TORCWA User Guide

Version 0.1.0

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Features

- TORCWA
  - **torc**h + **rcwa**
  - PyTorch implementation of rigorous coupled-wave analysis
  - GPU-accelerated simulation
  - Supporting automatic differentiation for optimization

- Units: Lorentz-Heaviside
  - Speed of light: 1
  - Permittivity and permeability of vacuum: both 1

- Notation: $\exp(-j\omega t)$

Installation

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- Requirements
  - Python version 3.8 or higher
  - PyTorch version 1.10.1 or higher
  - For GPU operation, GPUs that support CUDA operations

- After installing the above requirement, run the following command at the command prompt.

  $ pip install torcwa

- If the PyTorch version is lower than the required, it will automatically install PyTorch 1.10.1 or higher, but the CPU-only PyTorch or incompatible version may be installed.
- Therefore, **before installing using the above command, please install PyTorch version that is compatible with GPU**.

Example list

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- Example 0: Fresnel equation
- **Example 1: Simulation with rectangular meta-atom**
  Normal incidence / Parametric sweep on wavelength / View electromagnetic field
- Example 2: Simulation with square meta-atom
  Oblique incidence / View electromagnetic field
- Example 3: Simulation with rectangular meta-atom
  Normal incidence / Parametric sweep on geometric parameters
- Example 4: Gradient calculation of cylindrical meta-atom
  Differentiation of transmittance with respect to radius
- Example 5: Shape optimization
  Maximize anisotropy
- **Example 6: Topology optimization**
  Maximize 1st order diffraction

Simulation

- 1. Define simulation parameters

```python
# Import
import numpy as np
import torch
from matplotlib import pyplot as plt
import scipy.io

import torcwa
import Materials

# Hardware
# If GPU support TF32 tensor core, the matmul operation is faster than FP32 but with less precision.
# If you need accurate operation, you have to disable the flag below.
torch.backends.cuda.matmul.allow_tf32 = False
sim_dtype = torch.complex64
geo_dtype = torch.float32
device = torch.device('cuda')
```

❖ Only PyTorch is required to run the simulation, but other **additional libraries are required for data plotting and saving**. (Here, matplotlib and SciPy are utilized.)

❖ ‘torch.backends.cuda.matmul.allow_tf32’

- **RTX 3090 or later models** support TF32 core operation for matrix multiplication. This is faster than the conventional computation with less accuracy. It is **recommended to set to False for accurate operation**.

Simulation

- 1. Define simulation parameters

```python
# Import
import numpy as np
import torch
from matplotlib import pyplot as plt
import scipy.io

import torcwa
import Materials

# Hardware
# If GPU support TF32 tensor core, the matmul operation is faster than FP32 but with less precision.
# If you need accurate operation, you have to disable the flag below.
torch.backends.cuda.matmul.allow_tf32 = False
sim_dtype = torch.complex64
geo_dtype = torch.float32
device = torch.device('cuda')
```

❖ ‘sim_dtype’
- This is a data type that requires **complex number operation** and is used when declaring simulation.

❖ ‘geo_dtype’
- This is a data type that requires **real number operation** and is used when declaring geometric parameters, wavelength, and incident angles.

❖ ‘device’
- Choose ‘cpu’ (CPU operation) or ‘cuda’ (GPU operation).

Simulation

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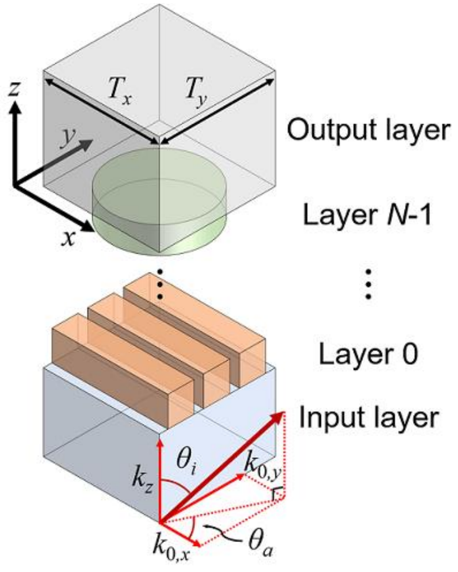
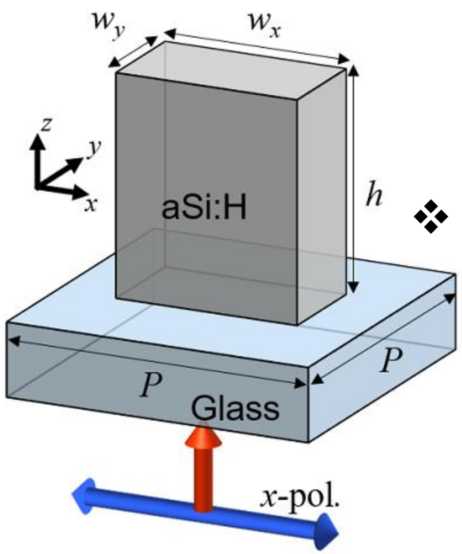
- 1. Define simulation parameters

```python
# Simulation environment
# light
inc_ang = 0.*(np.pi/180)     # radian
azi_ang = 0.*(np.pi/180)     # radian

# material
substrate_eps = 1.46**2

# geometry
L = [300., 300.]                 # nm / nm
torcwa.rcwa_geo.Lx = L[0]
torcwa.rcwa_geo.Ly = L[1]
torcwa.rcwa_geo.nx = 300
torcwa.rcwa_geo.ny = 300
torcwa.rcwa_geo.grid()
torcwa.rcwa_geo.edge_sharpness = 1000.
torcwa.rcwa_geo.dtype = geo_dtype
torcwa.rcwa_geo.device = device
z = torch.linspace(-500,1500,501,device=device)

x_axis = torcwa.rcwa_geo.x.cpu()
y_axis = torcwa.rcwa_geo.y.cpu()
z_axis = z.cpu()

# layers
layer0_geometry = torcwa.rcwa_geo.rectangle(Wx=180.,Wy=100.,Cx=L[0]/2.,Cy=L[1]/2.)
layer0_thickness = 300.
```





❖ Variables

- inc_ang: incident angle (θi in above image)
- azi_ang: azimuthal angle of incidence (θa in above image)
- substrate_eps: permittivity of substrate
- L: Lattice constant ([Tx, Ty] in above image)
- layer0_geometry: rectangle with Wx = 180, Wy = 100
- layer0_thickness: height of structure (h in above image)

Simulation

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- 1. Define simulation parameters

```python
# Simulation environment
# light
inc_ang = 0.*(np.pi/180)    # radian
azi_ang = 0.*(np.pi/180)    # radian

# material
substrate_eps = 1.46**2

# geometry
L = [300., 300.]            # nm / nm
torcwa.rcwa_geo.Lx = L[0]
torcwa.rcwa_geo.Ly = L[1]
torcwa.rcwa_geo.nx = 300
torcwa.rcwa_geo.ny = 300
torcwa.rcwa_geo.grid()
torcwa.rcwa_geo.edge_sharpness = 1000.
torcwa.rcwa_geo.dtype = geo_dtype
torcwa.rcwa_geo.device = device
z = torch.linspace(-500,1500,501,device=device)

x_axis = torcwa.rcwa_geo.x.cpu()
y_axis = torcwa.rcwa_geo.y.cpu()
z_axis = z.cpu()

# layers
layer0_geometry = torcwa.rcwa_geo.rectangle(Wx=180.,Wy=100.,Cx=L[0]/2.,Cy=L[1]/2.)
layer0_thickness = 300.
```

❖ ‘torcwa.rcwa_geo’

- If the lattice constant (L) and sampling number (n) are specified, basic geometry such as rectangle and circle and functions such as union and intersection can be used.
- The generated geometry is expressed as 1 or 0 on the grid.
- The edge sharpness of the geometry also can be specified. The higher this value, the sharper the edge.

Simulation

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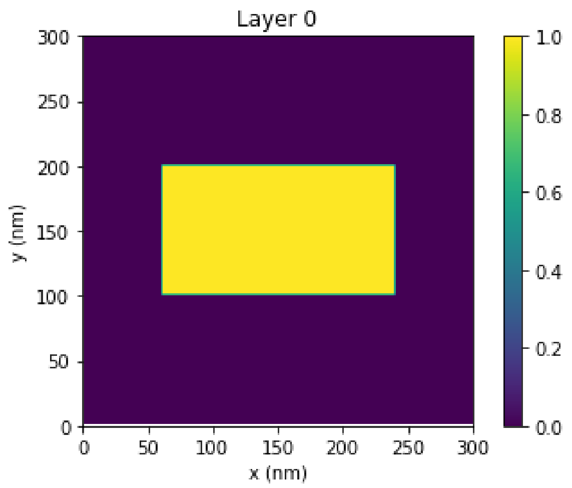
- 2. View internal layer geometry

```
# View layers
plt.imshow(torch.transpose(layer0_geometry,-2,-1).cpu(),origin='lower',extent=[x_axis[0],x_axis[-1],y_axis[0],y_axis[-1]])
plt.title('Layer 0')
plt.xlim([0,L[0]])
plt.xlabel('x (nm)')
plt.ylim([0,L[1]])
plt.ylabel('y (nm)')
plt.colorbar()
```



❖ View with matplotlib
❖ Other plotting library can be utilized.

Simulation

- 3. Generate and perform simulation (**Only get S-paramters** without electromagnetic field)

```python
# Generate and perform simulation
order_N = 15
order = [order_N,order_N]
lamb0 = torch.linspace(400.,700.,61,dtype=geo_dtype,device=device)

txx = []
for lamb0_ind in range(len(lamb0)):
    lamb0_now = lamb0[lamb0_ind]
    sim = torcwa.rcwa(freq=1/lamb0_now,order=order,L=L,dtype=sim_dtype,device=device)
    sim.add_input_layer(eps=substrate_eps)
    sim.set_incident_angle(inc_ang=inc_ang,azi_ang=azi_ang)
    silicon_eps = Materials.aSiH.apply(lamb0_now)**2
    layer0_eps = layer0_geometry*silicon_eps + (1.-layer0_geometry)
    sim.add_layer(thickness=layer0_thickness,eps=layer0_eps)
    sim.solve_global_smatrix()
    txx.append(sim.S_parameters(orders=[0,0],direction='forward',port='transmission',polarization='xx',ref_order=[0,0]))
txx = torch.cat(txx)
```

❖ Variables

- order: truncated Fourier order [x-direction, y-direction]
- lamb0: wavelength for parametric sweep

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- 3. Generate and perform simulation (**Only get S-paramters** without electromagnetic field)

```
# Generate and perform simulation
order_N = 15
order = [order_N,order_N]
lamb0 = torch.linspace(400.,700.,61,dtype=geo_dtype,device=device)

txx = []
for lamb0_ind in range(len(lamb0)):
    lamb0_now = lamb0[lamb0_ind]
    sim = torcwa.rcwa(freq=1/lamb0_now,order=order,L=L,dtype=sim_dtype,device=device)
    sim.add_input_layer(eps=substrate_eps)
    sim.set_incident_angle(inc_ang=inc_ang,azi_ang=azi_ang)
    silicon_eps = Materials.aSiH.apply(lamb0_now)**2
    layer0_eps = layer0_geometry*silicon_eps + (1.-layer0_geometry)
    sim.add_layer(thickness=layer0_thickness,eps=layer0_eps)
    sim.solve_global_smatrix()
    txx.append(sim.S_parameters(orders=[0,0],direction='forward',port='transmission',polarization='xx',ref_order=[0,0]))
txx = torch.cat(txx)
```

❖ Sequence – 1. Declare simulation

- freq: Frequency
- order: Truncated Fourier order
- L: Lattice constant
- dtype: Simulation data type
- device: Simulation device

❖ Sequence – 2. Add input and output layer (This step can be skipped if both layers are free space)

- eps, mu

Simulation

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- 3. Generate and perform simulation (**Only get S-paramters** without electromagnetic field)

```
# Generate and perform simulation
order_N = 15
order = [order_N,order_N]
lamb0 = torch.linspace(400.,700.,61,dtype=geo_dtype,device=device)

txx = []
for lamb0_ind in range(len(lamb0)):
    lamb0_now = lamb0[lamb0_ind]
    sim = torcwa.rcwa(freq=1/lamb0_now,order=order,L=L,dtype=sim_dtype,device=device)
    sim.add_input_layer(eps=substrate_eps)
    sim.set_incident_angle(inc_ang=inc_ang,azi_ang=azi_ang)
    silicon_eps = Materials.aSiH.apply(lamb0_now)**2
    layer0_eps = layer0_geometry*silicon_eps + (1.-layer0_geometry)
    sim.add_layer(thickness=layer0_thickness,eps=layer0_eps)
    sim.solve_global_smatrix()
    txx.append(sim.S_parameters(orders=[0,0],direction='forward',port='transmission',polarization='xx',ref_order=[0,0]))
txx = torch.cat(txx)
```

❖ Sequence – 3. Set incident angle
- inc_ang: Incident angle
- azi_ang: Azimuthal angle of incidence
- angle_layer: Reference layer to incident and azimuthal angle (default: ‘input’)

❖ Sequence – 4. Add internal layer(s)
- eps, mu (grid / scalar) (default: both 1)

Simulation

- 3. Generate and perform simulation (**Only get S-paramters** without electromagnetic field)

```python
# Generate and perform simulation
order_N = 15
order = [order_N,order_N]
lamb0 = torch.linspace(400.,700.,61,dtype=geo_dtype,device=device)

txx = []
for lamb0_ind in range(len(lamb0)):
    lamb0_now = lamb0[lamb0_ind]
    sim = torcwa.rcwa(freq=1/lamb0_now,order=order,L=L,dtype=sim_dtype,device=device)
    sim.add_input_layer(eps=substrate_eps)
    sim.set_incident_angle(inc_ang=inc_ang,azi_ang=azi_ang)
    silicon_eps = Materials.aSiH.apply(lamb0_now)**2
    layer0_eps = layer0_geometry*silicon_eps + (1.-layer0_geometry)
    sim.add_layer(thickness=layer0_thickness,eps=layer0_eps)
    sim.solve_global_smatrix()
    txx.append(sim.S_parameters(orders=[0,0],direction='forward',port='transmission',polarization='xx',ref_order=[0,0]))
txx = torch.cat(txx)
```

❖ Sequence – 5. Solve global S-matrix

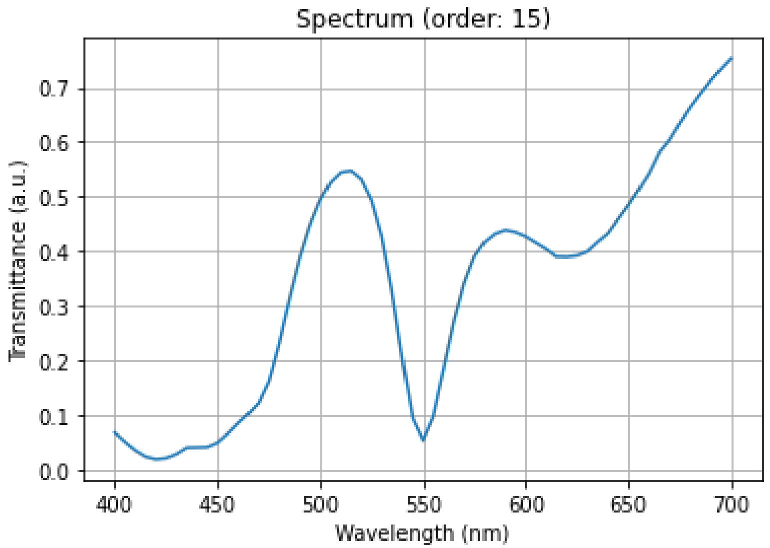
❖ Sequence – 6. Get S-parameter

- orders
- direction (forward/backward)
- port (transmission/reflection)
- polarization (xx/xy/yx/yy)
- ref_order: Reference order to calculate S-paramters

Simulation

- 4. View spectrum and export data

```python
# View spectrum
plt.plot(lamb0.cpu(),torch.abs(txx).cpu()**2)
plt.title('Spectrum (order: '+str(order_N)+')')
plt.xlabel('Wavelength (nm)')
plt.ylabel('Transmittance (a.u.)')
plt.grid()
```



❖ Saving as .mat file with SciPy.

```python
# Export spectrum data
ex1_data = {'lamb0':lamb0.cpu().numpy(),'txx':txx.cpu().numpy()}
scipy.io.savemat('Example1_spectrum_data_order_'+str(order_N)+'.mat',ex1_data)
```

Simulation

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- 5. Generate and perform simulation (**Get electromagnetic field**)

```
# Generate and perform simulation
lamb0 = torch.tensor(532.,dtype=geo_dtype,device=device)    # nm

order_N = 15
order = [order_N,order_N]
sim = torcwa.rcwa(freq=1/lamb0,order=order,L=L,dtype=sim_dtype,device=device)
sim.add_input_layer(eps=substrate_eps)
sim.set_incident_angle(inc_ang=inc_ang,azi_ang=azi_ang)
silicon_eps = Materials.aSiH.apply(lamb0)**2
layer0_eps = layer0_geometry*silicon_eps + (1.-layer0_geometry)
sim.add_layer(thickness=layer0_thickness,eps=layer0_eps)
sim.solve_global_smatrix()
sim.source_planewave(amplitude=[1.,0.],direction='forward')
```

```
# View XZ-plane fields and export
[Ex, Ey, Ez], [Hx, Hy, Hz] = sim.field_xz(torcwa.rcwa_geo.x,z,L[1]/2)
Enorm = torch.sqrt(torch.abs(Ex)**2 + torch.abs(Ey)**2 + torch.abs(Ez)**2)
Hnorm = torch.sqrt(torch.abs(Hx)**2 + torch.abs(Hy)**2 + torch.abs(Hz)**2)
```

❖ Sequence – 7. Set light source
- amplitude
- direction (forward/backward)

- source_planewave
- source_fourier is also possible.

❖ Sequence – 8. Get electromagnetic field
- *x*, *y*, *z* axis or point

Simulation

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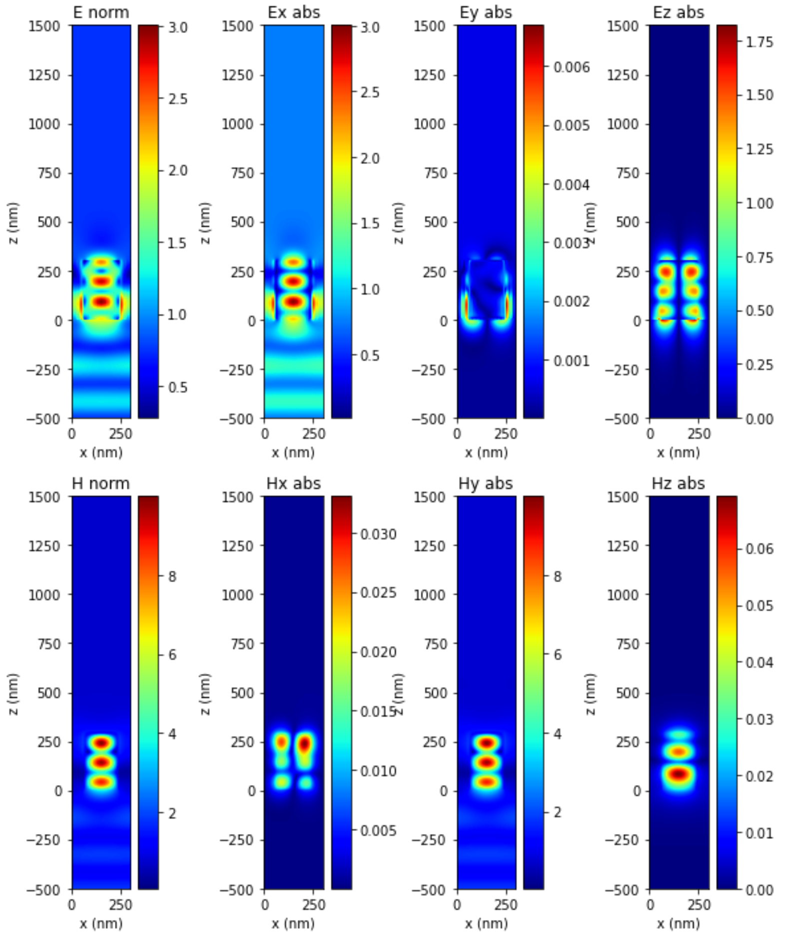
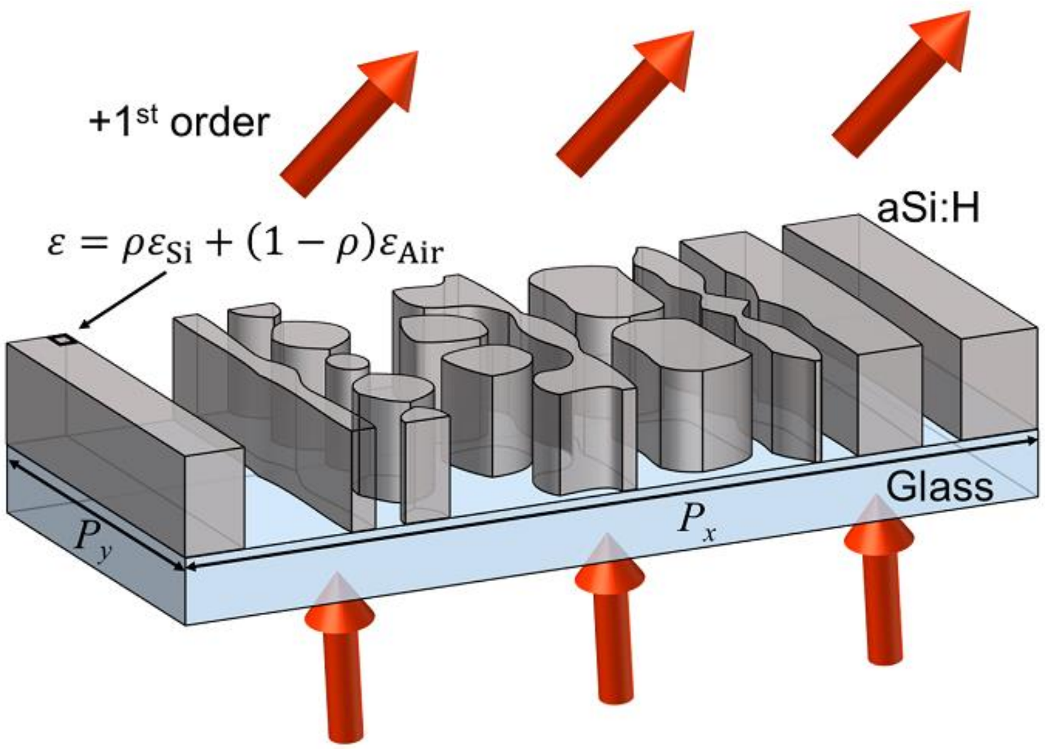
- 6. View electromagnetic field and export data

```python
# View XZ-plane fields and export
[Ex, Ey, Ez], [Hx, Hy, Hz] = sim.field_xz(torcwa.rcwa_geo.x,z,L[1]/2)
Enorm = torch.sqrt(torch.abs(Ex)**2 + torch.abs(Ey)**2 + torch.abs(Ez)**2)
Hnorm = torch.sqrt(torch.abs(Hx)**2 + torch.abs(Hy)**2 + torch.abs(Hz)**2)

fig, axes = plt.subplots(figsize=(10,12),nrows=2,ncols=4)
im0 = axes[0,0].imshow(torch.transpose(Enorm,-2,-1).cpu(),cmap='jet',origin='lower',extent=[x_axis[0],x_axis[-1],z_axis[0],z_axis[-1]])
axes[0,0].set(title='E norm',xlim=(0,L[0]),xlabel='x (nm)',ylim=(z_axis[0],z_axis[-1]),ylabel='z (nm)')
im1 = axes[0,1].imshow(torch.transpose(torch.abs(Ex),-2,-1).cpu(),cmap='jet',origin='lower',extent=[x_axis[0],x_axis[-1],z_axis[0],z_axis[-1]])
axes[0,1].set(title='Ex abs',xlim=(0,L[0]),xlabel='x (nm)',ylim=(z_axis[0],z_axis[-1]),ylabel='z (nm)')
im2 = axes[0,2].imshow(torch.transpose(torch.abs(Ey),-2,-1).cpu(),cmap='jet',origin='lower',extent=[x_axis[0],x_axis[-1],z_axis[0],z_axis[-1]])
axes[0,2].set(title='Ey abs',xlim=(0,L[0]),xlabel='x (nm)',ylim=(z_axis[0],z_axis[-1]),ylabel='z (nm)')
im3 = axes[0,3].imshow(torch.transpose(torch.abs(Ez),-2,-1).cpu(),cmap='jet',origin='lower',extent=[x_axis[0],x_axis[-1],z_axis[0],z_axis[-1]])
axes[0,3].set(title='Ez abs',xlim=(0,L[0]),xlabel='x (nm)',ylim=(z_axis[0],z_axis[-1]),ylabel='z (nm)')
im4 = axes[1,0].imshow(torch.transpose(Hnorm,-2,-1).cpu(),cmap='jet',origin='lower',extent=[x_axis[0],x_axis[-1],z_axis[0],z_axis[-1]])
axes[1,0].set(title='H norm',xlim=(0,L[0]),xlabel='x (nm)',ylim=(z_axis[0],z_axis[-1]),ylabel='z (nm)')
im5 = axes[1,1].imshow(torch.transpose(torch.abs(Hx),-2,-1).cpu(),cmap='jet',origin='lower',extent=[x_axis[0],x_axis[-1],z_axis[0],z_axis[-1]])
axes[1,1].set(title='Hx abs',xlim=(0,L[0]),xlabel='x (nm)',ylim=(z_axis[0],z_axis[-1]),ylabel='z (nm)')
im6 = axes[1,2].imshow(torch.transpose(torch.abs(Hy),-2,-1).cpu(),cmap='jet',origin='lower',extent=[x_axis[0],x_axis[-1],z_axis[0],z_axis[-1]])
axes[1,2].set(title='Hy abs',xlim=(0,L[0]),xlabel='x (nm)',ylim=(z_axis[0],z_axis[-1]),ylabel='z (nm)')
im7 = axes[1,3].imshow(torch.transpose(torch.abs(Hz),-2,-1).cpu(),cmap='jet',origin='lower',extent=[x_axis[0],x_axis[-1],z_axis[0],z_axis[-1]])
axes[1,3].set(title='Hz abs',xlim=(0,L[0]),xlabel='x (nm)',ylim=(z_axis[0],z_axis[-1]),ylabel='z (nm)')
fig.colorbar(im0,ax=axes[0,0])
fig.colorbar(im1,ax=axes[0,1])
fig.colorbar(im2,ax=axes[0,2])
fig.colorbar(im3,ax=axes[0,3])
fig.colorbar(im4,ax=axes[1,0])
fig.colorbar(im5,ax=axes[1,1])
fig.colorbar(im6,ax=axes[1,2])
fig.colorbar(im7,ax=axes[1,3])

ex1_XZ_data = {'x_axis':x_axis.numpy(),'y_axis':y_axis.numpy(),'z_axis':z_axis.numpy(),\
    'Ex':Ex.cpu().numpy(),'Ey':Ey.cpu().numpy(),'Ez':Ez.cpu().numpy(),'Enorm':Enorm.cpu().numpy(),\
    'Hx':Hx.cpu().numpy(),'Hy':Hy.cpu().numpy(),'Hz':Hz.cpu().numpy(),'Hnorm':Hnorm.cpu().numpy()}
scipy.io.savemat('Example1_XZ_data.mat',ex1_XZ_data)
```



Optimization

- 1. Define simulation parameters




```python
# Simulation environment
# light
lamb0 = torch.tensor(532.,dtype=geo_dtype,device=device)    # nm
inc_ang = 0.*(np.pi/180)     # radian
azi_ang = 0.*(np.pi/180)     # radian

# material
substrate_eps = 1.46**2
silicon_eps = Materials.aSiH.apply(lamb0)**2

# geometry
L = [700., 300.]             # nm / nm
torcwa.rcwa_geo.Lx = L[0]
torcwa.rcwa_geo.Ly = L[1]
torcwa.rcwa_geo.nx = 700
torcwa.rcwa_geo.ny = 300
torcwa.rcwa_geo.grid()
torcwa.rcwa_geo.edge_sharpness = 1000.
torcwa.rcwa_geo.dtype = geo_dtype
torcwa.rcwa_geo.device = device

x_axis = torcwa.rcwa_geo.x.cpu()
y_axis = torcwa.rcwa_geo.y.cpu()

# layers
layer0_thickness = 300.
```

Optimization

- 2. Define objective function

```python
# Objective function
def objective_function(rho):
    order = [15,8]

    sim = torcwa.rcwa(freq=1/lamb0,order=order,L=L,dtype=sim_dtype,device=device)
    sim.add_input_layer(eps=substrate_eps)
    sim.set_incident_angle(inc_ang=inc_ang,azi_ang=azi_ang)
    layer0_eps = rho*silicon_eps + (1.-rho)
    sim.add_layer(thickness=layer0_thickness,eps=layer0_eps)
    sim.solve_global_smatrix()
    t1xx = sim.S_parameters(orders=[1,0],direction='forward',port='transmission',polarization='xx',ref_order=[0,0])
    t1yy = sim.S_parameters(orders=[1,0],direction='forward',port='transmission',polarization='yy',ref_order=[0,0])
    t1xy = sim.S_parameters(orders=[1,0],direction='forward',port='transmission',polarization='xy',ref_order=[0,0])
    t1yx = sim.S_parameters(orders=[1,0],direction='forward',port='transmission',polarization='yx',ref_order=[0,0])

    T1_sum = torch.abs(t1xx)**2 + torch.abs(t1yy)**2 + torch.abs(t1xy)**2 + torch.abs(t1yx)**2
    return T1_sum
```

❖ Objective function should return single scalar value.

Optimization

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- 3. Define hyperparameters and initialize

```
# Perform optimization
# optimizer parameters for ADAM optimizer
gar_initial = 0.02
beta1 = 0.9
beta2 = 0.999
epsilon = 1.e-8
iter_max = 800
beta = np.exp(np.arange(start=0,stop=iter_max)*np.log(1000)/iter_max)
gar = gar_initial * 0.5*(1+np.cos(np.arange(start=0,stop=iter_max)*np.pi/iter_max))

# blur kernel
blur_radius = 20.
dx, dy = L[0]/torcwa.rcwa_geo.nx, L[1]/torcwa.rcwa_geo.ny
x_kernel_axis = (torch.arange(torcwa.rcwa_geo.nx,dtype=geo_dtype,device=device)-(torcwa.rcwa_geo.nx-1)/2)*dx
y_kernel_axis = (torch.arange(torcwa.rcwa_geo.ny,dtype=geo_dtype,device=device)-(torcwa.rcwa_geo.ny-1)/2)*dy
x_kernel_grid, y_kernel_grid = torch.meshgrid(x_kernel_axis,y_kernel_axis,indexing='ij')
g = torch.exp(-(x_kernel_grid**2+y_kernel_grid**2)/blur_radius**2)
g = g/torch.sum(g)
g_fft = torch.fft.fftshift(torch.fft.fft2(torch.fft.ifftshift(g)))

torch.manual_seed(0)
rho = torch.rand((torcwa.rcwa_geo.nx,torcwa.rcwa_geo.ny),dtype=geo_dtype,device=device)
rho = (rho + torch.fliplr(rho))/2
rho_fft = torch.fft.fftshift(torch.fft.fft2(torch.fft.ifftshift(rho)))
rho = torch.real(torch.fft.fftshift(torch.fft.ifft2(torch.fft.ifftshift(rho_fft*g_fft))))
momentum = torch.zeros_like(rho)
velocity = torch.zeros_like(rho)

rho_history = []
FoM_history = []
```

❖ Hyperparameters
  - gar_initial: Initial learning rate
  - beta1: Momentum coefficients in ADAM optimizer
  - beta2: Velocity coefficients in ADAM optimizer
  - epsilon: Parameter for preventing division by zero
  - iter_max: Maximum number of iteration
  - beta: Binarize coefficient of pattern at each iteration
  - gar: Learning rate at each iteration

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- 3. Define hyperparameters and initialize

```python
# Perform optimization
# optimizer parameters for ADAM optimizer
gar_initial = 0.02
beta1 = 0.9
beta2 = 0.999
epsilon = 1.e-8
iter_max = 800
beta = np.exp(np.arange(start=0,stop=iter_max)*np.log(1000)/iter_max)
gar = gar_initial * 0.5*(1+np.cos(np.arange(start=0,stop=iter_max)*np.pi/iter_max))

# blur kernel
blur_radius = 20.
dx, dy = L[0]/torcwa.rcwa_geo.nx, L[1]/torcwa.rcwa_geo.ny
x_kernel_axis = (torch.arange(torcwa.rcwa_geo.nx,dtype=geo_dtype,device=device)-(torcwa.rcwa_geo.nx-1)/2)*dx
y_kernel_axis = (torch.arange(torcwa.rcwa_geo.ny,dtype=geo_dtype,device=device)-(torcwa.rcwa_geo.ny-1)/2)*dy
x_kernel_grid, y_kernel_grid = torch.meshgrid(x_kernel_axis,y_kernel_axis,indexing='ij')
g = torch.exp(-(x_kernel_grid**2+y_kernel_grid**2)/blur_radius**2)
g = g/torch.sum(g)
g_fft = torch.fft.fftshift(torch.fft.fft2(torch.fft.ifftshift(g)))

torch.manual_seed(0)
rho = torch.rand((torcwa.rcwa_geo.nx,torcwa.rcwa_geo.ny),dtype=geo_dtype,device=device)
rho = (rho + torch.fliplr(rho))/2
rho_fft = torch.fft.fftshift(torch.fft.fft2(torch.fft.ifftshift(rho)))
rho = torch.real(torch.fft.fftshift(torch.fft.ifft2(torch.fft.ifftshift(rho_fft*g_fft))))
momentum = torch.zeros_like(rho)
velocity = torch.zeros_like(rho)

rho_history = []
FoM_history = []
```

❖ 1. Define blurring kernel for fabrication feasibility of pattern

❖ 2. Initialize parameters

❖ PyTorch built-in optimization tool can be utilized instead.

Optimization

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- 4. Perform optimization

```python
start_time = time.time()
for it in range(0,iter_max):
    rho.requires_grad_(True)
    rho_fft = torch.fft.fftshift(torch.fft.fft2(torch.fft.ifftshift(rho)))
    rho_bar = torch.real(torch.fft.fftshift(torch.fft.ifft2(torch.fft.ifftshift(rho_fft*g_fft))))
    rho_tilda = 1/2 + torch.tanh(2*beta[it]*rho_bar-beta[it])/(2*np.math.tanh(beta[it]))

    FoM = objective_function(rho_tilda)
    FoM.backward()

    with torch.no_grad():
        rho_gradient = rho.grad
        rho.grad = None

        rho_history.append(rho_tilda.detach().cpu().numpy())
        FoM = float(FoM.detach().cpu().numpy())
        FoM_history.append(FoM)

        momentum = (beta1*momentum + (1-beta1)*rho_gradient)
        velocity = (beta2*velocity + (1-beta2)*(rho_gradient**2))
        rho += gar[it]*(momentum / (1-beta1**(it+1))) / torch.sqrt((velocity / (1-beta2**(it+1))) + epsilon)
        rho[rho>1] = 1
        rho[rho<0] = 0
        rho = (rho + torch.fliplr(rho))/2

        end_time = time.time()
        elapsed_time = end_time - start_time
        print('Iteration:',it,'/ FoM:',int(FoM*10000)/10000,'/ Elapsed time:',str(int(elapsed_time))+' s')
```

❖ 1. Declare 'requires_grad_(True)' for parameters to optimize
❖ 2. After some manipulation of the parameters, the FoM is derived by substituting it into the objective function.
❖ 3. Execute 'FoM.backward()' to calculate gradient
❖ 4. Gradient is obtained using 'rho.grad’.
❖ 5. Update the parameters according to the optimization algorithm.

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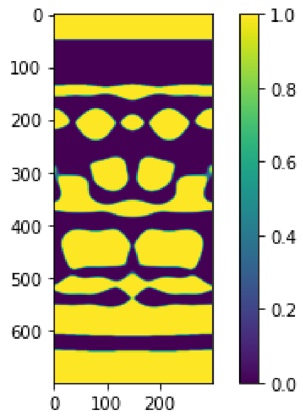
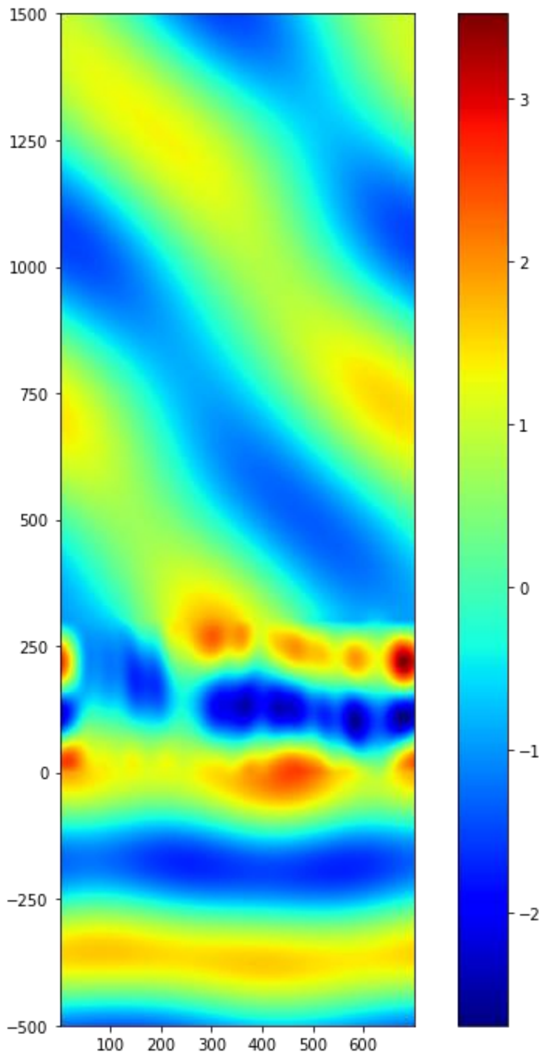
- 5. Get optimization results

```python
# Export data
filename = 'Example6_data.mat'
ex6_data = {'rho_history':rho_history,'FoM_history':FoM_history}
scipy.io.savemat(filename,ex6_data)

# Plot
plt.imshow(rho_tilda.detach().cpu().numpy())
plt.colorbar()
```




```python
# View XZ-plane fields and export for x-pol input
sim.source_planewave(amplitude=[1.,0.],direction='forward')
[Ex, Ey, Ez], [Hx, Hy, Hz] = sim.field_xz(torcwa.rcwa_geo.x,z,L[1]/2)
Enorm = torch.sqrt(torch.abs(Ex)**2 + torch.abs(Ey)**2 + torch.abs(Ez)**2)
Hnorm = torch.sqrt(torch.abs(Hx)**2 + torch.abs(Hy)**2 + torch.abs(Hz)**2)

plt.figure(figsize=(10,12))
plt.imshow(torch.transpose(torch.real(Hy),-2,-1).cpu(),cmap='jet',origin='lower',extent=[x_axis[0],x_axis[-1],z_axis[0],z_axis[-1]])
plt.colorbar()

ex6_Xpol_data = {'x_axis':x_axis.numpy(),'y_axis':y_axis.numpy(),'z_axis':z_axis.numpy(),\
    'Ex':Ex.cpu().numpy(),'Ey':Ey.cpu().numpy(),'Ez':Ez.cpu().numpy(),'Enorm':Enorm.cpu().numpy(),\
    'Hx':Hx.cpu().numpy(),'Hy':Hy.cpu().numpy(),'Hz':Hz.cpu().numpy(),'Hnorm':Hnorm.cpu().numpy()}
scipy.io.savemat('Example6_Xpol_data.mat',ex6_Xpol_data)
```



Advanced options

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```
def __init__(self,freq,order,L,*,
        dtype=torch.complex64,
        device=torch.device('cuda' if torch.cuda.is_available() else 'cpu'),
        stable_eig_grad=True,
        avoid_Pinv_instability=False,
        max_Pinv_instability=0.005
    ):
```

❖ Stable gradient of eigendecomposition

For degenerated eigenmodes, gradient calculation would be unstable due to division by zero.

- stable_eig_grad = True: Slightly sacrifices accuracy, but gains stability for gradient calculations

❖ Gradient calculation for layers with high order eigenmodes

For high order eigenmodes, transformation matrices (P and Q) are nearly singular matrix due to floating point error.

- avoid_Pinv_instability = True: If P is a nearly singular matrix, calculate the H-field eigenmode with Q.
- Max_Pinv_instability: Criteria for determining that P is a nearly singular matrix.

❖ More information can be found in the article.

Other Information

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- Citation
  - Chanhyun Kim, and Byoungho Lee, “TORCWA: GPU-accelerated Fourier modal method and gradient-based optimizations for metasurface” (2022).

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