



# pytheas Documentation

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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



## Installation

The easiest way to get started is to install via [PyPi](#):

```
pip install pytheas-pip
```





# 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 structures 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

<code>Periodic2D([analysis, pola, A, lambda0, ...])</code>	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”)) – Characteristic 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")*) – Characteristic 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

<i>femio</i>	Tools for gmsh/getdp control and input/output.
<i>utils</i>	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*



## Examples

### 4.1 Material examples

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

#### 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:

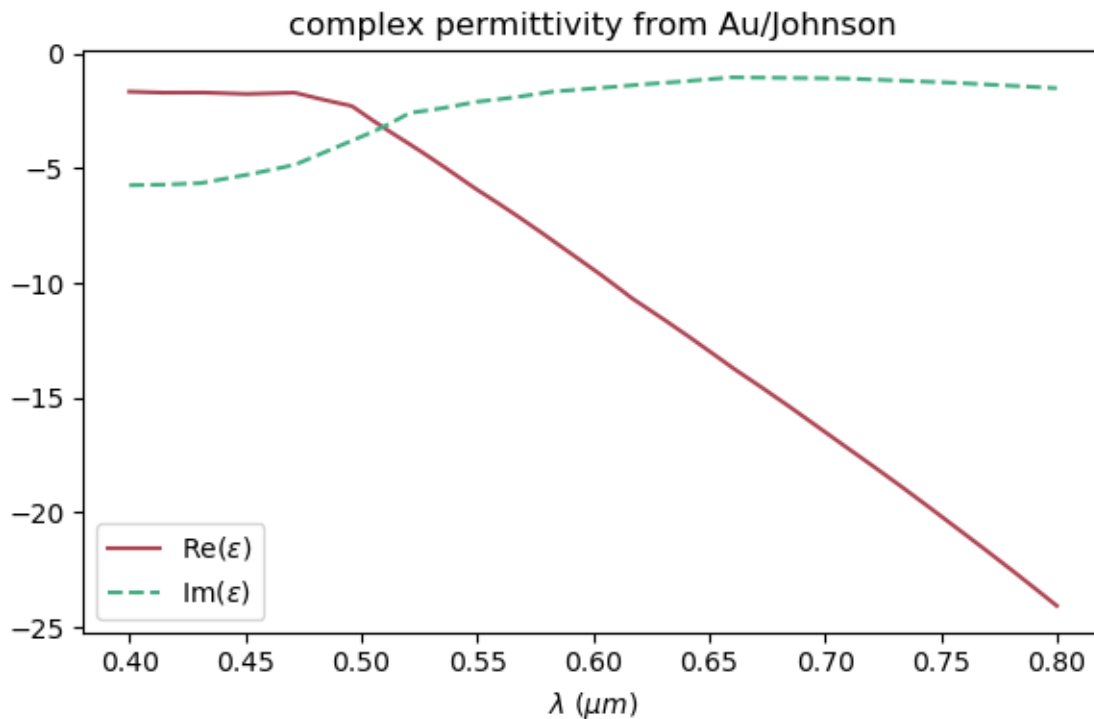
```
0.1879 1.937
```

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 0.447 seconds)

Estimated memory usage: 13 MB

## 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).

### 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
```

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```
from pytheas import genmat
from pytheas import Periodic2D
```

Then we need to instantiate 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
```

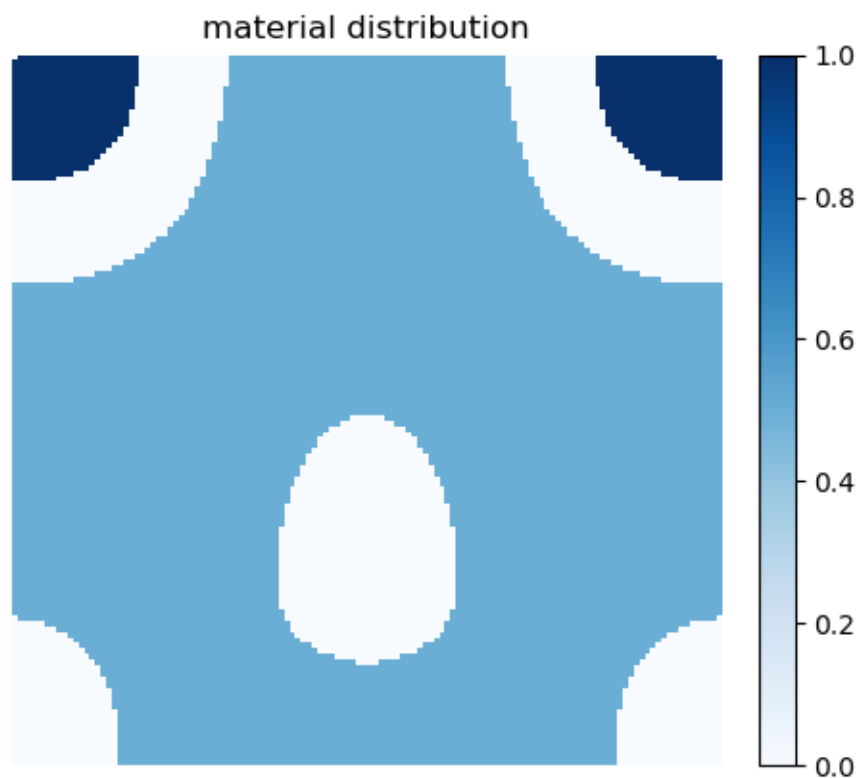
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```
fem.initialize()
mesh = fem.make_mesh()
```

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 2.599 seconds)

**Estimated memory usage:** 13 MB

## 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.

### 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 instantiate 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()
```

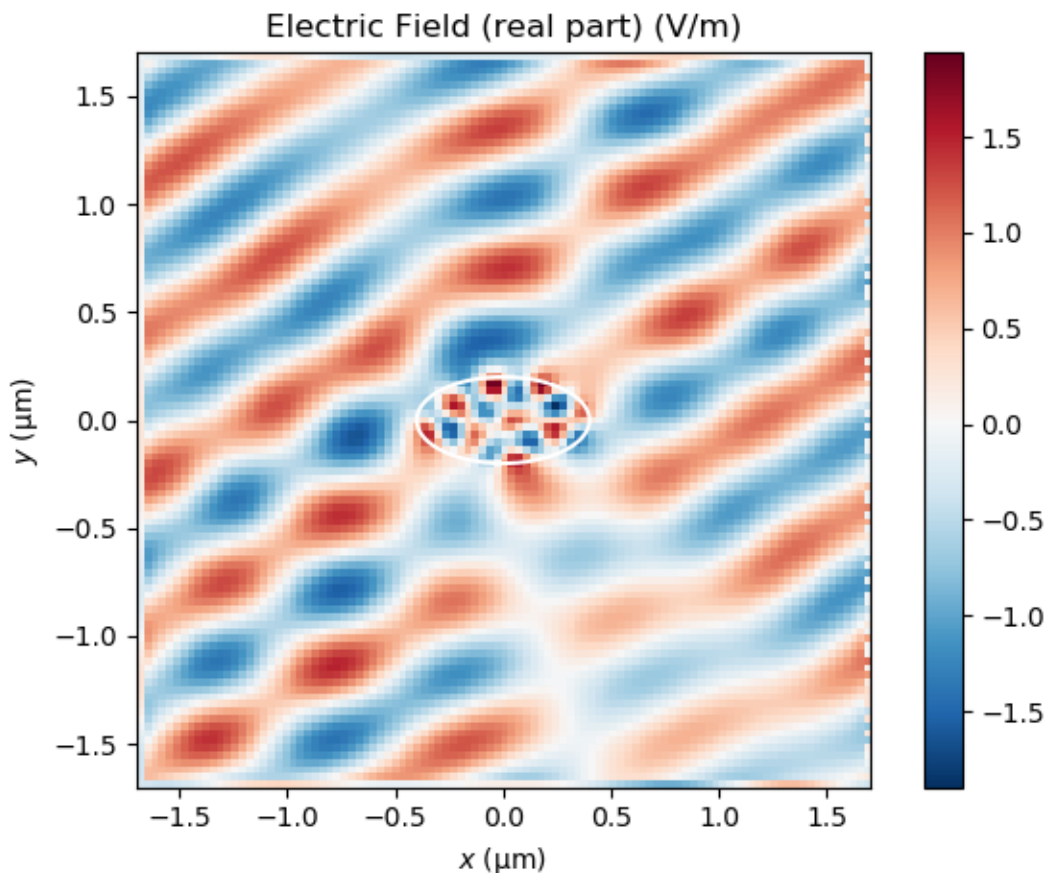
Get the electric field and plot it:

```
fem.postpro_fields()
u_tot = fem.get_field_map("u_tot.txt")
fig, ax = plt.subplots()
E = u_tot.real
```

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```
plt.imshow(E, cmap="RdBu_r", extent=(fem.domX_L, fem.domX_R, fem.domY_B, fem.domY_T))
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()
```

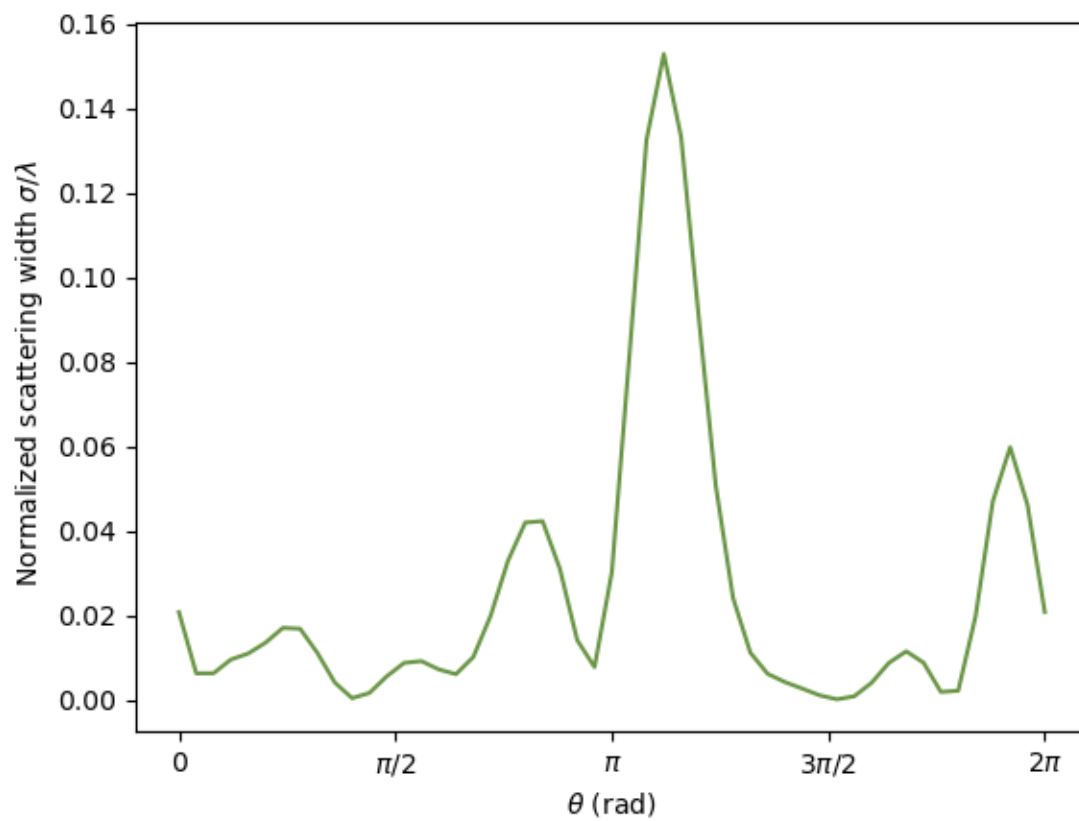


Do a near to far field transform and get the normalized scattering width:

```
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 14.643 seconds)

**Estimated memory usage:** 16 MB



# Bibliography

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



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