

recon_PUP_FF_SOFC_hires3_S2

February 8, 2019

1 Overview

This notebook provides detailed steps for the reconstruction (including data reduction and morphology reconstruction) of project PUP_FF_SOFC_hires3_S2, which was taken place back in 2015.

NOTE:

* Currently, only the first layer (out of seven valid layers) is analyzed. * The choice of the first layer is based on the fact that it contains the tip, the porosity of which has significant impact on the FC performance.

1.1 Preperation

Import modules and define user define functions.

```
In [1]: # -- import modules
import tomopy
import gc
import numpy as np
import scipy as sp
import numexpr as ne

import matplotlib.pyplot as plt

from tqdm import trange, tqdm_notebook
from tqdm import trange

from dxchange.reader import read_aps_1id_metafile
from dxchange.reader import read_tiff_stack
from dxchange.writer import write_aps_1id_report
from dxchange.writer import write_tiff_stack
from dxchange.writer import write_vtr

from tomopy.prep.alignment import find_slits_corners_aps_1id
from tomopy.prep.alignment import detector_drift_adjust_aps_1id
from tomopy.prep.alignment import remove_slits_aps_1id
from tomopy.prep.normalize import minus_log
from tomopy.misc.npmath import discrete_cdf
from tomopy.misc.npmath import gauss1d
```

```

from scipy.signal import medfilt
from scipy.signal import medfilt2d
# from scipy.signal import convolve
from scipy.optimize import curve_fit

from scipy.ndimage import gaussian_filter
from scipy.ndimage import shift
from scipy.ndimage import convolve

from scipy.special import erf, erfc

# --
import ipywidgets as widgets
from ipywidgets import interact, interactive, fixed, interact_manual, IntProgress
from IPython.display import display

# --
from matplotlib import animation, rc
from IPython.display import HTML, Image

```

```

/home/chenz3/.pyenv/versions/anaconda3-5.2.0/lib/python3.6/site-packages/skimage/transform/_warps.py:10: UserWarning: The default mode, 'constant', will be changed to 'reflect' in skimage 0.15.
  warn("The default mode, 'constant', will be changed to 'reflect' in ")

```

```

In [2]: # -- svd function
def svd_enhance(img, eigen_cut=20):
    U, S, V = np.linalg.svd(img, full_matrices=True)
    eigen_cut = min(eigen_cut, U.shape[1], V.shape[0])
    return np.dot(U[:, :eigen_cut]*S[:eigen_cut], V[:, :eigen_cut, :])

In [3]: # -- quick lambda function
val_atPercent = lambda ar, p: np.sort(ar.flatten())[int(np.prod(ar.shape)*p)]
wgt_histequal = lambda ar: (np.sort(ar.flatten()).searchsorted(ar) + 1)/np.prod(ar.shape)
wgts_binned = lambda wgts, bins: np.int64(np.floor(wgts * bins)).astype(wgts.dtype)

```

1.2 Metadata processing

Process/Parse the metadata (auto-generated during scan) to extract

- beam status (various stability)
- frame quality
- connectivity between rotation angle (ω) and the image sequence number
- group layers into dataframes

```

In [4]: # ----- CONFIG BLOCK ----- #
# -- change the following based on the sample
metaf1 = "PUP_FF_SOFC_hires3_S2_TomoStillScan.dat"
sampleImgName = "PUP_FF_SOFC_hires3_S2/PUP_FF_SOFC_hires3_S2_000008.tif"

```

```

write_base      = "PUP_FF_SOFC_hires3_S2_results/PUP_FF_SOFC_hires3_S2"
reportfn       = "PUP_FF_SOFC_hires3_S2_report/scanSummary.pdf"

# -- reconstruction config
recon_config = {'algorithm': 'gridrec',
                'filter'    : 'hann',
                }

# -- build data frame and generate report
df_layers = write_aps_lid_report(read_aps_lid_metafile(metaf1), reportfn)

layerIDs = df_layers['layerID'].unique()

print(f"Unique layers are: {layerIDs}")

```

Unique layers are: [6 7 8 9 10 11 12]

manual select the first layer, which contains the tip

In [5]: layerID = 6

```

df_layern = df_layers[df_layers['layerID'] == layerID]

df_layern.describe()

```

```

Out[5]:

```

	num	nSeq	exp	fOmega	Omega \
count	3631.000000	3631.000000	3.631000e+03	3631.000000	3631.000000
mean	1786.165244	1816.000000	1.500000e-01	-1.487194	-1.487225
std	1048.041119	1048.323741	1.015994e-14	104.810435	104.810434
min	1.000000	1.000000	1.500000e-01	-180.000000	-180.000000
25%	878.500000	908.500000	1.500000e-01	-92.250000	-92.250050
50%	1786.000000	1816.000000	1.500000e-01	-1.500000	-1.500080
75%	2693.500000	2723.500000	1.500000e-01	89.250000	89.249900
max	3601.000000	3631.000000	1.500000e-01	180.000000	180.000000

	ICint	IC-E1	IC-E2	IC-E3	IC-E4 \
count	3.631000e+03	3631.000000	3631.000000	3631.000000	3631.000000
mean	6.500000e-01	76380.527403	78185.773891	73212.141283	321.169375
std	4.441504e-14	4045.376572	4142.571960	3879.211524	15.836482
min	6.500000e-01	0.000000	0.000000	419.000000	284.000000
25%	6.500000e-01	76262.000000	78056.000000	72992.000000	309.000000
50%	6.500000e-01	76515.000000	78320.000000	73298.000000	320.000000
75%	6.500000e-01	76965.000000	78796.000000	73905.000000	334.000000
max	6.500000e-01	78201.000000	81453.000000	75524.000000	363.000000

	...	bpEds	LN2temp	SRcurrent	encoderX	seqNum \
count	...	3631.000000	3631.000000	3631.000000	3631.0	3631.000000
mean	...	-13.517194	84.220476	102.049297	0.0	1815.026990

std	...	1.058316	0.003734	0.174000	0.0	1048.324049
min	...	-13.574900	84.211000	101.639000	0.0	1.000000
25%	...	-13.573100	84.218000	101.927000	0.0	907.500000
50%	...	-13.572800	84.221000	102.052000	0.0	1815.000000
75%	...	-13.572400	84.223000	102.170000	0.0	2722.500000
max	...	7.125490	84.230000	102.508000	0.0	3631.000000

	layerID	TBS	VBS	BLS	BLT
count	3631.0	3631.000000	3622.000000	3631.000000	3631.000000
mean	6.0	0.987991	inf	2.105510	0.006412
std	0.0	0.052350	NaN	0.110042	0.039903
min	6.0	0.005654	0.949812	0.000000	0.004191
25%	6.0	0.985021	0.976874	2.107535	0.004288
50%	6.0	0.989150	0.977052	2.112055	0.004315
75%	6.0	0.997342	0.977191	2.114556	0.004344
max	6.0	1.019190	inf	2.147057	0.768496

[8 rows x 23 columns]

```
In [9]: # rotation related quantity (useful for reconstruction)
        thetas = np.radians(df_layern.loc[df_layern['type']=='still', 'Omega'].values)
        dn = int(np.pi/(thetas[1] - thetas[0])) # assuming equal spacing along omega
```

1.3 Data reduction

The raw data is way to large for regular computer server to handle, therefore data reduction is necessary before further analysis.

first, generate necessary folders for subsequent analysis

```
In [8]: %bash
```

```
mkdir -p PUP_FF_SOFC_hires3_S2_report
mkdir -p PUP_FF_SOFC_hires3_S2_results
mkdir -p PUP_FF_SOFC_hires3_S2_runtime
```

second, background normalization using collected dark and white field images

```
In [9]: print(f"Reading in tiff images")
        flat_pre = read_tiff_stack(sampleImgName, df_layern.loc[df_layern['type'] == 'pre_white'])
        flat_pst = read_tiff_stack(sampleImgName, df_layern.loc[df_layern['type'] == 'post_white'])
        dark_pst = read_tiff_stack(sampleImgName, df_layern.loc[df_layern['type'] == 'post_dark'])
        print(f"=> quick summary of background images for layer_{layerID}:")
        print(f"\tPre-flat image:{flat_pre.shape} as {flat_pre.dtype}")
        print(f"\tPost-flat image:{flat_pst.shape} as {flat_pst.dtype}")
        print(f"\tPost-dark image:{dark_pst.shape} as {dark_pst.dtype}")
```

Reading in tiff images

```
=> quick summary of background images for layer_6:
    Pre-flat image:(10, 2048, 2048) as uint16
```

```
Post-flat image:(10, 2048, 2048) as uint16
Post-dark image:(10, 2048, 2048) as uint16
```

```
In [10]: # interactively view the flat field image
        # 10 dark, 10 white_pre, 10_white_post
```

```
def viz_flat(n):
    fig, axes = plt.subplots(2, 3, figsize=(15, 10),)

    axes[0,0].imshow(flat_pre[n,:,:], 'jet')
    axes[0,0].set_title("white field (before)")
    xx,yy = discrete_cdf(flat_pre[n,:,:].flatten(), steps=500)
    axes[1,0].plot(xx,yy)
    axes[1,0].set_yscale('log')

    axes[0,1].imshow(flat_pst[n,:,:], 'jet')
    axes[0,1].set_title("white field (after)")
    xx,yy = discrete_cdf(flat_pst[n,:,:].flatten(), steps=500)
    axes[1,1].plot(xx,yy)
    axes[1,1].set_yscale('log')

    axes[0,2].imshow(dark_pst[n,:,:], 'jet')
    axes[0,2].set_title("dark field")
    xx,yy = discrete_cdf(dark_pst[n,:,:].flatten(), steps=500)
    axes[1,2].plot(xx,yy)
    axes[1,2].set_yscale('log')

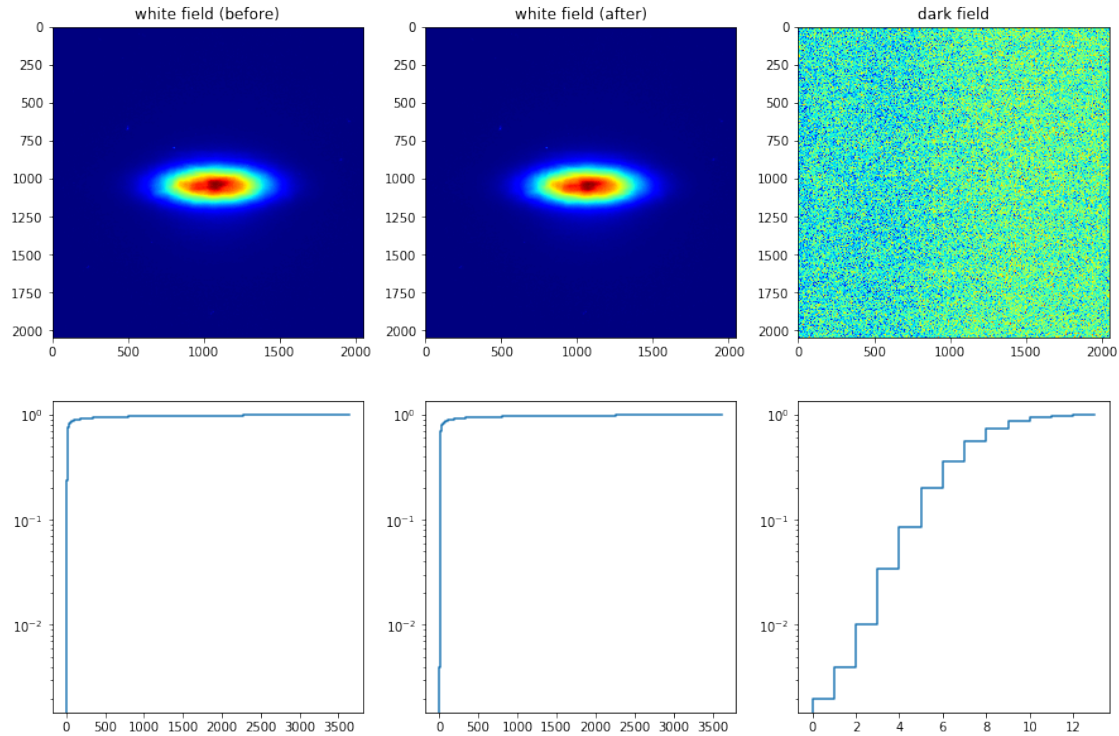
    # -- use the template
    interactive_plot = interactive(viz_flat, n=(0, flat_pre.shape[0]-1)) # still field

    output = interactive_plot.children[-1]
    interactive_plot
```

```
interactive(children=(IntSlider(value=4, description='n', max=9), Output()), _dom_classes=('wi
```

Static view (for non-interacitve notebook mode)

```
In [11]: viz_flat(4)
```



now, it is time to read in the raw projections

NOTE: careful with the memory usage (about **30.0G** per layer).

```
In [12]: projs = read_tiff_stack(sampleImgName, df_layern.loc[df_layern['type'] == 'still', 'I']
         print(f"=> quick summary of projection images for layer_{layerID}:")
         print(f"\tprojections image:{projs.shape} as {projs.dtype}")
```

```
=> quick summary of projection images for layer_6:
    projections image:(3601, 2048, 2048) as uint16
```

```
In [13]: # Interactive view of the projection images
```

```
def viz_proj(n):

    fig, axes = plt.subplots(1, 2, figsize=(10, 5))

    axes[0].imshow(projs[n,:,:], 'jet')

    xx,yy = discrete_cdf(projs[n,:,:].flatten(), steps=500)
    axes[1].plot(xx,yy)
    axes[1].set_yscale('log')

    # -- use the template
```

```

interactive_plot = interactive(viz_proj, n=(0, projs.shape[0]-1)) # still field

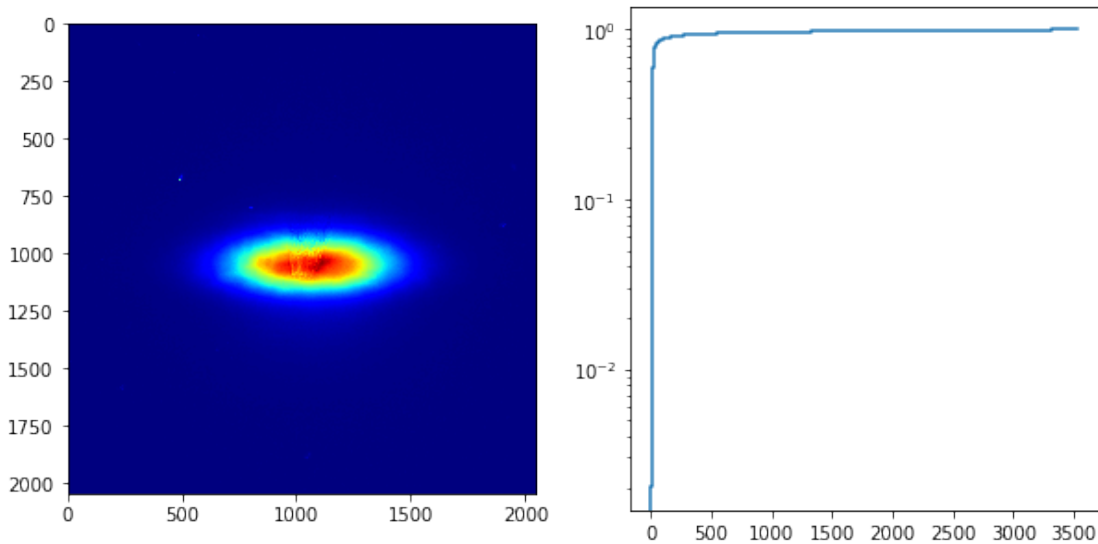
output = interactive_plot.children[-1]
interactive_plot

interactive(children=(IntSlider(value=1800, description='n', max=3600), Output()), _dom_classes=

```

static view of projeccio images (for non-interactive notebook session)

In [14]: viz_proj(1800)



since the majority of the image is empty, it is better to isolate the region with sample to reduce total data size.

After several interactive visual inspections, the following cropping limit is selected for this layer.

- Layer_6: img[750:1150, 800:1300]

1.3.1 Crop down images

```

In [16]: # get the background
          bg_white = np.median(flat_pre, axis=0).astype(float)
          bg_dark  = np.median(dark_pst, axis=0).astype(float)

In [17]: bg_white = bg_white[750:1150, 800:1300]
          bg_dark  = bg_dark[ 750:1150, 800:1300]
          projs    = projs[:, 750:1150, 800:1300]

```

```
In [20]: # remove the background using both white field and dark field
```

```
projs_clean = np.zeros(projs.shape)

for n in tqdm_notebook(range(projs.shape[0])):
    img = np.copy(projs[n,:,:]).astype(float)
    img = np.where(img-bg_dark>0, img-bg_dark, 0)
    bg = np.where(bg_white-bg_dark>0, bg_white-bg_dark, 1)
    img = img/bg
    img = -np.log(np.where(img>0, img, 1))
    projs_clean[n,:,:] = np.where(img>0, img, 0)
```

```
HBox(children=(IntProgress(value=0, max=3601), HTML(value='')))
```

```
In [21]: # Interactive view of the projection images
```

```
def viz_proj(n):

    fig, axes = plt.subplots(1, 2, figsize=(10, 5))

    axes[0].imshow(projs_clean[n,:,:], 'gray')

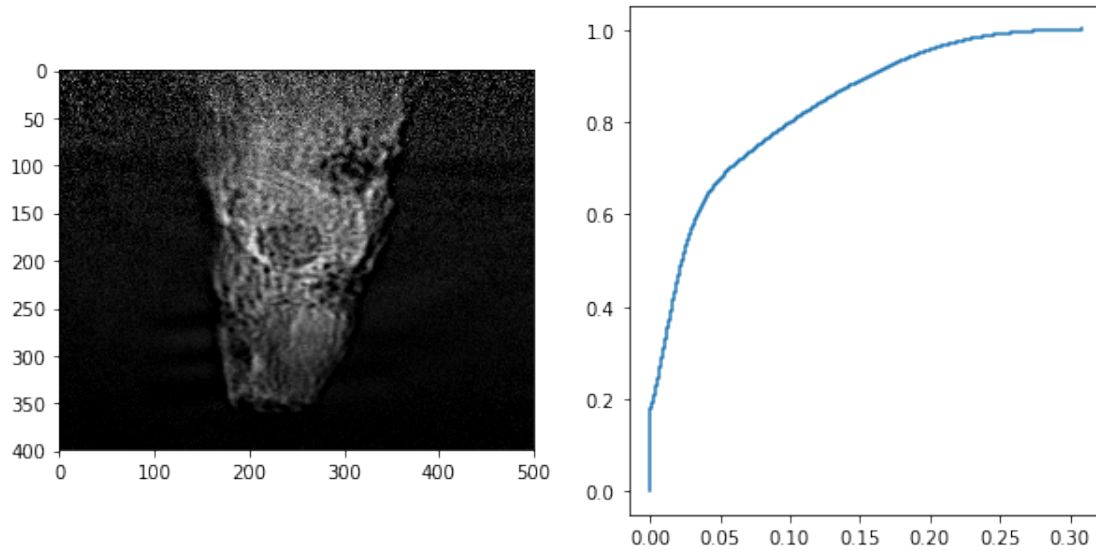
    xx,yy = discrete_cdf(projs_clean[n,:,:].flatten(), steps=500)
    axes[1].plot(xx,yy)

    # -- use the template
    interactive_plot = interactive(viz_proj, n=(0, projs.shape[0]-1)) # still field

    output = interactive_plot.children[-1]
    interactive_plot
```

```
interactive(children=(IntSlider(value=1800, description='n', max=3600), Output()), _dom_classes=
```

```
In [22]: # static view
viz_proj(1800)
```

save the reduced projections and **restart kernel (manual)**

```
In [23]: np.save('PUP_FF_SOFC_hires3_S2_runtime/layer6_projs_reduced', projs_clean)
```

1.4 Tomography reconstruction

With the reduced data set, it is now possible to perform the reconstruction.

1.4.1 Counter sample jittering

Due to the experiment setup, significant sample jittering (particularly horizontal one) is present in the data set. This poses a huge issue to the tomography reconstruction process which requires a common rotation axis for all image. Consequently, a phase correlation based correction process, termed “iterative pair-wise adjustment”, is used here to counter the **horizontal** sample jittering by forcing the rotation axis of all iamge to the center of the image.

Note: Although visible vertical sample jittering is also observed, there is currently no reliable way to counter its impact due to lack of common reference feature.

```
In [7]: # load the reduced data set
```

```
projs = np.load('PUP_FF_SOFC_hires3_S2_runtime/layer6_projs_reduced.npy')

for n in tqdm_notebook(range(projs.shape[0])):
    projs[n,:,:] /= projs[n,:,:].max()

print(projs.shape)
```

```
HBox(children=(IntProgress(value=0, max=3601), HTML(value='')))
```

(3601, 400, 500)

```
In [10]: # -- center the data using iterative pairwise adjustment
n_iters      = 10
rot_centers  = []

for i in tqdm_notebook(range(n_iters), desc='iter'):
    # adjust the images
    for n_img in tqdm_notebook(range(int(dn)), desc='adjust'):
        # locate the pair-wise center through PC
        _cnt = tomopy.find_center_pc(projs[n_img,:,:],
                                     projs[n_img+dn,:,:],
                                     rotc_guess=projs.shape[2]/2,
                                     )

        # adjust the pair images
        # NOTE:
        # make sure have order=1 to force using linear interpolation to avoid negative values
        val_shift = np.array([0, projs.shape[2]/2 - _cnt])
        projs[n_img,:,:] = shift(projs[n_img,:,:], val_shift, mode='constant', cval=0)
        projs[n_img+dn,:,:] = shift(projs[n_img+dn,:,:], val_shift, mode='constant', cval=0)

    # calculate the average rotation center
    tmp = []
    for n_img in tqdm_notebook(range(int(dn)), desc='calcAvg'):
        tmp.append(tomopy.find_center_pc(projs[n_img,:,:],
                                         projs[n_img+dn,:,:],
                                         rotc_guess=projs.shape[2]/2,
                                         )
                )

    # get the average rotation center
    _cnt = np.average(tmp)
    # if the average rotation center has been adjusted to middle, stop
    if abs(_cnt - projs.shape[2]/2)<0.1:
        break
```

```
HBox(children=(IntProgress(value=0, description='iter', max=10, style=ProgressStyle(description_text='iter')),
```

```
HBox(children=(IntProgress(value=0, description='adjust', max=1800, style=ProgressStyle(description_text='adjust')),
```

```
HBox(children=(IntProgress(value=0, description='calcAvg', max=1800, style=ProgressStyle(description_text='calcAvg')),
```

During the analysis, it was noticed that there are three corrupted frames, which will add unnecessary noise to the reconstruction results. Therefore, the pairs containing corrupted frames are excluded from the reconstruction process.

```

In [11]: # -- gather the horizontal jitter profile (rotation center distribution)
dict_rotcnts = {}

thetas = np.radians(df_layern.loc[df_layern['type']=='still', 'Omega'].values)
dn = int(np.pi/(thetas[1] - thetas[0])) # assuming equal spacing along omega

rot_centers = []
for n_img in tqdm_notebook(range(0, int(dn))):
    rot_centers.append(tomopy.find_center_pc(projs[n_img, :, :], projs[n_img+dn, :, :])

dict_rotcnts['iterPairWiseAdjust'] = rot_centers + rot_centers

# -- find the good/bad frames
rot_cnts = np.array(dict_rotcnts['iterPairWiseAdjust'])

idx_goodimg = np.where(abs(rot_cnts - 250) < 1)[0]
idx_badimg = np.where(abs(rot_cnts - 250) >= 1)[0]

projs_good = projs[idx_goodimg, :, :]
thetas_good = thetas[idx_goodimg]
rot_cnt = np.average(rot_cnts[idx_goodimg])

print(projs_good.shape, thetas_good.shape, rot_cnt, np.average(rot_cnts))

HBox(children=(IntProgress(value=0, max=1800), HTML(value='')))

(3594, 400, 500) (3594,) 249.99763494713412 249.98625

```

1.4.2 counter rotation axis tilt

Preliminary analysis (see below) indicate that the rotation axis is tilted, which is most likely caused by the mis-alignment between FF detector and the sample rotation stage. In theory, the most accurate correction would be in-plane rotation to bring the 180°-pair into a leveled position. However, due to lack of reference points, the exact rotation cannot be deterministically located. Therefore, an finite steps approximation is used where different rotation center is used for thin slice of data (two sinograms at a time).

```

In [12]: # testing for single pair

nimgs = [20, 100, 500, 1000]
for nimg in nimgs:
    cnts = []
    for nrow in range(0, projs.shape[1], 2):
        cnts.append(tomopy.find_center_pc(projs[n_img, nrow:nrow+2, :],
                                           projs[n_img+dn, nrow:nrow+2, :],
                                           rotc_guess=projs.shape[2]/2,
                                           ) - 250

```

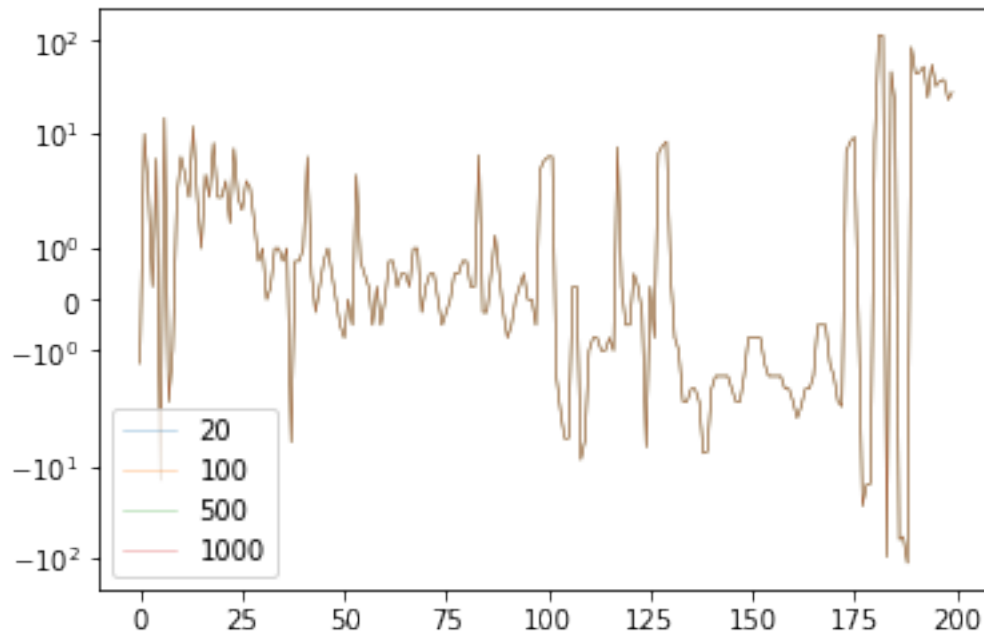
```

    )
    plt.plot(cnts, label=f"{nimg}", linewidth=0.5, alpha=0.5)

plt.yscale('symlog')
plt.legend()

```

Out[12]: <matplotlib.legend.Legend at 0x7f4718c83940>



```

In [ ]: # use slab of 16 pixels
        # [32, 16, 8, 4, 2,]

size_slab = 2
recon      = np.zeros((projs.shape[1], projs.shape[2], projs.shape[2]))
rotcnts    = []

for nrow in tqdm_notebook(range(0, projs.shape[1], size_slab), desc='slab'):
    # locate the rotation center
    _projs = projs[:,nrow:nrow+size_slab,:]
    _rotcnt = []
    for nimg in tqdm_notebook(range(dn), desc=f'r{nrow}_omega'):
        _rotcnt.append(tomopy.find_center_pc(_projs[nimg, :, :],
                                              _projs[nimg+dn, :, :],
                                              rotc_guess=projs.shape[2]/2,
                                              ),
        )
    _rotcnt = np.array(_rotcnt + _rotcnt) # 180 -> 360

```

```

# perform the reconstruction
recon[nrow:nrow+size_slab,:,:) = tomopy.recon(projs_good[:,nrow:nrow+size_slab,:],
                                                thetas_good,
                                                center=np.average(_rotcnt[idx_goodimg]),
                                                algorithm='gridrec', filter_name='han
                                                )
rotcnts.append(np.average(_rotcnt[idx_goodimg]))

# removal phase artifacts
recon = tomopy.circ_mask(recon, axis=0, ratio=0.6)

phase_recon = tomopy.retrieve_phase(recon,
                                    pixel_size=2e-5, # 200 nm pixel size on the dete
                                    dist=10,         # the notes said 36m !?
                                    energy=50,        # 45-50 keV, according to exist
                                    )

# output to disk
for n in tqdm_notebook(range(recon.shape[0])):

    img = np.copy(recon[n,:,:])
    pha = np.absolute(np.copy(phase_recon[n,:,:]))
    pha /= pha.max()

    img -= img.min()
    img /= img.max()

    msk = gaussian_filter(pha, sigma=20)

    recon[n,:,:) = img*msk*255

# -- write to disk
write_tiff_stack(recon,
                 overwrite=True,
                 fname=write_base,
                 start=0,
                 )

In [ ]: # quick sanity check
def peekrecon(n):
    fig, axes = plt.subplots(1, 2, figsize=(20,10))

    img = np.copy(recon[n,:,:])

    axes[0].imshow(img, 'gray')

    # plot the discrete rotation center

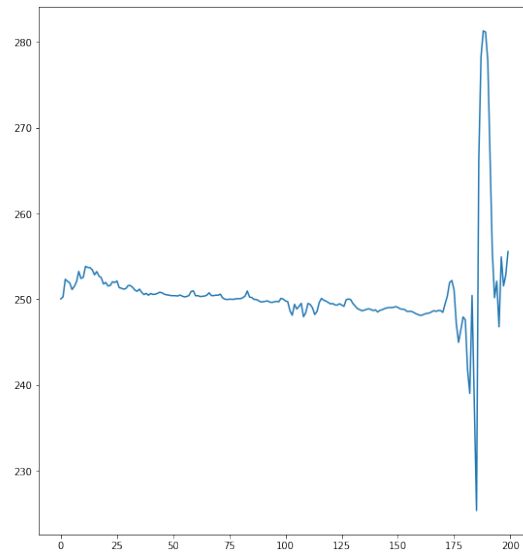
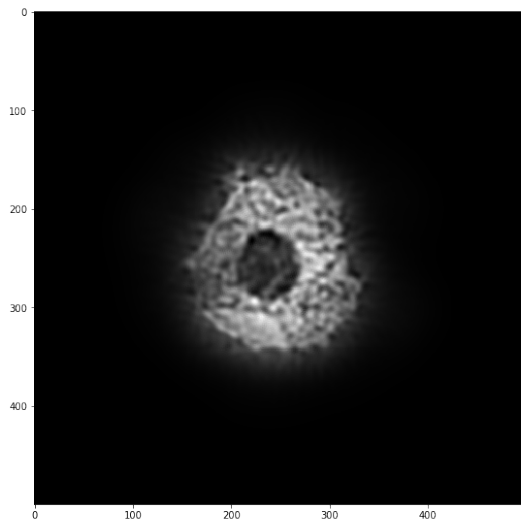
```

```
axes[1].plot(rotcnts)
```

```
# -- use the template
interactive_plot = interactive(peekrecon, n=(0, recon.shape[0]-1)) # still field

output = interactive_plot.children[-1]
interactive_plot
```

```
In [15]: # static view
         peekrecon(199)
```



1.5 Appendix

List versions of all the modules used in this notebook environment.

Note: Ensure reproducibility of the reconstruction results.

```
In [13]: # %load https://gist.github.com/kinverarity1/6038316/raw/loaded_modules.py
        '''List loaded modules and packages, and show their version numbers
        and/or Git repository's HEAD commit SHA.

        '''

        # Standard library modules
        import types

        # Third-party packages
        import git      # GitPython
        import os
```

```

def module_path(mod):
    '''Returns path to the file that module *mod* comes from.
    If it doesn't come from a file, return None.'''
    if hasattr(mod, '__file__'):
        return os.path.abspath(os.path.dirname(mod.__file__))
    else:
        return None

def from_git_repo(mod):
    '''Does the module *mod* reside in a Git repository?'''
    path = module_path(mod)
    if path:
        try:
            repo = git.Repo(path)
        except:
            return False
        else:
            return True
    else:
        return False

def git_path_sha(mod, slice=slice(0, 8, 1)):
    '''Return SHA hash for the HEAD commit for the repository
    that the module *mod* resides in.'''
    repo = git.Repo(module_path(mod))
    return repo.git_dir, repo.head.commit.hexsha[slice]

def module_version(mod):
    '''Return version string for module *mod*, or nothing if
    it doesn't have a "version" or "__version__" attribute.'''
    version = []
    if hasattr(mod, '__dict__'):
        keys = []
        for key in mod.__dict__.keys():
            if key.lower() == 'version' or key.lower() == '__version__':
                v = mod.__dict__[key]
                if isinstance(v, str):
                    version.append(v)
        if keys:
            print(mod, keys)
    if version:
        return ', '.join(version)
    else:

```

```

        return ''

def find_loaded_modules(only_versioned_modules=True):
    '''Return list of loaded modules for which there is a version
    number or a Git repository commit SHA.

    Return a list of *(name, version, path_to_git_repo, git_head_sha)*,
    which has an HTML property for pretty display in IPython Notebooks.

    '''

def list_of_lists_to_HTML(lists, header_row=None):
    '''Convert a list of a list of strings to a HTML table.'''
    s = '<table>'
    if header_row:
        s += '\n<tr>\n\t\t'
        s += ''.join(['<th>%s</th>' % item for item in header_row])
        s += '\n</tr>'
    for inner_list in lists:
        s += '\n<tr>\n\t\t'
        s += ''.join(['<td>%s</td>' % item for item in inner_list])
        s += '\n</tr>'
    s += '\n</table>'
    return s

class LoadedModules(list):
    '''Very simple wrapper for a list of lists of strings, with an attribute
    for display in IPython Notebooks.'''
    def __init__(self, *args, **kwargs):
        list.__init__(self, *args, **kwargs)

    @property
    def HTML(self):
        from IPython.display import HTML
        return HTML(
            list_of_lists_to_HTML(
                self, header_row=['Name', 'Version', 'Path', 'SHA']))

objs = LoadedModules()
for i, mod in enumerate(globals().values()):
    if isinstance(mod, types.ModuleType):
        if hasattr(mod, '__name__'):
            name = mod.__name__
        else:
            name = ''

        if from_git_repo(mod):
            path, sha = git_path_sha(mod)

```



```

else:
    path = ''
    sha = ''

version = module_version(mod)

if only_versioned_modules:
    flag = version or (path and sha)
else:
    flag = True

if flag:
    objs.append([mod.__name__, version, path, sha])
objs.sort(key=lambda r: r[0])
return objs

```

In [14]: find_loaded_modules().HTML

Out[14]: <IPython.core.display.HTML object>