

FOCUS manual pages

last updated July 2007.

these manual pages are meant to be as concise as possible.
they should not take you more than 20 minutes to read.
please let us know your comments.



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log into the instrument computer

FOCUS is run by the instrument computer *focus.psi.ch* next to the window of the hutch.
you log in as user 'focus' (the password will be provided to you by your local contact).

this is the instrument control computer, in order not to risk your own measurement:

- do not run applications other than from your local contact shown
- keep the directories clean, do not create directories and unnecessary files
(with the exception of job-files which reside in ~/batch)

we advice the users to run only the following programs on *focus.psi.ch*:
'sics', 'focus', 'sea', 'focusreport', 'focuscheck', 'setting', 'fit', 'nedit', 'six',
and standard unix commands as, e.g., 'less' etc.

there is another Linux computer *lnsl01.psi.ch* available near the rack. this computer is dedicated to
the visualization and analysis of your data. here you are invited to create your guest directory and
store your data. alternatively, we provide ethernet cables to connect your personal laptop to the
local network.

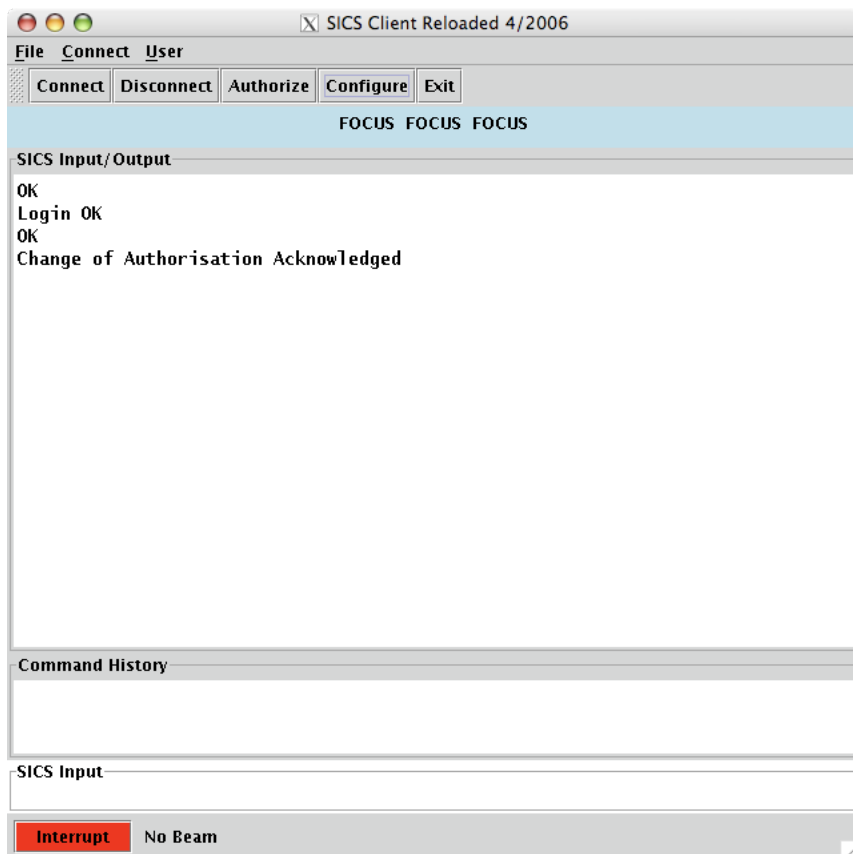
access to '*focus.psi.ch*' and '*lnsl01.psi.ch*' is only granted from within the PSI domain.

start/stop measurements with sics

measurements are controlled by the program 'sics'. invoke it from *focus.psi.ch*:

```
[focus@focus ~]$ sics &
```

then 'connect' to 'FOCUS' (from within the menu or menu buttons) [follow this link if you fail],
next 'authorize' by entering the username/password provided by your local contact.
then please fill in the respective fields in the 'configure' dialog (after having pressed the corresponding button).
you should get the following:



now you are able to start/stop measurements. normally, measurements are run from a job-file. these are tcl files and must be located in the directory '~/batch'. a typical job-file could look like this:

```
title dynamics of IF6 protein 6 AA, 300 K
sample buffer solution, T=300 K
drive temperature 300
wait 600
count monitor 20000
count monitor 20000
```

your local contact will be happy to help you writing the first job-file which you may then modify. as a convenient text editor you may use, e.g. 'nedit'.

it is good habit to check your file against syntax and spelling errors. this can be done with the syntax checker 'focuscheck' (invoked from the unix shell):

```
[focus@focus ~]$ focuscheck jobfile.tcl
```

once the job file is written and stored in '~/batch' you may execute it by invoking in 'sics':

```
batchrun jobfile.tcl
```

the status will correspondingly change to 'counting' in the 'sics' application (other states are listed below). a measurement can be stopped anytime by pressing the stop button, or by invoking 'stop' from within the command line of 'sics'.

P.S.: finally we note that sics commands can alternatively be entered within the 'focus' application (see below) or within the command-line version of 'sics' called 'six'. we refer to commands entered in the 'sics command line'.

supervising your running measurement

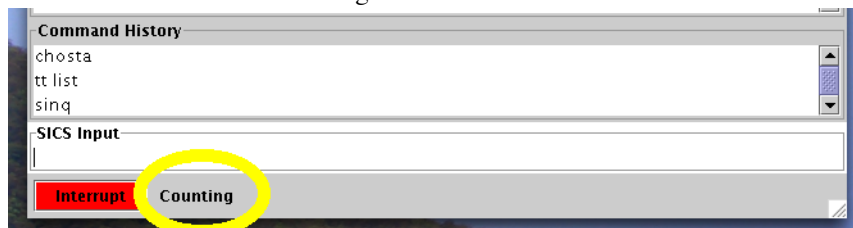
although your local contact will glance at the instrument from time to time, it is **your proper interest to check that the instrument is counting, data acquired and sample environment variables within setpoints**. we have taken care to make this task as transparent as possible for you and hope, the following guidelines will help.

you will sleep better, if you check before going to bed that:

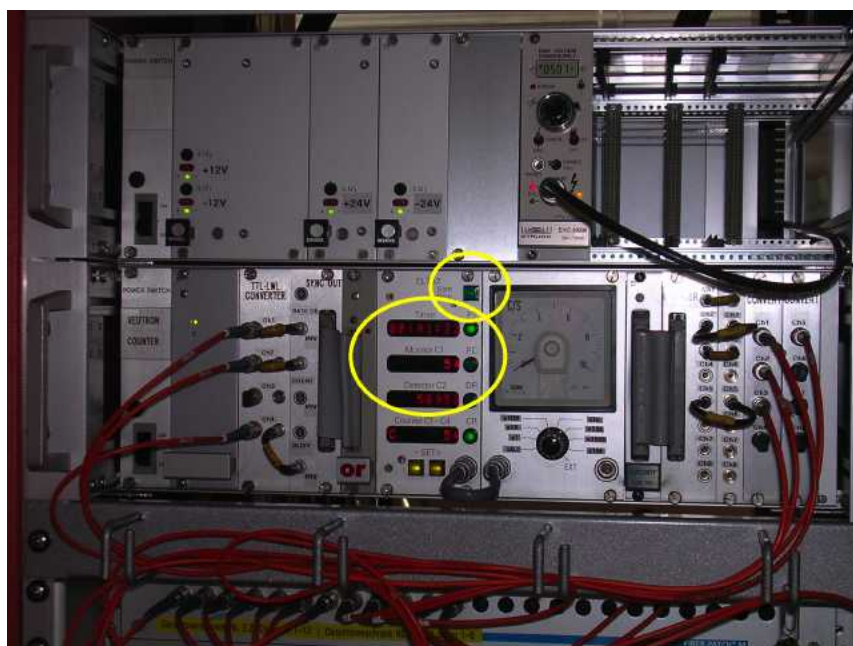
- (i) instrument is counting properly and chopper system is okay
- (ii) TOF spectrum looks reasonable
- (iii) sample environment variables are within setpoints
- (iv) data are saved accordingly to active job-file

(i) check that instrument is counting properly and chopper system is okay

the status of 'sics' reads 'counting':



the monitor values are increasing as seen, e.g., on the electronics rack in the instrument hutch:



if you happen to have no beam or beam below a certain threshold, the instrument is 'on-hold' with the start/stop light of the counter box (image) flashing. FOCUS will resume counting when beam is back. alternatively, you can check the monitor values by invoking in 'sics':

```
counter status
```

or by inspecting the monitor value with the 'focus' application (see below).

the status of the neutron source (and corresponding messages) can be checked with

```
sing
```

chopper states can be inspected by invoking from within 'sics'

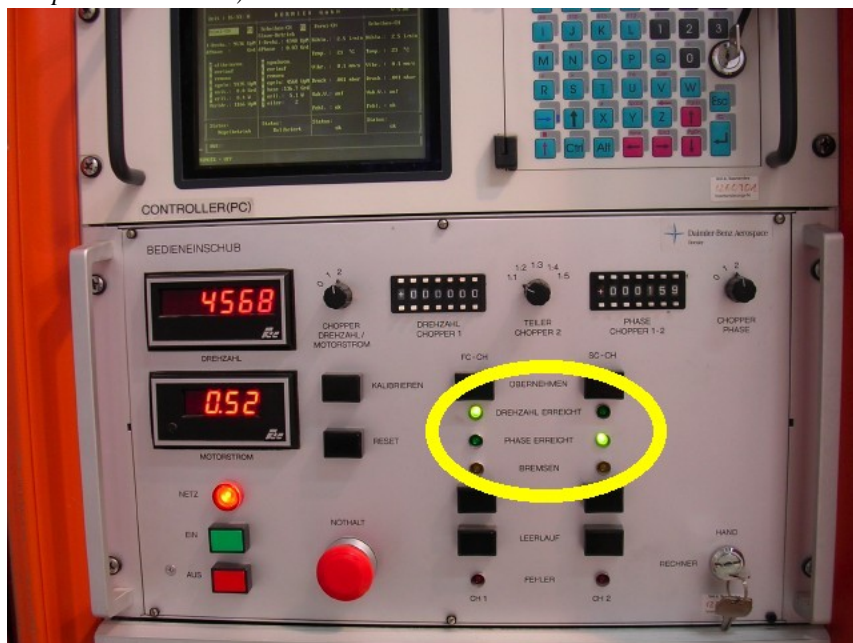
```
chosta
```

resulting, e.g., in:

Chopper Status		
Chopper in synch mode		
	Fermi Chopper	Disk Chopper
Actual Speed	16810	5603
Set Speed	16810	5603
Phase	0.0	21.2
Phase Error	0.0	0.02
Loss Current	0.4	5.1
Ratio	1	3
Vibration	0.2	0.2
Temperature	21.6	24.0
Water flow	2.7	2.7
Vakuum	0.0014	0.0019
Valve	1	1
Sumsi	0	0

vibrations should be within less than 0.5 mm/sec and water flow above 1.5 l/min.

a word of caution: actual values are read-out by a dedicated computer but are controlled by hardware. depending on the given setup the read-out might be erroneous and you may suspect a malfunction of chopper system - this however, is solely a problem of read-out (and a pretty old computer too). as long as the two LED lamps on the chopper rack (down stairs) are lightening in GREEN, you can be sure the speed and phase of the two choppers are okay. (errors in the read-out are linked to so-called 'XIX errors' displayed at the chopper read-out computer downstairs).

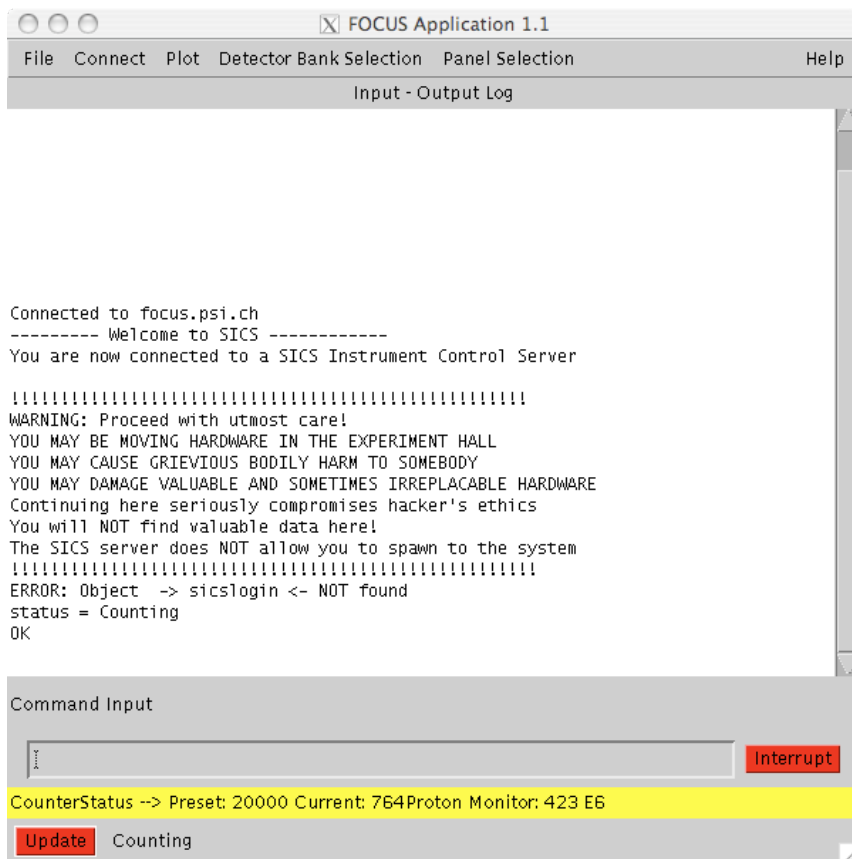


(ii) check that the TOF spectrum looks reasonable

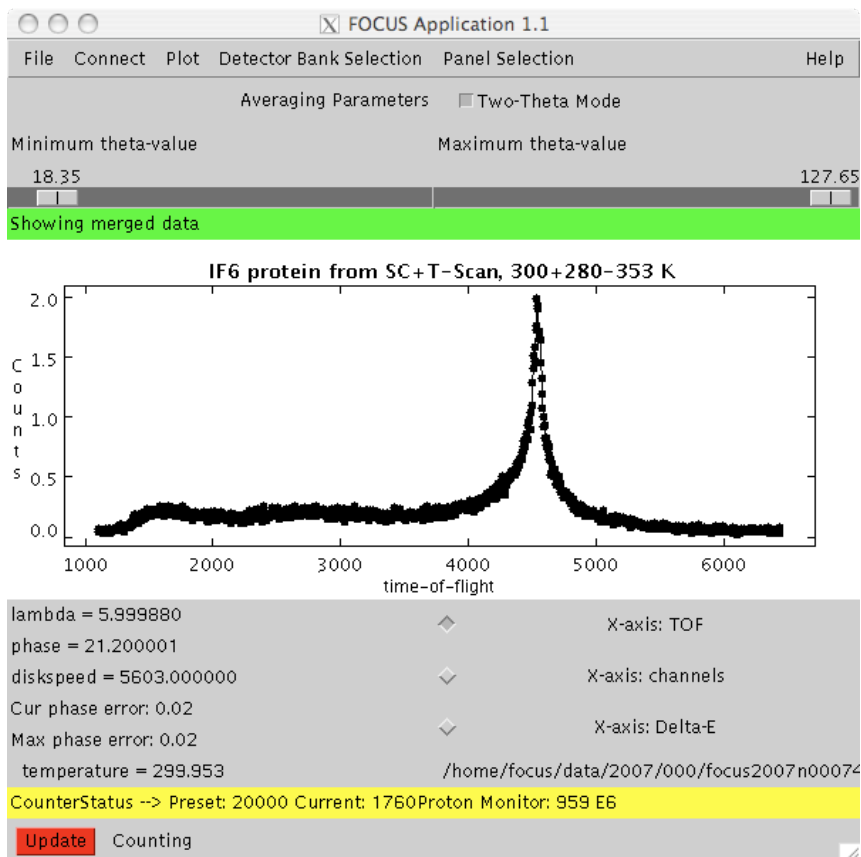
the application 'focus' invoked from *focus.psi.ch* gives you the possibility to visualize your current measurement.

```
[focus@focus ~]$ focus &
```

similar to 'sics', first 'connect' and optionally 'authorize' to FOCUS.



from within the command line you can invoke all FOCUS command as within the program 'sics' (we refer to commands typed into the 'sics command-line'). now choose the banks from the 'Detector Bank Selection' (choose merged), then in the 'Panel Selection' menu choose 'Status Panel' to get a view of the current spectrum (you may choose between TOF, energy and channel for the x-axis).



words of caution:

- (i) at the beginning of a measurement the conversion to energy may be wrong due to bad statistics since the elastic line cannot be fitted properly, be patient and collect for some more stats. also note that this program does not take into account $(k/k')^4$ correction of the measured intensity.
- (ii) chopper warnings may not be relevant since values may be read-out erroneously (see above) [we are working on this issue, but have no recipe yet].

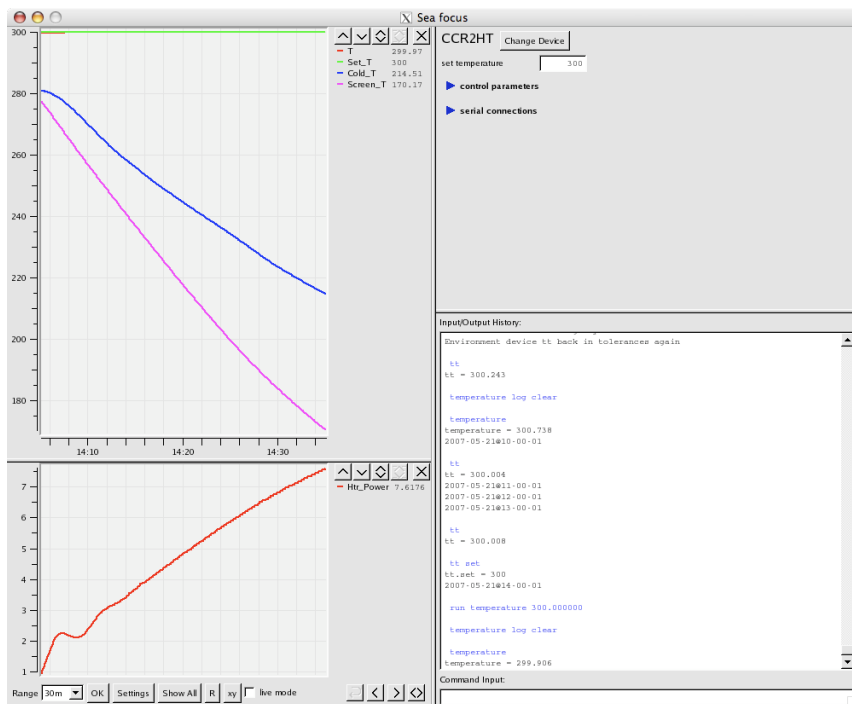
the monitor values are displayed at the bottom together with corresponding preset and the current state of the instrument. instrument states indicated by 'focus' and 'sics' are:

Eager to execute commands	the instrument is idle and awaits commands (you are wasting beam time)
Counting	the instrument is counting, beam above threshold
Driving	the instrument is driving a variable as, e.g., temperature - measurement is suspended until setpoint reached
No Beam	there is no beam (check the source is up, shutter open and choppers at speed/phase)

(iii) check that sample environment variables are within setpoints

sample environment variables (temperatures, magnetic field, helium level, etc.) are most conveniently checked from within the application 'sea', invoked from 'focus.psi.ch':

```
[focus@focus ~]$ sea &
```



alternatively you can invoke 'tt' or 'tt list' (or 'temperature' instead of 'tt' from within the 'sics' command-line) to get the current temperature value, setpoints etc.

sample environment variables can be either controlled by 'sics' or by 'sea'.

for running measurements we suggest using corresponding 'sics' commands as, e.g., 'drive tt 2.7'.

(iv) check that data are saved accordingly to active job-file

the command 'focusreport' lists monitor values, acquisition times, titles, temperatures, wavelengths and star dates/times of given run numbers, e.g.,

```
[focus@focus ~/thierry]$ focusreport 914 917
run-#  monitor  time                sample      T   WAV  Stardate
000914  50000  7248.29      NaCrO2, 5AA, T=1.8K  2.10  5.00  2007-05-29 22:59:19
000915  50000  7245.71      NaCrO2, 5AA, T=1.8K  1.90  5.00  2007-05-30 01:05:06
000916  50000  7204.13      NaCrO2, 5AA, T=35K  35.07  5.00  2007-05-30 03:17:44
000917  50000  7557.99      NaCrO2, 5AA, T=35K  34.90  5.00  2007-05-30 05:22:07
```

with SINQ running constantly, the monitor/time values should be approximately constant.

at the end of your measurements such list is also handy to print out and paste into your logbook.

```
[focus@focus ~/thierry]$ focusreport 914 917 | lp
[focus@focus ~/thierry]$ focusreport 914 917 > myfocusmeas.txt
```

visualizing your data in TOF

please: data analysis should be carried out on the computer *lns101.psi.ch* (closer to the electronics rack).
 the instrument computer *focus.psi.ch* is reserved for controlling the instrument.
lns101.psi.ch has access to all live datafiles.

Hint: in order to force an update of the current data file, invoke from within the sics command-line (on *focus.psi.ch*):

```
storefocus update
```

(this command should be invoked from an instance of the 'sics' or 'focus' application other than the one the job file has been launched from - otherwise you get a 'busy' error).

TOF spectra can be conveniently plotted using the program 'fit' available on all SINQ computers (now on *lnsl01.psi.ch*, please):

```
[focuslnsg@pc4689 ~/paolo]$ fit
```

```
Program FIT          Version 4.6 (2007-05-21 10:01:00)
```

```
-----  
Display device type: XWINDOW (X window window@node:display.screen/xw)  
Printer device type: CPS (Colour PostScript file, landscape orientation)  
print destination undefined  
one graph per page
```

```
Default for numors: focus:2007: (highest: 741)
```

```
Hit <RETURN> to continue with last data
```

```
Filename(s) or numor(s) (? to get help):
```

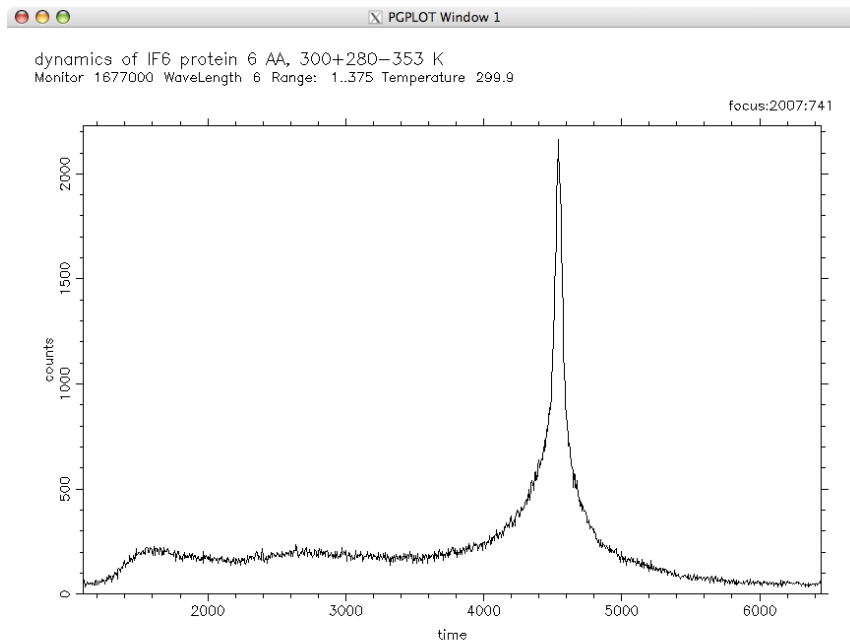
you are presented a welcome message with the number of the latest data run.
enter the run number of the data set you like to display (run numbers are displayed within 'sics' and 'focus'),
or alternatively press the [enter] key and load-in data with, e.g.

```
fit>dat 741
```

```
/afs/psi.ch/project/sinqdata/2007/focus/000/focus2007n000741.hdf opened  
lambda= 6.00; Temp= 300.74; Monitor=12913875.0; Counts=310539; Numor= 740  
Npkt= 1070; owner='Paolo Calligari'; Title='dynamics of IF6 protein 6 AA, 300 K'  
Date='2007-05-21 09:32:21'; sample='Cd, 300 K'
```

```
Files read: focus:2007:740
```

you get information on the read-in data file. typing in 'p'+[enter] (for plot) you get your data displayed:



you may zoom your data with the 'z' key ('x' key for autoscale), print with the 'p' key, get help with the '?' key and exit into the command line mode with the 'q' key.

'Fit' is a very versatile program and you may definitely find it worth to get further help by invoking 'help' from within 'Fit' or visiting the [html help-page](#).

Specific to FOCUS you will find the following commands useful:

```
dat 735-740      : reads in data of run numbers 735-740 separately (press the 'c' key to display i  
link 742        : links additional run to current set of runs (e.g. to type on top of each other)
```



```
merge          : sums (and if necessary rebins) all runs
mon 1000       : changes monitor to given value
sub 734        : subtract run number 734 (after normalizing to same monitor value)
dat 735[bank=b] : reads in middle bank of FOCUS only (alternatively use 'u'/'l' for upper/lower bank)
link &710-713  : merges 710-713 and links resulting dataset to present set
info          : additional information on read-in data
leg           : display legend (useful to distinguish multiple data sets)
file          : saves files in ascii-format (w/o header!)
```

note that 'Fit' automatically normalizes all subsequent data files to the monitor value of the first one read-in.

reducing your data into energy

please: data analysis should be carried out on the computer *lnsl01.psi.ch* (closer to the electronics rack).
the instrument computer *focus.psi.ch* is reserved for controlling the instrument.

Hint: in order to force an update of the current data file, invoke from within the sics command-line:

```
storefocus update
```

TOF data can be conveniently transformed into energy using the 'DAVE' suite of programs (we do have ports to other data reduction programs, such as, e.g., LAMP, INX, Nathan, etc. please ask your local contact if you needed any of these).

DAVE has been developed and is maintained by NIST, the FOCUS data reduction module has been written by Philip Tregenna-Piggott here at LNS/PSI.

here we only give a short introduction allowing you to take first steps with DAVE. for detailed information we refer to the corresponding manual.

with DAVE you are able to:

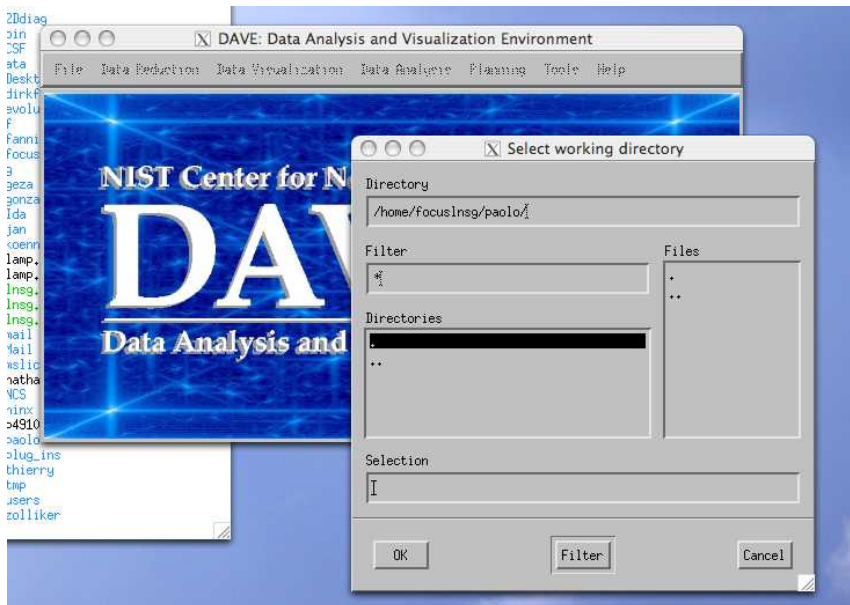
- convert your data from TOF to energy
- mask detectors containing Bragg peaks
- correct for background and detector efficiency
- rebin your data in E- and Q-space
- reconstruct a diffraction pattern
- further analyze your data in DAVE itself, export into
ascii, Igor or MSlice format

as a stand-alone program you are able to analyse your data back at home on your local Windows, Mac or Linux machine.

during your visit please use *lnsl01.psi.ch* to start DAVE:

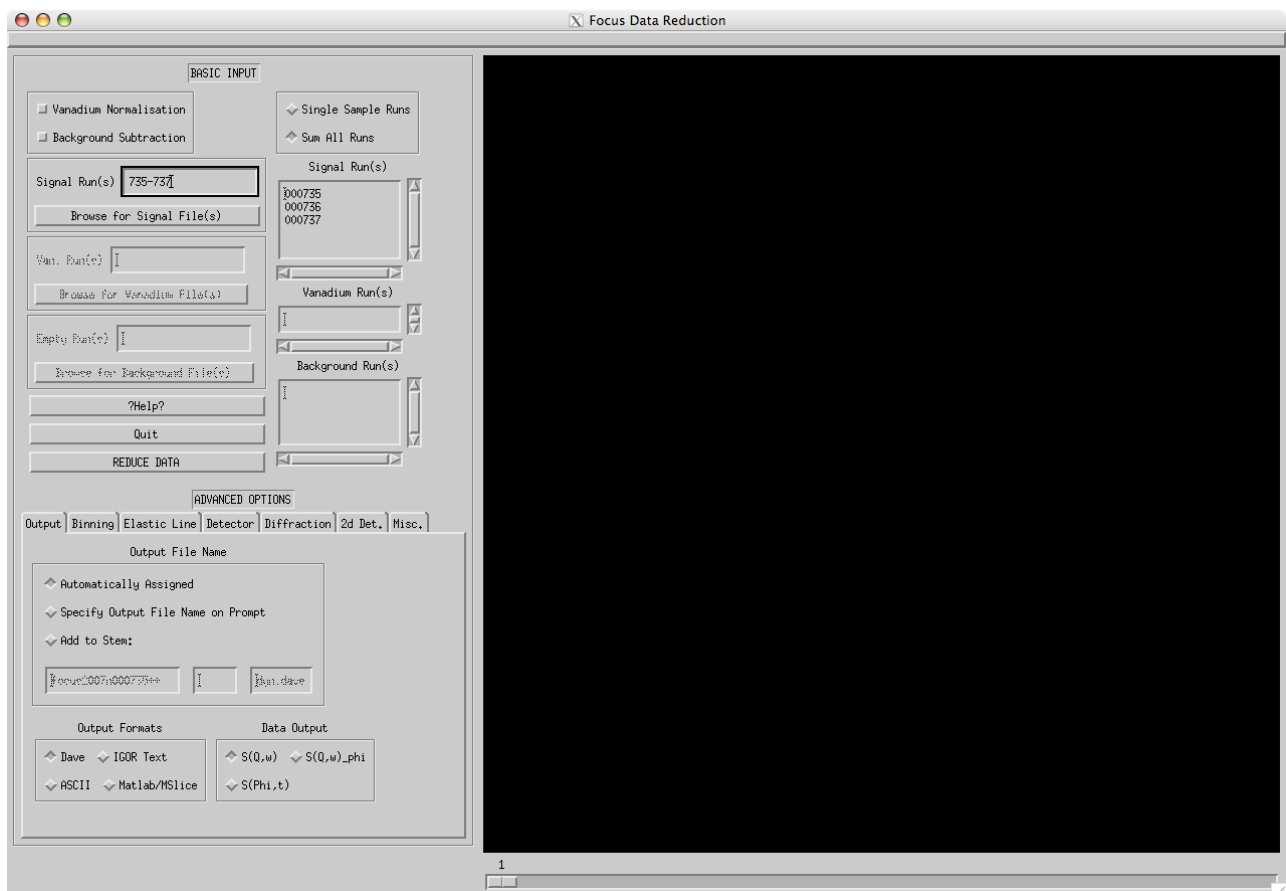
```
[focuslnsg@pc4689 ~/paolo]$ dave &
```

when you start DAVE for the first time, please make sure to change the current working directory (in order not to write DAVE's output into another user's directory), from the menu choose 'File -> Select working directory'.



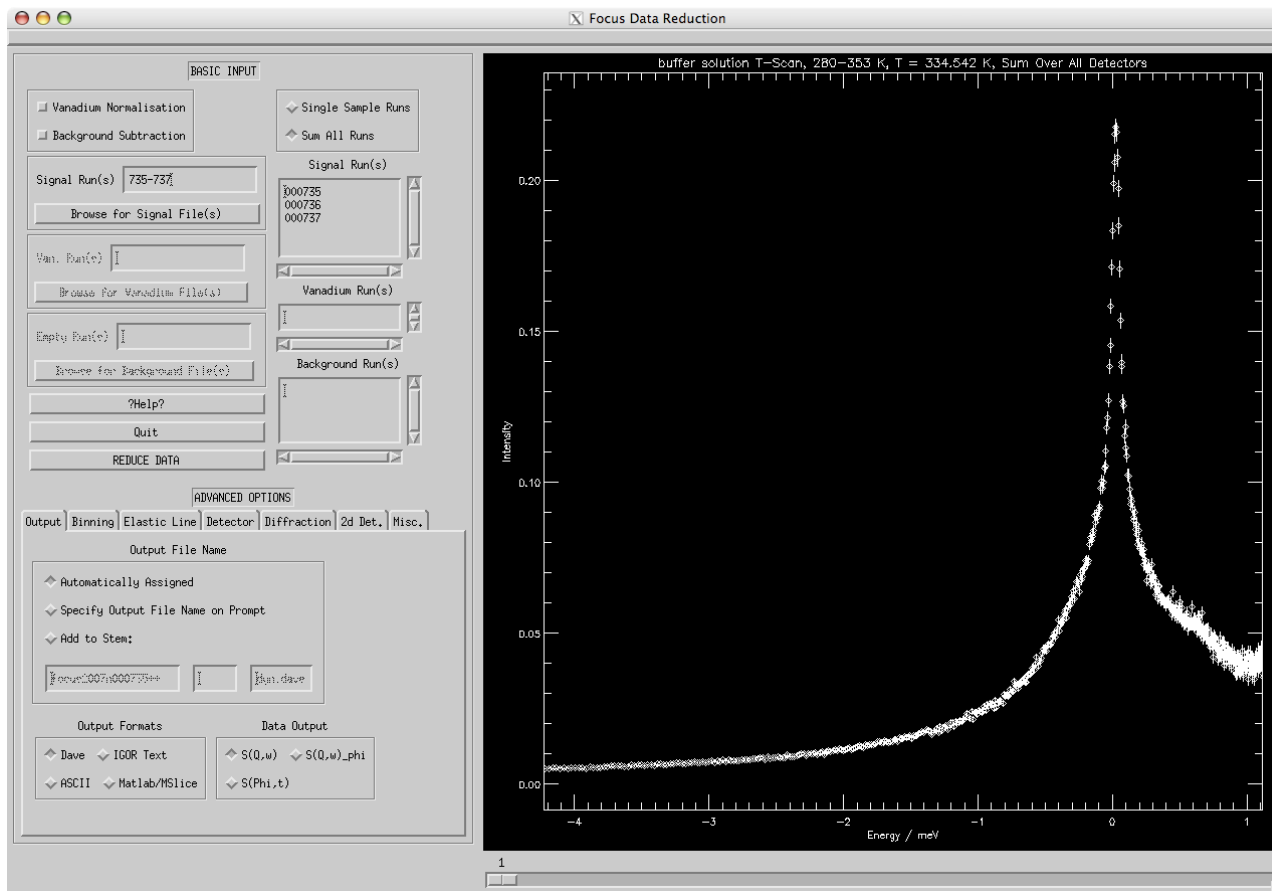
similarly, you can change the directory from where DAVE is taking the raw data. this directory should already be set correctly and read something like: /home/focusInsg/data/2007/000/ please note that data runs 0..999 are stored in /home/focusInsg/data/2007/000/, and 1000..1999 in /home/focusInsg/data/2007/001/ etc.

now you can launch the FOCUS data reduction module from within the 'Data Reduction' menu. in the up-coming window you may enter the file number(s) to reduce the data from (several files may be chosen with, e.g., 740-742). Please note that all input in DAVE needs confirmation with the [enter] key. The selected files are then echoed in the right column 'Signal run(s)', see e.g. below:



you may have a first rough look at your data by pressing the 'reduce data' button.

the reduced data are displayed in the right graphics space and binned into a single Q-group. use the mouse to zoom (double-click for autoscale).



the data are neither corrected for background (to be specified and activated in the main input mask, see above), nor for detector efficiency (vanadium runs must be specified and activated in the main input mask, see above). detector masking is possible within the 'Detector' sub-panel. Energy- as well as Q-binning is controlled within the 'binning' sub-panel, displayed Q-groups can be chosen with the horizontal scrollbar below the graphics space.

by default DAVE is normalizing all data to the monitor value and output is written in DAVE format. if you would like to have your reduced data in ascii format, please specify so in the 'output' sub-panel.

most of the options in the data reduction module are self-explanatory. for a detailed description we refer to the FOCUS data reduction manual.

Remains to be noted that DAVE is much more than a simple TOF-E converter since the converted DAVE files may be further analysed within DAVE (e.g. peak fitted, contour plotted, analysed for QENS, etc.). it is definitely worth to wander around DAVE and have a look at the data analysis modules such as, e.g., 'Data Visualization -> Data Browser', 'Data Analysis -> PAN', 'Data Analysis -> RAINS', modules within the menu 'Planning'.

analyzing your data

converted data can be analysed using 'Fit', 'DAVE', 'MSlice' or third party software depending on your specific context. make sure you do have chosen the correct output file format from within DAVE. if you do have specific questions on how to analyse your data, your local contact may advise you.

remember that depending on the way you analyse your data, you may find it useful to play with the exact reduction procedure of your data (e.g., binning). it hence is a good habit to make already during your visit at PSI sure that you are able to run DAVE locally on your personal computer you will use back at home.

if things go wrong - trouble shooting

*sometimes things go wrong - please have a look at our FAQ list
if you cannot readily ask your local contact:*

Q: I forgot usernames/passwords.

A: have a look around you.

Q: I cannot connect to FOCUS from within 'sics', 'focus' or 'six'

A: a program called 'sics_server' may not be running.

first check whether 'monit' is running by invoking (on 'focus.psi.ch'):

```
[focus@focus ~]$ monit status
```

this should bring up a list of all sub processes running, if not then start 'monit' by invoking:

```
[focus@focus ~]$ monit
```

allow it some time to start up, you may sporadically check with 'monit status' whether the sub processes are coming up.

if you find the 'sics_server' (first process in the list) keep staying in a state other than 'running' then invoke:

```
[focus@focus ~]$ monit restart sics_server
```

once you find the 'sics_server' running again, you may reconnect to FOCUS (make sure to 'authorize' again within 'sics' or 'focus').

Q: I still have troubles with 'monit'

A: there is help available via 'monit -h'. if things are all odd then invoke: 'monit restart all', or 'monit quit' followed by 'monit'. check the status of the sub processes with 'monit status'.

allow the sub process enough time to start-up.

if this does not help, then configurations may be wrong or hardware switched off.

call your local contact or the pikett service (off-hours).

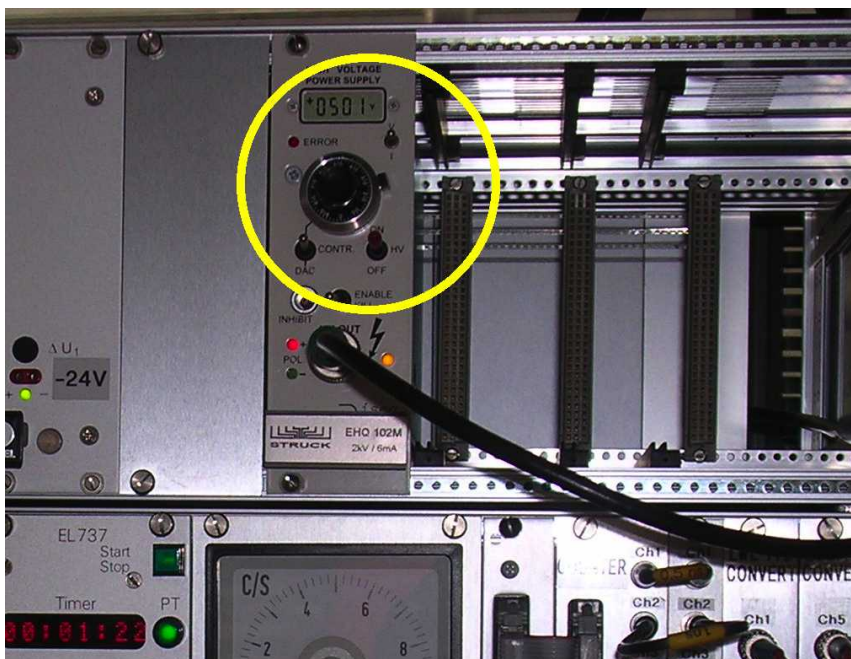
Q: the two green LEDs at the chopper electronics rack labelled

'Drehzahl erreicht' (at speed) and 'Phase erreicht' (in phase) are off.

A: the choppers must be reset and calibrated, please call your local contact.

Q: measurement does not start and 'sics' status reads 'no beam' even when SING is up.

A: (i) measurements only start above a certain threshold of neutron production (typically around 100 uAh), wait until SING is at full power, (ii) check that the shutter is OPEN, (iii) check the HV of the monitor is on



(iv) check choppers are at speed and in phase, (v) call your local contact.

Q: I cannot find my data with 'Fit'

A: tell 'Fit' to associate file numbers with FOCUS by invoking (only once needed), e.g.:

```
dat focus/741
```

(next time you are fine with 'dat 741' since 'Fit' remembers its settings.

Q: DAVE does not find the FOCUS raw data.

A: make sure the 'raw directory' is correctly set: 'File -> Display directories'. if not set it from 'File -> select raw directory'. also note that data runs 0..999 are stored in, e.g., /home/focusInsg/data/2007/000/, while 1000..1999 in /home/focusInsg/data/2007/001/ etc.

Q: I cannot find the output files created by DAVE.

A: DAVE is *not* writing its output in the directory it was launched from, but in the directory defined as the working directory. this directory can be displayed and set within the 'File' menu of the DAVE startup menu.

Q: SINQ is down, where do I get information when it will be back up again?

A: status messages, histories etc. can be obtained following this link, alternatively you may invoke 'sinq' from within the sics command line.

appendix I: list of most useful programs

application	description	example
sics	instrument control program	sics &
focus	instrument control/status program	focus &
sea	temperature control/status program	sea &
focusreport	reports parameters of data runs (e.g. titles, start/stop time, temperature, etc.)	focusreport 801 810 focusreport 801 810 2005

focuscheck	checks jobfile against syntax errors and typos	focuscheck jobfile.tcl
lt	similar to unix command 'ls' but most recent file printed last (handy to see changes in, e.g. ~/batch; corresponds to 'ls -lrt')	lt
sicstail	display last entries of logfile of sics	sicstail, sicstail 100
fit	plot, fit your data (raw data in TOF, reduced data in energy)	fit, fit 801 fit 801-810, fit 801,803
opsld	a collection of data visualization routines written in IDL (start it from within the ~/opsld directory)	opsld
nedit	general text editor (e.g. for editing job-files)	nedit &
idl	IDL (interactive data language)	idl, idlde &
octave	GNU Matlab clone	octave

appendix II: list of most important sics commands

command	description	example
batchrun	starts job-file (must be located in ~/batch)	batchrun prnio3.tcl
storefocus update	forces a read-out of the histogram and update of current data file	storefocus update
count monitor	starts counting to given preset	count monitor 10000
count time	starts counting given time (in seconds)	count time 3600
repeat	repeat counting to given preset several times (either in mode 'monitor' or 'time')	repeat 4 monitor 25000
sample	sets title of the sample (written in data file)	sample PrNiO3
title	sets general title (written in data file)	title PrNiO3, l=5AA, cooling
wait	waits given time (in seconds)	wait 600
drive tt	changes temperature & waits until within tolerance	drive tt 30
run tt	changes temperature & readily continues with next command (no wait)	run tt 30
chosta	prints out chopper status	chosta
setpar	prints out parameters of current instrumental setting	setpar
sampar	prints out parameters of current sample	sampar
vac	reads and prints out vacuum values	vac
tt	prints current temperature	tt
tt list	prints parameters of sample environment (e.g., helium level, setpoints, heating power,	tt list

| etc.)