# pytheas Documentation

## Release 1.1.1

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**Dec 02, 2019**

# Contents

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# Introduction

Pytheas is a Python package for creating, running and postprocessing electrodynamic simulations. It is based on open source software Gmsh for creating geometries and mesh generation, and GetDP for solving the underlying partial differential equations with the finite element method.

It features built in models of:

- periodic media in 2D and 3D with computation of diffraction efficiencies
- scattering analysis in 2D and 3D
- Bloch mode analysis of metamaterials
- treatment of open geometries with perfectly matched layers
- tools to define arbitrary permittivity distributions
- quasi-normal mode analysis
- two scale convergence homogenization
- tools for topology optimization in 2D
- built-in refractive index database

# 2 Installation

The easiest way to get started is to install via PyPi:

```
pip install pytheas-pip
```

# 3

# User guide

## 3.1 pytheas.periodic2D: 2D metamaterials

The pytheas.periodic2D module implements the resolution of the scalar wave equation for TE and TM polarization for mono-periodic stuctures in 2D:

- subject to an incident plane wave (diffraction problem) with calculation of the diffraction efficiencies, absorption and energy balance.
- eigenvalues and eigenmodes (modal analysis)

### 3.1.1 Classes

| | |
|---|---|
| Periodic2D([analysis, pola, A, lambda0, ...]) | A class for a finite element model of a 2D mono-periodic medium. |

#### pytheas.Periodic2D

```
class pytheas.Periodic2D(analysis='direct', pola='TE', A=1, lambda0=1, lambda_mesh=1, theta_deg=0, d=0.8,
                         h_sup=1, h_sub=1, h_layer1=0.1, h_layer2=0.1, h_des=1.0, h_pmltop=1.0, h_pmlbot=1.0,
                         a_pml=1, b_pml=1, eps_sup=(1+0j), eps_sub=(1+0j), eps_layer1=(1+0j), eps_layer2=(1+0j),
                         eps_des=(1+0j), eps_incl=(1+0j), mu_incl=(1+0j), mu_des=(1+0j))
```

A class for a finite element model of a 2D mono-periodic medium.

The model consist of a single unit cell with quasi-periodic boundary conditions in the x direction enclosed with perfectly matched layers (PMLs) in the y direction to truncate the semi infinite media. From top to bottom:

- PML top
- superstrate (incident medium)
- layer 2
- design layer: this is the layer containing the periodic pattern, can be continuous or discrete
- layer 1
- substrate

- PML bottom

**Parameters**

- `analysis` (`str`, `default "direct"`) – Analysis type: either "direct" (plane wave) or "modal" (spectral problem)
- `pola` (`str`, `default "TE"`) – Polarization case: either "TE" (E along z) or "TM" (H along z)
- `A` (`float`, `default 1`) – Incident plane wave amplitude
- `lambda0` (`float`, `default 1`) – Incident plane wave wavelength in free space
- `lambda_mesh` (`float`, `default 1`) – Wavelength to use for meshing
- `theta_deg` (`float`, `default 0`) – Incident plane wave angle (in degrees). Light comes from the top (travels along -y if normal incidence, `theta_deg=0` is set)
- `d` (`float`, `default 0.8`) – Periodicity
- `h_sup` (`float`, `default 1`) – Thickness superstrate
- `h_sub` (`float`, `default 1`) – Thickness substrate
- `h_layer1` (`float`, `default 0.1`) – Thickness layer 1
- `h_layer2` (`float`, `default 0.1`) – Thickness layer 2
- `h_des` (`float`, `default 1`) – Thickness layer design
- `h_pmltop` (`float`, `default 1`) – Thickness pml top
- `h_pmlbot` (`float`, `default 1`) – Thickness pml bot
- `a_pml` (`float`, `default 1`) – PMLs complex y-stretching parameter, real part
- `b_pml` (`float`, `default 1`) – PMLs complex y-stretching parameter, imaginary part
- `eps_sup` (`complex`, `default (1 - 0 * 1j)`) – Permittivity superstrate
- `eps_sub` (`complex`, `default (1 - 0 * 1j)`) – Permittivity substrate
- `eps_layer1` (`complex`, `default (1 - 0 * 1j)`) – Permittivity layer 1
- `eps_layer2` (`complex`, `default (1 - 0 * 1j)`) – Permittivity layer 2
- `eps_des` (`complex`, `default (1 - 0 * 1j)`) – Permittivity layer design
- `eps_incl` (`complex`, `default (1 - 0 * 1j)`) – Permittivity inclusion

`cleanup()`

Remove gmsh/getdp/python generated files from the temporary folder

`compute_solution()`

Compute the solution of the FEM problem using getdp

`diffraction_efficiencies(cplx_effs=False, orders=False)`

Postprocess diffraction efficiencies.

**Parameters**

- `cplx_effs` (`bool`) – If True, return complex coefficients (amplitude reflection and transmission). If False, return real coefficients (power reflection and transmission)

- `orders` (`bool`) – If True, computes the transmission and reflection for all the propagating diffraction orders. If False, returns the sum of all the propagating diffraction orders.

**Returns** A dictionary containing the diffraction efficiencies.

**Return type** dict

`get_field_map`(name)
Retrieve a field map.

**Parameters** `name` (`str`) – Choose between "u" (scattered field), "u_tot" (total field)

**Returns** A 2D complex array of shape (Nix, Niy)

**Return type** array

`initialize`()
Initialize the problem parameters.

`make_inclusion`(points, lcar='lc_incl', **kwargs)
Make a diffractive element geometry from points.

**Parameters**

- `points` (`array of size (Npoints, 2)`) – The points defining the simply connected 2D geometry of the object.
- `lcar` (`str (default "lc_incl")`) – Caracteristic length for the mesh.
- `**kwargs` (`dict`) – Extra arguments.

`make_mesh`(other_option=None)
Mesh the geometry using gmsh.

**Parameters** `other_option` (`str`) – Extra flag to pass to gmsh.

**Returns** The content of the .msh file.

**Return type** str

`mk_tmp_dir`()
Create a temporary directory

`open_gmsh_gui`(pos_list=None)
Open gmsh GUI to visualize geometry and postprocessing results.

**Parameters** `pos_list` (`list`) – A list of .pos files giving the views to load. By default it will render all the generated views.

`postpro_absorption`()
Compute the absorption coefficient

**Returns** **Q** – Absorption coefficient

**Return type** float

`postpro_fields`(filetype='txt', postop='postop_fields')
Compute the field maps and output to a file.

**Parameters**

- `filetype` (`str, default "txt"`) – Type of output files. Either "txt" (to be read by the method get_field_map in python) or "pos" to be read by gmsh/getdp.
- `postop` (`str, default "postop_fields"`) – Name of the postoperation

`postprocess(postop)`
Run getdp postoperation.

**Parameters** `postop` (`str`) – Name of the postoperation to run.

`rm_tmp_dir()`
Remove the temporary directory

`update_params()`
Update the dictionary of parameters and the corresponding file

#### Examples using `pytheas.Periodic2D`

- Simulating diffraction by a 2D metamaterial

## 3.2 `pytheas.scatt2D`: 2D scattering

The `pytheas.scatt2D` module implements the resolution of the scalar wave equation for TE and TM polarization in 2D:

- subject to an incident plane wave or line source (diffraction problem)
- eigenvalues and eigenmodes (modal analysis)

### 3.2.1 Classes

| | |
|---|---|
| `Scatt2D`() | A class for a finite element model of a 2D medium |

#### `pytheas`.Scatt2D

`class pytheas.Scatt2D`
A class for a finite element model of a 2D medium

`A = None`
incident plane wave amplitude

**Type** flt

`Ni_theta = None`
number of theta points for computing the angular dependance of the modal coupling coefficients

**Type** int

`Nibox_x = None`
number of x interpolation points on the design box

**Type** int

`Nibox_y = None`
number of y interpolation points on the design box

**Type** int

`Nin2f_x = None`
number of x interpolation points for near to far field calculations

**Type** int

`Nin2f_y = None`
number of y interpolation points for near to far field calculations

**Type** int

`Nix = None`
number of x points for postprocessing field maps

**Type** int

`a_pml = None`
PMLs parameter, real part

**Type** flt

`analysis = None`
analysys type (either "direct" or "modal")

**Type** str

`b_pml = None`
PMLs parameter, imaginary part

**Type** flt

`beam_flag = None`
beam?

`cleanup()`
Remove gmsh/getdp/python generated files from the temporary folder

`compute_solution(res_list=None)`
Compute the solution of the FEM problem using getdp

`dom_des = None`
design domain number (check .geo/.pro files)

`eps_des = None`
permittivity scattering box

**Type** flt

`eps_host = None`
permittivity host

**Type** flt

`eps_incl = None`
permittivity inclusion

**Type** flt

`eps_sub = None`
permittivity substrate

**Type** flt

`h_pml = None`
thickness pml

**Type** flt

`hx_des = None`
x - thickness scattering box (design)

**Type** flt

`hy_des = None`
y - thickness scattering box

**Type** flt

`initialize()`
Initialize the problem parameters.

`lambda0 = None`
incident plane wave wavelength in free space

**Type** flt

`lambda0search = None`
wavelength around which to search eigenvalues

**Type** flt

`lambda_mesh = None`
wavelength to use for meshing

**Type** flt

`ls_flag = None`
line source position

`make_inclusion(points, lcar='lc_incl', **kwargs)`
Make a diffractive element geometry from points.

**Parameters**

- `points` (`array of size (Npoints, 2)`) – The points defining the simply connected 2D geometry of the object.
- `lcar` (`str (default "lc_incl")`) – Caracteristic length for the mesh.
- `**kwargs` (`dict`) – Extra arguments.

`make_mesh(other_option=None)`
Mesh the geometry using gmsh.

**Parameters** `other_option` (`str`) – Extra flag to pass to gmsh.

**Returns** The content of the .msh file.

**Return type** str

`mk_tmp_dir()`
Create a temporary directory

`nb_slice = None`
number of y slices points for postprocessing diffraction efficiencies

**Type** int

`neig = None`
number of eigenvalues searched for in modal analysis

**Type** int

`open_gmsh_gui(pos_list=None)`
Open gmsh GUI to visualize geometry and postprocessing results.

**Parameters** `pos_list` (list) – A list of .pos files giving the views to load. By default it will render all the generated views.

`pola = None`
polarisation of the incident plane wave (either "TE" or "TM")

**Type** str

`postpro_fields(filetype='txt', postop='postop_fields')`
Compute the field maps and output to a file.

**Parameters**

- `filetype` (str, default "txt") – Type of output files. Either "txt" (to be read by the method get_field_map in python) or "pos" to be read by gmsh/getdp.
- `postop` (str, default "postop_fields") – Name of the postoperation

`postprocess(postop)`
Run getdp postoperation.

**Parameters** `postop` (str) – Name of the postoperation to run.

`rm_tmp_dir()`
Remove the temporary directory

`scan_dist_ratio = None`
such that scan_dist = min(h_sup, hsub)/scan_dist_ratio

**Type** flt

`theta_deg = None`
incident plane wave angle (in degrees). Light comes from the top (travels along -y if normal incidence, theta_deg=0 is set)

**Type** flt

`update_params()`
Update the dictionary of parameters and the corresponding file

`xpp = None`
coords of point for PostProcessing

`ypp = None`
coords of point for PostProcessing

#### Examples using `pytheas.Scatt2D`

- Simulating diffraction by an object in 2D

## 3.3 `pytheas.tools`: tools and utilities

Input/output and utilities.

### 3.3.1 Submodules

| | |
|---|---|
| femio | Tools for gmsh/getdp control and input/output. |
| utils | Shared utility functions used in pytheas. |

#### pytheas.tools.femio

Tools for gmsh/getdp control and input/output.

`pytheas.tools.femio.mesh_model(path_mesh, path_geo, mesh_format='msh2', dim=None, verbose=0, other_option='')`

Mesh the model using Gmsh

`pytheas.tools.femio.postpro_commands(postop, path_pro, path_mesh, path_pos=None, verbose=0)`

Generate a command list for postprocessing by GetDP (see main.pro file in ./base folder for default available postprocessings, or to add your own)

**Parameters**

- postop (str) – The name of the postoperation to perform.
- path_pro (str) – Path to the .pro file
- path_mesh (str) – Path to the .msh file
- path_pos (str , optional) – Path to a file to be read by gmshread.
- verbose (int) – verbosity level
- to None. (Defaults) –

**Returns** The list of strings to be oscommanded.

**Return type** list

#### pytheas.tools.utils

Shared utility functions used in pytheas.

`pytheas.tools.utils.normalize(x)`

Normalize an array between 0 and 1

**Parameters** x (array-like) – the quantity to be normalized

**Returns** **x_norm** – normalized array

**Return type** array-like

# 4

# Examples

## 4.1 Material examples

Examples to show how to retrieve complex refractive index from a database, generating material patterns.

**Note:** Click here to download the full example code

### 4.1.1 Importing refractive index from a database

Retrieve and plot the refractive index of a material in the refractiveindex.info data.

```
import numpy as np
from pytheas import refractiveindex as ri
import matplotlib.pyplot as plt
```

We can get the refractive index from tabulated data or a formula using the database in the `pytheas.material` module. We will import the measured data from the reference Johnson and Christy [JC1972]. We first specify the file `yamlFile` we want to import:

```
yamlFile = "main/Au/Johnson.yml"
```

We then get the wavelength bounds from the data (in microns) and create a wavelength range to interpolate:

```
bounds = ri.get_wl_range(yamlFile)
print(bounds[0], bounds[1])
lambdas = np.linspace(0.4, 0.8, 300)
```

Out:

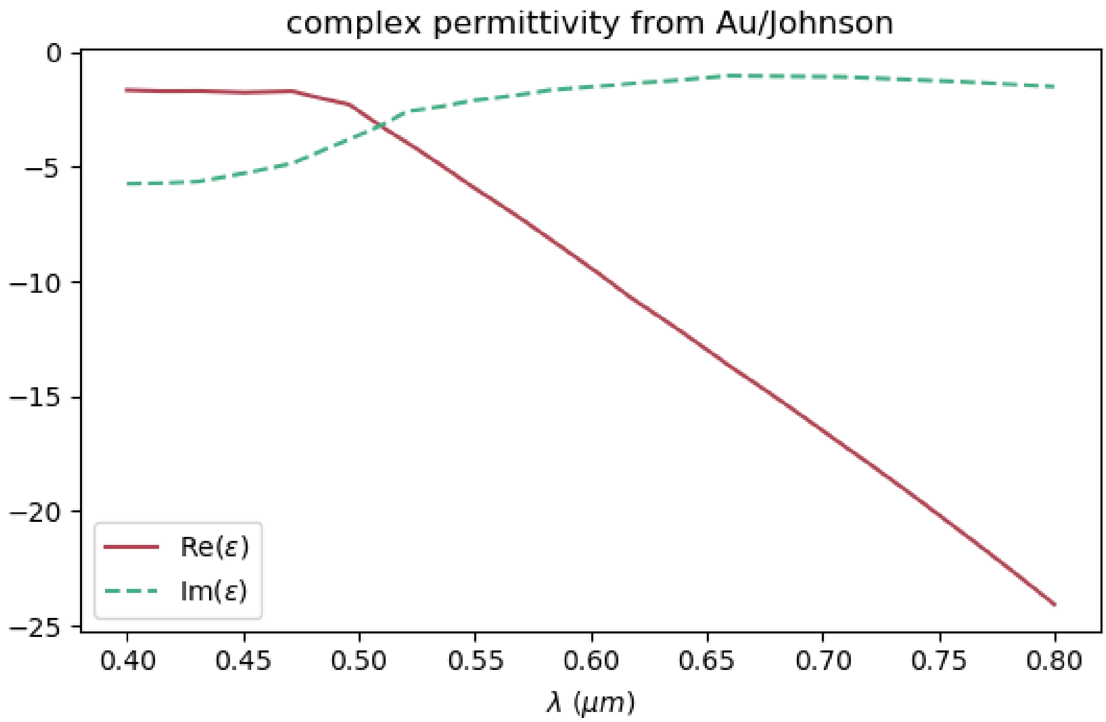
```
0.1879 1.937
```

Then get the refractive index data:

```
ncomplex = ri.get_complex_index(lambdas, yamlFile)
epsilon = ncomplex ** 2
```

And finally plot it:

```
fig, ax = plt.subplots(1, figsize=(6, 4))
ax.plot(lambdas, epsilon.real, "-", c="#ad4453", label=r"Re($\varepsilon$)")
ax.plot(lambdas, epsilon.imag, "--", c="#44ad84", label=r"Im($\varepsilon$)")
ax.set_xlabel(r"$\lambda$ ($\mu m$)")
ax.set_title("complex permittivity from " + yamlFile[5:][:-4])
ax.legend(loc=0)
plt.tight_layout()
```




**Total running time of the script:** ( 0 minutes 0.245 seconds)

## 4.2 Periodic 2D examples

Examples to show how to simulate a mono periodic medium (metamaterial) with the finite element method and postprocessing the results (fields maps and diffraction efficiencies).

**Note:** Click here to download the full example code

### 4.2.1 Simulating diffraction by a 2D metamaterial

Finite element simulation of the diffraction of a plane wave by a mono-periodic grating and calculation of diffraction efficiencies.

First we import the required modules and class

```
import numpy as np
import matplotlib.pyplot as plt
from pytheas import genmat
from pytheas import Periodic2D
```

Then we need to instanciate the class `Periodic2D`:

```
fem = Periodic2D()
```

The model consist of a single unit cell with quasi-periodic boundary conditions in the x direction enclosed with perfectly matched layers (PMLs) in the y direction to truncate the semi infinite media. From top to bottom:

- PML top
- superstrate (incident medium)
- layer 1
- design layer: this is the layer containing the periodic pattern, can be continuous or discrete
- layer 2
- substrate
- PML bottom

We define here the opto-geometric parameters:

```
mum = 1e-6  #: flt: the scale of the problem (here micrometers)
fem.d = 0.4 * mum  #: flt: period
fem.h_sup = 1.0 * mum  #: flt: "thickness" superstrate
fem.h_sub = 1.0 * mum  #: flt: "thickness" substrate
fem.h_layer1 = 0.1 * mum  #: flt: thickness layer 1
fem.h_layer2 = 0.1 * mum  #: flt: thickness layer 2
fem.h_des = 0.4 * mum  #: flt: thickness layer design
fem.h_pmltop = 1.0 * mum  #: flt: thickness pml top
fem.h_pmlbot = 1.0 * mum  #: flt: thickness pml bot
fem.a_pml = 1  #: flt: PMLs parameter, real part
fem.b_pml = 1  #: flt: PMLs parameter, imaginary part
fem.eps_sup = 1  #: flt: permittivity superstrate
fem.eps_sub = 3  #: flt: permittivity substrate
fem.eps_layer1 = 1  #: flt: permittivity layer 1
fem.eps_layer2 = 1  #: flt: permittivity layer 2
fem.eps_des = 1  #: flt: permittivity layer design
fem.lambda0 = 0.6 * mum  #: flt: incident wavelength
fem.theta_deg = 0.0  #: flt: incident angle
fem.pola = "TE"  #: str: polarization (TE or TM)
fem.lambda_mesh = 0.6 * mum  #: flt: incident wavelength
#: mesh parameters, correspond to a mesh size of lambda_mesh/(n*parmesh),
#: where n is the refractive index of the medium
fem.parmesh_des = 15
fem.parmesh = 13
fem.parmesh_pml = fem.parmesh * 2 / 3
fem.type_des = "elements"
```

We then initialize the model (copying files, etc...) and mesh the unit cell using gmsh

```
fem.getdp_verbose = 0
fem.gmsh_verbose = 0
```

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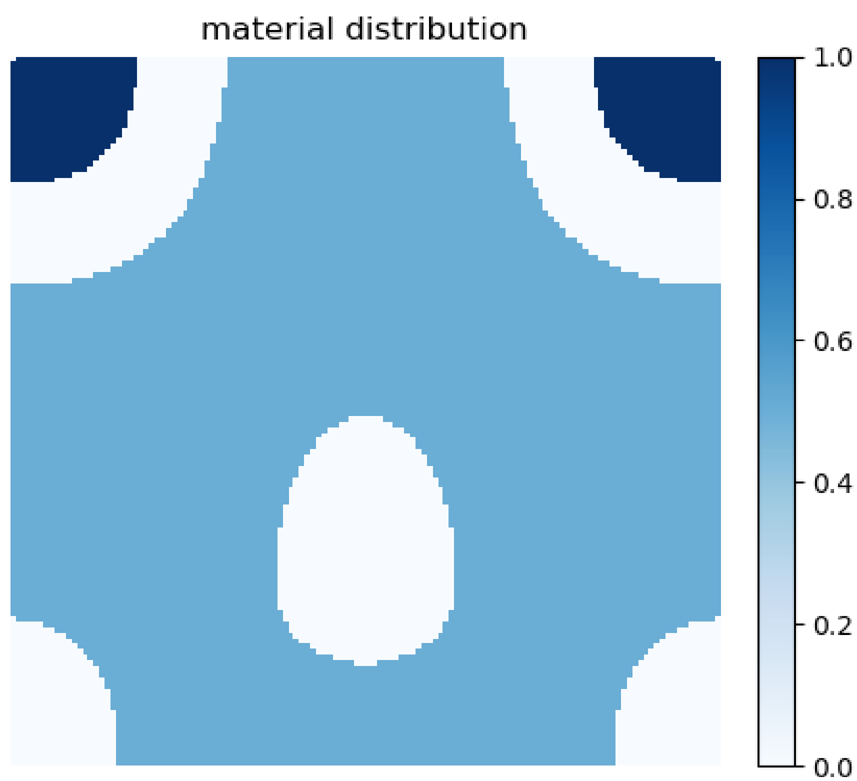
```
fem.initialize()
mesh = fem.make_mesh()
```

We use the `genmat` module to generate a material pattern

```
genmat.np.random.seed(100)
mat = genmat.MaterialDensity()  # instanciate
mat.n_x, mat.n_y, mat.n_z = 2 ** 7, 2 ** 7, 1  # sizes
mat.xsym = True  # symmetric with respect to x?
mat.p_seed = mat.mat_rand  # fix the pattern random seed
mat.nb_threshold = 3  # number of materials
mat._threshold_val = np.random.permutation(mat.threshold_val)
mat.pattern = mat.discrete_pattern
fig, ax = plt.subplots()
mat.plot_pattern(fig, ax)
```




We now assign the permittivity

```
fem.register_pattern(mat.pattern, mat._threshold_val)
fem.matprop_pattern = [1.4, 4 - 0.02 * 1j, 2]  # refractive index values
```

Now we're ready to compute the solution:

```
fem.compute_solution()
```

Finally we compute the diffraction efficiencies, absorption and energy balance

```
effs_TE = fem.diffraction_efficiencies()
print("efficiencies TE", effs_TE)
```

Out:

```
efficiencies TE {'R': 0.42749531344001657, 'T': 0.45592852708133014, 'Q': 0.1177478267191832, 'B
↪': 1.00117166724053}
```

It is fairly easy to switch to TM polarization:

```
fem.pola = "TM"
fem.compute_solution()
effs_TM = fem.diffraction_efficiencies()
print("efficiencies TM", effs_TM)
```

Out:

```
efficiencies TM {'R': 0.2052478291947634, 'T': 0.7359213200135426, 'Q': 0.05719724751542301, 'B
↪': 0.998366396723729}
```

**Total running time of the script:** ( 0 minutes 2.455 seconds)

## 4.3 Scattering 2D examples

Examples to show how to simulate a the 2D scattering off an object subject to a plane wave or line source harmonic excitation.

**Note:** Click here to download the full example code

### 4.3.1 Simulating diffraction by an object in 2D

Finite element simulation of the diffraction by an object illuminated by a plane wave or a line source. Calculation of scattering width and getting the field maps.

```
import numpy as np
import matplotlib.pyplot as plt
from pytheas import Scatt2D

plt.ion()

pi = np.pi
```

Then we need to instanciate the class `Scatt2D`:

```
fem = Scatt2D()
fem.rm_tmp_dir()
```

```
# We define first the opto-geometric parameters:

mum = 1  #: flt: the scale of the problem (here micrometers)
fem.lambda0 = 0.6 * mum  #: flt: incident wavelength
fem.pola = "TE"  #: str: polarization (TE or TM)
fem.theta_deg = 30.0  # 0: coming from top (y>0)
fem.hx_des = 1.0 * mum  #: flt: x thickness box
fem.hy_des = 1.0 * mum  #: flt: y thickness box
fem.h_pml = fem.lambda0  #: flt: thickness pml
fem.space2pml_L, fem.space2pml_R = fem.lambda0 * 2, fem.lambda0 * 2
fem.space2pml_T, fem.space2pml_B = fem.lambda0 * 2, fem.lambda0 * 2
fem.eps_des = 1  #: flt: permittivity design box
fem.eps_host = 1.0
fem.eps_incl = 11.0 - 1e-2 * 1j
#: mesh parameters, correspond to a mesh size of lambda_mesh/(n*parmesh),
#: where n is the refractive index of the medium
fem.lambda_mesh = 0.6 * mum  #: flt: incident wavelength
fem.parmesh_des = 10
fem.parmesh_incl = 10
fem.parmesh = 10
fem.parmesh_pml = fem.parmesh * 2 / 3

fem.Nix = 101
fem.Niy = 101
```

Here we define an ellipsoidal rod as the scatterer:

```
def ellipse(Rinclx, Rincly, rot_incl, x0, y0):
    c, s = np.cos(rot_incl), np.sin(rot_incl)
    Rot = np.array([[c, -s], [s, c]])
    nt = 360
    theta = np.linspace(-pi, pi, nt)
    x = Rinclx * np.sin(theta)
    y = Rincly * np.cos(theta)
    x, y = np.linalg.linalg.dot(Rot, np.array([x, y]))
    points = x + x0, y + y0
    return points


rod = ellipse(0.4 * mum, 0.2 * mum, 0, 0, 0)
fem.inclusion_flag = True
```

Initialize, build the scatterer, mesh and compute the solution:

```
fem.initialize()
fem.make_inclusion(rod)
fem.make_mesh()
fem.compute_solution()
```

Get the electric field and plot it:

```
fem.postpro_fields()
u_tot = fem.get_field_map("u_tot.txt")
fig, ax = plt.subplots()
E = u_tot.real
plt.imshow(E, cmap="RdBu_r", extent=(fem.domX_L, fem.domX_R, fem.domY_B, fem.domY_T))
```

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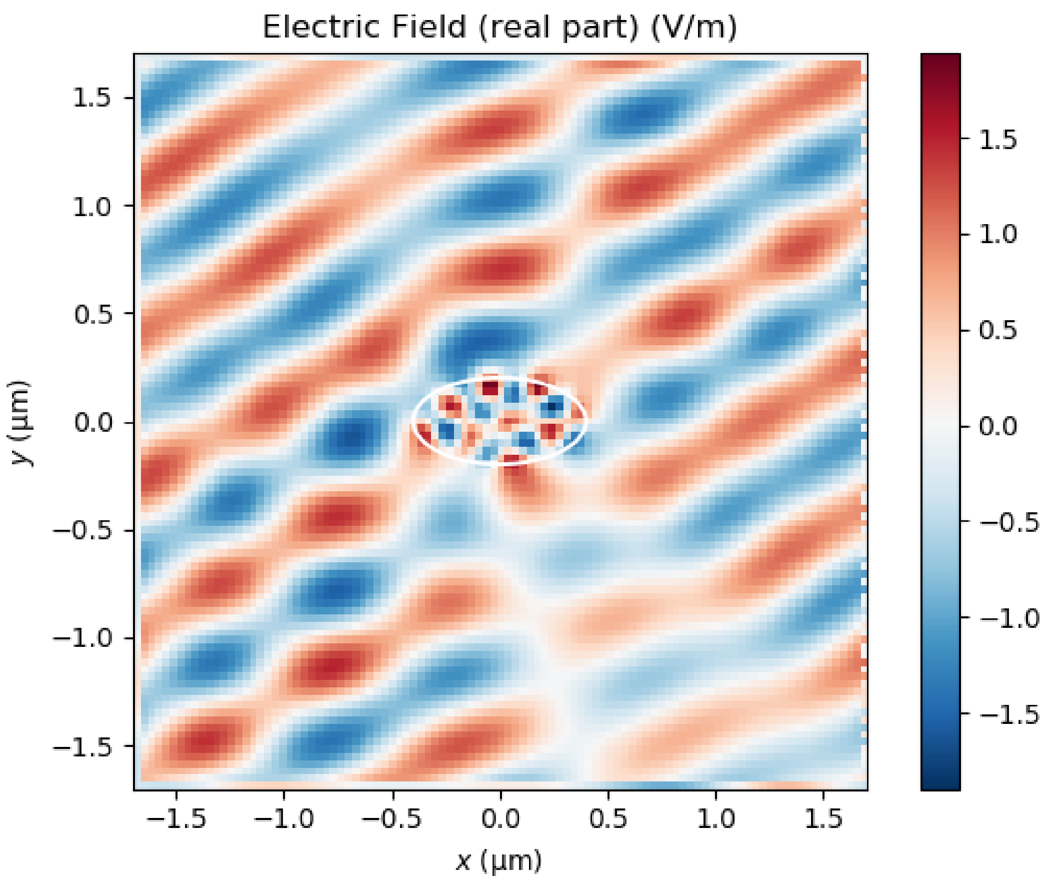
```
plt.plot(rod[0], rod[1], "w")
plt.xlabel(r"$x$ ($\rm \mu$m)")
plt.ylabel(r"$y$ ($\rm \mu$m)")
plt.title(r"Electric Field (real part) (V/m)")
plt.colorbar()
plt.tight_layout()
```

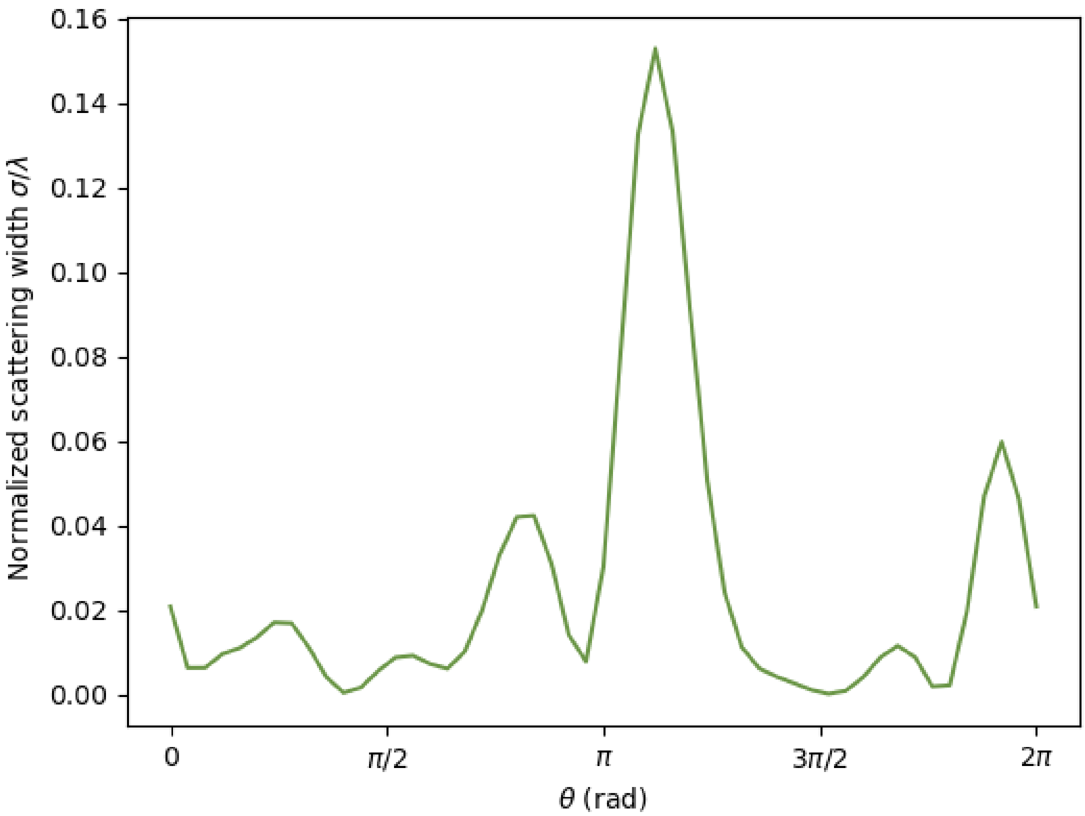



Do a near to far field transform and get the normalized scattering width:

```
ff = fem.postpro_fields_n2f()
theta = np.linspace(0, 2 * pi, 51)
scs = fem.normalized_scs(ff, theta)


fig, ax = plt.subplots()
plt.plot(theta / pi, scs, "-", c="#699545")
plt.xlabel(r"$\theta$ (rad)")
plt.ylabel(r" Normalized scattering width $\sigma/\lambda$")
ax.xaxis.set_ticks([0, 0.5, 1, 1.5, 2])
ax.xaxis.set_ticklabels(["0", "$\pi/2$", "$\pi$", "$3\pi/2$", "$2\pi$"])

scs_integ = np.trapz(scs, theta) / (2 * pi)
print("Normalized SCS", scs_integ)
```




Out:

```
Normalized SCS 0.02572717419074843
```

**Total running time of the script:** ( 0 minutes 17.162 seconds)

# Bibliography

[JC1972] (P. B. Johnson and R. W. Christy. Optical constants of the noble metals, Phys. Rev. B 6, 4370-4379 (1972)).

# Python Module Index

## p

# Index