# Second Harmonic Generation of a Gaussian Beam

Introduction

Laser systems are an important application area in modern electronics. There are several ways to generate a laser beam, but they all have one thing in common: The wavelength is determined by the stimulated emission, which depends on material parameters. It is especially difficult to find lasers that generate short wavelengths (for example, ultraviolet light). With nonlinear materials it is possible to generate harmonics with frequencies that are multiples of the frequency of the laser light. Coherent light with half the wavelength of the fundamental beam is generated with second-order nonlinear materials. This model shows how to set up second harmonic generation as a transient wave simulation using nonlinear material properties. A Nd:YAG ($\lambda = 1.06$ μm) laser beam is focused on a nonlinear crystal, so that the waist of the beam is inside the crystal.

Model Definition

To simplify the problem and to save some calculation time this model is not a full 3D simulation, but rather a 2D model. The model uses COMSOL Multiphysics' standard 2D coordinate system, assuming that the beam is propagating in the x direction, it has a transverse Gaussian intensity dependence in the y direction and that the electric field is polarized in the out-of-plane z direction.
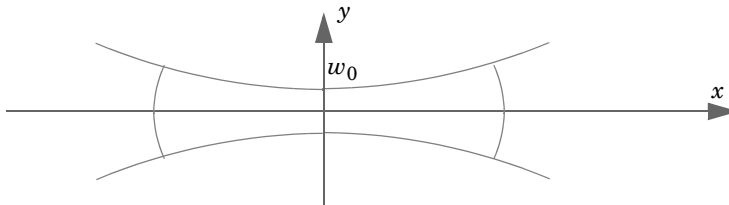
When a laser beam propagates, it travels as an approximate plane wave with a cross-section intensity of Gaussian shape. At the focal point, the laser beam has its minimum width, w_0. For a Gaussian beam with a minimum spot radius that is not too small compared to the wavelength ($w_0 > \lambda$), the solution of the time-harmonic Maxwell's equations for a 2D geometry[1] can be approximated by the following analytical solution of the paraxial wave equation[2]:

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1. Notice that the electric field is defined for a 2D Gaussian beam. In 2D, the amplitude is defined as the square root of the spot radius ratio and the Gouy phase shift $\eta(x)$ is defined with a factor $1/2$. In 3D the amplitude is defined using just the spot radius ratio and there is no factor $1/2$ for the Gouy phase shift.

$$\mathbf{E}(x, y, z) = E_0 \sqrt{\frac{w_0}{w(x)}} e^{-(y/w(x))^2} \cos\left(\omega t - kx + \eta(x) - \frac{ky^2}{2R(x)}\right) \mathbf{e}_z$$

where

$$w(x) = w_0 \sqrt{1 + \left(\frac{x}{x_0}\right)^2}$$

$$\eta(x) = \frac{1}{2} \text{atan}\left(\frac{x}{x_0}\right)$$

$$R(x) = x\left(1 + \left(\frac{x_0}{x}\right)^2\right)$$

In these expressions, w_0 is the minimum waist, ω is the angular frequency, y is the in-plane transverse coordinate, and k is the wave number. The wavefront of the beam is not exactly planar; it propagates like a spherical wave with radius $R(x)$. However, close to the focal point the wave is almost plane.

The laser beam is also modeled as a pulse in time, using a Gaussian envelope function. This produces a wave package with a Gaussian frequency spectrum.

These expressions are used as the input boundary conditions.

The nonlinear properties for second harmonic generation in a material can be defined with the following matrix,

$$\mathbf{P} = \begin{bmatrix} d_{11} & d_{12} & d_{13} & d_{14} & d_{15} & d_{16} \\ d_{21} & d_{22} & d_{23} & d_{24} & d_{25} & d_{26} \\ d_{31} & d_{32} & d_{33} & d_{34} & d_{35} & d_{36} \end{bmatrix} \cdot \begin{bmatrix} E_x^2 \\ E_y^2 \\ E_z^2 \\ 2E_z E_y \\ 2E_z E_x \\ 2E_x E_y \end{bmatrix}$$

where $\mathbf{P}$ is the polarization. The model only uses the d_{33} parameter for simplicity. To keep the problem size small the nonlinear parameter is magnified by some orders of magnitude. The crystal here has a value of 10^{-17} F/V, when the values for most materials usually are

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2. In the paraxial wave equation the second derivative with respect to the coordinate in the propagation direction is neglected. This approximation of the Helmholtz equation is not applicable for a strongly diverging beam, like a beam that is focused to a very small spot radius ($w_0 < \lambda$).

in the 10^{-22} F/V range. Without this magnification, to get a detectable second harmonics requires a much longer propagation distance, resulting in a large computational problem.

The mesh size is defined to resolve not only the fundamental wavelength, but also the second harmonic wavelength. Given the mesh size, the time step is calculated as

$$t_{\text{step}} = CFL \times h_{\text{max}}/c_0,$$

where CFL is the so called CFL number — named after Courant, Friedrichs, and Lewy — h_{max} is the maximum mesh element size, and c_0 is the speed of light. In this model, a CFL number of 0.15 is used. In general, it should be in the range 0.1 to 0.2. For more information on how to define the time step for the time-dependent solver, see Ref. 2.

Results and Discussion

The main purpose of this simulation is to calculate the second harmonic generation when the pulse travels along the 20 μm geometry. So you have to solve for the time it takes for the pulse to enter, pass, and disappear from the volume. The pulse has a characteristic time of 10 fs, and below you can see the pulse after it has traveled 61 fs.
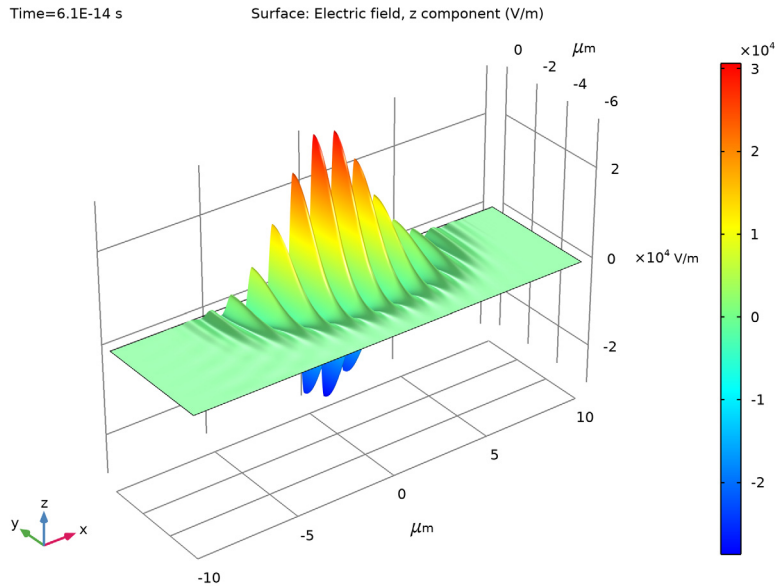

Figure 1: The pulse after 61 fs.

After **90** fs the pulse has reached the output boundary (see Figure 2). The simulation has to continue for another **30** fs until the pulse completely disappears.
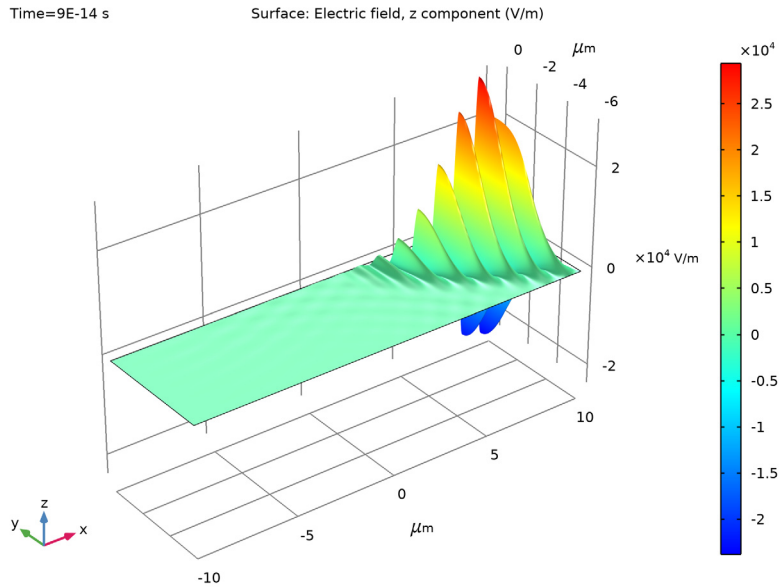

Figure 2: The pulse after 90 fs. It has now reached the output boundary.

The simulation stores the times between **60** fs and **120** fs, which is when the pulse passes the output boundary. The electric field at this boundary has a second harmonic component that can be extracted using a frequency analysis. The result appears in Figure 3. The small peak on the right side of the large peak is the second harmonic generation. To the left of the large peak is also a smaller peak, due to difference frequency generation. This optical rectification effect is also a second-order nonlinear optical process.
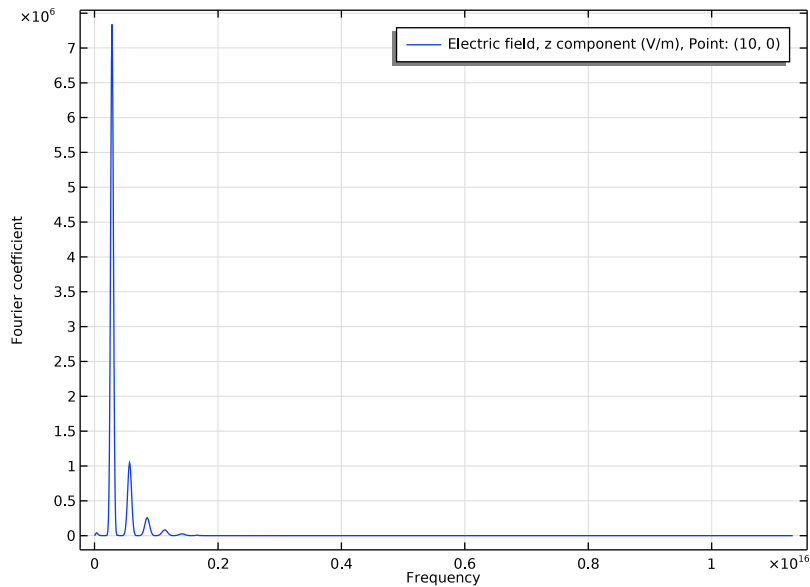
Figure 3: The frequency spectrum of the beam at the output boundary. The peak on the right side of the large peak is the second harmonic generation. You also find smaller peaks for higher harmonics. There is also a tiny peak close to zero frequency that is due to difference frequency generation.

Reference

1. A. Yariv, *Quantum Electronics*, 3rd Edition, John Wiley & Sons, 1988.

2. COMSOL Knowledge Base 1118, "Resolving time-dependent waves," https://www.comsol.com/support/knowledgebase/1118/.

Application Library path: Wave_Optics_Module/Nonlinear_Optics/second_harmonic_generation

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 Ω **2D**.

2 In the **Select Physics** tree, select **Optics>Wave Optics>Electromagnetic Waves, Transient (ewt)**.

3 Click **Add**.

4 Click → **Study**.

5 In the **Select Study** tree, select **General Studies>Time Dependent**.

6 Click ☑ **Done**.

GEOMETRY 1

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Geometry 1**.

2 In the **Settings** window for **Geometry**, locate the **Units** section.

3 From the **Length unit** list, choose **µm**.

GLOBAL DEFINITIONS

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 In the table, enter the following settings:

Name	Expression	Value	Description
w0	2[um]	2E-6 m	Minimum spot radius of laser beam
lda0	1.06[um]	I.06E-6 m	Wavelength of input laser beam
E0	30[kV/m]	30000 V/m	Peak electric field
x0	pi*w0^2/lda0	I.1855E-5 m	Rayleigh range
k0	2*pi/lda0	5.9275E6 I/m	Propagation constant
omega0	k0*c_const	I.777E15 I/s	Angular frequency
t0	25[fs]	2.5E-14 s	Pulse time delay
dt	10[fs]	IE-14 s	Pulse width
d33	1e-17[F/V]	IE-17 s^7·A³/ (kg²·m^4)	Matrix element for second harmonic generation
lda2	lda0/2	5.3E-7 m	Wavelength for second harmonic
hmax	lda2/6	8.8333E-8 m	Maximum mesh element size
CFL	0.15	0.I5	CFL number
tstep	CFL*hmax/c_const	4.4197E-I7 s	Time step

The last four parameters will be used for defining the maximum mesh element size and for defining the time step for the time-dependent solver.

Analytic I (anI)

1 In the **Home** toolbar, click $f(x)$ **Functions** and choose **Global>Analytic**.

2 In the **Settings** window for **Analytic**, type w in the **Function name** text field.

3 Locate the **Definition** section. In the **Expression** text field, type w0*sqrt(1+(x/x0)^2).

4 Locate the **Units** section. In the **Arguments** text field, type m.

5 In the **Function** text field, type m.

Analytic 2 (an2)

1 In the **Home** toolbar, click $f(x)$ **Functions** and choose **Global>Analytic**.

2 In the **Settings** window for **Analytic**, type eta in the **Function name** text field.

3 Locate the **Definition** section. In the **Expression** text field, type atan2(x,x0)/2.

4 Locate the **Units** section. In the **Arguments** text field, type m.

5 In the **Function** text field, type rad.

Analytic 3 (an3)

1 In the **Home** toolbar, click f(x) **Functions** and choose **Global>Analytic**.

2 In the **Settings** window for **Analytic**, type R in the **Function name** text field.

3 Locate the **Definition** section. In the **Expression** text field, type x*(1+(x0/x)^2).

4 Locate the **Units** section. In the **Arguments** text field, type m.

5 In the **Function** text field, type m.

GEOMETRY I

Create a rectangular calculation domain, where y = 0 is the symmetry plane for the laser beam.

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 20.

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

5 Locate the **Position** section. In the **x** text field, type -10.

6 In the **y** text field, type -6.

7 Click ▦ **Build All Objects**.

8 Click the ⊹ **Zoom Extents** button in the **Graphics** toolbar.

MATERIALS

Assume that the laser beam propagates through an artificial material with the properties of air except for an additional second-order optical nonlinearity. You will specify the nonlinearity later, when setting up the wave equation.

ADD MATERIAL

1 In the **Home** toolbar, click ▦ **Add Material** to open the **Add Material** window.

2 Go to the **Add Material** window.

3 In the tree, select **Built-in>Air**.

4 Click **Add to Component** in the window toolbar.

5 In the **Home** toolbar, click ▦ **Add Material** to close the **Add Material** window.

ELECTROMAGNETIC WAVES, TRANSIENT (EWT)

Only solve for the out-of-plane component.

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

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

3 From the **Electric field components solved for** list, choose **Out-of-plane vector**.

Perfect Magnetic Conductor 1

1 In the **Physics** toolbar, click ⬭ **Boundaries** and choose **Perfect Magnetic Conductor**.

2 Select Boundary 3 only.

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
0	y
E0*sqrt(w0/w(x))*exp(-y^2/w(x)^2)*cos(omega0*t-k0*x+eta(x)-k0*y^2/(2*R(x)))*exp(-(t-t0)^2/dt^2)	z

Scattering Boundary Condition 2

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

2 Select Boundary 4 only.

Wave Equation, Electric 1

1 In the **Model Builder** window, 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 **Remanent electric displacement**.

4 Specify the $\mathbf{D_r}$ vector as

0	x
0	y
d33*ewt.Ez^2	z

MESH I

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

Distribution 1
1 Right-click **Mapped 1** and choose **Distribution**.

2 Select Boundaries 1 and 4 only.

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

4 From the **Distribution type** list, choose **Explicit**.

5 In the **Relative placement of vertices along edge** text field, type sin(range(0,0.025* pi,0.5*pi)). This creates a denser mesh closer to the upper boundary.

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

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 hmax.

5 Click ⊞ **Build All**.

6 Click the ⊹ **Zoom Extents** button in the **Graphics** toolbar.
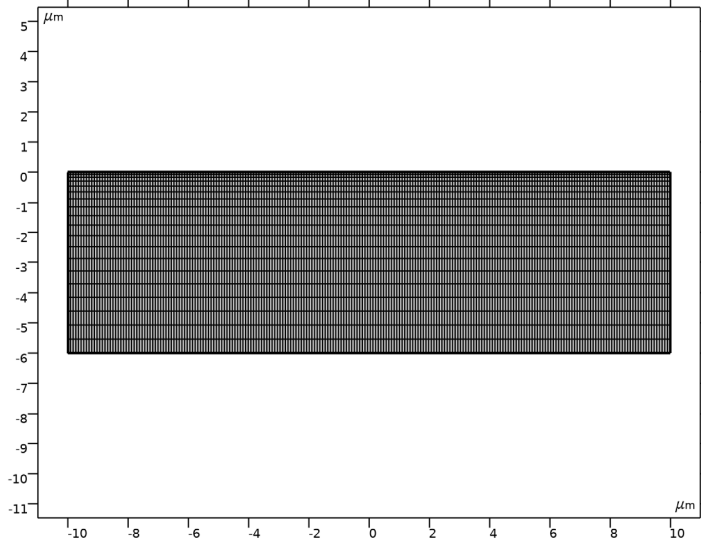
DEFINITIONS

To perform an FFT analysis, the number of time steps that have to be saved is very large. To store all solutions of the A-field results in a huge model file. However, for the FFT, it is only interesting to look at the field at the output boundary. You can take advantage of this fact by defining a Domain Point Probe that stores and displays the on-axis electric field at the output boundary, whereas the A-field is only stored at the times defined in the study.

Domain Point Probe 1

1 In the **Definitions** toolbar, click 🖊 **Probes** and choose **Domain Point Probe**.

2 In the **Settings** window for **Domain Point Probe**, locate the **Point Selection** section.

3 In row **Coordinates**, set **x** to 10.

Point Probe Expression 1 (ppb1)

1 In the **Model Builder** window, expand the **Domain Point Probe 1** node, then click **Point Probe Expression 1 (ppb1)**.

2 In the **Settings** window for **Point Probe Expression**, type Eout in the **Variable name** text field.

3 Click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1)>Electromagnetic Waves, Transient>Electric> Electric field - V/m>ewt.Ez - Electric field, z component**.

Step 1: Time Dependent

Now define the times for which to save the full field solutions.

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 **Output times** text field, type 0 61[fs] 90[fs] 120[fs].

4 Click to expand the **Results While Solving** section. Select the **Plot** check box.

Solution 1 (sol1)

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

 Set the solver to calculate the output field every 0.2 fs.

2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node, then click **Time-Dependent Solver 1**.

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

4 From the **Steps taken by solver** list, choose **Manual**.

5 In the **Time step** text field, type tstep.

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

RESULTS

2D Plot Group 1

Now define the surface plots, as displayed in Figure 1 and Figure 2.

Surface 1

1 In the **Model Builder** window, expand the **2D Plot Group 1** node, then click **Surface 1**.

2 In the **Settings** window for **Surface**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **ewt.Ez - Electric field, z component - V/m**.

Height Expression 1

Right-click **Surface 1** and choose **Height Expression**.

2D Plot Group 1

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

2 From the **Time (s)** list, choose **6.1E-14**.

3 In the **2D Plot Group 1** toolbar, click **Plot**. You should now see the plot in Figure 1.

4 From the **Time (s)** list, choose **9E-14**.

5 In the **2D Plot Group 1** toolbar, click 🔲 **Plot**. You should now see the plot in Figure 2.

Probe Table Graph 1

Finally, make a spectral analysis of the on-axis electric field at the output boundary.

1 In the **Model Builder** window, expand the **Results>Probe Plot Group 2** node, then click **Probe Table Graph 1**.

2 In the **Settings** window for **Table Graph**, locate the **Data** section.

3 From the **Transformation** list, choose **Frequency spectrum**.

4 Select the **Frequency range** check box.

5 In the **Probe Plot Group 2** toolbar, click 🔲 **Plot**.

Probe Plot Group 2

Now you should have a graph similar to the one in Figure 3.