


## SAXS USER BASICS

X-Ray generator is already ON (photo +



Computers are ON and softwares open (python , experiment.py)  
Control box on External

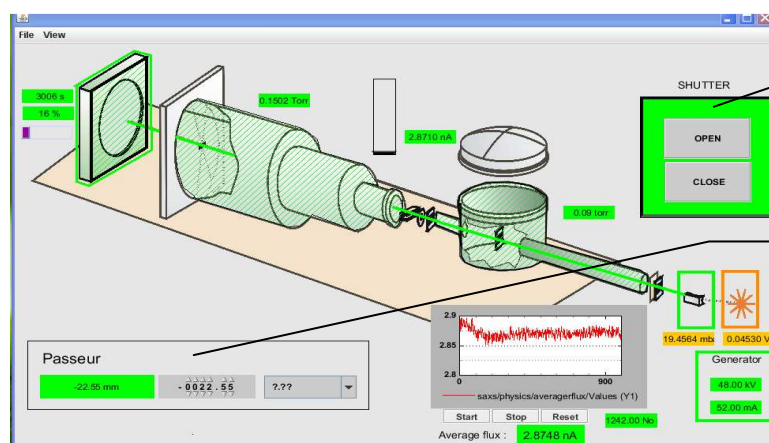


### Computers

- SAXS computer (left) : to conduct SAXS experiments

Python shell (Idle) = commands for acquisition with python

Synoptic = where the current values (transmitted flux, generator state, time left for experiment, etc) are displayed :



Command to open/close the shutter

Command to move the sample holder to a defined position

- MAR computer (right) : dedicated to the detector

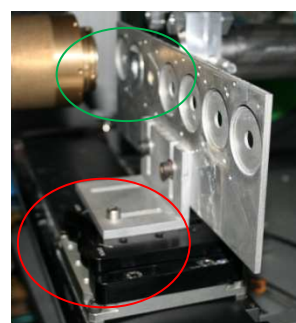
ATK panel displays the last image scanned. Raw images are saved in the computer (***data/mar/images***)

Green = ready; blue = scanning or erasing; yellow= not ready (need to reset)

- TANGO computer (back of the room): to treat the data with *ImageJ* and *GUI SAXS*

### Setting up samples

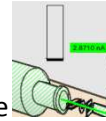
Lock/unlock carefully the sample holder (set position 120 mm = base closest to the user), screw/unscrew the vacuum "nose" to minimize the air thickness between sample and vacuum chamber.



Position 120 mm

## Running an experiment

- Place the sample holder containing your samples and/or references, close the door.



- Open the shutter (control the flux on the photodiode).
- If necessary use ScanPosi to find the exact position for “empty”, references and/or your sample :
  - o In Python Shell, write and `return` to run :

```
From experiment import *
scanPosi(type here the min position, type here the max position, type here the step)
```

- Open a previous script (Python Shell **file/open/recent file**) and save it under your initials (then overwrite for each modification).

### script\_MODELE.py

```
from experiment import *

#measure transmission
measureTempty(68,200)

#erase mar
saxs.mar.erase()

#start
count("samplename",3600,position=71.39,init='CG')
#count("Lupolen",1800,position=pos5,init='CG')

#measure transmission
measureTempty(68,200)

#erase mar
saxs.mar.erase()

#saxs.mar.off()
#stopGeneX()
#end
```

*Fill in empty position and counting time (s)*

*Fill in sample name, counting time (s), position (mm), user initials → generate the filename  
CG-2010-03-19-samplename-3600s*

*If necessary add command lines for other references or samples*

*Fill in empty position and counting time (s)*







*#count("Lupolen",1800,position=pos5,init='CG') → red= comment not read by TANGO*

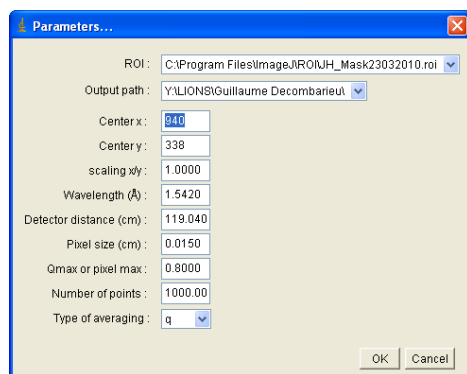
- **Run/run module** to run the experiment

**CRTL C to stop the running module**

- **Write the experiment parameters for each sample in the SAXS notebook**, together with the incident flux (“empty”) and the averaged transmitted flux displayed in the Python Shell window.

## Treating the data

- On MAR computer : copy-paste image file from **data/mar/images** to **laborx/communs/SIS2M/lions/saxsdata/saxs/mar** (password needed)
- On TANGO computer : Open ImageJ , **file/open** the image file
- **Image/look up tables/royal** and **Image/Adjust/Color Balance** to adjust the image
- **For the first reference (calibration in q-range) :**
  - o Adjust the center of the image  (around x= 940, y= 338)
  - o Define a mask , in ROI manager, open the most recent mask in **program file/ImageJ/ROI**, check the limits of the mask. To modify : right click/ **split**, delete previous one, use  to move the points, **update** , then right click/**combine**, create , then save under a new name.
  - o Radial average on q  :





Check mask file and output path to save the .rgr file

Detector-sample distance calibrated with the reference for q-range (octadecanol or tetradecanol)

 **creates a .rgr file**

- **For all the following images :**

Just open the image and radial average on q  (the parameters and the mask have been defined already).

With GUI SAXS  (scaling and normalization)

- open your .rgr file(s)
- **select** the data to be scaled, **Data treatment/SAXS/scaling**, open a previous set of parameters:

**SAXS Scaling Parameters**

Filename : Y:\LIONS\Camille Guio\param.par

Wavelength (Å) : 1.542

Detector to sample distance (cm) : 119.04

Pixel size (cm) : 0.015

q by pixel (-1 if not used) : -1.0

Exposition time (s) : 1800.0

Background by second : 0.00062

Background by pixel : 14.55

Total background (B by pixel + B by s \* time) : 15.666

Comment : 1.0

Incident Flux : 17.34

Transmitted Flux : 8.45

Transmission : 0.487312572088

Thickness : 1.0

Delta Omega : 1.58780323231e-008

K constant : 4647000.0

Total Flux = Incident Flux \* K (ph/s) : 80578980.0

Scaling :

☐ Scaling Q range

☒ Scaling I range

Data to apply scaling :

Data to apply scaling : CG-2010-03-31-kapton-1800s\_raw2000.rgr

Select data for background :

Select data for background :

Buttons: Compute, Apply, Save, Close

Fill in **exposition time, incident and transmitted flux** and check that the other parameters are correct, then click **compute** to automatically calculate internal background and transmission

K constant is defined by the intensity calibration with lupolen

Tick Scaling I range and **Apply** to generate the scaled curves

- Calibration : check the  $q_{\max}$  position for the references in q-range (octadecanol =  $0,1525 \text{ \AA}^{-1}$  tetradecanol =  $0,1583 \text{ \AA}^{-1}$ ), and the maximum intensity for the reference in intensity (Lupolen,  $6 \text{ cm}^{-1}$ ) (q-range is calibrated through the sample-detector distance and intensity is calibrated by K constant).
  - perform operations on curves (background subtractions, thickness normalization, etc)
- Edit/calculator**
- Save a .txt file for the ticked data (**file/save**), that can be later treated with excel, or save the set of data (**file/save all**) to open them later with pysaxs.