
pytheas Documentation

Release 1.1.1

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Jun 07, 2019

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

1.1 Classes

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

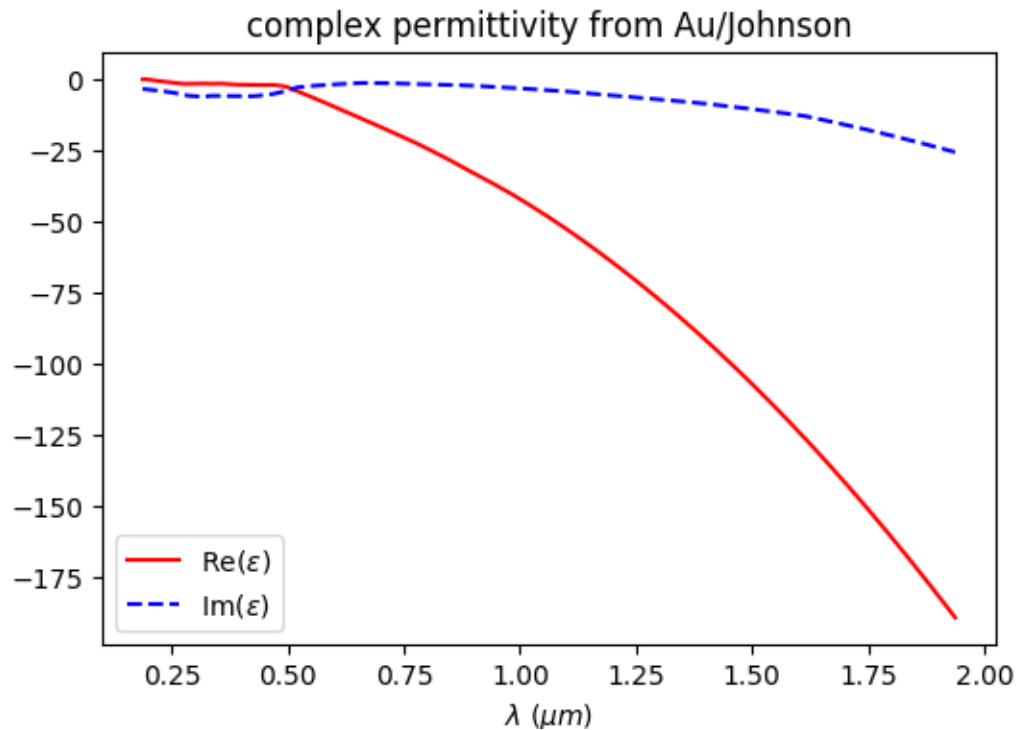
And finally plot it:

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

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```
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 0.268 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

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 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
```

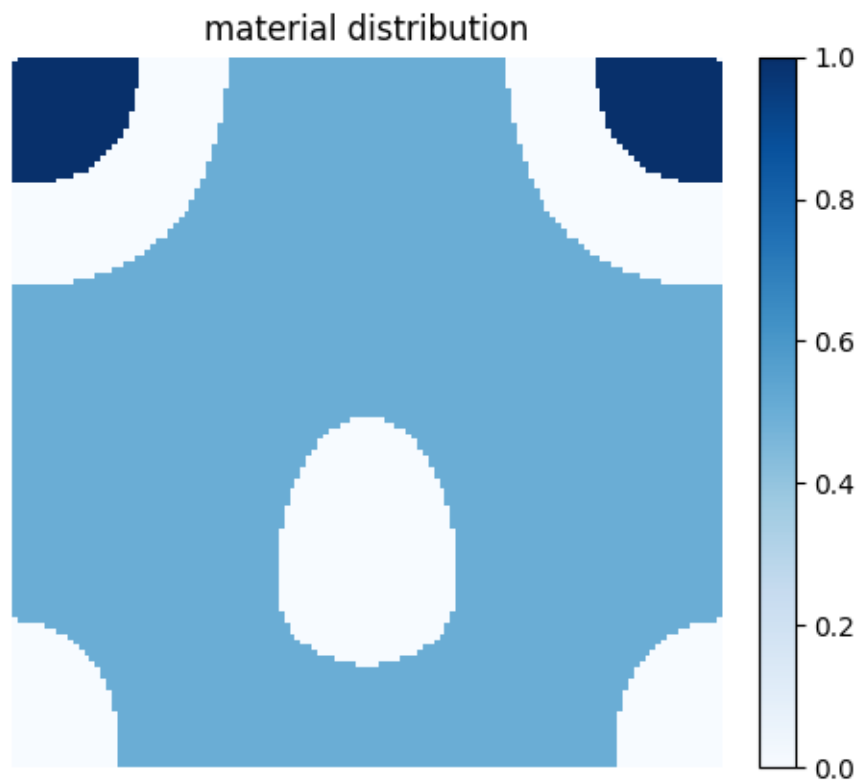
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```
fem.initialize()
mesh = fem.make_mesh()
```

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

```
genmat.np.random.seed(100)
mat = genmat.MaterialDensity() # 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': 0.359684236393363, 'T': 0.5279938129207201, 'Q': 0.
↪1128454301571147, 'B': 1.000523479471198}
```

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': 0.20523268509785825, 'T': 0.7489741597039322, 'Q': 0.
↪04426949819770286, 'B': 0.9984763429994933}
```

Total running time of the script: (0 minutes 3.035 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

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