A Tutorial: Computing QNMs for A Metallic Sphere in Air

1. Introduction

In this document, we give all the details on how to compute the QNMs of a classical example, a metallic sphere in an homogenous background, with **QNMEig** and COMSOL Multiphysics. Note that in the model libraries of COMSOL Multiphysics, there are already well-documented examples for computing modes for non-dispersive resonators. However, these examples cannot be directly applied for dispersive resonators, and **QNMEig** can be considered as an extension of the built-in solver in COMSOL Multiphysics for dispersive resonators.

Note: The solver computes the QNM eigenfrequencies $\tilde{f}_m$ in units of [Hz], which relate with QNM eigen-angular frequencies $\tilde{\omega}_m$, more popularly used in the nanophotonics community, by $\tilde{\omega}_m = 2\pi\tilde{f}_m$. In the following, we define a global variable ''*QNM_omega*" for representing $\tilde{\omega}_m$.

2. Model Definition

Geometry: a sphere with radius 40 nm.

Material parameters: the sphere has a dispersive permittivity described by the Lorentz-Drude model

$$\varepsilon_{\mathrm{Ag}} = \varepsilon_{\infty,\mathrm{Ag}}[1 - \frac{\omega_{p,\mathrm{Ag}}^2}{\omega^2 - \omega_{0,\mathrm{Ag}}^2 + i\omega\gamma_{\mathrm{Ag}}}], \quad (1)$$

with $\varepsilon_{\infty,\mathrm{Ag}} = 1$, $\omega_{p,\mathrm{Ag}} = 1.35\mathrm{e}16\ [\mathrm{rad/s}]$ corresponding to $\lambda_{p,\mathrm{Ag}} = 138$ nm in vacuum, $\gamma_{\mathrm{Ag}} = 0.0023\omega_{p,\mathrm{Ag}}$, and $\omega_{0,\mathrm{Ag}} = 0$.

The background is air, $\varepsilon_b = 1$.

3. Modelling Instructions

Open COMSOL Multiphysics. From its **File** menu, choose **New**.

NEW

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

MODEL WIZARD

1 In the Model Wizard window, click **3D**.

2 In the Select physics tree, select **Radio Frequency->Electromagnetic Waves, Frequency Domain (emw).**

3 Click **Add**.

4 In the Select physics tree, select **Mathematics->PDE Interfaces**, **Weak Form PDE**.

5 Click **Add**.

6 In the **Review Physics Interface** window, locate the **Dependent Variables** section. In the **Field name** text field, type ***P1***; in the **Number of dependent variables** text field, type ***3***; in

the **Dependent variables** text field, type ***P1x***, ***P1y***, ***P1z***. Locate the **Units** section. In the **dependent variable quantity** text field, choose **Electric Field V/m**.

7 Click **Study**.

8 In the Select study tree, select **Present Studies->Eigenfrequency.**

9 Click **Done**.

DEFINITIONS

Parameters

1 On the **Model** toolbar, click **Parameters**.

2 In the **Settings** window for **Parameters**, locate the **Parameters** section. In the table, enter the following settings:

- Material parameters for the sphere

Name	Expression	Description
omegap_Ag	1.3659E16 [rad/s]	Plasma frequency of Lorentz-Drude permittivity for silver
gamma_Ag	0.0023*omegap_Ag	Damping frequency of Lorentz-Drude permittivity for silver
omega0_Ag	0	Resonance frequency of Lorentz-Drude permittivity for silver
epsiloninf_Ag	1	Silver permittivity at infinite large frequencies

Here, omegap_Ag, gamma_Ag, omega0_Ag, epsiloninf_Ag correspond to $\omega_{p,\mathrm{Ag}}, \gamma_{\mathrm{Ag}}, \omega_{0,\mathrm{Ag}}$ and $\varepsilon_{\infty,\mathrm{Ag}}$ that appear in the Lorentz-Drude permittivity.

- Material parameters for the background

Name	Expression	Description
epsilonb	1	Background permittivity

- Parameters for perfectly-matched layers

Name	Expression	Description
lambda_pml	600 [nm]	Typical central wavelength for which PMLs should work properly

- Geometrical parameters

Name	Expression	Description
r0	40 [nm]	Sphere radius
rb	130 [nm]	Outermost background radius
tpml	80 [nm]	PML thickness

- Other parameters

Name	Expression	Description
lambda_N	100 [nm]	Normalization length for auxiliary-field equation

The parameter lambda_N is used in the auxiliary-field equation that we input in the **Weak Form PDE** module (see later) to make the two equations of the quadratic polynomial eigenproblem (see the User Guide document) have similar magnitudes, thereby increasing the numerical stabilities.

Variables

1 On the Model toolbar, click Variables->Global Varialbes.

2 In the **Settings** window, locate the **Variables** section. In the table, enter the following settings:

Name	Expression	Description
QNM_omega	(lambda/(–*j*)) [rad/s]	QNM eigen-angular frequencies

Here, "lambda" is the default notation used by COMSOL to represent eigenvalues in general. According to the COMSOL convention, $\widetilde{\omega}_m$, the QNM eigen-angular frequencies (in units of [rad/s]), equals to lambda/(–*j*)

GEOMETRY

The geometry consists of a metallic sphere in air background, surrounded by a PML.

Sphere 1

1 On the **Geometry** toolbar, click **Sphere**.

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

3 In the **Radius** text field, type 1.1*r0.

4 Locate the **Layer** section. In the **Thickness (m)** text field, type 0.1*r0.

We coat the metal sphere with a virtual thin layer made for refining the mesh elements close to the sphere surface, thereby allowing us to more accurately compute high-order QNMs.

Sphere 2

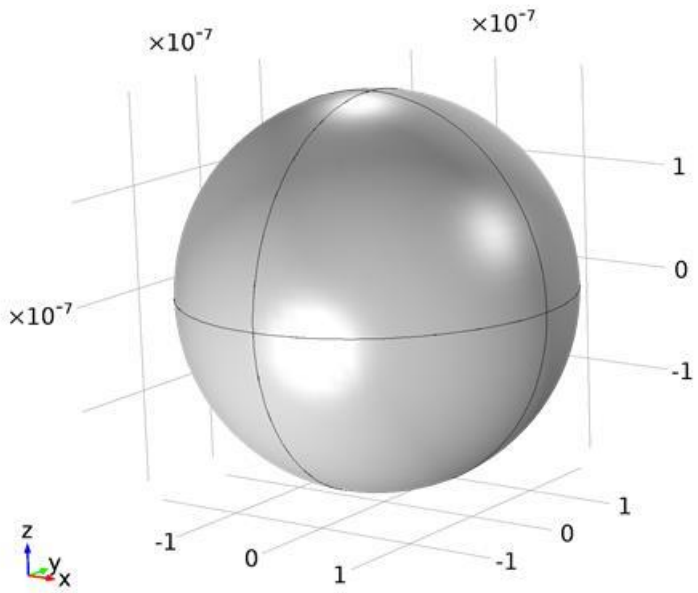
1 On the **Geometry** toolbar, click **Sphere**.

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

3 In the Radius text field, type rb+tpml.

4 Locate the **Layer** section. In the **Thickness (m)** text field, type tpml.

Click the **Build All Objects** button.



DEFINITIONS

Define PML domains and PML types. Define three variables, DP1x, DP1y, DP1z, which shall be used for QNM normalization and in the physics module, **ELECTROMAGNETIC WAVES, FREQUENCY DOMAIN (EMW).** Add two integration coupling operators: one for a volume integration in all domains including PML domains and the other one for volume integration in metal-domain only.

Domain Selection

1 On the **Definitions** toolbar, click **Explicit**.

2 In the Settings window for **Explicit**. In the **Label** text field, type **PML**.

3 Locate the **Input Entities** section, select PML domain, including 1, 2, 3, 4, 11, 12, 15, 18.

4 On the **Definitions** toolbar, click **Explicit**.

5 In the Settings window for **Explicit**. In the **Label** text field, type **Silver sphere**.

6 Locate the **Input Entities** section, select Silver domain, including 10.

7 On the **Definitions** toolbar, click **Explicit**.

8 In the Settings window for **Explicit**. In the **Label** text field, type **Air background and its attached PML**.

9 Locate the **Input Entities** section, select air background and also PML domains, including 1, 2, 3, 4, 11, 12, 15, 18, 5, 6, 7, 8, 9, 13, 14, 16, 17.

Perfectly matched layers

1 On the Definitions toolbar, click Perfectly Matched Layer.

2 In the **Settings** window for **Perfectly Matched Layer**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Explicit: PML**.

4 Locate the **Geometry** section. From the **Type** list, select **Spherical**.

5 Locate the **Scaling** section. From the **Typical wavelength from** list, choose **User defined**.

6 From Typical wavelength text field, type “lambda_pml”.

Integration 1 (intop1)

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

2 In the **Settings** window for Integration, type **intAll** in the **Operator name** text field.

3 Locate the **Source Selection** section. From the **Selection** list, choose **All domains**.

Integration 2 (intop2)

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

2 In the **Settings** window for Integration, type **intMetal** in the **Operator name** text field.

3 Locate the Source Selection section. From the Selection list, choose Explicit: Silver sphere.

Variables 1

1 On the **Definitions** toolbar, click **Variables**.

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

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

4 From the Selection list, choose Explicit: Silver sphere

5 Locate the **Variables** section. In the table, enter the following settings:

Name	Expression
DP1x	epsilon0_const*(emw.epsilonrxx*P1x+emw.epsilonrxy*P1y+emw.epsilonrxz*P1z)
DP1y	epsilon0_const*(emw.epsilonryx*P1x+emw.epsilonryy*P1y+emw.epsilonryz*P1z)
DP1z	epsilon0_const*(emw.epsilonrzx*P1x+emw.epsilonrzy*P1y+emw.epsilonrzz*P1z)

Variables 2

1 On the **Definitions** toolbar, click **Variables**.

2 In the **Settings** window for Variables, Locate the **Variables** section. In the table, enter the following settings:

Name	Expression
fdisp	2*omegap_Ag^2/(QNM_omega^2-omega0_Ag^2-j*QNM_omega*gamma_Ag)+QNM_omega*omegap_Ag^2*(2*QNM_omega-j*gamma_Ag)/(QNM_omega^2-omega0_Ag^2-j*QNM_omega*gamma_Ag)^2
QN	2*intAll((emw.Ex*emw.Dx+emw.Ey*emw.Dy+emw.Ez*emw.Dz)*pml1.detInvT)+intMetal((emw.Ex*emw.DP1x+emw.Ey*emw.DP1y+emw.Ez*emw.DP1z)*pml1.detInvT)*fdisp

QN is used for normalizing the QNM.

MATERIALS

Assign material properties on the model.

Material 1(metal)

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 **Geometric Entity Selection** section.

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

4 From the Selection list, select **Explicit: Silver sphere**

5 Locate the **Material Contents** section. In the table, enter the following settings:

Property	Name	Value
Relative permittivity	epsilonr	epsiloninf_Ag
Relative permeability	mur	1
Electrical conductivity	sigma	0

Note: the relative permittivity of metals here only includes the non-dispersive part, $\varepsilon_{\infty,\mathrm{Ag}}$; the dispersive part is captured by the introduced auxiliary fields.

Material 2(background, including PML)

1 In the **Model Builder** window, right-click **Materials** and choose **Blank Material**.

2 In the **Settings** window for Material, locate the **Geometric Entity Selection** section.

3 From the Geometric entity level list, choose Domain.

4 From the Selection list, choose **Explicit: Air background and its attached PML**.

5 Locate the Material Contents section. In the table, enter the following settings:

Property	Name	Value
Relative permittivity	epsilonr	epsilonb
Relative permeability	mur	1
Electrical conductivity	sigma	0

MESHES 1

According to the technical suggestion from COMSOL Multiphysics, it is recommended to define PMLs with a swept mesh with at least five elements across. Moreover, from many numerical tests, we find that it is better to also use a swept mesh across the thin background layer attached to the plasmonic nanosphere, if one wishes to compute high-order plasmonic modes more accurately.

Metal

1 In the **Model Builder** window, under **Component 1** (comp1) right-click **Mesh 1** and choose **Free Tetrahedral**.

2 In the **Settings** window for **Tetrahedral Free 1**, locate the **Domain Selection** section.

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

4 From the Selection list, choose Explicit: Silver sphere.

5 Right-click **Free Tetrahedral 1,** select **Size** option.

6 Locate **Element Size** section, select **Custom** option.

7 Locate **Element Size Parameters** section. In the **Maximum element size** text field, type "r0/3". In the **Minimum element size** text field, type "r0/6".

Thin-layer background

1 In the **Model Builder** window, under **Component 1** (comp1) right-click **Mesh 1** and choose **Swept**

2 In the **Settings** window for **Swept 1**, locate the **Domain Selection** section.

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

4 From the **Selection** list, choose **manual** and select thin background layer, including 6-9, 13-14, 16-17.

5 Right-click **Swept 1,** select ***Distribution*** option.

6 Locate the **Distribution** section. In the **Number of elements field** text field, type **1**.

Background

1 In the **Model Builder** window, under **Component 1** (comp1) right-click **Mesh 1** and choose **Free Tetrahedral**.

2 In the **Settings** window for **Tetrahedral Free 2**, locate the **Domain Selection** section.

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

4 From the **Selection** list, choose **manual** and select background domains excluding the thin layer background meshed above , including 5.

5 Right-click **Free Tetrahedral 1,** select **Size** option.

6 Locate **Element Size** section, select **Custom** option.

7 Locate **Element Size Parameters** section. In the **Maximum element size** text field, type "40 [nm]". In the **Minimum element size** text field, type "r0/3".

PMLs

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

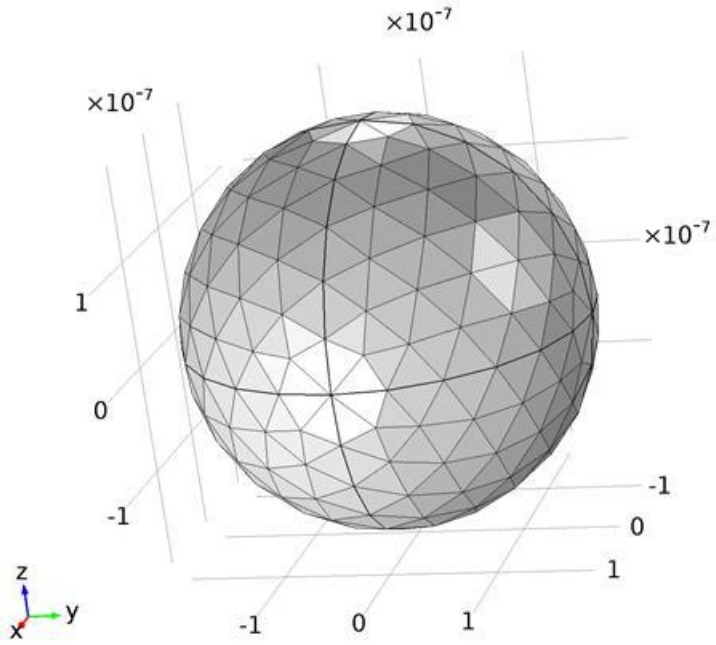
2 In the **Settings** window for **Swept 2**, locate the **Domain Selection** section.

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

5 Right-click **Swept 2,** select ***Distribution*** option.

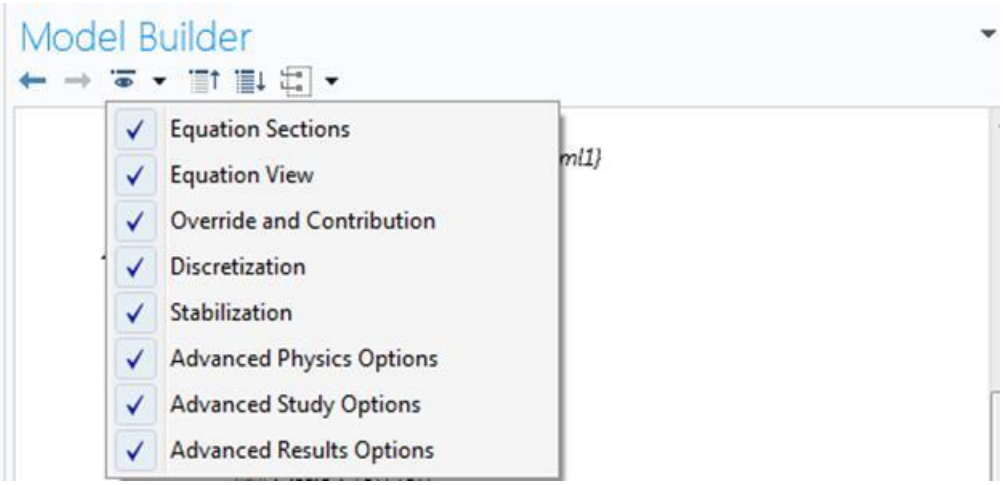
6 Locate the **Distribution** section. In the **Number of elements field** text field, type **8**.

Click the **Build All** button.



ELECTROMAGNETIC WAVES, FREQUENCY DOMAIN (EWFD)

1 On the top of the **Modal Builder** window, click show option (the one with an eye icon), select at least **Advanced Physics** and **Discretization** options.



2 On the Physics toolbar, select Electromagnetic Waves, Frequency Domain.

3 In the Settings window for Electromagnetic Waves, Frequency Domain, locate the Domain Selection section.

4 From the **Selection** list, choose **All Domains**.

5 On the **Physics** toolbar, from the **Domains** section list, choose **Weak Contribution**.

6 In the **Settings** window for **Weak Contribution**, locate **Domain Selection** section.

7 From the Selection list, choose Explicit: Silver sphere.

8 Locate the Weak Contribution section. In the Weak expression text field, type ***"mu0_const*QNM_omega^2*(test(emw.Ex)*DP1x+test(emw.Ey)*DP1y+test(emw.Ez)*DP1z) *pml1.detInvT"***

AUXILIARY FIELDS

1 On the Physics toolbar, select Auxiliary Fields.

2 In the **Settings** window for **Auxiliary Fields**, locate the **Domain Selection** section.

3 From the Selection list, choose Explicit: Silver sphere.

4 Locate the **Discretization** section. From the **Shape function type** list, choose **Curl type**.

5 In the **Modal Builder** window, under the **Auxiliary Fields** module, click **Weak Form PDE 1**.

6 In the **Settings** window for **Weak Form PDE 1**. Locate the **Weak Expressions** section, enter the following three expressions:

1/lambda_N^2*((test(P1x)*P1x+test(P1y)*P1y+test(P1z)*P1z)*(QNM_omega^2-j*gamma_Ag*QNM_omega-omega0_Ag^2)/omegap_Ag^2+(test(P1x)*emw.Ex+test(P1y)*emw.Ey+test(P1z)*emw.Ez))
0
0

STUDY 1

1 In the **Model Builder** window, expand the **Study** 1 node, then click **Step 1: Eigenfrequency**.

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

3 In the **Desired number** of eigenfrequencies text field, type **4**.

4 In the Search for eigenfrequencies around text field, type "omegap_D/(2*pi)*0.45".

We observe that, even though we ask the eigenfrequency solver for a given desired number of modes, N ($N = 4$ here), the final number of modes that the solver delivers after computations is $2N$. Furthermore, when resonators are made of non-dispersive dielectrics , and the auxiliary-field equation is not needed, the computed mode number is N.

5 On the Study toolbar, click **Compute**.

4. Results and Discussions

We compute 8 modes, which are QNMs, i.e., natural resonance states of the metal sphere in air. These modes are TM-polarized spherical waves, including three degenerate modes with spherical harmonic degree $\ell = 1$, and five degenerate modes with $\ell = 2$. Table 1 gives the computed eigenfrequencies (in units of Hz; not angular frequencies). Note that the mode degeneracy is slightly lifted because the numerical discretization breaks the spherical symmetry. We compare the COMSOL results with those obtained by finding poles of Mie's scattering coefficients (right column). Good agreement is achieved; the slight difference is due to inevitable numerical inaccuracies, introduced by numerical discretization and the inevitable imperfection of the numerical perfectly matched layers.

Spherical harmonic degree	Eigenfrequencies [Hz]	
	COMSOL	Mie's scattering theory
$\ell = 1$ (3 modes)	9.1860E14+1.5051E14i 9.1861E14+1.5046E14i 9.1869E14+1.5046E14i	9.1980E14+1.4953E14i

$\ell = 2$ (5 modes)	1.2351E15+2.2485E13i 1.2352E15+2.2450E13i 1.2352E15+2.2475E13i 1.2352E15+2.2480E13i 1.2353E15+2.2499E13i	1.2363E15+2.2476E13i

Table 1: 8 QNM eigenfrequencies computed with **QNMEig** for the metal sphere in air, and comparison with Mie's scattering theory.

The three components of the *normalized* QNM electric field are given by, Ex/sqrt(QN), Ey/sqrt(QN), Ez/sqrt(QN). Below, we plot the modulus of the normalized QNM electric-field, sqrt(abs(Ex^2+Ey^2+Ez^2/QN)), for the mode with the eigenfrequency 9.1826E14+1.5039E14i.