

---

# **pytheas Documentation**

***Release 1.1.1***

**Benjamin Vial**

**Nov 19, 2019**



# CONTENTS

- 1 pytheas.periodic2D: 2D metamaterials 3**
  - 1.1 Classes . . . . . 3
- 2 pytheas.tools: tools and utilities 7**
  - 2.1 Submodules . . . . . 7
- 3 pytheas.basefem: boilerplate class for FEM models 9**
  - 3.1 Classes . . . . . 9
- 4 Indices and search 13**
- 5 Examples 15**
  - 5.1 Material examples . . . . . 15
  - 5.2 Periodic 2D examples . . . . . 16
- Bibliography 21**
- Python Module Index 23**



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

### 1.1 Classes

---

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

---

#### 1.1.1 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 consists 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**(*res\_list=None*, *\*\*kwargs*)

Compute the solution of the FEM problem using getdp

**diffraction\_efficiencies**(*cplx\_effs=False*, *orders=False*)

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)

**get\_qty**(*filename*)

Retrieve a scalar quantity.

**Parameters** **filename** (*str*) – Name of the txt file to load.

**Returns** **qty** – The quantity to be loaded.



**Return type** array

**initialize()**

Initialize the problem: - make dictionary of parameters - write this dictionary entries to a .dat file - copy the .dat, .geo and .pro files to the temporary folder

**make\_param\_dict()**

Build dictionary of parameters. This will be later written to a parameter.dat file that is meant to be read by both gmsh and getdp

**mk\_tmp\_dir()**

Create a temporary directory

**postpro\_absorption()**

Compute the absorption coefficient

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

**Return type** float

**postpro\_choice(name, filetype)**

Run a postprocessing command with either pos or txt file output.

**Parameters**

- **name** (*str*) – Name of the post operation as defined in the .pro file.
- **filetype** (*str*) – File type to use (pos or txt)

**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

**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

**postprocess(postop)**

Run getdp postoperation.

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

**ppcmd(postop)**

Create a postprocessing command

**Parameters** **postop** (*str*) – Name of the post operation as defined in the .pro file.

**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*

## PYTHEAS . TOOLS: TOOLS AND UTILITIES

Input/output and utilities.

### 2.1 Submodules

<i>femio</i>	Tools for gmsh/getdp control and input/output.
<i>utils</i>	Shared utility functions used in pytheas.

#### 2.1.1 `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`

#### 2.1.2 `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

## PYTHEAS.BASEFEM: BOILERPLATE CLASS FOR FEM MODELS

The `pytheas.basefem` module implements a base class common for FEM models using `Gmsh` and `GetDP`. This should be used as a parent class and not directly.

### 3.1 Classes

---

`BaseFEM()`

Base class for Finite Element models

---

#### 3.1.1 `pytheas.BaseFEM`

```
class pytheas.BaseFEM
    Base class for Finite Element models

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

    bg_mesh_filename_ = None
        Gmsh geo filename for background mesh
        Type str

    cel = 299792458.0105029
        speed of light in vacuum
        Type flt

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

    compute_solution (res_list=None, **kwargs)
        Compute the solution of the FEM problem using getdp

    dim = None
        dimension of the problem

    epsilon0 = 8.854187817e-12
        vacuum permittivity
        Type flt

    geom_filename_ = None
        Gmsh geometry filename
        Type str
```

**get\_qty** (*filename*)  
Retrieve a scalar quantity.

**Parameters** **filename** (*str*) – Name of the txt file to load.

**Returns** **qty** – The quantity to be loaded.

**Return type** array

**getdp\_verbose** = **None**  
GetDP verbose (int between 0 and 4)

**Type** *str*

**gmsh\_verbose** = **None**  
Gmsh verbose (int between 0 and 4)

**Type** *str*

**initialize** ()  
Initialize the problem: - make dictionary of parameters - write this dictionary entries to a .dat file - copy the .dat, .geo and .pro files to the temporary folder

**make\_param\_dict** ()  
Build dictionary of parameters. This will be later written to a parameter.dat file that is meant to be read by both gmsh and getdp

**mk\_tmp\_dir** ()  
Create a temporary directory

**mu0** = **1.2566370614359173e-06**  
vacuum permeability

**Type** *flt*

**param\_filename** = **None**  
GetDP pro filename

**Type** *str*

**parmesh** = **None**  
global mesh parameter *MeshElementSize = lambda 0/(parmesh\*n) n*: refractive index

**Type** *flt*

**parmesh\_des** = **None**  
design subdomain mesh parameter

**Type** *flt*

**parmesh\_pml** = **None**  
PMLs mesh parameter

**Type** *flt*

**postpro\_choice** (*name, filetype*)  
Run a postprocessing command with either pos or txt file output.

**Parameters**

- **name** (*str*) – Name of the post operation as defined in the .pro file.
- **filetype** (*str*) – File type to use (pos or txt)

**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 gmsb/getdp.
- **postop** (*str*, default "postop\_fields") – Name of the postoperation

**postprocess** (*postop*)

Run getdp postoperation.

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

Create a postprocessing command

**Parameters** **postop** (*str*) – Name of the post operation as defined in the .pro file.**pro\_filename\_** = None

GetDP pro filename

**Type** *str***python\_verbose** = None

python verbose (int between 0 and 1)

**Type** *str***rm\_tmp\_dir** ()

Remove the temporary directory

**update\_params** ()Update the dictionary of parameters and the corresponding file

---





## INDICES AND SEARCH

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



## EXAMPLES

### 5.1 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

---

#### 5.1.1 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

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

Then get the refractive index data:

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

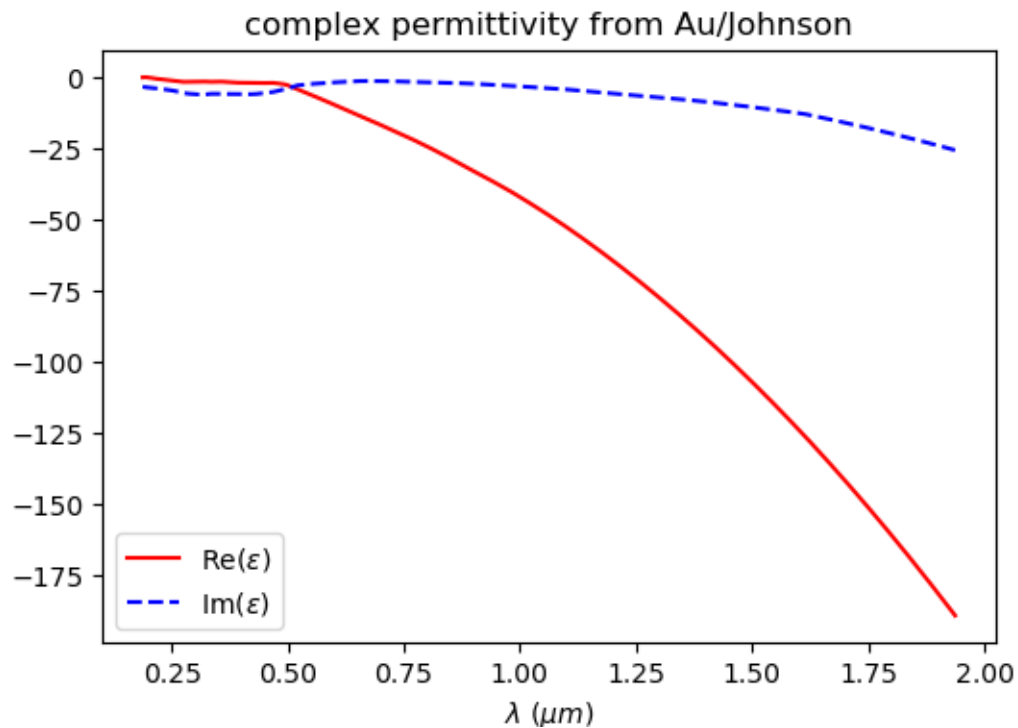
And finally plot it:

```
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($\varepsilon$)")
```

(continues on next page)

(continued from previous page)

```
plt.xlabel(r"$\lambda$ ($\mu$ m)")
plt.title("complex permittivity from " + yamlFile[5][:4])
plt.legend(loc=0)
plt.show()
```



Total running time of the script: ( 0 minutes 0.204 seconds)

## 5.2 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).

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

### 5.2.1 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 required modules and class

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

(continues on next page)

(continued from previous page)

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

Then we need to instantiate the class FemModel:

```
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:

```
# 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"
```

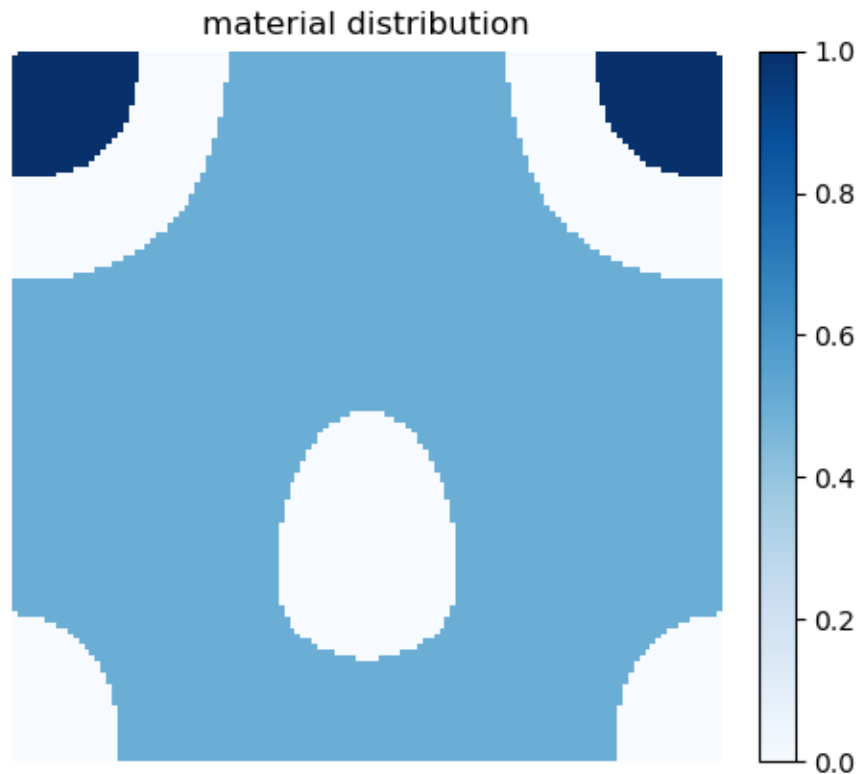
We then initialize the model (copying files, etc) and mesh the unit cell using gmsh

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

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
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 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': 0.34336372784519276, 'T': 0.5452602679212704, 'Q': 0.
↪1122393995886135, 'B': 1.0008633953550765}
```

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': 0.21048638011869789, 'T': 0.7435771802522158, 'Q': 0.
↪04312855666336047, 'B': 0.9971921170342741}
```

**Total running time of the script:** ( 0 minutes 2.928 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

- `pytheas.basefem`, 9
- `pytheas.periodic2D`, 3
- `pytheas.tools`, 7
  - `pytheas.tools.femio`, 7
  - `pytheas.tools.utils`, 7