Time-Domain Modeling of Dispersive Drude-Lorentz Media

Introduction

Plasmonic hole arrays have attracted a lot of scientific interest, since the discovery of extraordinary transmission through sub-wavelength hole arrays (c.f. Ref. 1). The classical Bethe theory predicts that transmittance through a sub-wavelength circular hole of diameter d in a PEC screen scales as $(d/\lambda)^4$, where λ is the wavelength. Yet, transmission through holes in realistic metallic films can exceed 50% and even approach 100%. This phenomenon was attributed to surface plasmon polaritons that can tunnel electromagnetic energy through the hole even if it is very much smaller than the wavelength.

This particular model is intended as a tutorial that shows how to model the full time-dependent wave equation in dispersive media, such as plasmas and semiconductors (and any linear medium describable by a sum of Drude-Lorentz resonant terms). The dispersion of the medium in the frequency domain is assumed to be of the form

$$\varepsilon_r(\omega) = \varepsilon_\infty - \frac{\omega_p^2}{\omega^2 - j\Gamma_i\omega - \omega_i^2}, \tag{1}$$

where the constant $\varepsilon_\infty > 1$ absorbs contributions from high-frequency contributions that are not modeled explicitly, ω_p is the plasma frequency, Γ_i is a damping coefficient, and ω_i is a resonance frequency, The particular case when the resonance frequency ω_i is zero is known as plasma (or Drude medium), and it covers most metals in the optical frequency range, from mid-IR to visible. For lossless plasmas, when the damping coefficient also is zero ($\omega_i = \Gamma_i = 0$), modeling simplifies significantly since then the polarization density is linearly related to the magnetic vector potential.

In this model, the wave equation for the magnetic vector potential

$$\nabla \times \mu_r^{-1}(\nabla \times \mathbf{A}) + \mu_0\sigma\frac{\partial \mathbf{A}}{\partial t} = \mu_0\frac{\partial \mathbf{D}}{\partial t}, \tag{2}$$

where the electric displacement field is defined by

$$\mathbf{D} = \varepsilon_0 \varepsilon_\infty \mathbf{E} + \mathbf{P}, \tag{3}$$

is solved together with an ordinary differential equation for the polarization field, obtained by a Fourier transformation of Equation 1,

$$\left(\frac{\partial^2}{\partial t^2} + \Gamma_i \frac{\partial}{\partial t} + \omega_i^2\right)\mathbf{P} = \varepsilon_0 f \omega_p^2 \mathbf{E}. \tag{4}$$

Here f is an oscillator strength (normally set to 1).

Notice that this model is not primarily intended to demonstrate the anomalously high transmission through hole arrays, but rather to demonstrate temporal dispersion modeling.

Model Definition

The geometry consists of a single dispersive slab of thickness 1 µm with a slit of width 0.5 µm in it. The wavelength used is 1 µm. Periodic boundary conditions are applied to make the structure physically appear as an array of slits. The source of electromagnetic radiation is a plane wave pulse with flat front and Gaussian temporal shape.

Results and Discussion

Figure 1 shows the probe plot of the y-component of the electric field at the input boundary. The left part of the curve represents the incoming wave, whereas the right part shows the reflected wave returning to the input boundary.

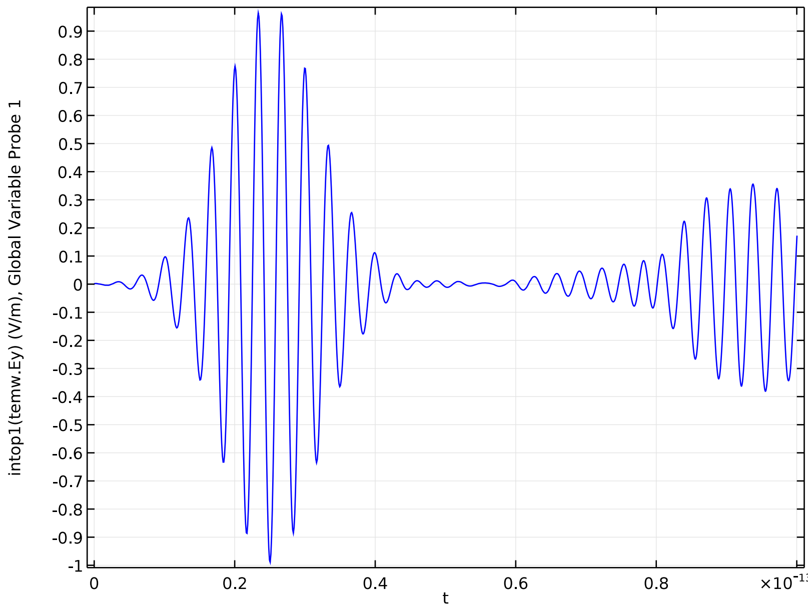


Figure 1: The y-component of the electric field at the input boundary. The left part shows the incident pulse and the right part shows the reflected pulse.

Figure 2 shows the probe plot of the y-component of the polarization at a point in the entrance of the slit. Notice the propagation delay between the incident field, shown in

Figure 1, and the onset of the polarization oscillations at this point.

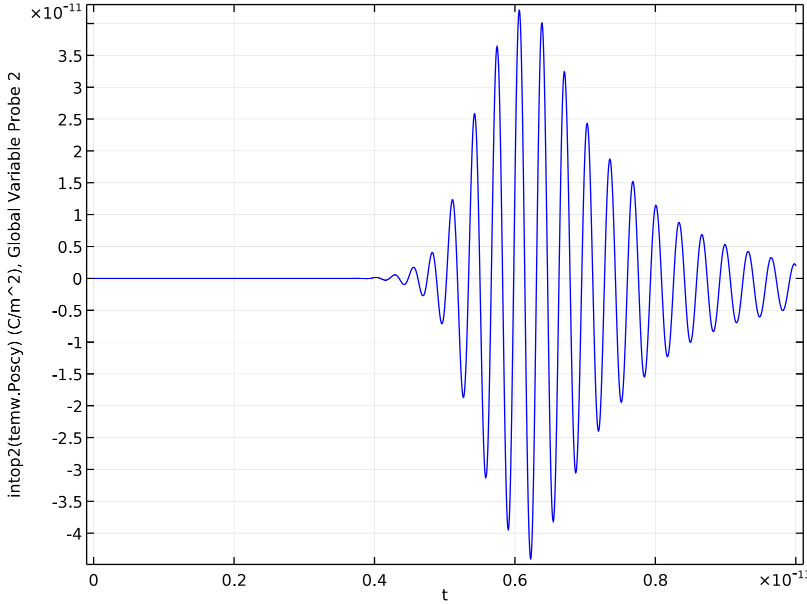


Figure 2: The y-component of the polarization at a point at the entrance of the slit.

Figure 3 shows the probe plot of the y-component of the polarization field at a point at the rear end of the slit.

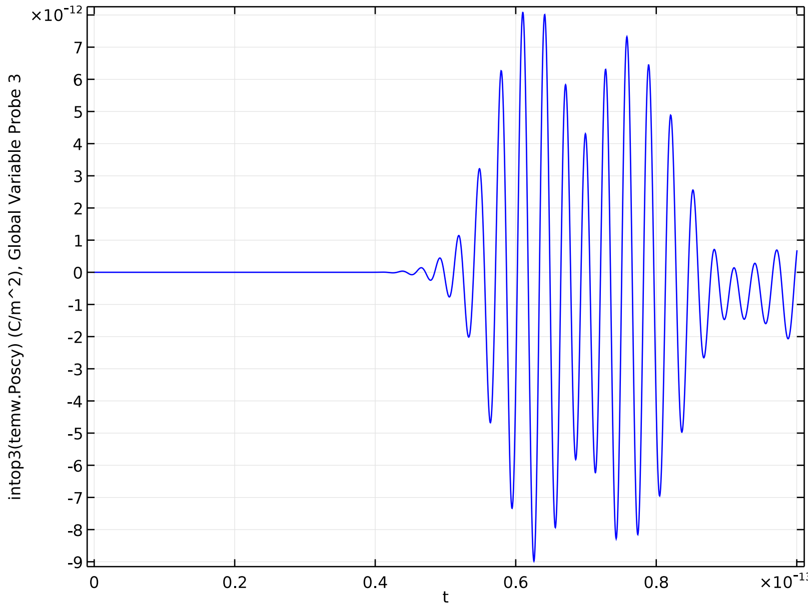


Figure 3: The y-component of the polarization at a point at the exit of the slit.

Figure 4 shows a field plot of the y-component of the polarization field after the last time step (100 fs).

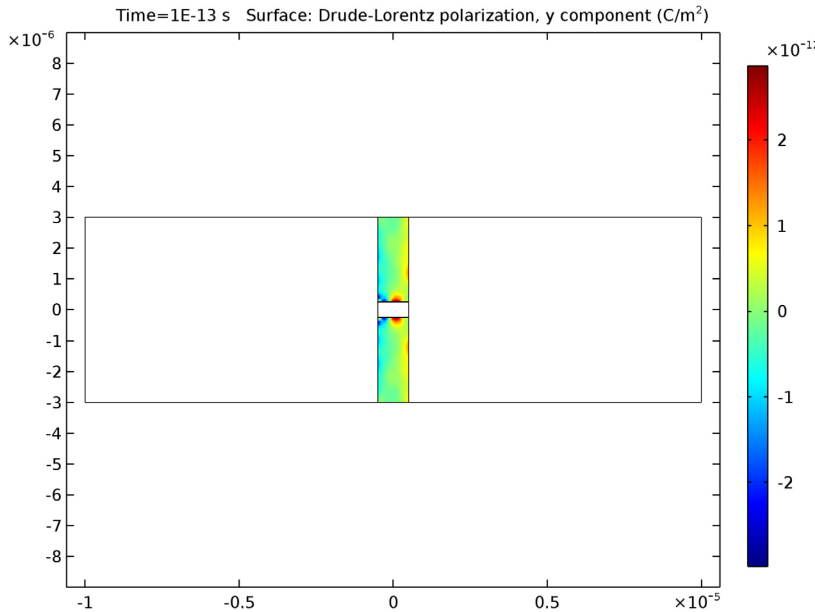


Figure 4: The y-component of the polarization field after 100 fs.

Finally, the out-of-plane component of the magnetic field and, as an overlaid contour plot, the y-component of the polarization field are shown in Figure 5, after 100 fs.

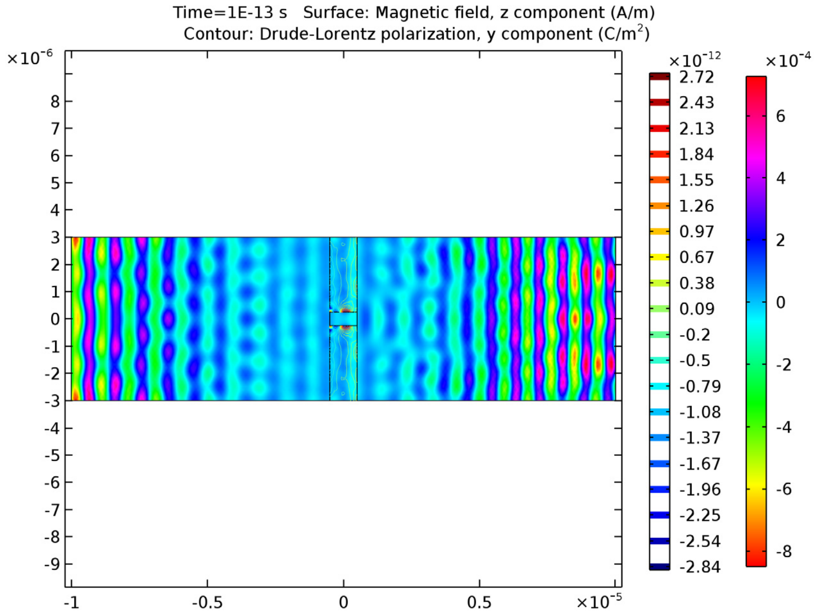


Figure 5: The out-of-plane component of the magnetic field and the y-component of the polarization field (contours) after 100 fs.

Reference

1. T. W. Ebbesen H. J. Lezec, H. F. Ghaemi, T. Thio, and P. A. Wolff, “Extraordinary Optical Transmission Through Sub-wavelength Hole Arrays,” *Nature*, vol. 391, pp. 667-9, 1998.

Application Library path: `RF_Module/Tutorials/drude_lorentz_media`

Model Instructions

From the **File** menu, choose **New**.

NEW

1 In the **New** window, click **Model Wizard**.

MODEL WIZARD

1 In the **Model Wizard** window, click **2D**.
2 In the **Select physics** tree, select **Radio Frequency>Electromagnetic Waves, Transient (temw)**.
3 Click **Add**.
4 Click **Study**.
5 In the **Select study** tree, select **Preset Studies>Time Dependent**.
6 Click **Done**.

GLOBAL DEFINITIONS

Parameters

1 On the **Home** toolbar, click **Parameters**. Add some parameters that will define the geometry and the properties of the incident field.
2 In the **Settings** window for Parameters, locate the **Parameters** section.
3 In the table, enter the following settings:

Name	Expression	Value	Description
lambda0	1[um]	1E-6 m	Wavelength
E0	1[V/m]	1 V/m	Electric field amplitude
k0	2*pi/lambda0	6.2832E6 1/m	Wave number in vacuum
t0	25[fs]	2.5E-14 s	Time delay
dt	10[fs]	1E-14 s	Pulse duration

DEFINITIONS

Variables 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Definitions** and choose **Variables**. Now add some variables that defines the incident field and the material properties.
2 In the **Settings** window for Variables, locate the **Variables** section.
3 In the table, enter the following settings:

Name	Expression	Unit	Description
omega0	2*pi*c_const/lambda0	1/s	Angular frequency
E_bnd	E0*cos(omega0*t-k0*x)	V/m	Plane-wave factor for electric field

Name	Expression	Unit	Description
E_pulse	exp(-(t-t0)^2/dt^2)		Temporal factor for electric field
omega_p	1.5*omega0	1/s	Plasma frequency
omega_1	0.5*omega_p	1/s	Resonance frequency
gamma_1	0.1*omega_1	1/s	Damping coefficient

GEOMETRY 1

The geometry is simple, consisting of only three centered rectangles.

Rectangle 1 (r1)

1 On the **Geometry** toolbar, click **Primitives** and choose **Rectangle**.

2 In the **Settings** window for Rectangle, locate the **Size** section.

3 In the **Width** text field, type `lambda0`.

4 In the **Height** text field, type `6*lambda0`.

5 Locate the **Position** section. From the **Base** list, choose **Center**.

Rectangle 2 (r2)

1 In the **Model Builder** window, right-click **Rectangle 1 (r1)** and choose **Duplicate**.

2 In the **Settings** window for Rectangle, locate the **Size** section.

3 In the **Width** text field, type `20*lambda0`.

Rectangle 3 (r3)

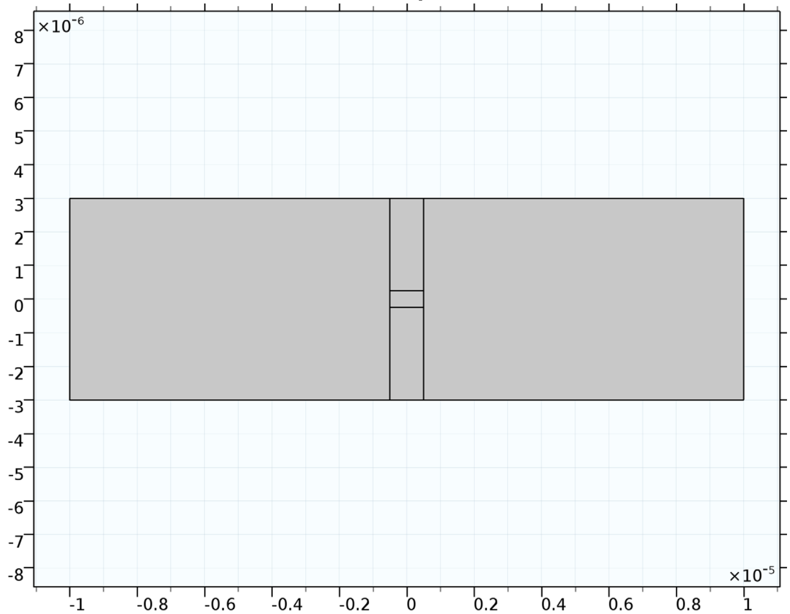
1 In the **Model Builder** window, under **Component 1 (comp1)>Geometry 1** right-click **Rectangle 1 (r1)** and choose **Duplicate**.

2 In the **Settings** window for Rectangle, locate the **Size** section.

3 In the **Height** text field, type `0.5*lambda0`.

4 Click the **Build All Objects** button.

5 Click the **Zoom Extents** button on the **Graphics** toolbar.



DEFINITIONS

Now, add three integration operator that will be used for probing the field and the polarization in three different points.

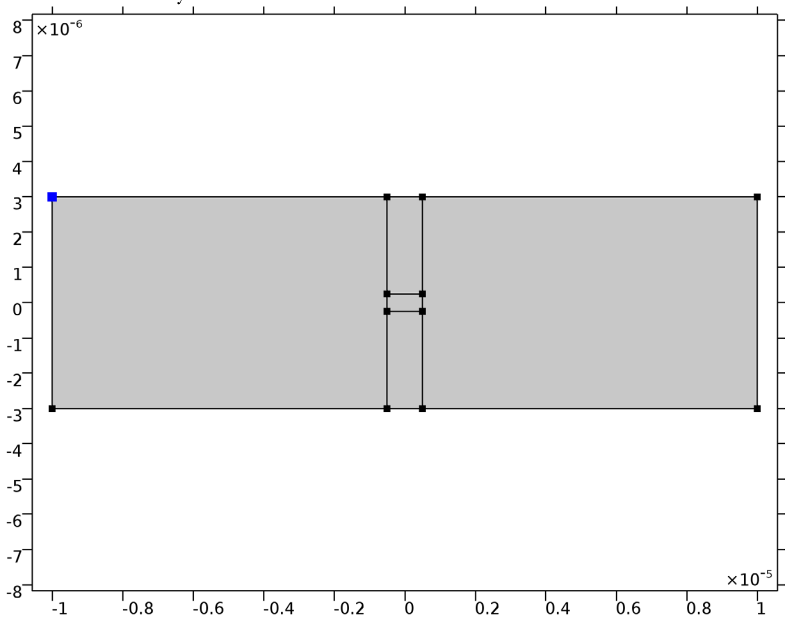
Integration 1 (intop1)

1 On the **Definitions** toolbar, click **Component Couplings** and choose **Integration**.

2 In the **Settings** window for Integration, locate the **Source Selection** section.

3 From the **Geometric entity level** list, choose **Point**.

4 Select Point 2 only.



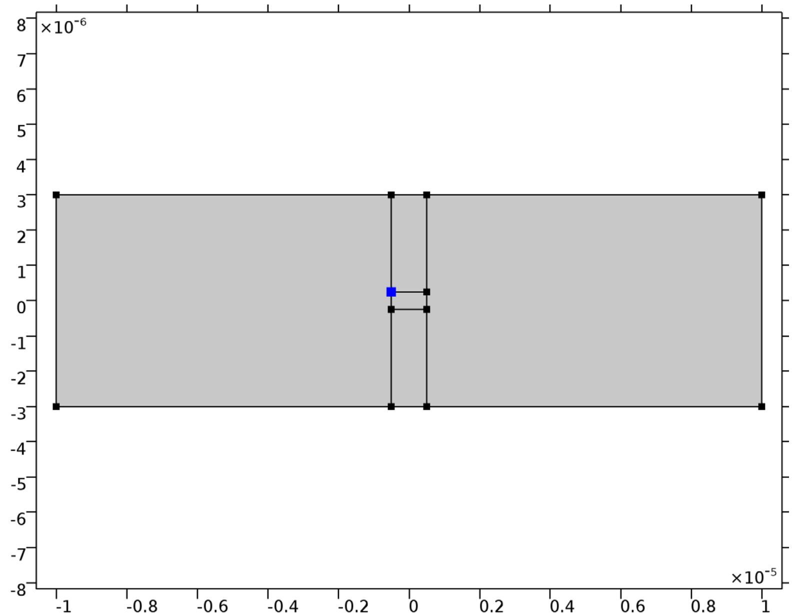
Integration 2 (intop2)

1 On the **Definitions** toolbar, click **Component Couplings** and choose **Integration**.

2 In the **Settings** window for Integration, locate the **Source Selection** section.

3 From the **Geometric entity level** list, choose **Point**.

4 Select Point 5 only.



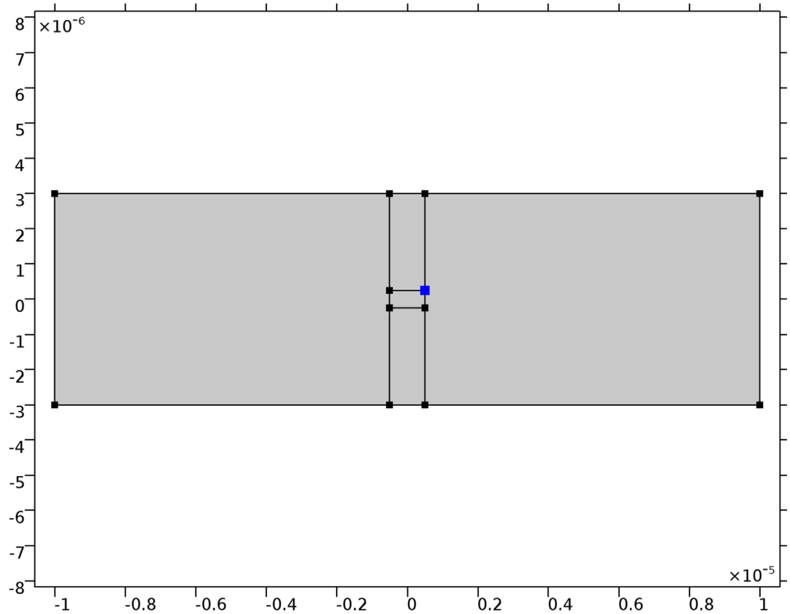
Integration 3 (intop3)

1 On the **Definitions** toolbar, click **Component Couplings** and choose **Integration**.

2 In the **Settings** window for Integration, locate the **Source Selection** section.

3 From the **Geometric entity level** list, choose **Point**.

4 Select Point 9 only.



ELECTROMAGNETIC WAVES, TRANSIENT (TEMW)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Electromagnetic Waves, Transient (temw)**.

2 In the **Settings** window for Electromagnetic Waves, Transient, locate the **Components** section.

3 From the **Electric field components solved for** list, choose **In-plane vector** to solve only for the in-plane components of the field.

Wave Equation, Electric 1

Define the first wave equation feature to use the Drude-Lorentz dispersion model. Later you will add another wave equation feature for the air domain.

1 In the **Model Builder** window, under **Component 1 (comp1)>Electromagnetic Waves, Transient (temw)** click **Wave Equation, Electric 1**.

2 In the **Settings** window for Wave Equation, Electric, locate the **Electric Displacement Field** section.

3 From the **Electric displacement field model** list, choose **Drude-Lorentz dispersion model**.

4 From the ε_∞ list, choose **User defined**. From the list, choose **Diagonal**.

5 In the ε_∞ table, enter the following settings:

4	0	0
0	4	0
0	0	1

6 In the ω_P text field, type `omega_p`.

7 Locate the **Magnetic Field** section. From the μ_r list, choose **User defined**. Locate the **Conduction Current** section. From the σ list, choose **User defined**.

Next, you add a Drude-Lorentz Polarization feature, as a sub-feature to the wave equation. There, more material parameters will be defined for the polarization field.

Drude-Lorentz Polarization 1

1 On the **Physics** toolbar, click **Attributes** and choose **Drude-Lorentz Polarization**.

2 In the **Settings** window for Drude-Lorentz Polarization, locate the **Drude-Lorentz Dispersion Model** section.

3 In the f_n text field, type `1`.

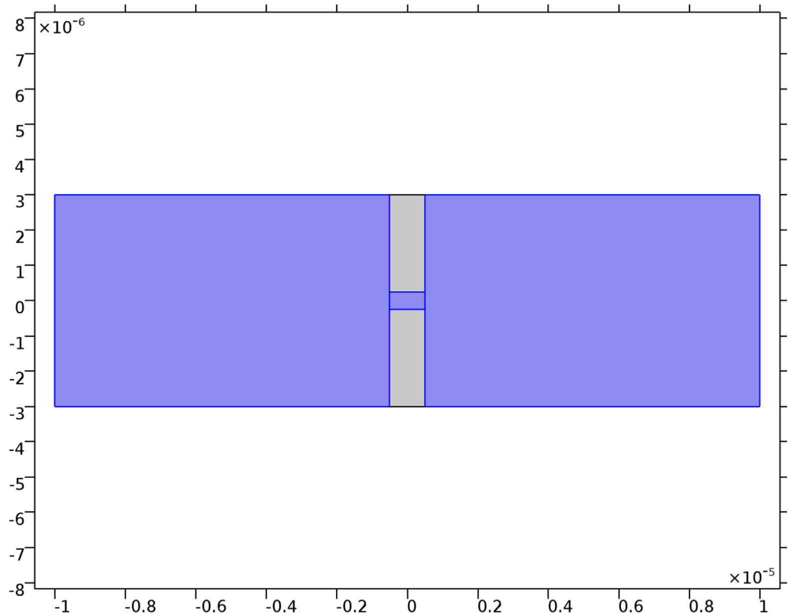
4 In the ω_n text field, type `omega_1`.

5 In the Γ_n text field, type `gamma_1`.

Wave Equation, Electric 2

1 On the **Physics** toolbar, click **Domains** and choose **Wave Equation, Electric**.

2 Select Domains 1, 3, and 5 only.



3 In the **Settings** window for Wave Equation, Electric, locate the **Electric Displacement Field** section.

4 From the ε_r list, choose **User defined**. Locate the **Magnetic Field** section. From the μ_r list, choose **User defined**. Locate the **Conduction Current** section. From the σ list, choose **User defined**.

Use scattering boundary conditions to excite the wave and to absorb it.

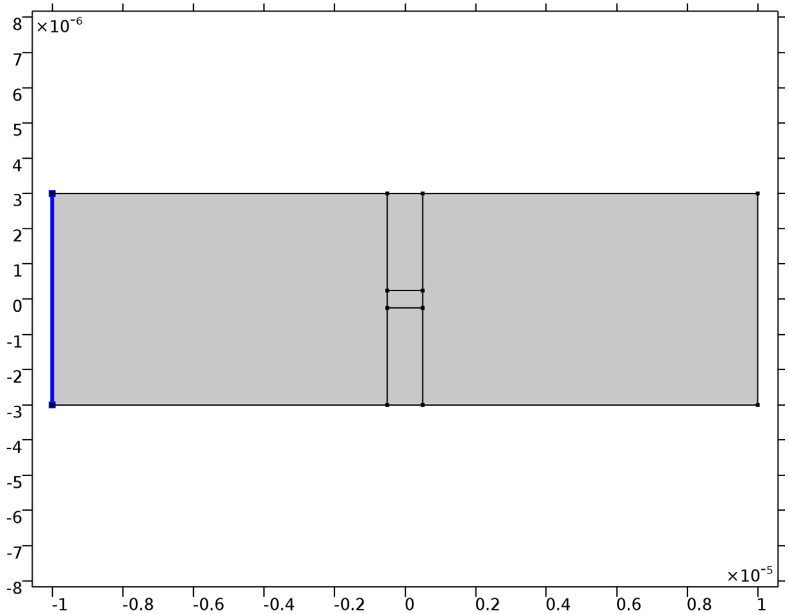
Scattering Boundary Condition 1

1 On the **Physics** toolbar, click **Boundaries** and choose **Scattering Boundary Condition**.

2 In the **Settings** window for Scattering Boundary Condition, locate the **Scattering Boundary Condition** section.

3 From the **Incident field** list, choose **Wave given by E field**.

4 Select Boundary 1 only.



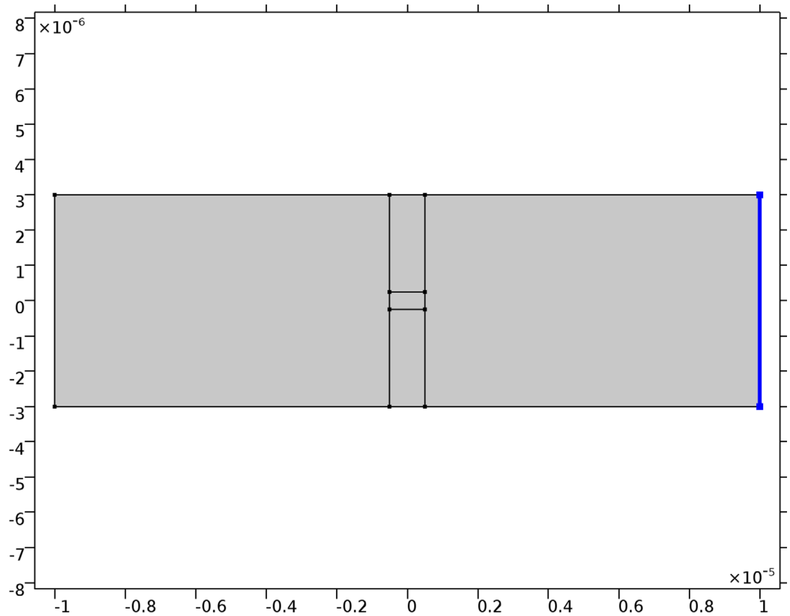
5 Specify the $\mathbf{E}_0$ vector as

0	x
E_pulse*E_bnd	y
0	z

Scattering Boundary Condition 2

1 On the **Physics** toolbar, click **Boundaries** and choose **Scattering Boundary Condition**.

2 Select Boundary 16 only.

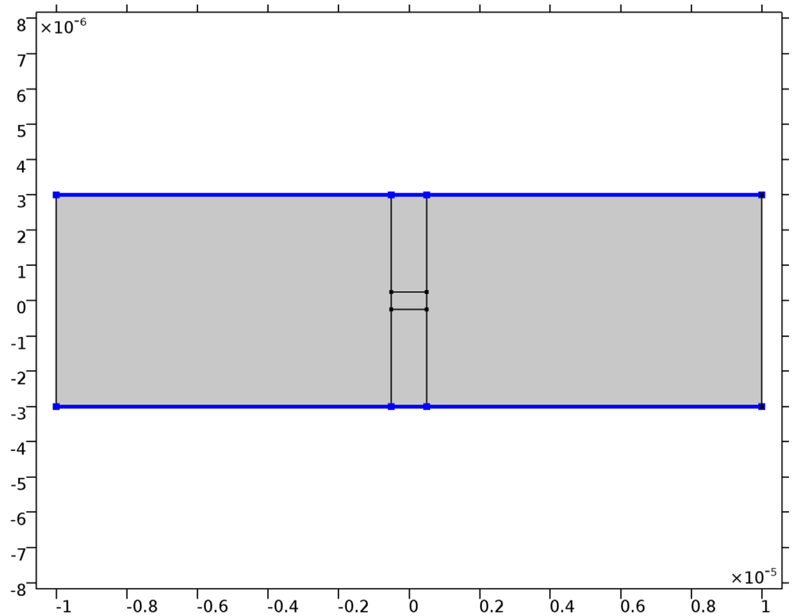


To model a hole array, periodic boundary conditions will be used.

Periodic Condition 1

1 On the **Physics** toolbar, click **Boundaries** and choose **Periodic Condition**.

2 Select Boundaries 2, 3, 5, 10, 12, and 15 only.



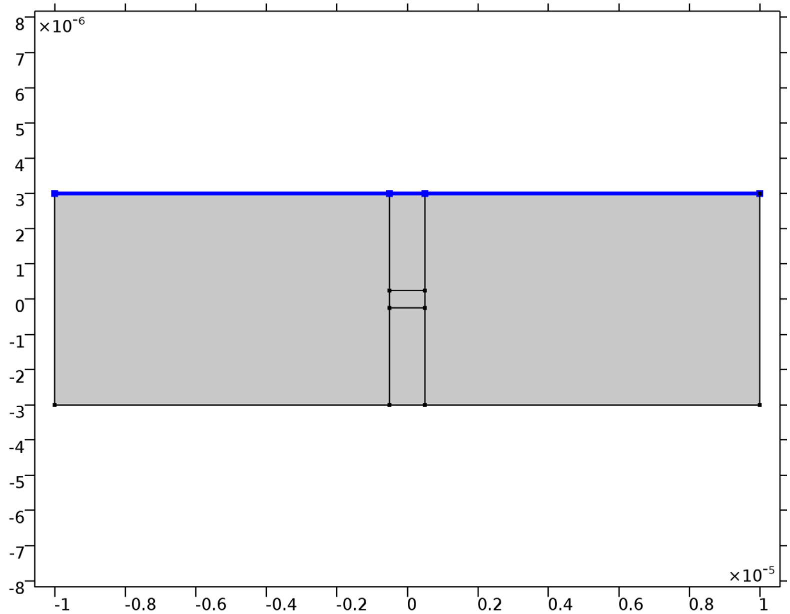
MESH 1

Since a periodic boundary condition is used, the mesh should also be the same on the top and bottom edge. Thus, add first an edge mesh and copy the mesh points to the opposite edge. Then add a triangular mesh.

Edge 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Mesh 1** and choose **More Operations>Edge**.

2 Select Boundaries 3, 10, and 15 only.



Copy Edge 1

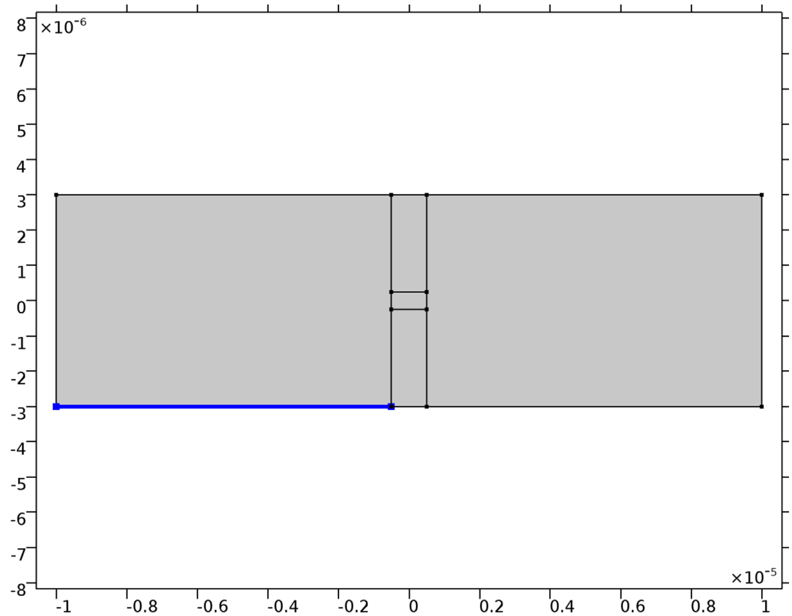
1 In the **Model Builder** window, right-click **Mesh 1** and choose **More Operations>Copy Edge**.

2 Select Boundary 3 only.

3 In the **Settings** window for Copy Edge, locate the **Destination Boundaries** section.

4 Select the **Active** toggle button.

5 Select Boundary 2 only.



Copy Edge 2

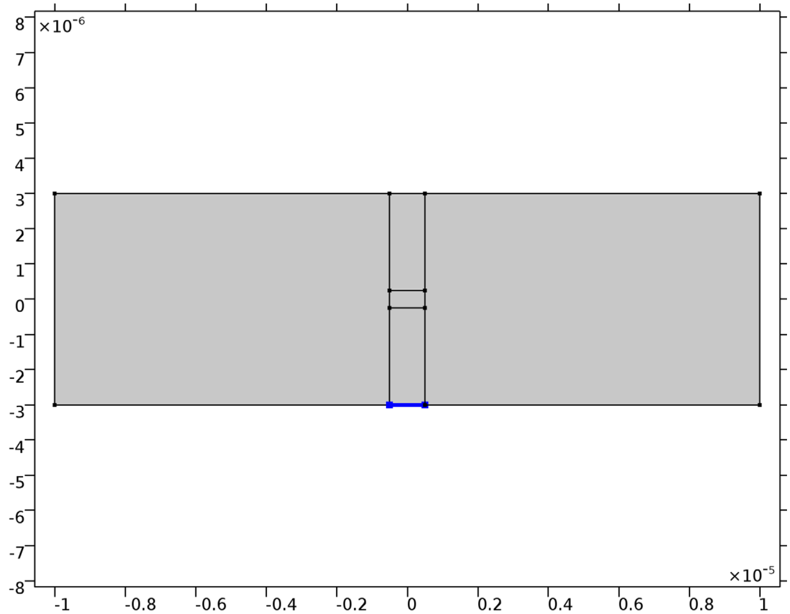
1 Right-click **Mesh 1** and choose **More Operations>Copy Edge**.

2 Select Boundary 10 only.

3 In the **Settings** window for Copy Edge, locate the **Destination Boundaries** section.

4 Select the **Active** toggle button.

5 Select Boundary 5 only.



Copy Edge 3

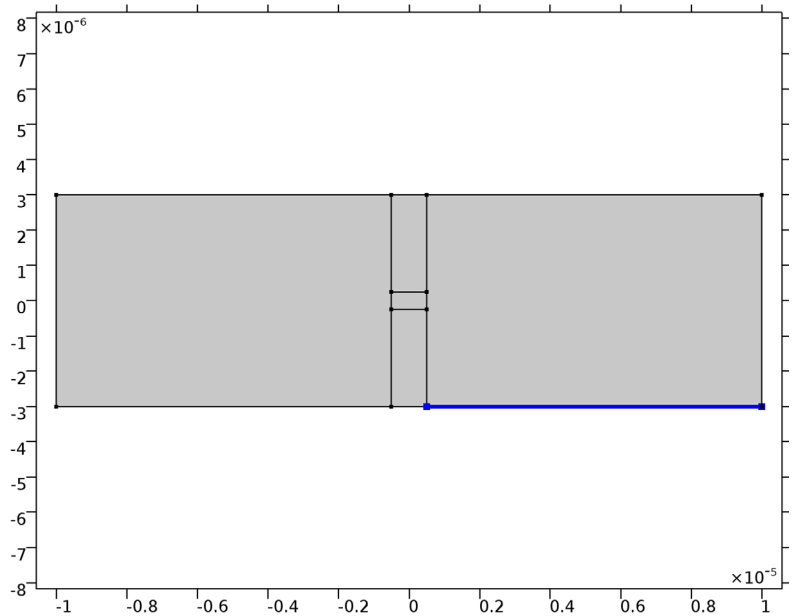
1 Right-click **Mesh 1** and choose **More Operations>Copy Edge**.

2 Select Boundary 15 only.

3 In the **Settings** window for Copy Edge, locate the **Destination Boundaries** section.

4 Select the **Active** toggle button.

5 Select Boundary 12 only.



Size

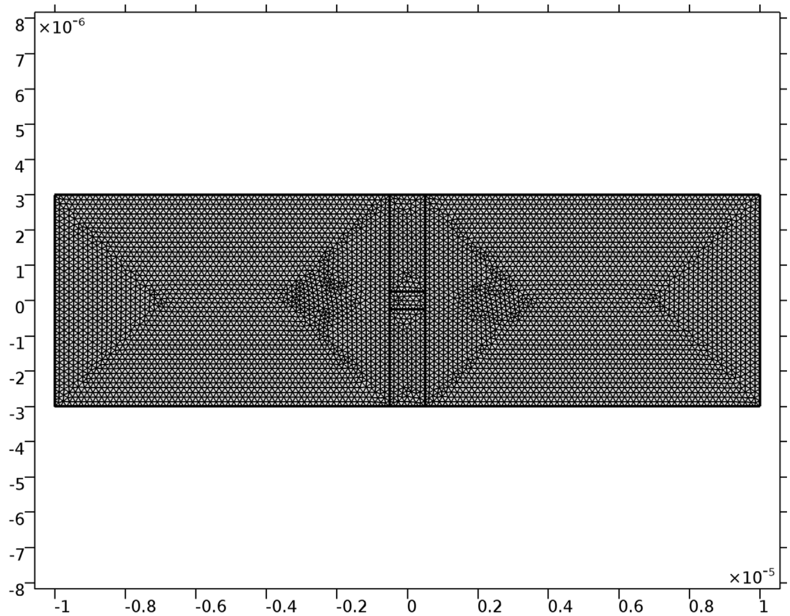
1 Right-click **Mesh 1** and choose **Free Triangular**.

2 In the **Settings** window for Size, locate the **Element Size** section.

3 Click the **Custom** button.

4 Locate the **Element Size Parameters** section. In the **Maximum element size** text field, type `lambda0/6`.

5 Click the **Build All** button.



STUDY 1

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 1** click **Step 1: Time Dependent**.

2 In the **Settings** window for Time Dependent, locate the **Study Settings** section.

3 In the **Times** text field, type `range(0,1[fs],100[fs])`.

4 On the **Study** toolbar, click **Show Default Solver**, to be able to make some modifications of the solver settings.

Solution 1

Force the solver to use a fixed small step size that resolves the temporal field oscillations.

1 In the **Model Builder** window, expand the **Study 1>Solver Configurations>Solution 1** node, then click **Time-Dependent Solver 1**.

2 In the **Settings** window for Time-Dependent Solver, click to expand the **Time stepping** section.

3 Locate the **Time Stepping** section. Select the **Initial step** check box.

4 In the associated text field, type `0.01[fs]`.

5 Select the **Maximum step** check box.

6 In the associated text field, type `0.1[fs]`.

DEFINITIONS

Before computing the solution, define the three Global Variable Probes that can be used for monitoring the computation progress.

1 On the **Definitions** toolbar, click **Probes** and choose **Global Variable Probe**.

2 In the **Settings** window for Global Variable Probe, locate the **Expression** section.

3 In the **Expression** text field, type `intop1(temw.Ey)`.

4 Click to expand the **Table and window settings** section. On the **Definitions** toolbar, click **Probes** and choose **Global Variable Probe**.

5 In the **Settings** window for Global Variable Probe, locate the **Expression** section.

6 In the **Expression** text field, type `intop2(temw.Poscy)`.

7 Locate the **Table and Window Settings** section. From the **Plot window** list, choose **New window**.

8 On the **Definitions** toolbar, click **Probes** and choose **Global Variable Probe**.

9 In the **Settings** window for Global Variable Probe, locate the **Expression** section.

10 In the **Expression** text field, type `intop3(temw.Poscy)`.

11 Locate the **Table and Window Settings** section. From the **Plot window** list, choose **New window**.

12 On the **Home** toolbar, click **Compute**.

RESULTS

Electric Field

Modify this surface plot to show the y-component of the Drude-Lorentz polarization.

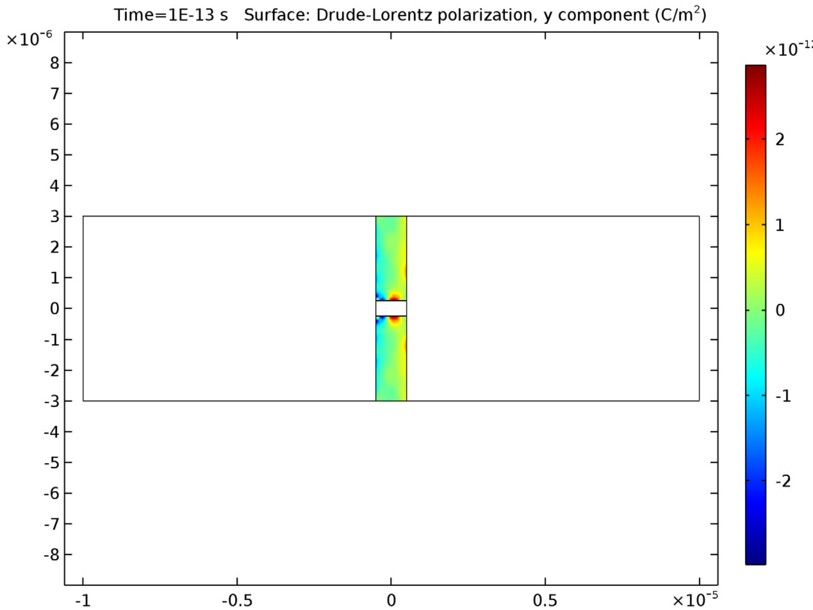
1 In the **Model Builder** window, expand the **Electric Field** node, then click **Surface 1.1**.

2 In the **Settings** window for Surface, locate the **Expression** section.

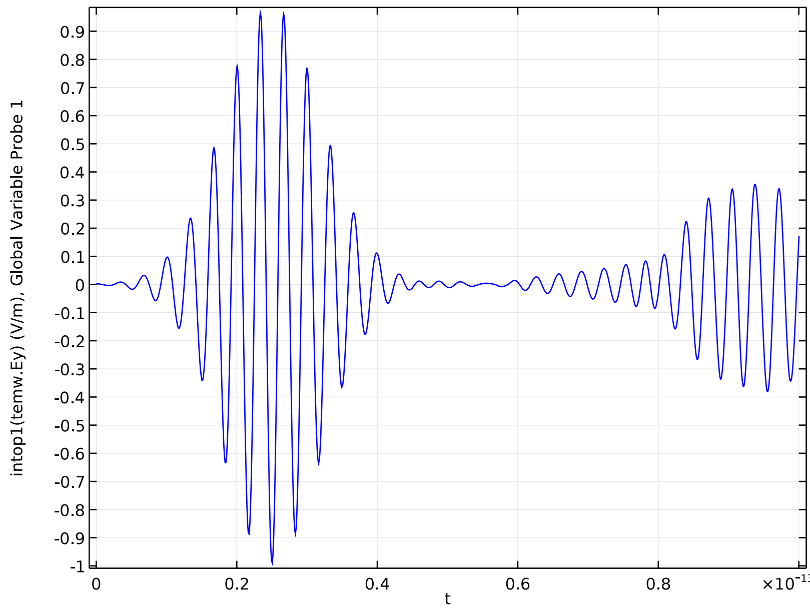
3 In the **Expression** text field, type `temw.Poscy`.

4 On the **Electric Field** toolbar, click **Plot**.

5 Click the **Zoom Extents** button on the **Graphics** toolbar.

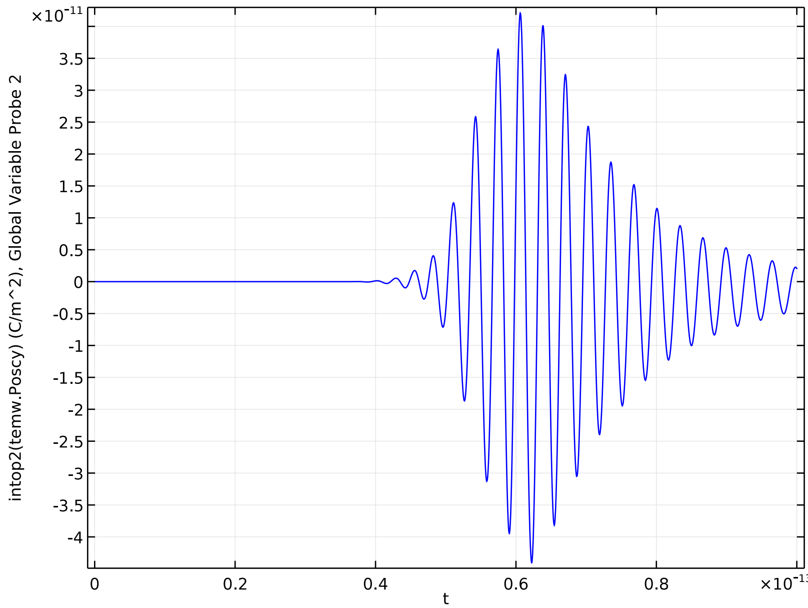


Probe Plot Group 2



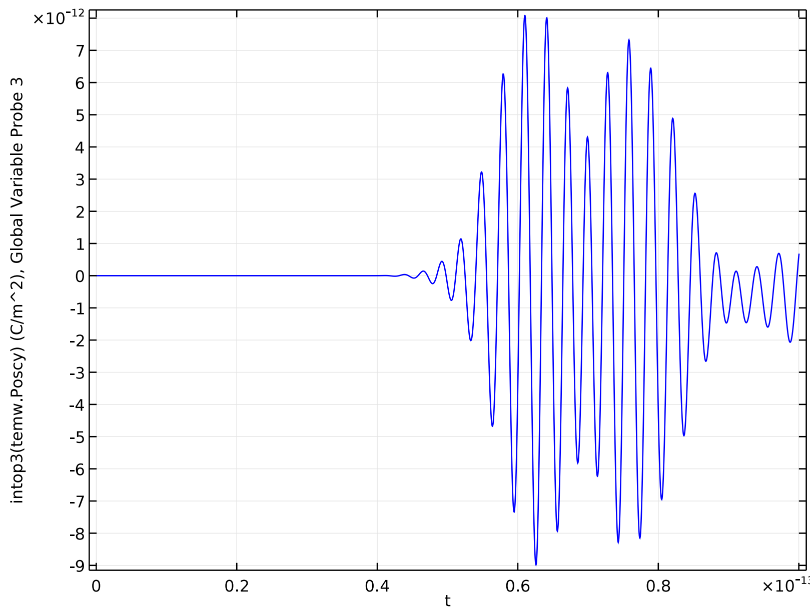
The first probe plot should look like the one above.

Probe Plot Group 3



The second probe plot should look like the one above.

Probe Plot Group 4



Finally, the third probe plot should look like the one above.

Now, add a surface plot of the z-component of the magnetic field and overlay a contour plot of the y-component of the Drude-Lorentz polarization.

2D Plot Group 5

1 On the **Home** toolbar, click **Add Plot Group** and choose **2D Plot Group**.
2 In the **Model Builder** window, under **Results** right-click **2D Plot Group 5** and choose **Surface**.
3 In the **Settings** window for Surface, locate the **Expression** section.
4 In the **Expression** text field, type `temw.Hz`.
5 Locate the **Coloring and Style** section. From the **Color table** list, choose **Cyclic**.
6 In the **Model Builder** window, right-click **2D Plot Group 5** and choose **Contour**.
7 In the **Settings** window for Contour, locate the **Expression** section.
8 In the **Expression** text field, type `temw.Poscy`.

9 On the **2D Plot Group 5** toolbar, click **Plot**.