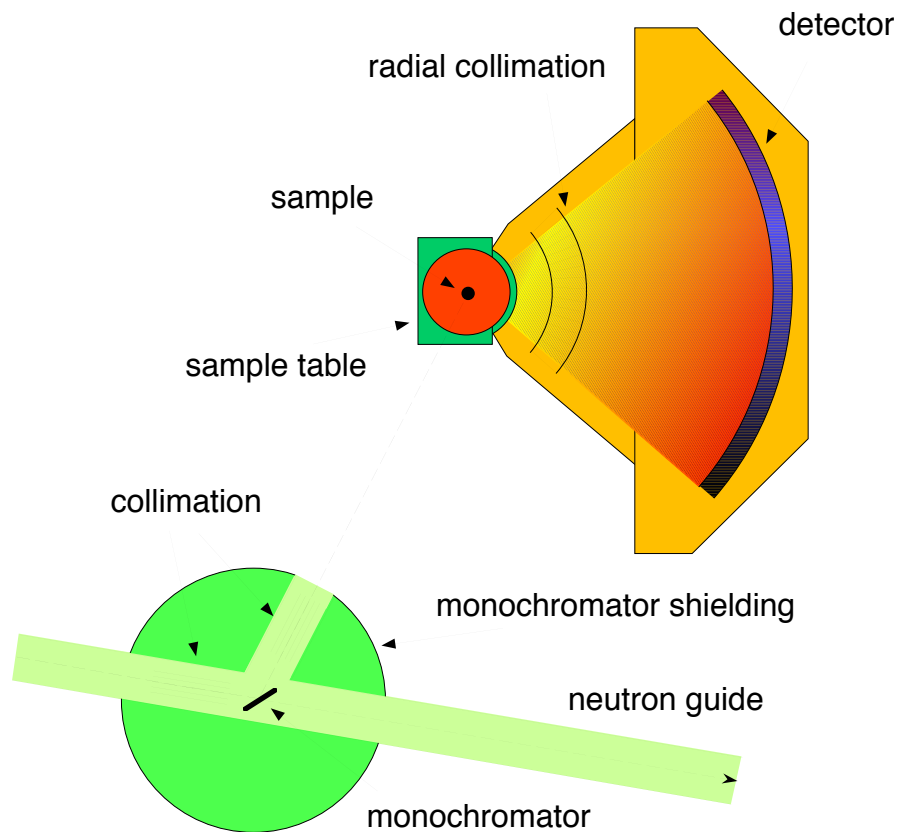


THE DMC ESSENTIALS



How to...

1.	... log in to the DMC computer	2
2.	... open the DMC status display	2
3.	... start the instrument control program SICS	4
4.	... start a measurement on DMC: the SICS commands	5
5.	... set up temperature controllers	7
6.	... edit the command file	8
7.	... add, subtract and convert data files	9
8.	... view data files	10

Appendix

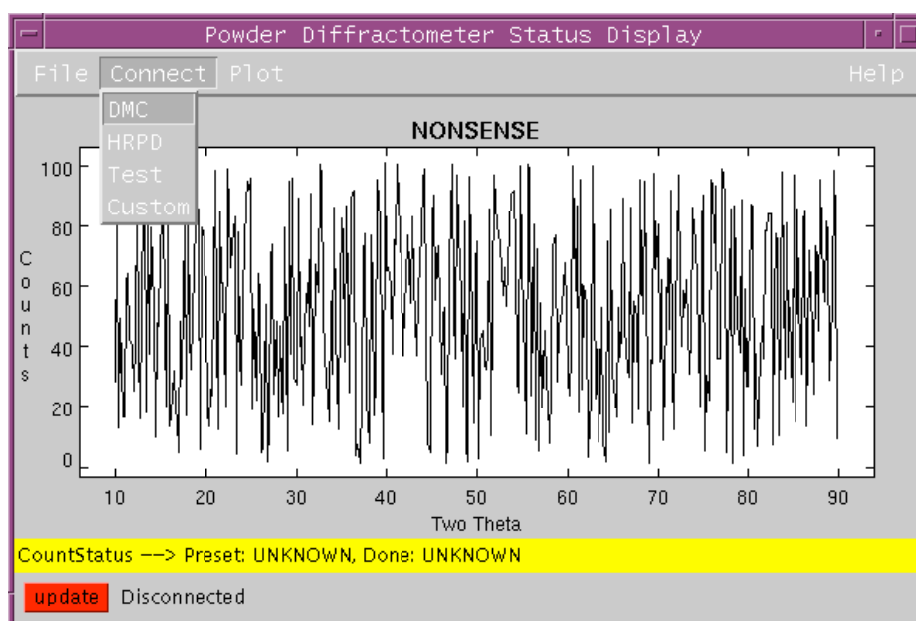
9.	Troubleshooting	13
10.	Definition of motors	13
11.	Refinement of the data	13
12.	Contact persons	14
13.	Safety procedure at SINQ	15

1. How to log in to the DMC computer

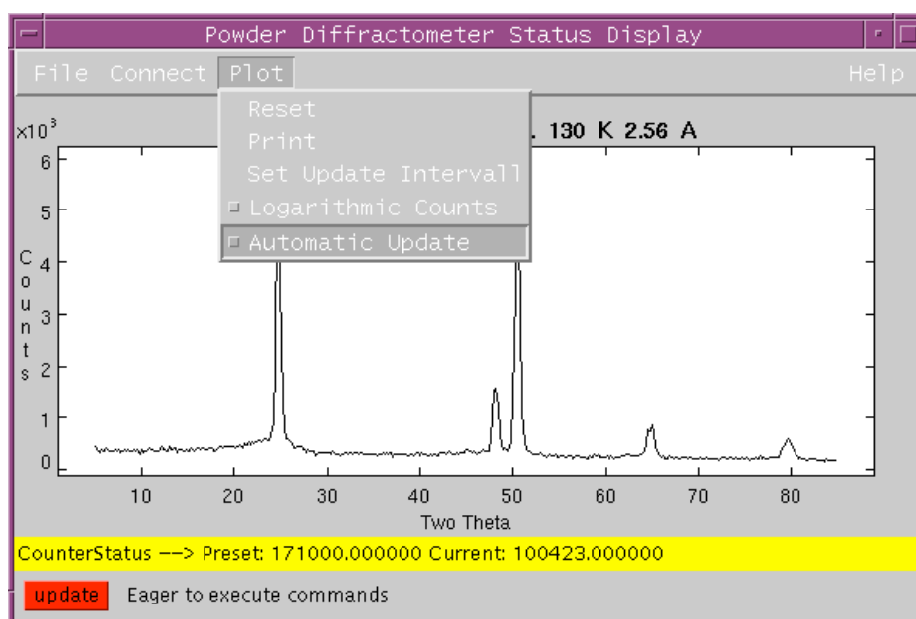
Open a terminal window on your workstation. Log in to `dmc.psi.ch` using `ssh` with username `****` and password `****` (case sensitive, this is a Linux machine). You will be asked for your name and a subdirectory `/home/dmclnsg/<your name>` will be created.

2. How to open the DMC status display

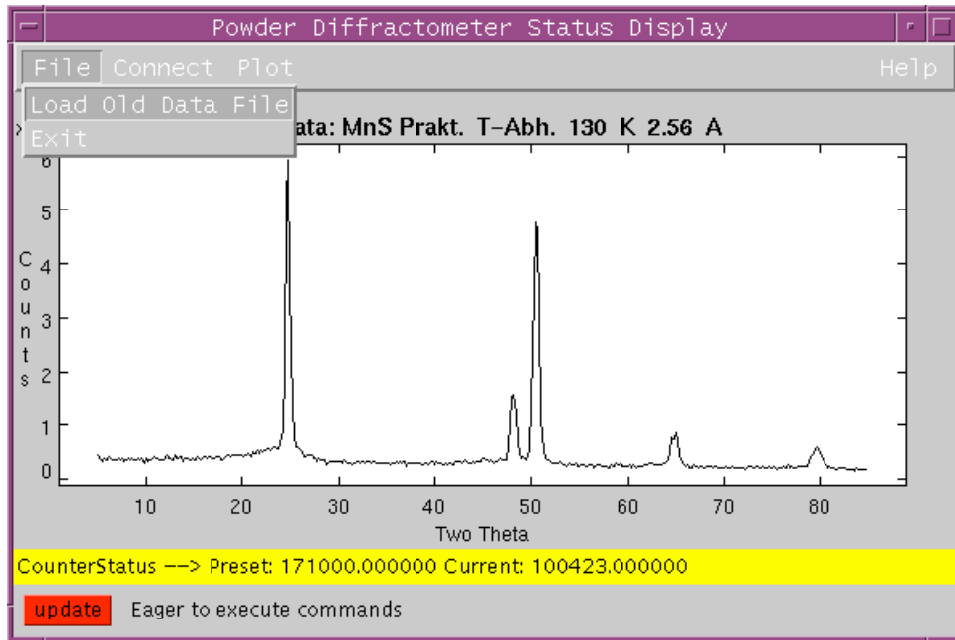
Type the command **powderstatus &** at the prompt or click on the `powderstatus` icon on the desktop of the workstation. After a few seconds the *Powder Diffractometer Status Display* appears on the screen. Connect to DMC.



The status display shows the current content of the histogramming memory. If the measurement is running you can update the display either by hitting the red *update* button in left bottom corner of the window or by activating the *Automatic Update* function of the *Plot* menu.



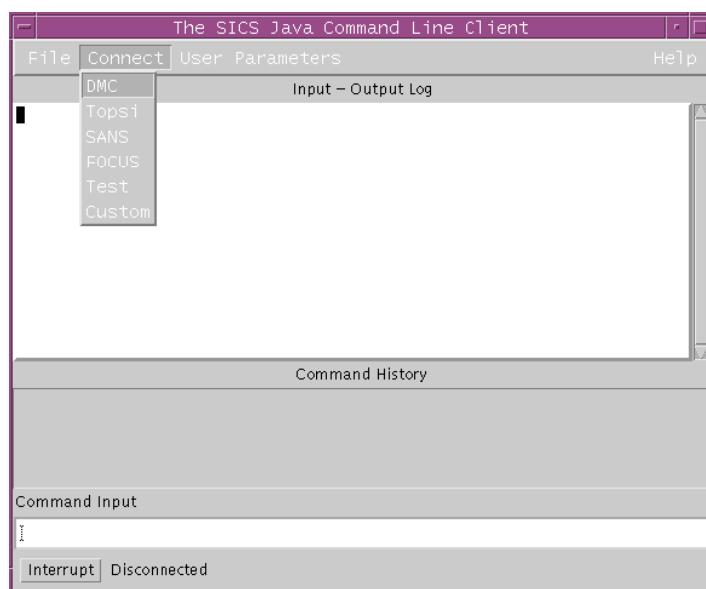
You can also use the status display to view old data files. To see previous measurements select *Load Old Data Files* in the *File* menu. You will be asked for the year and the file number of the data file. To view for example the file *dmc008252001.hdf* just choose the year 2001 and type 825.



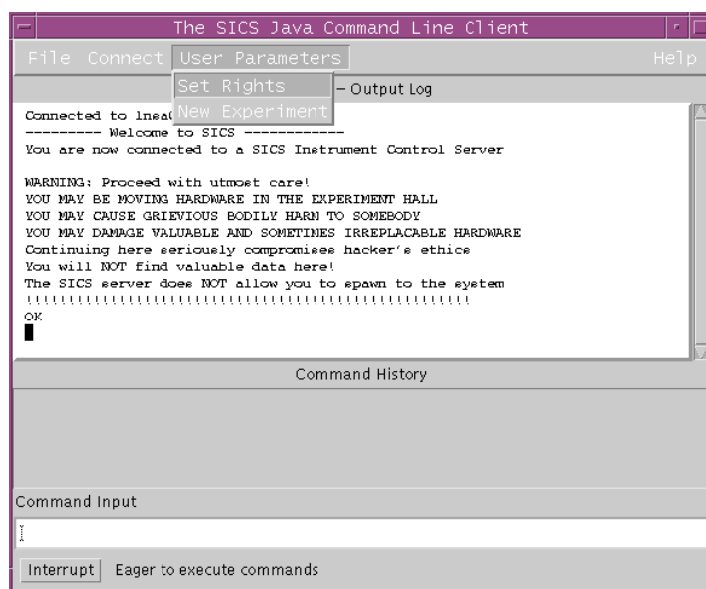
By hitting the red *update* button the display will return to the current measurement.

3. How to start the instrument control program SICS

Type the command **sics &** at the prompt or click on the sics icon on the desktop of the workstation. The *SICS Java Command Line Client* appears on the screen. Connect to DMC.



After connecting to DMC you are able to read out instrument parameters like motor positions and temperatures but you do not have the privilege to move the instrument or start the data collection, i.e. you have passive control of the experiment only. To get the privilege to control the instrument select *Set Rights* from the *User Parameters* menu.



With username ******** and password ******** you have the privilege to start measurements, change temperatures, run motors etc. Do not use this privilege on any other terminal than the one next to DMC in the guide hall.

Alternatively you may use the command line client *six*. Start it by typing **six** at the prompt.

4. How to start a measurement on DMC: the SICS commands

DMC can be controlled by typing SICS commands into the *Command Input* field of the *SICS Java Command Line Client*. A detailed description of the SICS command language and all SICS commands concerning DMC can be found on the world wide web addresses <http://lns00.psi.ch/sics/dmc.htm> and <http://lns00.psi.ch/sics/dmco.htm>, respectively. For most experiments the following few commands are sufficient.

<parameter>

Displays the current value of <parameter>. For example the command **temperature** displays the current temperature, the command **a4** shows the current position of angle 4 (which is the position of the detector bank, i.e. the scattering angle 2Θ of the first detector).

drive <motor> <new value>

Drives the selected motor to the new position. When rotating the sample table or moving the detector bank be careful and watch out for anything that might obstruct the movement. The movement can be stopped by clicking on the *interrupt* button in the left bottom corner of the *SICS Java Command Line Client* window (or by typing **stop** in the command line client *six*).

Examples: **drive a4 12** , **drive a3 180**

drive temperature <value>

Sends new set temperature to the temperature controller (see chapter 5).

Example: **drive temperature 2.5**

wait <seconds>

Example: **wait 300**

<variable> <new value>

Typing its name followed by the new value can set each variable. The variables *user*, *sample* and *title* must be set before every measurement.

Examples: **user Ruhnke** , **sample MnS** , **title MnS Praktikum**

count <mode> <preset>

Starts the counting. For monitor mode the preset is given in thousands (e.g. **count monitor 1** counts up to monitor 1'000), for timer mode the preset is given in seconds. After reaching the preset value the data will be automatically stored.

Examples: **count monitor 1** , **count timer 10**

mcount <mode> <preset> <angle> <start> <end> <step>

Starts the counting for multiple positions of <angle>. For every position <start>, <start>+<step>, <start>+2<step>, ... , <end> a file is stored.

Example: **mcount monitor 1 a4 5.0 6.9 0.1**

repeat <n> <mode> <preset>

Repeats the count command n times, n files will be stored.

Example: **repeat 4 monitor 1**

exe batchpath <path>

Sets the path to the directory with your command files.

Example: **exe batchpath /home/dmclnsg/ruhnke/**

exe <filename>

Runs a command file with the name <filename> located in the directory <path> (see command **exe batchpath**). The command file may contain any SICS command.

This is the regular way to perform a measurement on DMC.

Example: **exe ruhnke.job**

To start the measurement use the **count**, **mcount** or **exe** command. To stop the measurement click on the *interrupt* button in the left bottom corner of the *SICS Java Command Line Client* window (or by typing **stop** in the command line client *six*).

Example of a command file:

```
user Ruhnke
sample MnS
wavelength 2.4570

drive temperature 100
wait 300
title MnS Praktikum, 100 K, 2.45 A, DMC
mcount monitor 6 a4 3 4.9 0.1

drive temperature 130
wait 300
title MnS Praktikum, 130 K, 2.45 A, DMC
mcount monitor 6 a4 3 4.9 0.1

drive temperature 160
wait 300
title MnS Praktikum, 160 K, 2.45 A, DMC
mcount monitor 6 a4 3 4.9 0.1

exe ruhnke2.job
```

Note that you can link another (or the same) job file simply by using the **exe** command in your command file.

Other useful SICS commands:

counter status

Displays preset and current monitor.

sicsdatanumber

Displays number xxxxx of latest stored data file dmcxxxxxyear.hdf.

exe info

Displays the currently executing command file.

sinq

Displays the accelerator status and the proton current on the SINQ target.

counter getthreshold 1

Displays the threshold of the monitor. If the monitor count rate falls below this value [counts/0.5sec], then the measurement will be paused, e.g. if you close the shutter to enter the instrument area.

counter setthreshold 1 <value>

Sets the threshold [counts/0.5sec] of the monitor to this value.

Example: **counter setthreshold 1 2**

loadefficiency

Reads the most recent calibration file for data shown in **powderstatus**.

5. How to set up temperature controllers

After plugging in the connection to the temperature controller the system automatically recognizes the connected sample environment. Use the following SICS commands in the *Command Input* field of the *SICS Java Command Line Client*.

temperature

Displays the current sample temperature.

temperature device

Displays the sample environment device connected to the temperature controller. If no device is shown, type **temperature device 0** to force the program to check for the device used.

temperature list

Displays some parameters related to temperature controlling.

temperature tolerance <new value>

Defines the acceptable temperature interval around the set-temperature. If the temperature leaves the interval and the parameter **errorhandler** is set to 1, the measurement will be paused. The default for **errorhandler** is 0, i.e. a warning is printed but the measurement continues.

Examples: **temperature tolerance 2.5** , **temperature errorhandler 0**

temperature upperlimit <new value>

Defines the highest allowed set-temperature.

Example: **temperature upperlimit 300**

temperature lowerlimit <t>

Defines the lowest allowed set-temperature.

Example: **temperature lowerlimit 1.2**

drive temperature <new value>

Sends new set-temperature to the temperature controller. The program waits with the execution of the next command (e.g. in a command file) until the temperature is inside the tolerance interval. To allow the immediate execution of the next command, use **run temperature < new value>**.

Example: **drive temperature 10**

temperature list

Displays some parameters related to temperature controlling.

The temperature control software SEA

The temperature control software *SEA* is a stand alone program that enables to change all the parameters connected to temperature controlling independently of SICS, i.e. parameters like PIDs can be changed during the measurement without stopping the run.

To start *SEA* type the command **sea** at the prompt or click on the sea icon on the desktop of your workstation. In *SEA* you may change any parameters dealing with the sample environment. It uses a graphical user interface and is self-explaining.

6. How to edit the command file

There are several ways to create and/or edit a command file.

(i) Type **nedit <filename>** at the prompt. If the file <filename> does not exist, a new file will be created.

(ii) Type **joe <filename>** at the prompt. The joe editor will open the file <filename>, if the file doesn't exist joe creates a new file. To get the help feature with a description of the editor commands use <ctr>k <ctr>h in the editor window.

```
Help Screen      turn off with ^KH      more help with ESC . (^[.)
CURSOR          GO TO          BLOCK          DELETE          MISC          EXIT
^B left ^F right ^U prev. screen ^KB begin ^D char. ^KJ reformat ^KK save
^P up ^N down ^V next screen ^KK end ^Y line ^T options ^C abort
^Z previous word ^A beg. of line ^KM move ^W >word ^R refresh ^KZ shell
^X next word ^E end of line ^KC copy ^O word< ^@ insert FILE
SEARCH          ^KU top of file ^KW file ^J >line SPELL ^KE edit
^KF find text ^KV end of file ^KY delete ^_ undo ^[N word ^KR insert
^L find next ^KL to line No. ^K/ filter ^A redo ^[L file ^KD save
IW t.t Row 1 Col 1 6:08 Ctrl-K H for help
```

Use this editor if you are logged in through a telnet session and are not able to use one of the graphic based editors.

(iii) Type **pico <filename>** at the prompt. the pico editor will open the file <filename>, if the file doesn't exist pico creates a new file.

7. How to add, subtract and convert data files

The DMC raw data files *dmcyearnxxxxx.hdf* (e.g. dmc2007n008252.hdf) are stored in the NeXus format. The program *addit* adds such files (or files in any other format used at SINQ), corrects the data for differences of efficiency of the 400 counters of DMC's position sensitive detector and transforms the result into the well known DMC data format.

```
DMC, MnS Praktikum T=130K l=2.5554A
Sample= MnS, T= 131.000, dT=0.013, Date= 1998-01-09 15:53:37
 5.000  0.200  84.800  150000., lambda=  2.55924
 387    379    350    325    360    348    378    360    341    344
 352    352    367    370    318    336    368    353    376    356
      ...
 216    198    214    176    183    189    214    203    202    188
 179    186    195    162    200    181    193    177    173    184
21.19  19.70  18.65  18.47  19.54  19.16  20.10  19.49  18.95  19.24
18.89  19.34  19.13  19.47  18.28  19.13  19.75  19.21  19.97  18.89
      ...
15.20  14.35  14.49  13.30  13.56  13.89  14.70  14.11  14.21  13.82
13.04  13.45  13.30  12.45  14.07  13.60  13.60  13.11  13.11  13.08
```

The DMC data format header consists of three lines. First line: Instrument and title of experiment; second line: sample name, average temperature, standard deviation of the temperature and date; third line: start value of scattering angle 2Θ , 2Θ step, 2Θ end value, monitor and wavelength. The block of intensities and the block of statistical errors of the corresponding intensities follow the header.

Add raw data files and/or files in DMC-format: *addit*

To start the program *addit* type the command **addit** at the prompt. The program will guide you interactively. To add for example the files 825, 835 to 839 and 841 to 850, just type "825,835-839,841-850" when you are asked for the files to add.

The data will be automatically corrected for the detector efficiencies of the 400 counters. The data sets to add are not required to have the same scattering angle range, i.e. sums of low and high angle data sets or measurements with intermediate steps are supported. In the final sum the data points are normalized to the same monitor. If necessary the program interpolates data points in order to get a final sum with equal steps between the data points.

Subtract two raw data files and/or files in DMC-format: *subit*

Use the program *subit* for subtract data files, e.g. to create difference pattern. To start the program type the command **subit** at the prompt. The program will guide you interactively.

Convert raw data files to DMC-format: *conv*

To start the program *conv* type the command **conv** at the prompt. The input syntax is similar to the program *addit* (see above). The input “825,835-839,841-850” will do the detector efficiency correction for every single raw data file and saves them in the files 000825.dat, 000835.dat, 000836.dat, ... , 000850.dat in the DMC format.

8. How to view data files

To view raw data files *dmcyearnxxxxx.hdf* use the status display as described in chapter 2 or type **fit** at the prompt. You will be asked for the numor(s) to be read in. The input syntax is similar to the program *addit* (see above). You will be sked fot the file (or the file list) to read in. If no default for the instrument is set then type “dmc/<year>/825,835-837” to view the files 825, 835, 836 and 837. The data is automatically corrected for detector efficiencies of the 400 counters. With the command **scale** at the fit prompt you may change the range of the plot, with **plot** the files are displayed.

The program fit has much more features than just displaying data sets. Type **help** at the fit prompt for more information.

To view converted files with DMC format type **fit** at the prompt. You will be asked for the filename. Follow the instructions given by the program.

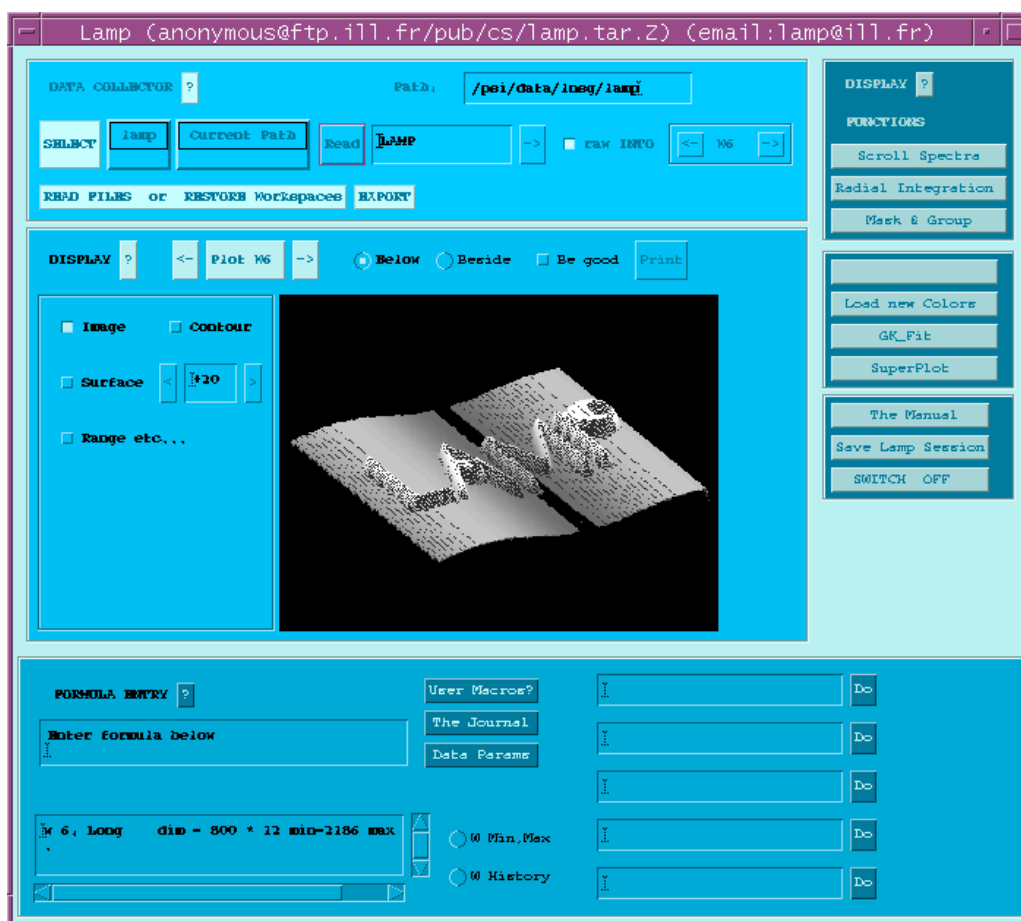
To print a **file** on the printer next to the DMC cabin type **lp -d sinq_lho_1 <filename>** at the prompt.

Alternatively you can use the refinement program FULLPROF to print the data. FULLPROF recognizes the DMC data format (instr=8).

Create 3D-plots using *lamp*

To create "three-dimensional" plots of your diffraction data (e.g. temperature dependency of the diffraction pattern), the data sets must be converted into a special data format using the program *clamp* (convert to *lamp* format). To start *clamp* activate the window *dterm* and type the command **clamp** at the prompt. The program will guide you interactively. *clamp* is able to convert the same file formats that are recognized by the program *fit*, in particular raw data format as well as DMC format. Scattering angle range and monitor are expected to be the same for all data files. Two output files are created: **LAMP** and **LAMPascii**.

To start the program *lamp* type first the command **idlinit** and then **lamp** at the prompt. Now hit the *START LAMP* button in the *lamp* desktop window. After the main *lamp* window has opened, click on *DATA Access*. Choose *lamp* in the file format list and type in **LAMP** to read in the files created by the conversion program *clamp*. After hitting the *Read* button the data is read into a workspace and can be plotted.



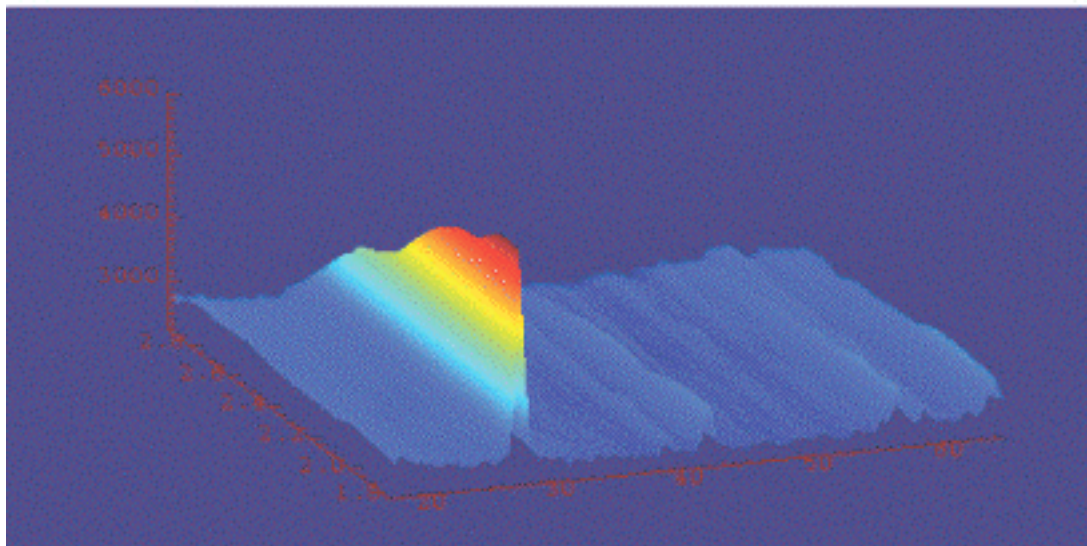
Click on *The Manual* for details of the features of *lamp*. Here are the most important ones:

Click on *Range etc...* to set the plot range; always select *Regular Grid*!

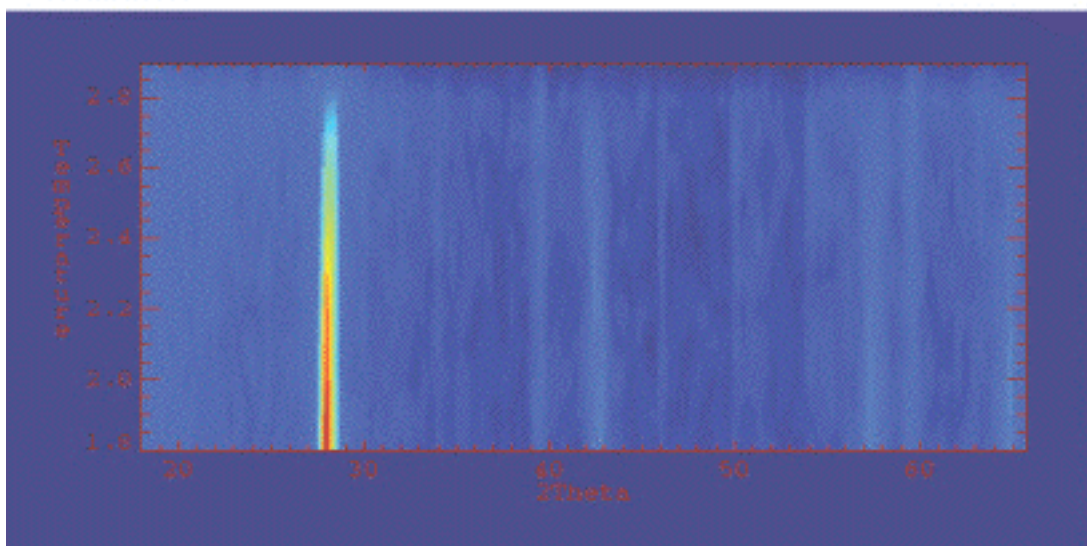
Click on *Be good* to control several plot options like shading of the surface, plot angle, title etc.

Select *Below* to view the plot in the main window, *Print* for a postscript file of this plot.

Select *Beside* to view the plot in a separate window, to change the color settings and to create postscript files for print outs on color printers.



Select *Surface* for three-dimensional surface plots.



Select *Contour* for contour plots, i.e. the projection onto the xy-plane (in this example: the 2 Θ -Temperature plane).

Appendix

9. Troubleshooting

If there are problems concerning the temperature controller or the connection to the temperature controller, then check if the connection is plugged in and if the controller is set to *remote*. If the wrong sample environment device is set, type **temperature device 0** in *SICS* (or choose the right sample environment in *SEA*) to force the program to check for the connected device. Then wait two minutes to let the controller download the proper calibration curves.

If there is no connection to the histogramming memory, the motor controller or the counter box then turn them off and on again.

All actions of the *SICS* client are stored in a log file. A check of this file might help to solve your problem. To view the last 20 lines of the log file type **commandlog tail** in *SICS*. With **commandlog tail <n>** you will see the last n lines of the file.

For more trouble shooting hints concerning the *SICS* software check out the www page <http://lns00.psi.ch/sics/trouble.htm>.

10. Definition of the motors

- a1 monochromator Θ
- a2 monochromator take-off angle
- a3 sample table rotation
- a4 scattering angle 2Θ of detector no. 1 (then no. 400 is at $2\Theta+79.8^\circ$)
- a5, a6 monochromator translations
- a7, a8 monochromator tilting angles
- a9 monochromator curvature

Users must not move any angles other than a3 and a4.

11. Refinement of the data

The program *fullprof* is installed on the DMC computer. The manual is accessible under <http://sinq.web.psi.ch/sinq/doc/fullprof.pdf>.

12. Contact persons

Instrument responsables

Lukas Keller, WHGA/135, Tel. 4007
Antonio Cervellino, WHGA/131, Tel. 4611

Software, Computing

Mark Könnecke, WHGA/249, Tel. 2512
Uwe Filges, WHGA/249, Tel. 4606
Heinz Heer, WHGA/145, Tel. 2093

Detector electronics

Thomas Gahl, WHGA/248, Tel. 4311

Electronics

Roman Bürge, WHGA/243, Tel. 4299
Urs Greuter, WMHA/C46, Tel. 3112

Sample environments

Markus Zolliker, WHGA/135, Tel. 2089
Stephan Fischer, WLGA/130, Tel. 4118

13. Safety Procedure at SINQ

Before the Experiment:

<http://lns00.psi.ch/safety/safety.htm>

Safety sheet has to be signed and posted at the experiment.

NOTE:

All active material has to be shipped according to international law using specialized companies to:
Paul Scherrer Institute, Att. SU (Active Samples),
Bldg. OSUA, CH-5232 Villigen PSI
You are not allowed to ship such items to your local contact. You have to bring them in by yourself.



After the Experiment:

http://lns00.psi.ch/safety/samples_at_sinq.pdf

NOTE:

All active material has to be shipped according to international law using the SAR-company (for questions: Contact H.U. Aebersold, Tel. 4294)

You are not allowed to remove active material from PSI on your own.

All material brought into the SINQ-halls (TH/LH) is **considered to be active** as long as not stated inactive by a safety official (SU) from PSI. The instrument responsible is not allowed to make this safety procedure for you.

Samples must be stored temporarily in the special cabinet in the guide hall WNLA opposite of TASP (every instrument responsible has a key). You are not allowed to take them to the hutches or to the offices.

Store the sample in the transparent plastic boxes (-> one sample per box!) as shown to the right. Include a label with the following information:

- Name, Adress/Phone/FAX, E-Mail
 - Date, Experiment Number
 - Instrument
 - Material, Amount [g]
 - Local Contact
- Activity will be measured by SU.*

Please **distinguish** between samples and material

- to stay at PSI (West and East)
- to exit PSI
- to exit Switzerland



Sample Storage after the Experiment:

The cabinet in Zone I (next to DMC and TASP) is locked; the cabinet in Zone 0 is always accessible (next to the south exit of the guide hall).

Alle samples have to go into the cabinet to the left after the experiment.

Samples are separated by the instrument.

The diagram illustrates the sample storage workflow between Zone 1 and Zone 0. Zone 1 is located in the SINQ guide hall WNLA, close to DMC/TASP. Zone 0 is the accessible cabinet area. A yellow arrow points to 'New samples: (Input by instrument scientist)' in Zone 1. A red arrow points to 'Destination PSI' in Zone 0. A green arrow points to 'Destination CH/World' in Zone 0. A green arrow also points to 'checked samples: (may be removed) (Check and transfer to this cabinet done by PSI SU-staff only)' in Zone 0. A yellow arrow points to 'active samples: we have to wait!!' in Zone 1. Two photographs show the cabinets: one in Zone 1 and one in Zone 0. Text at the bottom right reads 'Questions: J.Schefer # 4347' and 'Sample Storage.CDR/PC2360/May2000'.

- unchecked new material
TO LEAVE PSI
(RED BOXES)**
- unchecked new material
TO STAY AT PSI
(GREEN BOXES)**
- checked but active material
(YELLOW BOXES)**
- material to stay at SINQ
(open shelf)**

- checked material
TO LEAVE PSI
(BLUE BOXES)**
- checked material
TO STAY AT PSI
(GREY BOXES)**

Samples_at_SINQ.doc/PC2953
[Ins00.psi.ch/safety/samples_at_sinq.pdf](https://ins00.psi.ch/safety/samples_at_sinq.pdf)
J. Schefer/Tel. 4347 - Nov.2000