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# **pytheas Documentation**

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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

The complete project is documented for every submodule.



## 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) and calculation of the diffraction efficiencies, absorption and energy balance.
- eigenvalues and eigenmodes (modal analysis)

### 1.1 Classes

---

<code>periodic2D.FemModel([analysis, pola, A, ])</code>	A class for a finite element model of a 2D mono-periodic medium.
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#### 1.1.1 `pytheas.periodic2D.FemModel`

```
class pytheas.periodic2D.FemModel (analysis='diffraction', 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))
```

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 "diffraction") – Analysis type: either diffraction (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**()

Clean gmsh/getdp generated files

**diffraction\_efficiencies**()

Postprocess diffraction efficiencies

**get\_field\_map**(*name*)

Retrieve a field map.

**Parameters** *name* (*str* {'u', 'u\_tot'}) – u (scattered field), u\_tot (total field)

**Returns** *field*

**Return type** array, shape (self.Nix, self.Niy)

**postpro\_absorption**()

Compute the absorption coefficient

**Returns** *Q* – Absorption coefficient

**Return type** float

**postpro\_fields**(*filetype*='txt')

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`.

**postpro\_fields\_cuts** ()

Compute the field cuts in substrate and superstrate

**Returns**

- `u_diff_t` (*array-like*) – Transmitted field cuts
- `u_diff_r` (*array-like*) – Reflected field cuts

### Examples using `pytheas.periodic2D.FemModel`

- *Simulating diffraction by a 2D metamaterial*
-



## 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)

### 2.1 Classes

---

<code>scatt2D.FemModel()</code>	A class for a finite element model of a 2D medium
---------------------------------	---

---

#### 2.1.1 `pytheas.scatt2D.FemModel`

```
class pytheas.scatt2D.FemModel
    A class for a finite element model of a 2D medium

    A = None
        flt – incident plane wave amplitude

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

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

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

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

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

    Nix = None
        int – number of x points for postprocessing field maps

    a_pml = None
        flt – PMLs parameter, real part

    analysis = None
        str – analysys type (either diffraction or modal)
```

**b\_pml = None**  
*flt* – PMLs parameter, imaginary part

**beam\_flag = None**  
beam?

**cleanup()**  
Clean gmsl/getdp generated files

**dom\_des = None**  
design domain number (check .geo/.pro files)

**eps\_des = None**  
*flt* – permittivity scattering box

**eps\_host = None**  
*flt* – permittivity host

**eps\_incl = None**  
*flt* – permittivity inclusion

**eps\_sub = None**  
*flt* – permittivity substrate

**h\_pml = None**  
*flt* – thickness pml

**hx\_des = None**  
*flt* – x - thickness scattering box (design)

**hy\_des = None**  
*flt* – y - thickness scattering box

**lambda0 = None**  
*flt* – incident plane wave wavelength in free space

**lambda0search = None**  
*flt* – wavelength around which to search eigenvalues

**lambda\_mesh = None**  
*flt* – wavelength to use for meshing

**ls\_flag = None**  
line source position

**nb\_slice = None**  
*int* – number of y slices points for postprocessing diffraction efficiencies

**neig = None**  
*int* – number of eigenvalues searched for in modal analysis

**pola = None**  
*str* – polarisation of the incident plane wave (either TE or TM)

**scan\_dist\_ratio = None**  
*flt* – such that  $scan\_dist = \min(h\_sup, h\_sub)/scan\_dist\_ratio$

**theta\_deg = None**  
*flt* – incident plane wave angle (in degrees). Light comes from the top (travels along -y if normal incidence, *theta\_deg=0* is set)

**xpp = None**  
coords of point for PostProcessing

**ypp = None**  
coords of point for PostProcessing

---



## INDICES AND SEARCH

- `genindex`
- `modindex`
- `search`





## EXAMPLES

### 4.1 Material examples

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

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**Note:** Click [here](#) to download the full example code

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#### 4.1.1 Importing refractive index from a database

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

```
# Code source: Benjamin Vial
# License: MIT

from pytheas.material.refractiveindex import *
from pytheas.tools.plottools import *
```

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 `ymlFile` we want to import:

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

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

```
bounds = getRange(ymlFile)
lambdas = np.linspace(bounds[0], bounds[1], 300)
```

Then get the refractive index data:

```
ncomplex = get_complex_index(lambdas, ymlFile)
epsilon = (ncomplex**2)
```

And finally plot it:

```
plt.close('all')
fig, ax = plt.subplots(1, figsize=(6, 4))
plt.plot(lambdas, epsilon.real, 'r-', label=r'Re($\varepsilon$)')
plt.plot(lambdas, epsilon.imag, 'b--', label=r'Im($\varepsilon$)')
plt.xlabel(r'$\lambda$ ($\mu$ m)')
```

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```
plt.title("complex permittivity from " + yamlFile[5:][:-4])
plt.legend(loc=0)
plt.show()
```



Total running time of the script: ( 0 minutes 2.714 seconds)

## 4.2 Periodic 2D examples

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

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**Note:** Click [here](#) to download the full example code

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### 4.2.1 Simulating diffraction by a 2D metamaterial

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

First we import the `femmodel` module and some utility functions:

```
# Code source: Benjamin Vial
# License: MIT

import numpy as np
```

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```

from pytheas.tools.plottools import *
from pytheas.material import genmat

from pytheas import periodic2D
from pytheas.periodic2D import FemModel, utils

```

Then we need to instantiate the class FemModel:

```
fem = FemModel()
```

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:

```

# 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. * mum  #: flt: "thickness" superstrate
fem.h_sub = 1. * 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. * mum  #: flt: thickness pml top
fem.h_pmlbot = 1. * 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 = 11  #: 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.  #: 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

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

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

```
genmat.np.random.seed(100)
mat = genmat.MaterialDensity() # instantiate
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
matprop = [1.4, 4 - 0.02 * 1j, 2] # refractive index values

mat._threshold_val = np.random.permutation(mat.threshold_val)
mat.pattern = mat.discrete_pattern
fig, ax = plt.subplots()
mat.plot_pattern(fig, ax, cmap=cmap)
```



We now assign the permittivity

```
fem.register_pattern(mat.pattern, mat._threshold_val)
fem.matprop_pattern = matprop
```

Now were 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': 0.6211041345785192, 'T': 0.22865897491724108, 'Q': 0.  
↪1635944609994113, 'B': 1.0133575704951716}
```

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': 0.4328988879579107, 'T': 0.4694257545635199, 'Q': 0.  
↪08455294909823927, 'B': 0.9868775916196699}
```

**Total running time of the script:** ( 0 minutes 5.457 seconds)



## 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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