

# cSAXS notes v1.02 (March 18th, 2011)

*When all else fails, read the instructions.*

For further questions please contact Ana Diaz, Andreas Menzel, or Oliver Bunk.

This document as PDF file:

[http://www.psi.ch/sls/csaxs/ManualsEN/csaxs\\_notes.pdf](http://www.psi.ch/sls/csaxs/ManualsEN/csaxs_notes.pdf)

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# 1 Common sense

Common sense and a certain sense of responsibility are essential for working at the cSAXS beamline. Examples are:

- There is no cleaning service apart from the floor being cleaned once a week. The local contacts try to bring the beamline in a reasonable state for you and we expect that you leave the beamline in a at least as reasonable state. In other words: Local contacts are researchers like you and not your private cleaning staff.
- cSAXS has no standardized experimental setup. Working at the beamline means research and in research you can not expect foolproof designs or a point-and-click way from the measurements to the final analysis. Please think before acting.
- Please think *before* acting ...!
- Each user is happy to find a well equipped toolbox and a well equipped chemistry lab. Please maintain this state by putting back all equipment to its original place before leaving.
- Please report all damage (whether it is caused by you or others).
- Please do not use or store chemicals in the control or user preparation room. Please do not mess around with chemicals in the experimental hutch. Please take care that all chemicals and samples are disposed in a proper way.
- Please remove all your belongings - not less and not more. One item more or less per user group makes a complete mess over one year ...

**There are many more examples and common sense means that we do not have to list them all.** Thank you for reading and following this section!

## 2 Preparation of your beamtime

Apart from discussing the experiment with your local contact well in advance some administrative tasks have to be completed before arrival at PSI.

### 2.1 Date of arrival and departure

For an efficient use of your beamtime you must arrive on the day before your beamtime starts and plan for some time in the end for removing your experiment, transferring data etc.

### 2.2 Dosimeter and badge

ALL users MUST apply for dosimeter and badge via the digital user office (DUO) PRIOR to their arrival at PSI: <http://duo.psi.ch>.

## 2.3 Guest house reservation

Please reserve your guest-house on-line:

<http://services.web.psi.ch/services/lodging/lodging.html>

## 2.4 Computer based safety training

A computer based safety training has to be attended on site. The course is available in PowerPoint format on-line as well under

[http://srp.web.psi.ch/su-introduction/Einfuehrung\\_Experimentatoren\\_englisch.pps](http://srp.web.psi.ch/su-introduction/Einfuehrung_Experimentatoren_englisch.pps). At the end of this course, printing the form confirming that you attended it can only be done from the single training PC set up for this. If you use the online version then please print the form directly from the pdf-file

[http://sls.web.psi.ch/view.php/beamlines/cs/manuals/proof\\_of\\_carrying\\_out\\_the\\_test.pdf](http://sls.web.psi.ch/view.php/beamlines/cs/manuals/proof_of_carrying_out_the_test.pdf).

## 2.5 Tea, espresso and guest network at the beamline

You will find facilities for preparing tea and espresso from capsules (currently 1 CHF/capsule) at the beamline as well as mugs and glasses. The opening hours of the cafeteria and canteen can be found in the appendix, [section E](#). A fridge for food and soft drinks is available at the beamline. Please use common sense in combining food, drink and work. Otherwise we will be forced to forbid this combination in general for all users in all rooms of the beamline.

An open wireless LAN is available, see appendix, [section C](#).

## 2.6 Power sockets in Switzerland

Voltage and frequency are 230 V, 50 Hz.

Switzerland has power sockets which differ from most other countries in the world including the US, Japan, France and Germany. Please search for 'SEV 1011' in [http://en.wikipedia.org/wiki/Power\\_socket](http://en.wikipedia.org/wiki/Power_socket) or have a look at the German pages [http://de.wikipedia.org/wiki/Stecker-Typ\\_J](http://de.wikipedia.org/wiki/Stecker-Typ_J). Two pin 'europlugs' will fit. We have a few adapters to the German/French 'Schuko' (Schutzkontakt) system CEE 7/4.

We can provide cables with Swiss plugs and IEC C13 connectors, see [http://en.wikipedia.org/wiki/IEC\\_connector](http://en.wikipedia.org/wiki/IEC_connector).

## 2.7 Guest bicycles

There is a limited number of bikes for users of the PSI large scale facilities available free of charge. Please ask at the user office near by the reception west.

## 2.8 Beamline web pages

The cSAXS home page can be found at

<http://www.psi.ch/sls/csaxs/csaxs>.

It includes among others a staff list with pictures  
<http://www.psi.ch/sls/csaxs/people> ,  
a brief description of standard experimental setup,  
<http://www.psi.ch/sls/csaxs/endstations> ,  
a section called manuals that includes the current document  
<http://www.psi.ch/sls/csaxs/manuals> ,  
our base package of Matlab macros, see also [section 5](#),  
<http://www.psi.ch/sls/csaxs/software> ,  
and a list of publications  
<http://www.psi.ch/sls/csaxs/manuals>.

## 3 Control system

The user front end of the control system is the command line driven program `spec` <http://www.certif.com>. Some hardware in the experimental hutch is controlled directly by `spec`. All other hardware is controlled by EPICS via the `spec` interface.

### 3.1 Console (PC) login: e-account

In the e-mail with the first invitation for your beamtime the main proposer received user name and password for a so called e-account. Log on with this account to all Linux PCs if your local contact has not already done this for you.

### 3.2 Data analysis PCs

There are four PCs in the control room, three running Linux and one running Windows. It is suggested to use `x12sa-cons-1` for experiment control and `x12sa-comp-1` and `x12sa-comp-2` for data analysis. The data analysis should be performed by logging on from these PCs to `x12sa-cn-1`, `-2`, or `-3`. Each compute node has twelve CPU cores, 96 GB of RAM and fast access to the file server, i.e., you can for example run several Matlab sessions in parallel or use parallel and distributed computing. The Windows PC is available to run specialized software like a frame grabber.

The file server is always accessible via your e-account home directory relative to the directory `~/Data10/`.

Standard software like Matlab and IDL is available. The cSAXS team provides Matlab routines for certain tasks. See [section 5](#) for details.

From the compute nodes you can not connect to any other system inside or outside the beamline network whereas a secure shell connection from the PCs at the beamline to other systems also outside PSI is possible.

### 3.3 Data storage

You must store all data in sub directories of `~/Data10/`. Directly in your home directory you have a very limited quota and it is very likely that you completely lock up the system (including your measurements) if you save data there. Please note, that files saved on

the Linux Desktop and moved to the Trash folder are stored in this limited quota home-directory as well.

### 3.4 Startup of `spec`

Open a terminal window (for example by clicking on the screen symbol bottom left). Log on to the `spec` PC: `ssh -X x12sa-rack-1`. Start `specES1`.

### 3.5 `spec` documentation and help

The complete `spec` manual is available online at <http://www.certif.com> and there is a `help` command in `spec`. The latest printed version is available at the beamline but ‘latest’ is much less up-to-date than the electronic pages. An overview over command lists with macros specific for cSAXS is displayed with the `spec` macro `cSAXS_help`. Some standard and some site specific macros are listed in [section 3.8](#).

### 3.6 `spec` log and data file

The `spec` ‘.log’ file contains all screen and file output from `spec`. The `spec` ‘.tlog’ file is a variant of the log file with file output suppressed and some additional line feeds to improve legibility. The `spec` ‘.dat’ data file contains the data columns of `spec` scans. If no data file exists upon startup then data and log file are created automatically in the directories `~/Data10/specES1/dat-files/` and `~/Data10/specES1/log-files/`. The `spec` ‘.elog’ file is an error log and currently not used at cSAXS by the cSAXS specific macros. The macro `new_std_files` can be used to create new log and data files. The old log file has to be closed manually. See also the macro overview `misc_help`.

The data directories for 2D detectors are set with other commands. Please refer to [section 3.7](#).

### 3.7 Data directories

Data directories for 2D detectors like the PILATUS 2M and also 1D detectors like a multi channel scaler are set by common commands. Usually the default settings are used and these macros are in that case not needed.

- `dir_base` [`<dir. relative to ~/Data10/detector-name/>`] sets the data directory relative to the file server directory
- `dir_grouping` [`<0-off, 1-on>`] controls grouping of directories in bundles of 1000 like `~/Data10/pilatus/S00000-00999/S...` rather than only `~/Data10/pilatus/S....`
- `dir_scan_no` sets the current scan number. `Spec` automatically increases this number by one for each new scan, but in case of a so-called ‘fresh’ restart the scan number is reset to 0 and then this macro should be used to restore its former value.

- `dir_ct_no` sets the current count number, i.e., the number for single exposures started via the `spec` macro `ct`. `Spec` automatically increases this number by one for each `ct`, but in case of a so-called ‘fresh’ restart the scan number is reset to 0 and then this macro should be used to restore its former value.
- `dir_show_all` displays a status overview
- `dir_help` displays a macro overview

### 3.8 Basic `spec` commands

Please note: **All commands, macros and motor movements can be canceled pressing <CTRL>-<C> in the `spec` window.** Tab completion is supported. Cursor up / down can be used to move in the command history. <CTRL>-<R> can be used to search backward in the command history.

- `wa` ‘where all’ displays all motor positions. The units are mm or degree by default.
- `wm` `<motor 1>` [`<motor name 2> ...`] ‘where motor’ displays the position(s) and limits of the specified motor(s). Wildcards can be used like `wm st*` to display all sample table motors.
- `umv` `<motor 1>` `<pos.1>` [`<motor 2>` `<pos.2>` ...] ‘update-move’ moves the specified motor(s) to the specified position(s)
- `umvr` `<motor1>` `<offs. 1>` [`<motor2>` `<offs. 2>` ...] ‘update-move relative’ moves the specified motor by the specified offset relative to its current position and displays the motor position(s) while moving
- `ascan` `<motor>` `<from>` `<to>` `<intervals>` `<c.time>`  
‘absolute scan’ This is a line scan using one motor. It scans the specified motor over the given range in the given number of intervals and counts at each position for the specified time in seconds, i.e., takes exposures in case of a 2D detector. When the scan is finished the motors stay at the final position.
- `a2scan` `<motor1>` `<from1>` `<to1>` `<motor2>` `<from2>` `<to2>`  
`<intervals>` `<c.time>`  
This is a line scan using two motors. It scans the specified motors over the given range in the given number of intervals and counts at each position for the specified time in seconds, i.e., takes exposures in case of a 2D detector. When the scan is finished the motors stay at the final position.
- `dscan` `<motor>` `<offs.from>` `<offs.to>` `<interv.>` `<c.time>`  
‘delta scan’ This is a relative line scan using one motor. It scans the specified motor over the given range like `ascan`, but the specified positions are relative to the current motor position rather than absolute. When the scan is finished or canceled then the motor returns to the original positions.



- `d2scan <motor1> <offs.from1> <offs.to1> <motor2>`  
`<offs.from2> <offs.to2> <interv.> <c.time>`  
This is a relative line scan using two motors. It scans the specified motors over the given range like `a2scan`, but the specified positions are relative to the current motor positions rather than absolute. When the scan is finished or canceled then the motors are returned to their original position.
- `cont_line <motor> <from> <to> <intervals>`  
`<c.time> [<readout time>]`  
This is an absolute scan like `ascan` but with the motor being scanned continuously while the detector takes an exposure series. See [section 3.10](#) for more information.
- `mesh <motor1> <from1> <to1> <intervals1> <motor2>`  
`<from2> <to2> <intervals> <c.time>`  
Opposed to the line scan `a2scan`, this is an area scan. For each position of `motor2` in the specified range it scans the `motor1` over the given range in the given number of intervals and counts at each position for the specified time in seconds, i.e., takes exposures in case of a 2D detector. When the scan is finished the motors stay at the final position.
- `dmesh <motor1> <offs.from1> <offs.to1> <intervals1>`  
`<motor2><offs.from2> <offs.to2> <intervals> <c.time>`  
This is an area scan like `mesh` but relative to the current motor positions.
- `cont_mesh <motor1> <from1> <to1> <intervals1> <motor2>`  
`<from2> <to2> <intervals> <c.time> [<readout time>]`  
This is an area scan with the fast axis, the first motor, being scanned continuously while the detector takes an exposure series. See [section 3.10](#) for more information.
- `round_scan <mot1> <mot2> <radius_i> <radius_f>`  
`<Rintervals> <THintervals> <c.time>`  
This is a scan along circles with radii in the specified range. The angular step size along each circle is specified by the number of theta intervals.
- `ct <counting time in seconds>` counts for the specified time which means in case of a 2D detector that an exposure is taken.
- `loopscan <no. of points> [<c.time> [<sleep time>]]` repeatedly takes exposures
- `timescan <c.time> [<sleep time>]` repeatedly takes exposures like `loopscan`, but until canceled using `<CTRL>-<C>` rather than for a specified number of points.
- `multexp_ctimes <c.time> [<c.time> ...]` activates multiple exposures at each point of standard scans. The specified exposure times are used additionally to the exposure time specified for the scan directly. `multexp_ctimes 0` deactivates this feature.

- `burst_scan` <number of exposures> <count time>  
 [<sleep/readout time>] an exposure series is started, similar to using `loopscan`, but once started recorded without interaction with `spec`. See also [section 3.9](#).
- `burst_at_each_point` <number of exposures>  
 [<sleep/readout time>] can be used to record an exposure series at each point of standard scans like `ascan`, `dscan`, etc. See also [section 3.9](#).
- The ‘tweak’ command `tw` can be used for optimizing a motor position. A cursor driven version ‘tweak cursor’ / `twc` is available:  
`twc` <motor1> <step size1> [<motor2> <step size2>]  
 [<count time>].  
 The position of the first motor is changed using cursor left/right. If a second motor is specified then its position can be optimized using cursor up/down. The step-size can be changed and the motors can be returned to their starting positions. Once you started the macro a brief help will be displayed that can be re-displayed by pressing ‘h’. If no count time is specified then no exposures are taken which may be useful when for example an x-ray eye is used. Other commands are available like pressing the <SPACE> bar to stop the current motion, ‘s’ to return to the start position etc. Please refer to the help text displayed by `twc`.
- All text output between the `pon` and the `poff` command is send to the printer when the `poff` command is given. This may be useful for documenting settings for the log book. The `pkill` command may be used to cancel a `pon` command without printing anything.

### 3.9 Burst scans

Some detectors support burst scans, i.e., scans where an exposure series is preprogrammed via `spec` and then running without any interaction with `spec` thereby reducing the overhead time considerably. Currently this kind of operation is supported for the:

1. PILATUS detectors, see [section 4.17](#)
2. multi channel scaler, see [section 4.21](#)

Macros available are:

- `burst_scan` <number of exposures> <count time>  
 [<sleep/readout time>] an exposure series is started, which is similar to using `loopscan`, but once started the series is recorded without interaction with `spec`
- `burst_at_each_point` <number of exposures>  
 [<sleep/readout time>] can be used to record an exposure series at each point of standard scans like `ascan`, `dscan`, etc. Contrary to `multexp_ctimes` the series is, once it has been started, recorded without interaction with `spec`.

### 3.10 Continuous scans

Data acquisition as a function of a motor position can be speeded up considerably if it is done ‘on the fly’ rather than in a stop-and-go manner. Currently this feature is only available for PILATUS detectors, see [section 4.17](#), and the multi channel scaler, see [section 4.21](#). The procedure is as follows: The PILATUS or MCS detector is set up for a burst mode data acquisition, see [section 3.9](#), and waits for a hardware trigger signal to start the data acquisition. The motor that shall be scanned is accelerated to the required speed. When both the required speed and the start position of the scan are reached a trigger signal is send to the detector and exposures are recorded while the motor moves continuously.

This procedure is implemented via the macros `cont_line` and `cont_mesh`. The macros take the same arguments as the stop-and-go equivalents `ascan` and `mesh`, see [section 3.8](#). Optionally a readout time can be specified as an additional, last argument. This readout time defaults to 0.003 sec. For using the full PILATUS 2M detector the sum of exposure and readout time must be at least 0.033 s, i.e., the maximum frame rate is 30 Hz.

Currently this feature is available for stepper motors controlled via EPICS and for piezo stages controlled via the digital E-710 controller, see [section 4.14](#). The Hexapod motors, see [section 4.12](#), and the air bearing rotation stage, see [section 4.13](#), are not supported.

For stepper motors the speed is calculated from the scan parameters, i.e., from the number of points, the exposure time and the readout time. To allow a broad range of scan speeds the local contact should set the speed of the continuous scan motor to the maximum allowed value and lower the starting speed to a small value. The motor is started at a point before the actual scan range so that the acceleration phase is outside the scan range. The end point of the motor movement is beyond the scan range to have the deceleration phase outside as well. There is no encoded feedback from the motors and therefore the trigger signal for starting the exposure burst is send to the detector after the calculated acceleration time. Time jitter may occur due to network delays when sending the trigger signal and due to imperfections of the scanning stage. The macros reset the speed after each scan to the initial, maximum one.

For piezo stages a ramp is programmed that covers the scan range at the calculated speed plus some startup and slow down phases. This ramp is repeated a few times and the dynamic digital linearization (DDL) of the piezo controller is used to optimize the piezo parameters for following the programmed ramp as closely as possible. Once the ramp is programmed and trained it is started and the piezo controller sends a trigger signal directly to the detector, when the starting point of the scan range is reached. No network is involved in this triggering and the time jitter is expected to be small.

Using the DDL feature of the piezo controller requires very accurate definition of the resonance frequencies of the piezo stage together with the current load on it. These frequencies are used in Fourier notch filters to avoid resonances as much as possible. The determination and definition of these resonance frequencies has to be done by your local contact. Improper setup or unreasonably fast scans can lead to very violent piezo movements and to sincere resonances. **Partial destruction of an expensive piezo system has been observed.** Please use this feature with care.

### 3.11 SMS notification

SMS text messages can be send to mobile phones either via a dedicated macro from within spec macros or in case the macro execution is canceled with an error.

Technically an e-mail is send to the sms.switch.ch gateway. Not all mobile phone networks will be reachable via this service. You may either just try it or check <http://www.switch.ch/mail/gw-spec.html#4> for additional information.

The SMS options are controlled via the following set of macros:

- `sms_numbers` <"space separated list of phone numbers"> [`<0-numbers only, 1-allow e-mail addresses>`] configure the destination numbers for the SMS messages. If the optional second parameter is specified as 1, then the syntax checking of the numbers is switched off and e-mail addresses may be specified as well. Text with an @ sign will be interpreted as an e-mail address whereas everything else will be interpreted as a number for SMS.
- `sms_send("message")` send a SMS message
- `sms_error` <0-no, 1-yes> activates automatic SMS message sending upon cancelation of execution. This feature can only be activated from within spec macros and is automatically deactivated upon return to the command prompt.
- `sms_no_beam` <0-no, 1-yes> controls automatic SMS sending if a scan has to wait for beam
- `sms_beam_back` <0-no, 1-yes> controls automatic SMS sending if a scan is resumed after waiting for the beam to return
- `sms_wait_for_beam` waits until the beam is back and sends a SMS then
- `sms_show_all` displays a status overview
- `sms_help` displays a macro overview

## 4 Beamline components and how to control them

See also <http://www.psi.ch/sls/csaxs/beamline-layout>.

### 4.1 Insertion device (U19 undulator)

In the short straight section 12S an U19 in vacuum undulator is installed.

### 4.1.1 Technical data

Length:	1.82 m
Period length:	19 mm
Minimum gap:	4.6 mm
Number of periods:	96
$K_{\max}$ :	2.46
Source size (at 12.4 keV):	$202 \mu\text{m} \times 18 \mu\text{m}$ (FWHM)
Source divergence:	$135 \mu\text{rad} \times 25 \mu\text{rad}$ (FWHM)

### 4.1.2 Control

The ID gap is operated via the `spec` pseudo motor `idgap`. If the gap is not under control of the experimentalist then changing its value will not succeed. In this case `spec` prints help texts how to enable the gap control. During machine beamtime or injections after beamdumps the gap will be permanently operator controlled and not be movable by the experimentalist. Further macros for the insertion device:

- `id_show_gap_E_keV <energy in keV>`  
[<1-use even harmonics,0-odd only (default)>]  
displays the smallest undulator gap that can be used to reach the specified energy.
- `id_gap_E_keV <energy in keV>`  
[<1-use even harmonics,0-odd only (default)>]  
moves the undulator gap to the smallest value that can be used to reach the specified energy.
- `id_show_all` displays a status overview
- `id_help` displays a brief macro overview.

Please note, that the gap value determined by the macros is approximate and should be optimized for example using `dscan` to scan the motor `idgap` by, say, plus/minus 0.05 mm.

## 4.2 Front end beam shutter

The front end shutter should stay open the whole beamtime to avoid changes in heat load on the optical components. If the shutter has been closed then the following opening procedure should be followed. If you are not absolutely sure about all steps then please inform your local contact.

1. Display the current status using the `spec` macro `bl_show_all`. This macro informs you if further steps are necessary to open the front end shutter, if there is no beam etc.
2. Search the optics hutch, if necessary, and open the front end shutter. Be patient after pressing the ‘open’ button: the shutter is slow.
3. Use `bl_show_all` to check the status.

See also the macro overview `bl_help` and [section 4.8](#) for information about the end station shutter.

### 4.3 CVD diamond filter

A water cooled CVD diamond filter can be inserted into the ‘white’ beam to absorb low energy radiation and reduce thereby the heat load on the monochromator. For all experiments so far this filter was inserted in the beam and it must only be operated by the local contact.

### 4.4 Slit systems

Five slit systems are permanently installed.

#### 4.4.1 Technical data

At 12.1 m from the source is a slit system that allows to limit the beam size in the horizontal direction. It can for example be used to symmetrize the source size and illuminate optics like a Fresnel zone plate with a ‘fully coherent’ beam. All other slit systems have four blades to limit the beam size both in the horizontal and the vertical direction.

In the optics hutch there is one water-cooled white-beam slit system in front of the monochromator with its center at 25.996 m from the source. The slit blades are water cooled and illuminated under grazing incidence to spread the heat load. The distance between the horizontal and vertical slit blades is 145 mm.

The second slit system is the first one for the monochromatic beam. It is located behind the mirror with its center at 30.664 mm from the source. The distance between the horizontal and vertical slit blades is 20 mm.

In the experimental hutch slits system three and four are installed in the so called exposure box on the sample table. The maximum opening of these slits is 2.5 mm. The blades of slit three are made of germanium whereas the blades of slit four are made of silicon, both sloped by  $10^\circ$  with respect to the x-ray beam. The standard exposure box ‘nose’ protrudes 300 mm, a short version 94 mm and a long version 428 mm from the end of the exposure box. The blades of slit system 4 are located 39 and 59 mm upstream from the end of the box (133 and 153 mm from the end of the standard nose). The blades of slit system 3 are located 320 and 340 mm from the end of the box (414 and 434 mm from the end of the nose). For both slit 3 and 4 the beam passes first the vertically and then the horizontally defining blades. The exposure box is motorized along the beam. The position of the slit systems 3 and 4 relative to the source can be measured using the known sample table position, see [section 4.9.1](#).

There are two ‘mobile’ slit systems of the JJ X-Ray ESRF type with KF40 flange (<http://www.jjxray.dk/-%20at-f7-hv%20%28esrf%29>) that can be installed by your local contact, if needed.

#### 4.4.2 Control

There are `spec` motors for the width and height of the slit opening and for the horizontal and vertical aperture position. Use the `spec` macro `slits_show_all` for an overview

including the motor names as well as `slits_help`.

Your local contact will optimize the slit settings together with you and in general it is wise to stay with these settings.

## 4.5 Front end filters

The white-beam filters in front of the monochromator are usually not needed and must only be operated by cSAXS staff. See also the macro overview `fil_op_help`.

The filters in the exposure box are for user operation. See [section 4.10](#) and `fil_help` for further details.

## 4.6 Monochromator

A liquid nitrogen cooled Si(111) double crystal monochromator defines the energy of the x-ray beam.

### 4.6.1 Technical data

The fixed exit Si(111) double crystal monochromator is located at 28.58 m from the source (position of the second crystal). The first crystal is liquid nitrogen cooled. The second crystal can be bend for horizontal focusing.

The accessible energy range is from about 4.0 to 18.6 keV. The energy resolution with Si(111) is about  $\Delta E/E \approx 2 \cdot 10^{-4}$ . The second monochromator crystal can be used to focus the beam horizontally by about 10:1 to approximately 20  $\mu\text{m}$  FWHM.

### 4.6.2 Control

Moving single motors of the monochromator can easily irreversibly damage the monochromator. This would be the end of not just your beamtime. Please do not operate the monochromator without introduction from your local contact and without exactly knowing what to do. To protect you from accidental movements of monochromator components are some of these motors password protected. Some monochromator spec macros:

- `mono_settings_E_keV <energy in keV>`  
displays the monochromator settings needed for the specified x-ray energy.
- `mono_E_keV <energy in keV>`  
moves the monochromator to the settings for the specified energy.
- `mono_offs <0-no, 1-yes>` controls the usage of empirical theta2 (motor `moth2`) offsets. In standard operation this feature should be active, see also [section 4.6.3](#).
- `mono_id <0-no, 1-yes>` controls the automatic setting of the ID gap if the x-ray energy is changed. In standard operation this feature should be active, see also [section 4.6.3](#).
- `mono_show_all` displays an overview of the monochromator state including the current energy.

- `mono_help` displays a macro overview including the position of all monochromator motors and the current x-ray energy.

The rotation of the second crystal needs to be optimized after it has been set using `mono_E_keV`, for example using the `dscan` command to scan `moth2` by plus/minus 0.010 degree. Due to top-up mode and the stability of the optics is it usually not necessary to re-optimize the second crystal position during a beamtime of a few days length.

The bender of the second crystal is accessible via the `spec` motor `mobd` and has, like most monochromator motors, no end switches, i.e., can be damaged.

### 4.6.3 Energy scans

For energy scans the pseudo motor `mokev` is available. This motor has not all safety features of the macro `mono_E_keV` and will therefore refuse to move by larger steps in energy at low energies, where crystal collision is an issue. The monochromator is not at all optimized for fast energy changes. If you plan to change or even scan the x-ray energy then please inform your local contact in advance.

To ensure the likelihood that the second crystal rotation `moth2` is exactly at the Bragg angle empirical corrections for the calculated rotation angles can be used. This feature is controlled via `mono_offs` and is active in standard operation.

To ensure that an undulator harmonic is at the current energy automatic ID gap setting should be activated via `mono_id`, which is the default setting.

## 4.7 Mirror

The mirror is used to reject higher harmonics and to focus in the vertical direction.

### 4.7.1 Technical data

The center of the plane mirror is located at 29.43 m from the source. The usable area is 400 mm long. The central 12 mm wide part of the mirror is uncoated, i.e., the fused silica is exposed to the beam here. Via the horizontal translation one can choose between this uncoated and 14 mm wide Pt and Rh coated stripes. The mirror can be bend for vertical focusing.

### 4.7.2 Control

As the monochromator, the mirror must not be operated by users without introduction from the local contact AND explicit permission. To protect you from accidental movements of mirror components these motors are password protected. Some mirror `spec` macros:

- `mirr_coat` [`<SiO2, Rh or Pt>`] positions the part of the mirror with the specified coating in the X-ray beam.
- `mirr_show_all` displays a status overview including all motor positions, the currently selected stripe and incidence angle.



- `mirr_help` displays a macro overview.

The bender is accessible via the `spec` motor `mibd` and has, like most mirror motors, no end switches, i.e., can be damaged.

## 4.8 End station beam shutter

In the compulsory safety training (see [section 2.4](#)) and the introduction from your local contact you learned how to operate the local access control (LAC) system. Additional to the LAC panel the end station shutter can be closed due to equipment protection system interlocks or simply by a software command issued, for example from `spec`:

- `bl_show_all` can be used to check the status of the shutter or to investigate why it can not be opened.
- `shclose` overrules the LAC panel. The end station shutter can not be opened until a `shopen` command is given.
- `shopen` enables opening of the end station shutter via the LAC panel.

The macros `shopen` and `shclose` act additional to the LAC panel in a safety-first way. This means, if either the panel or `spec` say that the shutter should be closed then it will stay closed. To open the shutter it has to be opened from both the panel and from `spec`. The order does not matter. The panel will not give LED feedback upon pressing the open button if the shutter is still disabled via `spec`. Effectively this all means that the shutter can be controlled from `spec` once it has been opened from the LAC panel.

See also the macro overview `bl_help` and [section 4.2](#) for information about the front end shutter.

## 4.9 Optical tables

Three optical tables are installed in the end station hutch ES1: the sample table, an auxiliary table that is for example used to motorize the detector flight tube entrance window and a detector table.

### 4.9.1 Technical data

The optical tables in the experimental hutch can be moved horizontally and vertically and can be tilted around the horizontal axis. They are specified for a maximum load of 500 kg.

By moving the tables one can damage detectors, vent the beamline vacuum for the incoming beam or the detector flight-tube. Please do not operate the tables without introduction from your local contact. To protect you from accidental movements all table motors are password protected, apart from the vertical motion of the detector table `dttry` and the horizontal movement of the whole detector bank `dettrx`. These two motions are needed to select and position a detector. Please handle them with care.

The sample table is an optical table, 2400 mm along the beam, 1200 mm perpendicular to it. It has a M6 x 25 mm grid of threaded holes and is stationary along the beam. The

distance from the table top to the beam position is typically about 500 mm. The most upstream threaded hole of the table is at about 34.12 m from the source. A so called exposure box with in-vacuum beam conditioning like two slit systems, [section 4.4](#), filters for attenuating the beam, [section 4.10](#), and a fast shutter, [section 4.11](#), is mounted on the optical table. The beam exits the exposure box through a ‘nose’ with a mica window that separates the beamline vacuum from the in-air sample environment. The standard ‘nose’ protrudes 94 mm from the end of the exposure box. The default ‘sample environment’ consists of about a cubic metre of air to be filled with whatever setup is needed.

The auxiliary table is 900 mm along the beam, 1500 mm perpendicular to it. Along the beam it is motorized on rails.

The detector table is 1200 mm along the beam, 1500 mm perpendicular to it. All detectors are located on a platform that can be translated horizontally using `dettrx`. Vertically the detectors can be positioned using the slow translation `dttry` of the whole detector table. Along the beam the detector table is motorized on rails.

## 4.9.2 Control

The spec macro `tables_show_all` displays an overview.

## 4.10 Exposure box filters

There are four filter wheels each containing different thicknesses of silicon and germanium filters and other calibration materials of different thicknesses. To avoid hardware damage the filters must be operated using the following macros rather than directly by moving the motors:

- `fil_find_trans <transmission between 0 and 1>`  
[<energy in keV>] displays a list of filter combinations with transmission closest to the specified one. If not specified, the current x-ray energy is used by default.
- `fil_trans [<transmission between 0 and 1>]`  
[<energy in keV>] moves the filter wheels to a combination that is closest to the specified transmission value. Without parameters a help text and the current transmission are displayed.
- `fil_installed` displays the currently installed materials
- `fil_comb <4-digit combination>`, like `fil_comb 1111` can be used to move a certain filter combination in the beam. With this macro calibration foils, which are not chosen by `fil_trans`, can be moved in the beam.
- `fil_show_all` displays the current filter setting.
- `fil_help` displays a macro overview.

## 4.11 Exposure box fast shutter

In the exposure box a magnet driven in vacuum fast shutter is installed. It should be switched on using `fshon` to avoid radiation damage for both the sample and the detector, which is therefore the default setting:

- `fshon` enables the automatic opening and closing of the fast shutter and closes the fast shutter
- `fshoff` disables the automatic opening and closing of the fast shutter
- `fshstatus` displays if the fast shutter is switched on
- `fsh_close_on_error` called from within a macro will close the fast shutter upon errors which cancel command execution, even if the automatic fast shutter closing is switched off. Upon successful macro completion this feature is deactivated.
- `fsh_on_on_error` called from within a macro will activate automatic fast shutter opening and closing and close the fast shutter upon errors which cancel command execution. Upon successful macro completion this feature is deactivated, i.e., the status of the automatic fast shutter opening and closing remains unchanged.
- `fshdelay <delay time in seconds>` should not be adjusted by users. See the discussion below.
- `fshutter_help` displays a command overview.

In scans without motor movements or with the movement of very fast motors like piezos is the time between closing and re-opening of the fast shutter very short. In that case the fast shutter becomes unreliable and it does not make sense to open and close it for each exposure rather than keeping it open all the time. To disable and re-enable the fast shutter automatically for such cases the following logic has been implemented in `spec`. Prerequisite is, that the automatic opening and closing of the fast shutter is switched on using `fshon`.

The first point of a scan is measured with opening and closing of the fast shutter. When the exposure for the second point shall be taken it is measured, how long the shutter has been closed. If this time is below the threshold defined via `fshdelay` then the fast shutter closing is delayed for the rest of the scan. By delaying rather than disabling the fast shutter it is ensured, that for example in a two motor scan with a fast first axis and a very slow second axis the fast shutter will still be closed when the slow second axis is moved.

Please do not change the timing of this automatically enabled delayed-closing feature without discussion with your local contact.

## 4.12 Hexapod

A PI M850.11 Hexapod is available. It emulates three degrees of translation and three degrees of rotation around a user-defined center of rotation. Its main purpose is the positioning of heavy equipment with micron precision. A smaller Hexapod M810 is for example used for positioning optical elements.

### 4.12.1 Technical data

Please see the separate description in

[http://www.psi.ch/sls/csaxs/ManualsEN/PI\\_Hexapod\\_M850p11\\_csAXS.pdf](http://www.psi.ch/sls/csaxs/ManualsEN/PI_Hexapod_M850p11_csAXS.pdf) for the large Hexapod M850 and

[http://www.psi.ch/sls/csaxs/ManualsEN/PI\\_Hexapod\\_M810\\_Datasheet.pdf](http://www.psi.ch/sls/csaxs/ManualsEN/PI_Hexapod_M810_Datasheet.pdf) for the smaller M810.

### 4.12.2 Control

The Hexapod related macros in `spec` need the internal number of the Hexapod that is addressed by issuing a command. The big M850 has the number 1 and the small M810 number 2.

After connecting the Hexapod and switching on the controller an initialization has to be performed using `hex_ini`. Please make sure that its save for the Hexapod to move in any direction since software limits will be ignored at this point.

- `hex_ini` initializes the controller, includes a search for the home position while ignoring software limits
- `hex_off` disables the Hexapod motors in `spec`. The Hexapod motors are then not listed by `wa`
- `hex_on` enables the Hexapod motors in `spec`. `hex_ini` executes this automatically.
- `hex_set_pivot_point` defines the center of rotation
- `hex_show_pivot_point` displays the current center of rotation
- `hex_help` displays a command overview

## 4.13 Air bearing rotation stage

A Micos UPR160F air bearing rotation stage is available upon request. It is for example part of the standard 3D setup for Ptychography and STXM, see also

<http://www.psi.ch/sls/csaxs/endstations>.

- `upr_ini` initializes the controller. This macro must be executed after switching on the controller, prior to using the stage in `spec`.
- `upr_on` enables the rotation stage for its use in `spec`.
- `upr_off` disables the rotation stage for its use in `spec`.
- `upr_speed <speed in deg/sec>` can be used to set the rotation speed.
- `upr_show_all` displays a status overview
- `upr_help` displays a brief macro overview

## 4.14 Piezo

A PI E710 piezo controller is available upon request. It is for example part of the standard 2D and 3D setups for Ptychography and STXM, see also <http://www.psi.ch/sls/csaxs/endstations>.

### 4.14.1 Macros

Some of the features of the E-710 piezo controller that go beyond the simple use as a positioning device have been implemented in `spec`. For continuous scans, see [section 3.10](#), or any other standard experiment one has not to deal directly with the macros below:

- `pz_on` activates all E-710 controlled piezo motors for use in `spec`. Upon errors the piezo motors may become deactivated and this command can be used to re-activate them.
- `pz_off` deactivates all E-710 controlled piezo motors for use in `spec`. This is useful to avoid error messages if the controller is switched off but the piezo motors are still configured in `spec`.
- `pz_auto_zero <motor>` recalibrates the zero position for the specified piezo axis. This should be performed after the controller has been switched on. Typically it will be defined in the controller setup that all connected axes are zeroed upon startup and manual zeroing via this macro will not be necessary.
- `pz_wait_settledown <0-off, 1-on>` If active, `spec` waits after motor movements until the controller signals that the piezo is settled at its destination position. This feature being active is the default.
- `pz_version` display the controller version
- `pz_status <motor>` displays the (error) status of the specified axis
- `pz_stop <motor>` stops all wave generators of the controller for the specified axis. This macro should for example be used after starting a wave form with `pz_run_waveform`.
- `pz_velocity <motor> [<velocity in mm/sec>]` set and display the velocity for the specified axis. Typical values are very high like 12.5 mm/sec.
- `pz_def_ramp <motor> <amplitude in mm> <time in seconds>` defines a waveform that ramps up linearly by the specified amplitude and back the same amplitude and rate plus intermediate sections as connections. The total time needed for the complete waveform is specified as parameter, i.e., this routine makes it easier to define the repeat frequency rather than the ramp speed.
- `pz_show_single_waveform <motor> [<output sampling>]` display the measured waveform. Prerequisite is the definition of a wave form, for example using `pz_def_ramp`. An output sampling greater than 1 can be used to suppress screen output of values to increase the speed of the screen output.

- `pz_run_waveform <motor> [<no. of repeats, 0 for infinity or 1-...>]`  
runs a previously defined waveform.
- `pz_step_response <motor> <step size in mm> [<no. of points to report>]`  
moves the specified axis by the specified step size (in mm) and records the position as a function of time. These data are read by `spec` and stored as a scan file. At least 500 points should be used for the report table to see the step, depending on the current speed settings.
- `pz_report_table <motor> <no. of points to report> [<output sampling>] [<start index>]`  
reads the report table of the piezo controller and stores the data as a scan file. All specified points are read but specifying a sample larger than 1 can be used to skip points for output to the screen and data file. The report table is for example filled using the `pz_step_response` or the `pz_def_ramp` macro.
- `pz_show_all` displays a status overview
- `pz_help` displays a macro overview

## 4.15 Detector flight tube lengths

Two detector flight tubes are available. The short flight tube is 2063 mm long, the long one 7000 mm. This is the nominal distance from the entrance window to the exit window position. The entrance window is a thin sheet of mica, separating the flight tube vacuum of a few mbar from the surrounding air. The exit window is made of a 350  $\mu\text{m}$  thick Mylar foil and has a clear aperture of 400 mm. A reduction flange to 120 mm clear aperture is available and adds 21.1 mm to the flight-tube length. This smaller diameter can be used with a 75  $\mu\text{m}$  Kapton window. A 13  $\mu\text{m}$  Kapton window of 600 mm diameter is available for flushing the flight tube with helium. The flight tube can be moved along the beam which allows to move its entrance close to the sample position. The total detector to sample distance should be measured at least. Ideally one measures a calibration sample with known spacings like the 58.380 Å of silver behenate:

<http://www.esrf.eu/UsersAndScience/Experiments/CRG/BM26/SaxsWaxs/Silverbehenate>.

## 4.16 Light curtain

In front of the detector table a light curtain is installed. If it is triggered then detector and auxiliary table motors are blocked in low level hardware. The effect is like triggered end switches. Some motions are blocked completely, others only in one direction. One can for example move the detector table away from the auxiliary table but not closer which allows to disentangle these two systems once the light curtain is triggered.

If the light curtain is triggered then:

- **Enter the hutch and investigate the problem.**
- Carefully resolve the problem by moving motors with `spec`.

## 4.17 PILATUS detector

The PILATUS 2M detector is the standard detector at the cSAXS beamline. A PILATUS 300k-W is available, for example as wide angle detector. A single 100k PILATUS module may be available upon request.

Several publications are describing PILATUS technology like, e.g., B. Henrich, A. Bergamaschi, C. Brönnimann, R. Dinapoli, E. F. Eikenberry, I. Johnson, M. Kobas, P. Kraft, A. Mozzanica, and B. Schmitt, *PILATUS: A single photon counting detector for x-ray applications*, Nucl. Instrum. Methods Phys. Res. A **607** 247-249 (2009).

### 4.17.1 Technical data

The PILATUS 2M detector has  $1475 \times 1679$  pixels of  $172 \times 172 \mu\text{m}^2$  resulting in an active area of  $253.7 \times 288.8$  mm. It consists of  $3 \times 8$  detector modules of  $487 \times 195$  pixels each. The area between the modules is not sensitive to x-rays and appears as simulated ‘dead’ pixels in the data frames, i.e., only 92 % of the 2.48 million pixels are real pixels, the other 8 % are simulated dead pixels between the modules. The horizontal separation of modules is seven and the vertical one 17 pixels.

The PILATUS 300k-W has  $195 \times 1475$  pixels. It consists of three modules in a row. See also <http://dectris.com/sites/pilatus300k-w.html>. The single module 100k has  $487 \times 195$  pixels.

If the count rate in a pixel reaches  $2^{20} = 1048576$  then the counter wraps over to 0 and continues counting. The detector is radiation tolerant but not radiation hard. It can not withstand the intensity of the direct beam. Long exposure to high intensity will alter the sensitivity of the exposed area.

The distance from the front surface of the detector housing to the surface of the detector modules is 20 mm.

Related information:

- PILATUS 2M on the DECTRIS web pages:  
<http://www.dectris.com/sites/pilatus2m.html>
- PILATUS pages of the SLS detector group:  
<http://pilatus.web.psi.ch/pilatus.htm>
- Effect of low, medium and high gain settings on the dead time:  
[http://pilatus.web.psi.ch/DATA/REPORTS/rate\\_scans.html](http://pilatus.web.psi.ch/DATA/REPORTS/rate_scans.html).  
See also the discussion in [section 4.17.6](#).
- energy threshold, see [section 4.17.6](#)

### 4.17.2 Control

Make sure that the detector is **protected from the direct beam** before opening the shutter for the experimental station.

### 4.17.3 Macro overview

The data directories are handled by general macros, see [section 3.7](#).

All PILATUS detector macros except `pilatus_show_all` need as the first parameter the detector number. The 2M detector is number 1, the 300k-W number 2, and the single 100k module is number 3.

- `pilatus_on <det.no.>` enables a PILATUS detector for use in `spec`. Both PILATUS detectors can be run in parallel.
- `pilatus_off <det.no.>` disables a PILATUS detector for use in `spec`.
- `pilatus_basename <det.no.> <base name>` sets the first part of the image filenames.
- `pilatus_file_format <det.no.> <base name>` sets the file format to either uncompressed edf or byte-offset compressed cbf.
- `pilatus_threshold <det.no.> <"full" or "partial"> [<threshold in keV>] [<1-low, 2-medium, 3-high gain>]` sets the energy threshold for detection, see [section 4.17.6](#).
- `pilatus_show_all` displays a status overview
- `pilatus_help` displays a command overview

### 4.17.4 Region of interest

The PILATUS 2M can be configured to be read out in

- eight banks ( $3 \times 8$  modules, i.e., full frame)
- four banks ( $3 \times 4$  modules)
- eight modules ( $2 \times 4$  modules)
- two banks ( $3 \times 2$  modules)
- two modules ( $1 \times 2$  modules)

mode. Switching between these modes is relatively fast but can NOT be done from `spec` in an automated way, see [section 4.17.5](#). Further region of interest features are currently not available.

### 4.17.5 Startup and shutdown procedure

The PILATUS 2M detector has to be started by your local contact according to the following procedure:

1. Switch on the Julabo chiller for the detector. Start it by pressing its enter button for several seconds. The temperature set-point is 23°C.



2. Switch on the power supply at the back side of the detector.
3. Log on to the detector PC: `ssh -X det@x12sa-pd-1`.
4. On the detector PC mount the file server via automount:  
`cd /sls/X12SA/Data10`
5. Still on the detector PC start `camserver` from its directory:  
`cd ~/p2_8bank`  
`./camonly_8b`. Wait until the `camserver` startup procedure is finished and a `'*'` prompt is displayed.
6. Activate use of the detector in `spec` using `pilatus_on 1`.
7. With the monochromator at the correct energy start  
`pilatus_threshold 1 "full"`  
in `spec`. See also [section 4.17.6](#).
8. You may define the base directory relative to the user home directory using `pilatus_basedir` and print an overview using `pilatus_show_all`.
9. If readout of less than the full frame is needed then perform additionally the following steps:
  - Switch the PILATUS detector off in `spec` using `pilatus_off 1`
  - `exit camserver`
  - On the detector PC run one of the following, from `~/p2_8bank`:
    - `./camonly_8b` (3x8 modules, full frame)
    - `./camonly_4b` (3x4 modules)
    - `./camonly_8m` (2x4 modules, center - left)
    - `./camonly_2b` (3x2 modules, center)
    - `./camonly_2m` (1x2 modules, center)
 Modules are specified horizontally  $\times$  vertically.
  - Enable the PILATUS detector in `spec` using `pilatus_on 1`
  - Call `pilatus_threshold 1 "partial"` in `spec`. The calibration can only be done for the full detector and is still active (if you did it before, as described above). The dead time correction is reset upon starting the sub-detector `camserver` version but activated again by `pilatus_threshold` with the `"partial"` parameter.

#### 4.17.6 Threshold

The PILATUS detector has energy threshold and gain settings. The default setting for the energy threshold is 55% of the x-ray energy for high counting efficiency but still no cross talk between neighbouring pixels. The threshold can be raised for example to suppress fluorescence from the sample.

The default gain setting is low gain for the highest count rates with a dead time of about 124.7 ns, see [http://pilatus.web.psi.ch/DATA/REPORTS/rate\\_scans.html](http://pilatus.web.psi.ch/DATA/REPORTS/rate_scans.html). At medium gain the dead time is about 200.4 ns and at high gain it is 338.8 ns. The lower the energy the higher the gain needed. At lower energies also energy threshold settings higher than 55 % of the current x-ray energy are needed. Otherwise the detector starts counting noise. This will be evident from an exposure without beam, if it happens. Larger areas of such hot pixels due to too low energy threshold will draw a high current and eventually damage the detector. The minimum threshold is currently 3.5 keV for high gain settings.

The spec macro `pilatus_threshold` can be called with only the detector number and "full" as parameters to use default settings. For user defined settings the energy threshold can be given as third command-line argument and the gain as fourth argument: '1' for low gain (high count rates), '2' for medium gain and '3' for high gain (low count rates). The PILATUS control program `camserver` may decide on its own to change the energy threshold setting. One should always check the settings that are really applied, for example, using `pilatus_show_all`.

If not the full detector is read out, see [section 4.17.5](#), then the energy threshold must be set first for the full detector using the "full" parameter and then for the sub-detector readout using the "partial" parameter. This is just a workaround: The energy threshold calibration can currently only be performed with the full detector. The sub detector `camserver` versions do not change the previously set threshold upon startup but unfortunately these versions do not report the previously applied threshold. Furthermore, the dead time correction has to be set in `camserver` after starting the sub-detector version. This is done by `pilatus_threshold` with the "partial" parameter. Additionally a warning in spec is switched off and the last known threshold setting is reported as the current one. If spec is restarted inbetween then these last known values are deleted and one must start with the full detector again to avoid useless warning messages.

## 4.18 Cyberstar scintillation point detector

The Cyberstar detector is often used as a kind of monitor, looking at air-scattering or sample back-scattering, or as point detector for photon correlation spectroscopy. It is available as counter in `spec`, typically as a channel called `mon`. Macros for setting the high voltage, gain and energy window are currently not available. If such macros are needed then please discuss this with your local contact well in advance.

## 4.19 Flat single APD

An APD of 10 mm × 10 mm active area and 200  $\mu\text{m}$  thickness mounted in a flat housing is available upon request. It is an APD0008 from FMB Oxford. It is controlled via the APD counter electronics NIM module ACE. The ACE module is connected via RS232 to `spec`. For a macro overview see `ace_help`.

## 4.20 Amptek XR-100CR detector and PX4 pulse processing unit

The Amptek XR-100CR is a two-stage Peltier cooled Si PIN diode used as energy dispersive detector. It is connected to the PX4 digital pulse processing unit. Additionally to the slow read out of full spectra, the PX4 unit has the option to integrate up to eight energy ranges and provides the resulting signals as TTL output that can be fed into a spec accessible counter card. The dynamic range of the detector is quite limited and its active area is  $6 \text{ mm}^2$  small. The active area is  $500 \mu\text{m}$  thick.

The PX4 unit is interfaced to spec via a serial RS232 connection. Currently it is assumed that the spec serial interface number 3 is connected to the PX4 unit and configured as 57600 baud, no parity, raw mode.

### 4.20.1 Maro overview

The data directories are handled by general macros, see [section 3.7](#).

- `px4_config <config. no.>` loads a configuration to the controller. Currently the configuration 1, the factory default for high energy resolution, the configuration 2 with shorter peaking time for higher count rates, and configuration 3 for even higher count rates with even worse energy resolution are available. Configuration 4 is for a different detector head with  $25 \text{ mm}^2$  sensor, not available at the beamline. This macro must be used first to initialize the PX4 unit.
- `px4_gain [<gain 3.1 - 703>]` sets the analog gain.
- `px4_peaking_time [<time in micro sec.>]` sets the peaking time in micro seconds.
- `px4_autotune` should be run after loading a new configuration or after changing parameters like gain or peaking time. The lower threshold for the discrimination of slow channel events, the lower threshold for the discrimination of fast channel events and the input voltage offset added to the pre-amplifier output are determined automatically.
- `px4_scaler_threshold [<scaler no.> <threshold low>  
<threshold high>]` sets the integration range in channels for the specified scaler output.
- `px4_scaler_enabled <scaler no.> <enabled 0-no, 1-yes>` enables or disables the output of the integrated scaler signal.
- `px4_count` starts a continuous data acquisition.
- `px4_plot [<log-y 0-no, 1-yes>]` reads and plots the current spectrum.
- `px4_set_basedir <relative directory>` sets the data directory relative to `~/Data10/px4/`. The directory is automatically created.
- `px4_set_basename <first part of the filename>` defines the fixed part of the file name for the energy spectra.

- `px4_on <level>` defines how the energy dispersive detector is used in `spec`:
  0. deactivates automatic use of the PX4 unit
  1. activates automatic use but without readout of spectra, i.e., only the scaler channels are used.
  2. activates full use of the unit including automatic read-out and storage of the energy spectra.
- `px4_off` deactivates the energy dispersive detector for automatic use in `spec`.
- `px4_show_config` displays the current configuration.
- `px4_show_status` displays the current status variables.
- `px4_show_all` displays both configuration and status.
- `px4_help` displays a macro overview.

#### 4.20.2 Startup procedure

Connect the detector head to the PX4 unit, this unit to the fan-out box and this box to `ttyS3` of the `spec` PC. In `spec` start `px4_config 2`, check `px4_show_status` until the detector head temperature is not printed in bold face anymore, i.e., reached 230 K. Without X-rays on the detector start `px4_autotune` to set the thresholds for the suppression of noise. Switch the detector on for usage in `spec` using `px4_on 2` and record a spectrum using `ct`. The spectrum can be displayed with the `spec` online plot and the Matlab macro `image_spec`, see [section 5](#). If the total number of counts in certain ranges of channels should be output as TTL pulses then use `px4_scaler_threshold` to define the ranges and `px4_scaler_enabled` to enable the outputs. The outputs may be connected to the multi channel scaler for continuous scans, see [section 4.21](#), or to the `spec` counter card accessible via the black fan-out box in the back-top of the rack.

### 4.21 Multi channel scaler (MCS)

A multi channel scaler can be used to count TTL pulses, for example output by the Amptek energy dispersive detector, see [section 4.20](#), in a burst scan or continuous scan.

Currently up to 31 input signals can be connected to the inputs 2-31. Input 1 is connected internally to the 50 Mhz timebase and must not be used. The control input 1 should be connected to the PILATUS trigger output. For each input channel currently up to 8192 values can be stored, i.e., this value defines the maximum number of exposures in a burst, see [section 3.9](#), or continuous scan, see [section 3.10](#).

#### 4.21.1 Macro overview

The data directories are handled by general macros, see [section 3.7](#).

- `mcs_trigger` should be left at the automatic setting. In this mode the MCS is triggered either by the PILATUS detector or by `spec`, if the PILATUS is not active or not used in burst mode.

- `mcs_basename` [`<fixed part of filename>`] may be used to set the first part of the data file names
- `mcs_on` activates the MCS for use in `spec`
- `mcs_off` deactivates the MCS for use in `spec`
- `mcs_show_all` displays a status overview
- `mcs_help` displays a macro overview

## 4.22 X-ray eye and similar cameras

An x-ray eye is available at the beamline. It consists of a 100  $\mu\text{m}$  YAG scintillator that is monitored by a CCD camera using a 10 $\times$  microscope lens. The camera has a low dynamic range and therefore its gain must be adapted to the incident illumination either manually or automatically. The following `spec` macros all need as the first parameter the `spec`-internal number of the serial interface over which the camera is connected. For the x-ray eye this is usually 0, 9 or 10.

- `cam_manual_gain` `<interf.no.>` [`<gain 0-8>`] switches to manual gain mode and sets the gain
- `cam_shutter_speed` `<interf.no.>` switches to auto light control and sets the speed of the electronic shutter. This can be used to reduce the intensity if the minimum manual gain of 0 is not sufficient for this.
- `cam_senseup` `<interf.no.>` [`<0-off, 1-12 for 2x to 128x>`] on-sensor integration
- `cam_zoom` `<interf.no.>` [`<-1-off, 0-8>`] provides an electronic zoom feature
- `cam_hmirr` `<interf.no.>` [`<0-off, 1-on>`] mirror images horizontally
- `cam_vmirr` `<interf.no.>` [`<0-off, 1-on>`] mirror images vertically
- `cam_show_all` `<interf.no.>` displays a status overview
- `cam_help` displays a command overview including here unlisted options for title display etc.

## 4.23 Fingerlakes Instrumentation ProLine CCD

A ProLine PL1001E CCD with Kodak KAF-1001E class 1 sensor, 1024  $\times$  pixels, may be available upon request. It can be connected via USB 2.0 to the `spec` PC. Please see `fli_help` for an overview on the available macros.

## 4.24 Analog and digital I/O

Analog -10 to 10 V input (ADC) and output (DAC), TTL (5 V) input and output and opto coupler input and output (24 V maximum) connections are available in the experimental hutch. If you need any of these then please discuss this with your local contact before your beamtime. The following `spec` macros are provided to control these IO channels:

- `ttl_out <ch.no.> [<0 or 1>]` optionally sets and displays the state of the specified output channel
- `ttl_out_auto <ch.no.> [<value while counting>]` controls automatic setting of the output channel. If a value of 0 or 1 is specified then the output channel is brought to this state before the counting starts and reset to the inverse state afterwards. This feature is deactivated with a negative value.
- `ttl_in <ch.no.>` displays the state of the specified input channel.
- `ttl_show_all` displays the status of all input and output channels and of the automatic output channel setting.
- `opt_out <ch.no.> [<0 or 1>]` optionally sets and displays the state of the specified output channel
- `opt_out_auto <ch.no.> [<value while counting>]` controls automatic setting of the output channel. If a value of 0 or 1 is specified then the output channel is brought to this state before the counting starts and reset to the inverse state afterwards. This feature is deactivated with a negative value.
- `opt_in <ch.no.>` displays the state of the specified input channel.
- `opt_show_all` displays the status of all input and output channels and of the automatic output channel setting.
- `dac_out <ch.no.> [<voltage in V>]` optionally sets and displays the state of the specified output channel
- `adc_in <ch.no.>` displays the voltage at the specified input channel.
- `adcdac_show_all` displays the status of all analog input and output channels.
- `io_show_all` displays the status of all digital and analog input and output channels and their automatic setting.
- `io_wait [<time in seconds>]` optionally sets and displays the wait time that is applied after all automatic IO channels are set before the counting starts. This wait time is for example needed by the fast shutter. It is not applied if no automatic channel setting is active.
- `io_help` displays a macro overview

The automatic TTL output is for example used for triggering the in-vacuum fast shutter that is installed in the exposure box.

#### 4.24.1 DAC pseudo motor

The -10 to +10 V output of the digital to analog converters can be controlled via a pseudo motor in `spec`. This can be used for controlling a device via an analog voltage. Examples are power supplies and analog piezo controllers. If you need such a feature then please arrange this with your local contact and see `dac_mot_help` in `spec`.

#### 4.25 Digital delay generators

Two Stanford Research Systems digital delay generators DG645 are available. Each has eight channels. Please see `ddg_help` for an overview over the available macros.

#### 4.26 Temperature controller

A LakeShore 336 temperature controller is available upon request. Please see `ls_help` for an overview over the available macros.

#### 4.27 Teslameter

A Group3 DTM-133 digital teslameter may be available upon request. It is connected via GPIB to the `spec` PC. A pseudo counter can be defined for reading the field strength. Please see `dtm_help` for an overview on the available macros.

#### 4.28 Syringe pumps

##### 4.28.1 Cetoni neMESYS syringe pumps

Three neMESYS syringe pumps are available at the beamline upon request. One pump is connected to the `spec` PC `x12sa-rack-1` via an RS232 interface and the other pumps are daisy chained using a CAN bus. On the control PC a server program is running independently of `spec` to optionally run programs in parallel to command execution in `spec`.

**4.28.1.1 Technical data** The neMESYS OEM module has a minimum velocity of 59.26 nm/s and a maximum velocity of 5.93 mm/s. The pulsation free minimum velocity is approximately twenty times the minimum velocity. The smallest step is 35 nm. The maximum force is 290 N. The stroke is 62 mm. The maximum syringe diameter is 30 mm. The pulsation free minimum and the maximum flow rate are for a 0.5  $\mu$ l/60mm syringe 10 pl/s - 49 nl/s, for a 100  $\mu$ l/60mm syringe 2 nl/s - 10  $\mu$ l/s, and for a 25 ml/60mm syringe 500 nl/s - 2.5 ml/s. PEEK valves with FFKM/FFPM sealing are available. They have an internal volume of 45  $\mu$ l and are suitable for a temperature range from 0 - 50°C, a pressure of up to 2 bar on the syringe and up to 0.5 bar on the experiment side. The valves have an UNF 1/4"-28 connection.

**4.28.1.2 Macro overview** After your local contact has connected the pumps they need to be initialized using `nem_init` and a following `nem_home` for the calibration of the zero position is recommended. Then one can run the pumps using `nem_...` macros or via pseudo motors and/or counters set up by your local contact.

Movements can be combined to programs that are stored and run on the syringe server program, independent of `spec`.

The `spec` macros for these pumps are:

- `nem_init` initializes the connection to syringe pump
- `nem_calibration` controls the syringe dependent mm/ $\mu$ l calibration
- `nem_velocity` controls the default syringe velocity
- `nem_home` performs a home movement to calibrate the position
- `nem_off` closes the connection to the server program
- `nem_valve_input` moves the valve to its input position. It can not be checked if a valve is connected and successfully moving.
- `nem_valve_output` moves the valve to its output position It can not be checked if a valve is connected and successfully moving.
- `nem_pos` displays the current position
- `nem_start_move_abs` starts moving to an absolute position without waiting for the completion of the movement
- `nem_move_abs` moves to an absolute position, waits until the syringe pump stops
- `nem_start_move_rel` starts moving relative to the current position without waiting for the completion of the movement
- `nem_move_rel` moves relative to the current position
- `nem_dose` moves permanently
- `nem_prog` selects the active program for programming
- `nem_cmd` sends a program string
- `nem_delete_last_cmd` deletes the last command from a program
- `nem_delete_prog` deletes an entire program
- `nem_display_programs` displays all programs on the server
- `nem_exec` executes a program on the server
- `nem_pause` programs a delay
- `nem_wait_stop` waits until the syringe motor stops



- `nem_mot_wait` controls macro motor and counter wait behavior
- `nem_cancel` stops all pumps immediately
- `nem_stop` programs a pump stop
- `nem_show_all` displays a status overview
- `nem_help` displays a macro overview

#### 4.28.2 Hamilton syringe pumps PSD/4

The PSD/4 syringe pumps from Hamilton are not available at the beamline. But if you bring such a pump with RS232 interface then the `spec` interface for controlling the pump is available. These pumps can be daisy-chained, i.e., only one RS232 connection to the `spec` PC is needed for controlling several pumps.

After your local contact has connected the pumps they need to be initialized using `hsp_init_out_right` or `hsp_init_out_left`. Then one can run the pumps using `hsp_...` macros or via pseudo motors and/or counters set up by your local contact. The `spec` macros for these pumps are:

- `hsp_init_out_right` initialize syringe and valve, output position is right
- `hsp_init_out_left` initialize syringe and valve, output position is left
- `hsp_wait` controls macro motor and counter wait behavior
- `hsp_calibration` controls the steps/ $\mu$ l calibration
- `hsp_velocity` controls the syringe velocity
- `hsp_backlash` controls the backlash correction
- `hsp_valve_input` moves the valve to its input position
- `hsp_valve_output` moves the valve to its output position
- `hsp_valve_bypass` moves the valve to its bypass position
- `hsp_start_move_abs` starts moving to an absolute position without waiting until this position is reached
- `hsp_move_abs` moves to an absolute position
- `hsp_start_move_rel` starts moving relative to the current position without waiting until this position is reached
- `hsp_move_rel` move relative to the current position
- `hsp_pos` display the current position
- `hsp_prg_begin` starts the programming of a command string

- `hsp_prg_wait` programs a wait time
- `hsp_prg_end` ends programming a command sequence
- `hsp_prg_cmd` sets directly the command string
- `hsp_prg_exec` executes a pre-programmed command sequence
- `hsp_show_all` displays status overview for the specified pump
- `hsp_help` displays a macro overview

## 4.29 EPICS interface

Much of the hardware access is controlled via EPICS, transparent to the user. The following macros for interaction with EPICS are for **use by the local contact rather than users**:

- `epics_dump_motor_par` displays the parameter of all EPICS motors that are configured in `spec`.
- `epics_holding_current <motor> [<0-off, 1-on>]` optionally sets and displays the holding current setting for the specified motor. A new setting becomes active once the motor is moved and is lost upon reboot of the corresponding VME crate. **Enabling holding current may damage a motor.**
- `epics_holding_current_show_all` displays the holding current setting for all motors that are configured in `spec`.
- `epics_reset_m1` resets position and limit for all EPICS\_M1 motors. This will only be useful in the initial phase of a beamtime when all motors are set up. The macro displays which motor positions are reset and with which command sequence this can be set back to the previous settings. This allows setting back a few selected motors using copy-paste.
- `epics_dump_encoder_par` displays the EPICS encoder settings
- `epics_set_encoder_offset <encoder no.> <offset value>` sets the offset parameter. The setting is lost upon reboot of the VME crate.
- `epics_set_encoder_dir <encoder no.> <dir. +1 or -1>` sets the direction parameter. The setting is lost upon reboot of the VME crate.
- `epics_boottime` displays the boot time of all known VME crates.
- `epics_load` displays the CPU load for the IOCs on the beamline VME crates. As a rule of thumb the load should not exceed 60 %.
- `epics_help` displays a macro overview

### 4.30 Julabo closed cycle water chillers

Integration of the sample table and detector chiller are planned. Please ask your local contact about the current status.

### 4.31 Oxford cryojet

Integration of the cryojet is planned. Please ask your local contact about the current status.

### 4.32 Lambda Genesys power supplies

Two 0-40 V, 0-19 A and one 0-60 V, 0-12.5 A power supplies are available. They can be controlled via their RS232 interface. Pseudo motors and counters can be defined in `spec` by your local contact to control voltage and current. See `lgen_help` for an overview. As startup procedure `lgen_init` or `lgen_init_cc` is needed to initialize the device.

## 5 Matlab (plotting and analysis)

Your local contact will provide some Matlab routines including a simple online viewer for 2D data, read and write functions for the data and macros for azimuthal integration. At the beamline the Matlab routines can be found in the directory `~/Data10/matlab/` of your e-account. From time to time we update the online available version at <http://www.psi.ch/sls/csaxs/software>.

The macros accept 'Name',value pairs for optional parameters. Calling the macros without parameters will display in most cases a help text and an example. Usually macros will accept parameters of sub-macros. An example is the online viewer `image_spec` that accepts the parameters of `image_read` and `image_show` since it is calling these functions to read and display the data.

Some of the Matlab functions:

- `image_read` can be used for reading PILATUS `cbf` and `edf` and other data files.
- `image_show` is a macro for reading and displaying an image data file.
- `image_spec` is an online viewer for spec, see [section 5.1](#)
- `spec_read` can be used to access the `spec` data file
- `spec_plot` can be used to plot data from the `spec` data file
- `scan_movie` can be used to view a whole scan or for writing this display as a video in AVI format.
- `prep_valid_mask` tries to identify the valid, i.e., neither dark nor hot pixels.
- `display_valid_mask` visualizes a valid pixel mask
- `beamstop_mask` cuts out the beamstop, i.e., a user specified region, from the list of valid pixels.

- `tune_valid_mask` can be used to remove remaining hot pixels by comparing median filtered integrated to raw data
- `get_beam_center` can be used to optimize the beam center in a  $7 \times 7$  grid around the specified good guess with sub-pixel precision. This macro is not very fast.
- `prep_integ_masks` is used to prepare the radial integration of SAXS data.
- `display_integ_masks` visualizes integration masks
- `radial_integ` performs the radial integration of SAXS data using the integration masks prepared beforehand.
- `integrate_range` integrates a range of scans as they become available
- `plot_radial_integ` can be used to display radially integrated data
- `mcs_mesh` displays multi channel scaler (MCS) data, see [section 4.21](#) for details on the MCS
- `stxm_online` is a viewer for scanning x-ray transmission microscopy (STXM) like raster scans

## 5.1 Online viewer

The Matlab online viewer for 2D detector data is typically started from a text-only Matlab session running on `x12sa-cn-1`. This text session typically runs in the second or third sub-window of the main text console (`spec` running in the first sub-window).

To start it from scratch log on to the compute node using `ssh -X x12sa-cn-1`. On the compute node change to the Matlab directory `cd ~/Data10/matlab` and start `matlab -nodesktop`. In Matlab start `image_spec`. The macro will display a brief help on its parameters. For displaying PILATUS 2M data with the default options use `image_spec(1);`

## 5.2 Example: how to get azimuthally integrated data

There are more options available than it is useful to list here. The following example demonstrates how one can get to integrated intensities, a common task in small-angle x-ray scattering (SAXS).

### 5.2.1 Valid pixel mask

To create a list of all valid pixels, called valid pixel mask, you should record a series of at least ten exposures of an unstructured intensity distribution for two well separated detector positions. Glassy carbon or air scattering may be options. One starts the macro once to create a new valid pixel mask for the first exposure series. This mask will not contain some of the pixels close to the beam stop since they have been sorted out due to high intensity variations. Calling the macro again for the second series of exposures with

the `Extend` parameter set to "or" will update the mask with the valid pixels from the second series and thereby add the beam-stop region to the valid pixels:

```
prep_valid_mask('~Data10/pilatus/S05000-05999/S05716/');  
prep_valid_mask('~Data10/pilatus/S05000-05999/S05717/', ...  
  'Extend', 'or');
```

The valid pixel mask is stored in `~/Data10/analysis/data/` if nothing else has been specified.

## 5.2.2 Including the beamstop in the valid pixel mask

The function `beamstop_mask` can be used to cut out the beamstop and its support from the valid pixel mask. The user needs to specify the name of an example data image and the (x,y) coordinates of the beamstop area. The example image is displayed with the user-defined beamstop area in reduced intensity to aid judging if the coordinates are sufficient. If the result is satisfying then the updated mask can be saved by setting the `'SaveData'` parameter to 1:

```
beamstop_mask(['~/Data10/pilatus/S05000-05999/S05715/' ...  
  'e12612_1_05715_00000_00000.cbf'], ...  
  'xyCoord', [705 0; 712 619; 715 699; 720 699; 720 619; 721 0], ...  
  'SaveData', 1);
```

The original valid pixel mask will be overwritten.

## 5.2.3 Determining the beam center

Using silver behenate or any other strong scatterer one can determine the beam center by minimizing the standard deviation of the intensity integrated over a ring as a function of the ring center position. One needs to specify the name of the data file, a good guess for the beam center position and the radius range for the ring over which the macro will integrate:

```
get_beam_center(['~/Data10/pilatus/S05000-05999/S05715/' ...  
  'e12612_1_05715_00000_00000.cbf'], ...  
  'GuessX', 717, 'GuessY', 708, 'RadiusFrom', 80, 'RadiusTo', 100);
```

It is not recommended to increase the area over which this macro searches for the optimum beam center beyond the default value of  $\pm 3$  pixels since this macro is quite slow. The beam center that is returned has usually sub pixel precision.

## 5.2.4 Preparing the integration masks

The coordinates for the azimuthal integration are determined once and stored in a data file. As parameters one needs to specify the name of a raw data file for the final quality control display and the beam center as for example determined using `get_beam_center`:

```
prep_integ_masks(['~/Data10/pilatus/S05000-05999/S05715/' ...  
  'e12612_1_05715_00000_00000.cbf'], ...  
  [ 716.901 707.951 ], 'NoOfSegments', 16);
```

The number of azimuthal segments is by default 1. If the SAXS data exhibit azimuthal asymmetry then this may be captured by integrated in a certain number of segments like 16 in the present case. The integration masks are stored in `~/Data10/analysis/data/` if nothing else has been specified.

### 5.2.5 Integrating a range of scans

Azzimuthal integration of data can be done using `radial_integ`. To integrate a range of scans as they become available a wrapper function is available:

```
integrate_range(5714,5915);
```

This call integrates the scans 5714 up to and including 5915. Without further parameters the default input path `~/Data10/pilatus/...` is used and the default output path `~/Data10/analysis/radial_integration/` for the integrated data in Matlab data format. The integrated data of all files of a scan are stored in a single data file. The file name is deduced from the name of the first file of raw data that is read and integrated.

### 5.2.6 Plotting radially integrated data

By default the plotting routine displays the mean of all points, i.e., of all integrated intensities stored in a file and also of all azimuthal segments:

```
plot_radial_integ(['~/Data10/analysis/data/' ...  
                  'radial_integration/' ...  
                  'e12612_1_05714_00000_00000_integ.mat']);
```

This plotting function returns the plotted data, i.e., it can be used for simple averaging tasks.

### 5.2.7 Removing hot pixels from the valid pixel mask

If one notices that the azimuthal integration has artificial spikes then these are most likely related to hot pixels that have not been recognized so far. One can mask them by comparing the median filtered azimuthally integrated data against the raw data, if the raw data exhibit a smooth intensity distribution:

```
tune_valid_mask('~/Data10/pilatus/S05000-05999/S05720/', ...  
               'SaveData',1);
```

In the present example all `*.cbf` files from the specified PILATUS directory are compared against the radially integrated data stored under the default name in the default location. A quality control plot is displayed and if the result is satisfying then one can set the 'SaveData' parameter to 1 to update the stored valid pixel mask. For this updated mask to take effect the integration masks need to be generated again, see [section 5.2.4](#).

### 5.2.8 Determining the sample to detector distance using silver behenate

If one records the SAXS signal of silver behenate, integrates the data and determines the position of a ring of intensity by clicking on the plot displayed by the plotting function, see [section 5.2.6](#), then one can calculate the sample to detector distance as  $r \cdot 0.172 \text{ mm} / \tan(n \cdot \arcsin(\lambda / (2 \cdot 58.380 \text{ \AA})) \cdot 2)$  which may be approximated by  $r \cdot 0.172 \text{ mm} \cdot 58.380 \text{ \AA} / (n \cdot \lambda)$ . Here  $r$  is the radius of the ring of intensity in pixels,  $n$  is the order of the silver behenate diffraction ring and  $\lambda$  is the x-ray wave length as displayed by `mono_show_all` in `spec`. The detector pixel size of 0.172 mm and the silver behenate spacing of 58.380 Å are the remaining parameters.

## 6 Chemistry lab.

A small chemistry lab is located directly at the beamline to help you preparing your samples for the measurements. The lab is not suitable for handling, e.g., ultra toxic or radioactive hazards. Among others the following equipment is available:

- solvent cabinet (with exhaust)
- fume hood: width 1.5 m, max. 500 m<sup>3</sup>/h, nitrogen and argon gas supply upon request
- horizontal laminar flow box as local cleanroom environment (in the user preparation room, not in the chemistry lab): Skanair HFX90, 0.9 m width
- fridge freezer combination with not too much space: Dometic ML305C, fridge set to 5°C, freezer to -20°C, min. -35°C possible
- Millipore Milli-Q Gradient water purification
- stereo microscope Zeiss Stemi 2000 with Schott KL1500 LCD cold light source (the latter with ring light adapter and alternatively double goose neck light guide)
- Leica DM2500 M high resolution microscope with camera and sample position encoder attached (in the user preparation room, not in the chemistry lab)
- Hettich Universal 320R centrifuge, relative centrifugal force up to 21382, temperature set point between -20°C and 40°C.
- heating cabinet: SalvisLab TC100, inner dimensions 450×500×460 mm<sup>3</sup> / 100 l useable volume, max. 200°C, microprocessor PID control
- digital RTD thermometer
- pH meter VWR symphony SB70P
- pH indicator paper, pH 1-14
- three weighing machines for different weight ranges: Sartorius BL210S with 0.1 mg reading and max. 200g, max. 4 kg and max. 50 kg weighing machines

- ultrasonic bath without heating option: Merck Eurolab, 35 kHz
- small magnetic stirrer
- magnetic stirrer and heating plate combination: IKA RCT basic, max. 1100 RPM and 250°C
- heating plate with digital control and external sensor option: Torrey Pines Scientific HP 30A-2, max. 400°C
- small membrane pump
- desiccators for vacuum or drying pad use
- hotmelt glue gun
- glassware washer
- demin. water and standard cold water from the tap
- Eppendorf safe lock tubes in 0.5 and 1.5 ml
- Eppendorf pipettes: Reference, 20, 100, 200 and 1000 ml
- basic glassware, spatulas, tweezers, scalpels, syringes
- glass capillaries with 10  $\mu\text{m}$  wall thickness, capillary wax and wax pen

Suggestions for improvements are welcome. Please report missing or almost out of stock items. Please arrange with your local contact if you need excessive amounts of certain consumables.

## 7 Troubleshooting / Frequently Asked Questions

- **Is the beam shutter open?**  
**Why can't I open the beam shutter?**  
**Is there beam available for the beamlines at all?**  
Please use `bl_show_all` in spec.
- **How do I get help?** Please contact your local contact using the PSI phone number from <http://www.psi.ch/sls/csaxs/people> or <http://www.psi.ch/sls/csaxs/contacts> or the mobile phone number 079 343 92 30 that is printed on the phone at the beamline as well. From within PSI dial a 0 first to get out. If this fails try to contact somebody else from the cSAXS staff page. You can phone the accelerator control room (5503) any time and briefly describe your problem. The control room has a phone list and will contact the appropriate person if needed.



- **The Matlab online viewer crashed or beeps when I move the mouse over it or I can not zoom in anymore. What shall I do?**

Search for the Matlab window. Typically this is in the main console window the second or third tabulator (the first being `spec`). Stop the online viewer there using `<CTRL>-<C>`. Close the online viewer plot window using the mouse or `close all` in Matlab. Restart the online viewer `image_spec` by pressing `<Cursor Up>` to get the previous command starting with `image_spec` and confirm with return. See also [section 5.1](#).

## A History

March 18th 2011	Oliver Bunk	v1.02, include slit 0, small Hexapod, PILATUS 300k-W, and indications of other pieces of hardware like teslameter, digital delay generators, temperature controller, Leica microscope, update links to new web page
June 17th 2010	Oliver Bunk	v1.01, include Cetoni and Hamilton syringe pumps, minor updates
May 21st 2010	Oliver Bunk	v1.00, include an example for azimuthal integration using Matlab and other minor updates
November 26th 2008	Oliver Bunk	v0.80, update x-ray energy range
September 23rd 2008	Oliver Bunk	v0.29, new name <code>epics_boottime</code> , document <code>pon</code> , <code>poff</code> and <code>pkill</code> , document new SMS features, update <code>pilatus_threshold</code>
August 7th 2008	Oliver Bunk	v0.28, new names <code>id_gap_E_keV</code> , <code>mono_settings_E_keV</code> , <code>mono_E_keV</code> , new macros <code>mono_offs</code> , <code>mono_id</code> , <code>dmesh</code> , section on continuous scans <code>cont_line</code> and <code>cont_mesh</code> , SMS features, delayed shutter closing, E-710 piezo controller macros
June 3rd 2008	Oliver Bunk	v0.27, add distance to PILATUS modules
May 28th 2008	Oliver Bunk	v0.26, add power socket and user bike information
May 26th 2008	Oliver Bunk	v0.25, add light curtain and slit 1 and 2 position, combine beamline layout with control section
May 23rd 2008	Oliver Bunk	v0.24, add information on the location of slit 3 and 4 and the sample table
May 19th 2008	Oliver Bunk	v0.23, add section on the beamline layout and sub-section on the beamline web pages, start the troubleshooting section
May 2nd 2008	Oliver Bunk	v0.22, rename <code>pilatus_set_threshold</code> and <code>pilatus_set_basename</code> , add <code>pilatus_file_format</code> , add Mythen macros, add basic chemistry lab. inventory
April 17th 2008	Oliver Bunk	v0.21, update data transfer section, add <code>rsync</code> for Windows
April 13th 2008	Oliver Bunk	v0.20, major update
December 12th 2007	Oliver Bunk	v0.17, last of several updates including among other Hexapod, fast shutter, exposure box slits and filters, PILATUS burst mode, camera and Matlab macro informations
August 23rd 2007	Oliver Bunk	include PILATUS threshold information
August 19th 2007	Oliver Bunk	several minor updates
August 8-9th 2007	Oliver Bunk	first draft

## B Phone list

The up to date phone-list is available online at

<http://www.psi.ch/sls/csaxs/contacts>. A printout can be found on the white-board in the control room.

## C Guest network

Connecting to the network or using any PSI IT resource requires agreement to the ‘Usage and Monitoring of IT Resources at PSI’ regulations available online at

<http://ait.web.psi.ch/regulations/>.

An open WLAN is available inside the SLS building and other selected areas. Using it should be ‘plug and play’.

See [http://ait.web.psi.ch/services/guest\\_net/](http://ait.web.psi.ch/services/guest_net/) for details.

Alternatively you may connect your laptop or PC via an ethernet cable to the beamline network provided

- it is in accordance with the security guidelines of our IT department, including an up-to-date virus scanner
- gets a network address via DHCP
- does not create heavy network load (no streaming of music and videos, IP-based phone calls etc.)

Your browser must be configured for using a proxy. In Mozilla you may use an automatic proxy configuration via <http://nedi.web.psi.ch/proxy.pac> (set this link in edit → preferences → advanced → proxy → automatic proxy configuration). Otherwise the proxy can be set manually to `proxy.psi.ch`, port 3128.

## D Data transfer

The amount of data created depends strongly on the application but please keep in mind that a single PILATUS frame means 10 MB of data typically compressed to 2.5 MB in CBF format. A typical run of 3-5 days creates between 100 GB and 15 TB. The data will compress well using tar+gzip which is the default for data transfer to user disks at cSAXS. Please bring a sufficient amount of sufficiently large USB or eSATA disks for your data. The data will be transferred using a ‘media station’ running Linux for transfer to ext3 or NTFS formatted disks. **We recommend that the data transfer is set up by your local contact and started while you measure, well before the end of your beamtime.**

### D.1 File systems

The disks will be formatted at the beamline or must be preformatted in either ext2 (Linux), ext3 (Linux), or NTFS (Windows). FAT32 is rather limited in the number of files per directory and the maximum file size and therefore not suitable for data transfer.

## D.2 Data transfer

Ideally you choose an ext3 or ext2 file system. Using FAT32 usually ends with running into one of its limitations, see [section D.1](#). Meanwhile NTFS is sufficiently supported under Linux to be used as well.

### D.2.1 Mounting drives

When an external hard-disk is connected then a popup window asks what to do. If you want to access a formatted disk then mount it via this popup. The drive will appear under `/media/`. If you want to format the disk then cancel this popup dialog.

If the auto mounting does not work follow the instructions at [https://intranet.psi.ch/Controls\\_IT/LinuxMediaStationUsage#manual\\_mount](https://intranet.psi.ch/Controls_IT/LinuxMediaStationUsage#manual_mount). These instructions are only available within the PSI network and need authentication with a PSI account.

### D.2.2 Formatting drives under Linux

A not mounted drive can be formatted using `sudo gparted`. **This tools allows formatting the system partitions as well, i.e., be sure what you do or you may crash the system unrecoverable.** Select the external disk in the list top-right. Most likely it is `/dev/sdb`. It is NOT `/dev/sda` or `/dev/md0`. If partitions of the external drive are mounted then unmount them using ‘Partition’, ‘Unmount’. If you want to completely erase all partitions and start from scratch with a new partition table then select ‘Device’, ‘Set Disklabel’.

Clicking on the unallocated disk space you can add a ‘New’ partition to it. This pending operation needs to be confirmed using ‘Apply’.

Mounting the drive can be done ending `gparted`, unplugging and plugging in the cable to the external drive and selecting ‘Open’ in the then emerging pop-up window.

### D.2.3 Access rights for pre-formatted Linux drives

If the e-account has not sufficient access rights to an ext2 or ext3 drive then `sudo usbdisk777` will flatten the access rights for all disks mounted as sub-directories of `/media/`.

### D.2.4 Compressing data

The PILATUS data will usually compress very well. A tar-bzip2 job for compressing the data could be run on `x12sa-cn-1`. Your local contact can start

```
~/Data10/bin/tar_pilatus_as_available
```

to compress data in bunches of a certain number of scans. At the end of the beamtime your local contact could run

```
~/Data10/bin/tar_pilatus_last and
```

```
~/Data10/bin/tar_non_pilatus_and_tar_files
```

for compressing the remaining data. You can read gzip compressed tar archive under Windows using helper applications like 7-Zip.

## D.2.5 Transferring data using rsync

Your local contact can start the script `~/Data10/bin/rsync_usbdisk` for you. The data transfer should be started at the beginning of the beamtime to run in parallel to the acquisition.

## D.2.6 Related informations

The mounted disks do not appear in `/etc/fstab`. The free space can be checked using `df -h`.

A `sudo umount` command for manual unmounting of disks is available, e.g., `sudo umount /media/disk`. Using `sudo gparted` and the ‘Partition’ menu with the ‘Unmount’ option is possible as well.

## D.3 Windows specific information

### D.3.1 Formatting drives

Either you need a local contact with sufficient access rights for the Windows PC or you have to prepare the hard disk on another PC or laptop where you have an account with sufficient access rights. On this machine the computer management should be started from the administrative tools menu or by running `compmgmt.msc /s`. Select ‘Disk Management’ and format the external disk to NTFS. Afterwards you can select ‘properties’ of this partition by right clicking on it and set under security sufficient access rights. Typically this means ‘Modify’ and related access right for ‘Everyone’.

### D.3.2 Mounting the e-account on the file server

Mount your e-account using the explorer: ‘Tools’, ‘Map Network Drive’, folder `\\x12sa\e-account` (replace with your e-account name), do not ‘Reconnect at logon’, ‘Connect using a different user name’ (your e-account and password), ‘Finish’.

## E Where to eat

The ‘personnel restaurant’ Oase offers lunch from 11:30 until 13:30 and dinner from 17:00 until 20:00, both Monday to Friday.

See <http://services.web.psi.ch/oase/menu.php> for the menu.

The cafeteria west, the ‘timeout’ is open from 8:00 - 16:00, Monday to Friday, see <http://log.web.psi.ch/verpflegungsbetriebe/oeffnungszeiten.shtml> for the up-to-date opening hours. Outside opening hours vending machines are available.

In Villigen, 10 minutes walk from PSI, you will find

- the restaurant ‘Zum Hirschen’ (closed on Tuesdays)
- a baker, Monday to Friday 6:30-12:00 and 15:00-18:00, Saturday 7:00-13:00
- a small Volg supermarket, Monday to Friday 7:30–18:30, Saturday 7:30-16:00

- and an ATP machine.

Towards Würenlingen is a large COOP supermarket easily reachable by bike.

By bus and car several restaurants in Brugg, Baden, Böttstein, Würenlingen etc. can be reached.

## **F Public transport**

Public transport in Switzerland is excellent. Even at PSI frequently buses are calling. Check for connections from and to 'Villigen PSI West' on the SBB home-page:

<http://www.sbb.ch/en/index.htm>

There are direct connections by train from Zurich airport to Brugg. From Brugg one can take the bus to get to PSI.

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