pytheas Documentation

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Benjamin Vial

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CONTENTS

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.

CHAPTER

ONE

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

1.1 Classes

periodic2D.FemModel([analysis, pola, A,])	A class for a finite element model of a 2D mono-periodic medium.

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 superstarte

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*

CHAPTER

TWO

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

scatt2D.FemModel()	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

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 diffraction or modal)

Type str

b_pml = None
PMLs parameter, imaginary part

Type flt

beam_flag = None
beam?

cleanup()
Clean gmsh/getdp generated files

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

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

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

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

Type str

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

xpp = None
coords of point for PostProcessing

ypp = None
coords of point for PostProcessing

CHAPTER

THREE

INDICES AND SEARCH

- genindex
- modindex
- search

CHAPTER

FOUR

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.

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

Then get the refractive index data:

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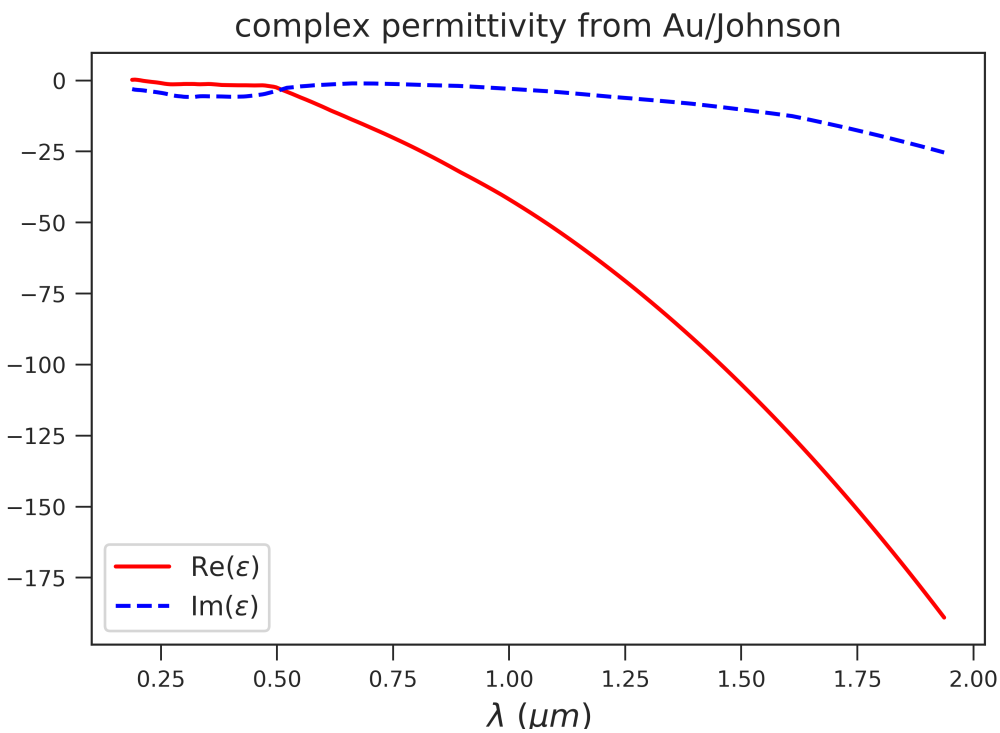
```
plt.title("complex permittivity from " + yamlFile[5:][:-4])
plt.legend(loc=0)
plt.show()
```



Total running time of the script: (0 minutes 2.055 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).

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 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 instanciate 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

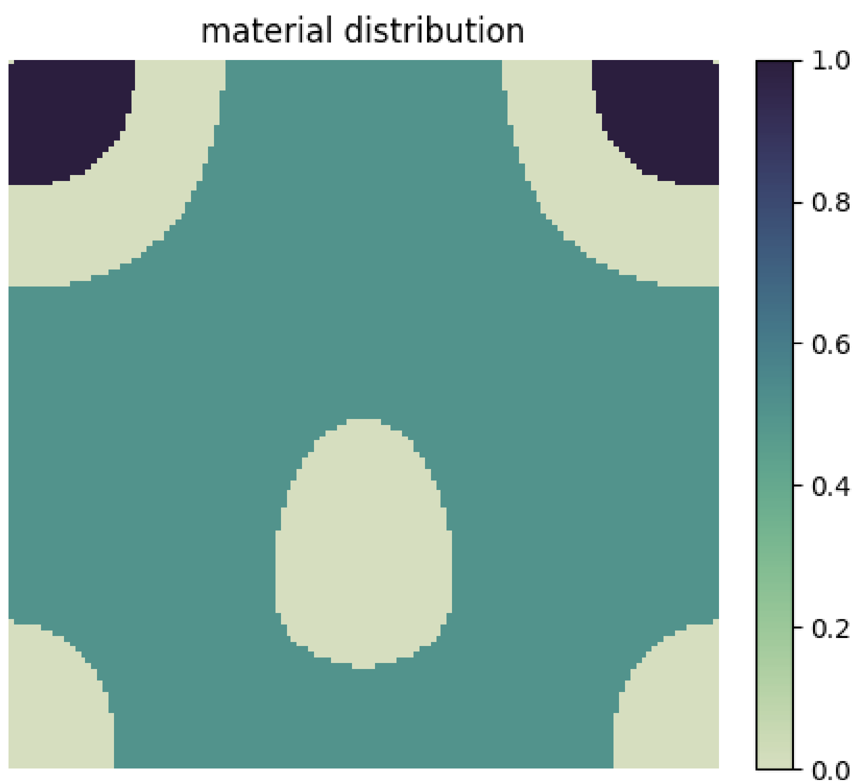
```
fem.getdp_verbose = 0
fem.gmsh_verbose = 0

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

We use the genmat module to generate a material pattern

```
genmat.np.random.seed(100)
mat = genmat.MaterialDensity()  # 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
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': 0.5731410517536096, 'T': 0.2974128553797291, 'Q': 0.
↪1409169091594835, 'B': 1.0114708162928223}
```

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': 0.49394494025915564, 'T': 0.4335054148256543, 'Q': 0.
↪0564858293592027, 'B': 0.9839361844440125}
```

Total running time of the script: (0 minutes 4.944 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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