Created in COMSOL Multiphysics 6.2

Second Harmonic Generation in the Frequency Domain

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Introduction

The emission spectra from different types of laser system cover a large part of the visible and near visible part of the electromagnetic spectrum. However, it is still more difficult to generate laser emission in the short-wavelength part of the spectrum than in the long-wavelength part. To circumvent this dilemma, it is common to use nonlinear frequency mixing to generate new wavelengths from the existing laser wavelengths. A common approach is to start with a Nd:YAG laser that emits at 1 064 nm wavelength and then frequency-double that wavelength to green at 532 nm. Given those two wavelengths, it is also possible to mix them, which results in the generation of light in ultraviolet (UV) at 355 nm — an effective frequency tripling of the original wavelength at 1 064 nm.

This model demonstrates how two frequency-domain interfaces can be coupled together to simulate the second harmonic generation process, where light from the fundamental wavelength (frequency) is injected in a nonlinear crystal that generates the second harmonic frequency, which is twice the fundamental frequency. The results are compared with analytical results obtained within the Slowly Varying Envelope Approximation (SVEA).

Model Definition

The geometry for the model is very simple, consisting only of a slender two-dimensional rectangle. The rectangle is many wavelengths long in the propagation direction, but consists of only one mesh element in the direction orthogonal to the propagation direction.

The first Electromagnetic Waves, Frequency Domain interface is defined for the fundamental frequency f_1 and the second Electromagnetic Waves, Frequency Domain interface is defined for the second harmonic frequency $2f_1$.

The only incident wave is polarized in the y-direction and launched at the fundamental frequency using a Scattering Boundary Condition feature.

The two interfaces are coupled using a Polarization feature added to each of the interfaces. For the fundamental interface, the polarization is given by

$$P_{1y} = 2dE_{2y}E^*_{1y} \tag{1}$$

and for the second harmonic interface the polarization is given by

$$P_{2y} = dE^2_{1y}, \tag{2}$$

where d is a nonlinear coefficient for the process, E_{1y} is the y-component of the electric field at the fundamental frequency, and E_{2y} is the y-component of the electric field at the second harmonic frequency. For more details regarding second harmonic generation, see for example Ref. 1.

The results from the simulation are compared with the analytical results obtained within the Slowly Varying Envelope Approximation (SVEA) (see Ref. 1). The analytical results for the photon flux density, assuming perfect phase matching, are for the fundamental wave

$$\phi_1(x) = \phi_1(0)\mathrm{sech}^2\left(\frac{\Upsilon x}{2}\right) \tag{3}$$

and for the second harmonic wave

$$\phi_2(x) = \frac{1}{2}\phi_1(0)\tanh^2\left(\frac{\Upsilon x}{2}\right), \tag{4}$$

where $\phi_1(0)$ is the incident photon flux density for the fundamental wave, the constant Υ is defined by

$$\Upsilon = 8d^2 Z_0^3 \omega^2 I_1(0), \tag{5}$$

Z_0 is the characteristic impedance of the medium, ω is the angular frequency, and $I_1(0)$ is the incident intensity for the fundamental wave. As seen from Equation 3 and Equation 4, when x goes to infinity the photon flux density for the fundamental goes to zero, whereas the photon flux density for the second harmonic approaches half of the initial fundamental photon flux density. Since the photon energy for the second harmonic is twice that of the fundamental, the energy is conserved in the process.

Results and Discussion

Figure 1 shows the y-component of the electric field of the fundamental wave. As shown, the amplitude decreases when the wave propagates through the medium and energy is transferred to the second harmonic wave. Figure 2 shows the y-component of the electric field for the second harmonic wave. For this wave, the initial amplitude is zero. Upon propagation, the amplitude increases, as energy is transferred from the fundamental wave.

Notice also that the wavelength for the second harmonic field is half that of the fundamental wave.

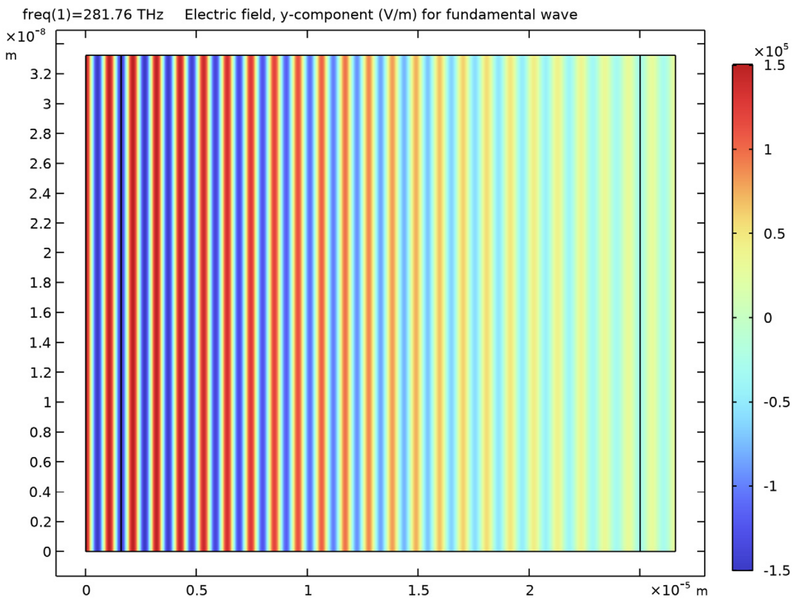


Figure 1: The electric field distribution of the fundamental wave (y-component).

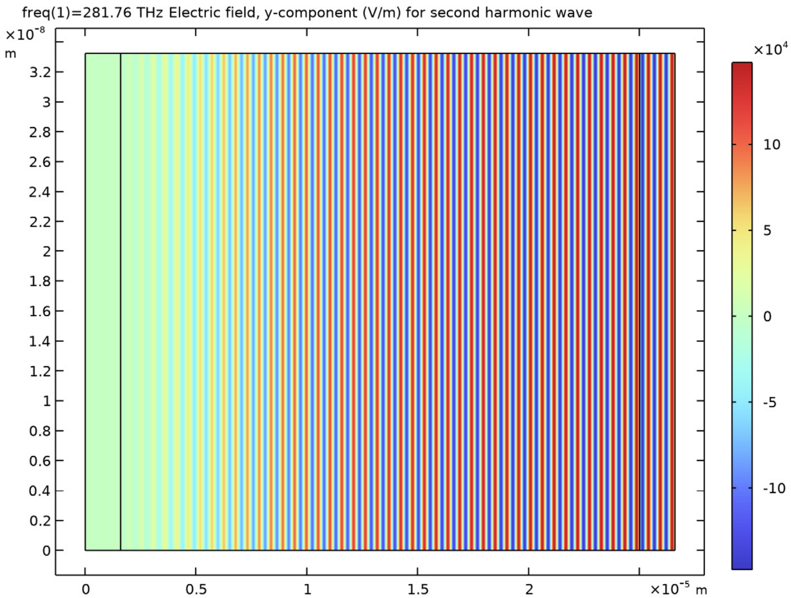


Figure 2: The electric field distribution of the second harmonic wave (y-component).

Figure 3 shows a comparison of the fundamental and the second harmonic, confirming the conclusions drawn from the comparison of the two previous figures.

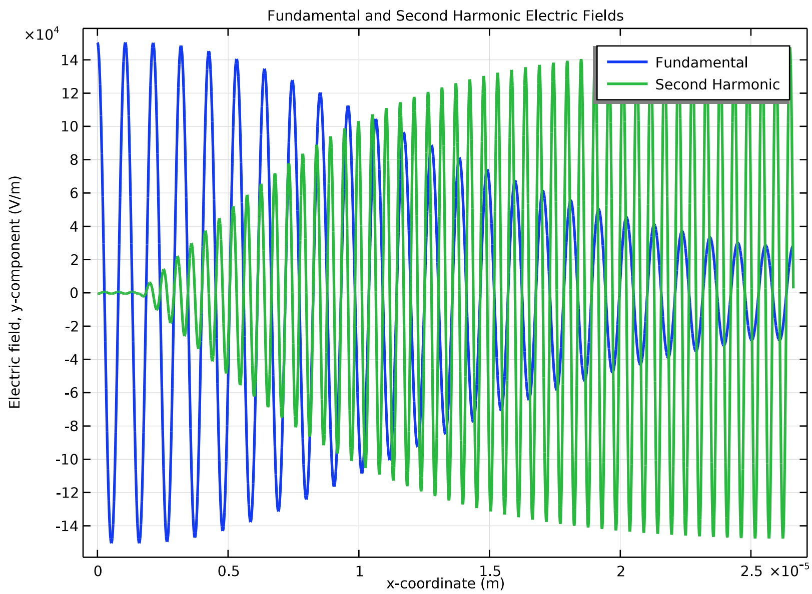


Figure 3: A comparison between the y-components of the electric fields for the fundamental and the second harmonic wave.

Finally, Figure 4 compares the results from the simulation with analytical results obtain by applying the Slowly Varying Envelope Approximation (SVEA) (see Equation 3 and Equation 4 in the Model Definition section above). As the energy for each photon in the second harmonic wave is twice that of the energy of the photons in the fundamental wave, the curves indicate that the energy is conserved in the second harmonic generation process.

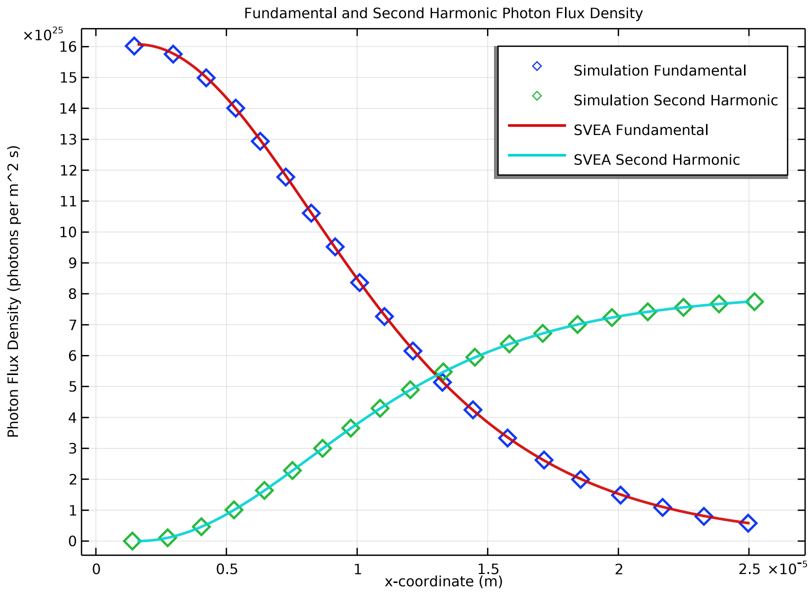


Figure 4: The photon flux density (in units of photons per m^2 and s) for the fundamental and the second harmonic wave. The diamonds represent the simulated results (blue diamonds representing the fundamental wave and green diamonds representing the second harmonic wave), whereas the red line represents the analytical result in Equation 3 *and the cyan line represents the analytical results in* Equation 4.

Notes About the COMSOL Implementation

The value for the nonlinear coefficient (d = 1×10^{-18} C/V^2) in this proof of concept model is intentionally chosen to be unphysically large, to allow for a small simulation domain. More typical values for realistic nonlinear materials are of the order of d = 1×10^{-24}–1×10^{-21} C/V^2.

As mentioned in Ref. 1, there exists different conventions for expressing the nonlinear coefficients in the series expansion of the polarization in terms of the electric field. In this model, the second order nonlinear coefficient follows the convention in Ref. 1.

Reference

1. B.E.A. Saleh and M.C. Teich, Fundamentals of Photonics, John Wiley & Sons, chap. 19, 1991.

Application Library path: `Wave_Optics_Module/Verification_Examples/second_harmonic_generation_frequency_domain`

Modeling Instructions

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

NEW

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

MODEL WIZARD

1. In the **Model Wizard** window, click **2D**.
2. In the **Select Physics** tree, select **Optics>Wave Optics>Electromagnetic Waves, Frequency Domain (ewfd)**.
3. Click **Add**.
4. Click **Add**.
5. Click **Study**.
6. In the **Select Study** tree, select **General Studies>Frequency Domain**.
7. Click **Done**.

GLOBAL DEFINITIONS

Start by importing the parameters from a file.

Parameters 1

1. In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.
2. In the **Settings** window for **Parameters**, locate the **Parameters** section.
3. Click **Load from File**.
4. Browse to the model's Application Libraries folder and double-click the file `second_harmonic_generation_frequency_domain_parameters.txt`.

GEOMETRY 1

In the **Geometry** toolbar, click **Sketch**.

Rectangle 1 (r1)

1 In the **Geometry** toolbar, click **Rectangle**.

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

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

4 In the **Height** text field, type `sim_h`.

5 Click to expand the **Layers** section. In the table, enter the following settings:

Layer name	Thickness (m)
`Layer 1`	`offset`

6 Select the **Layers to the left** check box.

7 Select the **Layers to the right** check box.

8 Clear the **Layers on bottom** check box.

DEFINITIONS

In the **Model Builder** window, expand the **Component 1 (comp1)>Definitions** node.

Axis

To get a more interesting aspect ratio for the graphics, set the **View scale** for the **Axis** to **Automatic**.

1 In the **Model Builder** window, expand the **Component 1 (comp1)>Definitions>View 1** node, then click **Axis**.

2 In the **Settings** window for **Axis**, locate the **Axis** section.

3 From the **View scale** list, choose **Automatic**.

4 Click **Update**.

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

MATERIALS

Material 1 (mat1)

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Materials** and choose **Blank Material**.

2 In the **Settings** window for **Material**, locate the **Material Contents** section.

3 In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Refractive index, real part	n_iso ; nii = n_iso, nij = 0	1	1	Refractive index
Refractive index, imaginary part	ki_iso ; kiii = ki_iso, kiij = 0	0	1	Refractive index

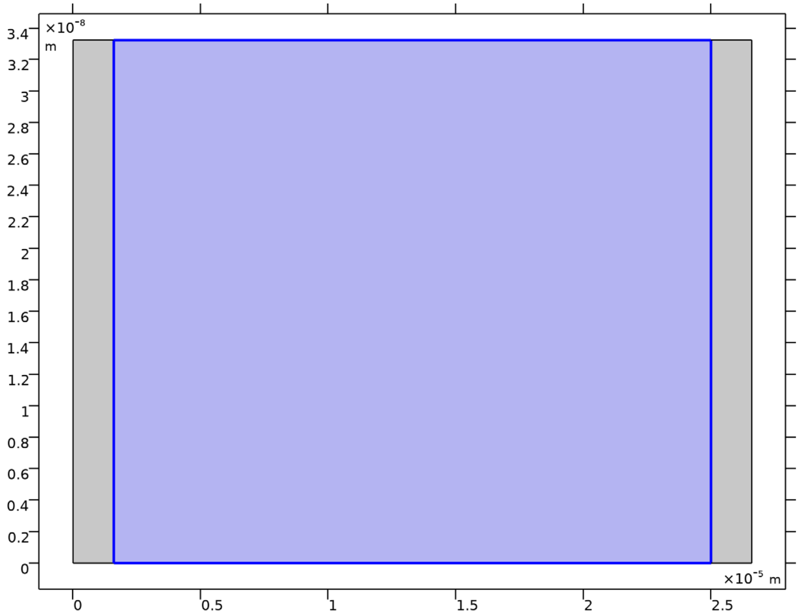
FUNDAMENTAL

1. In the **Model Builder** window, under **Component 1 (comp1)** click **Electromagnetic Waves, Frequency Domain (ewfd)**.
2. In the **Settings** window for **Electromagnetic Waves, Frequency Domain**, type `Fundamental` in the **Label** text field.
3. In the **Name** text field, type `ewfd1`, as we denote the fundamental wave with the number 1.
4. Locate the **Components** section. From the **Electric field components solved for** list, choose **In-plane vector**, as only the in-plane polarization will be included in the simulation.

Polarization 1

1. In the **Physics** toolbar, click **Domains** and choose **Polarization**.

2 Select Domain 2 only, as the nonlinear domain does not start at the exterior boundaries.



3 In the **Settings** window for **Polarization**, locate the **Polarization** section.

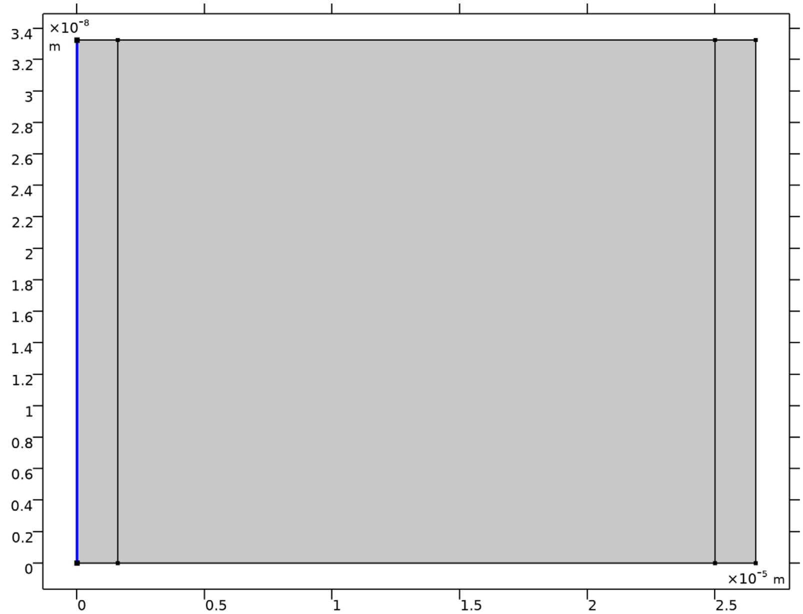
4 Specify the $\mathbf{P}_i$ vector as

`0`	x
`2*d*ewfd2.Ey*conj(ewfd1.Ey)`	y
`0`	z

Scattering Boundary Condition 1

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

2 Select Boundary 1 only.



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

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

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

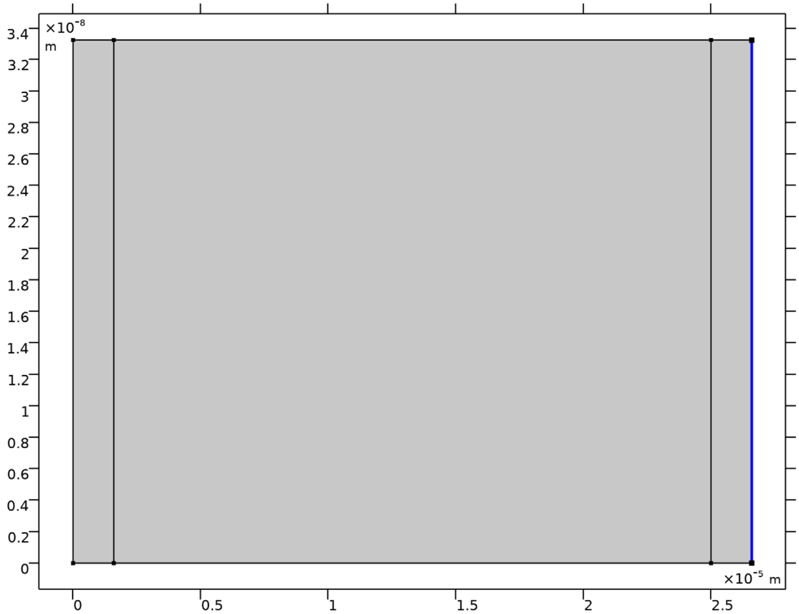
0	x
E1	y
0	z

This is the input field, driving the nonlinear process.

Scattering Boundary Condition 2

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

2 Select Boundary 10 only.



SECOND HARMONIC

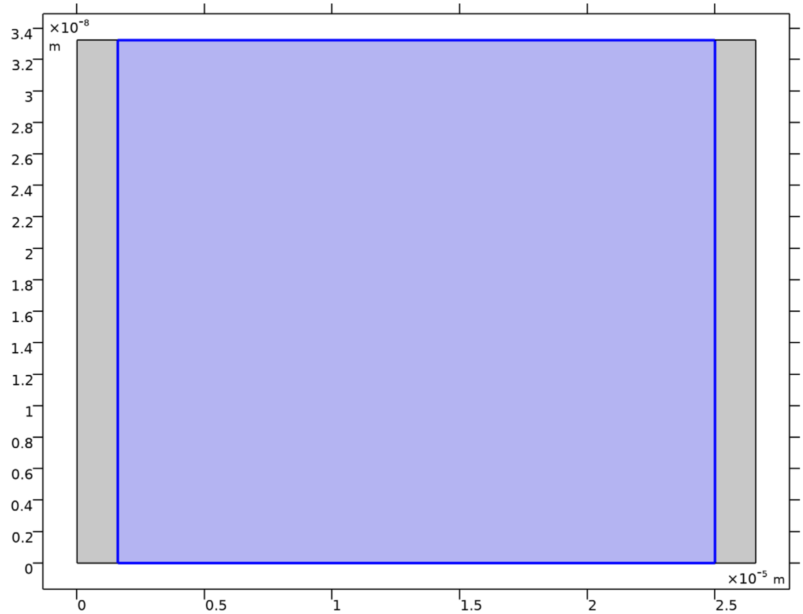
The second interface should use the second harmonic frequency. This will be set below in the **Equation** settings for the interface.

1. In the **Model Builder** window, under **Component 1 (comp1)** click **Electromagnetic Waves, Frequency Domain 2 (ewfd2)**.
2. In the **Settings** window for **Electromagnetic Waves, Frequency Domain**, type `Second Harmonic` in the **Label** text field.
3. Locate the **Components** section. From the **Electric field components solved for** list, choose **In-plane vector**.
4. Click to expand the **Equation** section. From the **Equation form** list, choose **Frequency domain**.
5. From the **Frequency** list, choose **User defined**. In the *f* text field, type `f2`.

Polarization 1

1. In the **Physics** toolbar, click **Domains** and choose **Polarization**.

2 Select Domain 2 only.



3 In the **Settings** window for **Polarization**, locate the **Polarization** section.

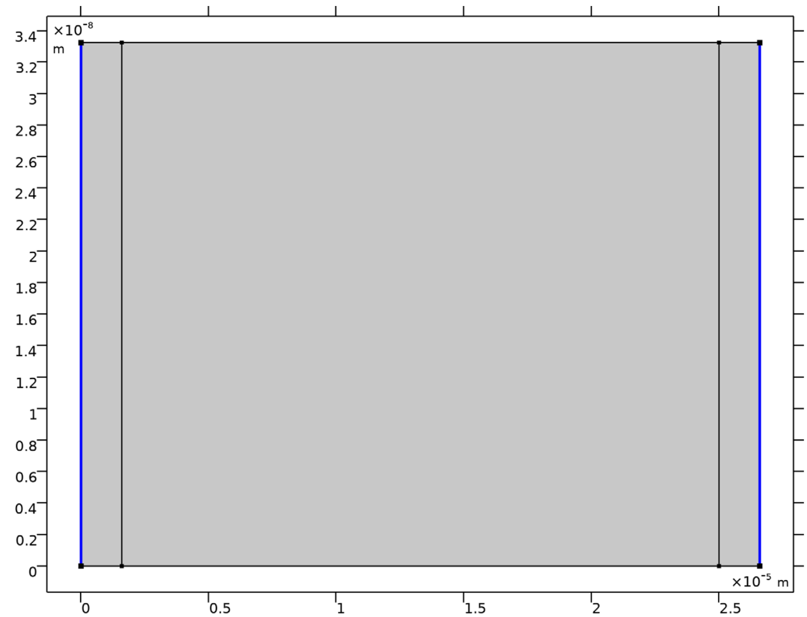
4 Specify the $\mathbf{P}_i$ vector as

0	x
`d*ewfd1.Ey*ewfd1.Ey`	y
0	z

Scattering Boundary Condition 1

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

2 Select Boundaries 1 and 10 only.



MESH 1

Mapped 1

1 In the **Mesh** toolbar, click **Mapped**.

2 In the **Model Builder** window, under **Mesh 1** click **Size**.

Size

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

2 Click the **Custom** button.

3 Locate the **Element Size Parameters** section. In the **Maximum element size** text field, type `sim_h`.

4 In the **Minimum element size** text field, type `sim_h`.

The settings above create a mapped mesh with only one element in the height direction.

DEFINITIONS

Variables 1

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Definitions** and choose **Variables**.

2 In the **Settings** window for **Variables**, locate the **Variables** section.

3 In the table, enter the following settings:

Name	Expression	Unit	Description
gamma	sqrt(8*d^2*Z0_const^3*(2*pi*ewfd1.freq)^2*I1)	1/m	Coupling coefficient

This variable will be used when comparing the simulated results with the analytical results from the Slowly Varying Envelope Approximation (SVEA).

STUDY 1

Step 1: Frequency Domain

1 In the **Model Builder** window, under **Study 1** click **Step 1: Frequency Domain**.

2 In the **Settings** window for **Frequency Domain**, locate the **Study Settings** section.

3 In the **Frequencies** text field, type `f1`.

Solution 1 (sol1)

1 In the **Study** toolbar, click **Show Default Solver**.

2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node, then click **Compile Equations: Frequency Domain**.

3 In the **Settings** window for **Compile Equations**, locate the **Study and Step** section.

4 Select the **Split complex variables in real and imaginary parts** check box.

5 In the **Model Builder** window, under **Study 1>Solver Configurations>Solution 1 (sol1)** click **Stationary Solver 1**.

6 In the **Settings** window for **Stationary Solver**, locate the **General** section.

7 In the **Relative tolerance** text field, type `0.001`.

8 In the **Study** toolbar, click **Compute**.

Since the polarization expression for the fundamental harmonic contains the complex conjugate of the electric field, it is advisable to split complex variables in real and imaginary parts in order to improve convergence. Moreover, the tolerance has been manually decreased to 0.001 to ensure that the nonlinear solver has converged to a solution and not just incidentally reached below the tolerance.

RESULTS

Fundamental

In the **Settings** window for **2D Plot Group**, type `Fundamental` in the **Label** text field.

Surface 1

1 In the **Model Builder** window, expand the **Fundamental** node, then click **Surface 1**.

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

3 In the **Expression** text field, type `ewfd1.Ey`.

Fundamental

Before finishing the plot, update the plot title.

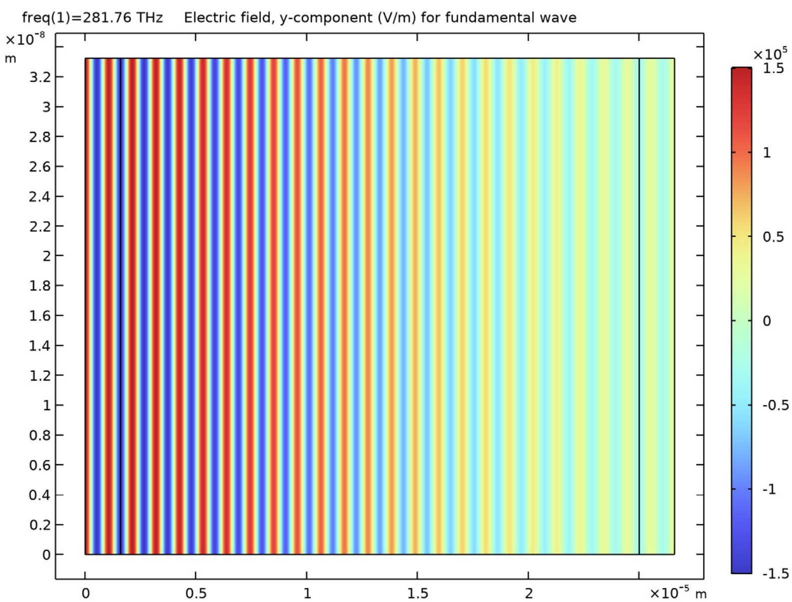
1 In the **Model Builder** window, click **Fundamental**.

2 In the **Settings** window for **2D Plot Group**, click to expand the **Title** section.

3 From the **Title type** list, choose **Manual**.

4 In the **Title** text area, type `Electric field, y-component (V/m) for fundamental wave`.

5 In the **Fundamental** toolbar, click  **Plot**.



Second Harmonic

1 In the **Model Builder** window, under **Results** click **Electric Field (ewfd2)**.

2 In the **Settings** window for **2D Plot Group**, type `Second Harmonic` in the **Label** text field.

Surface 1

1 In the **Model Builder** window, expand the **Second Harmonic** node, then click **Surface 1**.

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

3 In the **Expression** text field, type `ewfd2.Ey`.

Second Harmonic

Again, update the plot title.

1 In the **Model Builder** window, click **Second Harmonic**.

2 In the **Settings** window for **2D Plot Group**, locate the **Title** section.

3 From the **Title type** list, choose **Manual**.

4 In the **Title** text area, type `Electric field, y-component (V/m) for second harmonic wave`.

5 In the **Second Harmonic** toolbar, click **Plot**.

Notice that the wavelength is half of that displayed in the **Fundamental** plot group for the fundamental wave.

Electric Fields

Now create a line graph showing the electric fields for the fundamental and the second harmonic waves.

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Electric Fields` in the **Label** text field.

Fundamental

1 Right-click **Electric Fields** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, type `Fundamental` in the **Label** text field.

3 Select Boundaries 2, 5, and 8 only.

4 Locate the **y-Axis Data** section. In the **Expression** text field, type `ewfd1.Ey`.

5 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

6 In the **Expression** text field, type `x`.

7 Click to expand the **Coloring and Style** section. From the **Width** list, choose **2**.

8 Click to expand the **Legends** section. Select the **Show legends** check box.

9 Find the **Include** subsection. Select the **Label** check box.

10 Clear the **Solution** check box.

11 Right-click **Fundamental** and choose **Duplicate**.

Second Harmonic

1 In the **Model Builder** window, under **Results>Electric Fields** click **Fundamental 1**.

2 In the **Settings** window for **Line Graph**, type `Second Harmonic` in the **Label** text field.

3 Locate the **y-Axis Data** section. In the **Expression** text field, type `ewfd2.Ey`.

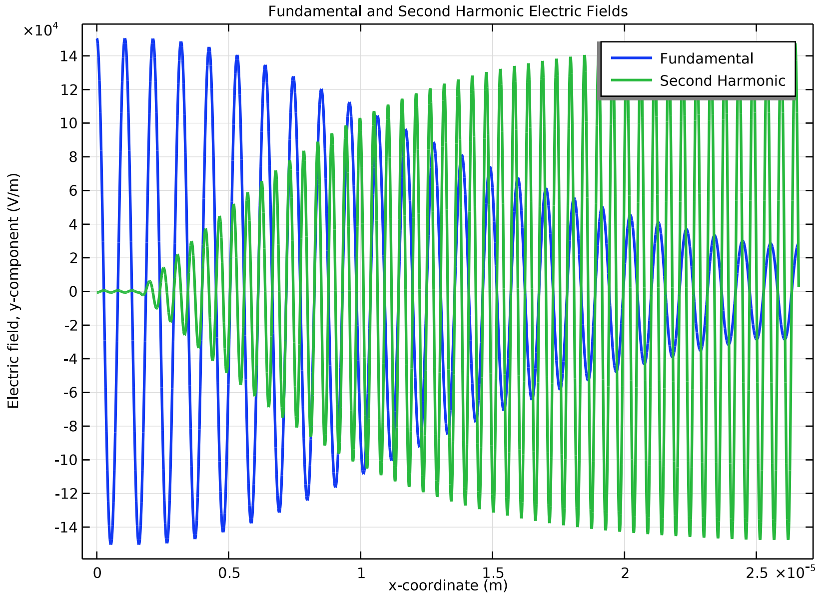
Electric Fields

1 In the **Model Builder** window, click **Electric Fields**.

2 In the **Settings** window for **1D Plot Group**, click to expand the **Title** section.

3 From the **Title type** list, choose **Manual**.

4 In the **Title** text area, type `Fundamental and Second Harmonic Electric Fields`.



Photon Flux Density

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Photon Flux Density` in the **Label** text field.

Simulation Fundamental

1 Right-click **Photon Flux Density** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, type `Simulation Fundamental` in the **Label** text field.

3 Select Boundaries 2, 5, and 8 only.

4 Locate the **y-Axis Data** section. In the **Expression** text field, type `ewfd1.Ey*conj(ewfd1.Ey)/(2*Z0_const)/hbar_const/(2*pi*ewfd1.freq)`.

5 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

6 In the **Expression** text field, type `x`.

7 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **None**.

8 From the **Width** list, choose **5**.

9 Find the **Line markers** subsection. From the **Marker** list, choose **Diamond**.

10 From the **Positioning** list, choose **Interpolated**.

11 In the **Number** text field, type `20`.

12 Locate the **Legends** section. Select the **Show legends** check box.

13 Find the **Include** subsection. Select the **Label** check box.

14 Clear the **Solution** check box.

15 Right-click **Simulation Fundamental** and choose **Duplicate**.

Simulation Second Harmonic

1 In the **Model Builder** window, under **Results>Photon Flux Density** click **Simulation Fundamental 1**.

2 In the **Settings** window for **Line Graph**, type `Simulation Second Harmonic` in the **Label** text field.

3 Locate the **y-Axis Data** section. In the **Expression** text field, type `ewfd2.Ey*conj(ewfd2.Ey)/(2*Z0_const)/hbar_const/(2*pi*ewfd2.freq)`.

4 Right-click **Simulation Second Harmonic** and choose **Duplicate**.

Slowly Varying Envelope Approximation (SVEA) Fundamental

1 In the **Model Builder** window, under **Results>Photon Flux Density** click **Simulation Second Harmonic 1**.

2 In the **Settings** window for **Line Graph**, type `Slowly Varying Envelope Approximation (SVEA) Fundamental` in the **Label** text field.

The analytic expression is only valid in the nonlinear domain. Thus, remove the selections for the edges surrounding the nonlinear domain.

3 Locate the **Selection** section. Click to select the **Activate Selection** toggle button.

4 In the list, choose **2** and **8**.

5 Click **Remove from Selection**.

6 Select Boundary 5 only.

7 Locate the **y-Axis Data** section. In the **Expression** text field, type `(sech(gamma*(x - offset)/2))^2*I1/hbar_const/(2*pi*ewfd1.freq)`.

8 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Solid**.

9 From the **Width** list, choose **2**.

10 Find the **Line markers** subsection. From the **Marker** list, choose **None**.

11 Locate the **Legends** section. From the **Legends** list, choose **Manual**.

12 In the table, enter the following settings:

Legends
`SVEA Fundamental`

13 Right-click **Slowly Varying Envelope Approximation (SVEA) Fundamental** and choose **Duplicate**.

Slowly Varying Envelope Approximation (SVEA) Second Harmonic

1. In the **Model Builder** window, under **Results>Photon Flux Density** click **Slowly Varying Envelope Approximation (SVEA) Fundamental 1**.
2. In the **Settings** window for **Line Graph**, type `Slowly Varying Envelope Approximation (SVEA) Second Harmonic` in the **Label** text field.
3. Locate the **y-Axis Data** section. In the **Expression** text field, type `(tanh(gamma*(x - offset)/2))^2*I1/hbar_const/(2*pi*ewfd2.freq)`.
4. Locate the **Legends** section. In the table, enter the following settings:

Legends
`SVEA Second Harmonic`

Photon Flux Density

1. In the **Model Builder** window, click **Photon Flux Density**.
2. In the **Settings** window for **1D Plot Group**, locate the **Title** section.
3. From the **Title type** list, choose **Manual**.
4. In the **Title** text area, type `Fundamental and Second Harmonic Photon Flux Density`.
5. Locate the **Plot Settings** section.

6 Select the **y-axis label** check box. In the associated text field, type `Photon Flux Density (photons per m^2 s)`.