Operators Manual

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Introduction

Dear User,

You are about to use the most advanced and versatile laboratory-based Small Angles X-Ray Scattering system in the world (of 2013). That such an instrument is available for the laboratory usage is the result of a number of very recent and significant advances in x-ray generators and detectors. Without these advances the performance, functionality and unprecedented up-time would not have been possible.

Given these advances, SAXSLAB (previously named JJ X-Ray Systems) applied their extensive knowledge in instrumentation, precision motion, automation, and SAXS experimentation to come up with a SAXS instrument like no other commercially available system:

1) The motion of the detector allows the user to make measurements over a very large q-range.
2) The complete motorization of the system, allows for ease of use and a high degree of automation in alignment and experiment execution.
3) The integrated data management (with detailed system information being carried over in date-headers interpretable by the data-reduction software) facilitates the task of monitoring, data-collection, data-reduction and data-interpretation

Based on a close collaboration with the Life Science Department of the University of Copenhagen the prototype came to life in 2010, and was the basis for the first series of production instruments installed in 2012.

Your instrument is one of the first 6 production instruments, and as such one of the very first of these 3rd Generation laboratory-based SAXS systems.[1]

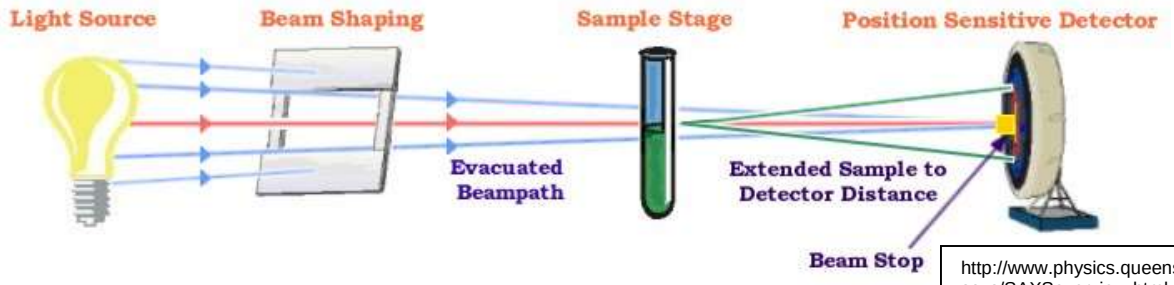
We trust that you will find the instrument useful for your analysis needs and hope that you will contact us with both praise and criticism.

Karsten Joensen
SAXSLAB Aps
Copenhagen, January 2013

[1] 1st generation systems were 2-pinhole systems offered by Bruker. 2nd generation systems were 3-pinhole systems offered by Bruker(Nanoviewer), Rigaku(nanoviewer), Molecular Metrology (SMAX),

System Overview

A schematic illustration of a 2-dimensional SAXS system is seen below:



http://www.physics.queensu.ca/~saxs/SAXSoverview.html

In the Ganesha, each item is truly state-of-the-art, with hardware and software integration, as well as full motorization and extended automation, allowing the strengths of the individual components to live out their full potential.

As examples we can mention:

The x-ray source is a High Brilliance Microfocus Sealed Tube with shaped multilayer optics, yielding a monochromatic high intensity beam at very low power.

The beam shaping is initially handled by the shaped multilayer, and then further collimated by 3 sets of 4-bladed slits, the last of which contains single crystal “Scatterless” blades.

The beam path is evacuated by an oil-free high speed pump allowing full pump-down to clean operating pressures in 4 minutes.

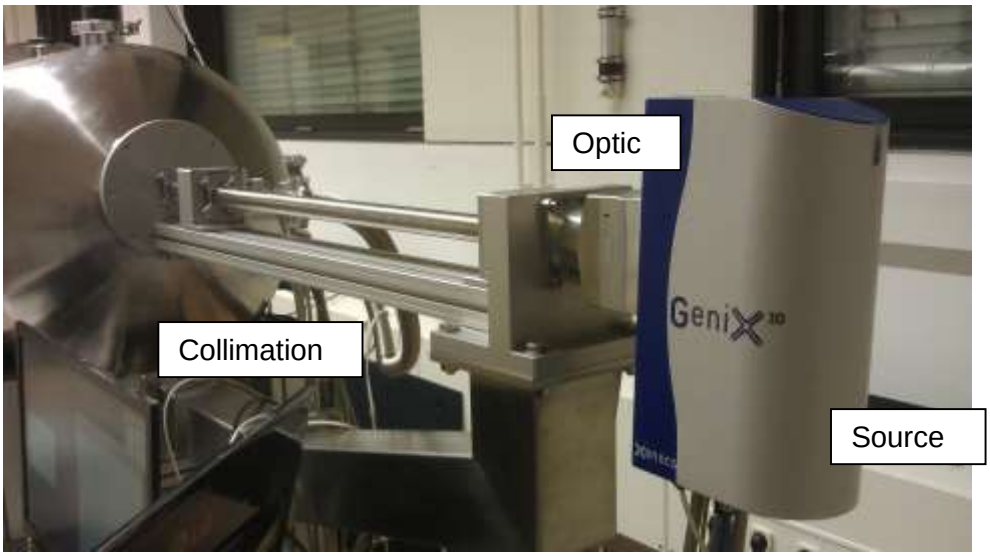
The sample area comes with an XY-theta goniometer for alignment and position of samples for both transmission and grazing incidence work. A large number of sample stages can be inserted into the large sample environment

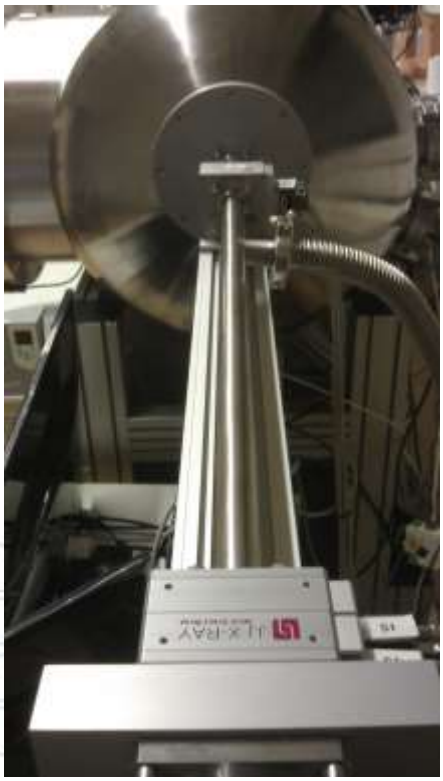
The position sensitive detector is a Pilatus detector, combining the best of single photon counting, dynamic range and robustness. The detector can be moved over 1300 mm allowing for measurement in WAXS, MAXS, SAXS and Extreme-SAXS.

The beam stops (there are 3) can be inserted and retracted for various purposes. The same holds true for a large pin-diode immediately in front of the beam stop.

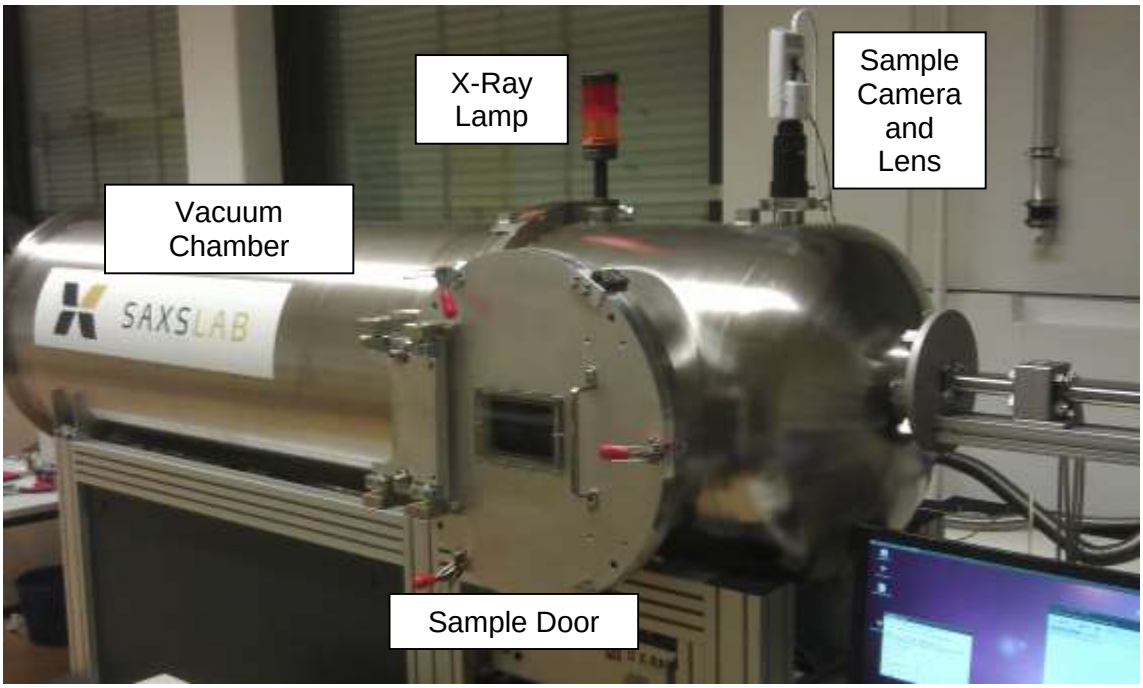
Getting Oriented on the System

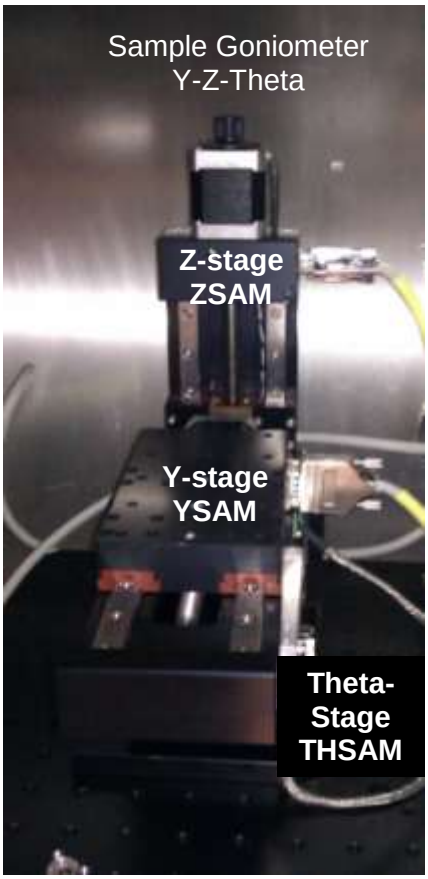
Source, Optic, and Collimation

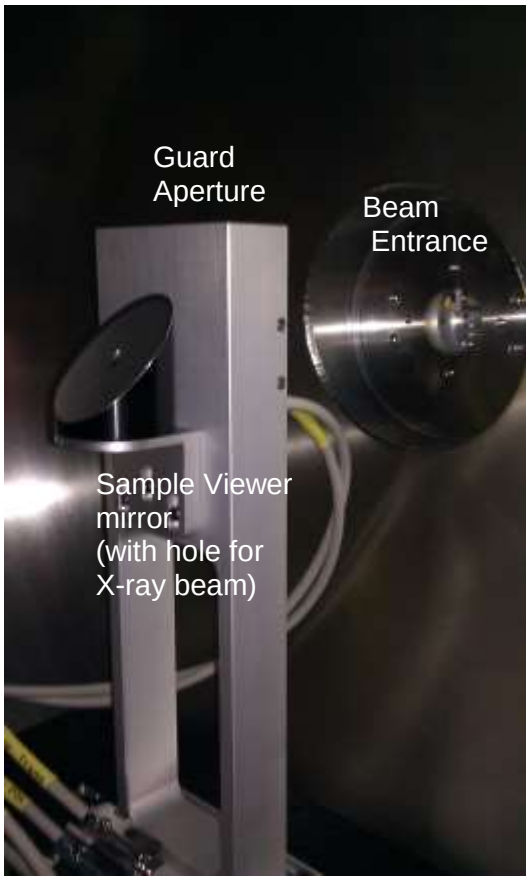




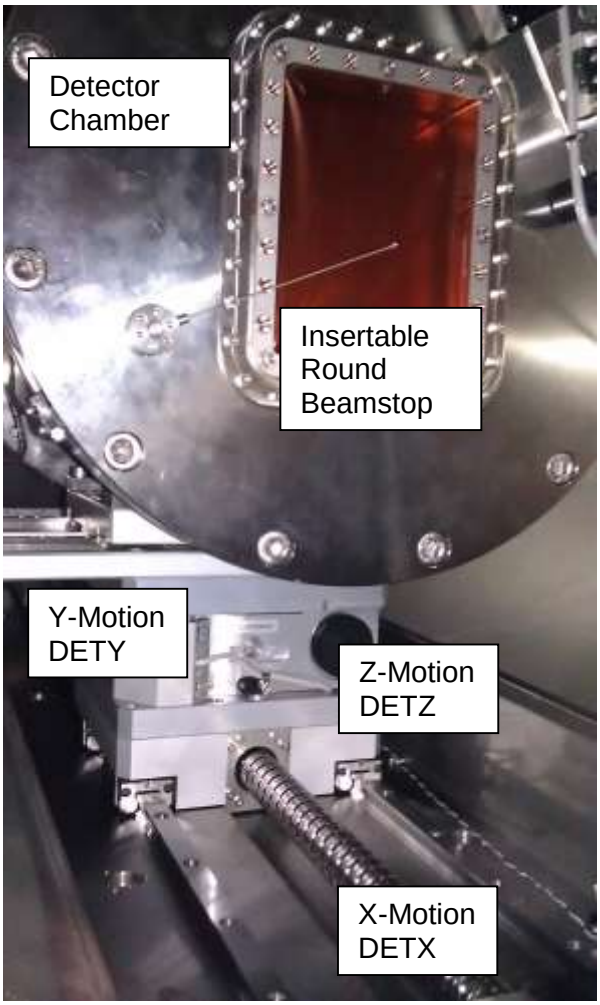
Sample Area

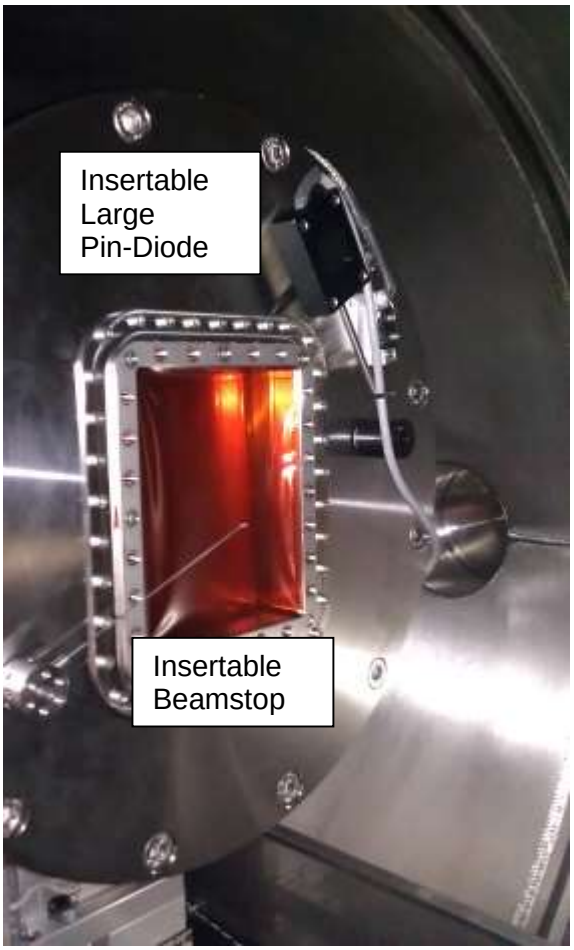

X-Ray Lamp
Sample Camera and Lens
Vacuum Chamber
SAXSLAB
Sample Door


Sample Goniometer
Y-Z-Theta
Z-stage
ZSAM
Y-stage
YSAM
Theta-
Stage
THSAM

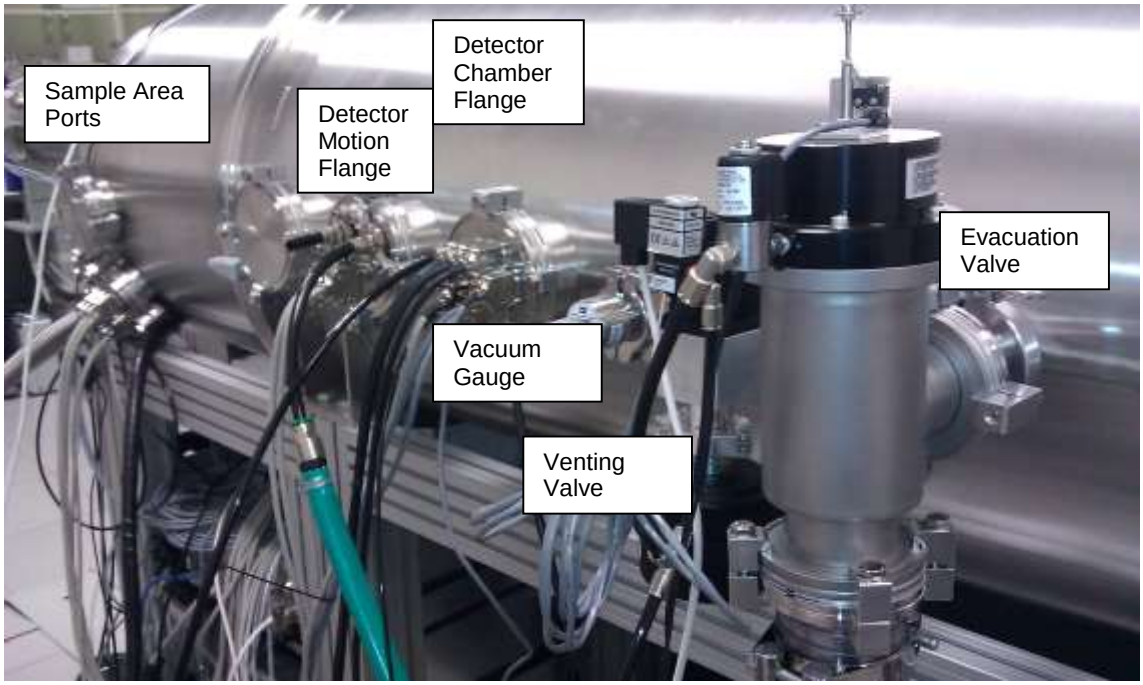

Guard
Aperture
Beam
Entrance
Sample Viewer
mirror
(with hole for
X-ray beam)

Detector Chamber, Motion, Beam Stop and Pin-diode



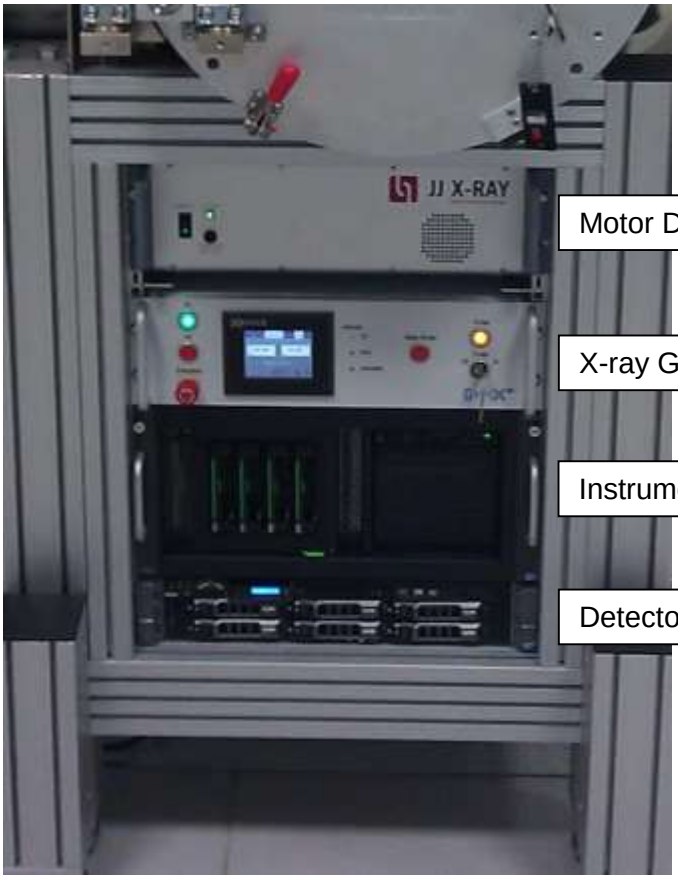


Ports and Valves



-

Electronics

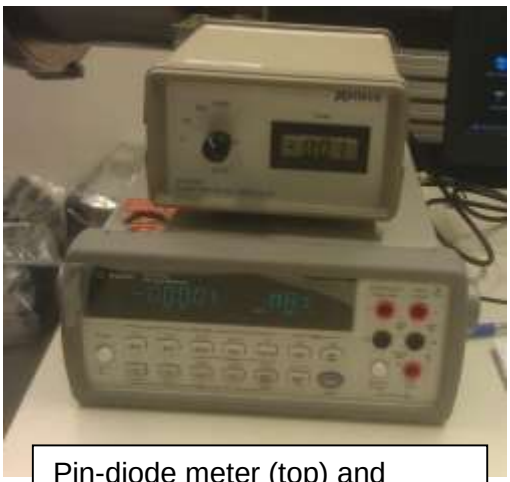


Motor Drive and Controller

X-ray Generator and Controller

Instrument Control Computer

Detector Control Computer



Pin-diode meter (top) and Voltage Analyser

Vacuum Meter

Vacuum Pumps (2 options)

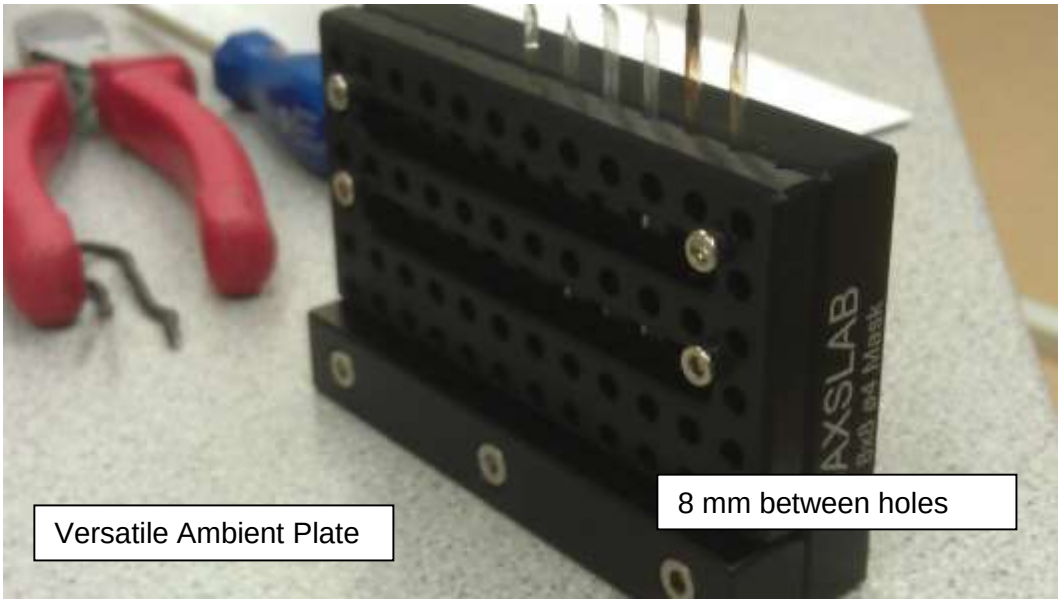
n-Volume Dry-

Coolers (Source, Detector and Pump)

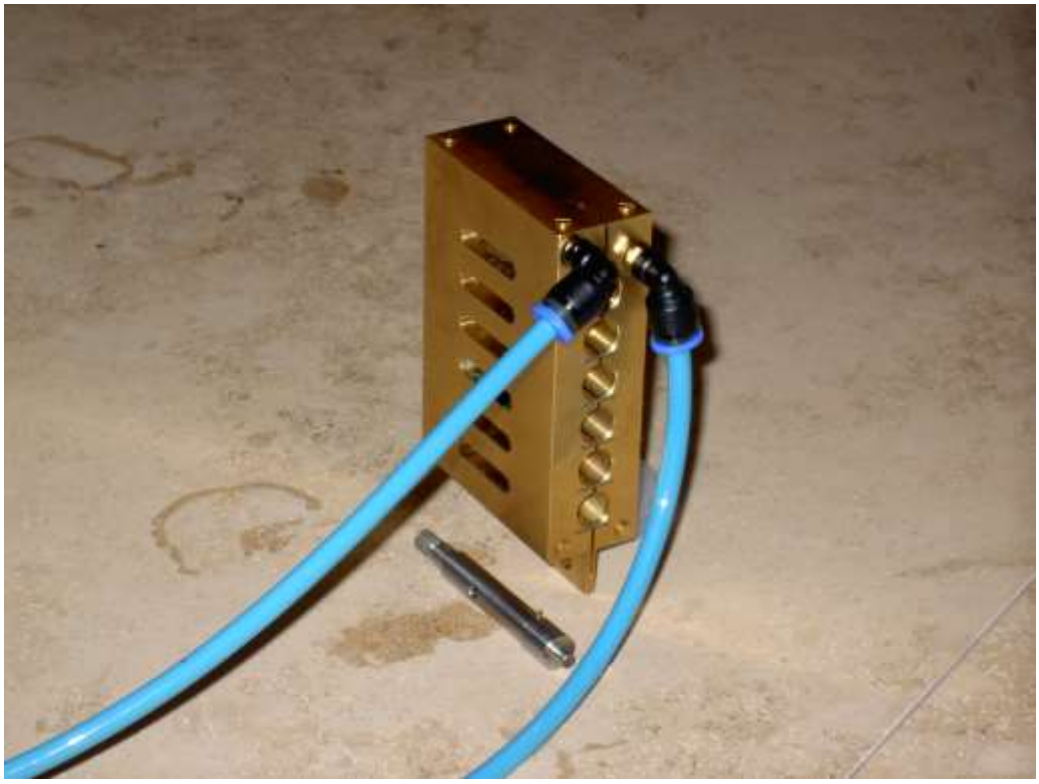
Detector and Source Cooler

Dry Pump Cooler

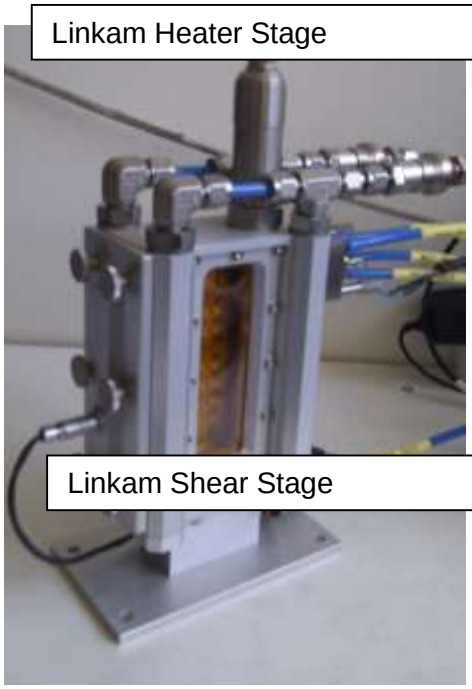
Sample holders and stages (not all may be available for your system):



ween



Linkam Heater Stage

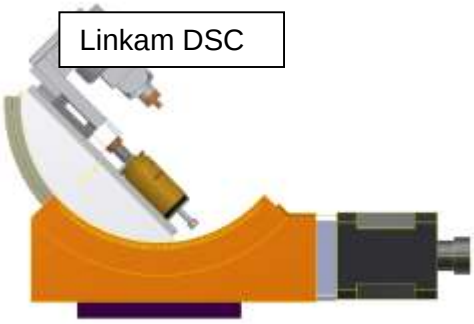


Linkam Shear Stage

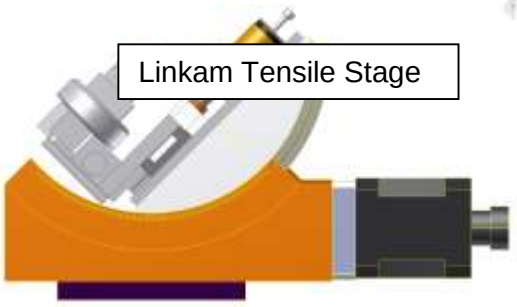
tal/Humidity Cell

er Segment

Linkam DSC



Linkam Tensile Stage



Getting Oriented on the Computer Desktop

Startup Screen

The Instrument controlling computer (ICC) is a linux computer running Ubuntu 12.04 LTS.

The login prompt will look like the image on the right.

The account is

saxslab

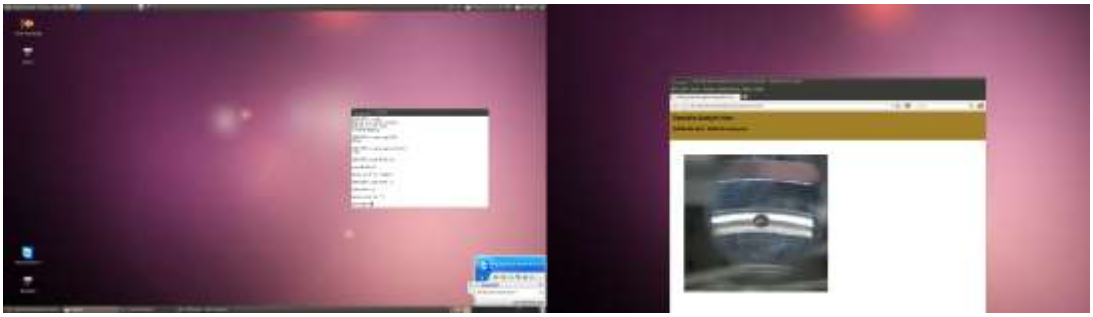
And the password is

saxslab12

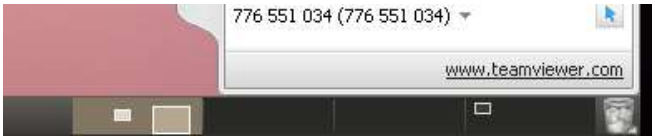
There are a number of looks that one may choose. The one we use is “gnome-classic without features”

The 4 desktops and the 2 screens

Most instruments will have 2 side-by-side screens, where one screen will normally be used for interacting with the programs and the others for monitoring. In this example we have the control program “spec” in the leftmost window and the sample viewer in the rightmost screen



In addition to these screens there are actually 4 individual desktops which can be accessed by clicking on the icon in the lower right corner of the left screen.

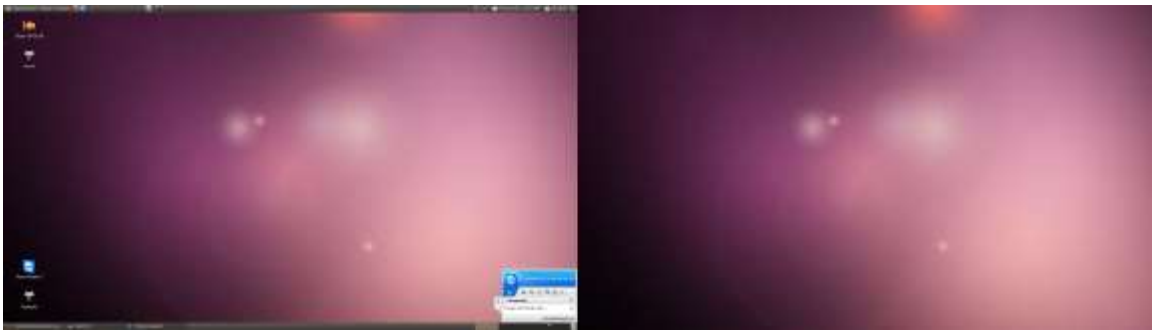


1 2 3 4
Desktops

Such 4 screens are useful when one has many windows open.

Minimizing windows

Windows can be closed, minimized or maximized by clicking on the small icons in the upper left corner of the window. The cross is closing, the “V” is minimizing and the “upside-down V” is maximizing. When minimized the windows can be found in the bar on the bottom of the leftmost screen



General Organization Suggestions

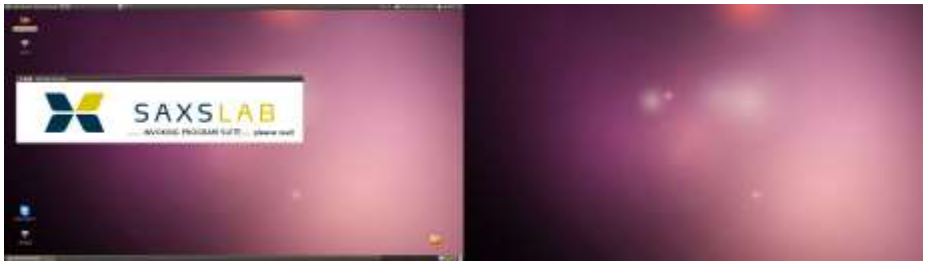
Generally it is a good idea to keep similar tasks running in the same desktop.
Per default

- Desktop 1 is used for interactive instrument control and monitoring
- Desktop 4 is used for windows where various background processes are running and reporting. These may be useful in case of trouble, but would otherwise not be needed
- Desktop 2 and 3 could be used for data analysis and web-access.

Starting up the SAXSLAB programs

On the desktop you will find an icon called “Start SAXSLAB”.
Right click this..and choose “open”. This action will first splash up a SAXSLAB banner and then open up a whole array of programs and windows needed to run the SAXS system. While this is happening the user should let the computer be.

When the banner disappears, the user can take control of the computer again.

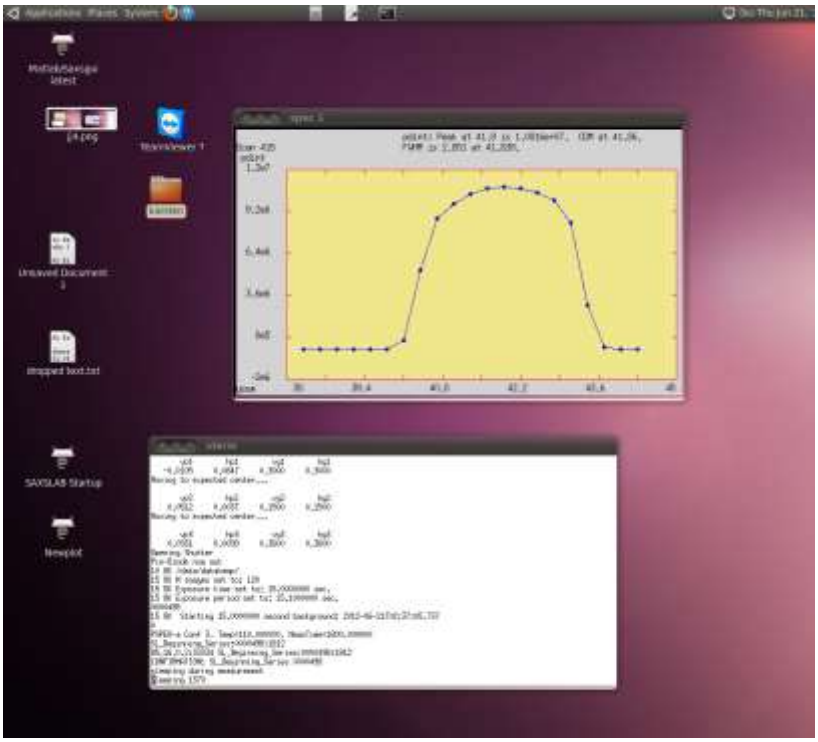


Important SAXSLAB Programs and Windows

All the important programs, required for running the instrument are invoked when you open the “Start SAXSLAB” Icon on the desktop.

If some of these are missing you can simply open “Start SAXSLAB” again.

Spec and c-plot



Spec (shown here in the white terminal- may also be a purple terminal) is the main program for controlling the instrument.

Control is exercised through writing commands on the line at the prompt. This command line approach is extremely flexible and powerful. Higher level commands for the SAXS system are available and are typically defined in macros residing in files in the directory /usr/local/lib/spec.d. An incomplete list of useful commands can be found in Appendix 5, which should at all times serve as a “cheat sheet” and be available in hardcopy near the computer.

A typical action is to scan over a part of you sample and record the transmitted intensity. The results of such a scan are plotted by the program C-plot, which is shown in the upper part of the image above. The C-plot window will not normally be displayed when Spec is started.

Sample Viewer (RayCam)

A completely standard and very useful feature of the Ganesha SAXS system is the Sample Viewer which has an on-axis view to the sample.

The combination of camera, lens and curved optic (with a hole in it to let the x-ray through), actually provide a microscope view of the sample that is streamed to a small dedicated viewer.

The RayCam viewer is a new internal development and has only been with users since November 2012. Please report problems and bugs so that we may address them.

The viewer allows one to position a while a cross, which can then be used as a reference for the beam position when aligning samples.

When you have defined the cross you may lock the position, so that it cannot be moved (unless it is unlocked again). Several crosses can be defined, but only one shown at a time.

One can calibrate the viewer so that the scale is actually represent real sizes.

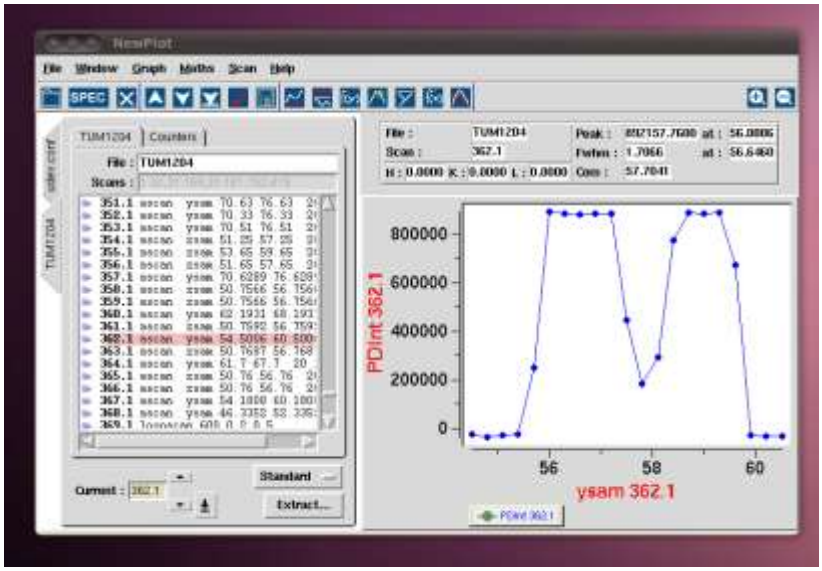
Also one may use the viewer to zoom. It zooms in around the cross.

For documentation purposes one may also use the viewer to take a snapshot or even to record the video stream.

Note: Due to curvature of the mirror straight lines may look curved. This is

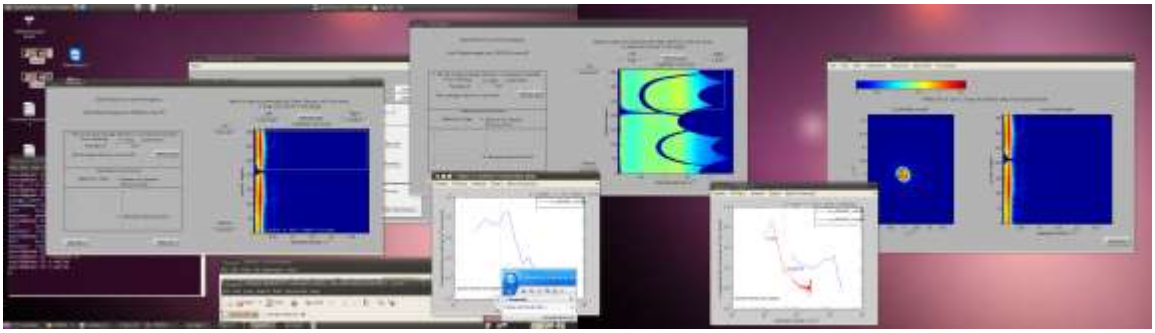
PyMCA

If one wants to look at the results from previous scans, one can use the program PyMca, to look for scans saved in the log-files. All scans are saved in the current log-file. (You can change the name of the log-file by using the spec command “newsample”)



SAXSGUI

SAXSGUI is the data-monitoring and data-reduction program that gives you the possibility to image, reduce, plot and save your data manually…….or in the case you have a large number of files…do the same automatically (based on the information in the header and your reduction selections)



The various Servers:

Various servers are required to run in the background in order for everything to work correctly:

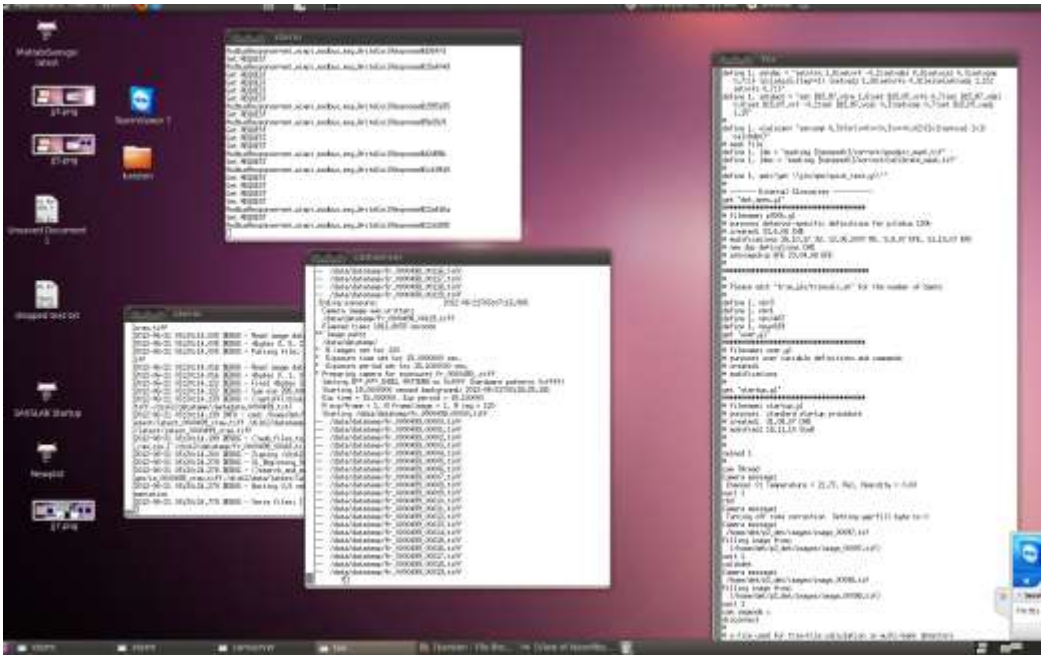
Camserver – this server runs on the detector computer and talks directly to the Detector. Should not be needed by the operator

Tvx- this server runs on the detector computer and can provide low-level communication to Camserver if needed. Should not be needed by the operator.

Sl_server – this server runs on the detector computer and handles all of the processing of the data in a measurement producing cumulative files and making sure correct headers are included in the files. As of January 2013 this server also does advanced noise-reduction.

Modbus_server – This server runs on the instrument control computer and handles communication from spec to the Xenocs source generator…controlling for example the opening and closing of the shutter and the High voltage and current settings.

These various servers are usually reporting in Desktop 4



If any programs are missing you can get them back by invoking the “Start SAXLAB” icon.

Data Output

Image data is saved in tiff format and should be readable by most data-handling packages. However, since the header (see Appendix 1 for details on the header) is stuffed with information about the measurement, full utilization of this information requires SAXSGUI, or a dedicated customer header-interpreter

The measurements are numbered consecutively with pre-fix and suffixes indicating the actually type of tile.

A measurement is actually a string of measurements

Per default, we have chosen that instead of making one long exposure for each measurement, we will make many short measurements and then add these short measurements together. We save both the summed image and the complete measurement history.

There are a couple of advantages to this approach:

1) The dynamic range of the measurement becomes higher
2) We can observe the experiment progression each time the short measurement is finished
3) We can use a time-slice of the data, if at some point the measurement fails
4) We can track the scattering as a function of time
5) We can perform advanced noise reduction, by comparing the short measurement with each other in various ways.

For practical purposes we have chosen a time interval for the short measurements of 15 seconds. A 3600 second measurement therefore actually consists of 240 images.

As a result of the measurement the following files are generated:

Filename	Description
/disk2/data/latest/latest_nnnnn_craw.tiff	A tiff-file that is all the time updated to include the latest taken data…i.e. this file is the “real-time” sum of all the short measurements. This file has the full header information inserted.
/disk2/data/images/im_nnnnn_craw.tiff	A tiff-file that is created at the end of the measurement and is the sum of all the data taken during the short measurements. It should therefore be equal to the latest_nnnnn_craw.tiff. This file has the full header information inserted.
/disk2/data/frames/frames_nnnnn_craw.zip	A zip-file containing the short measurements as well as a file with the Metadata. This file is not readable by SAXSGUI..but may be processed for cosmic background reduction from SAXSGUI.

A Measurement

Initial Preparation

In the following we will assume that you (the user) will be running the system on your own, but that the instrument responsible has made sure the instrument is prepared for you…i.e. that the instrument is turned on, aligned, calibrated and basically ready to go.

However before commencing you will need to think a little about the experiment, prepare the sample, check the instrument and mount the sample in the system.

Planning your measurement what are you looking for?

Before getting access to the instrument you should think about your measurement.

1) What q-range are you interested in?
2) How strongly does your sample scatter?
3) What are you looking for?
    a. Peak Positions and peak-width?
    b. Particle sizes?
    c. Data that can be accurately modeled over a large q-range.

The answers to the above questions will determine how you run your experiment and for how long you will run it.

Appendix 2 has a table of the available standard configurations for this system. It shows aperture sizes, detector distances, q-range and intensities. In planning your measurement understanding this table is crucial.

The first thing to realize is that in the routine running of the instrument you have a unique chance to trade off resolution for intensity. The intensity available in the WAXS configuration (configuration 1) is a factor of 4-5 higher than in the MAXS-configuration and again a factor 4-5 higher than in the SAXS-configuration, and once again a factor 4-5 more than in the extreme SAXS regime. Flux is one of the most expensive things in an x-ray instrument, so think about the resolutions (and the q-range) you need and run your measurement accordingly.

In general, it is also our impression that users who are looking for Peak Positions and Particle sizes spend much too much time measuring to get the low-intensity portions of the curve to look nice. Think about what you are looking for, measure it to the accuracy that you need and move on.

Checking the instrument performance

In order to use the system you need to make sure:

1) The instrument control computer is on
2) The detector control computer is on
3) The Motor Drive and controller is on
4) The SAXSLAB software environment is running
5) The pump and the pump-cooler are on
6) The x-rays are on and at full power
7) The pressurized air is on
8) The camera is on
9) That the remote disk containing the data is accessible.

If any of these are not satisfactory, you can contact the instrument responsible or try to fix it yourself as outlined in Appendix 3.

If the system is not running at all you should contact the instrument responsible or try to start it yourself as outlined in Appendix 4

Preparing and mounting the sample

Samples need to be prepared for measurement in vacuum. Depending on the samples this may mean inserting them in disposable capillaries, putting them in sandwich cells, inserting them in refillable capillaries or doing nothing at all. Please see Appendix 4 for some inspiration.

Sample Alignment

Establishing a vacuum

When samples are mounted and everything is ready to go, the system should be evacuated. This can be done with the spec command:

>evacuate_system

It will take roughly 4 minutes to reach the operating pressure of 2E-1 mbar. It is possible to measure data long before this level has been reached, but the background scattering from residual air will be too high for weakly scattering samples.

The vacuum will continue to improve over the evacuation time, but this will not affect the measurements.

If 2E-1 cannot be reached please try to look for unattached hoses or other leaks or a lack of pressurized air (which means the evacuation valve can not be opened)

Alternatively have the instrument responsible take a look.

Telling spec what sample holder is mounted

In order to make sure that the calibration holds for different sample holders it is important that spec “knows” which stage is mounted.

The spec command:

>change_sample_stage

will give you a list of stages to choose from. Choose the correct one and proceed.

Note: There may be sample stages that have not been calibrated)

Goniometer Motions

The standard motors (and motions) in the sample goniometer are:

- zsam--- Vertical motion (Z-axis) – A total travel of ~80 mm is available
- ysam--- Horizontal motion (Y-axis) – A total travel of ~80 mm is available
- thsam--- Rotation around the vertical Axis (thetat-motion) +-180 mdegrees.

The position of these motors (and all the others) can be seen by the spec-command:

>wu

The motors can be moved with the commands (examples):

>mv zsam 10
>umv ysam 40
>mvr zsam -5
>umvr thsam 1

The place where the beam hits the sample can be scanned by the command

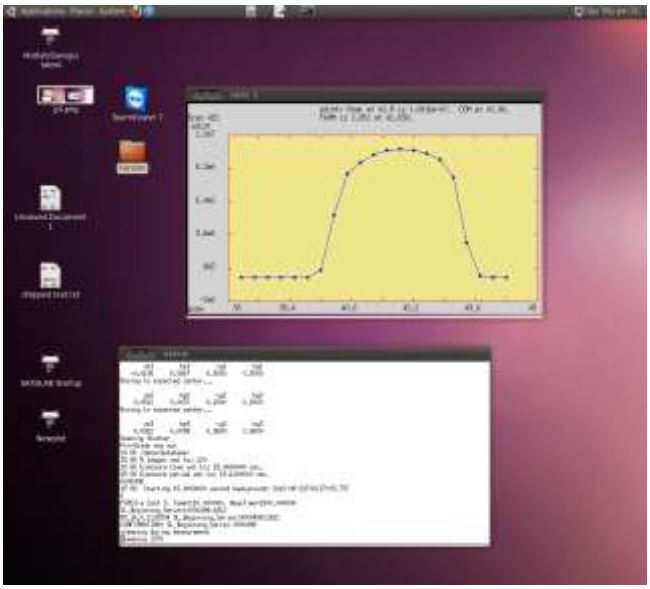
>ascan zsam 30 45 15 1 (which scans zsam from pos 30 to 45 in 15 intervals counting 1 second per interval)

>dscan ysam -3 3 12 1 (which scans ysam relatively from relative pos -3 to relative position 3 in 12 intervals counting 1 second per interval)

However do remember to insert the pin-diode, and open the x-ray shutter, so the overall measurement will have the following command flow:

>pd_in
>o_shut
>dscan ysam -3 3 12 1
>c_shut
>pd_out

A scan of a hole in a sample in a block could look like this.



<u>Aligning the sample –by using the on-axis camera</u>

The on-axis camera helps to obtain a rough idea of where the sample is.

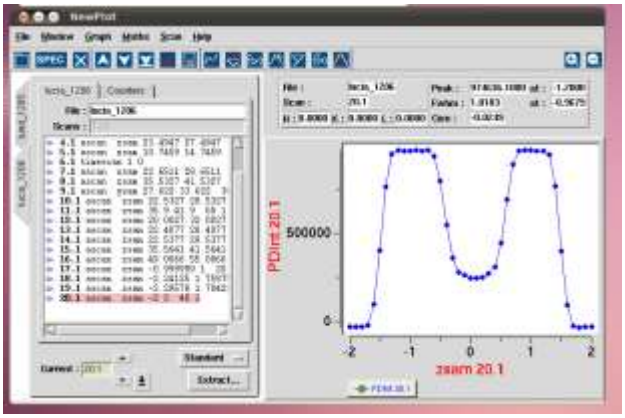
The cross indicates where the beam is. And one can then use a transmission measurement combined with a scan (as immediately above) to do a fine alignment.

Aligning the sample – by using the pin-diode and scanning motors

After having performed the rough alignment with the camera, one can perform a scan like this.

>pd_in
>o_shut
>dscan ysam -3 3 12 1
>c_shut
>pd_out

This could yield this plot, which we could analyze to determine the best sample position.



However, for capillaries there is a dedicated routine, that does the same

>capalign ysam -3 12 1

AND moves to the best spot by itself. Very useful.

Where's the blank?

In order to make transmission measurements, we need to measure the transmitted intensity through the sample. But we also need to measure the intensity without any absorption, i.e. the Io.. So we need to define a blank spot, where there is no sample (if we want to measure transmission). We do this with these spec commands

>mv ysam 12.4
>mv zsam 35.4
>blankpos_def

Please note that the stage is first moved to a position and then this position is defined as the blank position. This is to make sure that you do not make an error and specify a position that cannot be moved to.

Pre-measurement Actions

Choosing a q-range /configuration

Based on the table of the various configurations in Appendix 2, one can decide which combination of resolution, q-range and intensity is desired. Once this has been decided, one can go to this configuration using the spec command:

>conf_ugo N…..where N is the number of the configuration (forexample conf_ugo 1)

Letting the computer adjust the beam stop position

It has been our experience that the most sensitive alignment is the location of the detector with respect to the beam, which ultimately means the location of the beam stop with respect to the beam. In order to correct for this, the system has a small routine which can be executed on its own.

So if you wish, you may run the spec command:

>mv_beam2bstop

to center the beamstop on the beam.

Note: This routine relies on the beamstop being centered on a reference position on the detector. If for some reason it is not centered on here (someone bumped or similar) then one will have to redefine either motor positions or this reference positioned as described in the "Expert Users FAQ"

Measuring Io and the sample transmission

If a blank position has been defined, one can issue the command:

>transmission_measure

to measure the Izero as well as the transmission, using the pin-diode.

The Izero is stored in the spec variable I0 and the transmission is stored in the variable SAMPLE_TRANS.

Describing the measurement

For entering into the header, as well as the super log file (master.dat) one may define the value of the spec variable SAMPLE_DESCRIPTION like this:

>SAMPLE_DESCRIPTION=”This is my sample in configuration 3 measured for 300 seconds”

This string is then saved to the file header and displayed in SAXSGUI when the file is loaded.

Additional Reduction Parameters

In addition to these measured parameters one can also enter the following parameter

>SAMPLE_THICKNESS=0.1 #where thickness is given in cm

Beam Stop Mask

To facilitate quick data-reduction one can also specify a beamstop mask that will be applied to the data when reduced in SAXSGUI. A beamstop mask particular to each configuration has been defined. To invoke this feature one can write

>use_bsmask

NOTE: All these reduction parameters SAMPLE_DESCRIPTION, SAMÅLE THICKNESS and use_bsmask are reset after a successful measurement.

Telling SPEC that it is for real

The command

>saxson

is a necessary command to tell spec that this measurement is for real and that it needs to establish connection to the detector computer. It can be entered anytime and is assumed “on” until a saxsdiscconnect command is given.

Pre-measurement routine

So the preparation of a measurement could look like:

>evacuate_system
>do_sleep (250)

>conf_ugo 2
>saxson
>mv_beam2bstop
>mv ysam ysamblank
>mv zsam zsamblank
>blankpos_def
>mv ysam ysam_roughpos
>mv zsam zsam_roughpos
>capalign ysam 2 40 1
>transmission_measure
>SAMPLE_DESCRIPTION=”my sample”
> use_bsmask
> SAMPLE_THICKNESS=0.1

The Measurement

The Measurement command and on-screen feedback

Given all the preparation from before we now just need to issue the command

>saxsmeasure *time*

Where *time* is the desired exposure time in seconds.

Once the measurement has started, a number of messages are output to the spec window. One should just look at the output screen to make sure that a file is actually recording.

If it is not recording it is likely that one has forgotten the

>saxson

spec-command.

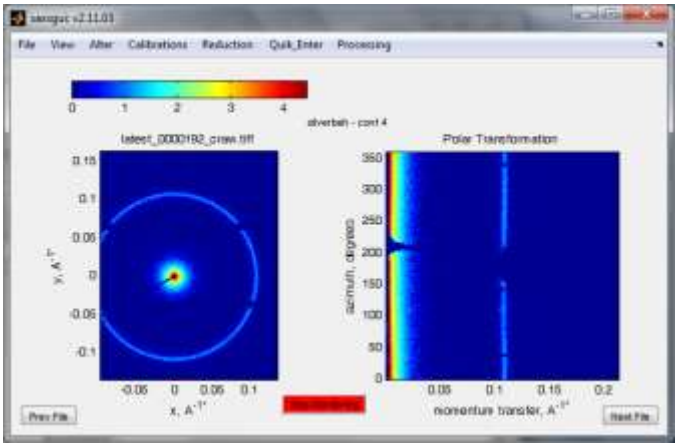
Monitoring the measurement from SAXSGUI

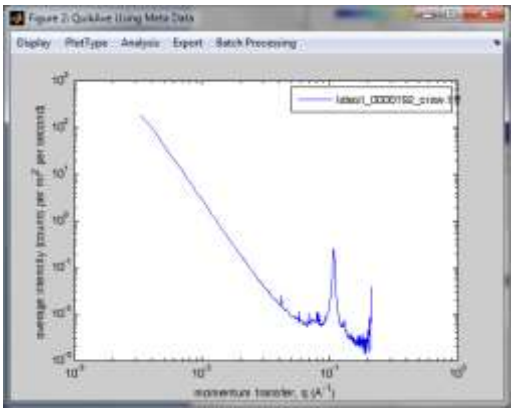
SAXSGUI has recently been upgraded to allow it to monitor the development of the data-gathering both in a 2D image and in a 1D plot.

This functionality can be obtained by accessing the menu:

>File >Open Latest (cont)

In SAXSGUI



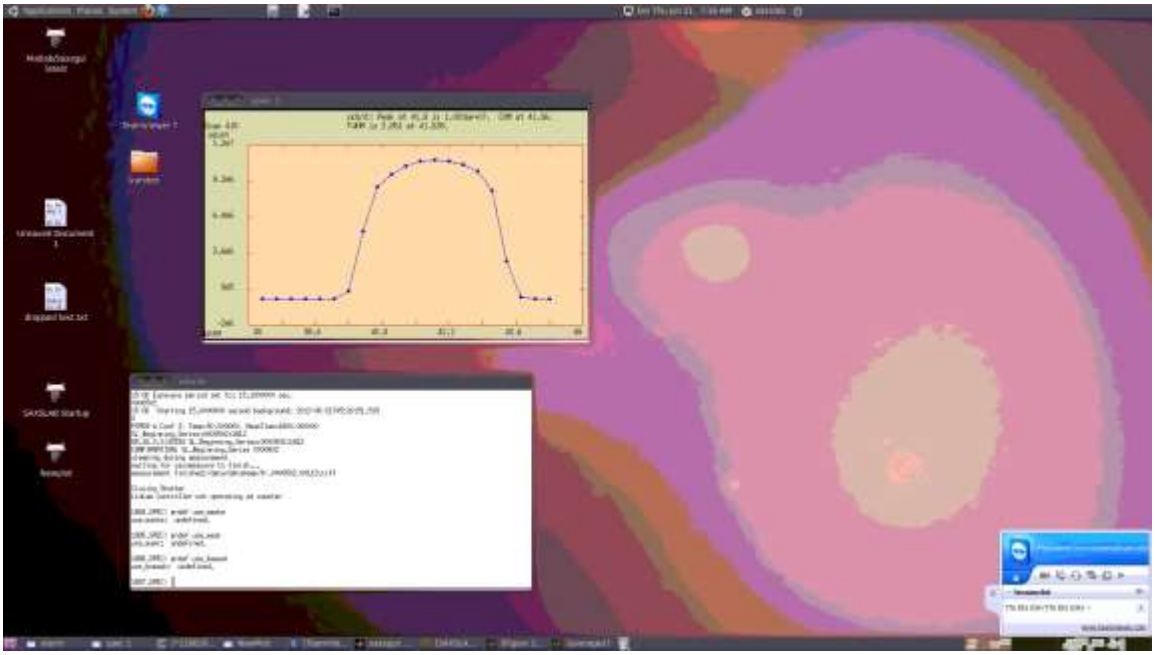


Monitoring the measurement remotely by Teamviewer

All systems come with Teamviewer installed. Teamviewer is a state of the art desktop sharing software, with free usage for non-commercial use.

With Teamviewer, the operator may monitor the system from a remote location.

Naturally such access is dependent on the internet access policy of the organization



Interactive Data Reduction

SAXSGUI is the main data-reduction tool available with the system. It has its own manual and even its own basic website (www.saxsgui.com).

The source-code can be found at

http://www.saxsgui.com/latest_saxsgui_saxslab.zip

The latest executables can be found at

http://www.saxsgui.com/latest_saxsgui_SLlinux32.zip (linux 32-bit)

and

http://www.saxsgui.com/latest_saxsgui_SLwin32_prg.exe (windows 32-bit))

If one already has the appropriate Matlab Runtime Library one can choose to download instead

http://www.saxsgui.com/latest_saxsgui_SLwin32.exe

which is just the program.

The latest manual (often not completely current) can be found at

http://www.saxsgui.com/latest_manual.pdf

or

http://www.saxsgui.com/latest_manual.doc

Viewing the data

SAXSGUI was originally created for very interactive viewing of data collected on less automated instrumentation. It therefore features a long list of interactive methods to visualize, alter, center and calibrate the data.

However, it has been adapted to make extensive use of the header information available in the Ganesha data file.

As a result when a file is opened, both the image, the polar plot and the radial average will be displayed. Each window has a range of tools and menus for displaying the data.

Interactive Centering and Calibrating

Due to the program history there is a long list of interactive methods to visualize, alter, center and calibrate the data, which will normally not be required, as the relevant information is usually already in the metadata header.

Reductions

Some reductions are presently available in the metadata

- transmission correction
- intensity correction
- sample thickness correction
- beam stop mask

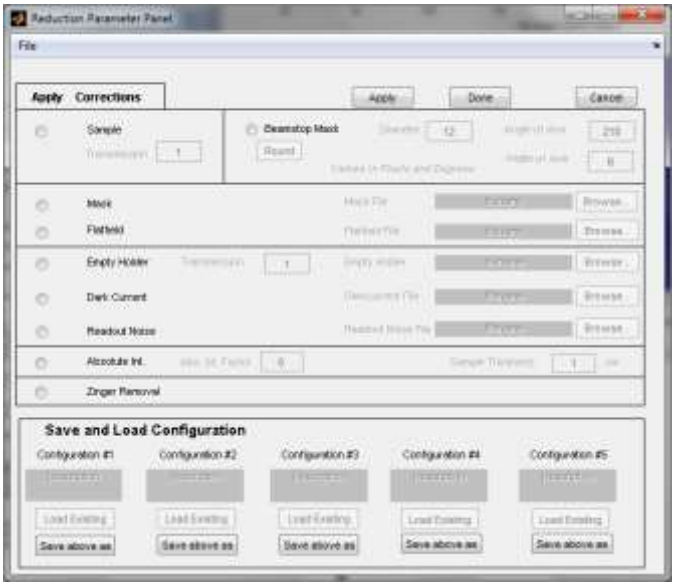
However relational reductions (relating to other files) such as

- empty holder reduction
- darkcurrent reduction
- zinger reduction

are not presently supported in the Ganesha meta-data format.

To reduce the data further one may therefore use the Reduction Panel in the Reduction Menu.

This panel will be filled with parameters from the metadata header and relational files can be added.



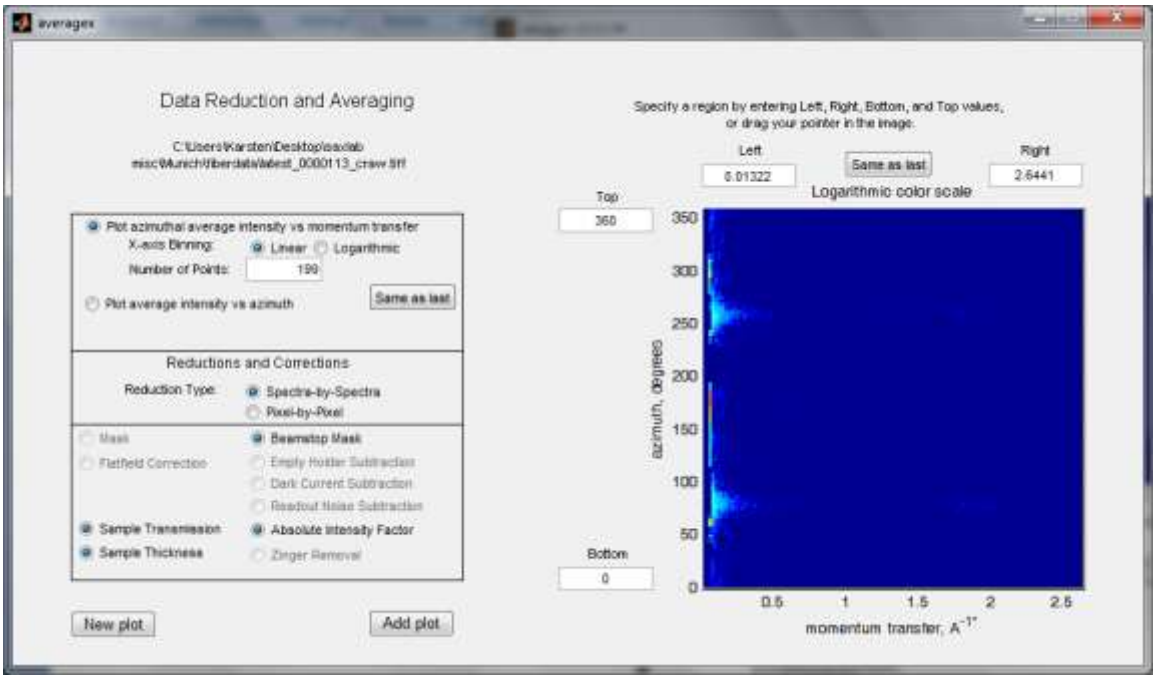
Masking

In the reduction panel “File” menu there is a Create Mask item. This will open up MaskMaker which is a mask-building tool for SAXSGUI.

Averaging

Averaging is performed from the processing menu. The GUI gives the options to choose the averaging parameters and reductions interactivey.

Basic Analysis



From the averaged plot one may inspect the data and perform simple analysis such as peak-fitting and Guinier fitting.

Exporting the data

From the averaged plot the data may be exported in various formats. The GRAD format is the most comprehensive. See Appendix 6 for a complete description of this format.

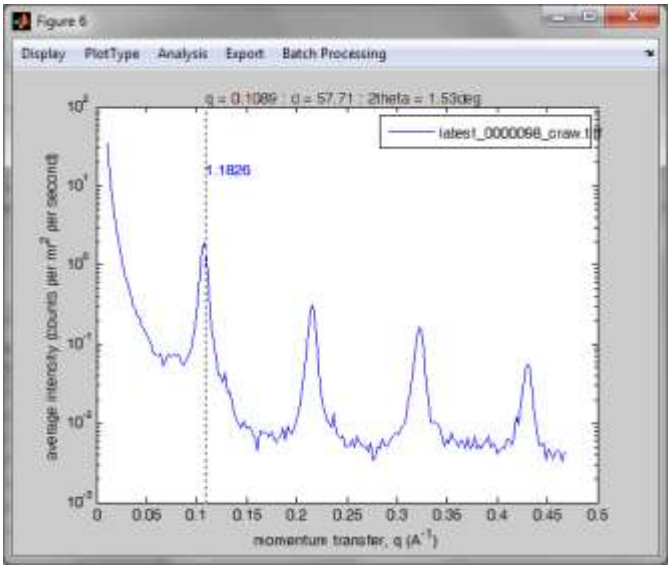


Figure 6
Display
PlotType
Analysis
Export
Batch Processing
q = 0.1089 ; d = 57.71 ; 2theta = 1.53deg
latest_0000098_craw.tif
1.1826
average intensity (counts per mm² per second)
momentum transfer, q (A⁻¹)
0
0.05
0.1
0.15
0.2
0.25
0.3
0.35
0.4
0.45
0.5

Automated Processing(AP) (based on the metadata header)

SAXSGUI has been expanded to automate a lot of the tedious tasks associated with data reductions, using the information in the metadata-header.

Quick Experiment Overview
If one uses the “Next” and “Previous” buttons in the panel, one can quickly investigate a series of measurements.

The radial average plot of each new image is added to the plot.
Note. If the number of datasets plotted become too large simply close the window.

Exporting the AP data
When many files are generated, the interactive reduction becomes tedious. However, using the metadata information, it is possible to automatically process the files and save

- 2D images
- 1D plots
- Data in SAXSLAB GRAD format (see Appendix 7 for examples)

This can be done by going to Processing->Autoprocess-AP with Metadata. Then you will be prompted for which files to process and which directory to save the processed data to.

Tips for Exporting the AP-data
The automated processing uses the sizes of the windows to generate the images. If you find that the plots in the automated images do not look nice, try making the size of the window larger.

Known Limitations in AP on the Ganesha

SAXSGUI (as in any other software package) in always in development, with a timeframe determined by priority and difficulty.

Many Measurements

In the previous sections, we showed how to prepare and measure a single sample in a single measurement.

Of course normally one would want to investigate the sample for a broader range of q-values than accessible with a single measurement or measure several samples. Both examples are explored below

Examples of many measurements

Changing configurations
The command for changing configurations was

```
conf_ugo configuration_number
```

which becomes useful, for example, with many measurements of a capillary over many configurations:

```
evacuate_system  #Evacuate the system
do_sleep (250)          #Waits for the evacuation
conf_ugo 2              #Go to configuration 2
saxson                  #Make sure spec knows we want to communicate
mv_beam2bstop           # Adjust the detector
mv ysam ysamblank # Move to the Y-position of the blank sample position
mv zsam zsamblank #Move to the Y-position of the blank sample position
blankpos_def            #Define this position as the blank
mv ysam ysam_roughpos       #Move to the sample Y position (nominal)
mv zsam zsam_roughpos       #Move to the sample Zposition (nominal)
catalign ysam 2 40 1        #Align the capillary
transmission_measure        # Measure the sample transmission and Izero
SAMPLE_DESCRIPTION=”my sample in conf 2”
 use_bsmask                 #Use a beamstop mask for processing
 SAMPLE_THICKNESS=0.1 #Use a sample thickness in cm for processing”
saxsmeasure time            #Measure for an amount of time

#Now for new configuration
conf_ugo 2              # Go to configuration 2
mv_beam2bstop           # Adjust the detector
transmission_measure        #Measure Sample transmission and Izero
SAMPLE_DESCRIPTION=”my sample in conf 2”
use_bsmask                  #Use a beamstop mask for processing
 SAMPLE_THICKNESS=0.1 #Use a sample thickness in cm for processing”
saxsmeasure time            #Measure for an amount of time
```

Changing Samples

Another example is moving to a different location:

```
evacuate_system  #Evacuate the system
do_sleep (250)          #Waits for the evacuation
conf_ugo 2              #Go to configuration 2
saxson                  #Make sure spec knows we want to communicat
mv_beam2bstop           # Adjust the detector
mv ysam ysamblank # Move to the Y-position of the blank sample position
mv zsam zsamblank #Move to the Y-position of the blank sample position
blankpos_def            #Define this position as the blank
mv ysam ysam_roughpos1    #Move to the sample Y position (nominal)
mv zsam zsam_roughpos1    #Move to the sample Zposition (nominal)
catalign ysam 2 40 1            #Align the capillary
transmission_measure          # Measure the sample transmission and Izero
SAMPLE_DESCRIPTION=”my sample #1 in conf 2”
 use_bsmask                   #Use a beamstop mask for processing
 SAMPLE_THICKNESS=0.1 #Use a sample thicknes in cm for processing”
saxsmeasure time              #Measure for an amount of time

#Now for new sample
ysam ysam_roughpos2         #Move to the sample Y position (nominal)
mv zsam zsam_roughpos2    #Move to the sample Zposition (nominal)
catalign ysam 2 40 1            #Align the capillary
transmission_measure          # Measure the sample transmission and Izero
SAMPLE_DESCRIPTION=”my sample #2 in conf 2”
 use_bsmask                   #Use a beamstop mask for processing
 SAMPLE_THICKNESS=0.1 #Use a sample thicknes in cm for processing”
saxsmeasure time              #Measure for an amount of time
```

Constructing advanced sample descriptions

From the 2 examples above you can see there is a lot of repetition involved in these cases. Yet, generally, you want the sample description to be quite specific about the measurement, so here is a way to construct a very specific header.

Let's say

```
myconf=2
conf_ugo myconf
saxson                  #Make sure spec knows we want to communicat
mv_beam2bstop           # Adjust the detector
mv ysam ysamblank # Move to the Y-position of the blank sample position
mv zsam zsamblank #Move to the Y-position of the blank sample position
blankpos_def            #Define this position as the blank
mv ysam ysam_roughpos1    #Move to the sample Y position (nominal)
mv zsam zsam_roughpos1    #Move to the sample Zposition (nominal)
catalign ysam 2 40 1      #Align the capillary
transmission_measure      # Measure the sample transmission and Izero

strtmp=sprintf("Blah conf %i , IO=%i, T=%f" (myconf, Io,SAMPLE_TRANS))
SAMPLE_DESCRIPTION=strtmp
saxsmeasure 300
```

The sprintf command prints the values of myconf, izero and SAMPLE_TRANS to the Sample Description String.

Sprintf uses the same syntax for formatted output as the common computing commands sprint and fprintf.

Constructing a macro for multiple actions (with gedit)

Rather than writing all of these commands on the spec command line, they can be put in a txt-file. There is a decent text editor available (gedit) which can be used to write the series of command

Executing a macro from Spec

With the file is saved it is possible to call this "macro-function" by the following spec command

```
qdo directory/filename
```

An Experiment

The nature of an experiment

The above examples have all been examples of simple measurements, i.e.

1) Measure a sample for a certain amount of time in one configuration
2) Measure a sample in a number of different configurations
3) Measure many samples in one or more configurations

But often there is a need to do more complicated measurements, where typical characteristics of the sample are altered. For example, performing measurements at different temperatures.

In these more complicated scenarios, we speak of experiments. Due to their complexity, the experiments yield themselves well to inserting the command sequences into macros

Free-form or loops in SPEC

An experiment can of course be written into a macro as a series of individual measurements (the freeform – commands shown are not actual spec command)

```
Prepare experiment
Set temperature to 10 degrees
Describe Sample
Measure
Set temperature to 12 degrees
Describe Sample
Measure
```

But one can also use the loop structures available in spec

```
Prepare experiment
For (icnt=1;icnt<5;icnt++) {
        Mytemp =( icnt-1)*2+10
        set temperature to Mytemp
        Describe Sample
        Measure
}
```

This loop will measure 5 times, starting at 10 degrees and finishing at 18.
In such cases, it is very useful to construct the advanced sample descriptions as discussed above as for example:

SAMPLE_DESCRIPTION=sprintf(“My Great Sample Temp=%d”;Mytemp)

Varying position

To vary the position or angle of the sample one can use the commands

mv, umv, mvr, umvr

as discussed earlier in this manual.

The sample motors that can be manipulated are

ysam, zsam, and thsam

So a position scan could look as follows

```
for (icnt=0;icnt<10; icnt++) {
        ysamstart=42
        ysamstep=1
        ysampos=ysamstart+icnt*ysamstep
        mv ysam ysampos
        SAMPLE_DESCRIPTION=sprint("Mysample ysam=%d",A[ysam])
        use_bsmask
        saxsmeaure 600
}
```

And of course one could make a 2D scan by enclosing the above loop within another loop

```
for (icnt1=0;icnt1<10; icnt1++) {
        zsamstart=10
        zsamstep=1
        zsampos=zsamstart+icnt1*zsamstep
        mv zsam zsampos
        for (icnt2=0;icnt2<10; icnt2++) {
                ysamstart=42
                ysamstep=1
                ysampos=ysamstart+icnt2*ysamstep
                mv ysam ysampos
                tmp= sprint("Mysample xsam=%d, ysam=%d", A(ysam), A(zsam))
                SAMPLE_DESCRIPTION=tmp
                use_bsmask
                saxsmeaure 600
        }
}
```

Varying Temperature with the Julabo Circulating Heater/Chiller

Useful Commands for the Julabo

Julabo Thermostated Bath	
julabo_start	Switches ON the Julabo Unit
julabo_end	Switches OFF the Julabo Unit
julabo_stabilise *s_p stabilization_time maxtime*	Sets setpoint to *s_p* and logs temperature until the temperature is reached. After the temperature is reached it stabilizes for the given time. If reaching the temperature takes more than *maxtime* then the command is stopped
_julabo_get_temperature()	Returnt the temperature of Julabo stage
julabo_get_temperature	Prints out the current temperature to the screen

An example macro

```
julabo_start
for (icnt=0;icnt<10; icnt++) {
        mytempstart=42
        mytemstep=0.5
        mytemp=mytempstart+icnt*ysamstep
        julabo_stabilise mytemp 300
        tmp= sprint("Mysample temp=%d",_julabo_get_temperature())
        SAMPLE_DESCRIPTION=tmp
        use_bsmask
        saxsmeaure 600
}
julabo_end
```

Varying Temperature with the Linkam Heater stage

Useful Commands for the Linkam Heater Stage

Linkam Thermal Stage Commands	
linkam_start	Switches ON communication with Linkam Controller (overhead cost = 4 seconds)
linkam_end	Switches OFF communication with Linkam Controller
linkam_pump_auto	Start the Linkam pump in auto mode. Manual mode can also be set Linkam_pump_manual, and then Linkam_set_pumpspeed. But this is not recommended
linkam_stabilise *s_p maxtime*	Sets setpoint to *s_p* and logs temperature until the temperature is reached. Unless *maxtime* is exceeded.
_linkam_get_temperature()	Returns current temperature of Linkam stage
linkam_get_temperature	Get current temperature of Linkam stage
linkam_get_rate	Get current ramp rate for Linkam stage
linkam_get_setpoint	Get current setpoint for Linkam stage
linkam_set_rate *rate*	Sets the temperature ramp rate to *rate degrees per minute*
linkam_set_setpoint *temp*	Sets the temperature to *temp* degrees
linkam_set_pumpseed *nn*	Sets the pumpspeed to nn%
linkam_watch *maxtime*	Logs the temperature for *maxtime*
linkam_cool	Cools the Linkam stage as fast as possible

An example macro

```
linkam_start
linkam_pump_auto
linkam_set_rate 10
for (icnt=0;icnt>10; icnt++) {
        mytempstart=80
        mytemstep=5
        mytemp=mytempstart+icnt*ysamstep
        linkam_stabilise mytemp 180 900
        tmp= sprint("Mysample temp=%d",_linkam_get_temperature())
        SAMPLE_DESCRIPTION=tmp
        use_bsmask
        saxsmeaure 600
}
linkam_end
```

Appendix 1: The SAXSLAB metadata-header

```
# <SAXSLAB METADATA START>
# datatype: tiff
# detectortype: PILATUS 300K
# start_timestamp:
# end_timestamp:
# save_timestamp:
# realtime:
# livetime:    1800.00
# pixelsize: 0.172 0.172
# beamcenter_nominal:     338.50    201.50
# beamcenter_actual:     338.47    201.42
# <DATA METADATA START>
# data_mean:
# data_min:
# data_max:
# data_rms:
# data_p10:
# data_p90:
# <DATA METADATA END>
# <CALIBRATION METADATA START>
# calibrationtype: geom
# kcal:
# pixelcal:
# koffset:
# wavelength: 1.5408
# detector_dist: 1056.2000
# <CALIBRATION METADATA END>
# <CONFIGURATION METADATA START>
# saxsconf_r1:
# saxsconf_r2:
# saxsconf_r3:
# saxsconf_l1:
# saxsconf_l2:
# saxsconf_l3:
# saxsconf_l4:
# saxsconf_wavelength: 1.5408
# saxsconf_dwavelength: 0.01
# saxsconf_Izero: 211338
# saxsconf_det_offx: 0
# saxsconf_det_offy: 0
# saxsconf_det_rotx: 0
# saxsconf_det_roty: 0
# saxsconf_det_pixsizez: 0.172
# saxsconf_det_pixsizey: 0.172
```

```
# saxsconf_det_resx_0:
# saxsconf_det_resy_0:
# saxsconf_abs_int_fact:
# <CONFIGURATION METADATA END>
# <SAMPLE METADATA START>
# sample_transfact:    0.00000
# sample_thickness:
# sample_xpos:
# sample_ypos:
# sample_angle1:
# sample_angle2:
# sample_angle3:
# sample_temp:
# sample_pressure:
# sample_strain:
# sample_stress:
# sample_shear_rate:
# sample_concentation:
# <SAMPLE METADATA END>
# <SPEC METADATA START>
# hg1: 0.299975
# hp1: 0.084741
# vg1: 0.299975
# vp1: -0.010509
# hg2: 0.149987
# hp2: 0.003747
# vg2: 0.149987
# vp2: 0.051181
# hg3: 0.360010
# hp3: 0.009861
# vg3: 0.360010
# vp3: 0.093097
# ysam: 41.840000
# zsam: 39.290000
# thsam: 0.000000
# detx: 950.000000
# dety: -0.815313
# detz: 0.890944
# bstop: 42.120000
# pd: 10.000000
# <SPEC METADATA END>
# <GENERATOR METADATA START>
# source_type: MM002+
# source_runningtime:
# source_kV: 42 kV
# source_ma: 0.95 mA
# <GENERATOR METADATA END>
```

```
# <DEFAULT REDUCTION RECIPE START>
# xaxis:
# xaxisfull:
# yaxis:
# error_norm_fact: 1
# xaxisbintype: lin
# log:  log
# reduction_type: s
# reduction_state:
# raw_filename:
# mask_filename:
# flatfield_filename:
# empty_filename:
# solvent_filename:
# darkcurrent_filename:
# readoutnoise_filename:
# zinger_removal: 0
# data_added_constant: 0
# data_multiplied_constant: 1
# <DEFAULT REDUCTION RECIPE END>
# <SLDS START>
# Img.Class:
# Img.MonitorMethod:
# Img.ImgType: 2D
# Img.Site: KU-LIF
# Img.Group:
# Img.Researcher:
# Img.Operator:
# Img.Administrator:
# Img.Description
# Meas.Description: PSPEO-a Conf 3, Temp=110.000000,
MeasTime=1800.000000
# <SLDS END>
# <SAXSLAB METADATA END>
```

Appendix 2: Standard Configurations

Conf	Mne	Description	DETX	Sample Det-Dist	Ideal beam stop	Aperture size (mm)	qmin	qmax	Io Mphs
0	Open	Open Apertures	50	NA	NA	4-4-5			80
1	WAXS	Wide Angle	50	~180	2mm	0.7-0.4-1.0	0.05	2.5	20
2	MAXS	Medium	350	480	2mm	0.4-0.3-0.7	0.012	0.67	6
3	SAXS	SAXS	950	1080	2mm	0.3-0.15-0.4	0.006	0.26	1.5
4	E-SAXS	Extreme SAXS	1400	1540	2mm	0.2-0.1-0.3	0.003	0.21	0.3

Appendix 3: Checking that the instrument is ready

Before you can measure with the instrument the following have to be fullfilled:

1) The instrument control computer is on
2) The detector control computer is on
3) The Motor Drive and controller is on
4) The SAXSLAB software environment is running
5) The pump and the optional pump-cooler are on
6) The x-rays are on and at full power
7) The pressurized air is on
8) The camera is on
9) That the remote disk containing the data is accessible.

Checking if the instrument control computer is on:
The green light on the upper right hand corner is on.

If it is Orange, press it for a couple of seconds to start the computer.

If it is green, but you have no signal on the monitors, move the mouse a bit, to see if the monitors liven up. If not then try the standard things: mouse-batteries, loose cables, etc.

If nothing helps, it may be necessary to turn off the Instrument Control Computer by holding the on-button in for 8 seconds and then restarting

Checking if the detector control computer is on
There is here a button on the left side of the detector control computer, which is green if it is on.

If not…press it.

Checking if the Motor Drive and controller is on

The Motor Drive and Controller is on if the green light on the front panel toggle button is on. There should also be a clearly audible hum from the fan. If it is not on, turn it on.

Checking if SAXSLAB software environment is running

Press “Start Saxslab” to start opening the all the software.
If you later notice that something has not started this indicates a serious fault and you should contact your instrument responsible.

Checking if the pump and cooler is on

You will be able to hear, if these are on. If the pump cooler for the dry pump is not on, the dry pump will stop after a couple of minutes.

Checking if the x-rays are on and at full power

If X-rays are on, the orange lamp on top of the instrument will be lit.
If the generator is at full power the settings should be close to 50kV, 60mA (but slightly below).
You can also inquire about these values by using the spec commands

>p genix_get_HT()

>p genix_get_current()

Checking if the pressurized air is on

Pressurized air is required for purging the detector (clean dry air) and providing power to open the ventilation and evacuation valves.

You should hear a slight hissing from the pipes, if the air is on. You can also try to operate the vent valve by using the spec commands:

>ventvalve_open
>ventvalve_close

and listening for the sound of air hissing as the valve changes state.

Checking to see if the camera is on
There will be 2 green lights on the camera underside. Power and Communication. Of course the image should also be displayed in the sample viewer window.

Checking to see if the remote disk (/disk2) is mounted
Data is located on the detector computer disk, which is remotely mounted for access.

To check if the remote disk has mounted correctly, open a terminal on the linux desktop and write

ls /disk2/data

This command should list the directories latest, images, frames and stats

If not please run the command

sudo mount –a

and test again. If it still fails contact the instrument responsible

Appendix 4: Sample Preparation for the Ganesha SAXS system

With heavy inspiration from Ronit Bitton, Ben Gurion University

Preparing the sample(s)

Powder samples

If the samples are powders, they can conveniently be mounted in a capillary or in between two pieces of tape. Sometimes using the hole of a small washer (with tape on both side of the washer is a good simple way to prepare a thicker powder sample. 3M Scotch tape is fairly good but does have some weak low-q scattering.

Alternatively, one can use the "Sandwich Cells" provided for the Linkam stage, and fill them as described for Viscous Liquid Samples

Non-viscous Liquids samples

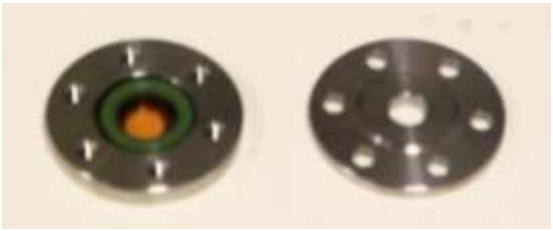
Non-viscous liquids can be inserted into a capillary. The capillary should be sealed either by wax, glue or flame-sealing, or by using one of the "reusable" capillary holders where sealing is done with an O-ring.The capillary should ideally be free of bubbles; containing as little air as possible (the pressure from the residual air has been known to break some capillaries). Please treat capillaries with care. Free-standing capillaries are typically 3-4 € per piece and reusable capillaries are more than 500€ (up to 1000 € by some vendors)

Viscous Liquids samples

Viscous liquids are difficult to get in and out of capillaries. As a consequence we use holders where the viscous liquids are sandwiched between 2 thin sheets of either Mica or Kapton (10 mm diameter). These are intended for use with the Linkam stage, but can be mounted anywhere.

We prefer Mica windows, since scattering is very low and very uniform. However, since absorption is high in Mica, the windows must be very thin, and thus unfortunately become costly. ~4 € for 5-7 micron thick window.

SAXSLAB can supply the required Mica sheets.



Mounting the sample(s)

The systems would normally be supplied with this stage

- A 2D ambient temperature stage, where 42 sample positions are provided

And may then contain the following optional stages

- A JSP multi-capillary holder for capillaries (both refillable and non-refillable) with temperature control (5-70C).

- A special vacuum adapted Linkam thermal stage for thermal analysis, which allows for mounting one flat solid sample, one capillary inserted into the thermal block or one sandwich cell. Temperature range is -150C-300C
  The maximum heating/cooling rate of 30 C/min.

Generic Stage:

Samples can be fixed to the generic stages by using tape, vacuum grease, wax or holes in the sample holder that fit the pins on the generic stage.

Capillaries should be mounted vertically.

The sample holder is inserted into the chamber by sliding it into the gap in the sample stage

The writing on the side of the sample holder should be facing the chamber door (you)

GISAXS in generic holder

Tape the sample in the middle of the sample holder sticking out on top

The sample holder is inserted into the chamber by sliding it into the gap in the sample stage

Multi-capillary holder:

This holder fits 6 capillary metal cartridges. The cartridges should be filled, capped and inserted all the way into the holder. A pin will ensure that they are placed reproducibly.

Linkam thermal stage:

The stub below the thermal block should be fitted with a spring which forces the sample or the sandwich holder up against the block. The springs supplied by Linkam have a “lollipop” shape and there is 1 such “lollipops” provided

It should be possible to change samples without taking out the block

For samples in capillaries an alternative mounting approach is used, in that the capillary can be inserted horizontally into a small (1.6 mm) hole in the block. 1 and 1.5 mm capillaries should fit. With a little bit of care the capillary can be inserted from outside the stage body.

Alternatively one can screw a small lid on the heater plate, and insert the capillary into this lid.

Appendix 5: Ganesha SAXS installation- SPEC Quick Reference (12/06/20)

Most used Commands	
vent_system, evacuate_system	Vent and evacuate the SAXS system
c_shut, o_shut	Close and Open the Shutter
conf_go, conf_ugo, what_conf	Go to a predefined configuration, update
mv, umv, mvr, umrv	Moves motors in different ways
wu	Shows motor positions
ascan, dscan, lup	Different types of motor scans
pd_in , pd_out	Move pin diode detector into the beam
SAMPLE_DESCRIPTION="hello"	Sets a parameter that is written to master.dat and image header
saxsmeasure , killsaxsmeasure	Takes and image and saves it, kill the saxsmeasurement completely
transmission_measure, blankpos_def	Measures the transmission of a sample, define blank position
qdo *macro-file*	Execute the commands in the macrofile (quiet do)
mv_beam2bstop	Centers the beam on the beamstop
Light_on, Light_off	Centers the beam on the beamstop
Standard SPEC Commands	
>spec	to run *spec-session* from UNIX window
wa	list of all defined motors with its user and dial values
wu	list of all defined motors with its user values
wm *motor-name1 motor-name2 ...*	where motors: user and dial values, soft limits of motors
mv *motor-name number*	absolute move of a motor by *number* [mm] or [º]
mvr *motor-name number*	relative move of a motor by *number* [mm] or [º]
umv *motor-name number*	updated absolute move of a motor by *number* [mm] or [º]
umvr *motor-name number*	updated relative move of a motor by *number* [mm] or [º]
ascan *motor-name init_value final_value nº_of_steps time_per_step*	absolute scan – remember to open shutter before running this
dscan *motor-name init_value final_value nº_of_steps time_per_step*	relative scan – remember to open shutter before running this
lup *motor-name init_value final_value nº_of_steps time_per_step*	relative scan, which goes to the peak afterwards
counters	define your counters
setplot	define parameters of the plot on the screen
plotselect	define counters to be plotted
Ctrl-**C**	stop execution of a command
newsample	Allows to define parameters for new sample (filename, plot window etc)

prdef *macro-name*	listing of commands in a known macro
lsdef *name*	list of known macros conatining string *name*

Beam stop and Pin-diode Related Commands	
change_bstop_conf	Change the desired beam stop position/configuration
bstop_in	Move the beam stop into nominal position
bstop_out	Move the beam stop out of the detector area
pd_in	Move Pin-diode into beam
pd_out	Move Pin-diode out of beam
Configuration Related Commands	
what_conf	Ask what configuration is most likely the present
conf_go *conf#*	Go to the configuration specified (using configuration variables)
conf_ugo *conf#*	Go to the configuration specified (using configuration variables) – updating positions
conf_lineup *conf#*	Create lineup procedure for configuration specified
full_conf_lineup *conf#*	Create lineup procedure for configuration specified including detector alignment
detpos_go *conf#* **detpos_ugo** *conf#*	Go to the detector position in the specified configuration
conf_save *conf#*	Save the present pinhole location to the pinhole configuration variables
conf_save2disk	Saves the present pinhole configuration variables to a file that can later be reloaded
conf_load_latest	Loads latest saved pinhole positions
conf_load_default_positions	Loads old default positions
Source and Detector-Related Commands (remember “remote mode” for generator)	
o_shut	Open X-ray Shutter
c_shut	Close X-ray Shutter
x_start	Starts X-ray generator and goes to standby mode
x_ramp	Ramps the X-ray generator and goes to full power
x_standby	Moves the X-ray generator to standby values
x_off	Turns the generator off

SAXS-Related Commands	
saxson	Prepares SPEC for SAXS image measurements
saxsconnect	Connect and control Pilatus Camserver
saxsdisconnect	Releases control of the Pilatus Camserver
saxsoff	Releases SPEC from SAXS image measurements
saxsmeasure *time*	Measures for a total of time seconds saving an images each 15 seconds (FRAME_TIME=15). Filename is consecutive
saxsmeasure_free *time*	Measures for time seconds and saves the image. Filename is consecutive number
saxsmeasure_temp *time*	Measures for time seconds and saves the image in a temporary file called temp.tiff
saxsmeasure_cont *time*	Continuously measures images time seconds long and saves the images in a temporary file called temp.tiff (which are continuously overwritten)
saxsmeasure_freefile *time filename*	Measures for time seconds and saves the image in a file called filename.tiff
SAMPLE_DESCRIPTION=sprintf("bla")	Gives the next saved file a brief description
blankpos_def	Defines a blank position (no sample)
Transmission_measure	Measure the relative transmission at this location (with respect to the blank)
Vacuum Related Commands	
evacuate_system	Evacuate the SAXS system
vent_system	Vent the SAXS system
Misc commands	
Capalign *motor half-range #intervals*	Performs an absorption scan of a capillary in a hole and move to the capillary center

Julabo Thermostated Bath	
julabo_start	Switches ON communication with Julabo Controller (overhead cost = 4 seconds)
julabo_end	Switches OFF communication with Julabo Controller
julabo_counter_on	Start using Julabo as a counter (to Julabos and Julaboe)
julabo_counter_off	Stop using Julabo as a counter
julabo_get_temperature	Get current temperature of Julabo stage
julabo_get_setpoint	Get current setpoint for Julabo stage
julabo_set_setpoint(temp**)**	Sets the temperature setpoint to *temp*
julabo_stabilise *s_p stabilization_time maxtime*	Sets setpoint to *s_p* and logs temperature until the temperature is reached. After the temperature is reached it stabilizes for the given time. If reaching the temperature takes more than *maxtime* then the command is stopped
julabo_watch *maxtime*	Logs the temperature for *maxtime*
julabo_cool	Cools the Julabo stage as fast as possible

Command for Time-sequences	
timescan *counting-time sleep-time*	Counts until it is stopped. In-between each counting time there is a sleep time.
loopscan *npoints counting-time sleep-time*	As timescan but stops after *npoints*

Linkam Thermal Stage Commands	
linkam_start	Switches ON communication with Linkam Controller (overhead cost = 4 seconds)
linkam_end	Switches OFF communication with Linkam Controller
linkam_pump_auto	Start the Linkam pump in auto mode. Manual mode can also be set Linkam_pump_manual, and then Linkam_set_pumpspeed. But this is not recommended
linkam_stabilise *s_p maxtime*	Sets setpoint to *s_p* and logs temperature until the temperature is reached. Unless *maxtime* is exceeded.
_linkam_get_temperature()	Returns current temperature of Linkam stage
linkam_get_temperature	Get current temperature of Linkam stage
linkam_get_rate	Get current ramp rate for Linkam stage
linkam_get_setpoint	Get current setpoint for Linkam stage
linkam_set_rate *rate*	Sets the temperature ramp rate to *rate degrees per minute*
linkam_set_setpoint *temp*	Sets the temperature to *temp* degrees
linkam_set_pumpseed *nn*	Sets the pumpspeed to nn%
linkam_watch *maxtime*	Logs the temperature for *maxtime*
linkam_cool	Cools the Linkam stage as fast as possible

Appendix 6: SAXSLABS GRAD format

Generalized Radial Format Example of a single file
The file starts out with a 3 lines describing the data in the file.
Then a line indicating that the data is starting (but first some lines with denominations)
The data is comma separated in q,I and deltaI format.
After the data, the complete header is given in XML format

See an example here:

```
……..
  1,"Number of Datasets"
  3,"Number of Columns per Dataset"
  400,"Maximum Number of Rows for Any Dataset"
  #DATASETS q-units: Angstrom I-units: A.U.
  latest_0000183_craw,"silverbeh - Conf 3",
  q,I,dI,
   1.830175e-003, 4.187610e-002, 3.738704e-004
   2.563712e-003, 3.768850e-002, 2.367372e-004
   3.297249e-003, 3.195810e-002, 1.896544e-004
   4.030787e-003, 6.404026e+001, 1.235938e+001
   4.764324e-003, 1.916254e+002, 6.681762e+001
   5.497861e-003, 1.342785e+002, 3.474193e+001
   6.231398e-003, 7.794415e+001, 1.452430e+001
   6.964935e-003, 4.848007e+001, 7.050067e+000
  …….
   2.864426e-001, 1.687502e-003, 2.013602e-006
   2.871761e-001, 1.004504e-003, 1.009028e-006
   2.879097e-001, 1.004542e-003, 1.009105e-006
   2.886432e-001, 1.240952e-003, 1.539963e-006
   2.893767e-001, 0.000000e+000, NaN
   2.901103e-001, 0.000000e+000, NaN
   2.908438e-001, 0.000000e+000, NaN
   2.915773e-001, 0.000000e+000, NaN
   2.923109e-001, 0.000000e+000, NaN
   2.930444e-001, 1.055054e-002, 1.113139e-004
   2.937780e-001, NaN, NaN
   2.945115e-001, NaN, NaN
  #HEADERS
  latest_0000183_craw,"silverbeh - Conf 3"
```

<?xml version="1.0" encoding="utf-8"?><ROOT> <det_pixel_size>[0.000172
0.000172]</det_pixel_size> <det_thickness>0.00032</det_thickness>
<det_exposure_time>1800</det_exposure_time>
<det_exposure_period>1812</det_exposure_period> <det_tau>3.838e-007</det_tau>
<det_count_cutoff>1077896</det_count_cutoff>
<det_threshold_setting>4024</det_threshold_setting>
<det_n_excluded_pixels>19</det_n_excluded_pixels>
<det_excluded_pixels>badpix_mask.tif</det_excluded_pixels>
<det_flat_field>FF_p300k0138_E8048_T4024_vrf_m0p15.tif</det_flat_field> <det_trim_directory>:
p300k0138_E8048_T4024_vrf_m0p15.bin</det_trim_directory> <detectortype>PILATUS
300K</detectortype> <start_timestamp/> <end_timestamp/> <save_timestamp/> <realtime/>
<livetime>1800</livetime> <pixelsize>[0.172 0.172]</pixelsize> <beamcenter_nominal>[201.5
279.5]</beamcenter_nominal> <beamcenter_actual>[0 0]</beamcenter_actual> <data_mean/>
<data_min/> <data_max/> <data_rms/> <data_p10/> <data_p90/>
<calibrationtype>geom</calibrationtype> <kcal/> <pixelcal/> <koffset/>
<wavelength>1.5408</wavelength> <detector_dist>1056.2</detector_dist> <saxsconf_r1/>
<saxsconf_r2/> <saxsconf_r3/> <saxsconf_l1/> <saxsconf_l2/> <saxsconf_l3/> <saxsconf_l4/>
<saxsconf_wavelength>1.5408</saxsconf_wavelength>
<saxsconf_dwavelength>0.01</saxsconf_dwavelength> <saxsconf_Izero>1</saxsconf_Izero>
<saxsconf_det_offx>0</saxsconf_det_offx> <saxsconf_det_offy>0</saxsconf_det_offy>
<saxsconf_det_rotx>0</saxsconf_det_rotx> <saxsconf_det_roty>0</saxsconf_det_roty>
<saxsconf_det_pixsizez>0.172</saxsconf_det_pixsizez>
<saxsconf_det_pixsizey>0.172</saxsconf_det_pixsizey> <saxsconf_det_resx_0/>
<saxsconf_det_resy_0/> <saxsconf_abs_int_fact/> <sample_transfact>0</sample_transfact>
<sample_thickness/> <sample_xpos/> <sample_ypos/> <sample_angle1/> <sample_angle2/>
<sample_angle3/> <sample_temp/> <sample_pressure/> <sample_strain/> <sample_stress/>
<sample_shear_rate/> <sample_concentation/> <hg1>0.299975</hg1> <hp1>0.276384</hp1>
<vg1>0.299975</vg1> <vp1>-0.018415</vp1> <hg2>0.149987</hg2> <hp2>0.037719</hp2>
<vg2>0.149987</vg2> <vp2>-0.04299</vp2> <hg3>0.5</hg3> <hp3>-0.008191</hp3>
<vg3>0.5</vg3> <vp3>-0.084303</vp3> <ysam>73.64</ysam> <zsam>53.6</zsam>
<thsam>0</thsam> <detx>950</detx> <dety>-0.606719</dety> <detz>0.4006</detz>
<bstop>42.12</bstop> <pd>10</pd> <source_type>MM002+</source_type>
<source_runningtime/> <source_kV>42 kV</source_kV> <source_ma>0.95 mA</source_ma>
<xaxis/> <xaxisfull/> <yaxis/> <error_norm_fact>1</error_norm_fact>
<xaxisbintype>lin</xaxisbintype> <log>log</log> <reduction_type>s</reduction_type>
<reduction_state/> <raw_filename/> <mask_filename/> <flatfield_filename/> <empty_filename/>
<solvent_filename/> <darkcurrent_filename/> <readoutnoise_filename/>
<zinger_removal>0</zinger_removal> <data_added_constant>0</data_added_constant>
<data_multiplied_constant>1</data_multiplied_constant> <Img> <Class/> <MonitorMethod/>
<ImgType>2D</ImgType> <Site>KU-LIF</Site> <Group/> <Researcher/> <Operator/>
<Administrator/> </Img> <Meas> <Description>silverbeh - Conf 3</Description>
</Meas></ROOT>

Example of a multiple plot file

Multiple plots can also be saved in GRAD files…in this case the format is the same, with the multiple data sets put into additional “column”, and the additional meta-data sets listed one after the ohter.

See an example here:

……

3,"Number of Datasets"

3,"Number of Columns per Dataset"

400,"Maximum Number of Rows for Any Dataset"

#DATASETS q-units: Angstrom I-units: A.U.

latest_0000165_craw,"silverbeh - Conf 1","","latest_0000174_craw","silverbeh - Conf 2","","latest_0000183_craw","silverbeh - Conf 3","",

q,I,dI,q,I,dI,q,I,dI,

1.557831e-002, 2.646137e-004, 7.002041e-008, 4.202093e-003, 6.391972e-003, 1.667992e-005, 1.830175e-003, 4.187610e-002, 3.738704e-004

2.182212e-002, 6.048441e-004, 1.829182e-007, 5.886299e-003, 8.788975e-003, 1.994485e-005, 2.563712e-003, 3.768850e-002, 2.367372e-004

2.806593e-002, 4.981209e-004, 1.240622e-007, 7.570505e-003, 8.018028e-003, 1.783050e-005, 3.297249e-003, 3.195810e-002, 1.896544e-004

3.430975e-002, 4.457028e-004, 9.932547e-008, 9.254711e-003, 9.081331e+000, 4.937561e-001, 4.030787e-003, 6.404026e+001, 1.235938e+001

4.055356e-002, 5.962245e-002, 1.203130e-004, 1.093892e-002, 4.295231e+001, 5.304727e+000, 4.764324e-003, 1.916254e+002, 6.681762e+001

4.679737e-002, 1.556202e-001, 5.338377e-004, 1.262312e-002, 2.351147e+001, 1.904302e+000, 5.497861e-003, 1.342785e+002, 3.474193e+001

5.304118e-002, 4.234801e-002, 8.020123e-005, 1.430733e-002, 1.314908e+001, 8.061074e-001, 6.231398e-003, 7.794415e+001, 1.452430e+001

…….

2.475640e+000, 2.080022e-003, 1.529646e-006, 6.677792e-001, 2.711755e-003, 5.199792e-006, 2.908438e-001, 0.000000e+000, NaN

2.481884e+000, 1.778828e-003, 1.415086e-006, 6.694634e-001, 1.525676e-003, 2.327689e-006, 2.915773e-001, 0.000000e+000, NaN

2.488128e+000, 5.609853e-004, 3.147045e-007, 6.711476e-001, 0.000000e+000, NaN, 2.923109e-001, 0.000000e+000, NaN

2.494372e+000, 0.000000e+000, NaN, 6.728318e-001, 6.105230e-003, 3.727383e-005, 2.930444e-001, 1.055054e-002, 1.113139e-004

2.500615e+000, NaN, NaN, 6.745160e-001, NaN, NaN, 2.937780e-001, NaN, NaN

2.506859e+000, NaN, NaN, 6.762002e-001, NaN, NaN, 2.945115e-001, NaN, NaN

#HEADERS

latest_0000165_craw,"silverbeh - Conf 1"

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<det_count_cutoff>1077896</det_count_cutoff> <det_threshold_setting>4024</det_threshold_setting>
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279.5]</beamcenter_nominal> <beamcenter_actual>[0 0]</beamcenter_actual> <data_mean/> <data_min/> <data_max/> <data_rms/> <data_p10/>
<data_p90/> <calibrationtype>geom</calibrationtype> <kcal/> <pixelcal/> <koffset/> <wavelength>1.5408</wavelength>
<detector_dist>106.2</detector_dist> <saxsconf_r1/> <saxsconf_r2/> <saxsconf_r3/> <saxsconf_l1/> <saxsconf_l2/> <saxsconf_l3/> <saxsconf_l4/>
<saxsconf_wavelength>1.5408</saxsconf_wavelength> <saxsconf_dwavelength>0.01</saxsconf_dwavelength> <saxsconf_lzero>1</saxsconf_lzero>
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