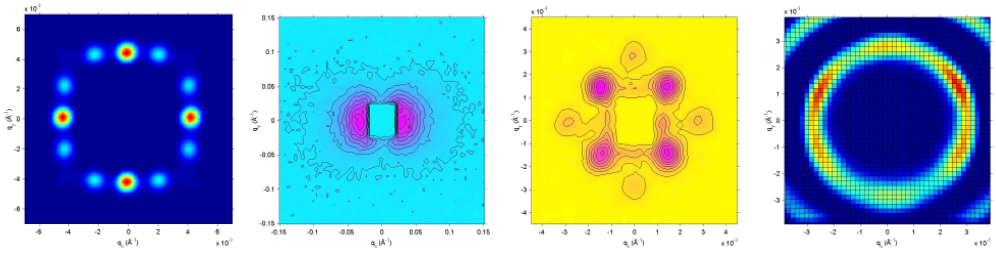
GRASANSP

Manual Version 2.0

Software Version 3.40

April 2003

User Manual



Graphical Reduction and Analysis SANS Program for Matlab™

www.ill.fr/lss/grasp/

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Acknowledgements

The existing suite of ILL SANS software created and maintained by Ron Ghosh (ILL) and co-workers has served as a benchmark standard during testing of *GRAS$_{ans}$P*. Don McK Paul (University of Warwick) provided the initial impetus and highlighted the requirement for a graphical software package tailored for anisotropic or diffraction-based SANS measurements. Bob Cubitt, Giovanna Fragneto, Isabelle Grillo, Roland May, Simon Levett, Ross Stewart and Johannes Zipfel (ILL) have carried out further testing and gathering of user feedback. Thanks also go to Peter Timmins and the ILL direction for allowing me to pursue this project, based upon some of my own ideas about data analysis and without a formal demonstration of the project case. It is now clear that the expanding user-base of *GRAS$_{ans}$P* demonstrates the validity and usefulness of this project. Special thanks go to *GRAS$_{ans}$P*'s first users and early believers.

Table of Contents

Overview

GRAS$_{ans}$P is a Matlab™ script application designed for the graphical inspection, analysis and reduction of multi-detector data produced by the Small-Angle Neutron Scattering (SANS) instruments of the Institut Laue Langevin (ILL). *GRAS$_{ans}$P* presents a modern package and general purpose suite of tools to deal with the diverse requirements for reduction and analysis of two-dimensional small angle scattering and diffraction data. Data from the two ILL SANS instruments, D11 and D22 as well as that from the small-angle diffractometer D16 are catered for in the *GRAS$_{ans}$P* package.

Since its first release in early 2001 *GRAS$_{ans}$P* has attracted significant attention and support both within the user community and from responsibles of similar multi-detector-based instruments at other neutron and X-ray facilities. Some of these instruments are now catered for within *GRAS$_{ans}$P* including SINQ SANS I & II and HMI V4 data. In principle the architecture and coding of *GRAS$_{ans}$P,* combined with the matrix handling abilities, graphics and other advantages of the Matlab™ environment should allow continued development of this software and be able to provide more general aspects of multi-detector and complex data set handling.

A major milestone in the development and distribution of *GRAS$_{ans}$P* came in mid 2001 when Matlab™ compilers were bought for PC, Linux, SGI and now Macintosh OSX platforms. By compiling the Matlab™ script code into a 'runtime' or 'stand-alone' application we are now able to distribute *GRAS$_{ans}$P* freely without obligation to buy the costly Matlab™ package. Compiled *GRAS$_{ans}$P* is freely available and distributed via the *GRAS$_{ans}$P* web site www.ill.fr/lss/grasp/.

This manual is the second to be written, the first being with the first release of the software in early 2001. The software has evolved considerably over the course of the last year (more so than the manual!), fine-tuning some of the tailor made routines and applications for different types of SANS data analysis. Comments and suggestions are always welcome and should be e-mailed directly to me at dewhurst@ill.fr. You 'the user' are instrumental in the development of *GRAS$_{ans}$P* by continuing to support this project, by reporting bugs or suggestions for improvements. Users are also encouraged to actively participate in the development of *GRAS$_{ans}$P* by the contribution of 'user modules' and 'fitting functions' to tailor *GRAS$_{ans}$P* to specific needs and can be easily and almost seamlessly integrated into the *GRAS$_{ans}$P* interface without modification to the main code (m-code version only).

Software Download, Installation and Configuration

Software Download

Up-to-date 'Runtime' and 'm-code' versions of *GRAS$_{ans}$P* can be downloaded from the Institut Laue Langevin web site at:

www.ill.fr/lss/grasp/

The web site also includes download for this manual in PDF format, example data and other utilities as well as news on *GRAS$_{ans}$P* developments and bug-fixes.

System Requirements

- 500 Mhz or higher processor
- 64 megabytes of RAM (recommended 128 MB)
- 30 megabytes of free disk space
- Screen graphics resolution of 1024 x 768 or higher (1280 x 1024 recommended)

Runtime or Matlab™ 'm-code' *GRAS$_{ans}$P*?

- Matlab™ 'm-code' versions of *GRAS$_{ans}$P* run on any platform with Matlab™ version 6.0 or higher.
- Compiled 'Runtime' versions of *GRAS$_{ans}$P* exist for:
  - Windows 95, 98, NT4, 200, XP
  - Linux
  - SGI
  - MacOSX

  and are **licence free 'freeware'**.

Installation: Runtime version

The runtime version of *GRAS$_{ans}$P* offers users the opportunity to use *GRAS$_{ans}$P* with all the associated graphic features of Matlab™ without having to purchase the costly Matlab™ package. *GRAS$_{ans}$P* is frequently tweaked, modified and improved with new versions regularly appearing on the *GRAS$_{ans}$P* web site **www.ill.fr/lss/grasp/**. Runtime *GRAS$_{ans}$P* is licence free and freely distributable.

PC Windows 95/98/NT4/2000/XP

1. Download **grasp_pc.exe** from the *GRAS$_{ans}$P* website.
2. Double-click the **grasp_pc.exe** file and follow the installation instructions on screen that will guide you through the installation procedure.
3. *GRAS$_{ans}$P* can now be run be clicking on the shortcut placed in the windows start menu.

Linux / Unix

1. Download **grasp_linux.tar.gz** from the *GRAS$_{ans}$P* website.
2. Unzip and un-tar the contents of the compressed archive file in to new directory, e.g. /grasp_runtime/
3. Use **setenv LD_LIBRARY_PATH $LD_LIBRARY_PATH/:$home/grasp_runtime/bin/glnx86/** for tcsh or csh shells. Use **export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:$home/grasp_runtime/bin/glnx86/** for bash shells, to set the Linux / Unix environment variable.
4. Launch *GRAS$_{ans}$P* by typing '**grasp**' in the terminal window in the '/grasp_runtime/' directory.

SGI

1. Download **grasp_sgi.tar.gz** from the *GRAS$_{ans}$P* website.
2. Unzip and un-tar the contents of the compressed archive file in to new directory, e.g. **'/grasp_runtime/'**
3. Use **setenv LD_LIBRARY_PATH $LD_LIBRARY_PATH/:/grasp_runtime/bin/sgi/**, as described in the packaged **readme.txt** file, to sent the environment variable.
4. Launch *GRAS$_{ans}$P* by typing '**grasp**' in the terminal window in the **'/grasp_runtime/'** directory.

Tip: The default instrument configuration and general *GRAS$_{ans}$P* environment settings can be modified by editing the **grasp.ini** configuration file.

Installation: Matlab™ 'm-code' version

GRAS$_{ans}$P m-code is a Matlab™ script application and therefore requires the commercial Matlab™ package in order to run. The script code is system independent and can run on both PC, Unix/Linux and Macintosh_OSX Matlab™ versions. The main advantage of using Matlab™ and the m-code version is that users have complete control over the *GRAS$_{ans}$P* analysis environment allowing the addition of User Modules, User Fitting Functions, *GRAS$_{ans}$P*-Script (soon) and direct access to data and parameters from the Matlab™ command line.

PC Windows 95/98/NT4/2000/XP

1. Download **grasp_m.exe** from the *GRAS$_{ans}$P* website
2. Double-click the **grasp_m.exe** file and follow the installation instructions on screen that will guide you through the installation procedure.
3. Create a new, or copy an existing shortcut to the Matlab™ application. Edit the shortcut properties such that Matlab™ immediately runs the m-code *GRAS$_{ans}$P* startup script '**grasp_startup.m**' and *GRAS$_{ans}$P* application upon launching Matlab™ from this shortcut. E.g. Shortcut target **' *"C:\Program Files\Matlab\bin\win32\matlab.exe" -r run(['c:\progra~1\grasp_m\grasp_startup']);grasp* '**.
4. Alternatively to (3), **grasp_startup.m** followed by **grasp.m** can be run directly from the Matlab™ command prompt.

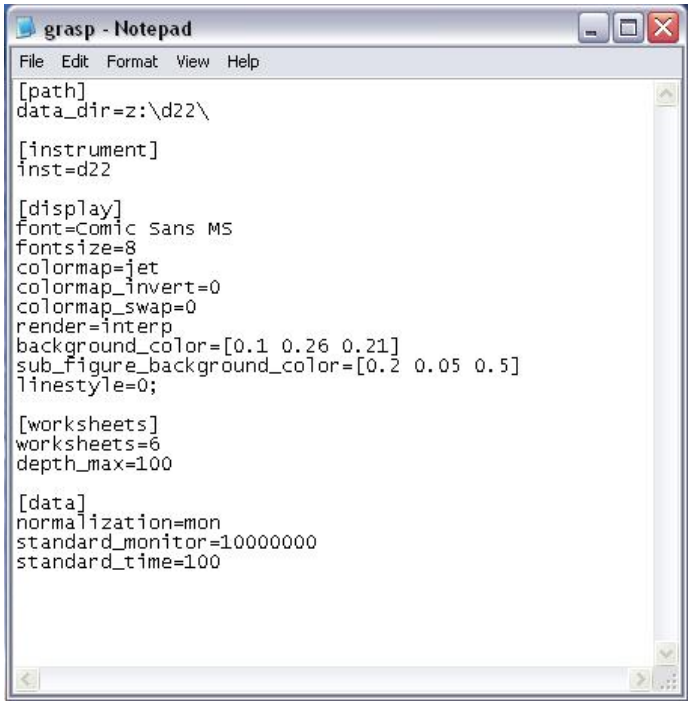
Important: The **grasp_m.exe** PC installer by default offers to install *GRAS$_{ans}$P* into the *'C:\Program Files\Grasp_m\'* directory. If the *GRAS$_{ans}$P* m-code is installed into any other directory the grasp_root path must be set accordingly by editing the file **grasp_startup.m**, e.g. grasp_root = 'c:\program files\grasp\'.

Linux, SGI, Unix, Macintosh_OSX and other Operating Systems

1. Download **grasp_m.zip** from the *GRAS$_{ans}$P* website.
2. Un-zip the application into a new directory.
3. Open and edit the file **grasp_startup.m**. Set the 'grasp_root' path variable to the directory where you have un-zipped the *GRAS$_{ans}$P* m-code. E.g. grasp_root = '/home/grasp_m/'.
4. Launch Matlab™ and manually run **grasp_strartup.m** followed by **grasp.m** from the Matlab™ command prompt.

Customisation and Optional Edits to the 'grasp.ini' Initiation File

The following edits can be made to the *GRAS$_{ans}$P* initiation file, **grasp.ini**, to customise the appearance, operation, default instrument, and data directory paths for *GRAS$_{ans}$P*. **grasp.ini** can be found in the root of the grasp_m or grasp runtime directories.



[path]

- **data_dir** Default directory path to the SANS data, e.g. data_dir=z:\d22\, data_dir=d:\sans_data\ etc.

[instrument]

- **inst** Default *GRAS$_{ans}$P* instrument configuration at start-up, e.g. inst = d22, inst = d11, inst = SINQ_sans.

[display]

- **font** Font used for the main display, e.g. font=arial, font=comic sans ms etc.
- **fontsize** Font size used for the main display, e.g. fontsize=9.
- **colormap** Default color map used for the main 2D data display, e.g. colormap=hot, colormap=jet, colormap=cool, etc.
- **colormap_invert** Invert up-down the color map matrix (1=on, 0=off).
- **colormap_swap** Swap left-right the color map matrix (1=on, 0=off).
- **render** Default image render, i.e. interp, flat or faceted.

- **background_color** Background color of the main display window [RGB].
- **sub_figure_background_color** Background color of the 1D plotter and associated tools windows [RGB].
- **linestyle** Default line-connect style of 1D plotter (0 = none, 1 = '—', 2 = ':', 3 = '-.', 4= '--').

[worksheets]

- **worksheets** Number of data worksheets (try not to exceed 6, system depending).
- **depth_max** Max number of allowed worksheet depths (try not to exceed 100, system depending).

[data]

- **normalisation** Data normalisation setting, e.g. 'mon', 'time', 'none'.
- **standard_monitor** Reference standard monitor value for data normalisation.
- **standard_time** Reference standard time value for data normalisation.

Tip: The default instrument configuration that *GRAS$_{ans}$P* starts up in can be overridden from that described in **grasp.ini** by typing 'grasp *inst*' on the either the Matlab™ command line, command prompt or icon shortcut for runtime versions, where *inst* is the instrument name e.g. d22, d11, d16, SINQ_sans_I etc.

Data access at Institut Laue Langevin

Data measured on ILL instruments is transferred automatically from the local instrument control computer to the network data server, SERDON, regularly every few minutes. *GRAS$_{ans}$P* reads current cycle and older data directly from SERDON and not from the instrument control computer.

PC

Current cycle data on the network server SERDON can be found directly via the local neighborhood network via the path '**\\SERDON\data*inst***', where *inst* is the ILL instrument name. On many user PC's at ILL the network drive '**Z:*inst***' is already attached to the network data drive. '**Y:*inst***' is configured to the previous cycle.

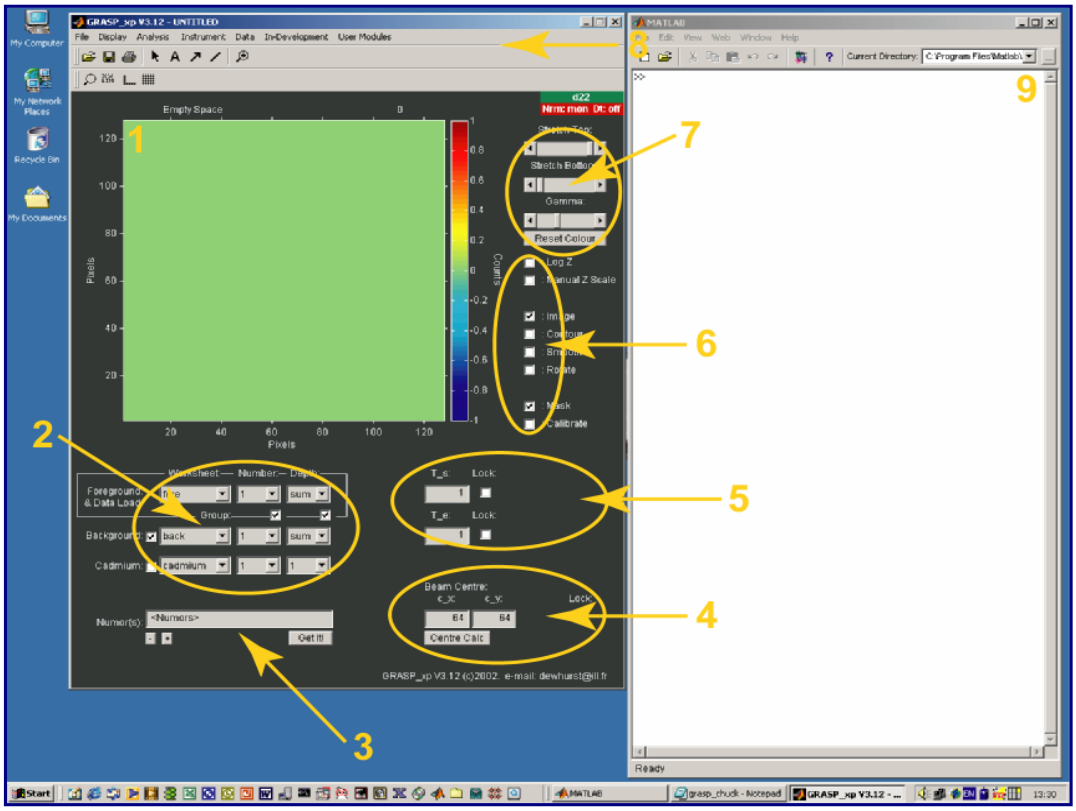
Linux / Unix / SGI

Current cycle data on the network server SERDON can be found via the path '**/usr/illdata/data/*inst*/**', where *inst* is the ILL instrument name.

Tip: If recently measured data does not appear on the SERDON data server, (i.e. within the preceding few minutes), a transfer of recent data can be forced from the instrument control computers by typing the command '**transfer**' from the UNIX command prompt.

Main Program Interface

The main *GRAS$_{ans}$P* graphical interface window appears at the left and side of the screen, as shown in the figure below. The graphical interface looks like that of a typical modern style application including drop down menus, push buttons, edit boxes and a graphical data display. Key features of the interactive display are described briefly below while a detailed description is given later in this manual.



Key Features of the Main User Interface

1 **Main Graphical Data Display:** The result of 2D data treatment is displayed in graphical form in the main display window. The displayed data is the result of the sample scattering data minus the sample background and cadmium background as indicated by the data selectors (see 2) while taking account of the sample and sample holder transmission values (see 5). A choice of display styles is available including pixelated, faceted or interpolated colour surface plots and / or contour plots, as determined by the main display options.

2 **The Data Selector:** The data selector is an important concept for the efficient use of *GRAS$_{ans}$P* and is essentially an index to the large data storage arrays, or worksheets. During operation of the program the data selector serves two principle uses:

- Directing newly loaded data to the required worksheet for storage. **Only the top 'Foreground / Data Load' selector determines where the newly load data should be placed in the storage data arrays**. Other selectors have no effect.

- Once the data worksheets have been filled the appropriate foreground, background and cadmium background worksheets for data treatment can be selected. Subtraction of the sample background and cadmium background is enabled/disabled by checking/un-checking the subtraction checkboxes. Accurate values of the sample and sample holder transmissions (see 4) are imperative for the correct subtraction of background scattering.

The following worksheets have been pre-allocated to accept data from measurement types common to most SANS experiment:

Worksheet	Number Available	Depths Available	Description
'fore'	6	1-100 + Sum	Sample scattering or foreground scattering data.
'back'	6	1-100 + Sum	Sample or sample holder background scattering.
'cad'	6	1	'Cadmium' or 'electronic noise' background data.
'empty beam'	6	1	Image of the direct beam on the multi-detector.
'trans smpl'	6	1	Direct beam attenuated by the sample + holder.
'trans emty'	6	1	Direct beam attenuated by the sample holder only.
'water'	6	1-100 + Sum	Water or Calibration sample scattering.
'water_back'	6	1-100+ Sum	Background scattering to accompany the 'water' measurement.
'water_cad'	6	1	'Cadmium' or 'electronic noise' background measurement to accompany the 'water' measurement.
'wtr emty beam'	6	1	Direct beam attenuated by the sample + holder.
'wtr trans'	6	1	Direct beam attenuated by the sample + holder.
'wtr trans emty'	6	1	Direct beam attenuated by the sample holder only.
'masks'	6	1	Bad data masks are built and stored in this location.
'det_eff'	1	1	Detector efficiency map determined by analysis of a nominally flat scatterer at small angles, e.g. Water.

Worksheet Number: Data storage is available for several different worksheets of the same type. Using several worksheets the user can, for example, store data measured at several different instrument configurations (e.g. *q*-ranges) in the worksheets 'fore' <1>, 'fore' <2>, 'fore' <3> etc. Worksheets can be '**grouped**' together such that changing the Foreground worksheet number automatically toggles and updates the Background and Cadmium worksheet number as well as the current mask, beam centre and transmissions associated with the current worksheet. Ungrouped worksheets can be toggled independently.

Worksheet Depth: The worksheet 'depth' allows many individual measurements made under the same instrumental configuration but with varying sample environment such as temperature, magnetic field etc., to be collected together and stored as individual frames making a single larger measurement. The worksheet 'depth' is effectively a 3rd dimension to the 2D data arrays. Depths can be '**grouped**' in a similar manner to worksheets. Toggling the current Foreground Worksheet Depth toggles the background depths accordingly to match (if they exist). Analysis algorithms that automatically search though the Foreground worksheet depth will only scroll equivalently though the background depths if the depth grouping option is checked.

Advanded Tip: The number of worksheets and worksheet depths available to *GRAS$_{ans}$P* is essentially system memory limited. Default settings in **grasp.ini** provide for 6 worksheets and maximum depths of 100 worksheets. The can be modified by the user if necessary by setting the values for '**worksheets**' and '**depth_max**' in **grasp.ini**.

3 **Data Load Control:** Enter the run number or range of the data to be loaded into the data load edit box. Pressing the 'GetIt!' button then loads the data into the workspace indicated by the 'Foreground / Data Load' worksheet selector (see 2). The use of several deliminators (e.g. '>' ':' ',' '+' etc.) between ranges allows flexibility in the loading of groups of run numbers to be stored incrementally in the worksheet depth. For a single file number indicated in the data load edit box, the **+** and **–** buttons beneath allow incremental/decremental scrolling though file numbers.

4 **Transmission Indicator:** Displays the current sample and sample holder (empty cell) transmission values T_s and T_e respectively. The option to calculate transmissions becomes available when transmission type worksheets are displayed. Transmission values are calculated, for example, from the zoomed area of the display by comparison of the 'trans_smpl' and 'trans_emty' (for T_s) or 'trans_emty' and 'empty_beam' (for T_e) worksheets. Alternatively, transmission values can be entered directly into the T_s and T_e edit boxes. The transmission can be '**locked**' at it's current value using the 'lock' checkbox such that subsequent scrolling of worksheet number or depths do not toggle the transmission value in use.

5 **Centre of Mass Indicator:** Displays the current centre of mass associated with the current group or individual worksheet number. It can either be calculated from a zoomed area of the current displayed data (direct beam on the detector) or entered directly into the *c_x* and *c_y* edit boxes (*c_θ* also for D16 detector angle). The centre of mass can be '**locked**' at is current value using the 'lock' checkbox such that subsequent scrolling of worksheet number or depths do not toggle the centre of mass value in use.

6 **Display Image Options:** Options to manipulate characteristics of the current displayed data. These include log-z, manual z-scale, correction for detector efficiency, masking, data smoothing, surface and contour displayed data.

7 **Colour Control:** Stretch top and bottom of colour scale and adjust colour gamma.

8 **Menu and Tool Bar:** The *GRAS$_{ans}$P* menu items offer access to File, Display, Analysis, Instrument Characteristics and Data organisational tools and options. Some of these are reproduced as short-cut icons on the tool bar or have quick CTRL key shortcuts.

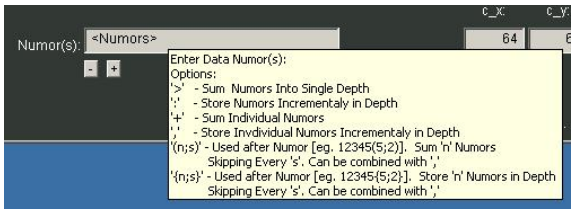
9 **Matlab™ Command Window or Text Output Window (Runtime version):**

The Matlab™ command window (m_code version) or Text Output Window (Runtime version) window displays an summary of data and analysis parameters, warning messages etc. each time the main *GRAS$_{ans}$P* display is updated. Using the full Matlab™ m_code version users have the advantage of direct access to the Matlab language with access to the *GRAS$_{ans}$P* global variables, data store and subroutines for further development or one-off procedures.

Online Help

A pop-up 'tool-tip' based help system accompanies many of the interactive buttons, menus and edits items in the main *GRAS$_{ans}$P* interface. To activate the quick pop-up help leave the mouse pointer over the object for a second and pop-up help should appear.

e.g.



Quick-Start Guide to Data Inspection and Analysis

This 'Quick-Start' section contains step-by-step instructions for data analysis in some of the more simple cases. Following the several examples presented (see 'Data Analysis Examples') will help the user in the operation and capabilities of *GRAS$_{ans}$P*.

Principle Data Reduction Steps:

Treatment of the Calibration Standard Data (e.g. Water)

1. **Calibration and Scaling:** Load the calibration measurement (e.g. Water Scattering), background and cadmium background into the 'water', 'water_back' and 'water_cad' workspaces. Use the 'Detector Efficiency Calculator' option to generate a calibration scaling value (counts/pixel/standard monitor) and detector efficiency map.

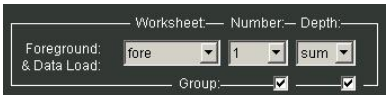
Treatment of the Sample Scattering

2. **Scattering Data:** Load foreground, background and cadmium data sets into the relevant workspace areas, 'fore', 'back' and 'cad'.
3. **Sample Transmission:** Load sample transmission and reference empty cell transmission into the 'trans_smpl' and 'trans_emty' worksheets. Calculate sample transmission, T_s, using the graphical zoom and transmission calculator.
4. **Empty Cell Transmission:** Load empty cell transmission and reference empty beam into the 'trans_emty' and 'empty beam' worksheets. Calculate empty cell transmission, T_e, using the graphical zoom and transmission calculator.
5. **Beam Centre:** Use the 'Centre of Mass' calculator to determine the beam centre coordinates from a zoomed area of the transmission or reference beam measurement.
6. **Mask:** Use the 'Mask Editor' to create a bad-data mask of pixels to eliminate from further analysis. This is combined with an 'instrument mask' that eliminates permanently inactive regions of the multi-detector from analysis.
7. **Isotropic Analysis:** Radial Average (I vs. $|q|$) etc.
8. **Anisotropic Analysis:** Sectors, Boxes, Strips, Sector-Radial Average, Azimuthal Average, 2D data fitting etc.
9. **Reduced 1D or 2D data:** Data Export, Graphical Export, Print.

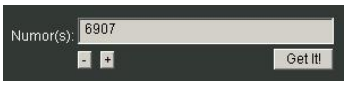
GRAS$_{ans}$P Data Correction Procedures

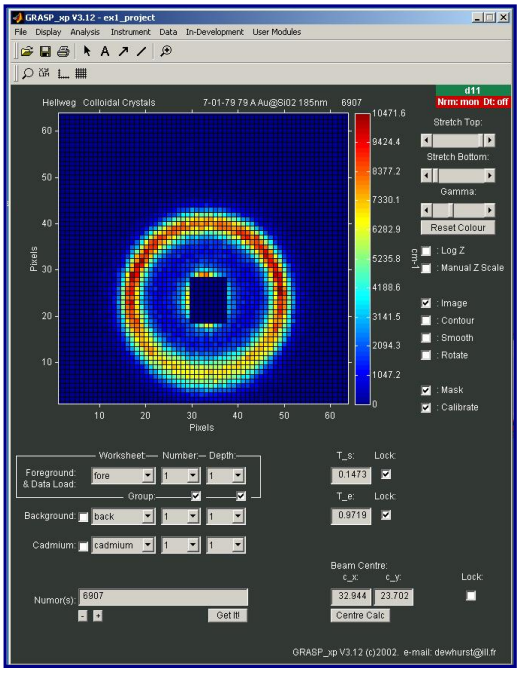
Loading Data and Visual Inspection

1 Select the worksheet and worksheet number of the appropriate data workspace where you wish to load the data. For example, to load the sample scattering data into Foreground 1, set the set the 'Foreground / Data Load' selector to read: <fore> <1> <sum>.

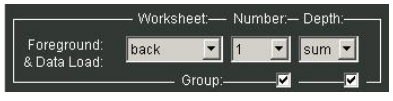


2 Enter the run number of the data to be loaded and press the 'Get It!' button to read the data. The newly loaded data is displayed in the main figure window.





3 Repeat this process to load the Sample Background and Cadmium Background data files in the relevant workspace areas. For example, load the sample background into the <back> <1> <sum> workspace



and the cadmium background into the <cadmium> <1> <1> workspace.

4 The sample transmission, T_S, and the transmission of the sample holder, T_e, (or empty cell, cryostat, furnace etc.) should be entered into the appropriate entry boxes (see 'Determination of Sample Transmission' for calculation of sample and empty cell transmissions).

Note: Data is <u>only</u> loaded into the workspace indicated by the 'Foreground & Data Load' selector while it is all three selectors that determine the final result of foreground – backgrounds.

Loading Combinations and Sequences of Run Numbers into a Single Worksheet

GRAS$_{ans}$P offers the ability to load various combination or sequences of run numbers. These can either be stored as combined or separate data sets. A detailed description of all the available, and sometimes complex data load modes is presented in 'Managing the Data Workspace' while a brief summary of the more common load modes is given below. For example, with '<Fore><1><sum>' displayed in the Data Load selector:

	Load String		
Single Run Number:	*'00001'*	→	*'GetIt'*
Immediate Specific Sum of Run Numbers	*'00001+00002+00005'*	→	*'Getit'*
Immediate Series Sum of Run Numbers	*'00001>00005'*	→	*'Getit'*

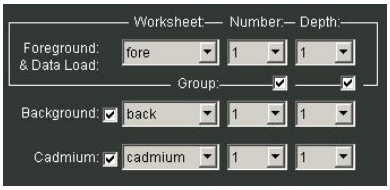
All the above result in a single combined 2D data set loaded into worksheet '<Fore><1><1>'.

Specific Load of Run Numbers into Depth	*'00001,00002,00005'*	→	*'Getit'*
Series Load of Run Numbers into Depth	*'00001:00005'*	→	*'Getit'*

Results all five run numbers, '00001' to '00005' being loaded and stored individually into the worksheet depth '<Fore><1>' depths <1>, <2>, <3>, <4> and 5. Although held together under the description of worksheet '<Fore><1>' the individually stored data in the worksheet depth can be viewed either as a '<sum>', referred to individually by toggling the depth indicator or areas of intensity cross referenced as a function of some varying experimental parameter though the series.

Corrected Sample Scattering Data (not Calibrated)

With the previous steps complete, all components necessary to calculate the scattered intensity, due only to the sample, are now in place. The corrected, but not calibrated, data can be viewed in the main display window by setting the 'Foreground', 'Background' and 'Cadmium' workspace indicators to their appropriate values and by ticking the checkboxes to the left of the 'Background' and 'Cadmium' data selectors. With these checkboxes ticked, all subsequent operation to the data will include correction for both types of background effects.



The corrected data is the result of the foreground minus the two background components taking into account the sample transmission. *GRAS$_{ans}$P* calculates this in the following manner for each element of the pixelated multi-detector data:

$$I_{Corrected} = \frac{1}{T_s T_e}\left[T_s - I_{Cd}\right] - \frac{1}{T_e}\left[I_{Bck} - I_{Cd}\right]$$

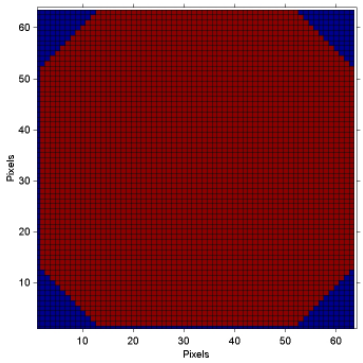
where $I_{Corrected}$ is the sample scattering corrected for background scattering, electronic noise, sample and empty cell transmission (i.e. attenuation effects) and other background effects. I_S is the measured scattering from the sample+holder. I_{Bck} is the measured background scattering from the sample holder. I_{Cd} is the 'electronic' background and T_s and T_e are the sample and empty cell transmissions.

A Note on Data Normalisation: The data correction procedure described above assumes each experimental data set to be either measured for the same time or beam monitor counts OR to have been normalised to a standard time or number of monitor counts. By default *GRAS$_{ans}$P* starts up with automatic normalisation of data to a standard monitor count of 10,000,000 (see 'Data Normalization').

Masking Data

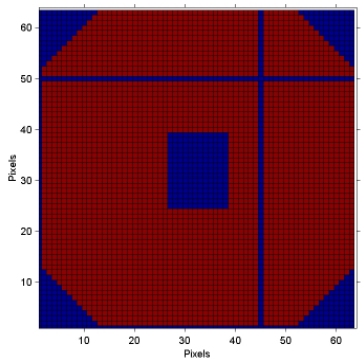
Instrument Mask

Some areas of multi-detector instruments may not exist as active pixel elements despite being included in the output data array. A good example is the D11 multi-detector that has inactive corners and therefore is masked by default when masks are applied using the in-build instrument mask.



Data Mask

Creating a data mask using the *GRAS$_{ans}$P* mask editor can eliminate elements of the multi detector data that are not to be included in subsequent analysis operations or display.



Using the Mask Editor

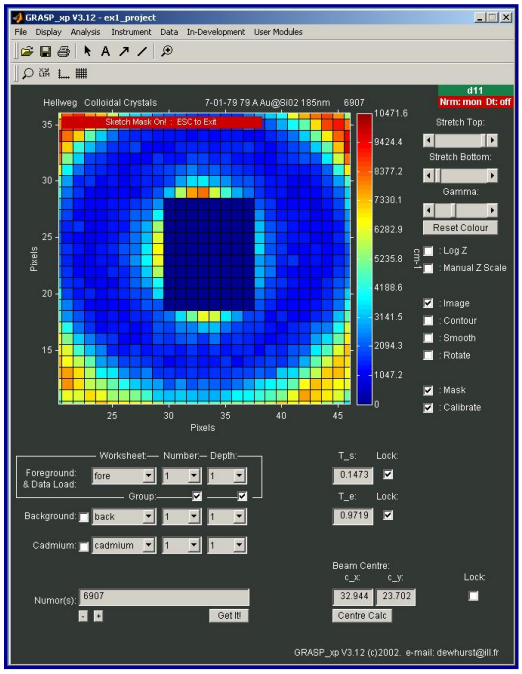
1. Launch the 'Mask Editor' from the 'Analysis>Mask Editor' menu (CTRL-M).
2. To view the Mask select the appropriate mask for display in the 'Foreground/Data Load' worksheet selector. Alternatively, leave the data to be masked on the main display ready to 'sketch' a mask directly over.
3. Simple masks may be built using the options presented in the Mask Editor window. These include:
   - Elimination of individual pixels.
   - Elimination of whole detector lines at constant *x* or *y*.
   - Elimination of rectangles of detector area.
   - Elimination of circles of detector area about a given centre.

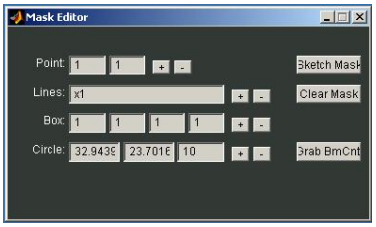
   All options use the [+] and [-] buttons to include or remove points from the mask.

4 'Sketch' rectangular masked areas using the mouse. This allows masks to be drawn directly over the top of the scattering data. To use the 'Sketch Mask' facility:

- Modify the foreground display selector such that the data to be masked is displayed in the main figure window.
- Click the 'Sketch Mask' button to enable the sketch mode. An indicator appears in the message box at the top left hand corner of the main display as a reminder that the sketch mode is active.
- Click and drag across the image to mask areas of the multi detector.
- To de-activate the sketch mask mode either click again the Sketch Mask' button or press ESC.

Tip: It is easier to accurately select regions of the image if the main display is set to 'Faceted' in the 'Display>Image Render>Faceted' menu options.





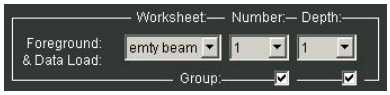
Import / Export of Mask Flies

Mask files can be Exported or Loaded into *GRAS$_{ans}$P* using the 'File>Export Data' and 'File>Import' menus from the main window. Mask files are stored, loaded and saved in the standard ILL format.

Determination of the Beam Centre

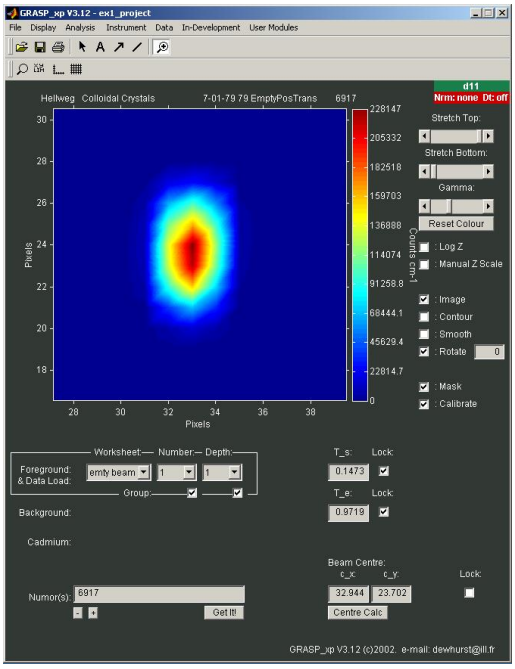
The beam centre is important to know since it is about this position that all radial symmetries are based for both isotropic and anisotropic scattering data. *GRAS$_{ans}$P* uses a centre-of-mass determination of the beam centre by analysis of the direct beam on the detector, as in an empty beam or transmission measurement.

1 Load an empty beam or transmission measurement into a suitable workspace. For example the <empty beam> <1> <1> workspace:



2 With the image of the empty beam on the main display use the 'Zoom' toolbar option to zoom in closely around the empty beam centre. Alternatively use the manual axis option to select a predefined detector area.

3 Click the 'Centre Calc' button to calculate the centre of mass of the displayed area of the image. The result will be stored as the current beam centre associated with the current worksheet number.



Note: If the 'lock' check box is checked all worksheets will use the same beam centre. This is useful when the several worksheets, <1>, <2>, <3> etc. contain data measured under the same instrument configuration.

Determination of Sample Transmission

Calculation of the corrected scattered intensity requires the transmission of the sample and sample holder (or empty cell, cryostat, furnace etc.) in order to correctly subtract the background contributions, as shown below. T_s and T_e refer to the transmission of the sample only (i.e. *not* the transmission of the sample + empty cell) and the transmission of the empty cell respectively. The corrected scattered intensity depends on the transmission values T_s and T_e and is given by:

$$I_{Corrected} = \frac{1}{T_s T_e}[I_s - I_{Cd}] - \frac{1}{T_e}[I_{Bck} - I_{Cd}]$$

Sample Transmission, T_s

The transmission of the sample, T_s, can be calculated by comparison of the transmitted beam through the sample + empty cell (or other sample holder) relative to the total counts for the empty cell.

$$T_s = \frac{Transmitted\ Neutrons\ through\ Sample\ +\ Empty\ Cell\ or\ Holder}{Transmitted\ Neutrons\ though\ Empty\ Cell\ or\ Holder}$$

Empty Cell or Holder Transmission, T_e

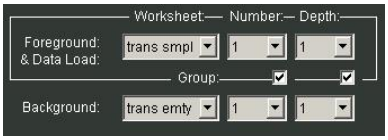
The empty cell transmission, T_e, can be calculated by comparison of the transmitted beam though the empty cell or other sample holder, relative to the total counts in the empty beam.

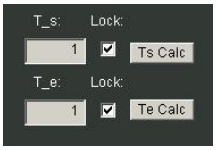
$$T_e = \frac{Transmitted\ Neutrons\ through\ Empty\ Cell\ or\ Holder}{Transmitted\ Neutrons\ in\ the\ Empty\ Beam}$$

Calculation of T_s and T_e using *GRAS$_{ans}$P*

1. Load an empty beam or transmission measurement into a suitable workspace. For example the <empty beam> <1> <1> workspace.
2. Load the empty cell (or sample holder) measurement into the allocated <trans emty> <1> <1> workspace.
3. Load the empty beam measurement into the allocated <emty beam> <1> <1> workspace.

4 To compare the total counts between the sample+cell transmission and empty cell transmission measurements set the main display selectors to <trans smpl> and <trans emty>.



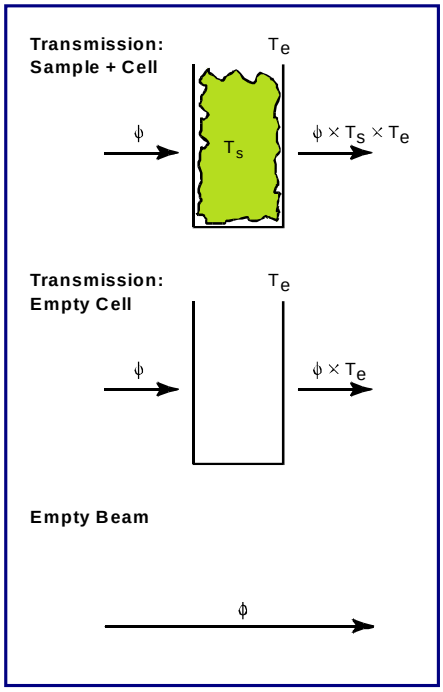


5 When the main display shows data in the transmission worksheets, <trans smpl> or <trans emty>, the option to calculate the sample transmissions T_s and T_e appears alongside the transmission values display.

6 Zoom around the required region of the transmitted beam to select the region from which the transmission calculation should be made, or use the manual axis option to select a predefined detector area.

7 Click the 'T_s Calc' button to calculate the sample transmission. The transmission value T_s is now associated with the current worksheet number.

8 Repeat the above procedure to calculate the empty cell transmission by comparison of the Empty Cell and Empty beam transmission measurements. Use the 'T_e Calc' button.



Note: If the 'lock' check box is checked next to the T_s or T_e indicators all worksheets will use the sample transmission. This is useful when the several worksheets, <1>, <2>, <3> etc. contain data from the same sample but measured under different instrument configurations e.g. different *q*-ranges or different sample environment conditions, e.g. different temperatures.

Data Normalisation: Standard Monitor, Time or Detector Counts

The correction procedure described above assumes each data set to be measured for the same time, beam monitor counts or to have been normalised to a standard time or number of monitor counts. Data normalisation is enabled / disabled from the 'Data>Normalisation' menu item.

Standard Monitor (e.g. 10,000,000 monitor counts)

Normalisation to a standard number of beam monitor counts is the most usual form of data normalisation and is enabled by default upon starting *GRAS$_{ans}$P*. All raw data counts, *n*, and errors, $\sqrt{n}$, are subsequently divided by the number of actual monitor counts for the duration of the measurement (stored within header information of the raw data file) and multiplied by the standard monitor. The resulting data counts in each pixel of multi detector data become counts or error_countrs per standard monitor. The value of the standard monitor can be modified by edits to **grasp.ini** or from the 'Data>Set Standard Monitor' menu.

Standard Time (e.g. 100 seconds)

Normalisation to a standard time results in the raw data counts, *n*, and errors, $\sqrt{n}$, being divided by the data measurement time (stored within header information of the raw data file) and multiplied by a standard time value. The resulting data counts in each pixel of multi detector data become counts or error_counts per standard time. The value of the standard time can be modified by edits to **grasp.ini** or from the 'Data>Set Standard Time' menu.

Total Detector Counts & Window Detector Counts

Raw data counts, *n*, and errors, $\sqrt{n}$, are divided by the total counts registered in the multi detector data array either over the detector or within a defined detector window, e.g. around the direct beam. This is particularly useful if reflectivities are to be calculated directly from measurements that include scattering and the direct beam.

None (absolute counts)

Raw data is untouched leaving counts, *n*, and errors, $\sqrt{n}$.

Detector Dead-Time Corrections

Neutron detectors typically operate on a charge avalanche principle whereby a neutron interacts with a ^{3}He nucleus, to form a ^{3}H nucleus releasing an energetic proton which subsequently ionises ^{3}He gas around it creating the charge avalanche that is detected. A typical detector requires a characteristic time in order to separate two detection events and distinguish the position associated with the neutron arrival. This characteristic time is the detector dead time, τ, and imposes an important experimental restriction for high counting rates. Essentially, within a time period, τ, after the arrival of a neutron further counting is inhibited.

Two models have been used to describe the relationship between the real number of neutrons arriving at the detector, n, and the apparent number actually recorded by the detector, n_m.

$$n_m = n/[1+n\tau] \qquad \text{(non paralysable model)}$$

$$n_m = n \cdot \exp(-n\tau) \qquad \text{(paralysable model)}$$

Both the non-paralysable and non-paralysable models are very similar and only begin to differ significantly for high count rates.

Dead time correction in *GRAS$_{ans}$P* using the non paralysable model is available but NOT activated by default. Dead time corrections can be enabled / disabled from the 'Data>Global Deadtime Correction' menu. A typical dead time for the D22 ^{3}He detector is of the order 1μs. If the dead time correction is significant implemented then the whole dataset is up scaled by the ratio n/n_m.

Note: *GRAS$_{ans}$P* default settings are data normalisation to standard monitor = 10,000,000 and dead time corrections off.

Calibration to Standards of Known Scattering Cross-Section

The previous section showed how data should be loaded into *GRAS$_{ans}$P* and how the background, transmission, normalised and dead time corrected sample scattered intensity can be achieved. The resulting quantity, $I_{sample}(Q)$, represents the real number of neutrons scattered by the sample per standard monitor, time etc.

If we measure and apply the same procedure to a standard sample of known scattering cross section, measured under identical conditions, then direct comparison with the unknown sample being investigated allows us to calculate the sample scattering cross section per unit volume per unit solid angle, $\partial\Sigma/\partial\Omega$, in units of cm^{-1}. For an incoherent scatterer such as water or single crystal vanadium then $\partial\Sigma/\partial\Omega$ can be expressed as a single number. Furthermore, since the scattering is incoherent and uniform over the spherical area 4π the measured and corrected scattering from the flat-scattering standard sample shows up fluctuations in efficiency of individual detector elements. Thus, measurement of a standard, incoherent flat scatterer such as water provides two important quantities:

Calibration Scalar

Detector Efficiency Map

GRAS$_{ans}$P's calibration procedure allows the calibration scalar and 2D detector efficiency map to be separated. In this way the calibration is made directly on the 2D sample data prior to further data reduction steps. *GRAS$_{ans}$P* is therefore ideal for analysis of anisotropic 2D data with full detector efficiency and calibration correction.

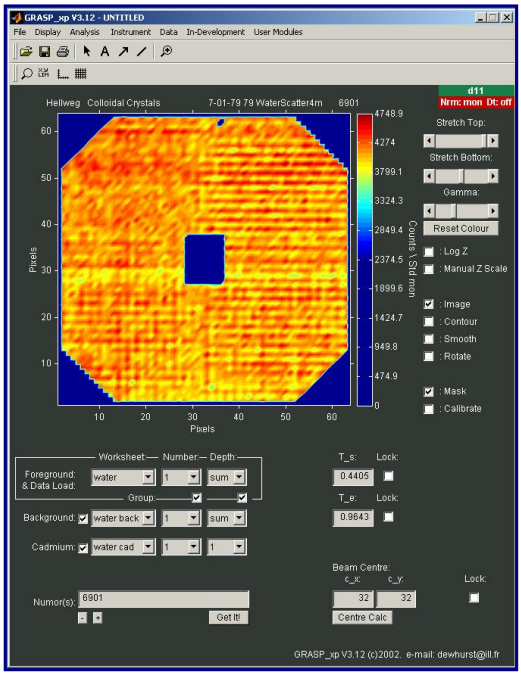
Assuming for the time being that both unknown sample and calibration sample have both been measured using the same instrument configuration (i.e. wavelength, collimation, detector distance – or *q*-range and resolution) and have been corrected for background, transmission etc. as described above. The scattering cross section of the unknown sample can be calculated by a simple division of the intensities measured in each pixel, multiplied by the known scattering cross section of the calibration sample as:

$$\frac{d\Sigma_{Sample}}{d\Omega} = \frac{I_{Sample}}{I_{Calibration}} \times \frac{d\Sigma_{Calibration}}{d\Omega}$$

Calculation of the Calibration Scalar & Detector Efficiency Map

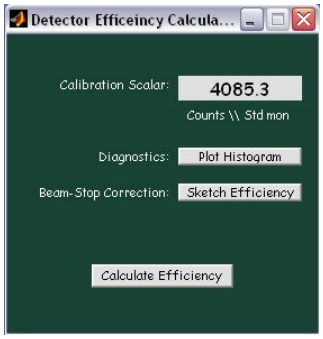
Prepare corrected standard sample scattering data (e.g. water):

- Load the water scattering, background and cadmium background into the relevant data workspace areas.
- Calculate or enter directly the water and empty cell transmissions T_s and T_e.
- Mask bad-data as required.



Separation of Calibration Scalar and Detector Efficiency Map:

- Open the 'Detector Efficiency Calculator' from the 'Analysis >Detector Efficiency Calculator' menu item or CTRL-W.



- The 'Calibration Scalar' is automatically calculated and displayed in the Detector Efficiency Calculator and represents the **average counts / pixel / standard monitor** (depending on the current normalisation selection) of the corrected data currently displayed in at it's measurement configuration (i.e. for it's detector distance, collimation setting, wavelength etc.)

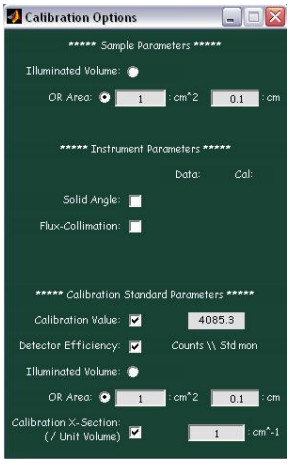
- The ‘Detector Efficiency Map’ can now be calculated by simply pressing the ‘Calculate Efficiency’ button. This takes the currently displayed calibration data and divides the 2D image by the calibration scalar. By definition, since the Calibration Scalar is the mean value of the counts in each pixel, the 2D Detector Efficiency map represents the deviations in detector efficiency with the efficiency value of each cell fluctuating about the mean value of 1. The 2D Detector Efficiency map can be applied to 2D sample scattering data to even distortions to the image due to the spatially varying detector efficiency.

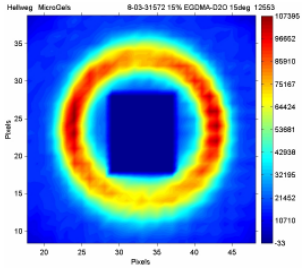
Using the Detector Efficiency Map and Calibration Scalar

Once the Detector Efficiency Map and Calibration Scalar have been calculated all subsequent data can be corrected by enabling the various calibration options in the ‘Calibration Options’ window (‘Analysis>Calibration Options’ menu item or CRTL-K).

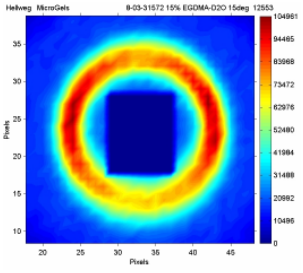
Detector Efficiency Correction

- Tick the ‘Detector Efficiency’ check box in the Calibration Options window. The displayed data is divided by the 2D detector efficiency map (with corresponding errors). This has the effect of smoothing out variations in efficiency of detector lines or pixels from the displayed data. Since the mean value of the detector efficiency map is (by definition) equal to 1, there is no corresponding change in the mean intensity of the corrected data. This means that correction by the detector efficiency map can still be made even if the detector efficiency map was deduced from calibration data measured in a configuration different to the data to be corrected.





No Det. Eff Correction

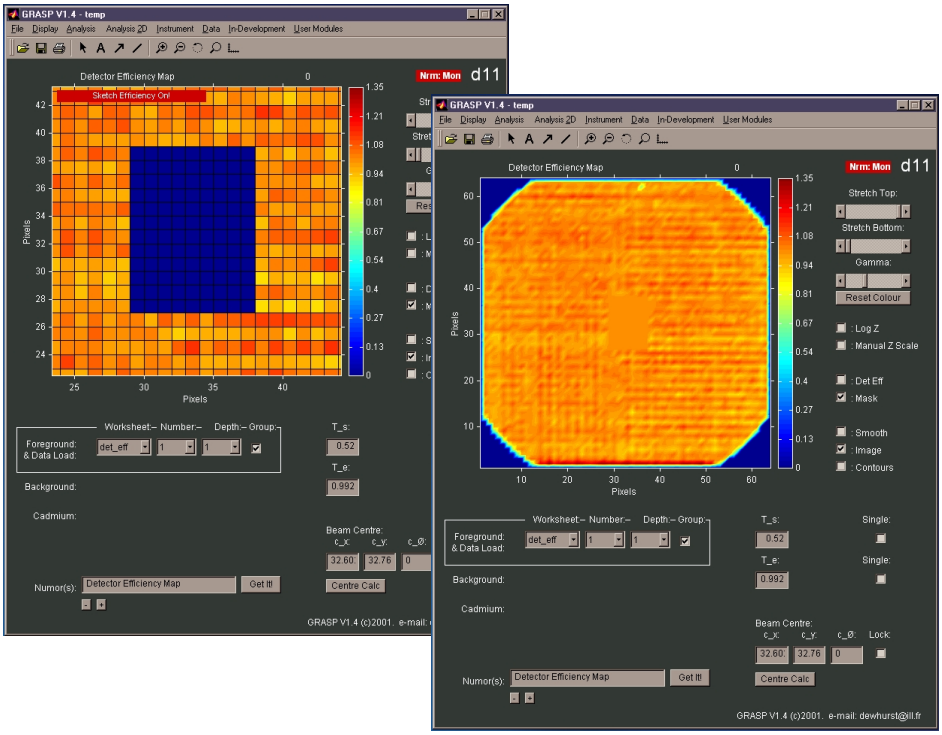


Det. Eff. Correction.

Using the Calibration Scalar

- Tick the 'Calibration Scalar' check box in the Calibration Options window to divided the displayed data by the calibration value.
- If the unknown sample and calibration sample volumes or illuminated areas differ these should be entered in the sample illuminated area or volume edit boxes.
- The scattering cross section of the known calibration sample should be entered in the relevant edit box, e.g. for Water the calibration cross section is close to 1cm^{-1}.
- Assuming calibration and sample data are measured under identical instrumental conditions (i.e. without further Flux and Solid Angle corrections - see 'Solid Angle and Incident Flux Corrections') the corrected data should now be presented in absolute units of cm^{-1}.

'Tweaking' of the Detector Efficiency Map (Optional)

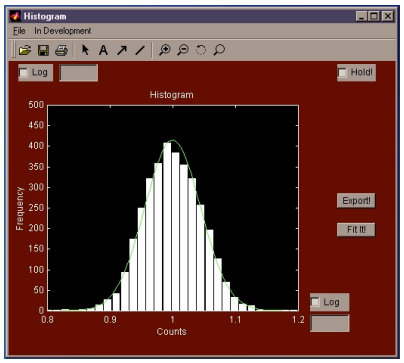


GRAS$_{ans}$P allocates a detector efficiency of 0 to areas of the multi detector masked by the bad-data or the internal instrument mask. This is clear from the example presented where the instrument mask has eliminated the inactive rounded detector corners of the D11 multi detector. The area about the beam

stop is also eliminated by the necessity of these masking pixels. On the other hand the central area of the detector does work and provides important low-*q* scattering information at long wavelengths and detector distances when the straight-through beam covers a lower region of the detector, or when the detector is translated (D22). If a detector efficiency map that was measured for short detector distances were used this central region of the multi detector would be allocated an efficiency of zero and masked. In this situation the central region of the multi detector can be recovered by allocating an efficiency value of 1 to this central region using the 'Sketch Efficiency' option. While information regarding the fluctuation of the detector efficiency in this central region does not actually exist in the calibration measurement, allocation of an efficiency of 1 and using the Calibration Scalar determined from the rest of the multi detector provides a reasonable approximation and recovery of this data.

Detector Efficiency Statistics
(Optional – Of Use Principally to Instrument Responsibles)

Using the 'Plot Histogram' option from the Water Analysis Window, statistics about the detector multi detector pixel elements are calculated as shown in the figure. Here, the detector efficiency map has been re-binned and a histogram plotted showing the extent of the multi detector efficiency variation. While this is not immediately useful for analysis of SANS data it does allow a certain check to be carried out as to the behaviour and quality of the SANS multi detector over time or following repairs etc.



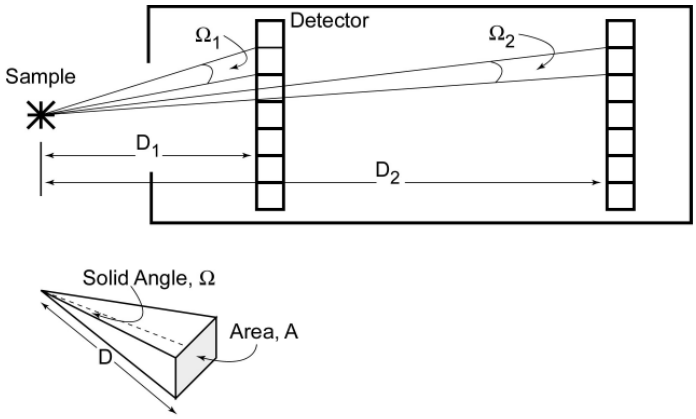
Solid Angle and Incident Flux Corrections

Merging Data Measured in Different Instrument Configurations

It is often useful if calibration data measured in one configuration can be used to correct and calibrate data measured in another configuration. This is, in fact, often essential since calibration by an incoherent scatter such as water cannot realistically be measured with any accuracy for long detector distances. Furthermore, it is unnecessarily time consuming to have to make a calibration measurement at each instrument configuration used for measurement of the unknown sample. Thus, ideally, a calibration measurement should be made an optimal instrumental configuration while the sample data may be measured one or more different instrument configurations (*q*-ranges) of interest. For example, at a given wavelength, measurements of a sample might be made at 3 different detector positions in order to achieve the maximum *q*-range at a fixed wavelength on the SANS instrument. Two important effects contribute the differences in scattered intensities at different instrument configurations. The first is the change in **solid angle** subtended by a detector pixel element on the sample as a function of detector distance. The second is the change in **incident flux** at the sample position as the instrument collimation is varied.

Solid Angle Correction (Detector Distance)

Consider two SANS scattering measurements made at two different detector positions, D_1 and D_2. The multi detector array is, of course, the same for the two measurement and consists of pixelated elements of size 7.5 x 7.5mm for D22 or 10 x 10mm for D11 for example. As the detector is moved further from the sample (for smaller *q*'s) each pixel subtends a smaller solid angle, $\Omega_1 = A/D_1^2$, on the sample, where A is the area of the detector pixel and D_1 is sample-to-detector distance. If this data is to be compared or calibrated to data measured in a second configuration with detector distance D_2, then each detector pixel element only registers neutrons over the solid angle, $\Omega_2 = A/D_2^2$. In other words, the counts **per pixel** from a sample measured at a closer distance, D_1, will be much greater than the counter per pixel measure for the same sample at a further detector distance D_2. For either case, however, the counts **per unit solid angle, Ω,** should be identical. Thus, comparison of the two data sets normalised by the solid angle subtended by each detector pixel should yield scattering data on comparable intensity scales.



Thus, comparison of the two data sets normalised by the solid angle subtended by each detector pixel should yield scattering data on comparable intensity scales.

To implement Solid Angle Corrections in *GRASansP*:

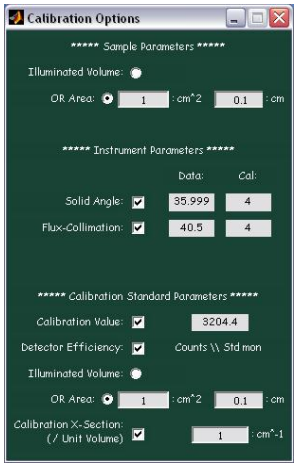
1. Open the Calibration Options Window from the 'Analysis>Calibration Options' menu item or CTRL-K.
2. Enable the Solid Angle Correction by ticking the appropriate checkbox. The value of the detector distance for the currently displayed data is displayed along with the reference detector distance used for measurement of the calibration sample.
3. Subsequent operations divide both sample and calibration (if it is present) data by their relevant pixel solid angles. Data measured for different detector distance configurations should now be corrected for the solid angle.

Incident Flux Correction (Flux vs. Collimation Distance)

Changing the instrument collimation length has the effect of modifying the incident flux at the sample position. This is simply due to the fact that as the collimation length increases the angular divergence criteria for a neutron to successfully make it though the system becomes tighter. Thus, when a sample is measured at several different detector distances (*q*-ranges) with the necessary changes in instrument collimation, the effective flux at the sample position is modified. In order to match scattering curves measured for in different instrument configurations (*q*-ranges) a correction for the effective flux at the sample position should be made as well as the aforementioned solid angle correction.

Since the collimation attenuation is not easily calculable analytically (due to the effects of gravity on the neutron flight path etc.) *GRAS$_{ans}$P* holds a database of measurements of the neutron flux as a function of both instrument collimation and neutron wavelength, currently for the instruments D11, D22 and SINQ_SANS_I (see Appendix 2). Rather than storing absolute values for the flux at the sample position which, in any case, varies between particular experiment and instrument setups, *GRAS$_{ans}$P* stores relative values for differences in flux between different collimation and wavelengths. For example, for D22 the relative flux difference between a collimation length of 4m and 2m (@ 10Å) is 3.0498. Using this relative collimation attenuation database means that the user should still measure the absolute flux at the sample position in at least one experimental configuration. This is usually provided by measurement of the calibration sample at a given collimation. The collimation attenuation database is relatively independent of the exact size of apertures used at the sample end of the collimation or the use of attenuators or apertures and the reactor end of the collimation tube (i.e. assumes a uniform flux density across the beam profile). Measurements made at wavelengths not given explicitly in the Grasp database calculate an interpolated flux-collimation-wavelength scaling value from adjacent points.

To implement flux-collimation scaling:



1. Open the Calibration Options Window from the 'Analysis>Calibration Options' menu item or CTRL-K.
2. Enable the Flux-Collimation scaling by ticking the appropriate checkbox. The value of collimation used for the currently displayed data is displayed along with the collimation value used for measurement of the calibration sample. If these two are equal then the relative flux ratio will be 1. When the two collimation lengths differ then the data is up- or down-scaled to match the same incident flux as that used for measurement of the calibration sample.
3. Subsequent operations up- or down-scale the currently displayed data intensity to match the same incident flux as that used to measurement of the calibration sample.

Tip: Example 1 gives a demonstration of full calibration and merging data measured at different collimations and detector distance.

GRAS$_{ans}$P Analysis Procedures

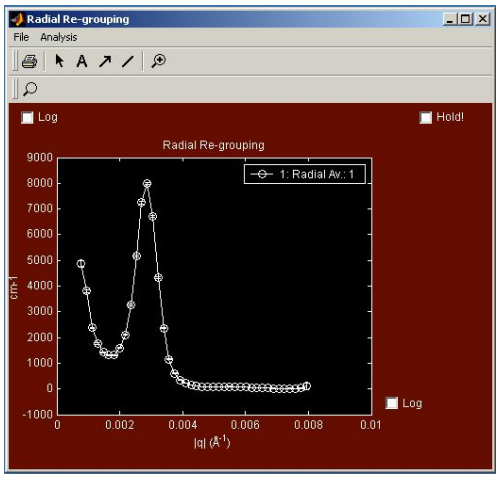
Isotropic Scattering: Averaging I vs. |q| and I vs. |2θ|

Once background corrected and calibrated data has been prepared, as described in the previous sections, isotropic scattering data can be further reduced to 1D plots of Intensity, *I*, vs. scattering vector, *q*, or angle, *2θ*. To calculate *I*, vs. |*q*| or *I* vs. |*2θ*|*:*

1 Open the 'Averaging' window from the 'Analysis>Averaging' menu.

2 Click the *I vs.* |*q*| or *I vs.* |*2θ*| button to produce radially averaged data. The average counts (per pixel or solid angle) around annuli of radius given by the radial bin size (pixels) as a function of pixel radius (|*q*|) across the detector is calculated (see 'Details of analysis procedures and algorithms).

3 The reduced data now appears in a separate graphic display window.



4 The resulting *I vs.* |*q*| or *I* vs. |*2θ*| data can now be:

- Exported as ASCII columns of data [|*q*| or *2θ, I, Err(I)*].
- Printed
- Curve Fitted

as a further analysis steps in *GRAS$_{ans}$P*.

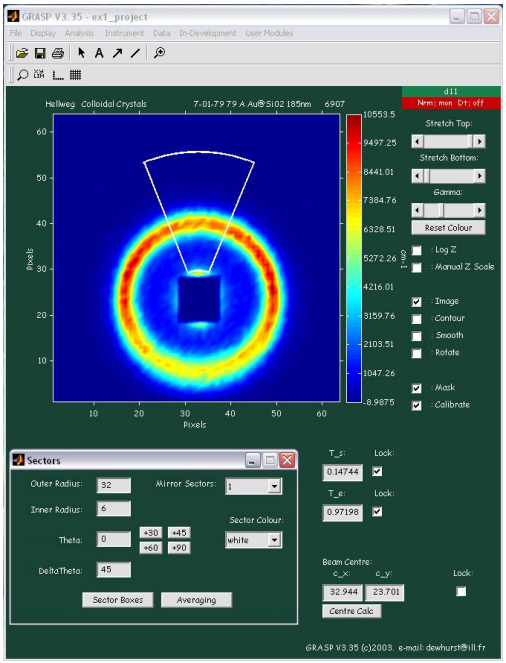
Anisotropic Analysis: Selective use of Multi-Detector Data

Analysis of anisotropic data with or without polar symmetry (i.e. symmetric about the beam centre) can be achieved easily and quickly by selective analysis of the multi detector data using Sectors, Ellipse, Strip and Box masks. Shaped masks can be designed, as described below, prior to reduction of the data only within the defined areas.

Sectors

- Open the 'Sectors' window from the 'Analysis>Sectors' menu. Enter the sector dimensions to position the sector appropriately over the region of interest of the multi-detector data. Sector dimensions are described in terms of:
  - Outer Radius (pixels)
  - Inner Radius (pixels)
  - Theta, sector angle to the vertical (degrees)
  - Delta Theta, sector opening (degrees)

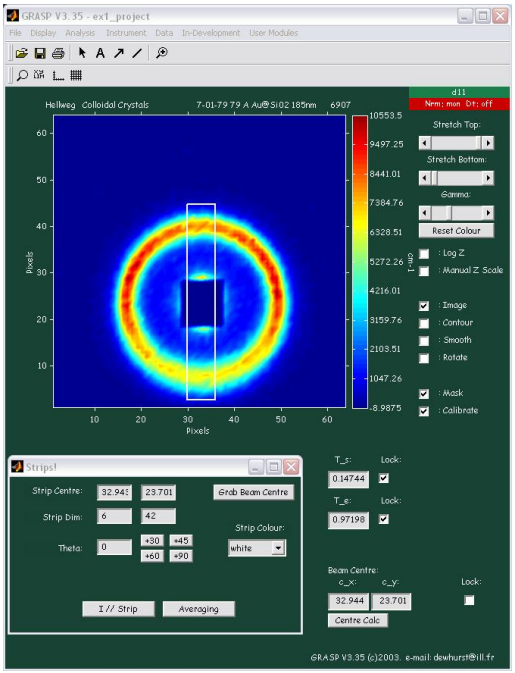
    as well as options for adding multiple sectors with 1 to 6-fold rotational symmetry.



- Use the Averaging or Sector Box tools to further reduce data defined by the Sector

Strips

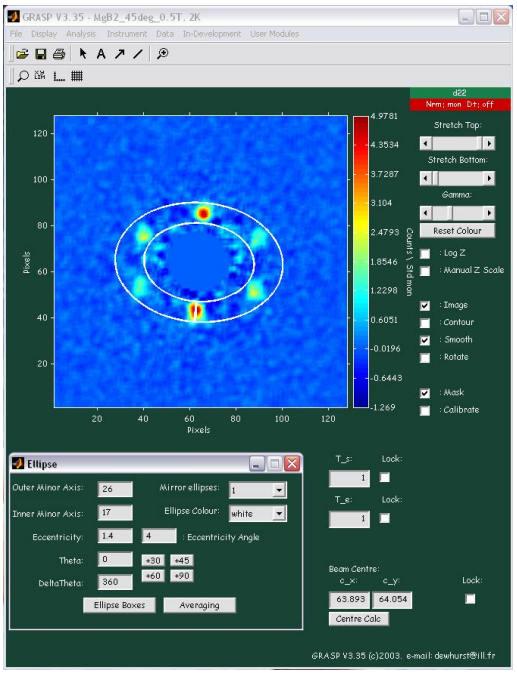
- Open the 'Strips' window from the 'Analysis>Strips' menu. Enter the Strip dimensions to position the strip over region of interest of the multi-detector data. Strip dimensions are described in terms of:



  - Strip Centre: Position of the centre of the strip, i.e. where the diagonals cross. An option is available to use the current beam centre.
  - Strip Width (pixels)
  - Strip Length (pixels)
  - Strip Angle, to the vertical (degrees)

Ellipse

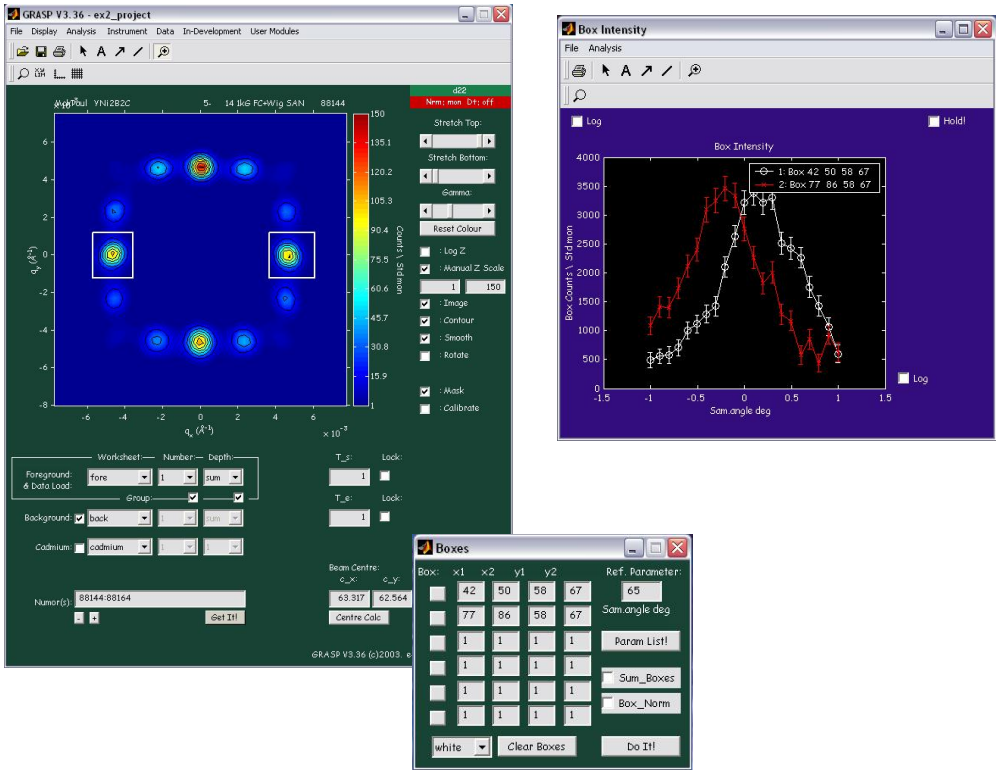
- Open the 'Ellipse' window from the 'Analysis>Ellipse' menu. Enter the Ellipse dimensions to position the ellipse over region of interest of the multi-detector data. Ellipse dimensions are described in terms of:



  - Outer-minor axis (pixels)
  - Inner-minor axis (pixels)
  - Ellipse eccentricity (major/minor) and eccentricity angle (minor axis angle to the vertical).
  - Theta, ellipse segment angle to the vertical (degrees)
  - Delta Theta, ellipse segment opening (degrees)

Boxes

- Open the ‘Boxes’ window from the ‘Analysis>Boxes’ menu. Use the zoom option of the main display to zoom in to the area of interest of the multi detector data. ‘Grab’ the coordinate of the zoomed area to one of the size box coordinate spaces.
- With stored boxes, sector boxes or ellipse boxes, summed intensities of selected multi detector areas can be extracted as a function of file stored in the worksheet depth.
- The resulting intensity can be plotted as a function of, for example, sample temperature, angle, magnetic field, time etc. or any other of the stored sample parameters.



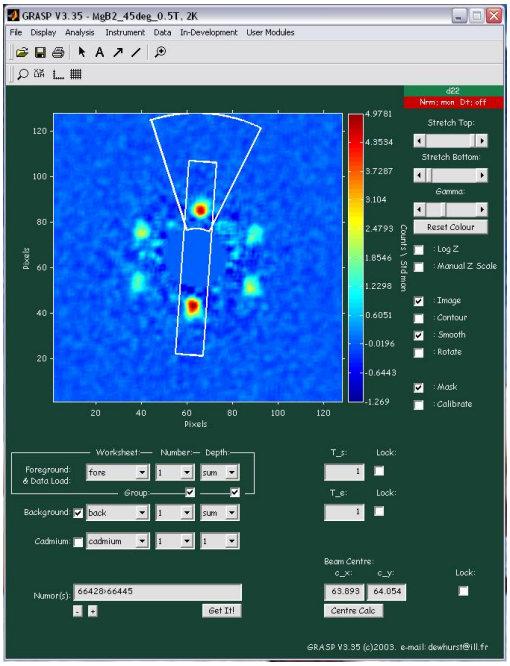
Using Sector, Strip and Ellipse Masks

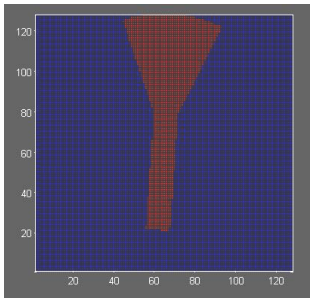
- Use the Averaging tools to further reduce data defined by the Sector, Strip or Ellipse

1. Open the 'Averaging' window from the 'Analysis>Averaging: Radial Azimuthal' menu item, CTRL-R or from the 'Averaging' buttons within the Sector, Strip or Ellipse windows.

2. Ensure the relevant checkbox is ticked to enable subsequent analysis using Sector, Strip or Ellipse masks.

Note: When combination of Sector, Strips and Ellipse masks are used simultaneously the resulting combined sector-strip mask is a logical 'OR' of the individual sector and strip definitions. E.g



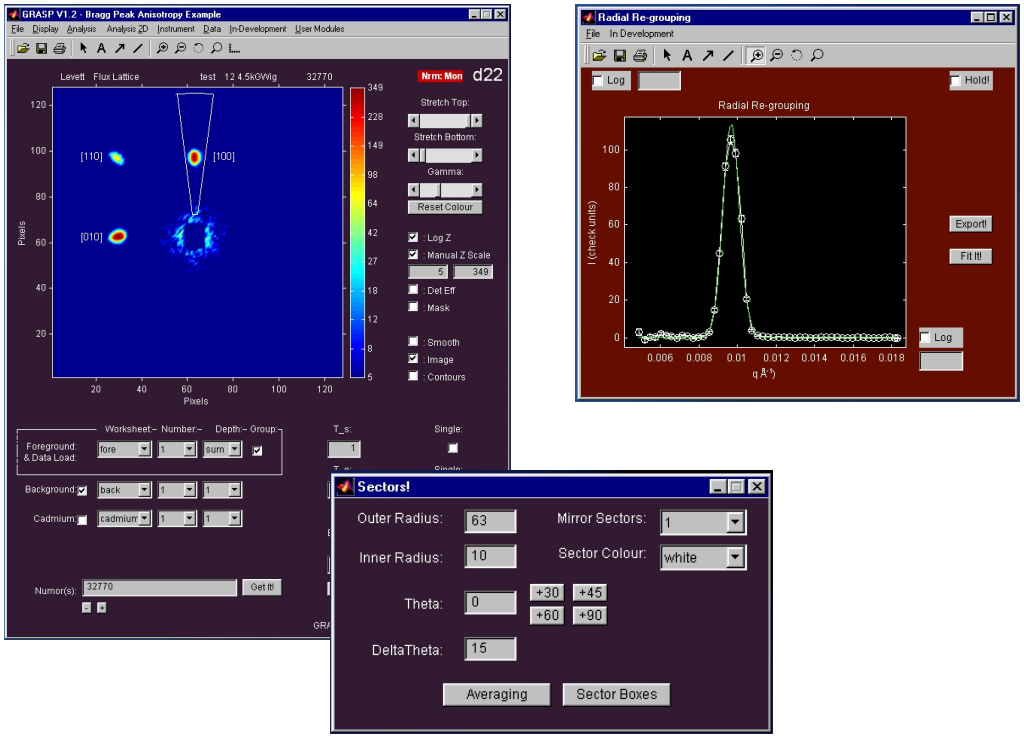


Example: Using Sectors with Averaging *I* vs. |*q*|

The sector defined and displayed in the figures below select a region of the multi detector encompassing a [100] Bragg diffraction peak from the superconducting flux-line lattice. The radial position, or |*q*|, of the Bragg peak can now be easily determined using sectors and the radial averaging routine, without contamination of the result from the unwanted regions of the multi detector.

1 From the 'Sectors' window, or from the 'Analysis>Averaging' menu, open the Averaging Window. The 'Use Sector Mask' check box should be checked instructing *GRAS$_{ans}$P* only to use the data within the defined sector.

2 Click the *I vs.* |*q*| button to produce the radial average within the defined sector. The |*q*| of the Bragg peak is now clearly visible in the *I vs.* |*q*| plot.



Remember: To use Sector or Strip 'masks' with many of the usual analysis check the 'Use Sector Mask' or 'Use Strip Mask' checkboxes where applicable.

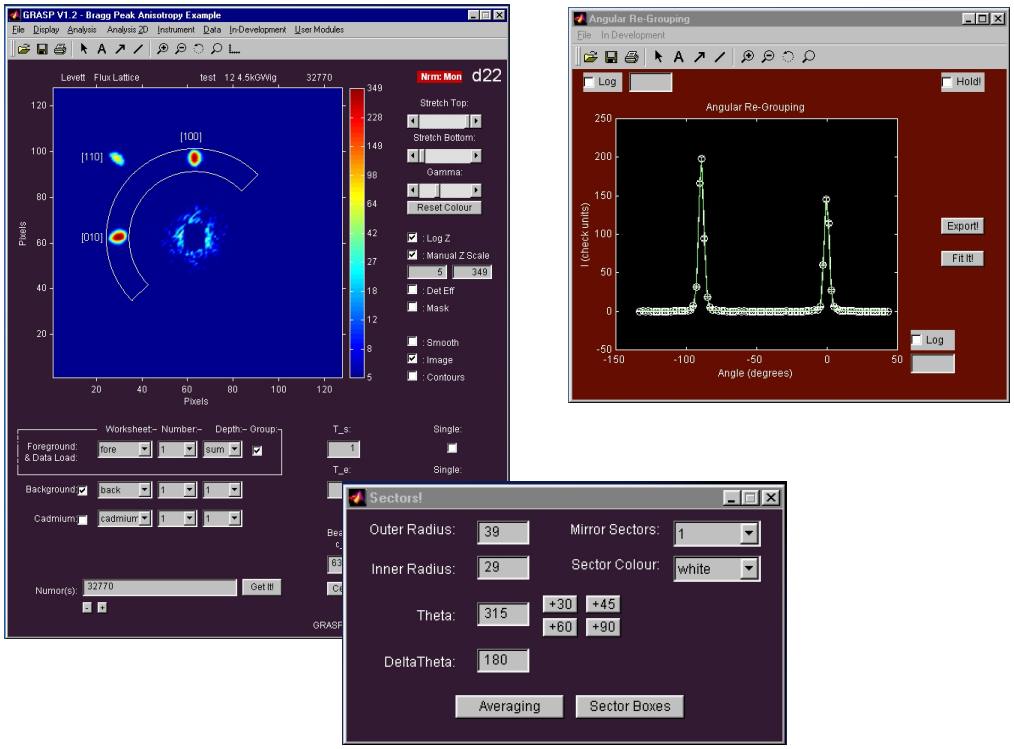
Example: Using Sector Masks with Azimuthal Averaging (*I vs. Ψ*).

The sector defined and displayed in the figures below selects an arc region of the multi detector image encompassing [100] and [010] Bragg peaks from the superconducting vortex. The Azimuthal, or angular variation of the diffracted intensity (*I vs. Ψ*) within the sector can now be easily determined using the Averaging: *I vs. Ψ* routine.

1. From the 'Sectors' window, or from the 'Analysis>Averaging' menu, open the Averaging Window.

2. The 'Use Sector Mask' check box should now be checked. This instructs *GRAS$_{ans}$P* only to use the data within the sector defined by the Sectors window.

3. Click the *I vs. Ψ* button to produce Azimuthally averaged data, *I vs. Ψ*, within the defined sector.



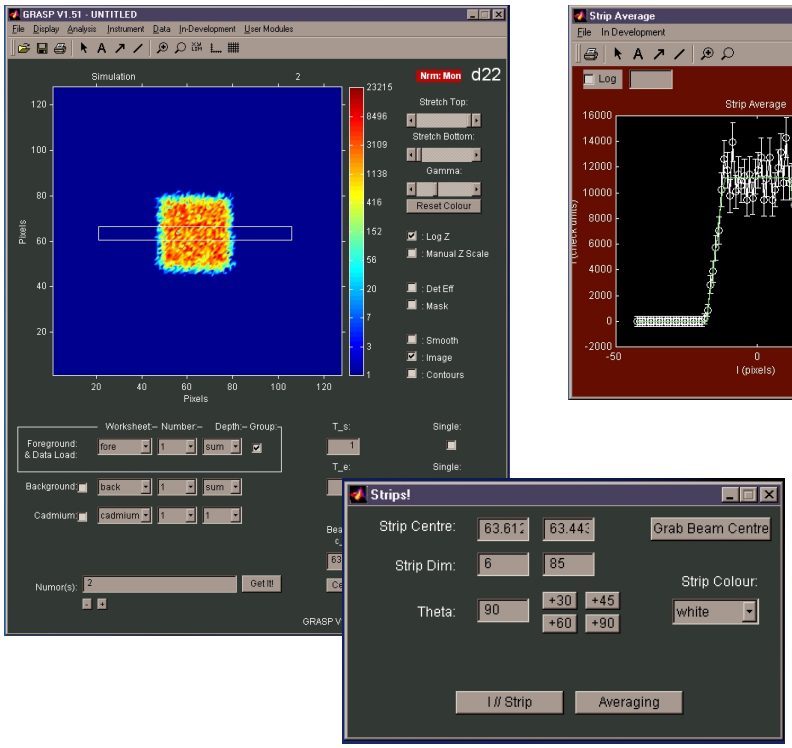
Remember: To use Sector or Strip 'masks' with many of the usual analysis check the 'Use Sector Mask' or 'Use Strip Mask' checkboxes where applicable.

Example: Using Strip Masks.

The data below shows the enlarged direct beam on the detector when the detector distance exceeds the collimation length (simulation data). Using 'Strip Masks' the profile of the direct beam can be extracted along a line in the chosen direction.

1 Use the 'Strips' window to define a strip across the multi detector data over the area of interest. For the data presented in the figure, the strip is centred at the beam centre with length 85 and width 6 pixels oriented horizontally in the detector plane.

2 Click the 'I//Strip' button in the strips to produce a plot of the average intensity across the strip width as a function of the strip length.



Remember: To use Sector or Strip 'masks' with many of the usual analysis check the 'Use Sector Mask' or 'Use Strip Mask' checkboxes where applicable.

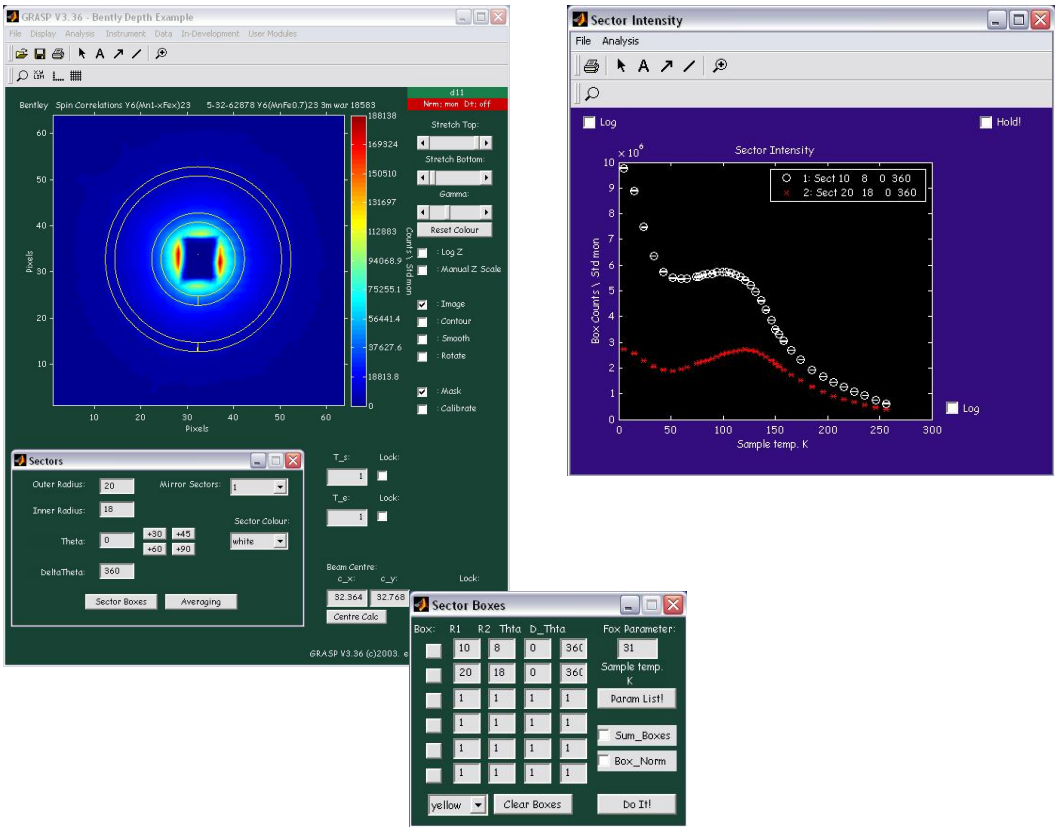
Extracting Intensity as a Function of Worksheet Depth: Boxes, Sector & Ellipse Boxes

Using the 'Boxes' tool or similarly defining 'Sector Boxes' or 'Ellipse Boxes' areas of intensity on the multi detector can be extracted and analysed as a function of a series of data files stored in the worksheet depth. This might be, for example, a series of data run numbers measured as a sample is rotated though it's rocking curve in small-angle diffraction experiment (see Example 2). Or, it might be a series of measurements made as the sample temperature, magnetic field, time or other environment condition is varied. The Boxes, Sector Boxes and Ellipse Boxes tool simply allow regions of the multi detector to be defined and the intensity within these 'boxes' to be extracted as a function of data file in the worksheet depth or sample environment parameter stored in the data file.

- Define a box, sector or ellipse region of the multi detector data of interest using the tools described previously.
- Open the appropriate box, sector or ellipse box window and 'grab' or enter manually the coordinates of the area of interest.
- With stored boxes, sector or ellipse coordinates summed intensities of the selected areas can be extracted as a function of file, or file parameter, stored in the worksheet depth.
- The resulting intensity can be plotted as a function of, for example, sample temperature, angle, magnetic field, time etc. or any other of the stored sample parameters.

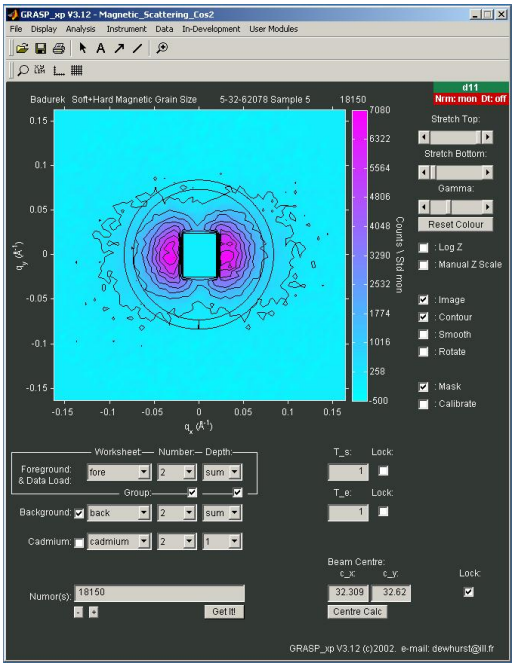
Example

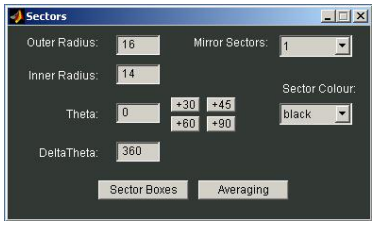
The example shows a series of data files recorded as a function of sample temperature and loaded into the worksheet depth. The sector window defines rings of multi detector data, the coordinates of which are recorded in the 'Sector Boxes' window. Selecting the sample temperature as the appropriate parameter (parameter 31 – use the 'Param List' button to display a list of all the data file header parameters) the ring intensities can be extracted as a function of temperature by pressing the 'Do It!' button.



Magnetic SANS: Ancos^2

Small-angle scattering from a magnetised ferromagnetic ribbon is shown in the figure below. The scattered intensity contains a mixture of isotropic nuclear scattering from the metal matrix and anisotropic magnetic scattering from the magnetic moments in the magnetic ribbon. Here the applied field is in the vertical direction and is sufficient to nominally fully saturate or polarise the ferromagnet along the field direction. In the ideal case (i.e. all magnetic moments aligned with the field in the vertical direction) there should be no magnetic scattering for *q*-vectors parallel to the magnetic moment direction (vertical) and a maximum in magnetic scattered intensity for *q*-vectors perpendicular to the moment direction. Around a circle of constant |*q*| the magnetic scattered intensity should vary as a Cosine^2 with angle around the multi detector image.

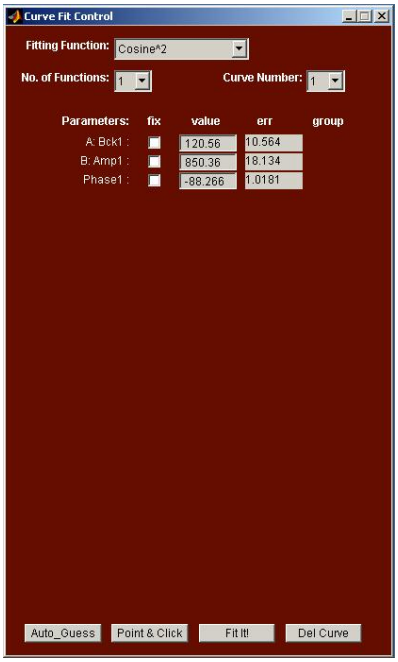


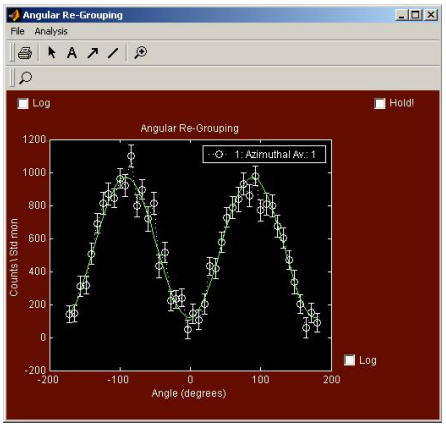


Inspection of Cosine^2 Magnetic Scattering at Constant *q*

With the corrected foreground – background combination and calibration already prepared in *GRAS$_{ans}$P*.:

1. Open the Sectors window and place a ring of width 1 or 2 pixels at a sensible position on the detector image opened to 360^o.
2. Open the Averaging window from the button within the Sectors window (opening Averaging from here ensures the 'Use Sector Mask' button is checked in the Averaging window).
3. Click the *'I vs. θ'* button to calculate the ring intensity as a function of angle around the chosen ring.
4. The Cosine^2 curve can be fitted by opening the Analysis>Curve Fit window.





Automated Cosine^2 curve fitting: Ancos^2 Module

The Ancos^2 module provides an automated procedure to repeat the above annulus selection and Cosine^2 curve fitting. The fit parameters to the Cosine^2 are then proportional to:

- Cosine^2 Offset : Nuclear scattered Intensity
- Cosine^2 Amplitude : Magnetic Scattered Intensity
- Cosine^2 Phase : Moment Direction

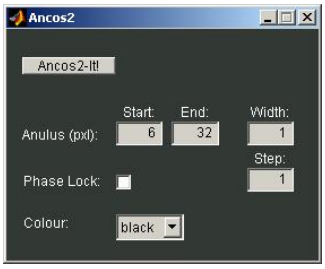
and are output as a function of *q*, as shown by the figures below.

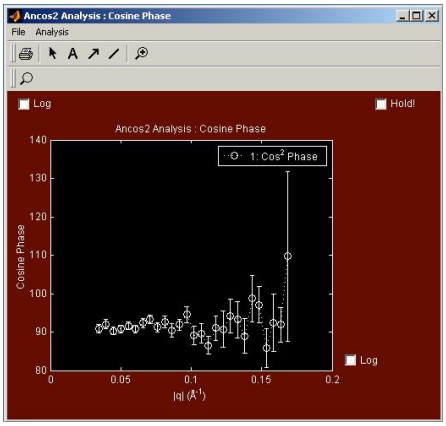
To extract the Nuclear and Magnetic scattered intensities using the Ancos^2 module:

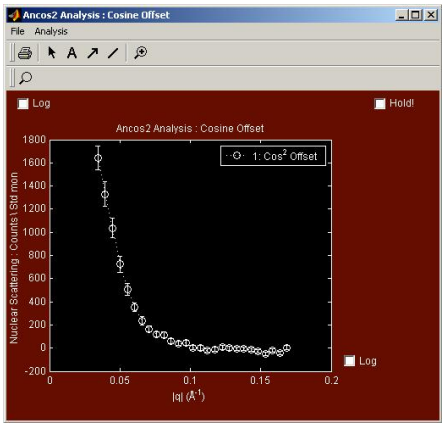
1 Open the Ancos^2 window from the 'Analysis>Ancos^2' menu.

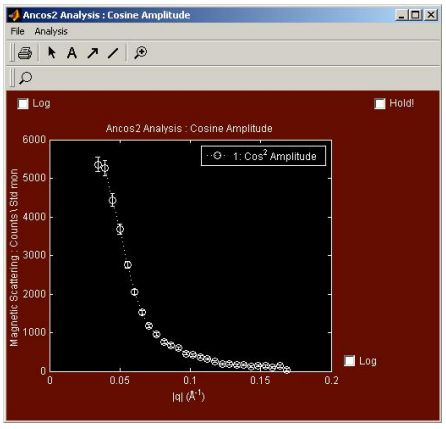
2 Enter the parameters over which the Cosine^2 curve fitting is to work:

- Start Radius: Normally the minimum radius just outside of the beam-stop.
- End Radius: Normally the maximum radius visible towards the edge of the detector.
- Width: Width of each annulus used for the Cosine^2 fit.
- Step: Annulus step between successive iteration. E.g. setting Width = 2 and Step = 1 effectively introduces a 'smoothing' to the data given to the Cosine^2 fit.
- Phase and Lock: If it is certain of the magnet moment direction then the phase can be held constant or locked at a given value during the fit.









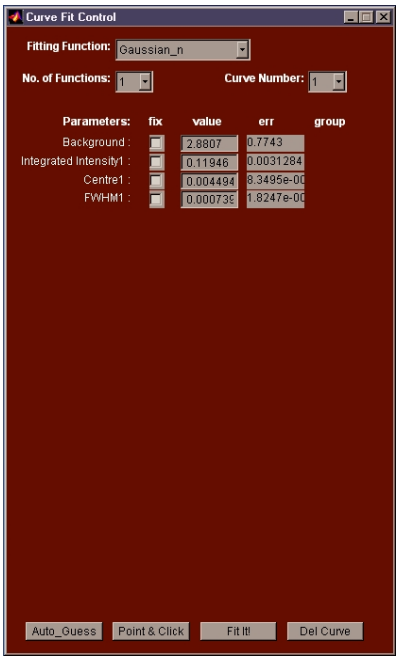
1D and 2D Curve Fitting in *GRAS$_{ans}$P*

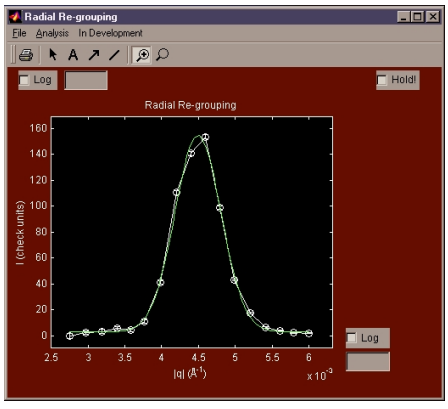
GRAS$_{ans}$P already contains several 1D and 2D curve fit functions available to the user from the 'Analysis>Curve Fit' menu items. The minimisation routine currently used by *GRAS$_{ans}$P* is the 'mf_lsqr.m', a Levenberg-Marquardt nonlinear regression routine by R. I. Shrager and modified more recently by A. Jutan and R. Muzac. 'mf_lsqf.m' is the routine used by the Risø and ILL TAS analysis program 'Mfit' (http://www.ill.fr/tas/). As such, fitting functions for *GRAS$_{ans}$P* are written in a very similar form to those of 'Mfit'. Given below are examples of how to use curve fitting within *GRAS$_{ans}$P* for both reduced 1D and 2D data. Parameters resulting from the last fit procedure can be accessed via the Matlab™ command line or users own programs and user modules.

Example: 1D Curve Fitting – A single Gaussian Function

The 1D data in the plot window shown below shows the result of a radial average over a set of data encompassing a Bragg peak centred around q= 4.45x10^{-3} Å^{-1}. The form of the data is close to that of a single Gaussian and can be fitted as such.

1. Open the 'Curve Fit Control' window from the 'Analysis>Curve Fit' menu item of the 1D output figure.
2. Select the Function type and number of simultaneous functions to be fitted. Here, the 'Gaussian_n' function is used with n set to 1.





3 Starting parameters for the curve fit can be either entered directly into the parameters edit boxes, auto guessed ('Auto_Guess' button) or chosen manually by clicking around particular points of the data to be fitted ('Point & Click' button), for example the background, peak intensity and position, width.

4 Once initial fit starting parameters have been provided the fit can commence by clicking the 'FitIt!' button. The final fit parameters are returned in the parameters edit boxes alongside their error. The Matlab™ edit window scrolls more detailed information from the 'mf_lsqr.m' minimisation function including the chi-squared, number of iterations etc.

Tip: The results from the last curve fit procedure can be accessed either on the Matlab™ command line, standard Matlab™ '.m' routines or user modules though the *GRAS$_{ans}$P* global variable structure 'fit_parameters'.

Example: 1D Curve Fitting – Two function fitted simultaneously

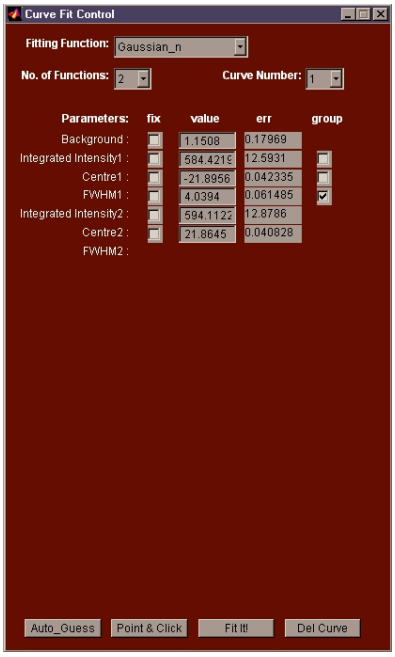
The example data presented below shows a strip average across a data set exhibiting two Bragg peaks at opposite sides of the multi detector. The two peaks are roughly Gaussian and should be of the same Gaussian full-width-half-max (FWHM). The two peaks could be fitted individually, as in the previous example, by zooming in on the region of the interest of the data. On the other hand, if the two peaks are fitted simultaneously the FWHM for the peaks can be forced to be common. This is one of the advantages of simultaneously fitting multiple similar functions. Other advantages might be where two peaked functions overlap significantly and cannot be easily resolved.

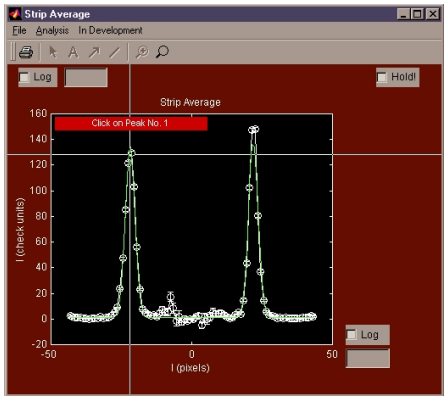
1 Using the 'Gaussian_n' function, set the number of simultaneous functions, n, to 2.

2 Starting parameters for the curve fit can be either entered directly into the parameters edit boxes or chosen manually by clicking around particular points of the data to be fitted ('Point & Click' button), for example the background, peak intensity and position, width. (NOTE: Auto guess currently only works for single peaked functions and is not yet implemented for multiple peaked functions).

3 To 'group' the FWHM of the two Gaussian functions, tick the checkbox to the right hand side of the first Gaussian FWHM parameter. Both fitted Gaussian will be forced to share a common FWHM.

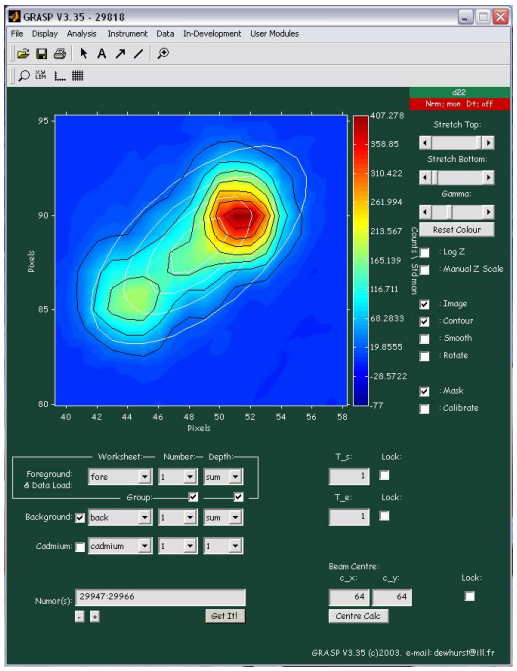
4 Once initial fit starting parameters have been provided the fit can commence by clicking the 'FitIt!' button. The final fit parameters are returned in the parameters edit boxes alongside their error. The Matlab™ edit window scrolls more detailed information from the 'mf_lsqr.m' minimisation function including the chi-squared, number of iterations etc.

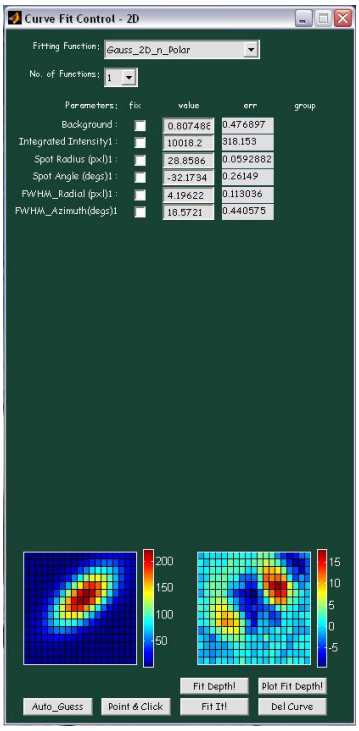




Example: Small-Angle Diffraction: Bragg Peaks and Fitting to 2D Multi detector Data

In the following example fitting of 2D functions to corrected 2D multi detector data is presented. The main figure window below shows a Bragg peak on the D22 multi detector from the superconducting vortex lattice. Closer graphical inspection of the data actually suggests that the vortex lattice may actually be split into 3 domains slightly miss-orientated to each other. To begin with, let's try to fit a single 2D Gaussian to the data, even though we can clearly see that this is a very bad approximation!





1. Open the '2D Curve Fit Control' window from the 'Analysis>2D Curve Fit' main menu item.
2. Select the Function type and number of functions to be fitted. Here a single 2D Gaussian with Polar Symmetry has been selected (i.e. major and minor axes are radial and azimuthal to the beam centre).
3. Starting parameters for the curve fit can be either entered directly into the parameters edit boxes, auto guessed ('Auto_Guess' button) or chosen manually by clicking around particular points of the data to be fitted ('Point & Click' button), for example the background, peak intensity and position, width.
4. When initial fit starting parameters have been provided or calculated the fit can commence by clicking the 'Fit It!' button. The final fit parameters are returned in the parameters edit boxes alongside their error. The Matlab™

edit window scrolls more detailed information from the mflsqr.m minimisation function including the chi-squared, number of iterations etc.

5 The resulting 2D curve fit is plotted on top of the original data as a contour plot.

6 The bottom of the '2D Curve Fit' control window shows the fitted function (left) and error map (right) as 2D images. The error map shows the difference between the curve fit and the real data divided by the error in the real data. The error map provides a useful graphical illustration as to the accuracy of the fitted 2D curve. For the example presented above it clear from the error map that the single Gaussian curve is not a good description of the data and that furthermore, three overlapping Gaussian functions would make a better description (see following example).

Example: 2D Curve Fitting – Multiple 2D Gaussians

The same data as in the previous example can be more appropriately fitted with 3 simultaneous 2D Gaussian curves by setting the 'number of functions' selector to equal 3. Since the three Bragg peaks come from three slightly miss-oriented, but otherwise similar domains, it is reasonable to assume that both the radial and azimuthal widths of the Gaussian should be similar. This 'grouping' the FWHM for the three curves reduces the number of fitting parameters. Furthermore, since the data shows is already background corrected we can fix the 'background' fitting parameter to zero, reducing further the number of fit parameters.

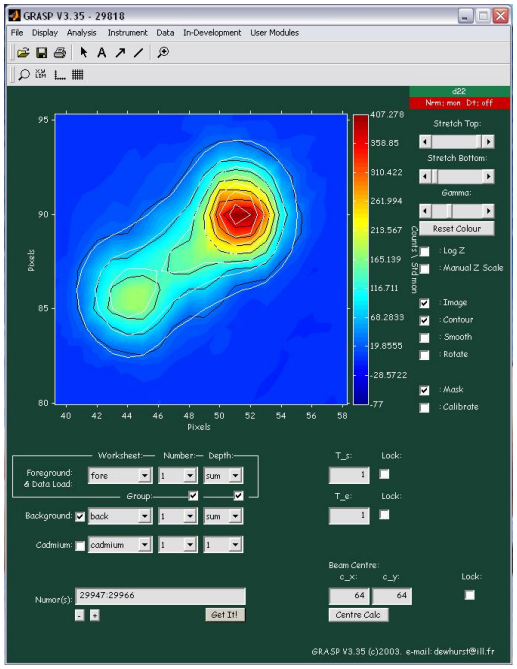
1 Select the Function type and number of functions to be fitted. Three simultaneous 2D Gaussian's with Polar Symmetry has been selected.

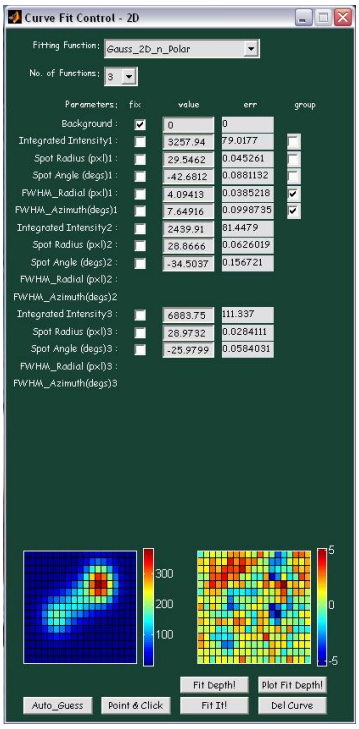
2 The starting parameters for the curve fit should either entered directly into the parameters edit boxes or chosen manually by clicking around particular points of the data to be fitted.

3 Click the 'Fit It!' button to start the fit. The final fit parameters are returned in the parameters edit boxes alongside their error. The Matlab™ edit window scrolls more detailed information from the mflsqr.m minimisation function including the chi-squared, number of iterations etc.

4 The resulting 2D curve fit is plotted on top of the original data as a contour plot.

5 The error map shows that, in this example, three simultaneous 2D Gaussian curves make a good fit to the data. This is apparent from the error map that now displays a much 'flatter' profile and therefore a much closer agreement with between the fit and the real data.





For more complicated curve fitting examples, the final fit result may need to be carefully approached by selective minimisation of different parameters or groups of parameters at one time. Use the 'Fix' and 'Group' parameters options in the curve fit control window to fix constant, or group parameters of a similar type together.

Accessing *GRAS$_{ans}$P*'s Fit Parameters in Matlab™

The results from the last curve fit procedure can be accessed either on the Matlab™ command line, standard Matlab™ '.m' routines or user modules though the *GRAS$_{ans}$P* global variable structure 'fit_parameters'. 'fit_parameters' is a structured array with fields:

fit_parameters.name	[char]	Function name
.pnames	[char]	Parameter names
.params	[double]	Fit Parameters
.error	[double]	Fit Parameters Error
.err_non_cov_check	[double]	Fit Parameters Error

To access 'fit_params', declare it as 'global' in your programs.

Writing Fit Functions for *GRASansP*

Users of the Matlab™ version of *GRASansP* (not runtime compiled version) can write their own 1D or 2D curve fitting functions to suit their own particular analysis needs. The fit function should be written in the same manner as the example presented and described below. These should then be placed in the 'grasp/fit_functions/functions/' or 'grasp/fit_functions/functions2D/' depending upon wither they are to be used by the 1D or 2D fitting routine respectively. *GRASansP* will automatically pick-up the new functions and add them to the function menu in the curve fit window. Common and useful fitting functions should be submitted to dewhurst@ill.fr for permanent inclusion in future versions of *GRASansP*.

Principles of the Function Program

GRASansP fit functions perform two important roles: The first is to calculate *y*-data for a given array of *x*-data according the fit function formula and the input parameters. This is used by the 'mf_lsqr.m' minimisation routine during the actual fit process. Once the fit is complete the function is re-called with the *x*-data and final fit parameters such that a plot of the fitted function can be created. The second role of the fit function is to contain routines dedicated to the guessing of initial fit parameters. Clearly, in order to guess fit parameters the function must be provided with both the real x and y data. Using this, a guess of the starting parameters can be made tailored to the details of the fitting function.

Multiplicity of Functions

Most functions currently provided with *GRASansP* aim to include a 'multiplicity' option such that many functions of the same type can be fitted simultaneously to a data set, as shown in the examples above. The multiplicity factor ('Number' in the example below.) is contained in params(1) and is not actually a fit parameter and as such is not varied during the minimisation process. The function parameters follow, and contain the once-only parameters first ('Number' and 'Background' in the example below) followed by parameters that are repeated for multiple functions ('Integrated Intensity1','Centre1', 'FWHM1', 'Integrated Intensity2', 'Centre2' ….etc.). The parameters array is then extended by a list of flags (0's or 1's) that determined whether certain parameters are grouped. Grouped parameters are copied from the first position where they occur in the 'params' array to the other equivalent positions.

Example: *GRAS$_{ans}$P* (modified Mfit) Fitting Function

```
function [y, name, pnames, pin]=gauss_n(x,p, flag, ydat)
% gauss_n     : Multiple Gaussian
% [y, {name, pnames, pin}]=gauss_n(x,p, {flag}, ydat);
% GRASP Gaussian fitting function (Modified from MFIT)
% p = [number Background Amp1 Centre1 Width1 etc.....]
% Author:  MZ <mzinkin@sghms.ac.uk>
% Modified: by Chuck (dewhurst@ill.fr) 4/5/00

%***** Function Name, as will be reported in 'name'; *****
name='Gaussian_n';

%***** Function Parameter Names, as reported by pnames *****
pnames = str2mat('Number','Background');
for n = 1:p(1);
   ns = num2str(n);
   pnames = str2mat(pnames,['Integrated Intensity' ns],
            ['Centre' ns],['FWHM' ns]);
end

%***** Check to: Use function or Guess Initial params *****
if nargin==2;

   %***** Use the formula to generate Gaussians from x data *****

   %***** Copy primary parameters to secondary position *****
   param_off_set = 2;
   param_repeat_unit = 3;

   no_params = size(pnames);
   for n = 1:no_params(1);
      if p(no_params(1)+n) == 1
         for m =1:p(1)
            p(n+((m-1)*param_repeat_unit)) = p(n);
         end
      end
   end

   %***** This is the Gaussian function: *****
   %y = y0 + [I / (fwhm*sqrt(pi/2) / sqrt(log(4)))] *
              exp((-2(x-xc)^2)/(fwhm^2/log(4)))

   %***** Loop and add n Gaussian Functions together *****
   y = p(2); %Background
   for n = 0:(p(1)-1)
      y = y + (p(3+n*3)/(p(5+n*3)*sqrt(pi/2)/(sqrt(log(4)))))
              *exp(-2*((x-p(4+n*3)).^2)/((p(5+n*3).^2)/log(4)));
   end

else

   %***** If 'flag' parameter is provided guess parameters *****

   %flag = 1 :  Computer 'intelligent' guess at params
   if flag==1
      if p(1) ~=1 %number of functions in the fit.
         disp('Auto Parameters Only works for a single Gaussian');
         flag = 2; %i.e. go to manual select
      else
         [amp i_amp] = max(ydat); %Peak Intensity
         cen = x(i_amp);          %Centre Position
         bg = min(ydat);          %Background
                                  %Width estimation fwhm
         half_height = (amp - bg)/2; %Half height of data
         i_y = find(ydat > half_height); %Find indices >fwhm
         xmin = x(i_y(1)); xmax = x(i_y(length(i_y)));
         width = (xmax - xmin)/2;

         %Put estimated parameters into the output array.
         pin=[p(1) bg amp cen width];
      end
   end
```

Function declaration

x = x-data array
p = function parameters
flag = determines the job to, i.e. fit or guess params.
ydat = y-data array, used only for guessing params.

Function Name

Parameter Names
1-only params
repeated params

Generate Gaussian from x-data

Number of 1-only params
Number repeated params

Copy any grouped params into the correct repeated position.

******* THIS IS THE GAUSSIAN FUNCTION *******

Loop and add n functions together.

Guess or Click-Enter Starting Parameters

Auto computer guess

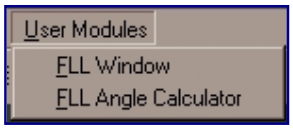
```
   %flag = 2 :  Point and click Option
   if flag==2

      %Grasp Text Message
      text_handle = message(['Click on Background'],1,'sub');
      [x bg]=ginput(1); %Mouse input
      delete(text_handle);
      pin = [p(1) bg];

      for n = 1:p(1)
         text_handle = message(['Click on Peak No. '
                       num2str(n)],1,'sub');  %Grasp Text Message
         [cen amp]=ginput(1); %Mouse input
         delete(text_handle);

         %Grasp Text Message
         text_handle = message(['Click on Width No. '
                       num2str(n)],1,'sub');
         [width y]=ginput(1); %Mouse input
         delete(text_handle);

         width=abs(width-cen);
         amp=amp-bg;

         %Put estimated parameters into the output array.
         pin=[pin amp cen width];
      end
   end
end
```

Point and Click Option

End

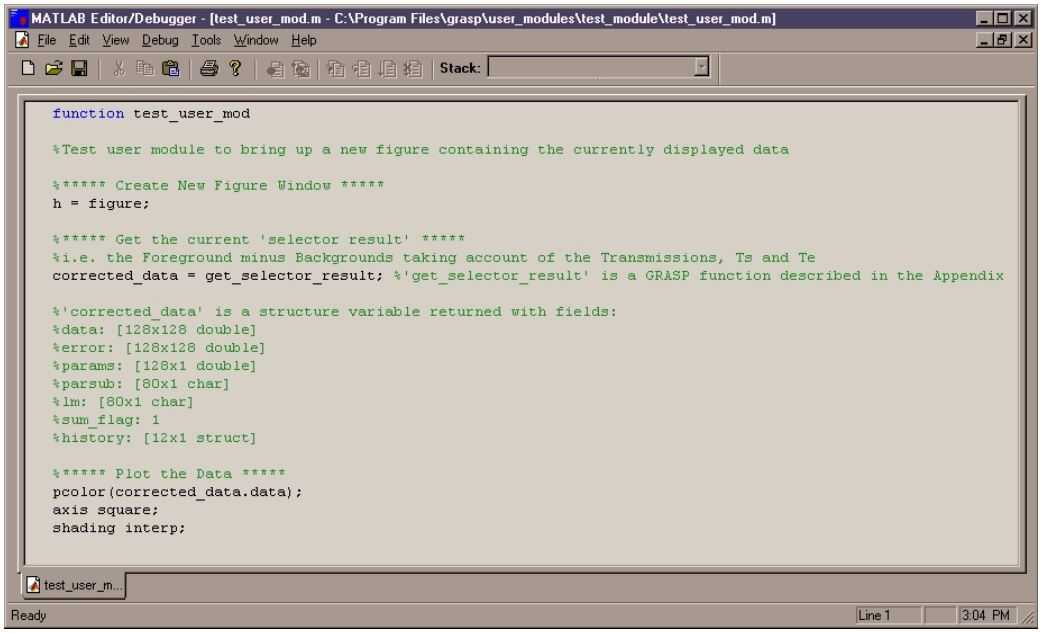
User Modules

User modules allow *GRASansP* users to develop their own functions, modules, control windows etc. and have the callback for execution to be added to the main *GRASansP* interface (Matlab™ version only, i.e. not runtime version ….since it is already compiled…obviously!). Creating user modules is simply a matter of writing standard Matlab™ code. An edit is then made to the 'grasp\usermodules\usermodules.m' file to add a description of the file and it's location. Upon launching *GRASansP* a menu item is added to the *GRASansP* 'user modules' menu bar. Many *GRASansP* global variables and important functions and available to grasp developers either at the Matlab™ command prompt or declared within user '.m' files. These are tabulated in Appendix 3.

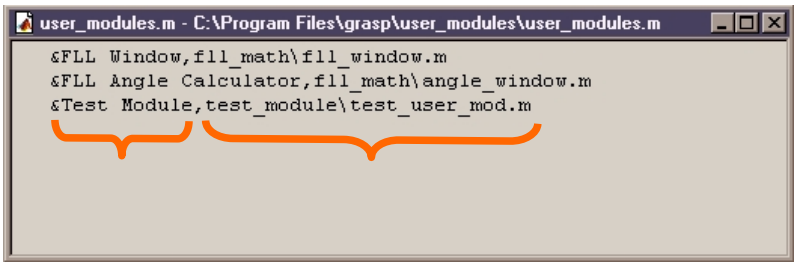


Example: Creating a *GRASPansP* User Module

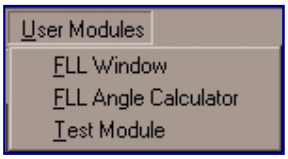
1 Write the user module e.g. 'test_user_mod.m': The example below re-displays the main image in a separate figure window.



2 Edit the 'user_modules.m' description file to *GRASansP.* The first part before the comma is the name of the user module as it will appear in the *GRASansP* user module menu. The second part after the comma is the path and filename to the user module Matlab™ '.m' file.



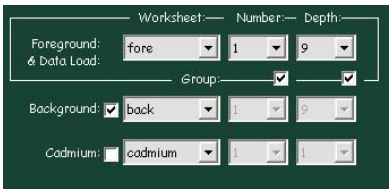
3 Restart *GRASansP* and the new user module 'Test Module' now be available from the user modules menu.

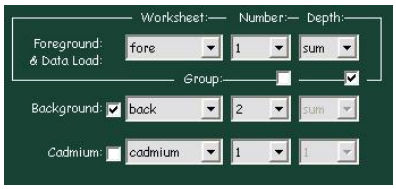


Managing the Data Workspace

Grouped Worksheets & Depths

Below the 'Foreground & Data Load' selector are two checkboxes, 'Group Number' and 'Group Depth'. These perform an important and commonly used data grouping procedure and are enabled in *GRAS$_{ans}$P* by default. With the 'Number Group' checkbox ticked all worksheet numbers are grouped together such that the Background and Cadmium 'Number' selectors are disabled and automatically follow the Foreground Worksheet Number. Likewise, with the 'Depth Group' checkbox ticked, all worksheet depths are grouped and are controlled only by the Foreground Worksheet Depth. If the Group checkboxes are un-ticked, then the relevant Number or Depth selectors are enabled and can be toggled independently to allow subtractions of different worksheets or worksheet depths.

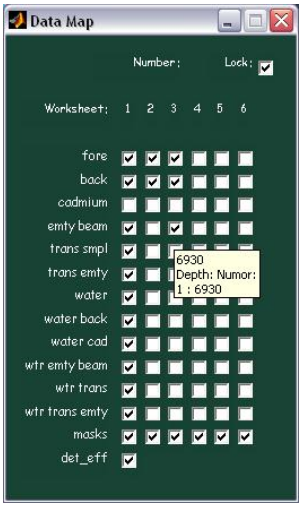




Data Map

To keep track of the many data run numbers, Sample Scattering, Backgrounds, Transmission measurements, etc. loaded into *GRAS$_{ans}$P* the 'Data Map' gives a visual representation of which workspaces have been filled with data. Holding the mouse over each of the checked elements displays a tool tip containing the run number(s) contained within the worksheet and the organisation of the worksheet depth.

If the 'Lock' checkbox in the top right hand corner is un-checked, then workspaces can be cleared selectively by un-checking the relevant checkbox.



Run Number Load Deliminators

'>' Sum run numbers between given range. The resulting summed data is stored in 'Depth 1' with an equivalent copy stored in the 'Depth Sum'.

e.g. 90125>90130

Depth:	Numors
1	90125>90130
Sum	90125>90130

':' Store run numbers between given range incrementally in the worksheet Depth. The individual data files are stored in the worksheet Depths from 1 to *n*. A sum of the data is stored in the worksheet 'Depth Sum'.

e.g. *90125:90128*

Depth:	Numors
1	90125
2	90126
3	90127
4	90128
Sum	90125>90128

'+' Sum individual run numbers. The resulting summation is stored in 'Depth 1' with an equivalent copy stored in the 'Depth Sum'.

e.g. *90125+90126+90128*

Depth:	Numors
1	90125+90126 +90128
Sum	90125+90126 +90128

',' Store individual run numbers incrementally in the worksheet Depth. The individual data files are stored in the worksheet Depths from 1 to n. A sum of the data is stored in the worksheet 'Depth Sum'.

e.g. *90125,90130,90133*

Depth:	Numors
1	90125
2	90130
3	90133
Sum	90125+90130 +90133

'(n;s)' *n* sequential run numbers with a step *s* from and including the starting run number are summed and stored in the worksheet 'Depth 1' and 'Sum'.

e.g. *90125(3;2)*

Depth:	Numors
1	90125+90127 +90129
Sum	90125+90127 +90129

'{n;s}' *n* sequential run numbers with a step *s* from and including the starting run number are stored incrementally in the worksheet Depths form 1 to *n*. A sum of the data is stored in the worksheet 'Depth Sum'.

e.g. *90125{3;2}*

Depth:	Numors
1	90125
2	90127
3	90129
Sum	90125+90127 +90129

Combination of Load Deliminators

The run number load delimiters described above can be used in succession and in multi-combination to load a mixed series of measurements.

e.g. *90125>90130,90135>90140,90145>90150*

Each group of 5 run numbers would be summed with each summed group placed in Depth 1, 2 and 3.

Depth:	Numors
1	90125>90130
2	90135>90140
3	90145>90150

e.g. *90125:90128,90135:90138*

Each group of run numbers is stored incrementally in the Depth between the limits either side of the '**:**' deliminator.

Depth:	Numors
1	90125
2	90126
3	90127
4	90128
5	90135
6	90136
7	90137
8	90138

e.g. *90125+90127,90130:90135,90140>90142*

Each group of run numbers, separated by '**,**' will be placed into a separate Depth along with run numbers ranges within the '**,**' containing '**:**' that also instruct incremental loading of data into the Depth.

Depth:	Numors
1	90125+90127
2	90130
3	90131
4	90132
5	90133
6	90134
7	90135
8	90140>90142

e.g. *90125{3,2},90150{3,4}*

The second value within the brackets represents a 'skip' parameter. Thus, three run numbers, starting at 90125 and skipping every other run number will be stored in separate depths 1-3. A further three run numbers, starting at 90150 and taking every fourth run number will then be stored in separate depths 4-6.

Depth:	Numors
1	90125
2	90127
3	90129
4	90150
5	90152
6	90154

Details of Analysis Procedures and Algorithms

Data Correction: Subtraction of sample backgrounds and correction for sample transmission factors.

General Formula:

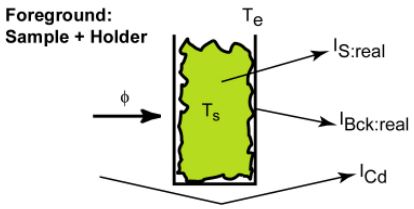
A general formula for correction of scattering for background scattering and cadmium background effects can be expressed as:

$$I_{Corrected} = \frac{1}{T_s T_e}[I_s - I_{Cd}] - \frac{1}{T_e}[I_{Bck} - I_{Cd}]$$

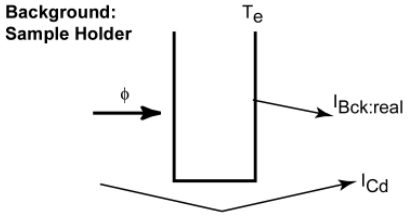
where $I_{Corrected}$ is the corrected sample scattering, I_s is the measured sample scattering, I_{Bck} is the measured background scattering, I_{Cd} is the cadmium background and T_s and T_e are the transmissions of the sample and sample holder. A wide range of experimental measurement procedures can all be corrected by this single general formula as described below:

Example: Sample, Sample Holder, with Removal of Sample for Background Measurement.

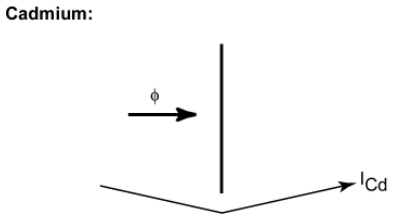
$$I_s = T_s T_e I_{s:real} + T_s T_e I_{Bck:real} + I_{Cd}$$



$$I_{Bck} = T_e I_{Bck:real} + I_{Cd}$$



$$I_{Cd}$$



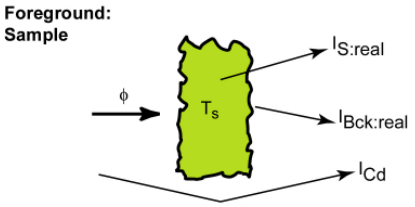
This is the most common situation for SANS measurements. A sample of transmission T_s is contained in a sample holder (e.g. Hellma cell) of transmission T_e. Measurements of the sample scattering, I_S, and background scattering, I_{Bck}, are made along with the cadmium background, I_{Cd}. The corrected sample scattering is given by the formula below, identical to the general formula.

$$I_{Corrected} = I_{S:real} = \frac{1}{T_s T_e}[I_s - I_{Cd}] - \frac{1}{T_e}[I_{Bck} - I_{Cd}]$$

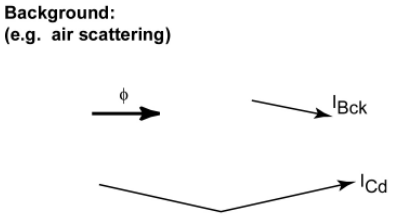
Summary: For this kind of analysis in *GRAS$_{ans}$P* load the foreground, background and cadmium measurements and calculate the sample and sample holder transmissions.

Example: Sample, No Holder, with Removal of Sample for Background Measurement.

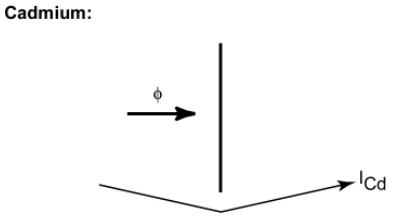
$$I_s = T_s I_{s:real} + T_s I_{Bck:real} + I_{Cd}$$



$$I_{Bck} = I_{Bck:real} + I_{Cd}$$



$$I_{Cd}$$



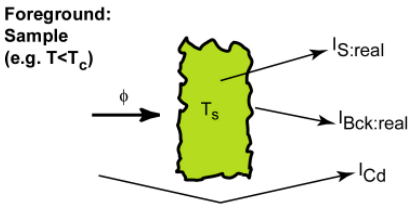
Here, a sample is placed in the neutron beam without being contained in a sample holder of any kind. For example, an under-illuminated freestanding solid sample. The background contribution to the measured sample scattering, I_{Bck}, is likely to be very small since a background is measured with the sample removed. Any residual background scattering may come, for example, from air scattering etc. combined with the cadmium background noise. We can still attempt to correct for these two rather small backgrounds given by the equation below:

$$I_{Corrected} = I_{S:real} = \frac{1}{T_s}[I_s - I_{Cd}] - [I_{Bck} - I_{Cd}]$$

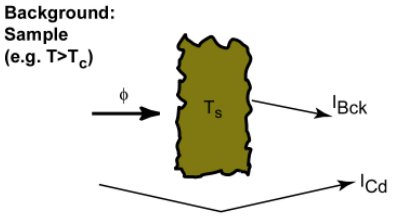
Summary: For this kind of analysis in *GRAS$_{ans}$P* load the foreground, background and cadmium measurements and calculate the sample transmission, T_s. Set the empty cell transmission value, T_e, equal to 1.

Example: Sample (with or without Holder), with non-removal of sample for background measurement. E.g. Magnetic scattering in a state $T<T_c$ that is completely absent in the state $T>T_c$.

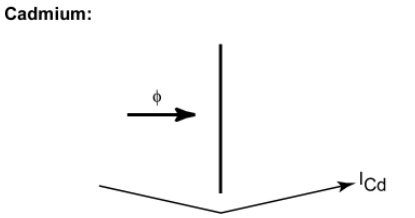
$$I_s = T_s I_{non-mag} + T_s I_{mag} + T_s I_{Bck:real} + I_{Cd}$$



$$I_{Bck} = T_s I_{non-mag} + T_s I_{Bck:real} + I_{Cd}$$



$$I_{Cd}$$



Here, the sample remains in the neutron beam for both the foreground and background scattering measurements. In the magnetic state the measured sample scattering consists of a nuclear non-magnetic part, $I_{non-mag}$, and a magnetic part, I_{mag}, as well as the usual background contributions. A background measurement is made with the sample still in the neutron beam but above the transition temperature, T_c. The formula for background correction in this case becomes:

$$I_{mag} = \frac{1}{T_s}\left[I_2 - I_{Bck}\right]$$

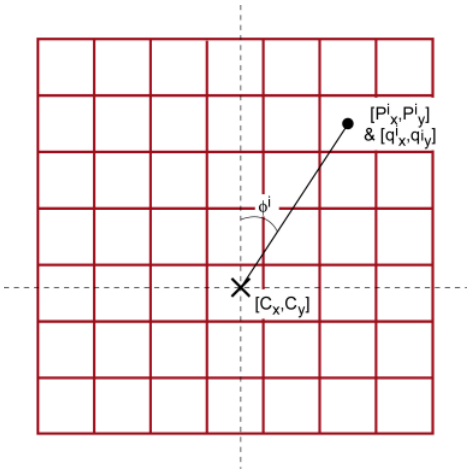
In other words, measurement of a cadmium background is not necessary!. In fact, in this case the physical sample can be considered as the 'sample holder' for the magnetism. Thus, the physical sample transmission should be used as the sample holder transmission, T_e, in *GRAS$_{ans}$P*. The transmission of the magnetic structure within the physical sample is assumed to be 1.

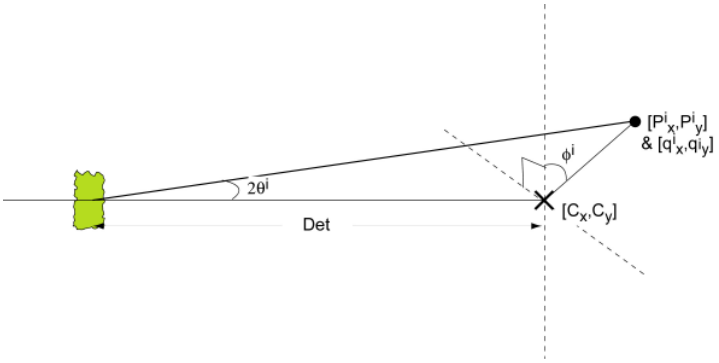
Summary: For this kind of analysis in *GRAS$_{ans}$P* load the foreground and background measurements. The physical sample transmission should be calculated and placed into T_e NOT T_s. Set T_s equal to 1.

Dealing with Pixelated Data

Definition of $|q|$, q_x, q_y and pixel-ϕ

Each data element or pixel, P^i, in the multi detector data array is allocated a q^i_x, q^i_y, $|q^i|$ and angle ϕ^i to the vertical, defined from the beam centre to the centre of pixel P^i.





Equations

Scattering angles:

$$\tan\theta^i_x = \frac{P^i_x - C_x}{Det} \qquad \tan\theta^i_y = \frac{P^i_y - C_y}{Det}$$

q's:

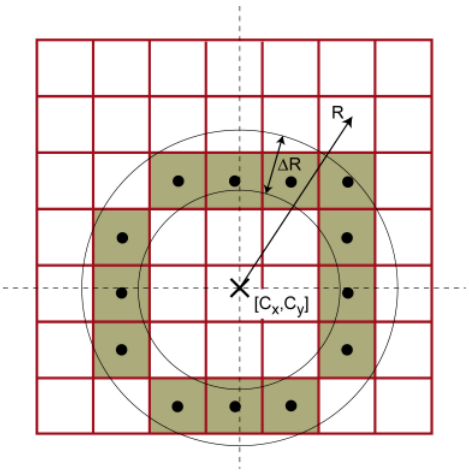
$$q^i_x = \frac{4\pi}{\lambda}\sin\theta^i_x \qquad q^i_y = \frac{4\pi}{\lambda}\sin\theta^i_y \qquad \tan\theta^i_x = \frac{P^i_x - C_x}{Det}$$

Pixel angle (from vertical):

$$\tan\phi^i = \frac{P^i_x - C_x}{P^i_y - C_y}$$

Radial Average

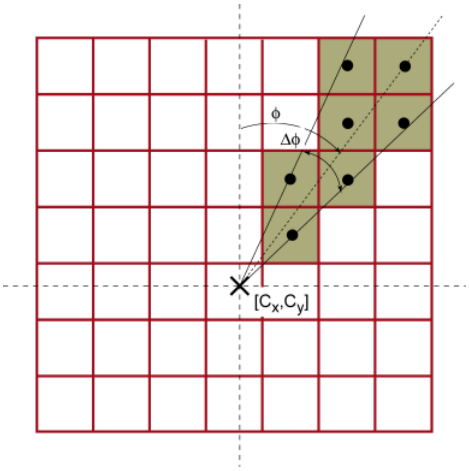
Where $[C_x,C_y]$ is the beam centre, and ΔR is the radial 'bin' step over which q-values are averaged at a given pixel radius R from the beam centre.



$$I_{|q|} = \frac{\left(\sum_{\text{Pixels within ring of constant } |q|} I\right)}{\text{Number of Pixels}}, \qquad Error\_I_{|q|} = \sqrt{I_{|q|}}$$

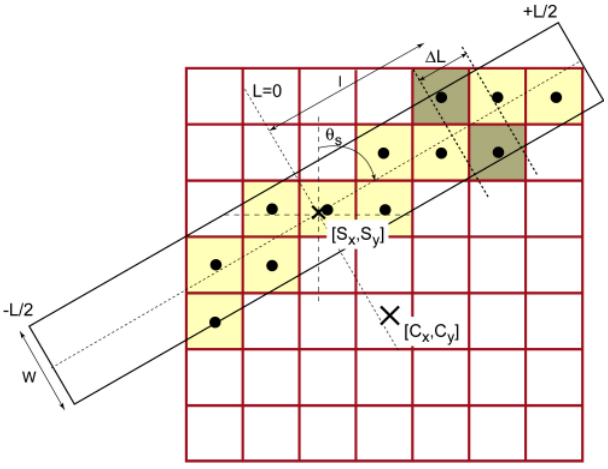
Azimuthal Average

Where $[C_x,C_y]$ is the beam centre, and $\Delta\phi$ is the azimuthal 'bin' step over which pixel intensities and their actual pixel angle, ϕ^j, values are averaged at a given angle ϕ from the beam centre.



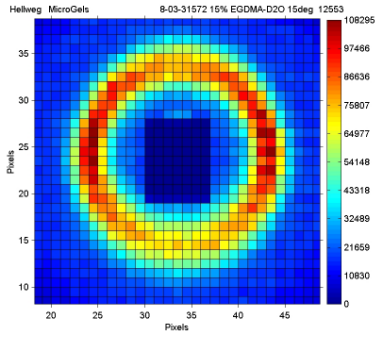
Strip Average

Where $[C_x,C_y]$ is the beam centre, $[S_x,S_y]$ is the strip centre, L is the strip length, W is the strip width and ΔL strip 'bin' step over which pixel intensities and their distance to the strip centre-line values are averaged at a given length, l, from the strip centre.

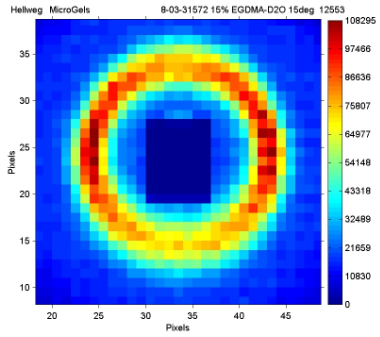


GRAS$_{ans}$P Interface, Graphics and Menus

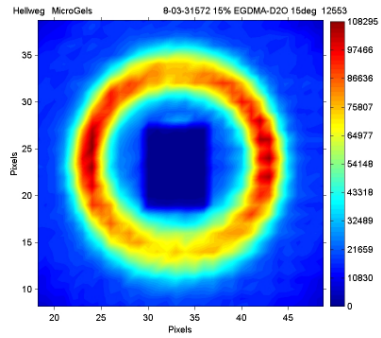
Image Render: (Matlab™ Pcolor Image properties)



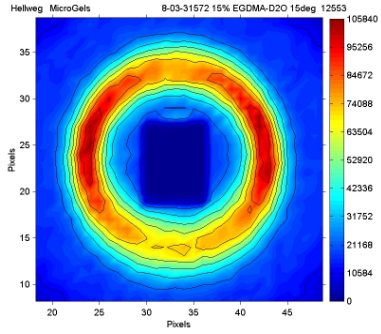
'faceted'



'flat'



'interpolated'



'interpolated + contour'

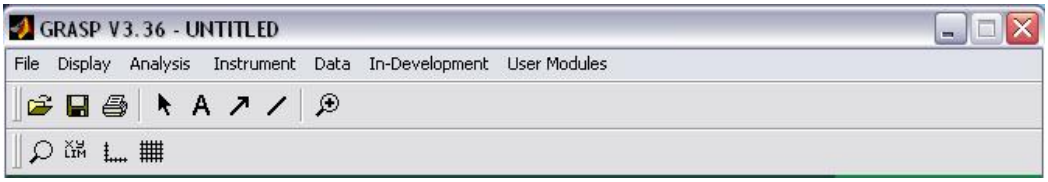
Display Control

- **Log Z:** Displays intensity data on a log10 intensity scale.
- **Manual Z Scale:** Allows entry of manual intensity scale limits.
- **Image:** Matlab™ Pcolor surface data display.
- **Contour:** Matlab™ Contours data display.
- **Smooth:** Apply box smooth convolution.
- **Rotate:** Rotate main image by a given angle.
- **Mask:** Apply bad-data and instrument mask.
- **Calibrate:** Enable calibration options, e.g. volume, solid angle, flux, calibration standard corrections.

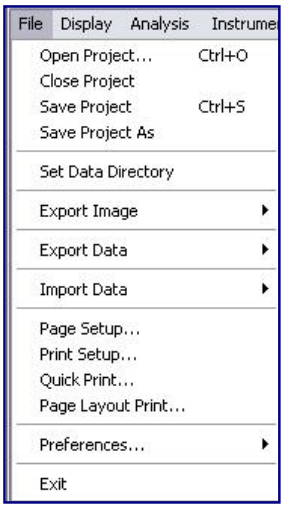
Colour Control

- **Stretch Top:** Modify the value at which the displayed data reaches the top colour of the colour map. (Used to enhance colour contrast for data well below the peak value).
- **Stretch Bottom:** Modify the value at which the displayed data reaches the bottom colour of the colour map. (Used to enhance colour contrast for data well above the minimum value).
- **Gamma:** Modify the manner in which the colour map is distributed across the range of z-values.
- **Reset Colour:** Resets the Colour Control Sliders to their default positions.

Menu Items

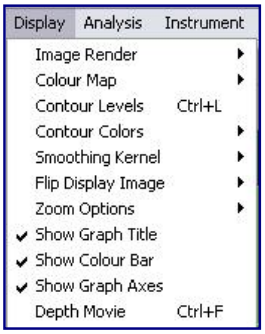


File Menu



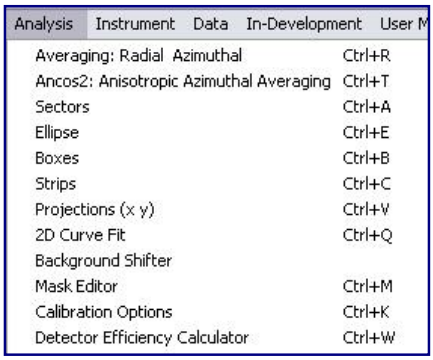
- **Open** / **Save** / **Close** *GRAS$_{ans}$P* projects.
- Set SANS Raw **Data Directory**.
- **Export** main display **image** as: Bmp, Jpg, Tiff, Eps, Adobe Illustrator.
- **Export Data:** Corrected 2D data, Mask files.
- **Page Setup:** Modify the position of the Export graphics on the page.
- **Print Setup:** Select Current Printer etc.
- **Quick Print:** Print main display image.
- **Page Layout Print:** Prepares layout page including main display image, summary of data parameters, analysis processes and parameters and any curve fit parameters.
- **Preferences:** Options to modify font, font size, line width and style.

Display



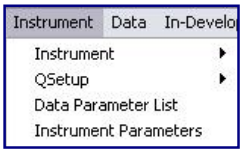
- **Image Render:** Flat (Pixelated), Interp (Interpolated Display), Faceted (Pixelated + Pixel facets).
- **Colour Map:** Choice of Standard Matlab™ Colour Maps, including options to reverse and flip the RBG colour map.
- **Contour Levels:** Auto / Manual contour options between given limits in either Absolute or Percent values.
- **Contour Colours**
- **Smoothing Kernel:** Box Kernels of 3x3, 5x5 & 7x7.
- **Zoom Options:** Manually set axes, Force Square Zoom: i.e. 1:1 aspect ratio based upon the largest of the axis dimensions.
- **Show Graph Title**
- **Show Colour Bar**
- **Show Graph Axes**
- **Depth Movie:** Generate a movie of the data files contained within the current worksheet depth.

Analysis



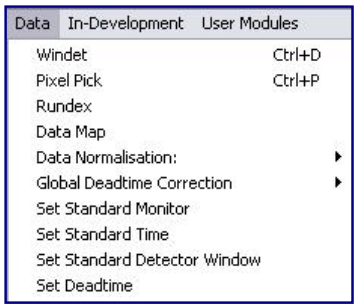
- **Averaging:** Radial and Azimuthal averaging.
- **Ancos2:** For magnetic Scattering.
- **Sectors:** Define sectors of multi detector data.
- **Elipse:** Define ellipse areas of multi detector data.
- **Boxes:** Define box areas of multi detector data.
- **Strips:** Define strip areas of multi detector data.
- **Projections(xy):** Vertical (y) or horizontal multi detector averaging.
- **2D Curve Fit:** Fit 2D functions to areas of multi detector data.
- **Background Shifter:** Allows subtle shifting of background relative to foreground data by fractions of a pixel. Also includes foreground-to-background minimisation routine.
- **Mask Editor:** Edit bad data masks.
- **Calibration Options:** Opens the calibration control window.
- **Detector Efficiency Calculator:** Analysis calibration data to determine detector efficiency map and calibration scalar.

Instrument



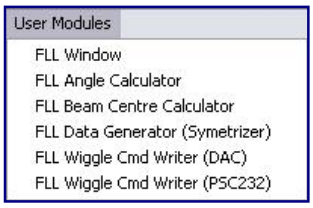
- **Instrument:** Select instrument corresponding to data to be analyzed. e.g. D11, D22, D16, SINQ_SANS_I etc.
- **QSetup:** Choose to use detector distance or detector distance + table offset to calculate *q*.
- **Data Parameter List:** Displays name and position of the parameters in the data file.
- **Instrument Parameters:** Displays characteristic parameters of the instrument. e.g. Allowed collimation values, attenuation factors and calculates relative flux decreases as a function of collimation.

Data



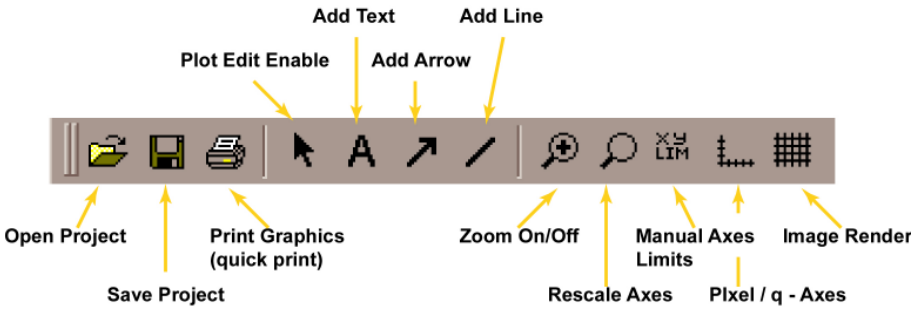
- **Windet:** Display listing of raw detector counts for the current displayed foreground.
- **Pixel Pick:** Allows pixel or groups of pixels values to be monitored by clicking or dragging over an area of the main display.
- **Rundex:** Produce a tabulated listing of Run Number, Title, User, and any one of the 128 data file parameters for data file.
- **Data Map:** Displays a map of the *GRAS$_{ans}$P* workspace and current data filling status.
- **Data Normalisation:** Choose from Standard Monitor (10 000 000 default), Standard Time (100 s default) or Absolute Counts (None).
- **Global Dead Time Correction:** Enable / Disable dead time corrections to all data.
- **Set Standard Monitor**
- **Set Standard Time**
- **Set Standard Detector Window:** Set the window area coordinates for detector counts normalisation.
- **Set Deadtime:** Set detector dead time for the current instrument.

User Modules



- User written modules and *GRASansP* routines appear here once registered in the user_modules.m description file.

Tool Bar

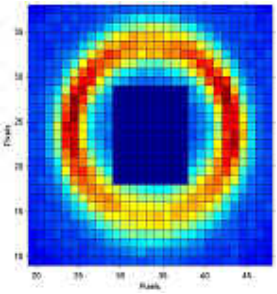


Data Analysis Examples

Example 1: Solution Scattering: e.g. Colloidal Nano-Particle Crystals

Experimental Data to be downloaded from www.ill.fr/lss/grasp/example1.html

Aims



- Combination of measurements at several *q*-ranges and instrument settings.
- Absolute calibration of scattered intensity.

Experiment Overview

- Instrument: D11
- Detector distances of: 2m, 8m, 36m
- Collimation distances of: 2m, 8m, 36m
- Wavelength: 10 angstroms
- *q*-ranges: 0.11 to 0.022, 0.033 to 6*10-3, 8*10-3 to 8*10-4

Scattering Measurements

Scattering	Sample	Empty Cell	Cadmium
2m	#6923	#6927	#6929
8m	#6918	#6922	----
36m	#6907	#6911	----

Transmission Measurements

Transmission	Sample	Empty Cell	Direct Beam
2m	----	----	#6930
8m	----	----	(missing)
36m	#6912	#6916	#6917

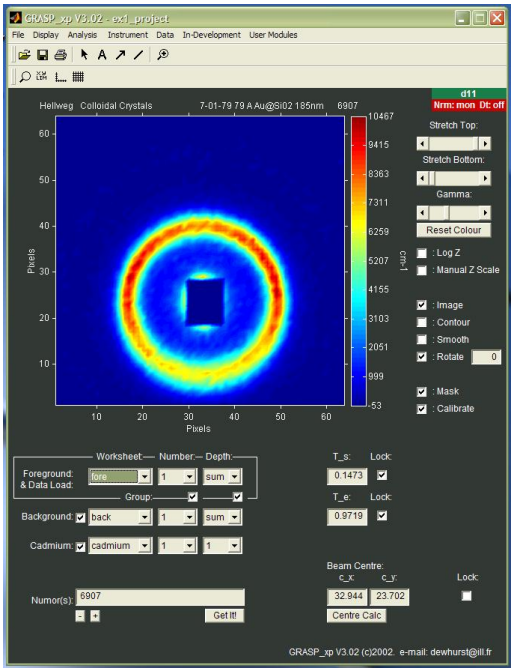
Calibration Measurements

	Water	Empty Cell	Cadmium/DB
Scattering 4m	#6901	#6902	#6903
Transmission	#6904	#6905	#6906

Data Reduction and Analysis Overview

1 Analyze the water calibration standard and calculate the detector efficiency map and calibration scalar.

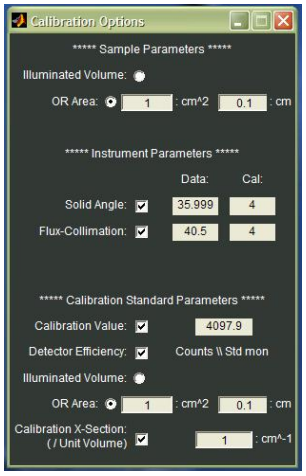
2 Load the sample data into the allocated workspaces. e.g. Load sample scattering, background and cadmium background into the allocated <fore>, <back> and <cadmium> worksheets. Use worksheet numbers <1>, <2> and <3> to store each data set measured at each instrument configuration i.e. 2m, 8m and 36m data.



3 Load the sample empty-beam data into the allocated workspaces. e.g. Load the empty beam data for the 2m, 8m, and 36m configurations into the <empty beam> <1>, <2> and <3> worksheets. Calculate the beam centre for each instrument configuration.

4 Load the sample transmission and empty cell transmission data into the allocated workspaces. These only needs to be measured once for each sample and does not depend on the instrument configuration used. Data can therefore be loaded into, for example, the <trans sample> and <trans empty> <1> worksheets. The sample transmission, Ts, and empty cell transmission, Te, can then be calculated. To apply these transmission values to all the data contained in all the worksheet numbers enable the 'Ts lock' and 'Te lock' check boxes.

5 Enable the required calibration options:



Solid Angle Corrections: taking into account the solid-angle subtended by each pixel in each case.

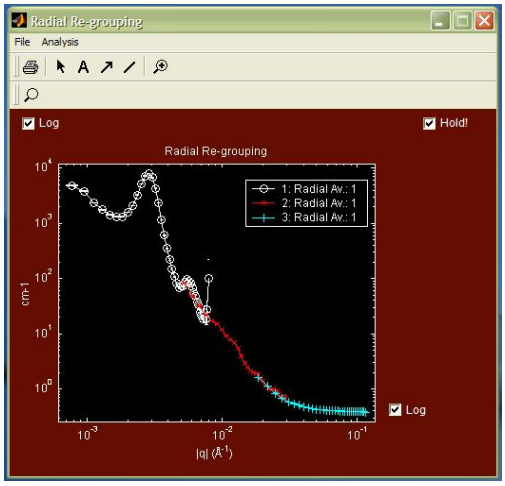
Flux vs. Collimation Corrections: taking into account the change in neutron flux at the sample position as the instrument collimation is varied to match the detector distance.

Calibration to a Known-Standard: The calibration scalar provides the relative intensity of the calibration data as measure in it's particular instrument setup.

Correcting for detector efficiency: Simply divides the scattering data by the measured detector efficiency as determined by analysis of a 'flat scatterer'. The detector efficiency has, by definition, a mean pixel value of 1 and therefore does not change the absolute intensity of the sample scattering data.

In the present example we only have one Water calibration measurement. This is even measured at a different instrument configuration to the rest of the sample scattering data. This should not matter. The Solid Angle and Flux-Collimation corrections described above should take care of all necessary data scaling.

6 Data reduction and Analysis: In this case the isotropic scattering would usually be reduced to a calibrated 1D I vs. |q| plot. Open the 'Averaging: Radial and Azimuthal' analysis window and perform an I vs. |q| operation for each of the data worksheets <1>, <2> and <3>. The resulting data can be overlaid in the same output plot by enabling the 'hold' checkbox in the output plot window.



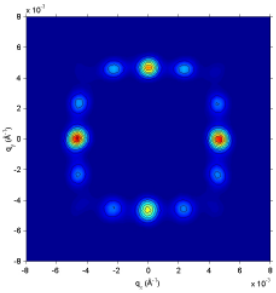
Acknowledgement

Many thanks to Thomas Hellweg for allowing this data to be used as *GRAS$_{ans}$P* example data.

Example 2: Small-Angle Diffraction: e.g. Superconducting Vortex Lattice

Experimental Data to be downloaded from www.ill.fr/lss/grasp/example2.html

Aims



- High resolution SANS measurements.
- Lattice structure, orientation and morphology.
- Rocking curves and integrated intensity and Bragg peaks.
- 2D Curve fitting.

Experiment Overview

- Instrument: D22
- Detector distance of: 17.6m
- Collimation distances of: 17.6m
- Wavelength: 10 angstroms
- Additional Entrance Aperture: Att 6 (20mm)

Vortex Lattice Scattering Measurements ($T<T_c$)

Rocking Curve Foreground: **Sample Angle from -1 to 1, step 0.1**
#88144 : #88164 (21 files)

Background Measurements ($T>T_c$)

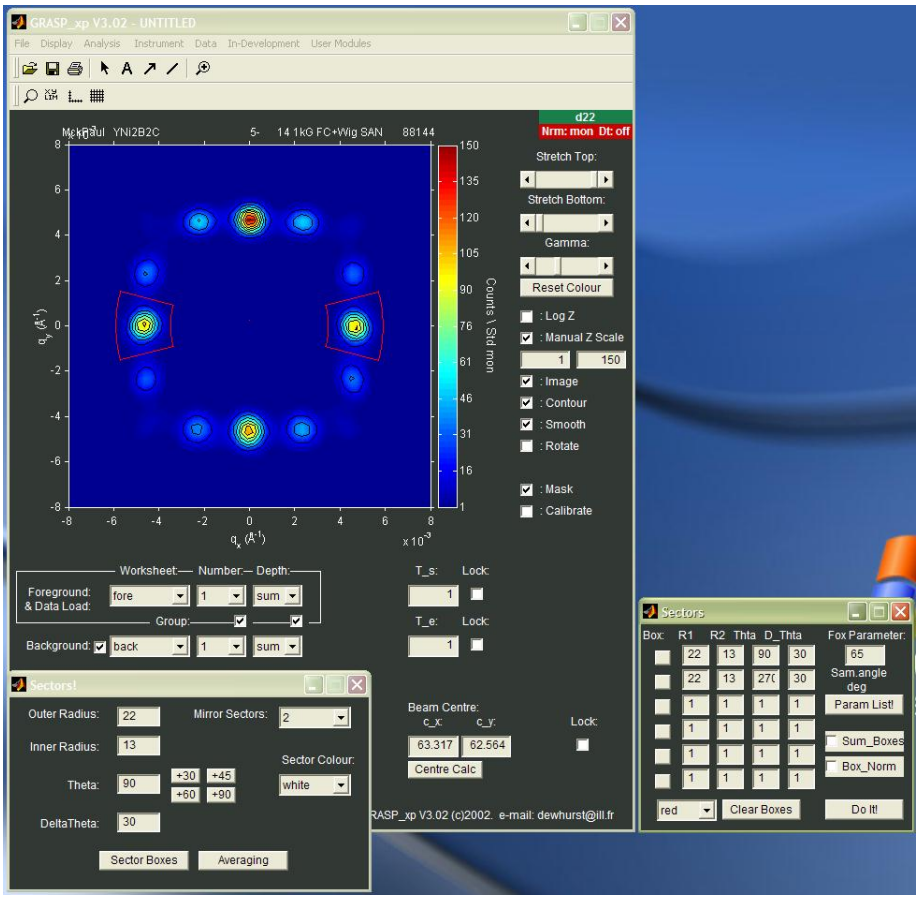
Rocking Curve Background: **Sample Angle from -1 to 1, step 0.1**
#88526 : #88546 (21 files)

Data Reduction and Analysis Overview

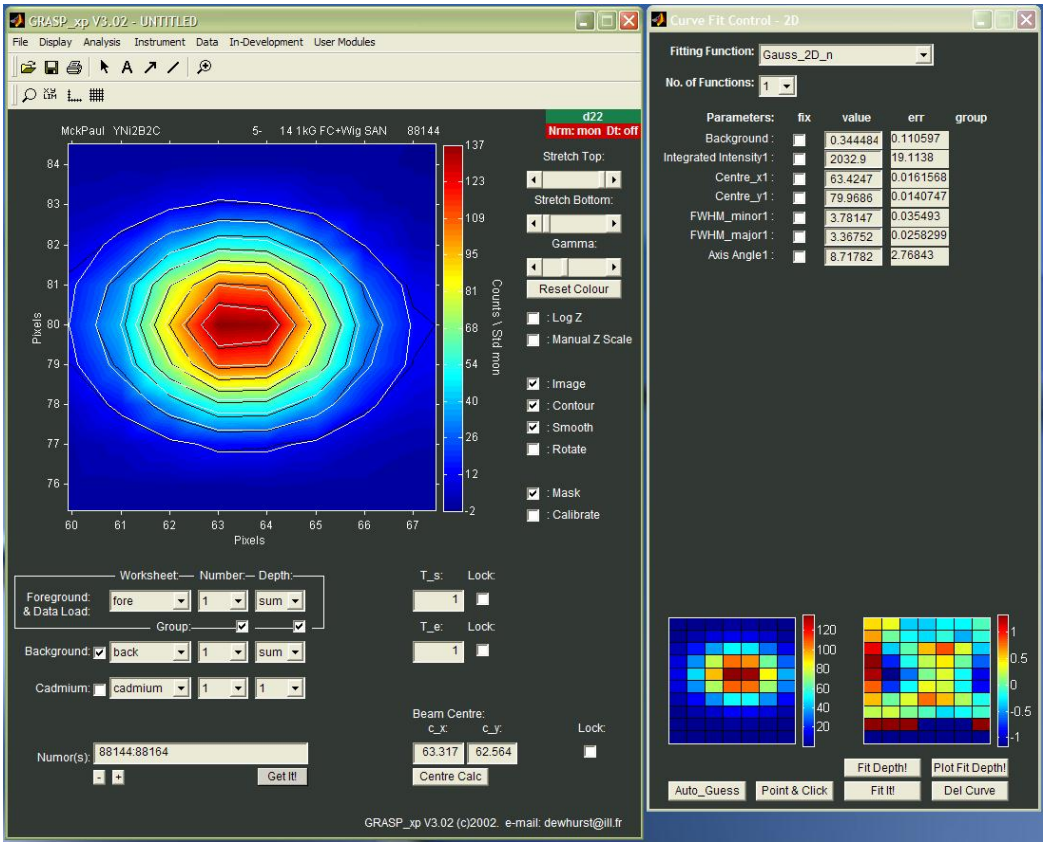
1 Load the 'foreground' scattering from the Vortex Lattice rocking curve data into the <fore> <1> workspace 'depth'. To fill load all the individual files into <fore> <1> but keep them separate for analysis as a function of sample angle use the ':' operator in the Numor Load string, e.g. '88144:88164'.

2 Load the 'background' nuclear scattering from the sample above the superconducting transition temperature, Tc. Again, the background rocking curve can be loaded into the 'depth' of worksheet <back> <1> using the ':' operator, e.g. '88526 :88546'.

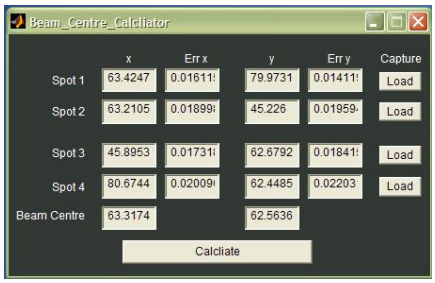
3 The resulting background subtracted image of the scattering from the Vortex Lattice can now be viewed and analyzed by selecting the worksheets to display, e.g. <fore> <1> <sum> - <back> <1> <sum>, in the worksheet selector.



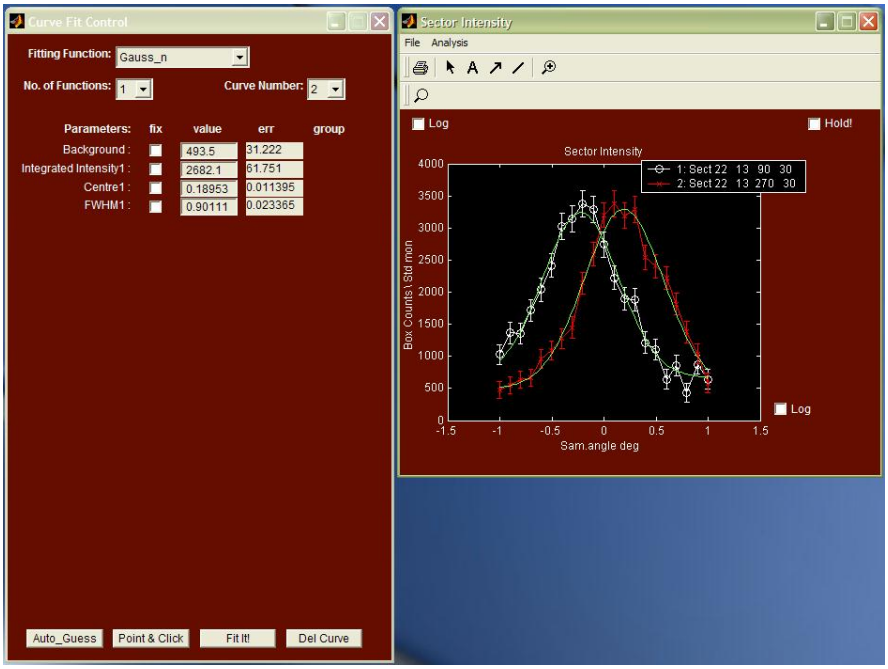
4 2D Curve Fitting Example: An accurate measure of the beam centre (centre of radial symmetry) for the diffraction image can be either measured directly by an attenuator measurement of the direct beam OR by calculation from the fitted diffraction spot positions of the symmetrical diffraction pattern. Open the 2D Curve Fitting Window and make a 2D curve fit to 2 pairs of Bragg peaks on opposite sides of the image.



5 A 'User Module' has been written to calculate the beam centre from the coordinates and pairs of Bragg peaks, assuming a symmetric diffraction pattern. Open the user module 'FLL Beam Centre Calculator'. As the Bragg peaks are fitted in turn, collect the spot co-ordinates in the beam centre calculator module. When you have fitted and collected the 2 pairs (4 spots) click 'Calculate' to calculate the new beam centre. This new value will be displayed in the user module window and also update the main beam centre value in the main display.



6 From now on, with an accurate beam centre, radially symmetric analysis operations can be reliably be performed. For example, to take a rocking curve of the two Bragg peaks on the horizontal axis, open the 'Sectors' analysis tool and place 2 opposing sectors (using the mirror tool) over the two Bragg peaks (see figure 1 above). When positioned correctly grab the sector co-ordinates using the 'Sector Box' tool, enter the data file parameter that is changing though the depth series of data (e.g. sample angle = 65, temperature = 31) and click 'Do It' to extract box intensity as a function of sample environment parameter. In the example below a rocking curve of the left and right horizontal Bragg peaks is extracted, fitted to a Gaussian function and can be printed or data exported.



Acknowledgement

Many thanks to Simon Levett for allowing this data to be used as a *GRAS$_{ans}$P* example.

Appendix 1: Input and Output Data and Graphic Formats

Support for 'gzip' Compressed Data

GRASansP offers the ability to load 'gzip' compressed data files directly without the user needing to uncompress the data prior to analysis. Compression of the ASCII raw data files makes enormous savings in disk space and is clearly an advantage when raw data is stored on the local machine. Furthermore, data stored at ILL is automatically compressed when older than 2 reactor cycles for archive on the ILL central data server. *GRASansP* can read this archived compressed data directly from the network server.

To implement compressed data compatibility in *GRASansP*, the freeware 'gzip' package must be installed on the local machine including addition of the gzip directory path to the default search path of the system. For example, on a PC, copy the 'gzip.exe' program into the system directory 'c:\windows\system'. *GRASansP* recognises compressed data by searching for the '.gz' or '.z' file extension. If a compressed file is found it is copied to a temporary file location, un-compressed and loaded into *GRASansP* before the temporary file is deleted.

To load compressed data files into *GRASansP* simply enter the run number in the data load area in the same way was for non-compressed files.

1D Data Export

Reduced 1D data can currently be exported either as an ASCII file with columns of data, for example ***q***, ***I***, ***Err_I***, with no header information for easy import into other plotting or analysis packages or as ILL standard 1D file format. From *GRASansP* use the 'File>Export Data' option.

2D Data Export

As a temporary solution to 2D data export *GRASansP* can export corrected 2D multi detector data as 'fake' ILL raw data format files. Data is actually exported as two files, the '.err' file contains the errors associated with the counts in the main file. From *GRASansP* use the 'File>Export Data' option.

Mask Files

Mask files can be Exported or Loaded into *GRAS$_{ans}$P* using the 'File>Export Data' and 'File>Import' menus from the main window. Mask files are stored, loaded and saved in the standard ILL format and offer full interchange ability with existing ILL SANS software.

Graphics File Export

Graphics from the main *GRAS$_{ans}$P* window or from the secondary 1D curve plotting window can be exported in one of the following standard graphic formats from the 'File>Export Image' menu:

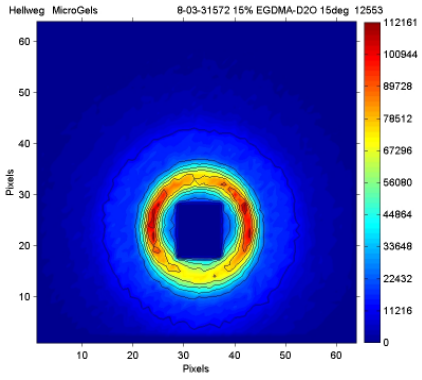
- Bmp
- Jpg
- Tiff
- Eps
- Adobe Illustrator

Printer Output Graphics

Graphics from the main *GRAS$_{ans}$P* window or from the secondary 1D curve plotting window can be printed in either one of two forms from the 'File>Quick Print' and 'File>Page Layout Print' menus.

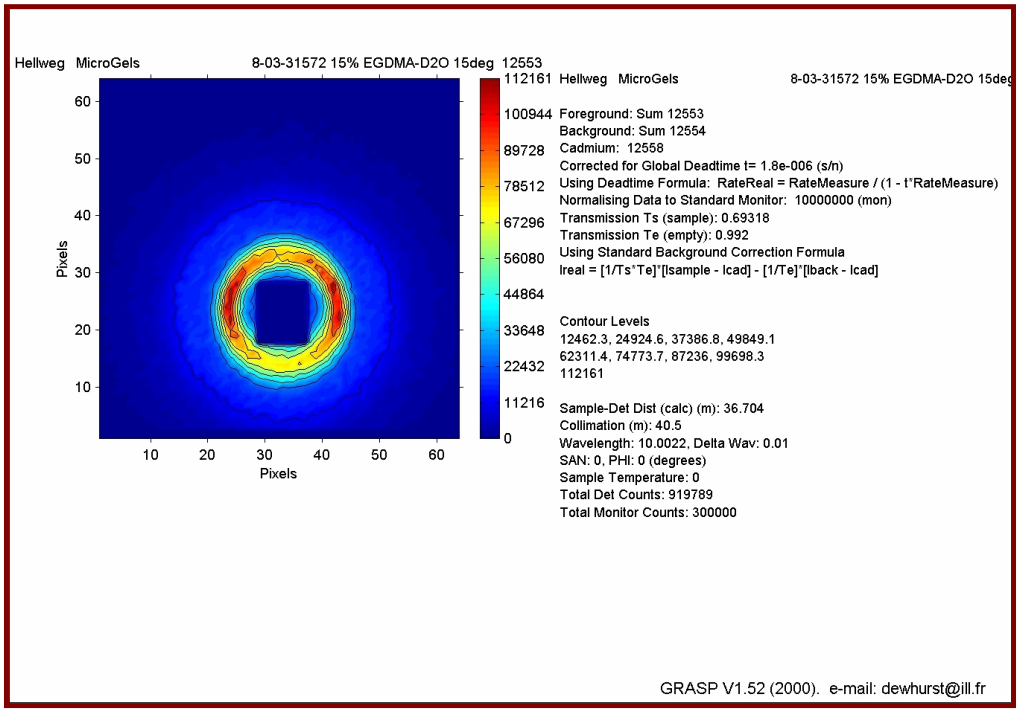
Quick Print

'Quick Print' sends only the current 2D detector image or 1D output graph to the default printer.



Page Layout Print

'Page Layout Print' prepares a layout page in a separate figure window prior to printing. The layout page includes additional details relevant to the data presented including the foreground, background and cadmium data files used, sample and holder transmissions, normalisation information, dead-time corrections, important instrument settings and a history of the data treatment process.



Appendix 2: Flux vs. Collimation Length Relative Flux

Tabulated below are values of the collimation attenuation factor (flux relative to flux @2m collimation) for both D22 and D11. To a first approximation the data follows an inverse square law expected for uniform divergence from a point source. This breaks down for long collimation lengths and long wavelengths where the neutrons parabolic flight-path (due to gravity) is blocked by the physical dimensions of the collimation tube and at short collimation lengths with small wavelengths due to the insufficient critical angle of the neutron guide.

Example: For D22, the relative flux change between 8Å, 4m and 8Å, 17.6m = 46.795 / 2.518 = 18.58. i.e. the neutron intensity at 8Å, 17.6m is 1/18.58 the intensity at 8Å, 4m.

Relative Collimation Attenuation Factors for D22.

Wavelength/ Collimation Length	5Å	8Å	10Å	14Å	17Å	20Å	25Å	30Å	35Å
2	1	1	1	1	1	1	1	1	1
2.8	1.074	1.448	1.672	1.733	1.735	1.810	1.816	1.803	1.707
4	1.398	2.518	3.050	3.175	3.203	3.336	3.269	3.445	3.185
5.6	2.213	4.654	5.876	5.859	5.931	6.167	5.883	6.428	6.035
8	4.031	9.291	11.535	11.223	11.349	11.962	11.940	12.652	11.942
11.2	7.914	18.017	22.962	21.233	21.735	22.929	22.913	24.620	23.091
14.4	14.337	31.744	41.187	38.149	37.575	36.958	36.371	40.952	41.542
17.6	21.538	46.795	57.370	61.7603	56.532	55.351	67.333	87.327	96.857

Relative Collimation Attenuation Factors for D11.

Wavelength/ Collimation Length	4.5Å	6Å	8Å	10Å	16Å	20Å	25Å
2.5	1	1	1	1	1	1	1
4	1.126	1.372	1.678	1.895	2.095	2.135	2.136
5.5	1.624	2.448	3.199	3.638	3.962	3.579	3.770
8	2.612	4.260	5.991	6.589	6.909	6.756	7.3779
10.5	3.890	6.714	8.995	9.805	11.193	11.090	12.535
13	5.960	10.213	14.709	15.485	16.929	17.229	20.272
16.5	8.311	14.905	20.376	23.003	24.245	24.539	32.107
20.5	12.083	23.340	32.304	36.507	39.200	37.860	∞
40.5	39.838	71.3438	94.320	128.544	678.550	∞	∞

Appendix 3: Notes for *GRAS$_{ans}$P* Contributors and Developers

Global Variables Available at the Matlab™ command line

Grasp System

Variable Name	Description	Type and Size	
grasp_root	Root directory where *GRAS$_{ans}$P* is installed.	String, e.g. 'c:\program files\grasp_m\'	
chuck_version	Program version number	Real	
font	Program font name	String, e.g. 'Arial'	
font_size	Program font size	Integer, e.g. 8	
background_color	Program window background color	Real [1,3], e.g. [0.2 0.2 0.2] i.e. Dark Grey	
sub_figure_background_color	Program sub-figure window color	Real [1,3], e.g. [0.4 0.05 0] i.e. Burgundy	
wks_nmbr	Number of available worksheets	Integer, e.g. 3	
wks_depth_max	Max number of worksheet depths	Integer, e.g. 50	
status_flags	Structured array containing almost all *GRAS$_{ans}$P*'s operating parameter status's and values.	**.axes**	Struct: current axes type, limits, and xy pixel mapping coordinates
		.color	Struct: colormap, stretching, gamma etc.
		.smooth	Struct: kernel name and kernel data
		.selector	Struct: values of the data selector foreground, background, cadmium
		.transmission	Struct: current transmission values and locked status
		.beamcentre	Struct: current beam centre and locked status
		.calibration	Strcut: parameters and checkbox status associated with the calibration window
		.render	Current image render type, i.e. inter, faceted, flat
		.normalization	Strcut: Normalizaton

			status
		.deadtime	Deattime correction status On/Off
		.display	Struct: Current display status, i.e. log, mask, smooth etc.
		.contour	Struct: Current contour level status, colour etc.
		.q	Flag indicating whether q-calculations should be based on detector distance or detector+table offset.

File

Variable Name	Description	Type and Size
data_dir	Directory path to data	String, e.g. 'z:\d22\'
working_data_dir	Directory path to working data directory	String e.g. 'c:\windows\desktop\'
project_dir	Directory path to current working project directory	String e.g. 'c:\windows\desktop\'
project_title	Title of current project	String e.g. 'someones data'

Instrument

Variable Name	Description	Type and Size	
inst	**Current Instrument, e.g. 'd11', 'd22', 'd16'**	String	
inst_params	**Structured array containing parameters associated with the instrument.**	**.att**	Attenuators
		.col	Collimations
		.det_size	Detector Size
		.imask	Instrument Mask
		.fparams	Parameter Names (from data file)
		.flux_col	Attenuation as fn. of Col and Wav.
		.pixel_size	p_x,p_y (mm)
		.pixel_anisotropy	p_x/p_y
		.wav_range	Wavelength range
		.default_fparams	Default parameter names.

Data

Variable Name	Description	Type and Size	
data	Store of all data arrays: e.g. foreground background cadmium empty beam transmission sample transmission empty masks detector efficiency etc. Note: Not all structure fields are used with each set.	**.name**	Worksheet name, e.g. 'fore'
		.nmbr	Number of worksheets of this type.
		.type	Type of worksheet, i.e. scattering data, transmission etc.
		.allowed_types	List of worksheet types allowed to be accessed in the selector with this worksheet.
		.sum_allow	Whether this worksheet has a Sum or not.
		.last_displayed	Positions of the Sub and Cad worksheets the last time this worksheet was selected as a Foreground
		.data	The actually multi detector array stored as RAW counts.
		.dpth	Current active depts of all the worksheets under this worksheet name.
		.dpth_max	Maximum allowed depth for this worksheet.
		.params	Data file parameters.
		.cm	Beam Centre of mass associated with each worksheet.
		.trans	Transmission value associated with each worksheet.
		.parsub	Data file experiment title information.
		.info	Structure containing data load string for, data file date, time etc.
		.error	Error data for the detector efficiency

			map.
		.effieincy_scale	Calibration Scalar.
		.efficiancy_scale_units	Units associated with the Calibration Scalar, e.g. Counts / Standard Monitor
		.calib_xsection	Known cross section of the calibration sample.
		.calib_xsection_units	Units associated with the Calibration Cross-section.
.displayimage	Data and information about the current image displayed in the main window.	**.data**	Image data
		.error	Error in the image data.
		.params	Data file parameters associated with the current foreground data.
		.parsub	Data subtitle associated with the current foreground data.
		.lm	Load string used to load the current foreground data.
		.sum_flag	Flag indicating whether the current display is a Sum or single depth.
		.units	Units of the current displayed data.
		.mask	Mask used for the currently displayed image.
		.history	Text history of data processing
standard_monitor	Standard Monitor Normalisation Value	Integer Default = 10 000 000	
standard_time	Standard Time Normalisation Value	Integer Default = 100 s	

GRAS$_{ans}$P Functions and Subroutines available at the Matlab™ command line

Display

Function / Subroutine Name	Description	Usage
display_params	Displays a summary of instrument and data parameters associated with the current foreground image in the Matlab™ command window.	"display_params"
display_param_list	Brings up a separate figure window displaying data file parameter number and name.	"display_param_list"
message	Displays a message in the top-left corner of either the main, or sub-figure axes.	"tag = message(<'text'>,<line>,<'window'>)" where 'window' = 'main' or 'sub' and 'line' is the line number. 'tag' is the Matlab™ tag to the newly created display object.
output_figure	Displays a data summary graph and history text of either the main figure window or the current sub-figure window ready for printing.	"output_figure(<'window'>);:" where 'windw' = 'main' or 'sub'.
plot_and_export2	*GRAS$_{ans}$P*'s own output graph plotting routine.	"plot_and_export2(<plotdata>, <'column_format'>, <additional_params>)" plotdata = [x,y,ErrY]; column_format = ['xye'] additional_params is specified as paired properties, e.g. 'plot_title','my graph', 'x_label','my x-axis', 'y_label','my y-axis' etc.
update_display	Updates the main *GRAS$_{ans}$P* interface window, including current displayed data and various drop-down menus, edit boxes, displayed text etc.	"update_display"

Data

Function / Subroutine Name	Description	Usage
get_numor	Low level basic SANS data read routine (ILL format).	"[data, param, parsub] = get_numor(<'directory'>,<numor>)" where 'data' is an [n*m] matrix, 'param' is a [128*1] list of data file parameters, and 'parsub' is the measurement subtitle string. Input parameters 'directory' is the data directory path string and 'numor' is the data file number (integer).
get_mask	Low level basic SANS data mask read routine (ILL format)	"[mask] = get_mask(<'directory'>,<'fname'>)" where 'mask' is an [n*m] matrix of '35's' (ascii '.' = masked) and '46's' (ascii '#' = not masked). Input parameters 'directory' is the mask file directory path string and 'fname' is the mask file name string.
get_selector_values	Reports the current reading of the main data selectors.	"[wks,nmbr,dpth,wks_tag,nmbr_tag,dpth_tag] = get_selector_values(<'selector'>)" where 'wks', 'nmbr', 'dpth' are the current reading of the selector (strings) and 'wks_tag', 'nmbr_tag' and 'dpth_tag' are the Matlab™ tags to the selector objects. Input parameter 'selector' is either: 'for', 'sub' or 'cad' for the relevant selector.
current_beam_centre	Reports the current Beam Centre values indicated by the main display.	"[bx,by,b_theta] = current_beam_centre"
current_mask	Reports the current mask data.	"[data] = current_mask"
current_transmission	Reports the current transmission values indicated by the main display.	"[ts,te] = current_transmission"

SANS Math

<table>
<tr><th>Function / Subroutine Name</th><th>Description</th><th>Usage</th></tr>
<tr><td>build_q_matrix</td><td>Builds an [nxmx4] matrix, where [nxm] is the same size as the data and contains qx, qy, mod_q and q_angle in [nxm] planes from depths to 4.</td><td>"[qmatrix]=build_q_matrix(params)"

where ‘params’ is a [128*1] column vector of data file parameters.</td></tr>
<tr><td>get_selector_result</td><td>Reports the result of the correct calculation of Foreground minus Background and Cadmium backgrounds, taking into account the Transmissions, Ts and Te.</td><td>“[intensity,flag] = get_selector_result”

where ‘intensity’ is a structure with fields:
<table><tr><td>.data</td><td>128 * 128</td></tr><tr><td>.error</td><td>128 * 128</td></tr><tr><td>.params</td><td>128 * 1</td></tr><tr><td>.parsub</td><td>Measurement subtitle string.</td></tr><tr><td>.lm</td><td>Load string</td></tr><tr><td>.sum_flag</td><td>‘Sum’ display flag</td></tr><tr><td>.history</td><td>Text history of data processing</td></tr></table></td></tr>
<tr><td>pixel_to_q</td><td>Reports q_x and q_y values for a given pixel_x and pixel_y based upon the current displayed data parameters and beam centre.</td><td>“[q]=pixel_to_q(pixel_x,pixel_y)”</td></tr>
<tr><td>q_to_pixel</td><td>Reports pixel_x and pixel_y values for a given q_x and q_y based upon the current displayed data parameters and beam centre.</td><td>“[pixel]=q_to_pixel(qx,qy,rnd_chk)”

if ‘rnd_chk’ = ‘yes’ the pixels are reported in integers.</td></tr>
<tr><td>err_add</td><td>Addition operator including errors based upon the propagation of errors standard formula:
If $Z = f(x, y)$
Then
$\Delta Z = \sqrt{\left(\frac{dz}{dx}\right)^2 (\Delta x)^2 + \left(\frac{dz}{dy}\right)^2 (\Delta y)^2}$</td><td>“[result,err] = err_add(a,da,b,db)”

where ‘result’ and ‘error’ are the result and associated error.

Input parameters are the numbers ‘a’ and its error ‘da’ and ‘b’ and it’s error ‘db’.</td></tr>
<tr><td>err_sub</td><td>Subtraction operator including errors based upon the propagation of errors standard formula:</td><td>“[result,err] = err_sub(a,da,b,db)”</td></tr>
<tr><td>err_multiply</td><td>Multiplication operator including errors based upon the propagation of errors standard formula:</td><td>“[result,err] = err_multiply(a,da,b,db)”</td></tr>
<tr><td>err_divide</td><td>Division operator including errors based upon the propagation of errors standard formula:</td><td>“[result,err] = err_divide(a,da,b,db)”</td></tr>
<tr><td>err_power</td><td>Power operator including errors based upon the propagation of errors standard formula:</td><td>“[result,err] = err_power(x,dx,a)”
where ‘a’ is the power.</td></tr>
</table>

err_acos	Arc_Cos operator including errors based upon the local gradient in Cos (i.e. Sin) about the point of interest.	"[result,err] = err_acos(a,da)"

Fit Functions

Function / Subroutine Name	Description	Usage
curve_fit_window	Brings up the 1D curve fitting control window (only works if a sub-figure exists).	
fit_control	Controls the 1D fitting procedure, i.e guessing of start parameters and fitting.	
curve_fit_window_2d	Brings up the 2D curve fitting control window.	
fit_control_2d	Controls the 2D fitting procedure, i.e guessing of start parameters and fitting	

Instrument

Function / Subroutine Name	Description	Usage
attenuation_scaler	Reports the attenuation setting for the supplied data parameters. The 'flux_scaler' factor has currently been disabled and is fixed at 1.	"[flux_scaler,message] = attenuation_scaler(params)" where 'flux_scaler' is the required up-scaleing to account for the current attenuator in the beam. 'message' is a text message describing the current attenuation state. Input parameter 'params' is the current data file parameter.
col_atten	Reports the relative attenuation of the beam using a certain collimation relative to a reference collimation.	[att] = col_atten(col, col_ref,wav)

User Modules

Function / Subroutine Name	Description	Usage
user_modules	User editable file containing a menu description and path to users own *GRAS$_{ans}$P* Modules.	

Appendix 4: *GRAS$_{ans}$P* - Script

GRAS$_{ans}$P-Script is a new development providing a 'backward' step in data processing software to allow common *GRAS$_{ans}$P* analysis tasks to be executed from the Matlab™ command line. *GRAS$_{ans}$P*-Script will be a collection of small commands that essentially operate *GRAS$_{ans}$P* by 'remote control' from the command widow or script file. The advantage of *GRAS$_{ans}$P* will be that repetitive analysis on large data sets, or highly complex and time consuming analysis on large data sets can be launched from a script file. Since the script is essentially Matlab™ functions and commands, the user has enormous flexibility in their analysis. *GRAS$_{ans}$P* script has only just begun and as such is not supported to the user community just yet…..watch this space!