input plane normal, anticlockwise around the tertiary axis. ϕ is measured anticlockwise around the secondary axis. See the image below, where the solid blue line is the propagation axis.



The right-hand rule is used to identify the secondary and tertiary axes, based on the direction of the input plane normal. For example, with a Z direction input plane, Z is the input plane normal (or primary axis), X is the secondary axis, and Y is the tertiary axis.

Note that the propagation axis is really the direction of the propagation constant $\vec{\gamma}$. If the material is *isotropic*, i.e. all three elements of the diagonal permittivity tensor are equal ($\epsilon_{xx} = \epsilon_{yy} = \epsilon_{zz}$), then the Poynting vector and the propagation constant are parallel. If the material is *anisotropic*, the Poynting vector and the propagation constant may not be parallel. In other words, the tilting angles θ and ϕ define the direction of the propagation constant which may not match the direction of the Poynting vector.

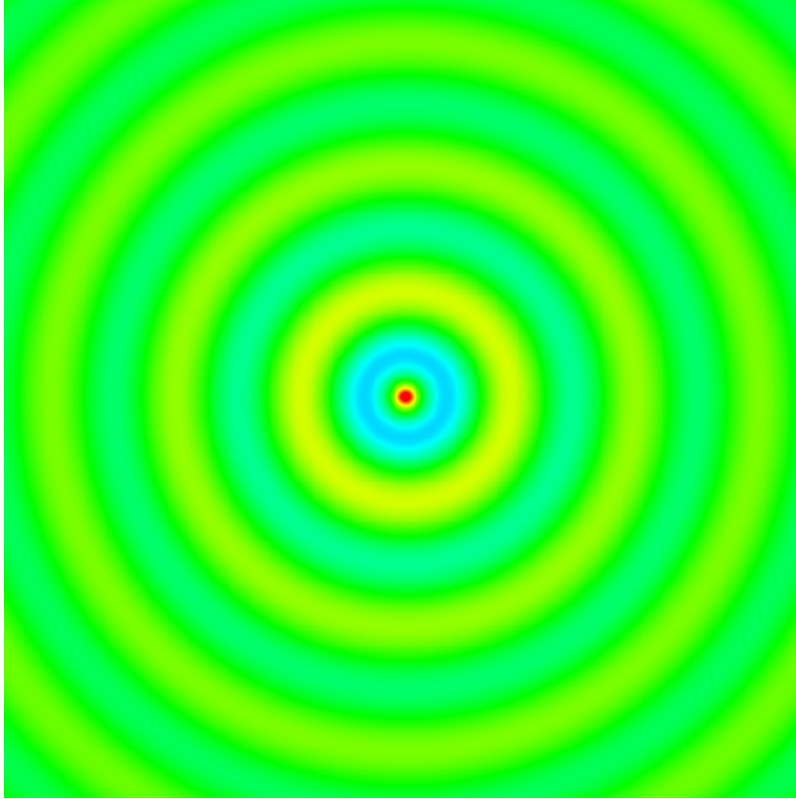
4.1.5 References

[1] Amnon Yariv and Pochi Yeh, *Photonics*, Oxford University Press, sixth edition, 2007.

4.2 Point Sources

A point source is used to model the situation of exciting a single point within the FDTD grid. This source can also be used to model dipole sources, because point sources induce dipole like field profiles in the other field components. In the correct plane the field component that is excited will radiate away from a single point in space

in a concentric spherical pattern as seen in the figure below. 2D simulations have the point source set to the E_y (TE) and H_y (TM) components while 3D simulations allow the user to select from the E field components.



18 A Point source (2D E_y)

The point source within OptiFDTD is created as a soft source, a source where the excitation is added to existing fields as opposed to enforcing a value. This is accomplished through the excitation of the current density J . For example Maxwell's curl equation for the E_z component becomes

$$\epsilon \frac{\partial E_z}{\partial t} = (\nabla \times H)_z - J_z$$

where J is defined from an analysis of the enclosed charge within the Yee cell and calculated as [1]

$$\begin{aligned} J &= \frac{I_{enclosed}}{Area} \\ &= \epsilon(\Delta x \Delta y + \Delta x \Delta z + \Delta z \Delta y) \frac{\partial E}{\partial t} \end{aligned}$$

where E is the desired excitation.

4.2.1 Continuous wave (CW) excitation

The field used in the above expression for J when modelling a CW source is expressed as:

$$F = A \cdot \left[1 - e^{(-t/t_r)} \right] \cdot \sin(\omega t + \theta_i)$$

where

- A is the field amplitude
- θ_i is the the initial phase offset which is the phase difference between points in the incidence plane. The phase offset can be adjusted to define the direction of the incident field.
- ω is the angular frequency of the input wave.
- t_r is a constant (equal to λ/c) which defines the rise time coefficient of the exponential function used to ramp the CW signal to full amplitude. In the CW case the optical wave propagates until it reaches the stationary state everywhere in the computational window.

4.2.2 Pulsed excitation

The field used in the above expression for J when modelling a pulsed source is expressed as:

$$F = A \cdot \exp\left[-1/2 \cdot (t - t_{delay})^2 / T^2\right] \cdot \sin[\omega(t - t_{delay}) + \theta_i]$$

where t_{delay} is the time delay for the signal and T is the standard deviation of the Gaussian function that forms the envelope of the pulse in time.



- Point sources can work with other kinds of sources (such as input planes).
- When a Point source is used as the key input. The normalized power calculation will be disabled in analyzer

4.2.3 References

1. Fumie Costen, Jean-Pierre Bérenger, Anthony K. Brown, "Comparison of FDTD Hard Source with FDTD Soft Source and Accuracy Assessment in Debye Media". IEEE Trans. on Ant. and Prop., Vol. 57, No. 7, July 2009.

5 S-Parameters

The S-Parameter functionality within OptiFDTD uses ports across input and output waveguides into a structure in order to provide the S-Parameter matrix. These S-Parameters are derived from the forward and reverse propagating modes obtained through eigenmode expansion.

5.1 Technical Background on the Eigenmode Expansion of an Electromagnetic Field

The total electric and magnetic fields propagating within a waveguide are equal to the summation of both the forward and reverse propagating fields

$$(1) \quad \vec{E}_T = \vec{E}_F + \vec{E}_R$$

$$(2) \quad \vec{H}_T = \vec{H}_F + \vec{H}_R$$

This can be represented as a linear expansion of the electric and magnetic fields, where T and R are complex weights of each forward and reverse propagating mode and m is an integer representing different modes supported by the waveguide.

$$(3) \quad \vec{E}_F = \hat{i} \sum_{m=0}^{\infty} T_m E_x^m + \hat{j} \sum_{m=0}^{\infty} T_m E_y^m$$

$$(4) \quad \vec{E}_R = \hat{i} \sum_{m=0}^{\infty} R_m E_x^m + \hat{j} \sum_{m=0}^{\infty} R_m E_y^m$$

$$(5) \quad \vec{H}_F = \hat{i} \sum_{m=0}^{\infty} T_m H_x^m + \hat{j} \sum_{m=0}^{\infty} T_m H_y^m$$

$$(6) \quad \vec{H}_R = -\hat{i} \sum_{m=0}^{\infty} R_m H_x^m - \hat{j} \sum_{m=0}^{\infty} R_m H_y^m$$

This in turn allows the total electric and magnetic fields to be expressed

$$(7) \quad \vec{E}_T = \hat{i} \sum_{m=0}^{\infty} (T_m + R_m) E_x^m + \hat{j} \sum_{m=0}^{\infty} (T_m + R_m) E_y^m$$

$$(8) \quad \vec{H}_T = \hat{i} \sum_{m=0}^{\infty} (T_m - R_m) H_x^m + \hat{j} \sum_{m=0}^{\infty} (T_m - R_m) H_y^m$$

For an orthonormal basis of guided modes m and n , the inner product is defined as,

$$(9) \quad \langle \vec{E}^m | \vec{H}^n \rangle = \int \int \vec{E}^m \times \vec{H}^n \cdot \hat{k} dA = \delta_{mn}$$

Where the cross product is equal to,

$$(10) \quad \vec{E} \times \vec{H} = (E_x H_y - H_x E_y) \hat{k}$$

In order to find the coefficients of the forward and reverse propagating fields (T_m and R_m) for a single mode we can start by using the cross product and place equation (7) into equation (10),

$$(11) \quad \vec{E}_T \times \vec{H}^n = \left(\sum_{m=0}^{\infty} (T_m + R_m) E_x^m H_y^n - \sum_{m=0}^{\infty} (T_m + R_m) E_y^m H_x^n \right) \hat{k}$$

$$(12) \quad \vec{E}_T \times \vec{H}^n = \sum_{m=0}^{\infty} (T_m + R_m) (E_x^m H_y^n - E_y^m H_x^n) \hat{k}$$

Placing equation (12) into equation (9) we get,

$$(13) \quad \langle \vec{E}_T | \vec{H}^n \rangle = \int \int \vec{E}_T \times \vec{H}^n \cdot \hat{k} dA = \sum_{m=0}^{\infty} (T_m + R_m) \int \int (E_x^m H_y^n - E_y^m H_x^n) dA$$

Using orthonormality (equation (9)) we get the following equation, using the fact that the inner product integral is equal to 1 when $m = n$ and 0 when $m \neq n$

$$(14) \quad \langle \vec{E}_T | \vec{H}^n \rangle = T_n + R_n$$

Following the same derivation for H_T we get,

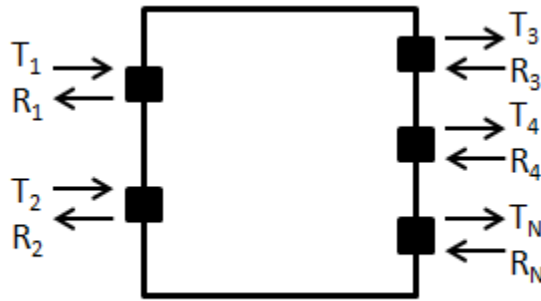
$$(15) \quad \langle \vec{E}^n | \vec{H}_T \rangle = T_n - R_n$$

T_n and R_n can now be obtained

$$(16) \quad T_n = \frac{\langle \vec{E}_T | \vec{H}^n \rangle + \langle \vec{E}^n | \vec{H}_T \rangle}{2}$$

$$(17) \quad R_n = \frac{\langle \vec{E}_T | \vec{H}^n \rangle - \langle \vec{E}^n | \vec{H}_T \rangle}{2}$$

Based on the definition of T_m and R_m , port to port scattering parameters can be calculated by using the coefficients of the guided modes at input (m) and output (n) ports.



The S parameter between port m and port n at a single frequency is given by,

$$(18) \quad S_{mn} = \frac{R_{mn}}{T_{mn}}$$

Once the s-parameters are calculated, an s-matrix can be formed to calculate the relationship between the input signals and the output signals of a device for a single wavelength/frequency.

$$(19) \quad \begin{bmatrix} O_1 \\ O_2 \\ \vdots \\ O_n \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} & S_{13} & \cdots & S_{1n} \\ S_{21} & S_{22} & S_{23} & \cdots & S_{2n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ S_{m1} & S_{m2} & S_{m3} & \cdots & S_{mn} \end{bmatrix} \begin{bmatrix} I_1 \\ I_2 \\ \vdots \\ I_m \end{bmatrix}$$

5.2 Calculate and Export S-Parameters with OptiFDTD

The S-Parameter port is a combination of an input plane and an observation area. Currently it is designed to be used with straight waveguides. The following procedure outlines the basic steps that can be followed to generate S-Parameter data from an OptiFDTD design.

1. Place one S-Parameter port for every input/output.
2. Configure the S-Parameter ports.
 - a. Select the input mode and direction (from the red line to the blue line) for every S-parameter port (Port Properties -> Reverse Direction)
 - b. Enter the input wavelength (Port Properties -> Input Field -> Wavelength). **All the ports need to have the same wavelength.**
 - c. Select the input type, CW for S-Parameters in a single frequency or Sine Modulated Gaussian for S-Parameters in a range of frequencies (Port Properties -> Input Field -> CW/Sine Modulated Gaussian). **All the ports need to have the same input type.**
3. Generate the S-parameter script (Scripting -> Scanning Script)
4. Run simulation
 - a. Open simulation settings under Simulation -> Simulate 3-D
 - b. Check Simulate Using Script. **Make sure that the simulation time window is sufficient enough to either reach steady state (CW) or there is no EM field left in the simulation domain (Gaussian)**
 - c. Click run to start the simulation. The simulation will run once for every S-Parameter Port placed in the design.
5. Once the simulation is complete open OptiFDTD analyzer file generated by the simulator.
6. To export the S-Parameters go to Tools -> S-Parameters and click on Export. The S-parameters are exported in polar coordinates.

6 Plane Wave Expansion (PWE) method

Maxwell's curl equations for the electric and magnetic fields in a transparent, time-invariant, source free, and non-magnetic medium can be combined in terms of the magnetic field and be written in the following form:

$$\nabla \times \frac{1}{\epsilon(\mathbf{r})} \nabla \times \mathbf{H}(\mathbf{r}) = \frac{\omega^2}{c^2} \mathbf{H}(\mathbf{r})$$

where

$\epsilon(\mathbf{r})$ is the space dependent dielectric function

c is the speed of light in vacuum

$\mathbf{H}(\mathbf{r})$ is the magnetic field vector of frequency ω and time dependence $e^{j\omega t}$

This equation is often referred to as the the Master Equation, and represents a Hermitian eigen-problem. The equivalent could not be said if the curl equations where combined such that the expression was in terms of the electric electric field.

Bloch theorem states that, assuming infinite periodicity, the magnetic field will take the form:

$$\mathbf{H}(\mathbf{r}) = e^{-j\mathbf{k}\mathbf{r}} \mathbf{h}_{\mathbf{k}}(\mathbf{r})$$

where

$$\mathbf{h}_{\mathbf{k}}(\mathbf{r}) = \mathbf{h}_{\mathbf{k}}(\mathbf{r} + \mathbf{R})$$

for all combinations of lattice vectors \mathbf{R} . Introducing the Bloch form into the master equation yields the master equation in operator form:

$$(\nabla - j\mathbf{k}) \times \left[\frac{1}{\epsilon(\mathbf{r})} (\nabla - j\mathbf{k}) \right] \times \mathbf{h}_{\mathbf{k}} = \frac{\omega^2}{c^2} \mathbf{h}_{\mathbf{k}}$$

This is the fundamental equation, which needs to be solved for a plane wave expansion calculation. The equation is transformed into a finite problem by expanding the magnetic field in a finite basis of simple plane waves. Different approaches can be explored to solve the final discretized problem. The result of solving the discretized problem is the dispersion relationship between the frequencies of the modes and wave vector \mathbf{k} , usually plotted in the form of a band diagram.

For an example of the application of this numerical method within OptiFDTD see the tutorial "Photonic Crystal Band Diagram".

6.1 References:

1. J.D. Joannopoulos, R.D. Meade, and J.N. Winn, "Photonic crystals, Molding the flow of light", Princeton University Press, 1995.
2. S.G. Johnson, J.D. Joannopoulos, "Block-iterative frequency-domain methods for Maxwell's equations in a planewave basis", Optics Express 8, no.3, p.173-190, 2000.
3. S.Guo, S.Albin, "Simple plane wave implementation for photonic crystal calculations", Optics Express 11, no.2, p.167-175, 2003.

7 Post-simulation Data Analysis

OptiFDTD consists of three primary software tools: Designer, Simulator, and Analyzer. While previous sections have discussed the Designer and the calculations within the Simulator, this section deals specifically with the post-processing capabilities made available through the Analyzer product.

7.1 Spectral response (Fourier transforms)

FDTD is a time domain numerical method and as such a single simulation can contain a broadband spectral response. This spectral response is obtain through the use of the Fourier transform, specifically in the case of a numerical method the solution is obtained through the discretized Fourier transform (DFT).

$$\begin{aligned} S(\omega) &= \int_0^T s(t)e^{-j\omega t} dt \\ &= \sum_{n=0}^N s(n)e^{-j\omega n\Delta t} \Delta t \end{aligned}$$

where $s(n)$ describes the discretized time domain response sampled in steps of Δt , N is the number of samples in time, and ω is the angular frequency.

OptiFDTD accomplishes the DFT through a fast Fourier transform algorithm where some accuracy is given up in the interest of ensuring computational speed. In the FFT algorithm the spectral response that is obtained is over the frequency range of $[0, f_s]$ where the f_s is the sampling frequency based on the step size in time and ensuring the Nyquist condition.

$$f_s = \frac{1}{2\Delta t}$$

The frequency domain sampling step size is therefore given by

$$\begin{aligned} f_s &= \frac{f_s}{N} \\ \Delta f_s &= \frac{1}{2N\Delta t} \end{aligned}$$

The parameters for the DFT spectral results can be preset within the simulation windows under *DFT Options* prior to running a simulation. These defined values will be used for the calculations for observation lines, and areas during the simulation and made available to the user from within OptiFDTD Analyzer. In contrast, observation points record the full time information for the fields and as such the DFT can be recalculated. Initial results will be based on the user defined values from prior to the simulation being run but can be changed within Analyzer.

7.2 Power calculation

Electromagnetic power can be calculated within OptiFDTD through the use of observation lines (2D) or observation areas (3D) and the OptiFDTD Analyzer. Power for propagating waves is a function of both the intensity over a given surface as well as the area over that surface. The intensity is the time-average of the quantity known as the Poynting vector.

7.2.1 Poynting Vector

The Poynting vector, \mathbf{S} , is given as

$$\mathbf{S} = \mathbf{E} \times \mathbf{H}$$

where \mathbf{E} and \mathbf{H} are complex vector fields. The complex vector fields can be expressed as

$$\begin{aligned}\mathbf{E} &= \mathbf{E}_0 e^{j(\omega t - \mathbf{k} \cdot \mathbf{r})} \\ \mathbf{H} &= \mathbf{H}_0 e^{j(\omega t - \mathbf{k} \cdot \mathbf{r})}\end{aligned}$$

where ω is the angular frequency, \mathbf{k} is the wave vector, and \mathbf{r} is the position vector. It should be noted that the quantities \mathbf{E}_0 and \mathbf{H}_0 are the complex field amplitudes and that other conventions use the RMS values for these quantities, which leads to a difference of 1/2 between the two conventions.

The time-average of the Poynting vector, using the complex quantities, yields

$$\begin{aligned}\langle \mathbf{S} \rangle &= \frac{1}{2} \text{Re}(\mathbf{E}_0 \times \mathbf{H}_0^*) \\ \langle \mathbf{S} \rangle &= \frac{1}{2} \text{Re}(E_{y0} H_{x0}^* - E_{x0} H_{y0}^*) \hat{x} \\ &\quad + \frac{1}{2} \text{Re}(E_{z0} H_{x0}^* - E_{x0} H_{z0}^*) \hat{y} \\ &\quad + \frac{1}{2} \text{Re}(E_{x0} H_{y0}^* - E_{y0} H_{x0}^*) \hat{z}\end{aligned}$$

Note that while these are complex quantities, the Poynting vector shown in OptiFDTD is the amplitude.

7.2.2 Intensity and power

The intensity of an electromagnetic field is defined as the the time-average of the Poynting vector and the power is the surface integral of the intensity. Focusing on the case where the power over the XY-plane is required, the Z-component of the Poynting vector is used, the power can be expressed as

$$\begin{aligned}
P_z &= \iint_s I_z dx dy \\
P_z &= \iint_s \langle S_z \rangle dx dy \\
P_z &= \frac{1}{2} \iint_s \text{Re}(E_{x0} H_{y0}^* - E_{y0} H_{x0}^*) dx dy
\end{aligned}$$

This derivation allows the power flowing through a plane parallel to the XY-plane to be expressed as the sum of two quantities: P_{z-x} which is based on the E_x component and P_{z-y} which is based on the E_y component.

$$\begin{aligned}
P_z &= P_{z-x} + P_{z-y} \\
P_{z-x} &= \frac{1}{2} \text{Re} \left(\iint_s E_{x0} H_{y0}^* dx dy \right) \\
P_{z-y} &= -\frac{1}{2} \text{Re} \left(\iint_s E_{y0} H_{x0}^* dx dy \right)
\end{aligned}$$

7.2.3 Power and field amplitude

The fields of a source can be scaled either by their amplitude or their power. For the cases of a Gaussian or rectangular transverse profile in a homogeneous medium, the power P and amplitude E_0 are related by simple expressions, given below. These equations are useful when defining a source in OptiFDTD Designer but they are not involved in the post-simulation data analysis performed by the software.

Gaussian in 2D:

$$P = \sqrt{\frac{\pi}{2}} \frac{c\epsilon_0 n w_0}{2} E_0^2$$

Gaussian in 3D, assuming $w_{0x} = w_{0y} = w_0$:

$$P = \frac{\pi c\epsilon_0 n w_0^2}{4} E_0^2$$

Rectangular in 2D:

$$P = c\epsilon_0 n w_0 E_0^2$$

Rectangular in 3D:

$$P = 2c\epsilon_0 n w_{0x} w_{0y} E_0^2$$

Note that the power in 2D and 3D simulations is measured in W/m and in W, respectively.

7.3 Far Field Transform

7.3.1 Fraunhofer approximation

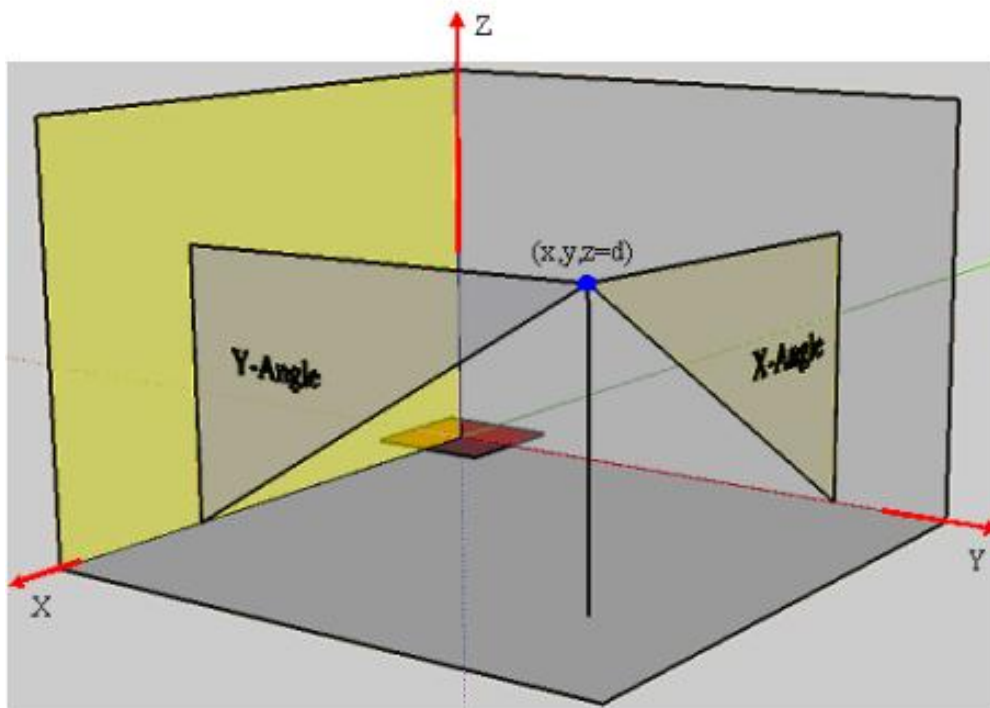
Narrow angle far-field transform being used in OptiFDTD is based on the Fraunhofer approximation:

$$E(x, y, z = d) \approx \frac{je^{jkd} e^{j\frac{k}{2d}(x^2+y^2)}}{\lambda d} \iint E(x', y', 0) e^{-j\frac{k}{d}(xx' + yy')} dx' dy'$$

At a large distance d , the far-field position can be expressed by the far-field angle approximation:

$$\tan(\theta_x) = \frac{x}{d}, \quad \tan(\theta_y) = \frac{y}{d}$$

Where the x-directional angle (θ_x) is the angle between the original YZ-plane and the shortest straight line connecting the point and the Y axis. The Y-directional angle (θ_y) is the angle between the original XZ-plane and the shortest straight line connecting the point and the x axis. The far-field angles are illustrated in the figure below.



19 Far-field angle

Using the angle approximation described above, the far-field formula can be simplified as:

$$E(\theta_x, \theta_y) \propto \iint E(x', y', 0) e^{-jn \frac{2\pi}{\lambda} [x' \tan(\theta_x) + y' \tan(\theta_y)]} dx' dy'$$

⚠ The above formula assumes that the far-field plane is far away from the near field. OptiFDTD uses the above equation to calculate the narrow angle far-field transform.

7.3.2 Fresnel-Kirchhoff Diffraction

The wide angle far-field transform is based on the Fresnel-Kirchhoff diffraction formula.

$$E(x, y, z = d) = -\frac{j}{\lambda} \iint E(x', y', 0) \frac{e^{jkR}}{R} \left[\frac{1 + \cos(\mathbf{R}, \mathbf{z})}{2} \right] dx' dy'$$

Where R is the vector from near-field to far-field.

The far-field position can be expressed using the far-field angle and the far-field distance d . Therefore in the wide angle far-field transform, the user needs to specify the far-field distance.

7.3.3 Far-field Transform - Surface Equivalence Theorem

For cases where the field cannot be approximated by a single scalar field, the far-field transform can be calculated using the surface equivalence theorem. This theory is a direct implementation of the theory presented in from Chapter 8.4 from Taflove [1], the complete theory can be found there.

The basis for this transformation is that knowledge of the electric and magnetic currents on any closed surface can be used to calculate the electromagnetic fields at any other point via an integration. In an FDTD algorithm, it is natural to choose a rectangular prism structure made from planes that match the Yee mesh. The surface currents are then given by:

$$\mathbf{J}_s = \hat{\mathbf{n}} \times \mathbf{H}_1$$

$$\mathbf{M}_s = -\hat{\mathbf{n}} \times \mathbf{E}_1$$

where \mathbf{J}_s is the electric current density and \mathbf{M}_s is the magnetic current density on the imaginary surface. Using the assumption that all but one of the planes detects any meaningful field amplitude, the six areas can be reduced to one plane. Note: This is for valid for either directional beams or when one plane captures most of the power from a scattering simulation. If the electric and magnetic fields are to be calculated at position \mathbf{r} and the source position is given by \mathbf{r}' , then the vector pointing from source to observation point is given by:

$$\mathbf{R} = \mathbf{r} - \mathbf{r}'$$

For large distances the following approximation can be made:

$$(20) \quad \mathbf{R} = [\mathbf{r}^2 - \mathbf{r}'^2 - 2\mathbf{r}\mathbf{r}'\cos\psi]^{\frac{1}{2}} \approx \mathbf{r} - \mathbf{r}'\cos\psi$$

where ψ is the angle between \mathbf{r} and \mathbf{r}' .

The electric and magnetic fields are then given by:

$$\begin{aligned} E_r &= 0 \\ E_\theta &= -\frac{jke^{-jkr}}{4\pi r}(L_\phi + \eta_0 N_\theta) \\ E_\phi &= +\frac{jke^{-jkr}}{4\pi r}(L_\theta - \eta_0 N_\phi) \\ H_r &= 0 \\ H_\theta &= +\frac{jke^{-jkr}}{4\pi r}(N_\phi - L_\theta/\eta_0) \\ H_\phi &= -\frac{jke^{-jkr}}{4\pi r}(N_\theta + L_\phi/\eta_0) \end{aligned}$$

where $\eta_0 = \sqrt{\mu_0/\epsilon_0}$ is the intrinsic impedance of free space, k is the wavenumber and r is the magnitude of the observation position vector. Finally, intermediate expressions L_θ , L_ϕ , N_θ , and N_ϕ are given by:

$$\begin{aligned} N_\theta &= \iint_S (J_x \cos\theta \cos\phi + J_y \cos\theta \sin\phi - J_z \sin\theta) e^{+jkr' \cos\psi} ds' \\ N_\phi &= \iint_S (-J_x \sin\phi + J_y \cos\phi) e^{+jkr' \cos\psi} ds' \\ L_\theta &= \iint_S (M_x \cos\theta \cos\phi + M_y \cos\theta \sin\phi - M_z \sin\theta) e^{+jkr' \cos\psi} ds' \\ L_\phi &= \iint_S (-M_x \sin\phi + M_y \cos\phi) e^{+jkr' \cos\psi} ds' \end{aligned}$$

The electromagnetic field can be calculated anywhere at large distances away from the near field plane, to satisfy assumption (20). To follow the far field calculation in the previous section, the fields are calculated on a plane at $z = d$, where d is the user supplied distance.

[1] A. Taflove and S. C. Hagness, Computational Electrodynamics: The Finite-Difference Time-Domain Method, Third Edition. 2005, ch. 8, sec. 4, pp. 338-343

7.4 Heat Absorption

It is known that the real electromagnetic power transmitted through a closed surface S into the volume V is equal to the power loss through Joule heating (conduction current) and the power loss resulting from the polarization damping forces.

From the complex Poynting vector theorem, the time-average heat absorption intensity is expressed as:

$$w(\lambda) = \frac{\sigma(\lambda)|E(\lambda)|^2}{2}$$

where σ is the wavelength dependant conductivity.

In OptiFDTD the heat absorption intensity for each polarization, for each cell within the observation area, can be expressed as:

$$\begin{aligned} w_{i,j}(\lambda) &= w_{x,i,j}(\lambda) + w_{y,i,j}(\lambda) + w_{z,i,j}(\lambda) \\ w_{x,i,j}(\lambda) &= \frac{\sigma_{x,i,j}(\lambda)|E_{x,i,j}(\lambda)|^2}{2} \\ w_{y,i,j}(\lambda) &= \frac{\sigma_{y,i,j}(\lambda)|E_{y,i,j}(\lambda)|^2}{2} \\ w_{z,i,j}(\lambda) &= \frac{\sigma_{z,i,j}(\lambda)|E_{z,i,j}(\lambda)|^2}{2} \end{aligned}$$

where the subscript letters x , y , and z represent the polarization while i and j indicate the position index.

The total heat absorption for one observation slice will be the integral of the heat absorption intensity in the volume

$$\begin{aligned} W(\lambda) &= W_x(\lambda) + W_y(\lambda) + W_z(\lambda) \\ W_x(\lambda) &= \frac{1}{2} \left(\iint_{obs} \sigma_{x,u,v}(\lambda) |E_{x,u,v}(\lambda)|^2 dudv \right) d\tau \\ W_y(\lambda) &= \frac{1}{2} \left(\iint_{obs} \sigma_{y,u,v}(\lambda) |E_{y,u,v}(\lambda)|^2 dudv \right) d\tau \\ W_z(\lambda) &= \frac{1}{2} \left(\iint_{obs} \sigma_{z,u,v}(\lambda) |E_{z,u,v}(\lambda)|^2 dudv \right) d\tau \end{aligned}$$

where du and dv are the mesh size in the observation plane, and $d\tau$ is the mesh size in the direction perpendicular to the observation plane. It is necessary for the heat absorption calculation that the material conductivity is known. The relationship between permittivity and conductivity can be expressed in terms of the complex refractive index:

$$\tilde{\epsilon}_r = \epsilon_r - j \frac{\sigma}{\omega \epsilon_0}$$

$$\tilde{\epsilon}_r = (n - j\kappa)^2$$

$$\epsilon_r = n^2 - \kappa^2$$

$$\sigma = 2n\kappa\omega\epsilon_0$$

For Lorentz-Drude dispersive materials,

$$\epsilon_r = \epsilon_{r\infty} + \sum_{m=0}^M \frac{G_m \Omega_m^2}{\omega_m^2 - \omega^2 + j\omega\Gamma_m}$$

$$\tilde{\epsilon}_r = \epsilon_{r\infty} + \sum_{m=0}^M \frac{G_m \Omega_m^2 (\omega_m^2 - \omega^2)}{(\omega_m^2 - \omega^2)^2 + (\omega\Gamma_m)^2} - j \sum_{m=0}^M \frac{\omega G_m \Omega_m^2 \Gamma_m}{(\omega_m^2 - \omega^2)^2 + (\omega\Gamma_m)^2}$$

As before the imaginary component of the relative permittivity can be used to determine the expression for the conductivity.

$$\epsilon_r = \epsilon_r - j \frac{\sigma}{\omega \epsilon_0}$$

$$\sigma = \epsilon_0 \sum_{m=0}^M \frac{\omega^2 G_m \Omega_m^2 \Gamma_m}{(\omega_m^2 - \omega^2)^2 + (\omega\Gamma_m)^2}$$