SAXS_toolbox Tutorial

I. Introduction

This tutorial is based on SAXS data acquired on a Xenocs/Xeuss2.0 device equipped with a Pilatus 1M detector from Dectris. In this tutorial, we will process SAXS data corresponding to nanoparticles dispersed in hexane.

The data set contains the transmission and scattering data for :

- water, used for intensity calibrations

- hexane used as reference

- 6 samples of nanoparticles.

Table 1 gives the correspondance between file numbers and type of measurements.

Empty beam		I0=22.89MPh/s
Calibration	Reference	4
	Calibrant	5
Sample	Reference	8
	sample files	14-19

Table 1 : Correspondance between file numbers and type of measurement

II. Procedure

I. Preliminaries

I.1 Set working directory

As a start, use **Menu/set Working Directory** to define the path to your data files. From now on, the program will use this directory as default path.

I.2 Check/perform detector calibration and transmission data

Before starting the data reduction, it is good practice to check wether the meta data from data file contain the calibration information and transmission data.

To do so, you can open an image using **Inspect Data/Open and view image,** and select a data file from your data set (in our case we use frame 005.edf). Check for the presence/absence of calibration information. If calibration information are present, take note of the text keys giving access to the following items: wavelength, distance, beam center coordinates, frame size, pixel size and TransmittedFlux. Fill the “Experiment Description” tab with the corresponding keys, select an image from your dataset, and click on the “Apply Calibration and generate poni file” button (see

Figure 2). Note that default text keys should correspond to most Pilatus detectors (SWING @ SOLEIL, SAXS @ LGC,…)

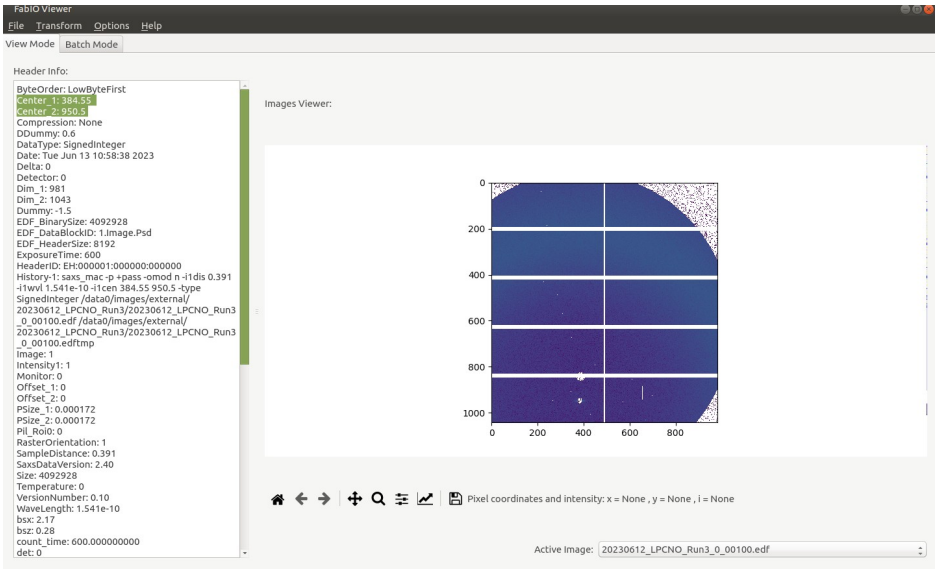


Figure 1 : Fabio_viewer interface and visualization of meta-data

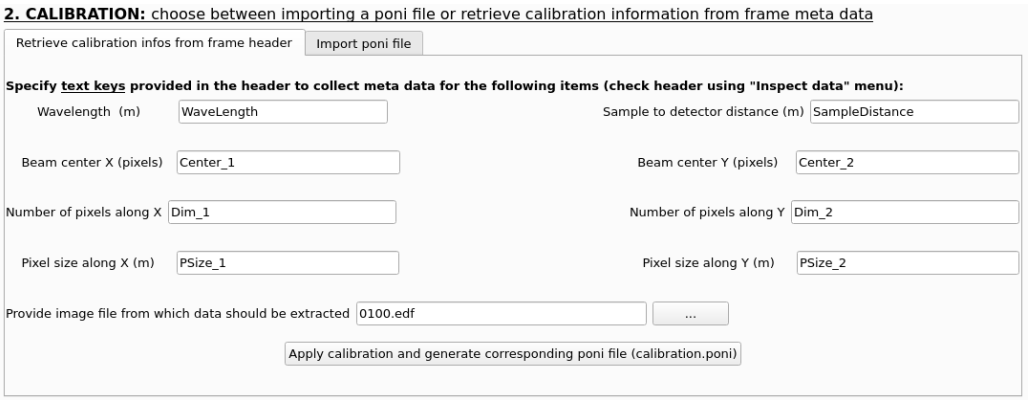


Figure 2: Calibration of images with meta data

When the calibration information are absent, it is necessary to perform the calibration using **pyFAI/Detector Calibration (**see SAXS_toolbox documentation for more details). In this step, a poni file can be creat”ed and further imported in SAXS_toolbox using the ‘Import poni file’ sub tab shown in Figure 3. Additional information such as apparent pixel sizes (different from physical pixel sizes if binning is performed to reduce the size of the datafile) and frame dimensions must be provided by the user. A good knowledge of the instrument is therefore required. This step is usually performed while reducing data from other sources (e.g. ESRF, Soleil,...)

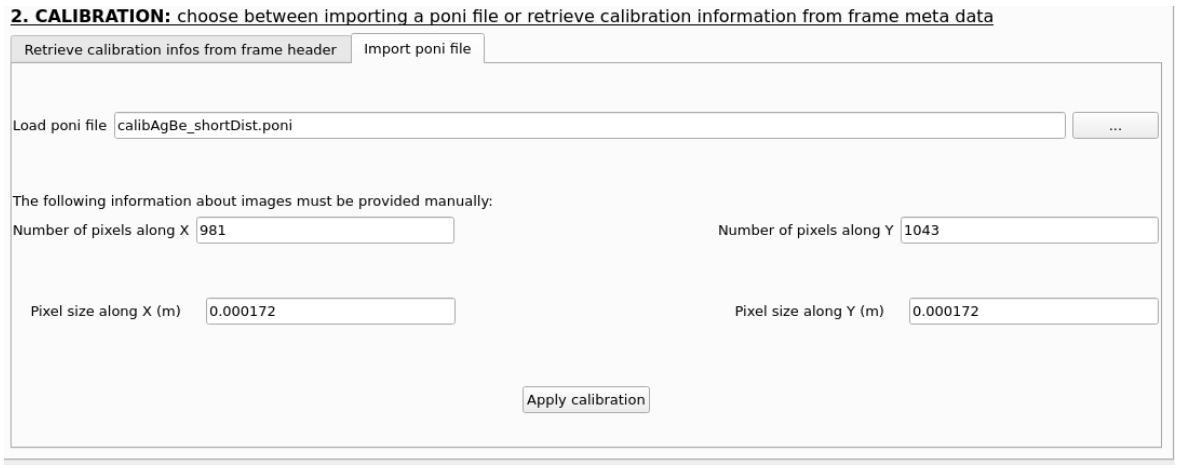


Figure 3: Calibration of data with a poni file

I.3 Generate mask and load it

A last preliminary step consists in providing a mask file, either using an image file via **pyFAI (pyFAI/Generate mask/using an image file),** either through the conversion of a foxtrot mask file **(pyFAI/Generate mask/convert foxtrot mask file)**.

In this tutorial, no mask file is available. Activate the function **pyFAI/Generate mask/using an image file** and select file 0018.edf (hexane measurement) to generate the mask. Here we select the file that contains a scattering signal as homogeneous as possible, in order to detect easily the bad pixels.

Perform the following steps

- mask below 0 intensity (automatically masks the dead zones of the detector + some of the dead pixels – but not all of them)

- create a circular mask around the beamstop

- use pencil tool to mask additional aeras (remaining bad pixels, shadows,…)

- inspect the frame using zoom tool and seek for bad/dead pixels

- use polygon tool to mask the shadowed areas in the frame corner

- save your mask in edf format by clicking the disk icon and then « Save mask and quit »

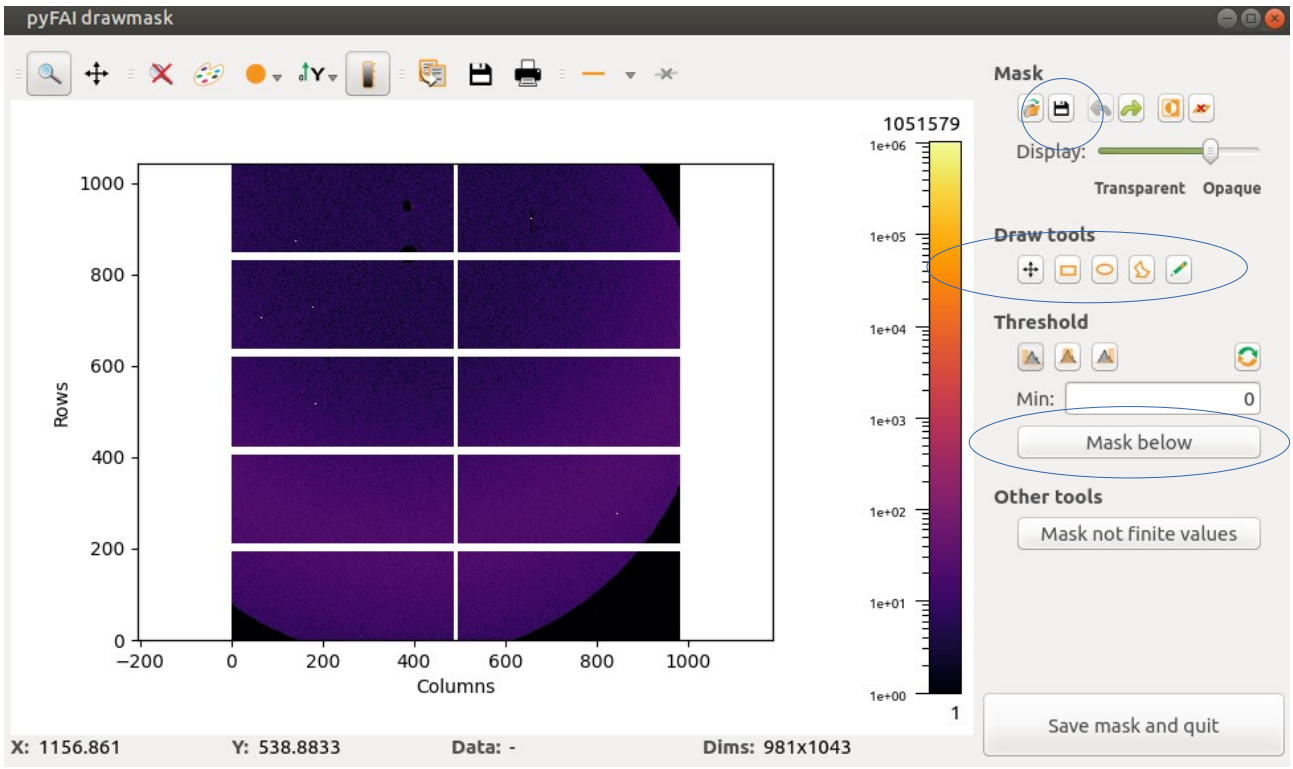


Figure 4 : pyFAI drawmask interface

After edition, the final mask shoud look like the one visible in the figure below :

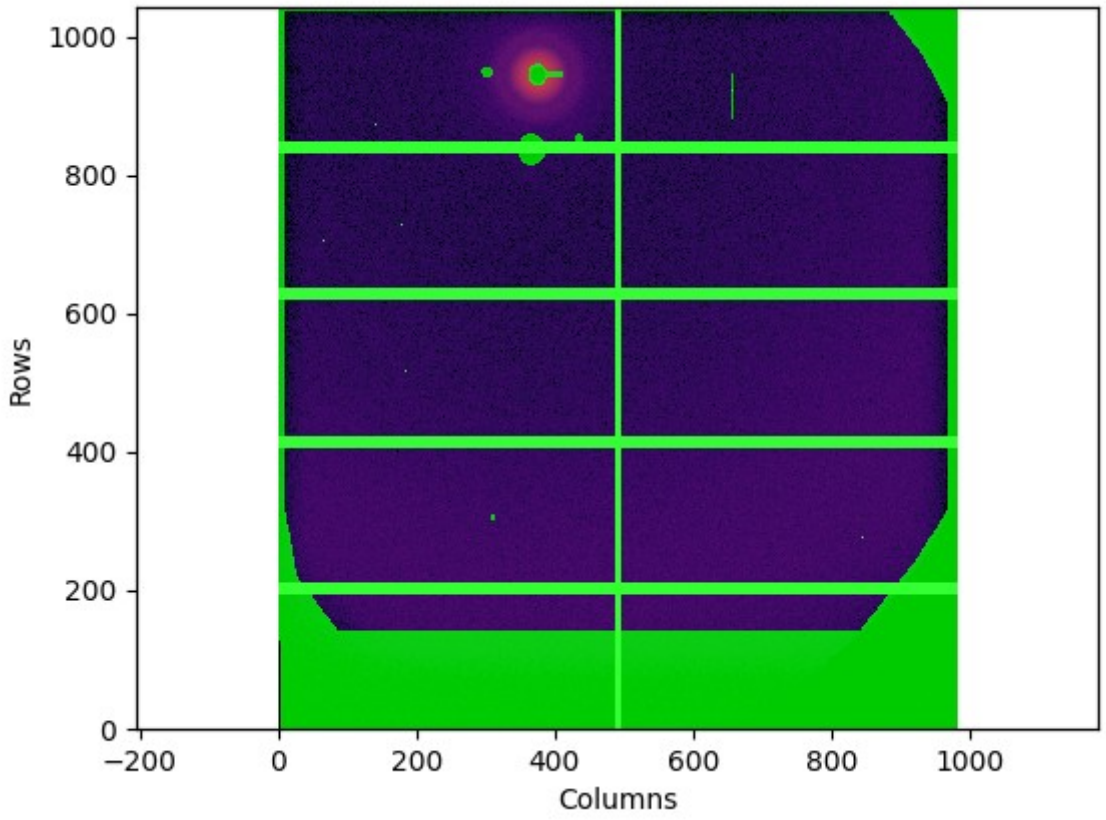


Figure 5 : View of the mask generated with pyFAI

Once the mask file is generated, load the mask file in the tab Experiment Description from SAXS_toolbox interface.

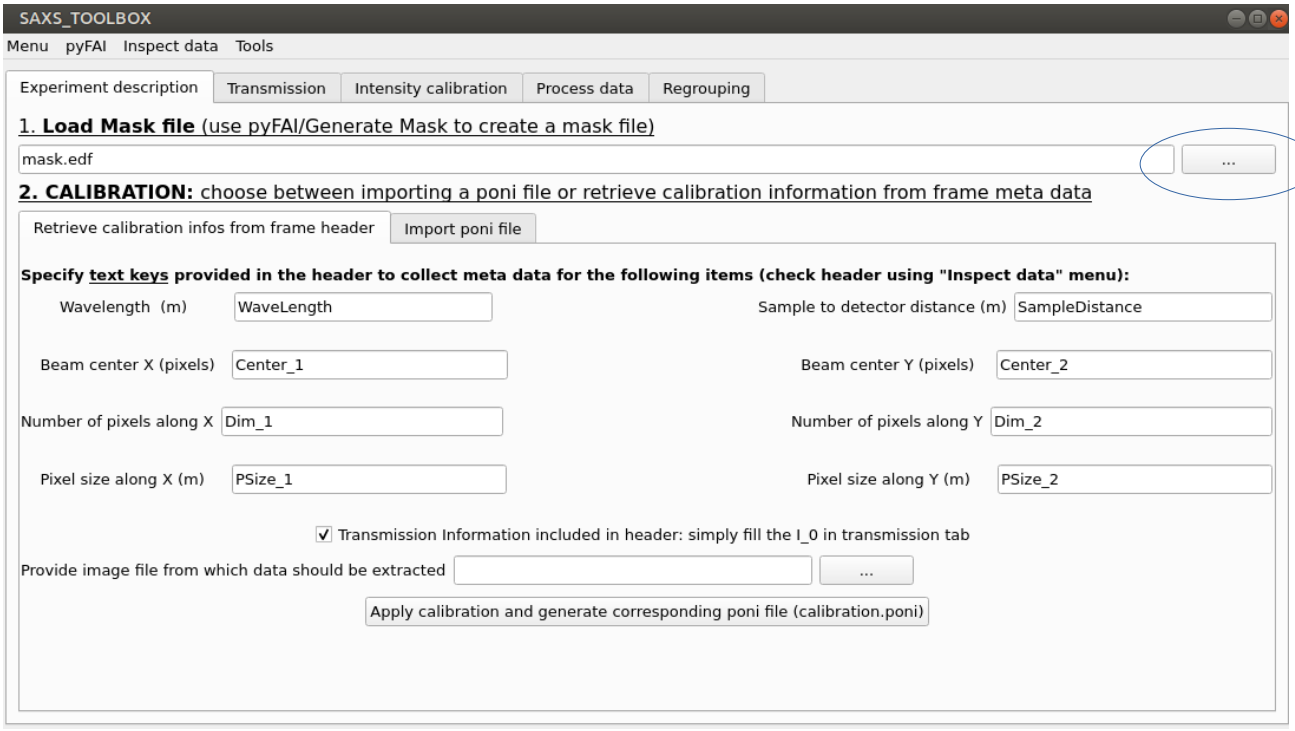


Figure 6 : Experiment description tab: load mask file + optional .poni file

When the mask is loaded, a confirmation message appears in the console (note that an error message also appears when the mask file is not provided)

II.2 Provide correction information

II.2.1 Transmission tab

In the « Transmission » tab, fill the I_0 field with appropriate value (here I_0=22.89*$10^{6}_{ph/sec.}$). Since transmission data is contained in the frame header, the remaining transmission values will be automatically updated as data files are loaded in the software.

II.2.2 Intensity calibration

In the intensity calibration tab (see Figure 9), select the water as a calibrant by checking the corresponding box.

Load data files corresponding to empty cell (file 0004.edf) and calibrant measurement (file 0005.edf) in the corresponding fields.

Click on the « Calculate calibration coefficient » button. During the computation, detailed information, such as mean intensity and standard deviations for each frame, are given in the console window. A small standard deviation (compare to mean value) indicate a good measurement statistics. In the provided example, the standard deviation is rather high due to insufficient exposure of the calibration measurement.

Figure 9 shows typical output of the intensity calibration, The most important bieng the calibration coefficient.

After computation, the calibration coefficient field is updated with the calculated value. Note that if you have already performed the intensity calibration for this experimental setup, the calculated value can be directly typed in this field. In this cas, there is non need to repeat the intensity calibration process, neither to provide transmissions files required by intensity calibration.

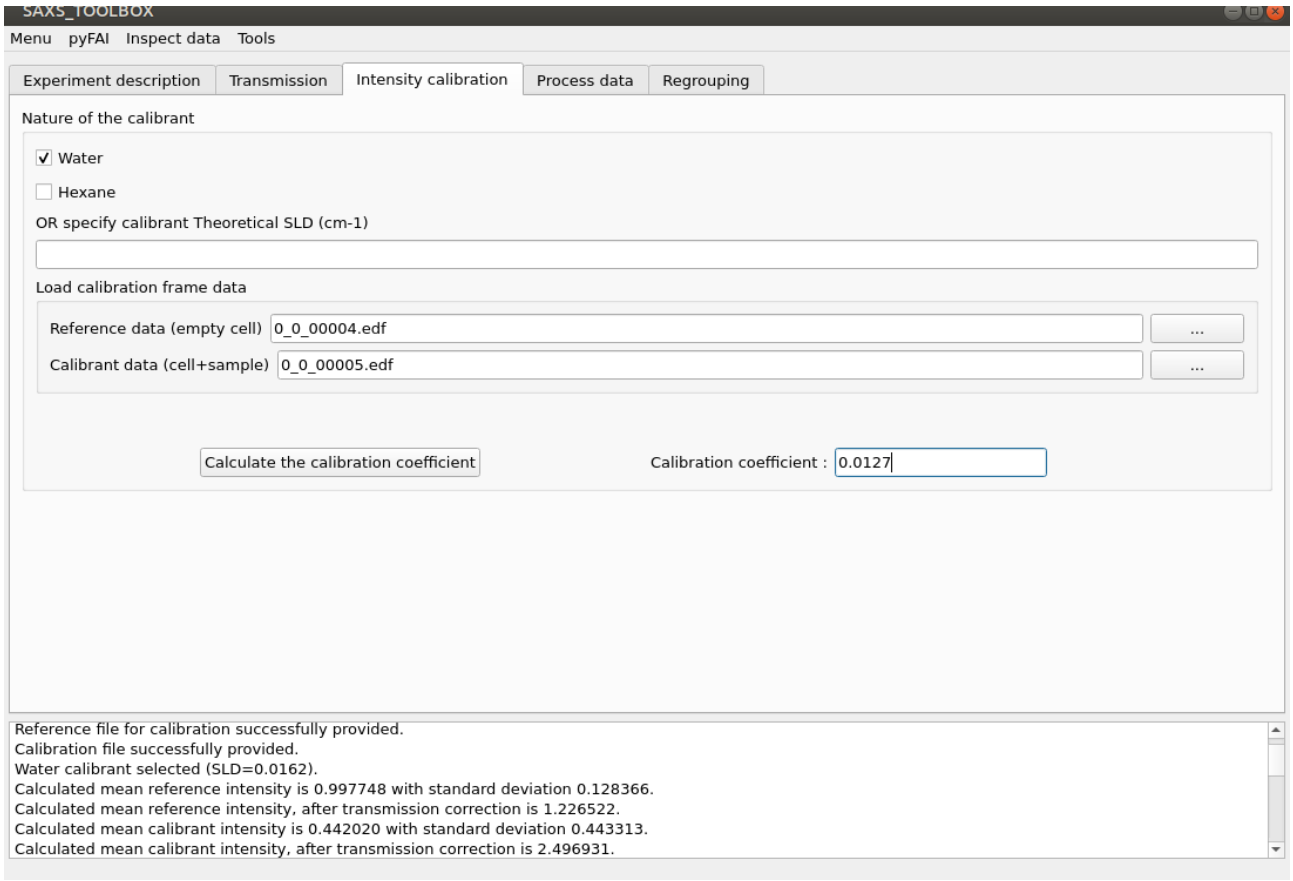


Figure 8: View of the intensity calibration tab

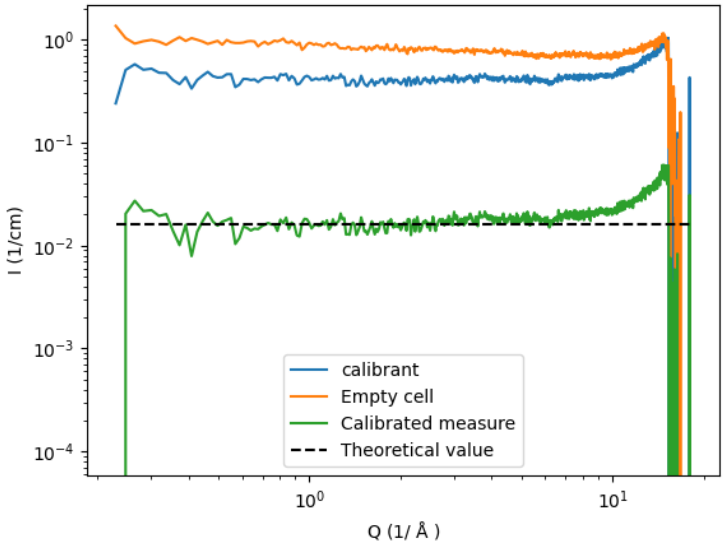


Figure 9: View of the intensity calibration results

At this stage, data are ready to be processed.

II.3 Process data tab

In this tab, the user can specify which files to use as a reference file (file 0008.edf- single file selection is possible), and which file(s) to use as specimen scattering data (files 0014.edf to 0019.edf). As there might be some dispersin in capillaries suzes, check the « Refine reference subtraction » magic box.

To process the data, simply click on « Process data » button. Corrected frames are saved in the destination folder : working_directory/corrected_edf_files.

OPTIONS :

Note that an option is available to skip reference substraction. In that case, all transmission values should be set to 1 (click the button « Set sample transmissions to1 »).

If the user wants to generate *.dat files in the Qx,Qy,I format (for input in sasview for instance), the checkbox « Convert edf to Qx,Qy,I for input in sasview » should be checked. This computation is time consuming, and should be performed only when necessary. 2D data files Qx,Qy,I are stored in working_directory/2D_dat_files

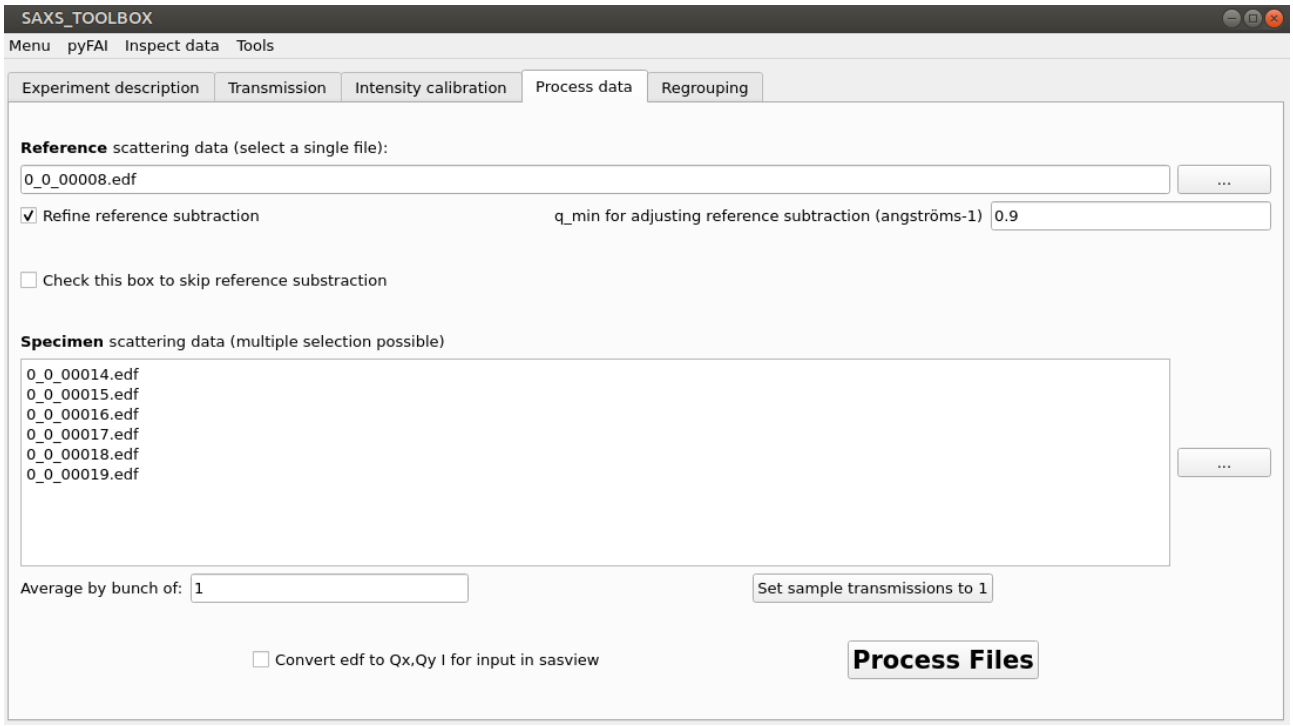


Figure 10: View of the process data tab

II.4 Integrate corrected frames

Data can be integrated using the « Regrouping tab ». For simple radial regrouping, simply click on the « Select, plot, and save file(s) » in the « Radial regrouping on the full azimuthal range » section.

1D data files are automatically stored in the working directory.

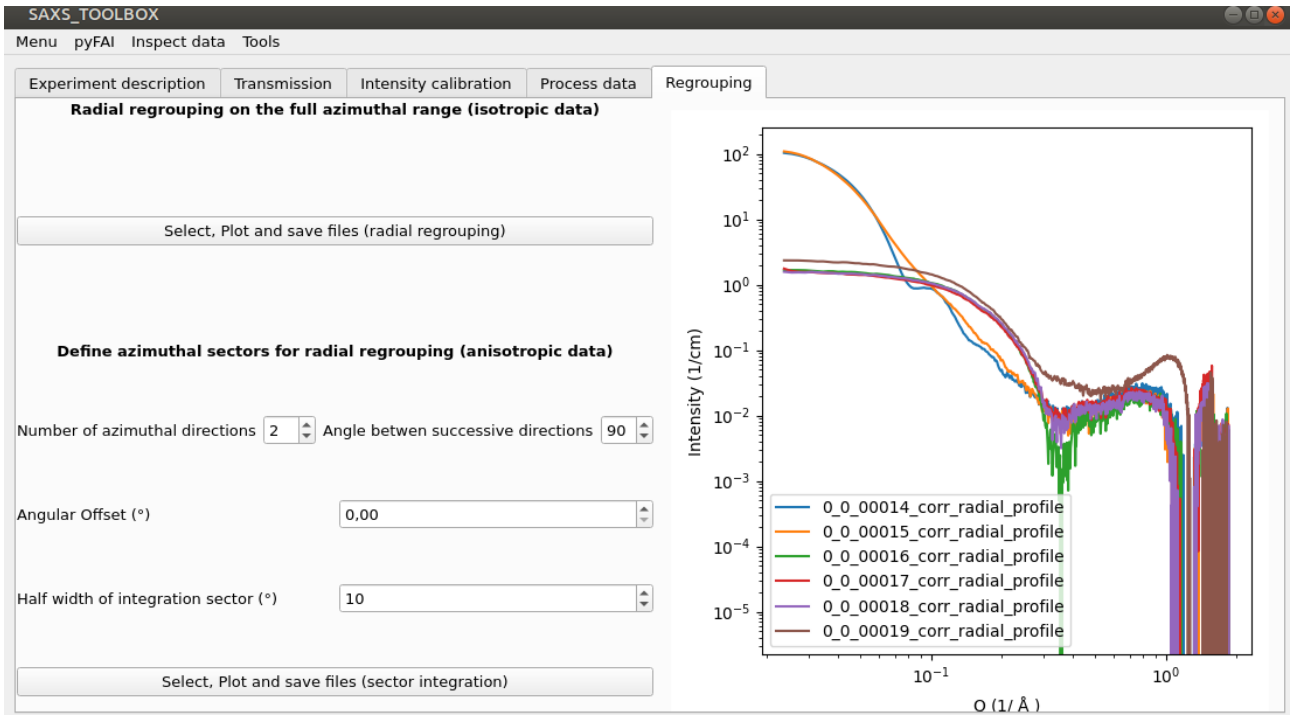


Figure 11 : View of the regrouping tab

III. Processing anisotropic data

The procedures for producing corrected and calibrated images is the same as the one described for isotropic cases (see chapter I and II).

In this tutorial, we will use an example of anisotropic data to test the cave function and sector integration. The corresponding file is 0029.edf. Since another setup is used, another mask file can be created using pyFAI/GenerateMask. It can be a good exercise for you to bluid the mask. In case you don't have the time, the corresponding mask file is « mask_medDist.edf », in the tutorial folder.

III.1 Caving function

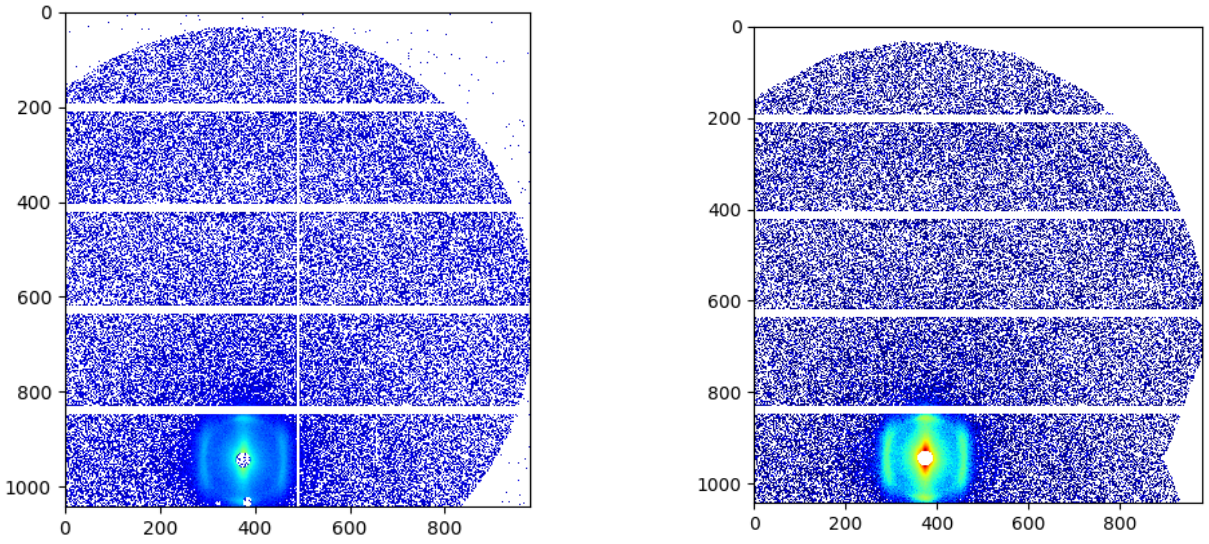
Caving allows to rebuild masked zones from an image, assuming horizontal and vertical symmetries on the scattering data. Given a masked pixel, the algorithm will seek fo a symetrically equivalent one to give a masked pixel an intensity value. It is therefore useful to remove dead zones from detector, bad pixels,...

The procedure is the following :

1. Provide a mask file in the « Experiment Decription tab »

2. Click in the menu Tools/cave_frames and select files you want to process

Resulting files are created in the working directory. The file names contain the suffix _cave.edf



a) before caving b) after caving

Figure 12 : Influence of caving on images (disparition of beamstops at the bottom, and vertical detector dead zone)

III.2 Sector regrouping

We will now perform vertical and horizontal azimuthal regrouping on the image produced after caving. We must therefore create a new mask corresponding to caving, using the menu PyFAI/GenerateMask/using an image file. The image used to create this mask is obviously the 0029_cave.edf file. Simply click on Mask Below 0, and save mask. This mask is saved as « mask_medDist_cave.edf »

The procedure for sector regrouping is the following :

0 (optional) : create mask

1. Load mask in the experiment descritpion tab

2. in the « Regrouping tab », click on « Select,plot and save files (sector integration) » in the bottom section entitled « Define azimuthal sectors for radial regrouping (anisotropic data)