1. Enter your user session

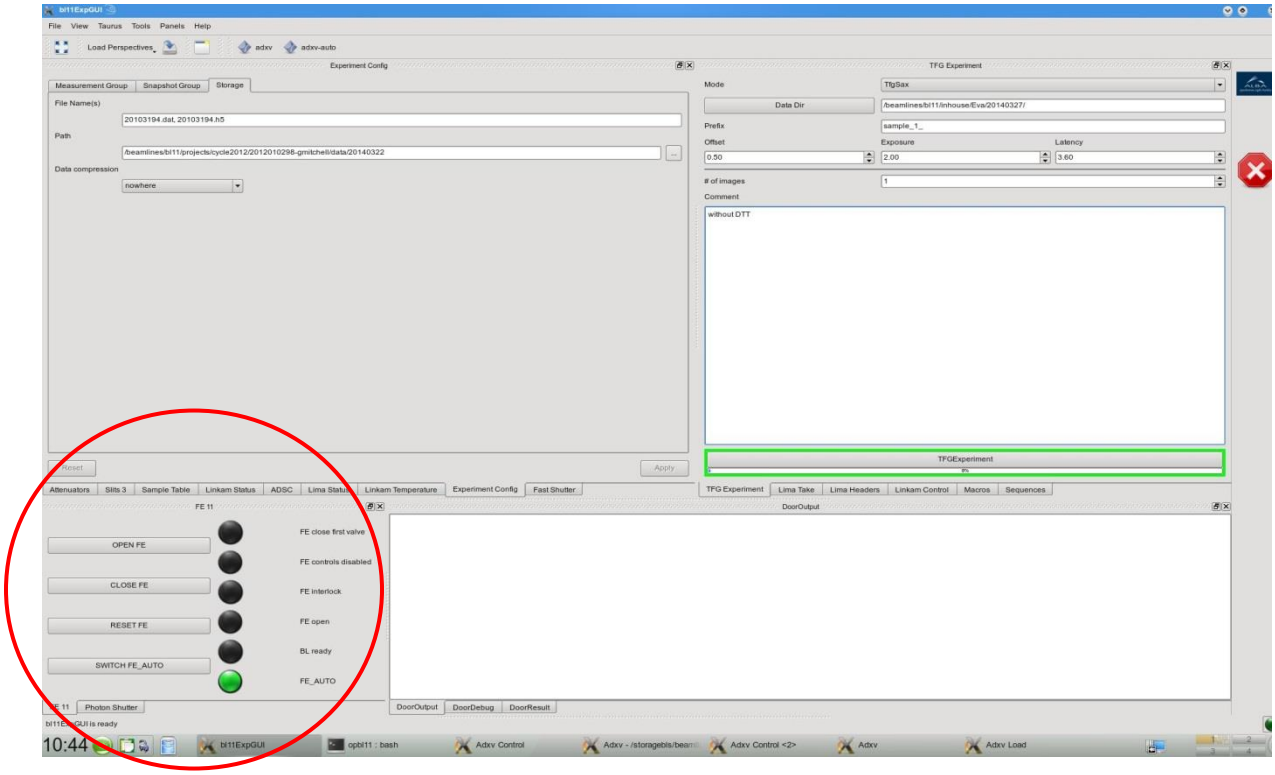
Enter the session with your user name (e.g. u2013030293) and password (you will be asked to change the default password; your local contact will help you to set a new password).

Once you have entered your session, click on the ALBA icon (normally at the top left of the desktop). A console named Experimental GUI (bl11ExpGUI) will open. This is a friendly user interface to perform your experiments.

You can also open bl11ExpGUI from a new terminal by typing `bl11ExpGUI` and pressing Enter (see **Section 1.3 – How to open a new terminal window**).

The Beamline is composed of an Optics and an experimental hutch. All elements that define energy, beam size etc… are located in the Optics hutch (OH). Users are not allowed to enter this part of the beamline. Samples are loaded on their holder in the experimental hutch (EH). A front end shutter located in the tunnel is normally always open except during reinjection (when in not top-up mode). Another shutter (Photon shutter, safety shutter or PSUH) located at the end of the optic hutch must be closed before entering the experimental hutch. The software bl11ExpGUI allows the users to open or close both shutters.

1.1. Front end tab

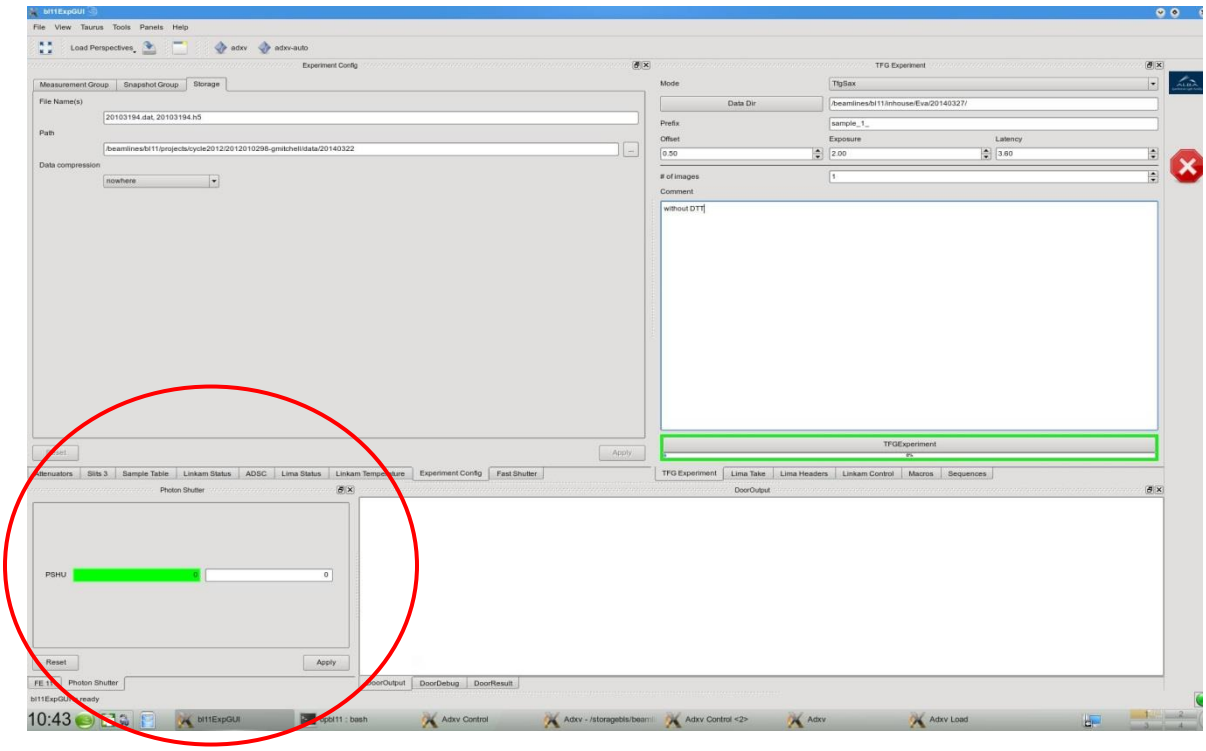


The front end (FE) must open before starting your experiment (FE open). For optimum stability in OH components, it is recommended to wait 20 minutes before you start your experiment once you open the front end. A lead light in green indicates that FE is open. You can also check the machine status in the big screen in the control room.

You can only open the front end when the beamline is ready (BL ready) indicated by a green light. If the light is black, call your local contact.

Front end auto should be enabled (**FE_AUTO**). A green lead light at the bottom of the panel indicates when this option is enabled. This means that FE will open automatically after the reinjection. If **FE_AUTO** is not enabled, you can do it by clicking **SWITCH FE_AUTO** and Apply. Nevertheless, if FE doesn't open due to unknown reason, call your local contact.

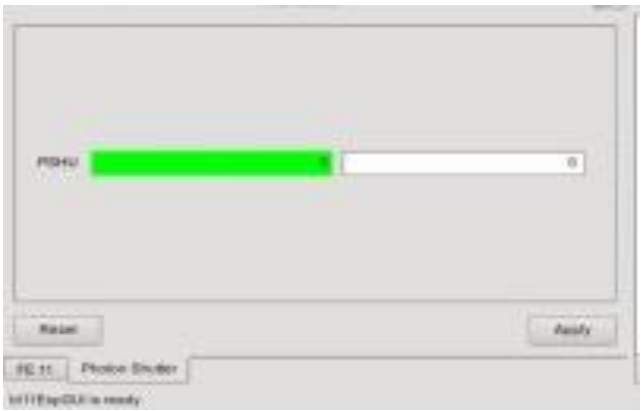
1.2. Photon shutter or Safety Shutter (PSHU)



The Photon Shutter or Safety Shutter (PSHU) is a safety element located between the Optics Hutch and the Experimental Hutch. You need to open it in order to let the beam enter the Experimental Hutch and hence be able to perform experiments. Please note that you do not have permission to open the PSHU unless you have interlocked the Experimental Hutch.

Once the Experimental Hutch is properly interlocked, print 1 into the right white box (input value) and press enter. The value inside the left box (readback value) will change from (0) to (1). The PSHU is only open when the readback value is 1.

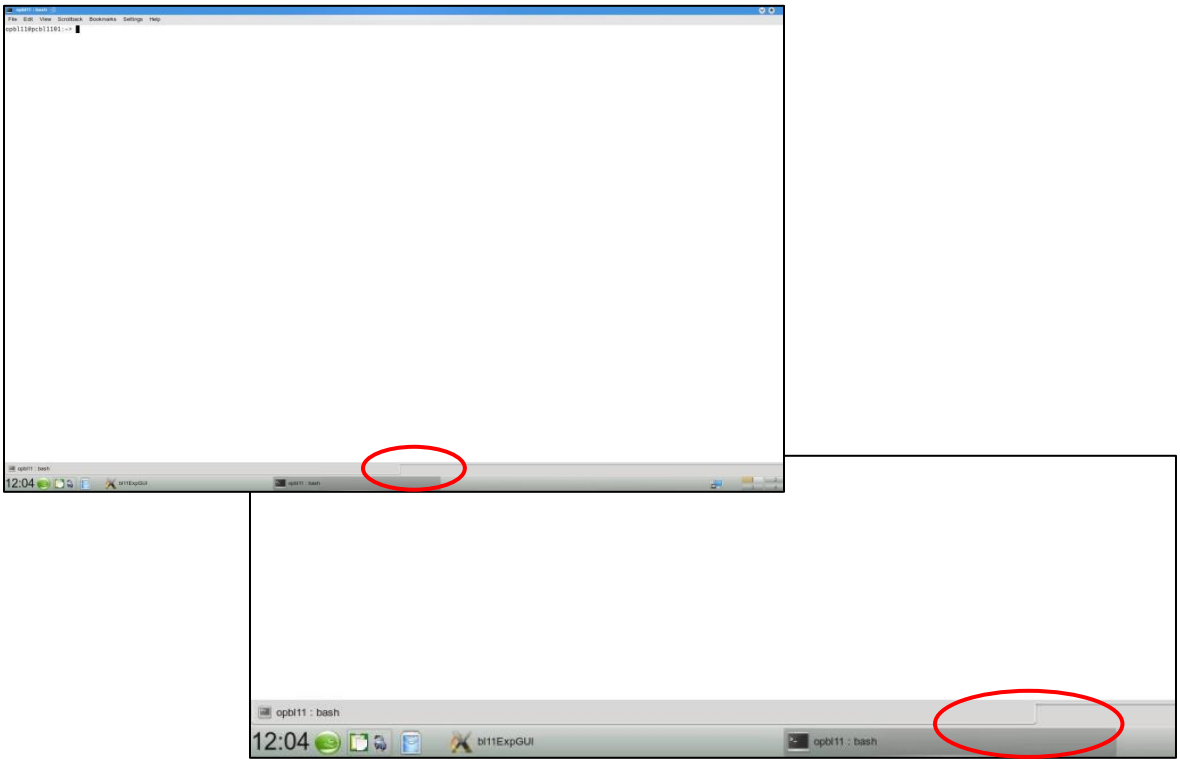
To close the PSHU, input 0 into the right box and press enter. The value inside the left box (readback value) will change from (1) to (0). This means that the PSHU is closed and you can open the Experimental Hutch.



1.3. How to open a new terminal window.

Click on the icon displaying a green chameleon circle at the bottom of the screen. Click on it to open the **Application Launcher**. A list of applications will appear. Click on the icon displaying a screen with a symbol like this: >_

A new terminal will open. You can add more terminal windows by repeating the same procedure or if you prefer to open just another tab in the same window you need to doucble-click at the bottom of any open terminal:

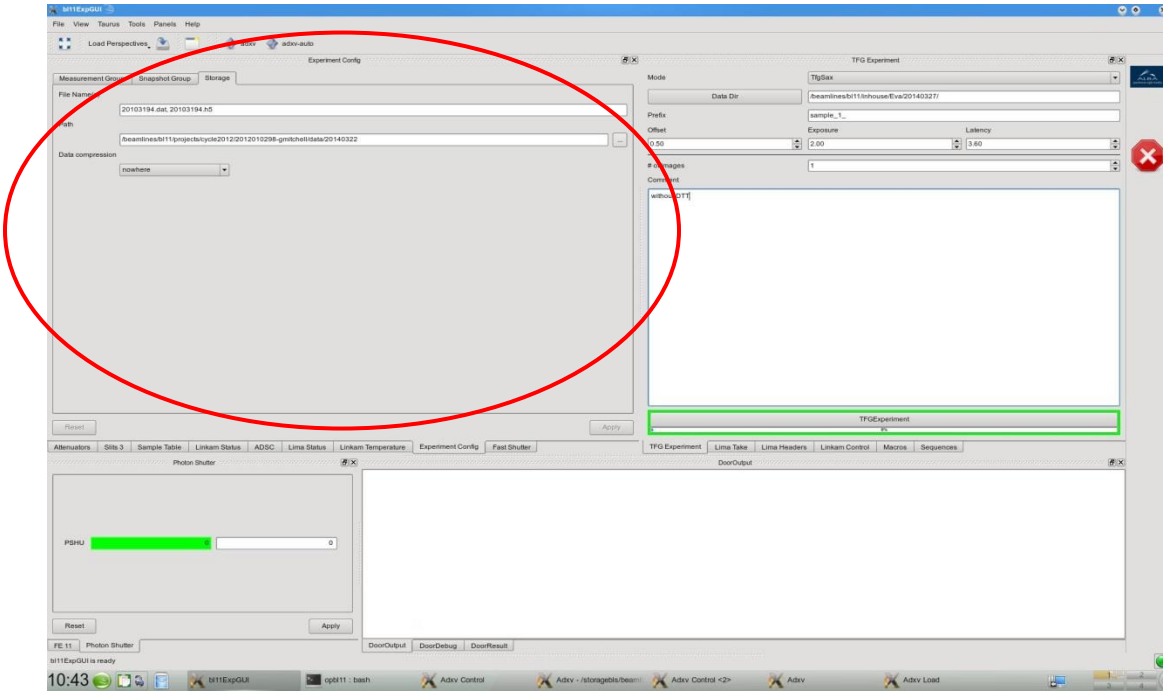


2. Data storage

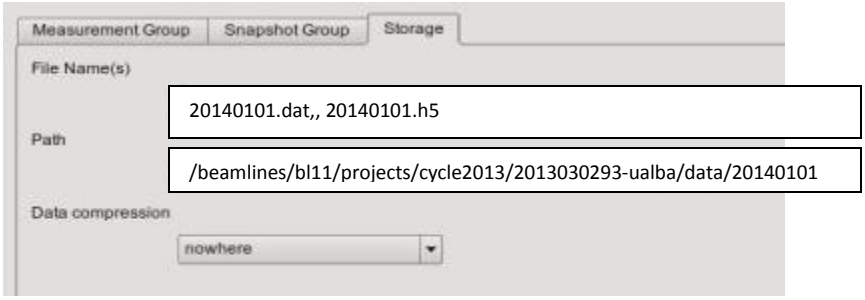
Your images can only be stored in the “DATA” folder or its subfolders of your directory. You have two ways of creating your directory, also including folders and subfolders.

2.1. Defining storage directory using the ExpGUI console

Go to the storage tab:



In the “File name(s)” field, type a useful file name (e.g. date of the experiment) with the extensions **.dat** and **.h5**. Whether you create your working directory via Data Manager (**Section 2.2.**) or LINUX, this step is essential for proper storage of your data.



In “Path” field, type the directory where you are going to store your data: your data must be stored inside the DATA directory because you will only have remote access to that directory and subdirectories.

You can create subfolders into your directory. For instance, if in “Path” field you type…

/beamlines/bl11/projects/cycle2013/2013030293-ualba/data/20140101/Experiment1

…you will create a subfolder named “Experiment1” inside the folder named “20140101”.

2.2. Defining storage directory by using Data Manager (“Windows-like” mode)

Click on the icon displaying a “green chameleon” at the bottom of the screen. Click on it to open the Application Launcher. A list of applications will appear. Click on the icon displaying a “blue file cabinet”. Search for the DATA folder inside your user directory. Here you can create folders and subfolders in an “MS Window-like” mode. Once you have created the directory, copy the path directory and paste it into the box directory of bl11ExpGUI (see section 2.1.). Your .edf files will be stored inside the “DATA” folder. You can choose either to create or not subfolders inside “DATA” to organize your measurements.

2.3. Suggestions for file names

• It is recommended to include an underscore after the file name; the system will start naming the files by putting 0000, 0001, 0002, etc. By doing it this way you can avoid mixing the sample number with the file number. Include also underscores to separate the name of sample from the number of sample, it will help you to locate the files:

e.g: sample_1_

• Do not use strange characters like accents, equals, percentages, etc. Some programs for data analysis may not work.

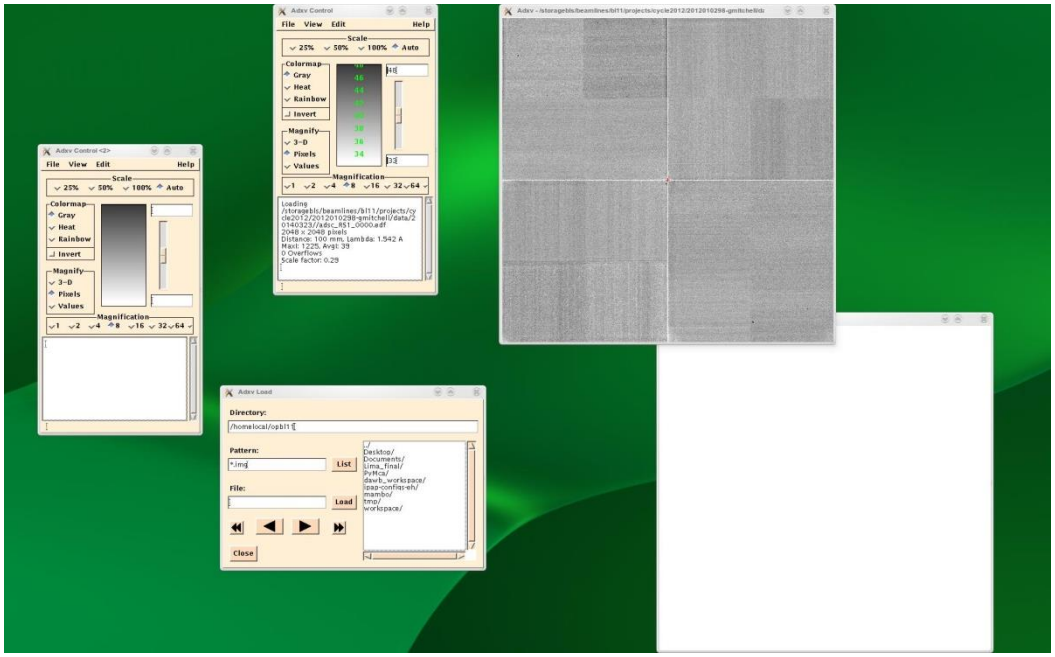
3. Image visualization

3.1. From LINUX

Before doing any acquisition, open the appropriate programs that allow you to view your SAXS and WAXS images.

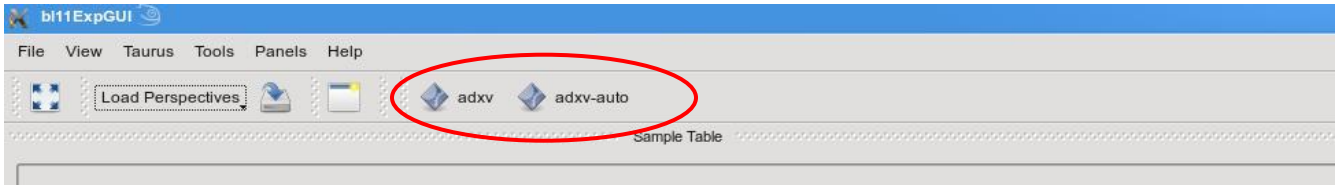
Open a new terminal window and type **adxv-auto** for SAXS (the new windows are named **adxv** and **adxv control**).

Open a new terminal window and type **adxv –q** for WAXS (the new windows are named **adxv2** and **adxv2 control**).



3.2. From bl11ExpGUI

By clicking the icons on the top left of ExpGUI console you can also open windows for visualization of SAXS and WAXS images. Click **adxv-auto** for SAXS and **adxv** for WAXS.



3.3. Image viewing

Once the acquisition is finished, SAXS images will be automatically loaded and displayed in the adxv window. For WAXS images this works differently as the program doesn't refresh the images automatically. In the window named **adxv load**, locate your directory (**Directory box**). Type ***.edf** into the **Pattern** box and click **List**. Select the file you want to visualize from the list, and click **Load**.

For clarity, **SAXS** images files are headed by **adsc**_filename and **WAXS** images files are headed by **rayonix**_filename (each one corresponds to the name of the detectors).

4. Running an experiment

If the sample is located in the beam path you can proceed following the instructions below. If not, please refer to section 5 (**Sample stages**).

You can choose to do your measurements by using the Experimental GUI (bl11ExpGUI) or by typing command lines from a console.

4.1. Running an experiment using sequences in Experimental GUI (ExpGUI)

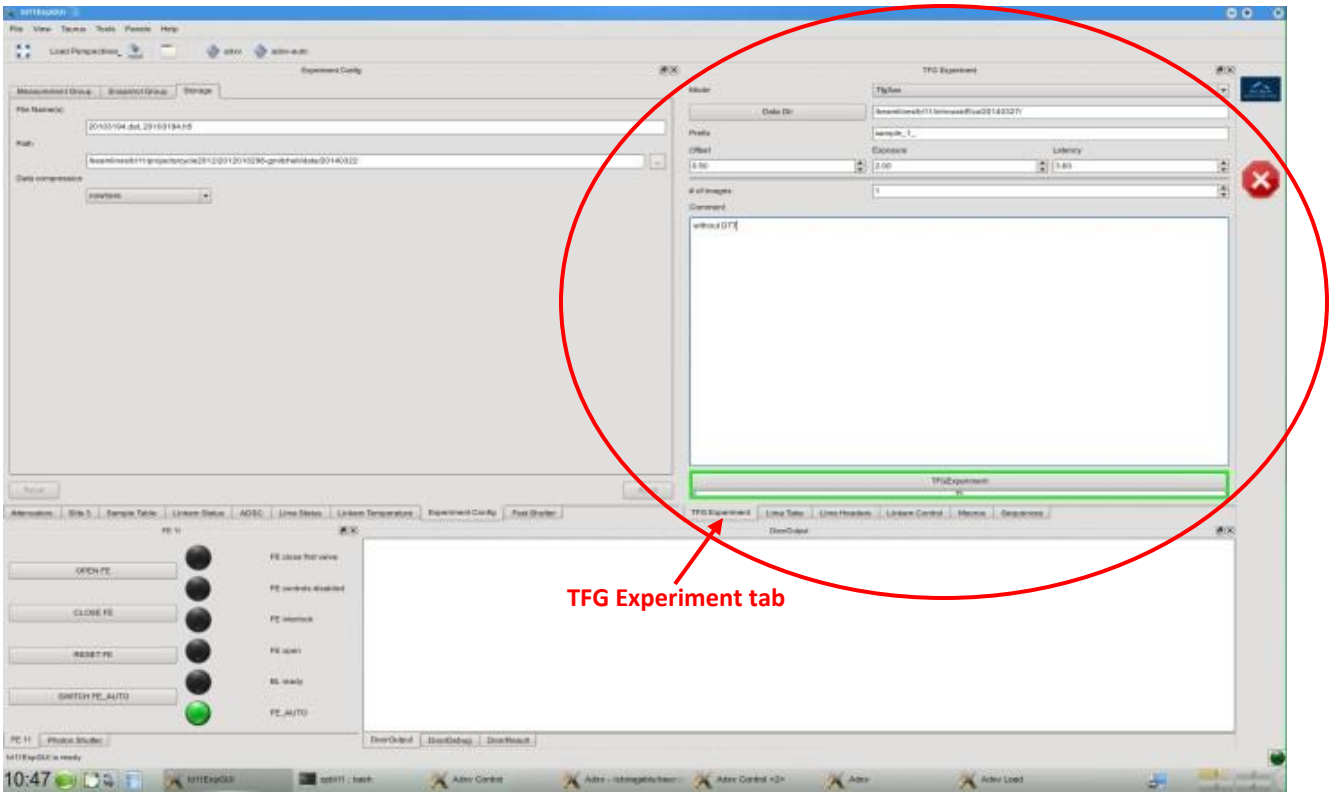
The following instructions explain how to run an experiment by using the user friendly interface bl11ExpGUI.

4.1.1. SAXS and SAXS/WAXS measurements

-The macro to run SAXS and SAXS/WAXS experiments is named TFG (Time Frame Generator).

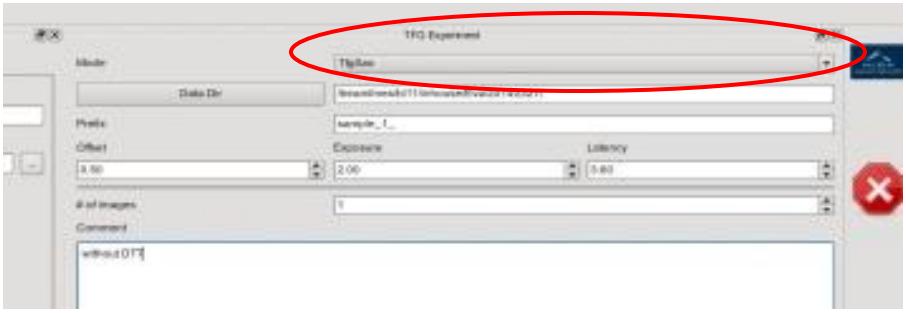
-You can run SAXS and SAXS/WAXS macros by using the sequencer.

-Go to TFG Experiment tab:



-Input the information for the following parameters into the corresponding fields. It's very important before running the experiment to press enter once you have written a value or parameter into each box.

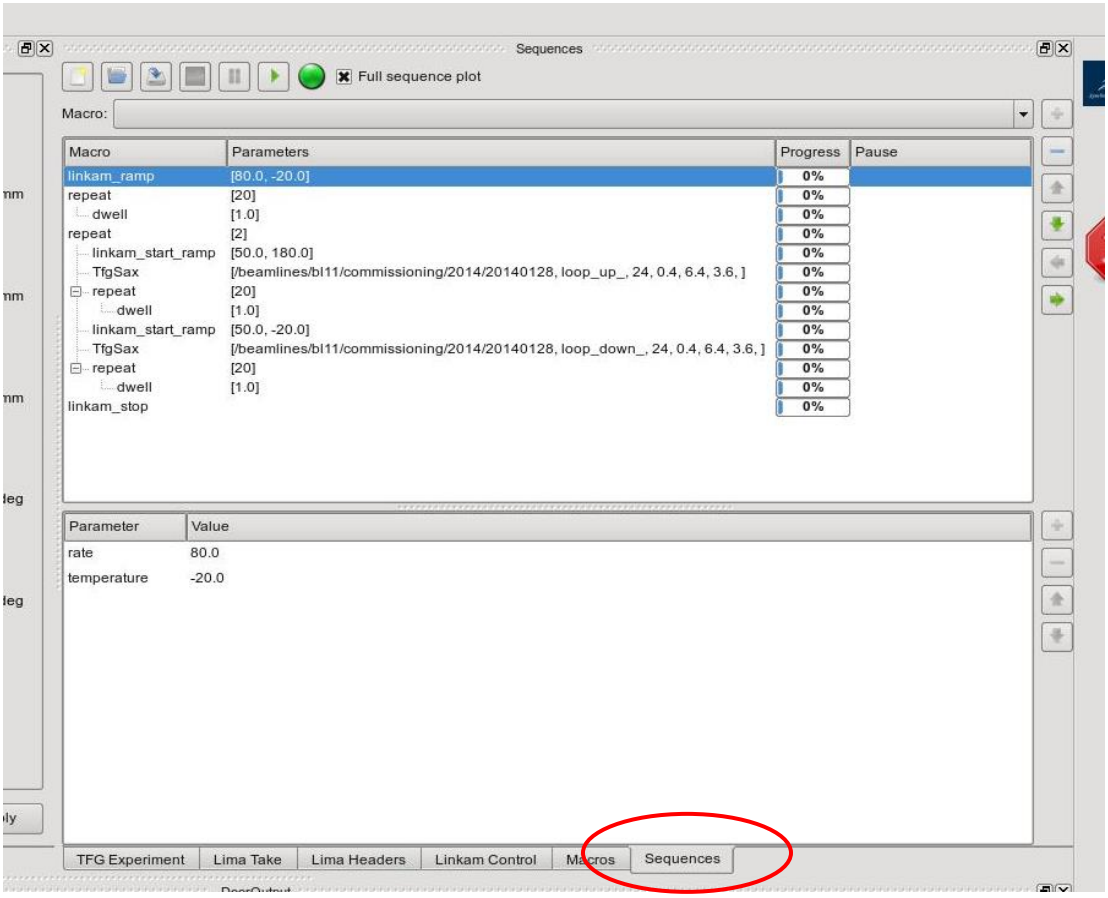
-First you have to select the type of experiment (TfgSax or TfgSaxWax):



- Base dir: directory where you would like to store the images.
- Prefix: name of the sample or experiment. It is advisable to include underscore to locate the files more easily; we strongly recommend including a final underscore: e.g. sample_1_
- Frames: number of images to acquire (e.g. 2)
- Offset: this value is always 0.4.
- Exp: Required exposure time in seconds (e.g. 5)
- Latency: this value is always 3.6 (it's the readout time; don't change it unless the beamline staff suggests another value).
- Comment: you can add some notes if you want; they will appear in the header of the file

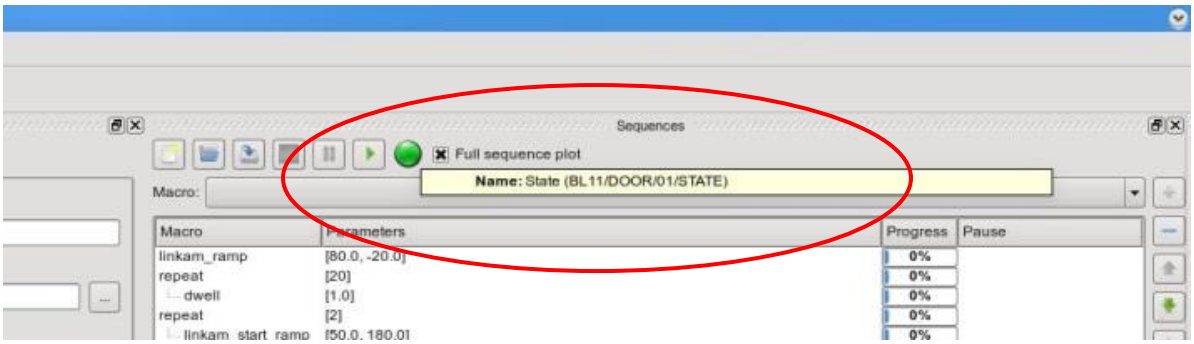
4.1.2. SAXS and SAXS/WAXS using LINKAM

-Click on the sequences tab.



-Click on the folder icon and open `/beamlines/bl11/controls/user-scripts/Linkam` and select a LINKAM sequence template.

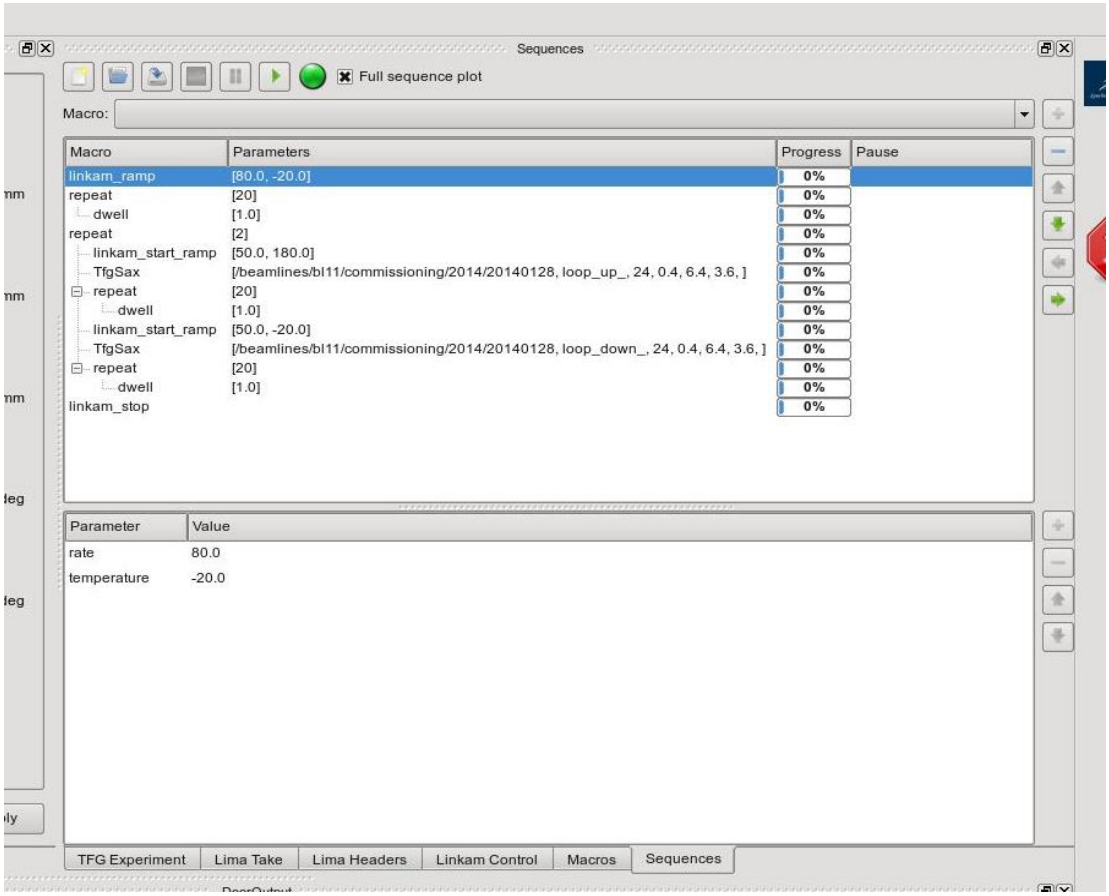
-Check if the circle next to the ▶ button is green. If not, right-click on the circle and afterwards click “check door state”.



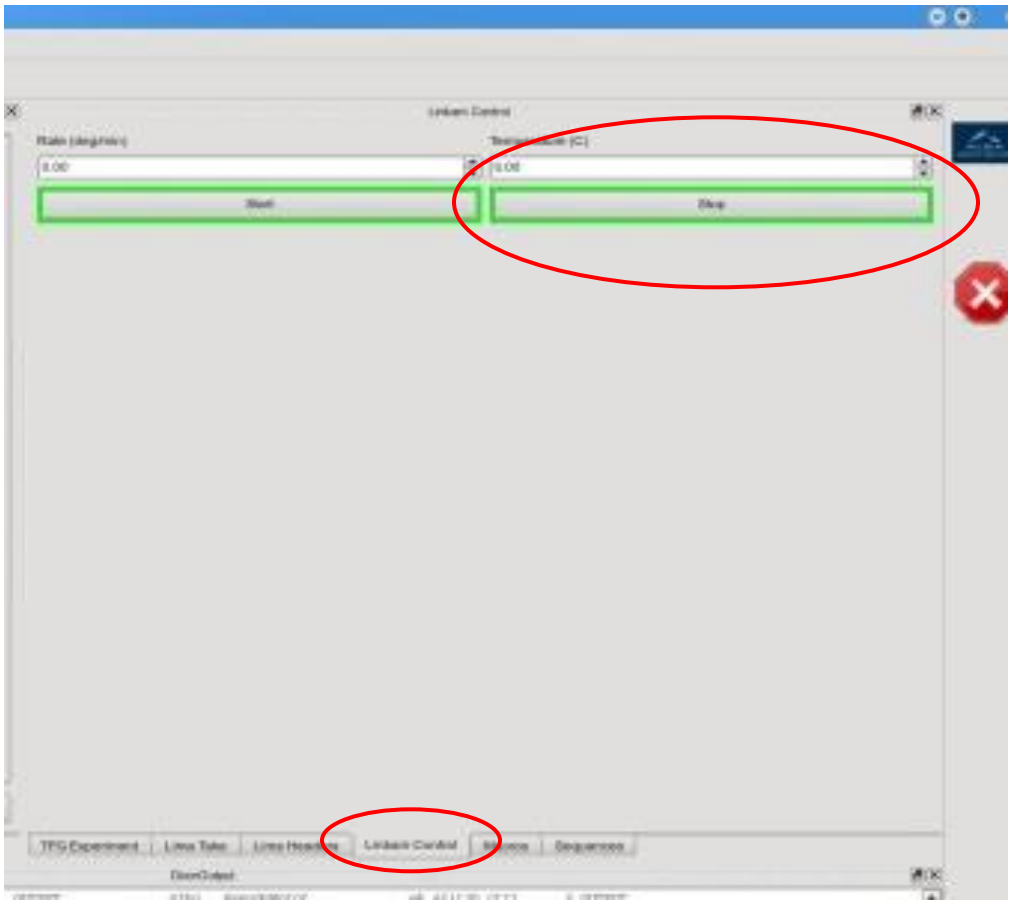
-When the green lead-light is green, you can press the ▶ button to start running your experiment.

VERY IMPORTANT:

-<u>Remember to activate submacros</u>: Submacros must be activated before starting to run the sequence. In the figure below, “dwell” is the submacro hanging from macro “repeat”. To activate submacros, right-click on the submacro (“hook places”) Click on the square next to the name of the submacro. A tick will appear on the square (☑ body).



-How to stop a sequence: You can stop sequences. However, this is not recommended as it often causes the detector server to crash. If you decide to stop the sequence, first click the ■ icon. Afterwards, go to “Linkam control” tab and click on the stop button with rectangular shape.

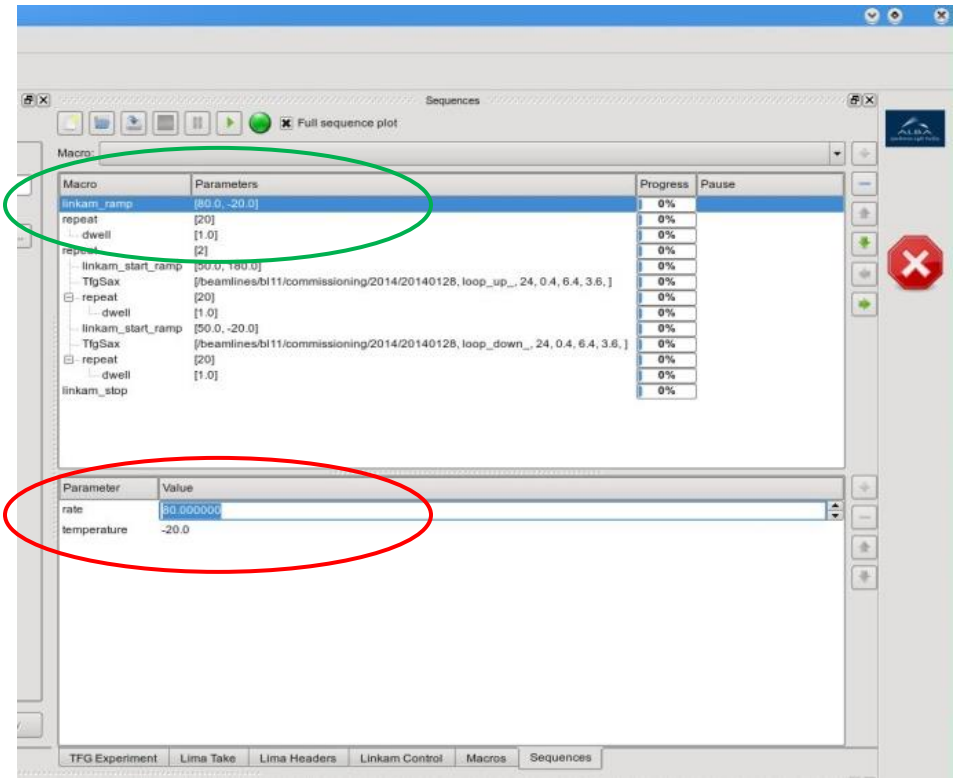


-How to restart a sequence (refreshing door state): You can restart sequences after stopping them. First, right-click on the green light next to the play button: a label will appear. Click on it to refresh door state. Now you can click on the play button.

4.1.3. How to edit LINKAM macros inside a sequence

4.1.3.1. From bl11ExpGUI console

Click on the parameter you want to edit on the upper panel (green circle), and edit the parameter on the bottom panel (red circle).



Remember to press enter after inputting the new value.

4.1.3.2. Using a text editor

From LINUX

-Open the directory `/beamlines/bl11/controls/user-scripts/Linkam` and select your LINKAM sequence template (.xml file). It is advisable to save your sequences in \DATA since that information can be very useful for your data analysis.

-Open the selected file with a text editor (KWrite in LINUX).

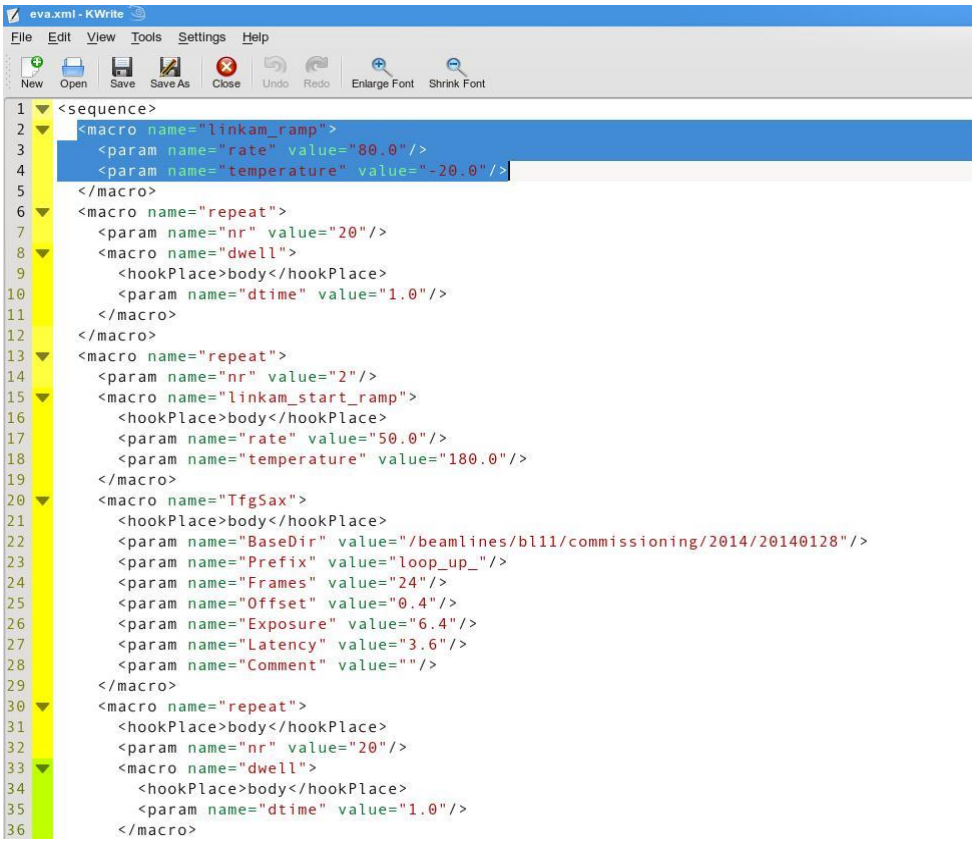
From Windows

-Open the directory `/beamlines/bl11/controls/user-scripts/Linkam` from file manager and select your LINKAM sequence.

-Open the selected file with a text editor, for instance Notepad++.

-You can delete, copy-paste, and edit the macros inside the sequence.

Either via LINUX or Windows, once you have opened the file you will be able to delete, copy-paste, or edit macros inside a sequence. Remember that every macro starts with **<macro …** and finishes with **</macro>.**



4.2. Running an experiment by executing commands from a console

Once you have executed a macro, you can recover history by using the upper arrows in your keyboard and execute the same macro without the need of writing it again. You can also retrieve a macro and edit it.

Remember that LINUX is case sensitive and care must be taken with capitals and lowercases.

To operate this way you must **Start a Spock session:**

-Open a new terminal (**Section 1.3.**).

-Type **Spock** and press **Enter.**

4.2.1. SAXS measurements

-Example: Performing a SAXS experiment with the following parameters:

Prefix: sample_1_

Base directory: /beamlines/bl11/projects/cycle2013/2013030293-ualba/data/20140101

Number of frames: 1

Offset: 0.4

Exposure time: 30

Latency: 3.6

The above parameters are the ones you would have indicated in bl11ExpGUI. Now, using the terminal option for macro execution you need to write the following macro:

```
TfgSax /beamlines/bl11/projects/cycle2013/2013030293-ualba/data/20140101 sample_1_ 1 0.4 30 3.6
```

and press **enter**.

4.2.2. SAXS/WAXS measurements

-Example: Performing a SAXS/WAXS experiment with the following parameters:

Prefix: sample_1_

Number of frames: 1

Offset: 0.4

Exposure time: 30

Latency: 3.6

-You will have to write the following macro:

```
TfgSaxWax /beamlines/bl11/projects/cycle2013/2013030293-ualba/data/20140101 sample_1_ 1 0.4 30 3.6
```

and press **enter**.

4.2.3. Useful commands

If you don't remember the syntaxes of a command you can type, for instance, **TfgSax?** or **TfgSaxWax?** and press enter. The computer will return a list of all commands involving these keywords, with indications of what you have to write to execute the macro.

```
bl11_sats [1]: TfgSax?
Type:           Magic function
Base Class:     <type 'instancemethod'>
String Form:    <bound method MatplotlibMTShell.TfgSax of <IPython.Shell.MatplotlibMTShell object at 0x173a790>>
Namespace:      IPython internal
File:           /homelocal/sicilia/lib/python/site-packages/sardana/spock/spockms.py
Definition:
Docstring:
    Syntax:
        TfgSax <BaseDir> <Prefix> <Frames> <Offset> <Exposure> <Latency> <Comment> ->

    Macro to run a SAX Experiment

    Parameters:
        BaseDir : (String) Base directory to store data.
        Prefix : (String) Prefix for the experiment.
        Frames : (Integer) Number of Sax frames.
        Offset : (Float) Waiting time before acquisition starts.
        Exposure : (Float) Exposure time.
        Latency : (Float) Latency time.
        Comment : (String) Comment to be stored in enviroment file

    Result:
```

5. Sample stages

If your sample it's not in the beam path, you have several motors that allow you to move the sample along the x (horizontal) and z (vertical) axis, in order to align it.

5.1. Samples stages by using Experimental GUI (ExpGUI)

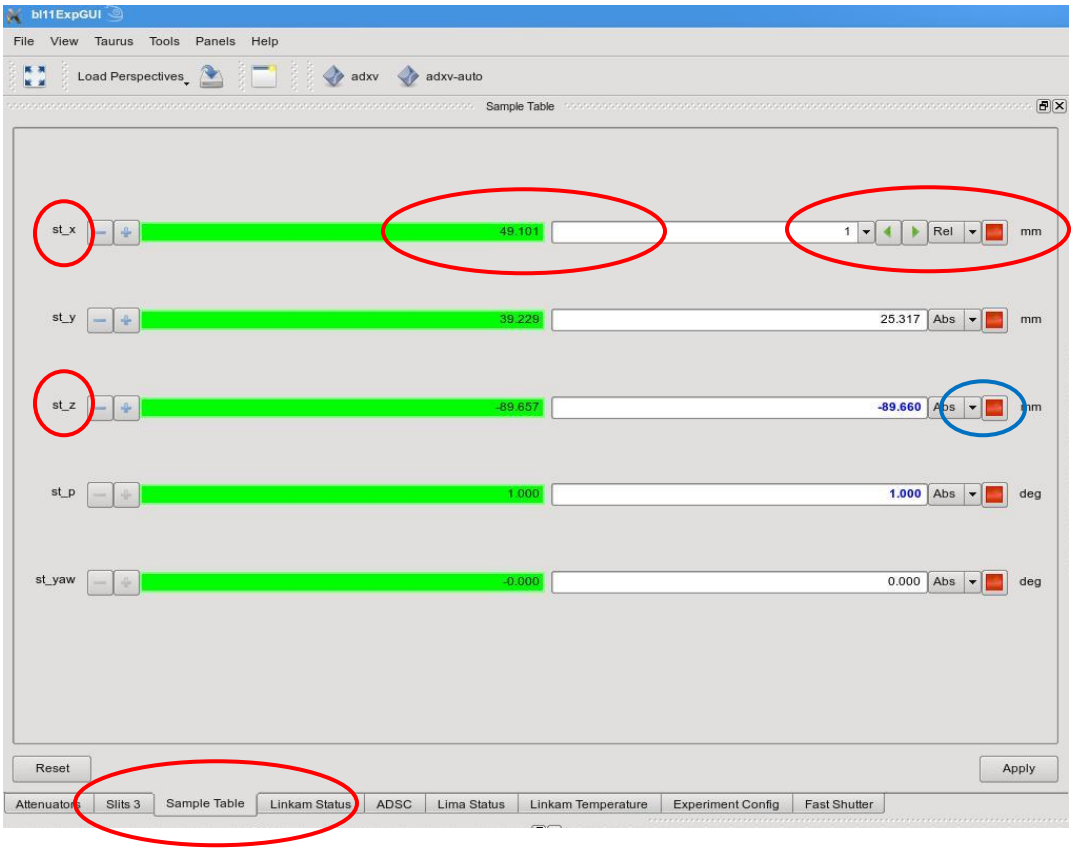
Go to “Sample stages” tab. You will usually use the following boxes:

5.1.1. Sample stage x

To move the sample stage in the **x direction** (horizontal movement):

1. Choose if you want an Abs (absolute) or Rel (relative) movement. If you print a value into the **Abs box**, the sample will move to this specific space co-ordinate position. If you print a value into the **Rel box** the sample will move this distance in mm relative to its original position. You can choose the absolute or relative movement option by clicking the black arrows (blue circle). Check the direction of the movement before you proceed. See step 2.

2. Consider the centre of ALBA storage ring as the reference point. The right green arrow moves the sample towards the centre of ALBA storage ring. The left green arrow moves the sample outwards the centre of ALBA storage ring.



3. Click the arrow to execute the movement.

<u>Example:</u>

-Current x position: 49.10. If you input 1 mm in the Rel box, the sample will move 1 mm to the position 50.10, towards the centre of ALBA storage ring (from position 49.101 to position 50.101).

VERY IMPORTANT: Remember that the actual position of the sample is the value in the green box at the left of the “Sample stage” panel.

5.1.2. Sample stage z

It moves the sample on the **z axis** (vertical movement). It works exactly as for sample stage x, but in this case you have to take into account that by clicking the right green arrow the sample will move upwards, and by clicking the left green arrow the sample will move downwards.

Example:

-Current z position: 48.00. If you input 47 mm in the Abs box, the sample will move downwards to position 47 mm.

5.2. Moving the sample stage by executing commands from the Spock terminal

5.2.1. Sample stage x

-From **Spock** (refer to section **4.2.** to see how to open a **Spock** session in a **new terminal**):

-Absolute movement: `mv sample_stage_x` (and type the desired value)

-Relative movement: `mvr sample_stage_x` (and type the desired value)

-If you type a positive value, the sample will move towards the centre of ALBA storage ring; if you type a negative value, the sample will move outwards the centre of ALBA storage ring.

5.2.2. Sample stage z

-From Spock (refer to section **4.2.** for details on this issue):

-Absolute movement: `mv sample_stage_z` (and type the desired value)

-Relative movement: `mvr sample_stage_z` (and type the desired value)

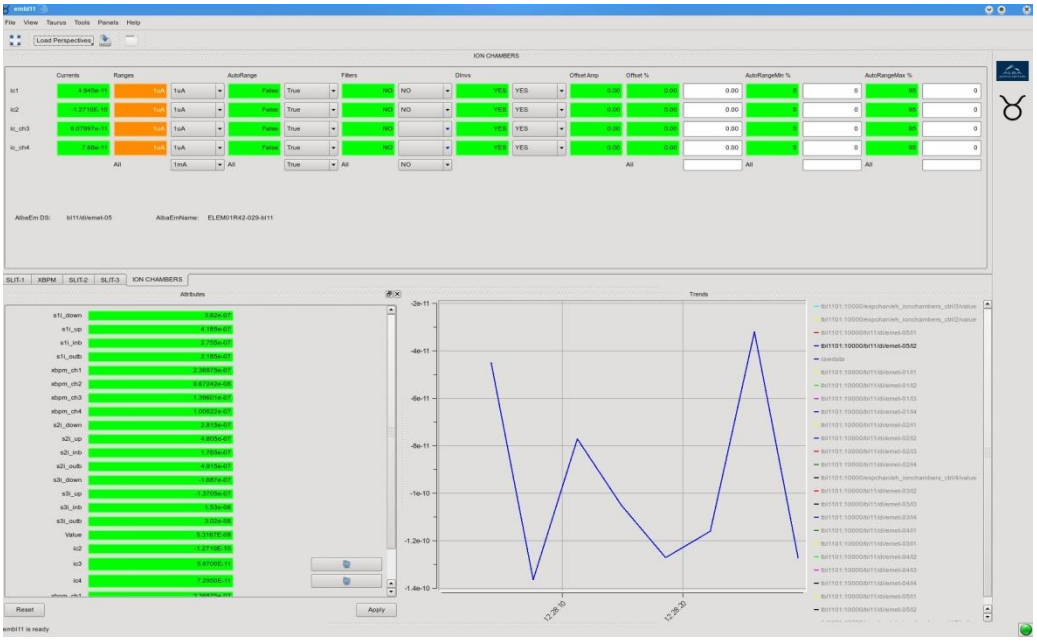
-If you type a positive value, the sample will move upwards; if you type a negative value, the sample will move downwards.

6. Locate a sample using the ion chambers

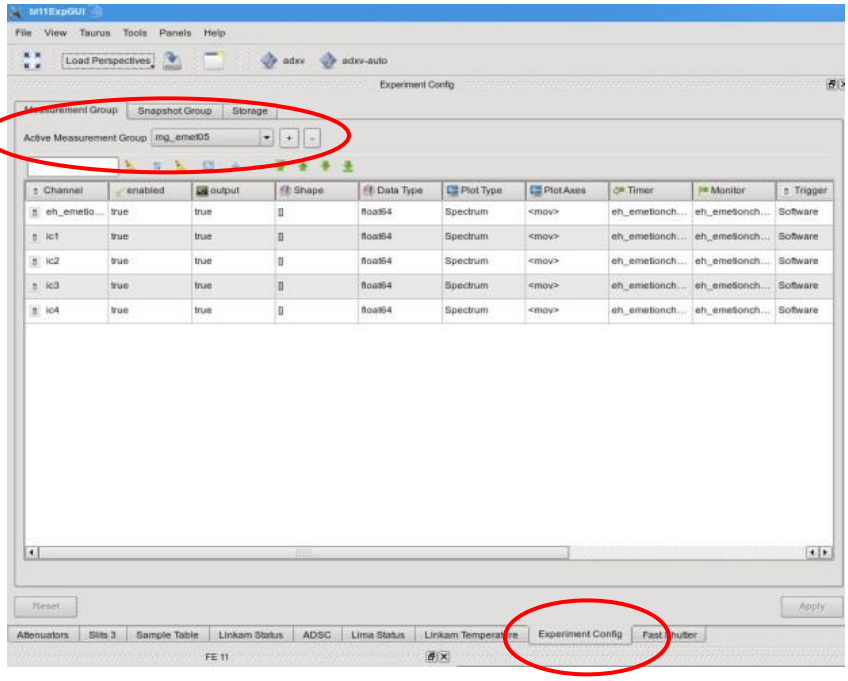
-Open a new terminal (see **Section 1.3.**) and ensure you are not in the /tmp directory.

-If yes, type cd .. and type `embl11` and press **enter**

-A new window will open displaying the current on the ion chamber 1 (IC1) and ion chamber 2 (IC2). IC1 is located before the sample and it is used to calibrate the current of the incident beam; IC2 is located after the sample and it is used to locate and/or calculate the transmission of the sample:



-In the bl11ExpGUI console on the left screen, click on “Exp Config” tab and select the Measurement group: **mg_emet05**:



-Go to bl11ExpGUI console and open the photon shutter or safety shutter (PSHU).

-Go to a terminal with a **Spock** session and open the fast shutter (please note: do not confuse the fast shutter with the safety shutter). To open the fast stutter type `tfg_shutter_open` and press **enter**.

-To locate your sample you have to follow IC2 current. In the terminal you have open, you will perform a differential scan or absolute scan by typing a command line:

`ascan sample stage x <motor starting position> <motor ending position> <number of intervals> <integration time>` (this option requires **absolute** motor values)

`dscan sample stage x <motor starting position> <motor ending position> <number of intervals> <integration time>` (this option requires **relative** motor values)

Once the sample is located in x, the same macros can be used for the sample_stage_z motor to locate the vertical direction.

This means that the motor is going to move along the x or z direction (this depends on what axis do you want to locate your sample), and you will observe that current on IC2 decreases when you sample blocks the beam. If you observe the same current on IC1 and IC2, the beam is not touching the sample. Normally the current in IC1 will be $\approx 10^{-7}$ A, and you will observe a decrease to $\approx 10^{-10}$ A in IC2 if the beam is touching your sample. If your sample is not in the beam path, you will observe more or less the same value of current in IC1 and IC2.

In order to view the current in both ion chambers and to observe the decrease in IC2 when the sample reaches the beam path it is very useful to use a real time graphical interface of the ion chamber currents. In bl11ExpGUI there is the <Trend1Dmove> panel where it plots automatically the ion chamber currents vs sample stage position (depending which sample stage was indicated in the ascan or dscan macro). Alternatively, once a terminal window is open, you can print **taurustrend -xe scan://bl11_sats** and a pop out window with the same graphical interface will appear.

Example

Performing a differential scan on the x axis of the sample stage from 5 mm at the left to 5 mm at the right of the current position of the sample. Since we are running a relative scan, the motor will return to its initial position once the scan is finished.

-Type `dscan sample_stage_x -5 5 100 1` and press **enter**. The motor will move on the x axis (horizontal) 5 millimetres at the left and will scan the IC1 and IC2 current from this position to 5 mm at right of the initial position, by measuring 100 points with an integration time of 1 second. This means, you have scanned 10 mm in total. You can follow the scan in Trend1D move (tab located in ExpGUI console).

-Once the scan is finished you will get a graph where you can observe the decrease of the current in IC2 as a Gaussian curve with a minimum where the sample has reached the beam path. The middle point of minimum of this Gaussian is the centre position of your sample.

-Now you have to move the sample to this position by using the corresponding motor. In our example we have moved in the x axis. You can move the motor via bl11ExpGUI console or via a command line from a Spock session. It is recommended to move the motor in the absolute

mode, it will avoid mistakes. Refer to **section 5** (Sample stages) to get instructions on this issue.

-Close the fast shutter by typing `tfg_shutter_close` and press **enter**.

-Now you are able to start your measurements as explained in **Section 4** (Running an experiment).

7. Troubleshooting

Sometimes you can have some problems that do not allow you to continue with your experiment. If it happens during the day, you have to call your local contact and he/she will try to solve it but in case it happens during the night (remember you will not have support), try to follow the next troubleshooting guide.

7.1 DETECTORS PROBLEMS

Definitions

ADSC: It is the name we use to refer to the SAXS detector

Rayonix: It is the name we use to refer to the WAXS detector

Symptoms

During the acquisition we got a message error (red colour) in the output of the GUI or in the spock session console and you have detected that some images are missing.

Solution

<u>If the Rayonix (WAXS) detector fails</u>

Execute the following commands from a spock session console:

`%lima_status rayonix` (it checks the detector status. It can be ON FAULT or ON READY)

If the status is ON FAULT do the following,

`%restartDS rayonix` (It will restart the device server)

Repeat the previous action:

`%restartDS rayonix` (Sometimes you have to restart the detector twice to get the ON READY status)

Check the status again by means of:

`%lima_status rayonix` (you will see the detector is in ON CONFIGURATION status)

Then, be sure that the safety shutter (also called photon shutter) is closed and type:

`%marccd_takebg rayonix` (it will take a background image)

Now, try to take an image again from the experimental GUI or from spock console session by means of the command:

`TfgWax /..../User1/DATA/Temporary Samle_test_ 1 0.4 1 4` (be sure you are trying to write the image in a directory you have permission to do it, for example inside you home directory and put a non-existing file name because when you restart the device server the control system resets the index counter)

If the status is ON READY but anyway you are no able to take images, try to do the following:

`%lima_stop rayonix` (It will stop the detector acquisition)

Or

`%lima_reset rayonix` (It will reset the detector acquisition)

and try to take an image again.

<u>If the ADSC (SAXS) detector fails</u>

Execute the following commands from a spock session console:

`%lima_status adsc` (it checks the detector status. It can be ON FAULT or ON READY)

If the status is ON FAULT do the following,

`%restartDS adsc` (It will restart the device server)

Repeat the previous action:

`%restartDS adsc` (Sometimes you have to restart the detector twice to get the ON READY status)

Check the status again by means of:

`%lima_status adsc` (you will see the detector is in ON CONFIGURATION status)

Then, be sure that the safety shutter (also called photon shutter) is closed and type:

`%adsc_takebg adsc 1` (it will take a background image of 1 second)

Now, try to take an image again from the experimental GUI or from spock console session by means of the command:

`TfgSax /..../User1/DATA/Temporary Samle_test_ 1 0.4 1 4` (be sure you are trying to write the image in a directory you have permission to do it, for example inside you home directory and put a non-existing file name because when you restart the device server the control system resets the index counter)

If the status is ON READY but anyway you are no able to take images, try to do the following:

`%lima_stop adsc` (It will stop the detector acquisition)

Or

`%lima_reset adsc` (It will reset the detector acquisition)

and try to take an image again.