# QNMtoolbox_grating: an openly available toolbox for computing the quasinormal modes and modal excitation coefficients of gratings

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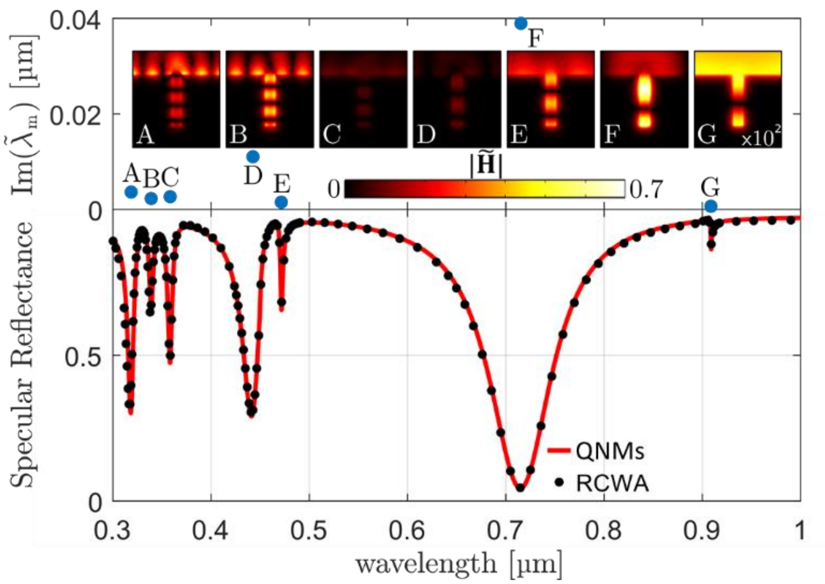


 It is composed of

- the present user guide document,
- **QNMtoolbox_grating.m**, a Matlab open-source script of the freeware package **MAN** (Modal Analysis of Nanoresonators) [1], built for extracting the normalized resonance modes (also called the quasinormal modes or QNMs) of periodic gratings [2], and computing the QNM excitation coefficients at real frequencies. **QNMtoolbox_grating.m** also computes the specular reflection, using QNM expansions. The script preferentially operates on the Matlab-COMSOL  Livelink environment with the solver **QNMEig** of the package **MAN**; however, the code would also work with QNMs computed with other software,

- **QNMEig_1DGrating_theta.mph**, a COMSOL model for operation with the **QNMEig** solver.



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# 1. INTRODUCTION TO QNMTOOLBOX_GRATING.M

**QNMtoolbox_grating.m** extracts the normalized QNMs of 1D-periodic gratings computed with the QNM solvers of the **MAN** package and computes the excitation coefficients associated to each QNM at real frequencies. The example is provided for a plane-wave excitation polarized along the $x$-axis propagating along the $z$-axis (TM polarization).

In this section, basic information about **QNMtoolbox_grating.m** is provided.

## 1.1 Download & Installation

**QNMtoolbox_grating.m** is a Matlab script to be used with the Matlab-COMSOL livelink environment, in conjunction with the solver **QNMEig** and the model **QNMEig_1DGrating.mph**. The script needs to be placed in your Matlab folder to be run.

## 1.2 How to acknowledge and cite

We kindly ask that you reference the **MAN** package from IOGS-CNRS and its authors in any publication/report for which you used it.

- The preferred citation for **QNMtoolbox_grating.m** is the following paper:
  [ref1] A. Gras, W. Yan, P. Lalanne, "Quasinormal-mode analysis of grating spectra at fixed incidence angles", Opt. Lett. **44**, 3494 (2019).
- The preferred citation for **MAN** is the following paper:
  [ref2] W. Yan, R. Faggiani, and P. Lalanne, "Rigorous modal analysis of plasmonic resonators", Phys. Rev. B **97**, 205422 (2018).

A brief description of the algorithm might be:
"The QNMs and the modal excitation coefficients are computed with the toolbox QNMtoolbox_grating [ref1] of the freeware MAN (Modal Analysis of Resonators) [ref2] under the COMSOL Multiphysics environment."

## 1.3 Units and conventions of input/output data

Unlike most of the models in the **QNMEig** package, the **QNMEig_grating_theta.mph** model and its companion script employ the following reduced units:

- The plasma frequency $\omega_p$ is entered into COMSOL as $2\pi$ and $c = \varepsilon_0 = \mu_0 = 1$.

- Every distance is divided by the wavelength $\lambda_p$ corresponding to $\omega_p$ and entered accordingly. For example, the period of the grating: $a = 600.0\ nm \cong 4.0107\ \lambda_p\ [SI] \rightarrow a = 4.0107$.

**Convention**. The time dependent terms $\exp(\mathrm{i}\omega\mathrm{t})$ used by COMSOL is adopted.

## 1.4 Outline of the theory and related key issues

**QNMtoolbox_grating.m** is dedicated to the design of periodic nanoresonator arrays and gratings. It relies on COMSOL Multiphysics®, its Mathematics Module, and MATLAB®.

Classically, to solve Maxwell's equations, one uses a particular excitation field with a given wavelength and polarization. However, the whole numerical simulation has to be redone each time the excitation field changes, in particular the wavelength. Then the numerical load may be heavy, and, above all, the computed results may still hide a great deal of knowledge about the physical mechanisms at play. Modes represent a powerful characteristic of the resonator. If one is able to find these modes (they are called quasinormal modes) and understand how they are excited, then it is possible to describe the interactions between the resonator and its environment much more easily and intuitively.

The approach adopted by **QNMtoolbox_grating.m** is exactly this one. It permits to compute the excitation coefficients of the normalized modes computed by **QNMEig**, simply by evaluating a surface integral [1]. This part is crucial as it results in a rapid and analytical method to calculate the electromagnetic field scattered by the grating, and all the associated physical quantities, such as the reflection spectra depicted in Fig. 1.

In the case of **periodic structures** such as gratings, the QNMs are computed for a given **directionality**, characterized here by the **angle of incidence** $\theta$ of the incoming plane wave upon the grating. The computed QNMs in this instance are the ones that are excited when the impinging wave has this directionality.

In more mathematical terms, we consider a plane wave $\mathbf{E}_{inc}(\mathbf{r},\omega)$ that is incident on the grating, propagating in the direction **characterized by the incidence angle** $\theta$. The optical response of the grating at that angle, e.g. the scattered field $\mathbf{E}_S(\mathbf{r},\omega,\mathbf{E}_b)$, is defined by a local change $\Delta\varepsilon(\omega,\mathbf{r})$ ($\Delta\varepsilon \neq 0$ for $\mathbf{r} \in V_{res}$) of a background permittivity $\varepsilon_b(\omega,\mathbf{r})$, so that $\varepsilon_b + \Delta\varepsilon$ is equal to the actual grating permittivity distribution (see figure 2). The background field $\mathbf{E}_b$ is the solution of Maxwell's equations for the background permittivity distribution upon illumination by $\mathbf{E}_{inc}$. The scattered field $\mathbf{E}_S(\mathbf{r},\omega,\mathbf{E}_b)$ can be written with a modal expansion of the form

$$\mathbf{E}_S(\mathbf{r},\omega,\mathbf{E}_b) = \sum_m \alpha_m(\omega,\mathbf{E}_b)\,\tilde{\mathbf{E}}_{m,\theta}(\mathbf{r},\tilde{\omega}_m), \tag{1}$$

where $\tilde{\mathbf{E}}_{m,\theta}$ denotes the electric-field map of the normalized QNM $m$ computed for the angle $\theta$, $\tilde{\omega}_m$ is the mode complex frequency, $2Q = \mathrm{Re}(\tilde{\omega}_m)\,/\,\mathrm{Im}(\tilde{\omega}_m)$, and the $\alpha_m$'s are the excitation coefficients that analytically depend on the background field. This implies that, once the resonant modes of the grating are calculated, the optical response is known *analytically* (i.e. by numerical computation of simple overlap integrals between the background field $\mathbf{E}_b(\mathbf{r},\omega)$ and the counter-propagative QNM field $\tilde{\mathbf{E}}_{m,-\theta}$ ) for any frequency $\omega$ of the excitation field and the physical understanding is immediate and unambiguous since the mode expansion explicitly depends on the excitation parameters [3].

For metal gratings whose permittivity follows a single Lorentz pole model, $\varepsilon(\omega) = \varepsilon_\infty\left(1 - \frac{\omega_p^2}{\omega^2-\omega_0^2+i\gamma\omega}\right)$, the modal excitation coefficient can be written [2]

$$\alpha_m(\omega) = \left(\varepsilon_b - \varepsilon_\infty - (\Delta\varepsilon(\tilde{\omega}_m))\frac{\tilde{\omega}_m}{\tilde{\omega}_m-\omega}\right) \iiint_{V_{res}} \mathbf{E}_b \cdot \tilde{\mathbf{E}}_{m,-\theta}\, d^3\mathbf{r}. \tag{2}$$

Note that if dispersion is not considered ($\omega_p = 0$), then Eq. 2 becomes $\alpha_m(\omega) = (\varepsilon_\infty - \varepsilon_\mathrm{b})\,\frac{\omega}{\tilde{\omega}_m-\omega}\iiint_{V_{res}} \mathbf{E}_b \cdot \tilde{\mathbf{E}}_{m,-\theta}\, d^3\mathbf{r}$.

The specular reflection of the grating at the frequency $\omega$ are plotted using the scattered field calculated with the QNM expansion and the background field. The 0-order reflectivity of the grating $r_0(\omega)$ is obtained from the Rayleigh expansion. We find

$$r_0(\omega) = \frac{1}{a}\frac{1}{H_0}\int_{x=-a/2}^{x=\frac{a}{2}}(\mathbf{H}_{tot}(\mathbf{r},\omega) - \mathbf{H}_{inc}(\mathbf{r},\omega))\cdot\hat{\mathbf{z}}\,dx = \frac{1}{a}\frac{1}{H_0}\int_{x=-a/2}^{x=\frac{a}{2}}(\mathbf{H}_s(\mathbf{r},\omega) + \mathbf{H}_b(\mathbf{r},\omega) - \mathbf{H}_{inc}(\mathbf{r},\omega))\cdot\hat{\mathbf{z}}\,dx, \quad (3)$$

where $\mathbf{H}_{tot} = \mathbf{H}_s + \mathbf{H}_b$ is the total magnetic field, $a$ is the grating's period along the $x$-direction, and $\mathbf{H}_{inc}$ is the TM-polarized field incident upon the grating system with an amplitude $H_0$ and an incident angle $\theta$. Expanding the scattered magnetic field $\mathbf{H}_s$upon the QNM basis gives the following expression of the 0-order reflectivity

$$r_0(\omega) = \frac{1}{a}\frac{1}{H_0}\left[\int_{x=-\frac{a}{2}}^{x=\frac{a}{2}}(\mathbf{H}_b(\mathbf{r},\omega) - \mathbf{H}_{inc}(\mathbf{r},\omega))\cdot\hat{\mathbf{z}}\,dx + \sum_{\mathrm{m}}\alpha_m(\omega)\int_{x=-\frac{a}{2}}^{x=\frac{a}{2}}\tilde{\mathbf{H}}_{m,\theta}(\mathbf{r})\ \cdot\hat{\mathbf{z}}\,dx\right]. \quad (4)$$

The specular reflectance of the grating is then

$$R_0(\omega) = |r_0|^2. \quad (5)$$

To summarize, the QNM computation and normalization (the prerequisite to using **QNMtoolbox_grating.m**) are performed with **QNMEig**, using COMSOL software. The script extracts the normalized QNM fields inside the grating domain, performs the overlap integral, and computes the modal excitation coefficients, and the specular reflection of the grating in a Matlab environment.

## 2. SET-UP: COMPUTATION OF THE EXCITATION COEFFICIENTS

We recommend that the user starts with the bowtie example that is provided to become familiar with **QNMtoolbox_grating.m**, before calculating the excitation coefficients for its own geometry. To calculate and normalize QNMs, follow the following steps:

**1/** Build on a COMSOL model sheet for your problem, or first use and modify the supplied grating model sheet **QNMEig_grating_theta.mph**.

**2/** Open the Matlab script **QNMtoolbox_grating.m**, and make sure that the COMSOL model in use is in the folder.

**3/** In **QNMtoolbox_grating.m**, check the parameters in the ***Input file name and Computing setting, Material parameters, and Computational settings*** sections of the program. In particular, please check the following parameters

- COMSOL.file: the name of the COMSOL file where the QNMs were computed.
- COMSOL.dataset: The tag of the data set of the QNM solution.
- COMSOL.resonator: the index of the resonator domain.

Details on how to correctly set these 3 parameters are given in section 4 of this document.

**4/** Run the script. For every real frequency $\omega$, $\alpha_m$ will be computed for a TM-polarized plane wave excitation of amplitude $H_0 = 1$ , propagating along incident direction characterized by the angle $\theta$. After that, the corresponding reflectance will be calculated.

## 3. FREQUENTLY ASKED QUESTIONS

**What are the reduced units used by the QNMEig model and the script?**

Unlike the other models in the QNMEig_package, **QNMEig_grating_theta.mph** employs only the mathematics module. Like the Matlab script **QNMtoolbox_grating.m**, it also uses the following reduced units:

The plasma frequency $\omega_p$ is entered into COMSOL as $2\pi$ and $c = \varepsilon_0 = \mu_0 = 1$.

Every distance is divided by the wavelength $\lambda_p$ corresponding to $\omega_p$ and entered accordingly. For example, the period of the grating: $a = 600.0\ nm \cong 4.0107\ \lambda_p\ [SI] \rightarrow a = 4.0107$.

**What does the QNM structure contain?**

When $N$ QNMs are computed by the COMSOL model, the QNM structure defined inside **QNMtoolbox_grating.m** contains the following elements.

| Name of variable | Description | Size |
|---|---|---|
| QNM.omega | QNM frequencies $\tilde{\omega}_m$ | $N \times 1$ |
| QNM.QN | QNM Normalization coefficients | $N \times 1$ |
| QNM.eps | Material permittivity evaluated at QNM eigenfrequency | $N \times 1$ |
| QNM.cord | Gauss pattern sampled $x$, and $y$, coordinates inside the perturbation domain. Column 1 is $x$, Column 2 is $y$ | $2 \times X$<br>$X$ depends on COMSOL mesh |
| QNM.cord_up | Gauss pattern sampled $x$, and $y$, coordinates in reflection integration region. Column 1 is $x$, Column 2 is $y$ | $2 \times X_2$<br>$X_2$ depends on COMSOL mesh |
| QNM.Ex | QNM Electric field $x$ component inside perturbation domain | $N \times X$ |
| QNM.Ey | QNM Electric field $y$ component inside perturbation domain | $N \times X$ |
| QNM.Ex_m | QNM Electric field x component for - $\theta$ incidence | $N \times X$ |
| QNM.Ey_m | QNM Electrix field y component for - $\theta$ incidence | $N \times X$ |
| QNM.Hz | QNM Magnetic field $z$ component inside perturbation domain | $N \times X$ |
| QNM.Hz_up | QNM Magnetic field $z$ component in reflection integration region | $N \times X_2$ |
| QNM.mesh_volume | "Weight" of sampled points inside perturbation domain (used for integration) | $1 \times X$ |
| QNM.mesh_volume_up | "Weight" of sampled points inside Reflection integration region (used for integration) | $1 \times X_2$ |

**How are the overlap integrals performed?**

The values of the QNM fields are extracted for the coordinates contained in QNM.coord. The incident Electric field that overlaps with the QNM fields is defined analytically using the $x, y$ coordinates in QNM.cord.

```
k=omega/Phy.c*sqrt(Mat.eps_b);                    % wavenumber in background
p=exp(1i*k*QNM.cord(1,:)*Comp.K(1)+...
```

```
    1i*k*QNM.cord(2,:)*Comp.K(2)+...
    1i*k*QNM.cord(3,:)*Comp.K(3));          % plane wave phase
E_inc_x=p*Comp.E(1); E_inc_y=p*Comp.E(2);  E_inc_z=p*Comp.E(3);          % incident
electric fields
```

The values of the overlap integral between a QNM mode and the incident field are stored inside the variable intE :

```
  % Field overlap integration between incident field and QNM field
intEx=QNM.Ex_m.*Ex_inc*QNM.mesh_vol.'; % Overlap integral x component
intEy=QNM.Ey_m.*Ey_inc*QNM.mesh_vol.'; % Overlap integral y component
% Overlap integral in resonator domain above the substrate
intE=intEx+intEy; % Total integral inside resonator domain performed with
Gaussian sampling
```

An overlap integral using this method entails the scalar product of the fields with QNM.mesh_volume. For example, the overlap integrals of the QNM fields with itself inside the resonator volume would be written:

```
int_E_self=sym_factor*(QNM.Ex.*QNM.Ex+QNM.Ey.*QNM.Ey+QNM.Ez.*QNM.Ez)*QNM.mesh_vol.';
```

**How may one extract the magnetic field?**

To extract a component of the QNM magnetic field from the COMSOL model use the following lines:

```
temp=mpheval(model, 'Hz', 'solnum', 'all','pattern','gauss','selection',
COMSOL.resonator_domain,'Complexout','on');
QNM.Hz=temp.d1;          % Magnetic field z component
```

Compared to the models that employ the RF module, there is no need for the “emw.” prefix when using mpheval to extract fields.

The lines to extract the magnetic field components are included in the **QNMtoolbox_grating.m** script, in the “Read data from COMSOL file” section, and these lines of code are simply commented.

**How are the modal excitation coefficients computed inside the program?**

The prefactors to the modal excitation coefficients at frequency $\omega$ are stored inside the variable “alpha_QNM” which is

$$\text{alpha\_QNM} = \left(\varepsilon_b - \varepsilon_\infty - \left(\Delta\varepsilon(\tilde{\omega}_m)\right)\frac{\tilde{\omega}_m}{\tilde{\omega}_m - \omega}\right)/N_\mathrm{m} = \frac{1}{\omega - \tilde{\omega}_m}\left(-\omega(\varepsilon_\infty - \varepsilon_b) - \tilde{\omega}_m(\varepsilon(\tilde{\omega}_m) - \varepsilon_\infty)\right)/N_m \quad ,$$ where

$N_m$ is the normalization coefficient of the $m^{th}$ QNM.

The modal excitation coefficients for a single frequency are obtained by the performing following product:

```
alpha_QNM*E_int      % Modal Excitation coefficients
```

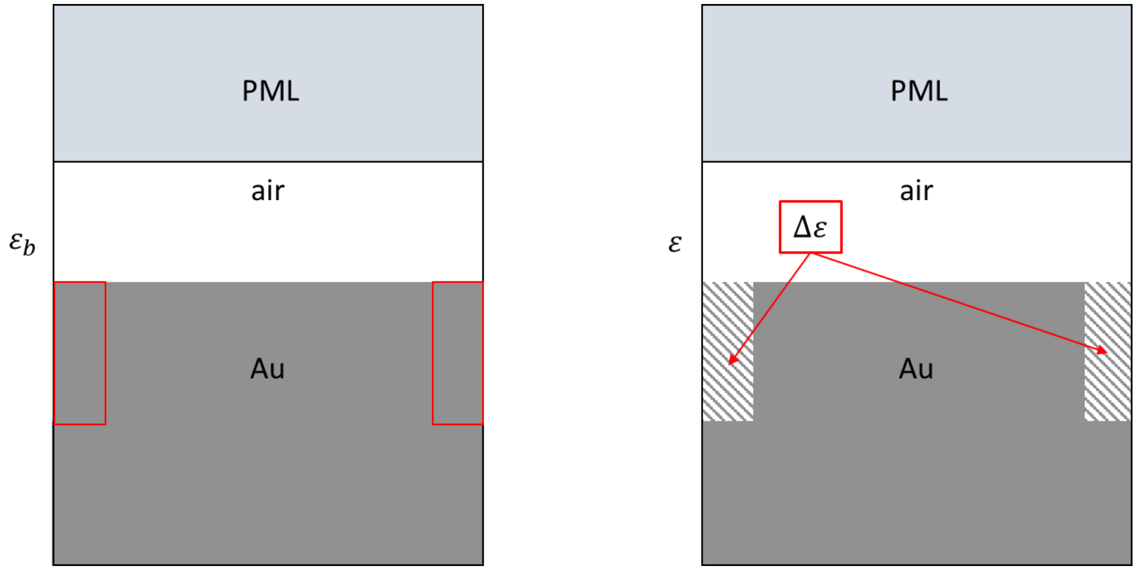



**Figure 2** Schematic of the unit cell of background medium(left) and of the grating obtained by adding the local permittivity perturbation $\Delta\varepsilon(\mathbf{r})$ to the background permittivity distribution $\varepsilon_b$ for QNMEig_grating_theta.mph.mph.

**How is the reflection computed inside the program?**

The script computes the reflectivity from the scattered field computed with QNMs. The scattering problem is described in [2].

Using the Rayleigh expansion, we can retrieve the $0^{\text{th}}$ order reflectivity of the grating by obtaining the mean value of the magnetic scattered field and the background field over a grating period. This value for the magnetic scattered field is computed using QNMs

$$\frac{1}{a}\frac{1}{H_0}\int_{x=-a/2}^{x=\frac{a}{2}} \boldsymbol{H}_s(\boldsymbol{r},\omega)\cdot\hat{\mathbf{z}}\,dx = \frac{1}{a}\frac{1}{H_0}\sum_m \alpha_m(\omega)\int_{x=-a/2}^{x=\frac{a}{2}} \widetilde{\boldsymbol{H}}_{m,\theta}(\boldsymbol{r})\cdot\hat{\mathbf{z}}\,dx\,.$$

This integral in the periodic direction $x$ is performed at a height $y$, designated by the "altitude" variable in both the script and the **QNMEig_grating_theta.mph** model. The mean value of the reflected background field is given analytically.

**Can the scattered field in space be plotted in space?**

The last part of the toolbox script "Plot scattered Magnetic field in space around grating" shows how to plot the reconstructed scattered field in space. In order to plot the scattered field in space, one needs to extract the QNM fields profiles from the COMSOL model. This can be done with the *mphinterp* command. An example of a use of this command would be:

```
numt=150;
[xss,yss]=meshgrid(linspace(-Geo.a/2,Geo.a/2,numt),linspace(-Geo.height/2-Geo.a/2,1.5,numt));
xsss=reshape(xss,1,numt^2); ysss=reshape(yss,1,numt^2);
[QNM.Hz_QNM]=mphinterp(model,{'Hz'},'solnum','all','coord',[xsss;ysss],'Complexout','on','dataset',COMSOL.dataset);   % read fields on your specified grids
```

```
QNM.Hz_QNM=reshape(QNM.Hz_QNM,length(QNM.omega),numt,numt);
```

where $numt^2$ is the number of sample points in the spatial domain specified by the spatial coordinates (xsss,ysss).

The variable QNM.Hz_QNM returned by the mphinterp function will be a matrix of size $N \times numt^2$ that contains the values of the QNM fields interpolated at various points in space. It is convenient to resize the matrix to a size of $N \times numt \times numt$.

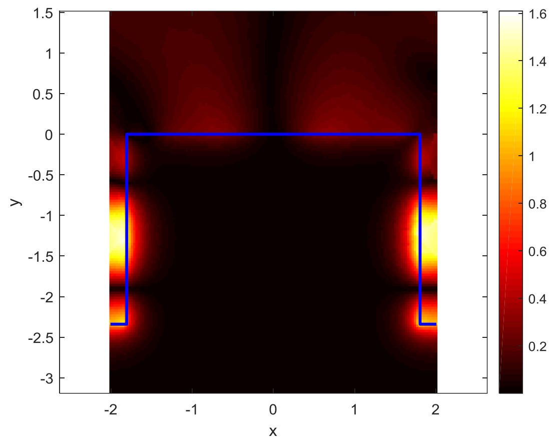



**Figure 3:** Reconstructed scattered Magnetic field at $\lambda = 500$ nm of the grating using 200 modes.

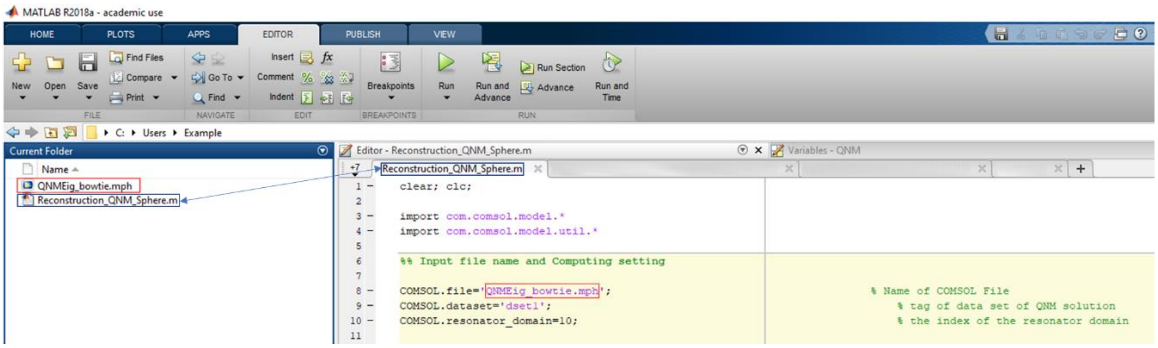
## 4. TROUBLESHOOTING

This section contains a few ways to find some of the COMSOL model information that you need to modify the **QNMtoolbox_grating.m** script to your liking.

The essential prerequisite step before you run **QNMtoolbox_grating.m** is to compute QNMs using the COMSOL model **QNMEig_grating_theta.mph** or a similar model implemented by you.

Once the QNM modes are computed inside the COMSOL model file, **QNMtoolbox_grating.m** needs to be modified for use with the specific COMSOL model.

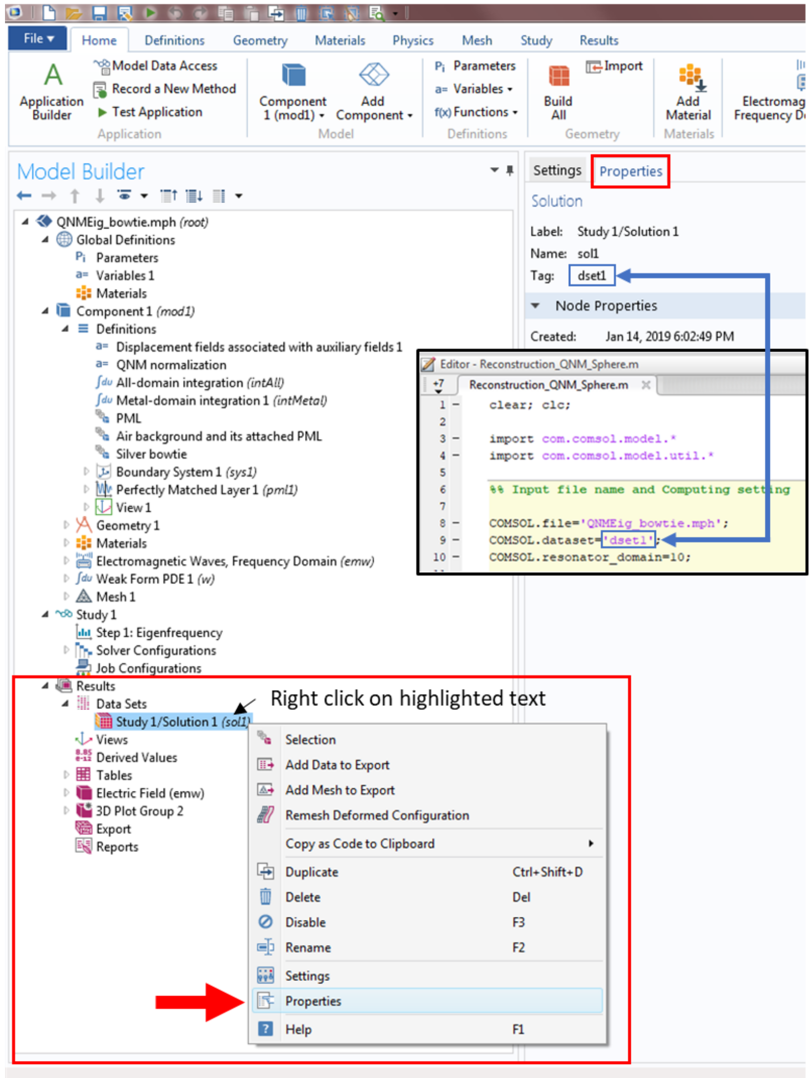
4.1/ The COMSOL model file should be placed in the same folder as **QNMtoolbox_grating.m** and the COMSOL.file variable should be defined with the complete name of the COMSOL file (file extension included).




The COMSOL model can be placed in another folder but you'll have to specify the location of the file in the COMSOL.file variable.

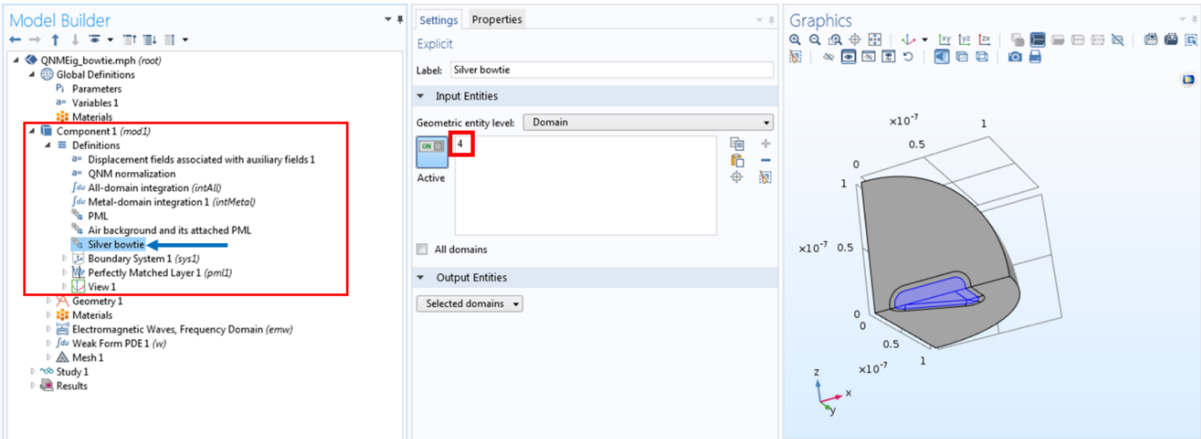
4.2/ The COMSOL.dataset variable must correspond to the name COMSOL dataset that contains the QNMs. This can be checked directly in COMSOL.

- Open the COMSOL model file using COMSOL.
- In the Model Builder window expand the "Results" section, by left clicking on the triangle on the left of "Results" line. This should make the "Data Sets" line appear. Click on the triangle on the left of the "Data sets" to expand the "Data Sets" section.
- Right click on the StudyX/Solution Y (solZ) line that corresponds to the QNM calculation (X,Y,Z are the numbers that correspond to the QNM data set) and select "Properties". It should bring up the Properties tab for the QNM dataset.
- The name of the dataset to be entered in **QNMtoolbox_grating.m.** is the **"Tag"**.




4.3/ COMSOL.resonator_domain corresponds to the numbered domain in the COMSOL model file that corresponds to the resonator domain. A way to check this would be to look inside the model in COMSOL. In the **QNMEig** model files, the different materials are split into different "explicit selections" to distinguish them.

In the Model Builder window, expand the "Component 1 (mod1)" section, then the "Definitions" section to reveal the "explicit selections" denoted by the  symbol. There should be one that corresponds to the **QNMEig** model's resonator domain (For example, the selection for the bowtie model is labeled "Silver Bowtie" and the corresponding domain is #4. This information can also be found inside the integration operators defined inside the COMSOL models, denoted by the  symbols. Here, "Metal-domain integration 1" should also contain that information.




## 5. References


[1] W. Yan, R. Faggiani, P. Lalanne, Phys. Rev. B **97**, 205422 (2018).
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[2] A. Gras, W. Yan, P. Lalanne, Opt. Lett. **44**, 3494 (2019).
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