QNMEig: a solver for calculating resonance modes of plasmonic nanoresonators and photonic microresonators (version 7 – January 2020)

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The present documentation provides the user guide of **QNMEig**, which, based on the commercial software COMSOL Multiphysics, computes and normalizes the natural resonance modes (also called quasinormal modes or QNMs) of plasmonic and photonic resonators [1]. It is deliberately short so that it can be a handy read.

1. INTRODUCTION

QNMEig computes and normalizes (the mode volume is provided) of resonance modes (also called the quasinormal modes or QNMs) of plasmonic and photonic resonators. With **QNMEig**, modes of resonators are computed by solving a standard linear eigenvalue problem derived from Maxwell's equations. Thus, a number of modes (the number is input by the user) is computed with a single computation without preconditioning. This makes **QNMEig** owns a superior numerical efficiency than **QNM**, our earlier developed QNM solver that computes QNMs one by one based on a pole-searching algorithm [2].

1.1 Download & Installation

QNMEig is a freeware that operates under COMSOL Multiphysics. To install it, copy and decompress the companion folder "**QNMEig.zip**".

1.2 How to acknowledge and cite

We kindly ask that you reference the **QNMEig** package from IOGS-CNRS and its authors in any publication/report for which you used it. The preferred citation for **QNMEig** is the following:

[ref] W. Yan, R. Faggiani and P. Lalanne, "Rigorous modal analysis of Plasmonic Nanoresonators", Phys. Rev. B **97**, 205422 (2018).

This article with its Suppl. Inf. is included in the package "**QNMEig.zip**".

1.3 Units and conventions of input/output data for QNMEig

Unit. All the input information requires to be in the SI unit (e.g., volts per meter for electric field E, amperes per meter for magnetic field H, …). Accordingly, the output information is given in SI unit as well.

Convention. **QNMEig** uses the time dependence $\exp j\omega t$ of COMSOL Multiphysics.

2. MATHEMATICAL BACKGROUND

The mathematical details on how **QNMEig** compute QNMs for the most general case of absorptive, dispersive nanoresonators by solving a standard linear eigenvalue problem is presented in Ref. [1], especially in Section II in the main text and Section 4.1 in the SI. Nevertheless, in the following, we give a minimum but self-contained description of key mathematical ingredients of **QNMEig**.

QNMs, the natural resonance modes of resonators, are eigenstates of Maxwell's equations

$$\nabla \times \mu_0^{-1} \nabla \times \tilde{\boldsymbol{E}}_m - \tilde{\omega}_m^2 \varepsilon(r, \tilde{\omega}_m) \tilde{\boldsymbol{E}}_m = 0, \tag{1}$$

supplemented by outgoing-wave conditions. Here, we assume that the resonators and their backgrounds are non-magnetic with vacuum permeability μ_0. $\tilde{\boldsymbol{E}}_m$ and $\tilde{\omega}_m$ denote the electric field and eigenfrequency of the m^{th} QNM, respectively, and $\varepsilon(r, \tilde{\omega}_m)$ denotes the permittivity that depends on both frequency and space. Apparently, when $\varepsilon(r, \tilde{\omega}_m)$ is non-dispersive, i.e., independent of frequency, Eq. (1) defines a standard, linear eigenvalue problem, which can be solved easily by COMSOL Multiphysis with its standard mode solver. However, when $\varepsilon(r, \omega)$ is dispersive for instance for plasmonic nanoresonators, Eq. (1) becomes a nonlinear eigenvalue equation; there is an additional difficulty in solving it.

Reference [1] shows that, if $\varepsilon(r, \omega)$ is modeled by a *N*-pole Lorentz-Drude permittivity, one can reformulate Eq. (1) into a linear eigenvalue problem by introducing auxiliary fields. Here, we demonstrate this numerical recipe by considering that $\varepsilon(r, \omega)$ is a single-pole Lorentz-Drude permittivity, i.e.,

$$\varepsilon(r, \omega) = \varepsilon_\infty [1 - \frac{\omega_p^2}{\omega^2 - \omega_0^2 - j\omega\gamma}]. \tag{2}$$

We introduce the auxiliary fields $\tilde{\boldsymbol{P}}_m$ are introduced by

$$\tilde{\boldsymbol{P}}_m = -\frac{\omega_p^2}{\tilde{\omega}_m^2 - \omega_0^2 - j\tilde{\omega}_m\gamma} \tilde{\boldsymbol{E}}_m. \tag{3}$$

Equations (1) and (3) together give us

$$\nabla \times \mu_0^{-1} \nabla \times \tilde{\boldsymbol{E}}_m - \tilde{\omega}_m^2 \tilde{\boldsymbol{E}}_m - \tilde{\omega}_m^2 \varepsilon_\infty \tilde{\boldsymbol{P}}_m = 0, \tag{4a}$$

$$\varepsilon_\infty \omega_p^2 \tilde{\boldsymbol{E}}_m - \omega_0^2 \varepsilon_\infty \tilde{\boldsymbol{P}}_m + i\tilde{\omega}_m \gamma \varepsilon_\infty \tilde{\boldsymbol{P}}_m + \tilde{\omega}_m^2 \varepsilon_\infty \tilde{\boldsymbol{P}}_m = 0. \tag{4b}$$

with eigenvectors $[\tilde{\boldsymbol{E}}_\mathrm{m}, \tilde{\boldsymbol{P}}_\mathrm{m}]$.

The full linearization of Eqs. (4) is not completely implemented in **QNMEig**. In fact, Eqs. (4a) and (4b) define a quadratic polynomial eigenvalue problem, and can be readily solved with COMSOL Multiphysics. Therefore, the full trivial linearization of Eqs. (4a) and (4b) is unnecessary, and we directly implement the weak formulations of Eqs. (4a) and (4b) (see Section 4.1 in the SI of Ref. [1]) in COMSOL Multiphysics: Eq. (4a) is implemented with the module ***ELECTROMAGNETIC WAVES, FREQUENCY DOMAIN,*** while Eq. (4b) is implemented with the module ***WEAK FORM PDE***. Details on how implementing Eqs. (4a) and (4b) can be found in another document "***QNMEig_Sphere.pdf***".

3. PROVIDED DOCUMENTS

Name	Description
QNMEig_Sphere.mph	COMSOL model sheet for computing QNMs of metal sphere in air.
QNMEig_Sphere.pdf	The PDF document provides all the details on how to build *QNMEig_Sphere.mph* from scratch.
QNMEig_CubeSubstrate.mph	COMSOL model sheet for computing QNMs of a metallic cube laying on a thin dielectric film deposited on a metallic substrate.
QNMEig_CubeSubstrate.pdf	The PDF document provides important details how to build *QNMEig_CubeSubstrate.mph*
QNMEig_1DGrating.mph	COMSOL model sheet for computing QNMs of a 1D silver grating in air
QNMEig_1DGrating.pdf	The PDF document provides important details how to build QNMEig_1DGrating.mph

REFERENCES

[1] W. Yan, R. Faggiani and P. Lalanne, "Rigorous modal analysis of Plasmonic Nanoresonators", Phys. Rev. B **97**, 205422 (2018).

[2] Q. Bai, M. Perrin, C. Sauvan, J. P. Hugonin and P. Lalanne, "Efficient and intuitive method for the analysis of light scattering by a resonant nanostructure", Opt. Express **21**, 27371-82 (2013).