Data analysis of Density measurements

Getting started :

On the current version, you have **MyDensity.py** (from MyDensity_development_29112023)

In a python terminal :

```
import sys
sys.path.append("/pathway/to/the/code/MyDensity/")


import MyDensity
md = MyDensity.Density()
md.setParameters()
```

USING INTERFACE :

```
######################################################################
DEFINE SETUP PARAMETERS FOR ACQUISITION AND ANALYSIS
######################################################################
```

Define the filename : Density_NMCLPSCl75_10

What is the sample diameter (in mm) : 1.2

What is the capsule diameter (in mm) : 2.5

Energy used for data analysis (in keV) : 37.7

Delta_E for data analysis (in keV) : 1

Initial guess for SAMPLE μ.ρ (g/cm^2): 7

Initial guess for capsule μ.ρ (g/cm2): .2

```
**********************************************************
LIMITING Ge ELEMENTS IN THE DATA ANALYSIS DUE TO THE ANVIL GAP
**********************************************************
```

counting with ch00 [y]/n ?

counting with ch01 [y]/n ?

counting with ch02 [y]/n ?

counting with ch03 [y]/n ?

counting with ch04 [y]/n ?

counting with ch05 [y]/n ?

counting with ch06 [y]/n ?

ANOTHER POSSIBILITY IS TO HAVE ALL PARAMETERS INSIDE BRACKETS :

```
md.setParameters(
filename = 'Density_PyroliteFe027_vertical_ref',
rsam = Sample_radius,
renv = Capsule_radius,
energy = Energy,
delta_E = delta_Energy,
mu_pho_abs = mu_pho_sample,
mu_pho_env = mu_pho_capsule)
```

Sample Geometry (mm)

Sample_radius = 1.8
Capsule_radius = 2.4

Energy parameters (in keV)

Energy = 22.4
delta_Energy = 0.5

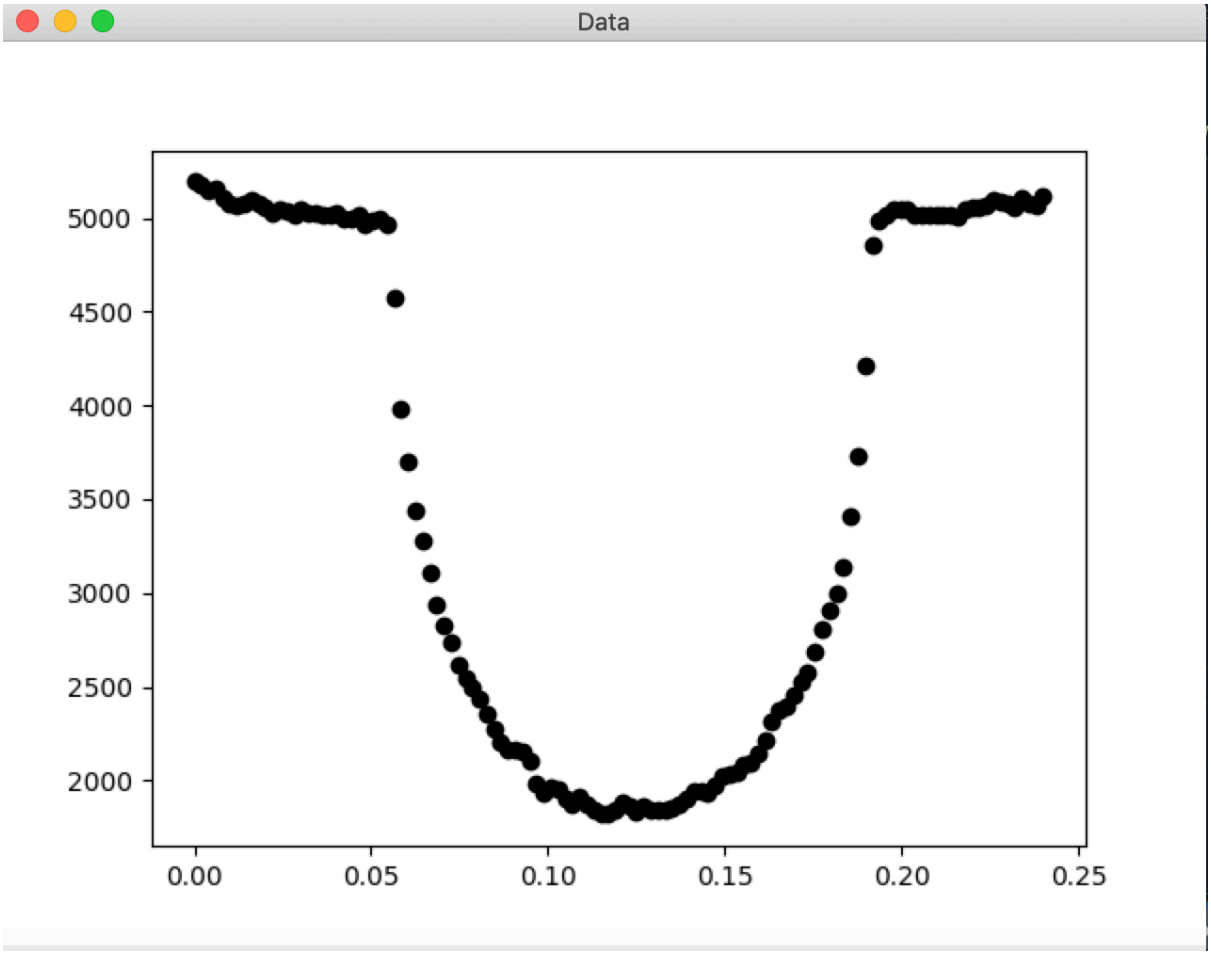
Estimated Value of mu_pho for sample and capsule
mu_pho_sample = 7
mu_pho_capsule = 2

```
md.setExpDir('/pathway/to/your/density/data/')
```

Loading data :

```
md.loadData()
```

#This will load the data from the md.setExpDir() and plot the absorption profile at the energy you put in the md.setParameters with the deltaE




```
md.crop(2, 3)
```

#This function can help you remove extra point outside the sample absorption that can cause problem in the fit. This is not mandatory as the capsule is also fitted. It is important to be consistent in your data treatment, which means that if you remove points in the first one, I suggest you always apply the same cropping to all the data from that run. The reason why is that you don't have a proper capsule with a known geometry and thus, we estimate that outside the sample, there is nothing (a.k.a I0). In practice, there is still the assembly part which is highly transparent to X-ray but still absorbs a few percent of the beam. If you crop differently, you impact the I0 from one data to the next one. We can discuss this more in depth if you want.

```
md.mirror()
```

#this is not necessary for you, it is for partial data acquisition which allows you to mirror the missing data.

To switch from different data file of the same run, you can use

```
md.nextPickle("new_file").                                    E.g.
: md.nextPickle('Density_NMCLPSCl75_11')
```

Fitting data :

```
md.function_fit()
```

#fits a cylinder and a capsule, fit the sample and capsule radius as well as the center of the absorption profile. I think this works quite well for your data

```
md.fit_trueGeometry(tomoFile = '0068_NMCLPSCl75_0_pag_512_512_128', extension = ".raw", tomoFilePath= '/Users/laurahenry/Library/Mobile Documents/com~apple~CloudDocs/Documents/soleil/Python/Density_dev/Thompson_0923/', dimZYX = [128,512,512], binning = 4, threshold_S = 10, pixelSize = 1.3, height = 0.1)
```

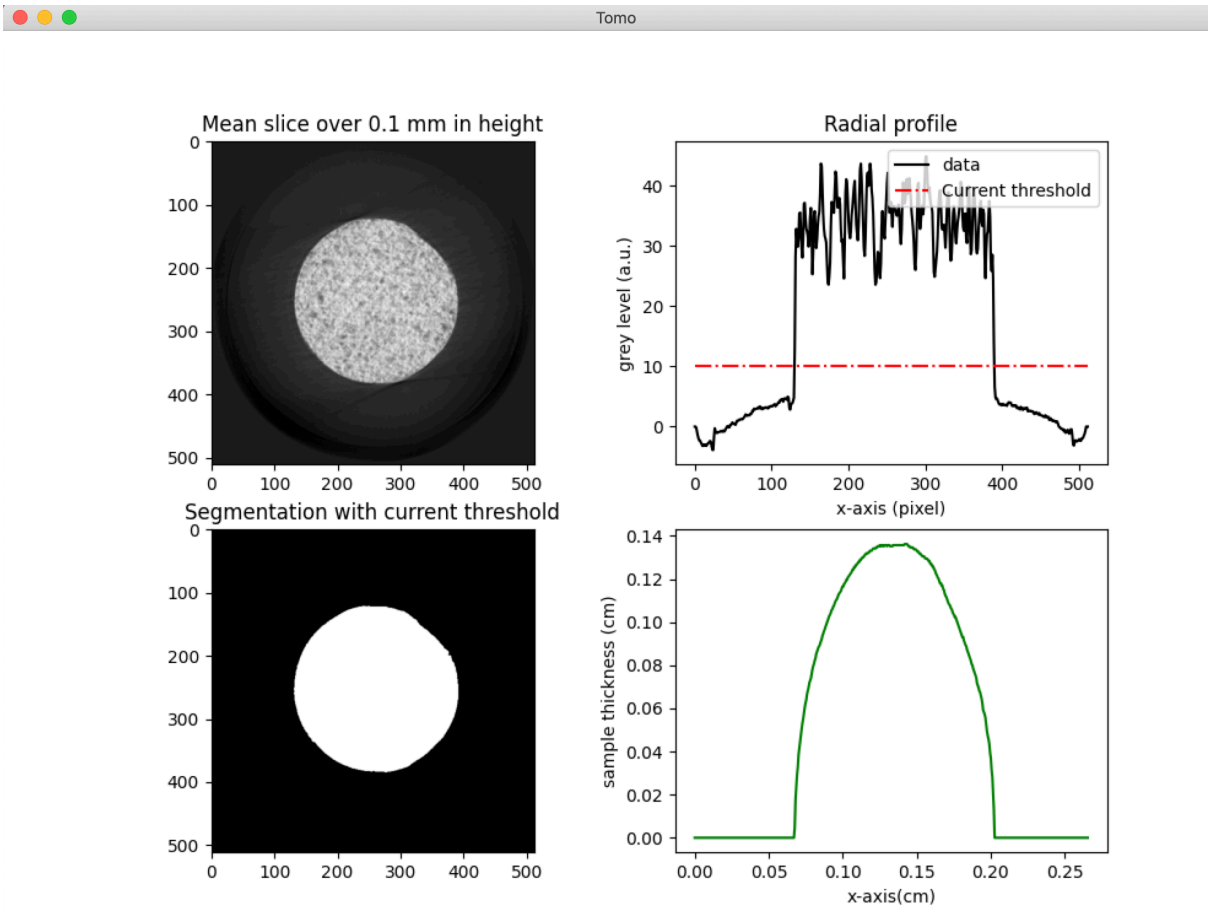
*#This is new, here are the args** of the function.*
***tomoFile** = 'name of the tomo without the extension'*
***extension** = '.vol' or '.raw' (needs to be float32 though if you're playing with the data before)*
***tomoFilePath** = '/pathway/to/the/tomo/file/'*
***dimZYX** = [dimZ, DimY, DimX] # size of your tomo data in Z, Y, X order*
***binning** = 1 (if this is not binned, or 2, 4 if you applied binning (to calculate new PixelSize)*
***threshold_S** = 10 (to threshold sample from environment and build geometry profile, this can be estimate by you after the first iteration, see below)*
***pixelSize** = 1.277 (from your experiment I believe)*
***height** = 0.1 (slit vertical gap for density measurement to select only the slices corresponding to the density).*

This gives you :
1 – Estimation of the density using the function_fit(). We keep the capsule size and absorption and r0 and reimplement with the new geometry.

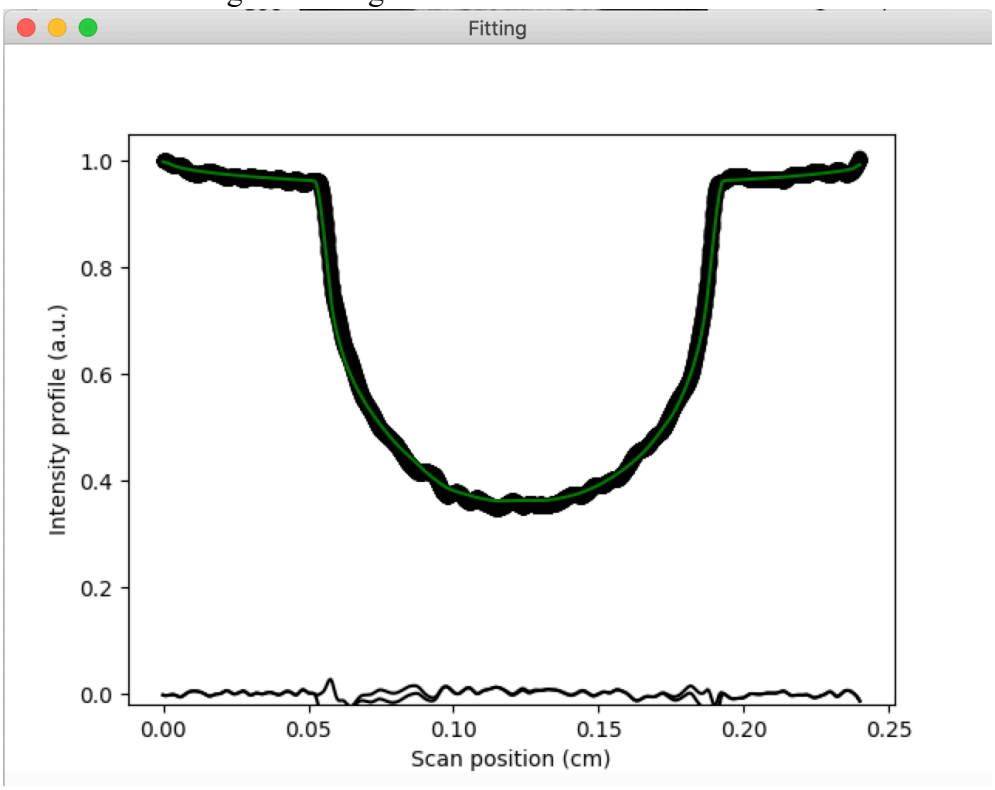
```
Fitting...# With the assumption of a cylinder
Standard deviation of residual is :  0.744 %
mu*pho(sample) =  7.528
mu*pho(capsule) =  0.189
sample radius(microns) =  665
capsule radius (microns) =  1217
```

2 – Tomo figure that build the profile as below

```
Now processing :  0068_NMCLPSCl75_0_pag_512_512_128
Building the average slice
Starting segmentation...  with sample threshold =  10
Building absorption profile with current threshold
```



3 – New fit on the same figure “fitting” :



Standard deviation of residual is : 1.185 %
mu*pho(sample) = 7.317 (**fitted** at this stage)
mu*pho(capsule) = 0.189 (not fitted at this stage)
offset r0 (cm) = -0.008 (**fitted** at this stage) (mismatch in x-axis between scan tomo et scan density)
capsule radius (microns) = 1217 (not fitted at this stage)