

DCS data reduction and analysis

Getting started

For the DCS data reduction and analysis you will be using the program DAVE (Data Analysis and Visualization environment). This software was developed at the NIST Center for Neutron Research. Every effort has been made to ensure that DAVE is supported under Linux, Windows, Mac-OS10 and SGI-Irix. It is available at no cost to users. For detailed information about the program including how to download it, please visit the official DAVE web site: <http://www.ncnr.nist.gov/dave>.

The aim of the experiment is to investigate the motion of the hydrogen atoms in $\text{Mn}[\text{N}(\text{CN})_2]_2 \cdot \text{pyrazine}$. In order to do this you must first reduce the data to obtain the incoherent scattering function $S_{\text{inc}}(\mathbf{Q}, \omega)$. You will then analyze the experimental $S_{\text{inc}}(\mathbf{Q}, \omega)$ by fitting it with appropriate combinations of mathematical functions (Gaussians and Lorentzians). The Q dependence of the amplitudes and widths of these functions can then be compared with predictions based on models representing different types of motion.

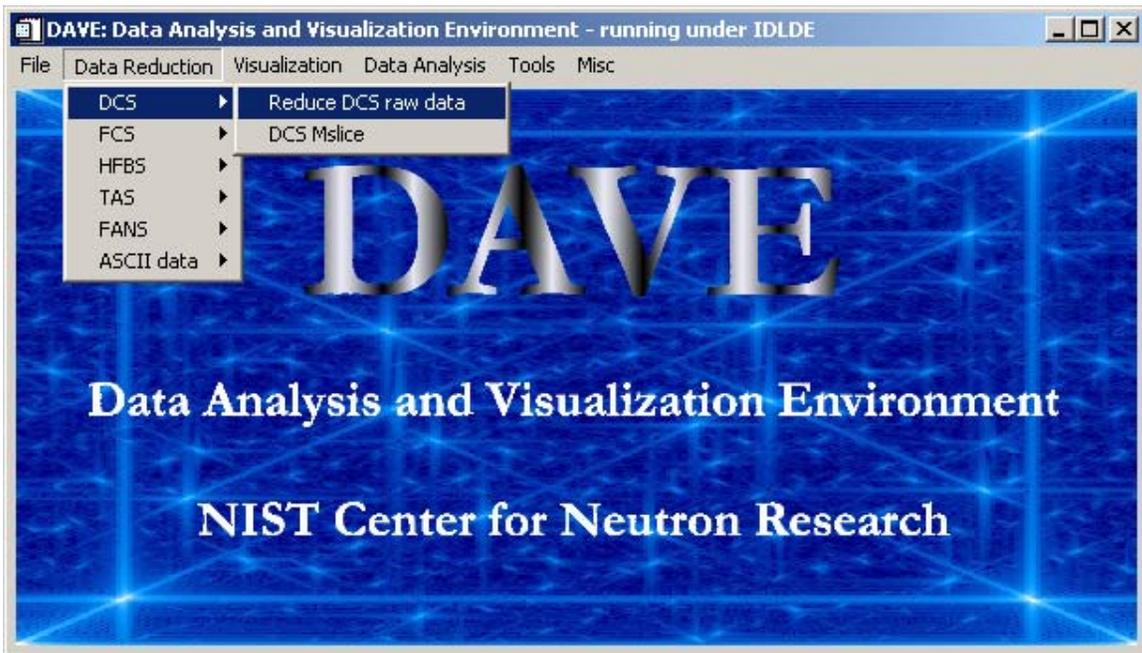
Data reduction

Before the summer school we made a series of measurements that you will use to reduce the data that you obtained using the protonated pyrazine compound. In what follows we shall describe the reduction of datasets that we obtained earlier, using 5.7g of the deuterated version of the compound.

The following table lists file names and temperatures for each of the data files that we shall use in the data reduction.

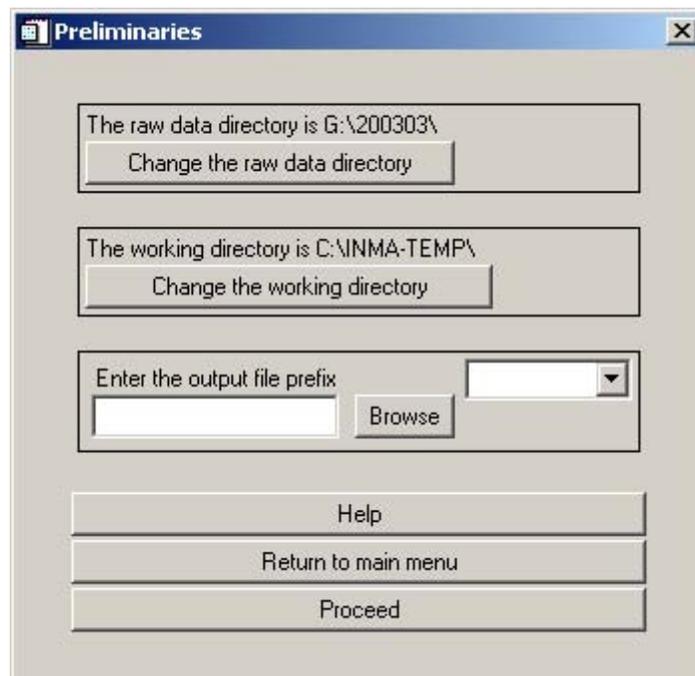
	File Name	T(K)
Deuterated sample	20030522_018.dcs.gz	390K
	20030523_003.dcs.gz	400K
	20030523_010.dcs.gz	300K
Vanadium	20030522_013.dcs.gz	Room temperature
Dark count	20030515_001.dcs.gz	(Room temperature)
(Fast background)	20030515_002.dcs.gz	(Room temperature)

■ Double-click on the appropriate icon to start the runtime development version of DAVE. The following screen will appear:

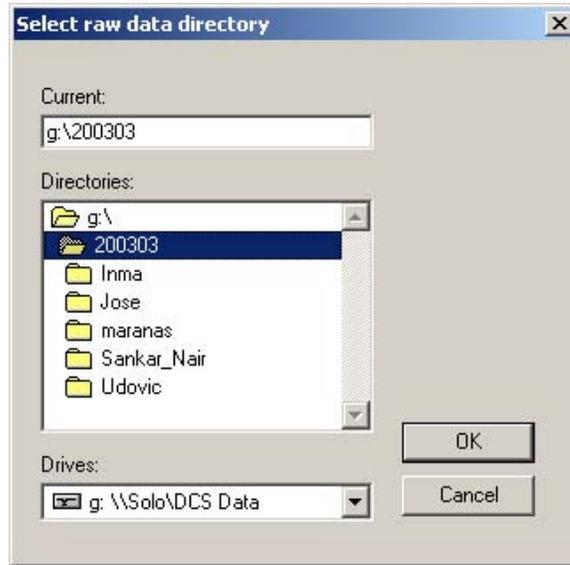


Click “Data Reduction→DCS→Reduce DCS raw data”.

■ Preliminaries



■ The raw data directory is the directory where the raw data files are located. The data for the present example are on the computer called “solo” (which should be mapped to your PC), in the directory /home/dcs/data/200305/. If this is not the current raw data directory, click “Change the raw data directory”.



Select the correct directory and hit “OK”.

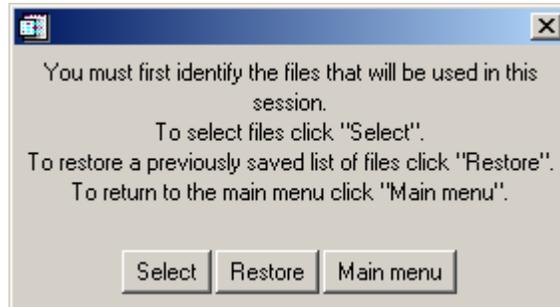
■ You will also need to define the working directory, which is where the files generated by the data reduction will be saved. Depending on the day, use one of the following: “C:\SS03\MonTue”, “C:\SS03\TueWed”, or “C:\SS03\WedThu”.

■ You must provide an “output file prefix” for your data reduction. This prefix will be common to all files generated during the data reduction session. For this example we have chosen “deuterated” as the prefix and we have chosen to reduce data for the sample at three different temperatures. This means that if we choose the symmetrized $S(Q, \omega)$ as final output the following list of files will be created in the working directory:

Intermediate files	deuterated_sam1sum.dave deuterated_sam2sum.dave deuterated_sam3sum.dave deuterated_bgdsum.dave deuterated_vansum.dave deuterated_sam1cor.dave deuterated_sam2cor.dave deuterated_sam3cor.dave
Final reduced files	deuterated_sam1SSQW.dave deuterated_sam2SSQW.dave deuterated_sam3SSQW.dave

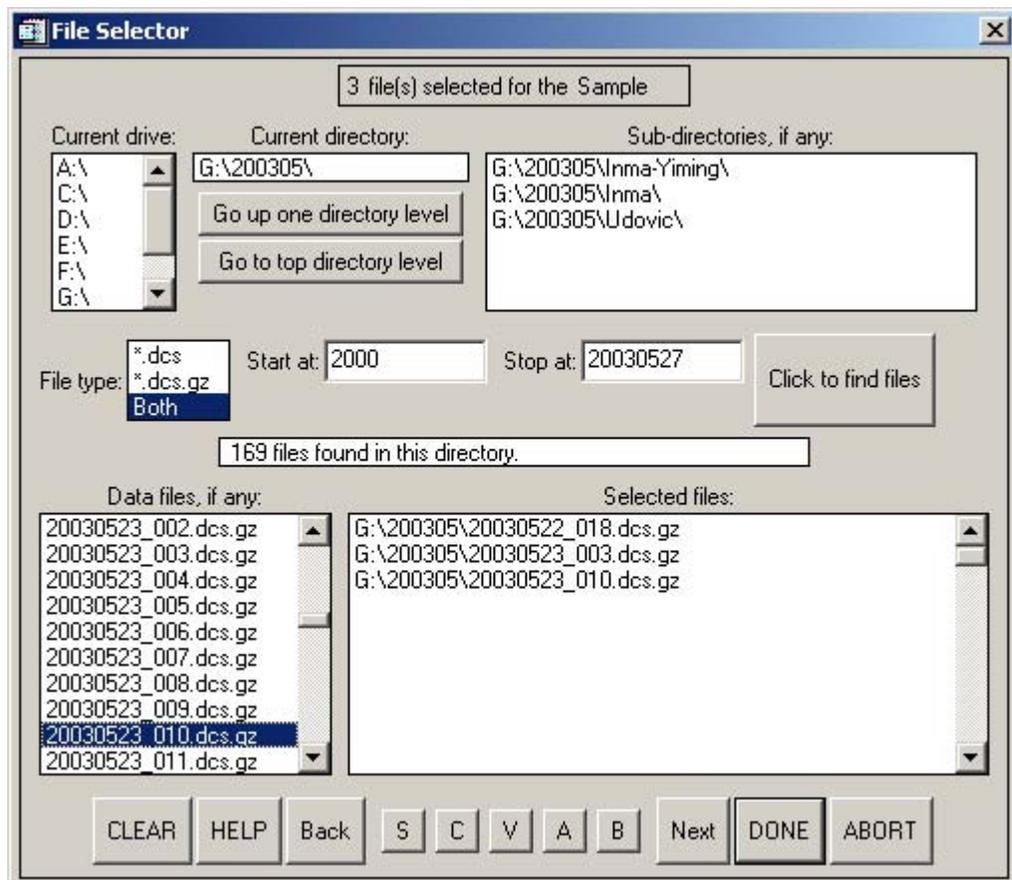
Enter the output file prefix in the box provided in the “Preliminaries” window, and then hit “Proceed”.

■ Specifying the raw data input files



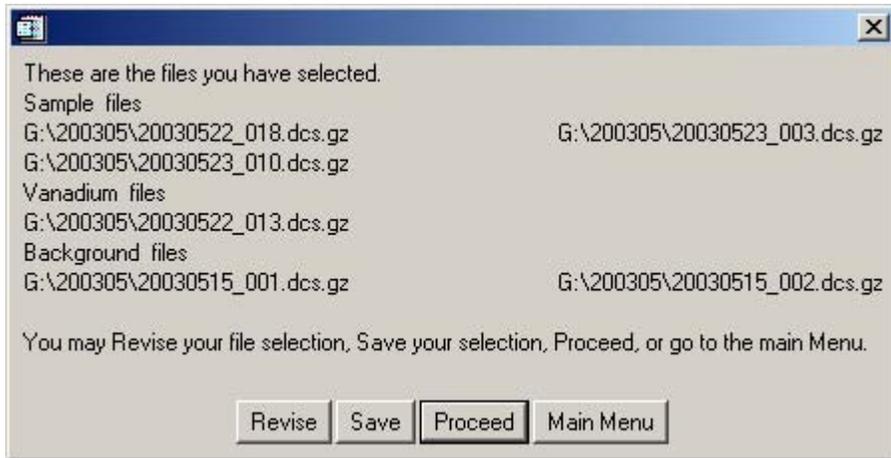
If this is the first time you are reducing the data files, you must click “Select”. If you are redoing the data reduction and have previously saved the list of files (the file name will be “deuterated.flis”) you can instead click “Restore”.

■ Choose the files for the sample. Click “Help”, or ask for help, if you have problems using this widget.



To select the vanadium (background) files, click “V” (“B”) and then double-click on the appropriate file names.

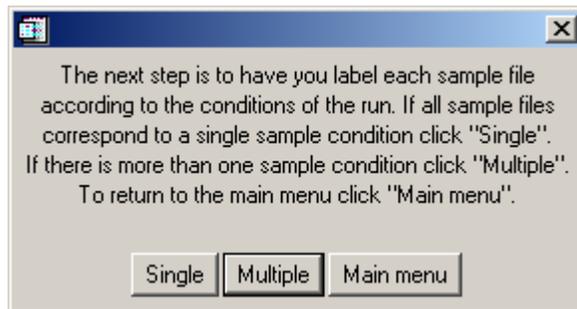
Once you are satisfied, click “DONE”. You will get the following type of screen.



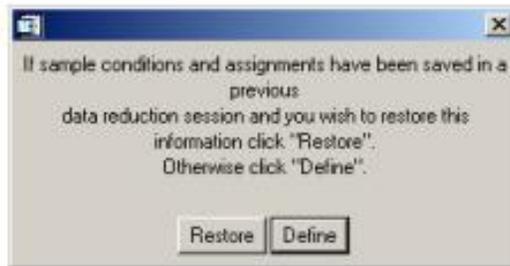
Check the names of the files and revise the selection if necessary. Once you are satisfied you may wish to save the list of files (which can be very useful and time-saving). You can then proceed to the next step in the data reduction. You may have to wait a short time while various operations are performed on the raw datasets.

■ Multiple sample conditions

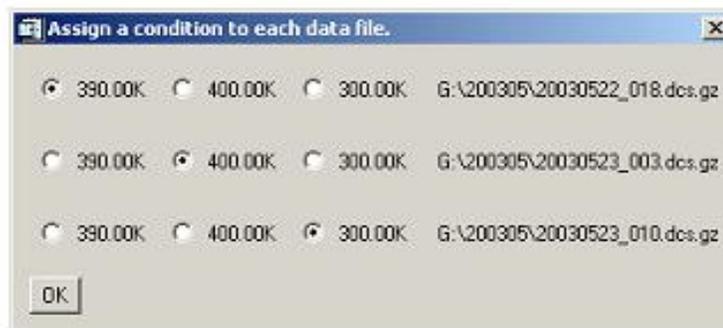
The DCS reduction software allows you to reduce multiple sample datasets in parallel (multiple sample datasets meaning datasets obtained under different sample conditions), as long as the same auxiliary datasets (empty container, vanadium, background, etc) are used with all sample datasets.



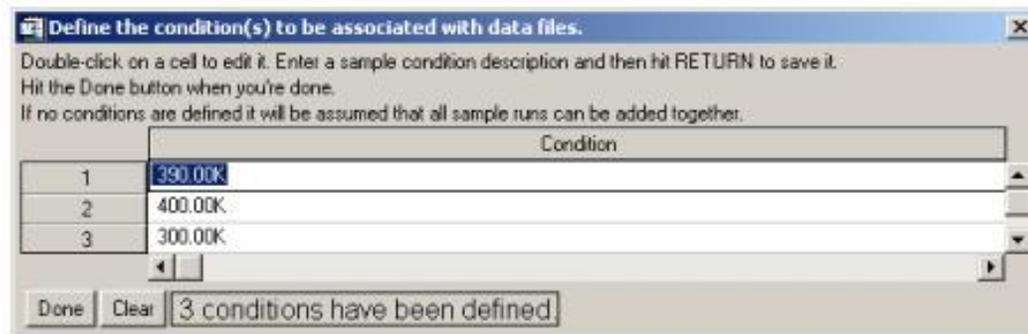
In this example we are simultaneously reducing sample data at three different temperatures, so we select “Multiple”.



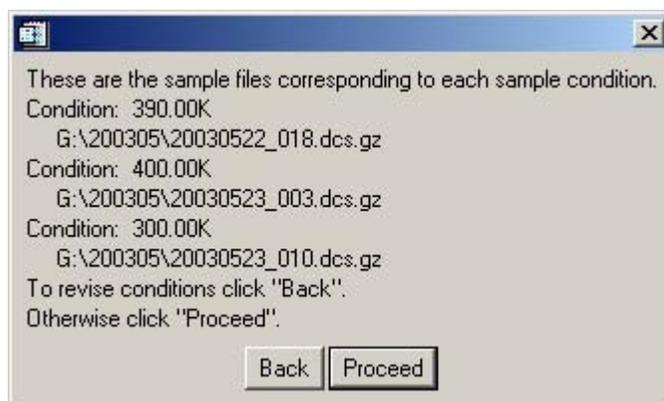
We must now define the conditions to be associated with the different files. Alternatively we could restore this information if it had been saved previously. Presuming that this is not the case, click “Define”.



The default assumption is that the different sample conditions are distinguished by their temperature set points. Since this is the case, click “Done”.



The table (shown above) relates each sample data file to one of the sample conditions. Assuming it is correct, click “OK”.



A list of sample conditions and associated files now appears. The first listed (*n*'th listed) condition corresponds to output files with names containing the string “sam1” (“sam*n*”) (see above). Thus in this example the output files “deuterated_sam1sum.dave”, “deuterated_sam1cor.dave” and “deuterated_sam1SSQW.dave” correspond to the 390K data. It may be useful to record separately the order of the entries in this list.

If the list of conditions and files is correct, click “Proceed”.

The next window (not shown) affords you the opportunity to save the sample conditions and assignments to a file. This can be useful if you expect to redo the data reduction.

■ Detector masking

The next window (not shown) asks you to decide whether or not you wish to define a detector mask. Masked detectors are excluded from the data reduction. Since we wish to omit detectors that contain Bragg peak intensity (and possibly other detectors), click on “Generate/restore”. The following widget appears.

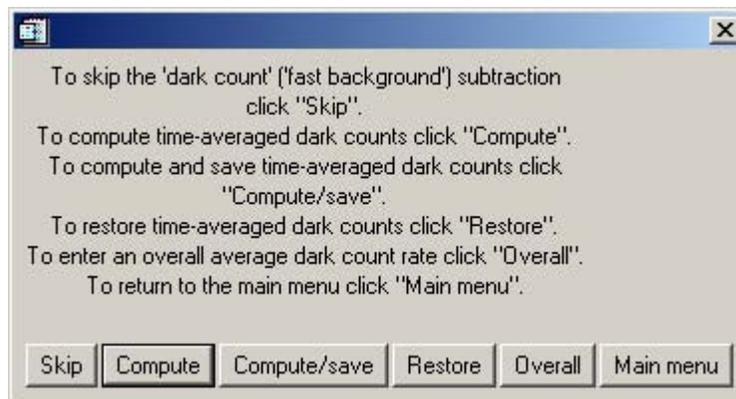


This widget allows you to define detectors to be masked by typing their numbers following the phrase “MASK DETECTORS”. A more practical approach is to plot detector sums, i.e. sums over all time channels as a function of detector number for one or more of the input raw data files, and then select the detectors to be masked using the

mouse. You may save the list of masked detectors in order to be able to restore the list in future data reduction sessions. For general help click the “Help” button. To use the graphical approach click “Plot sums” and then select one or more files. When the plot appears you may wish to click the “Help” button for additional help. When you are satisfied with the mask, and have possibly saved the list of masked detectors, click “Proceed”.

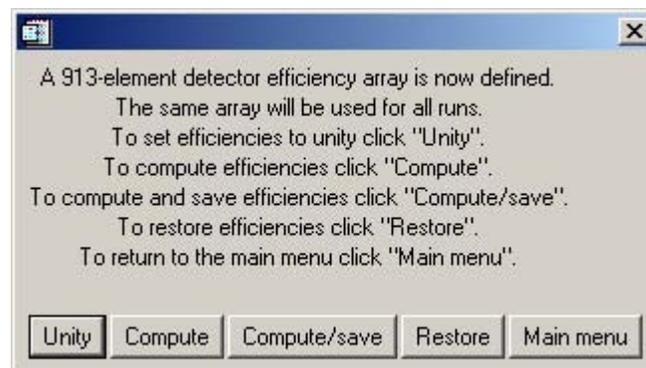
At this stage any so-called “bitflips” are corrected, the detector mask is applied, the counts in each time channel are divided by the time channel width, nominally identical files (in this example files 20030515_001 and 20030515_002) are summed, and the results are saved to disk in the DAVE format (with names containing the string “sum.dave”). Please be patient.

■ Dark count subtraction



The next step is to decide whether or not to correct all datasets for the “dark count” (beam closed) background, and if so how. Since we have dark count data files and we wish to perform this correction, click “Compute”.

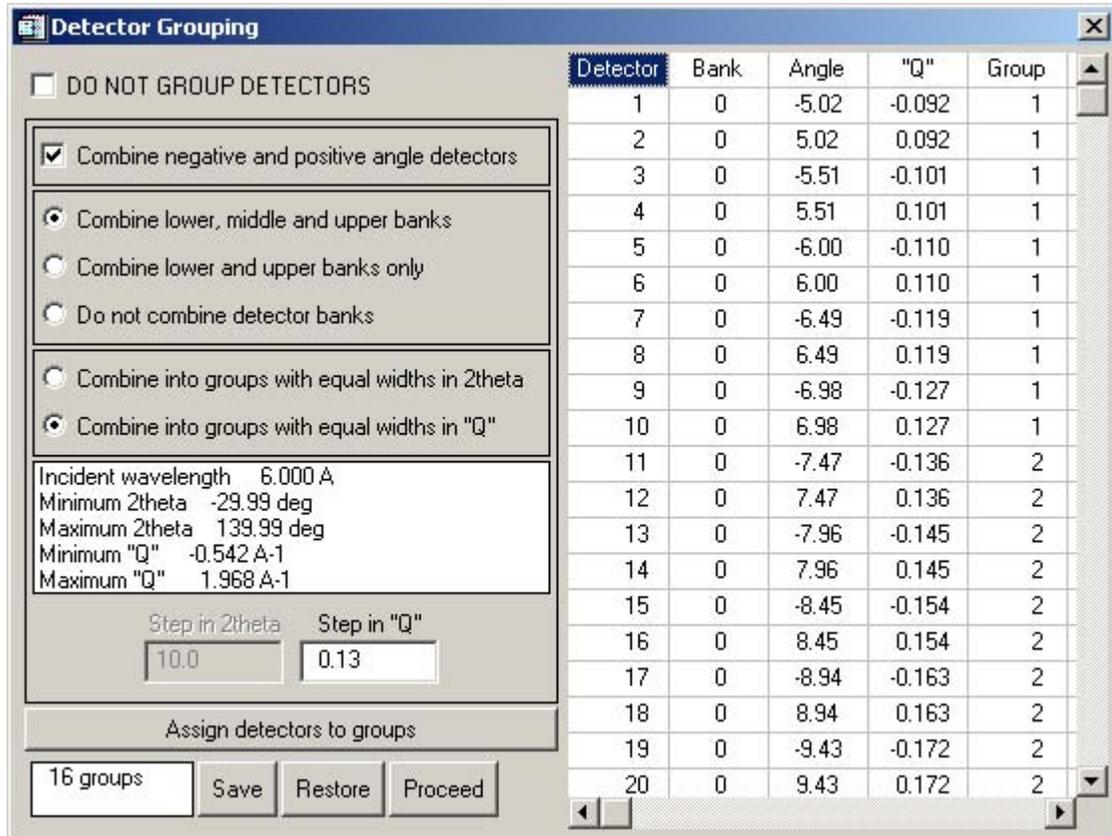
■ Detector efficiencies



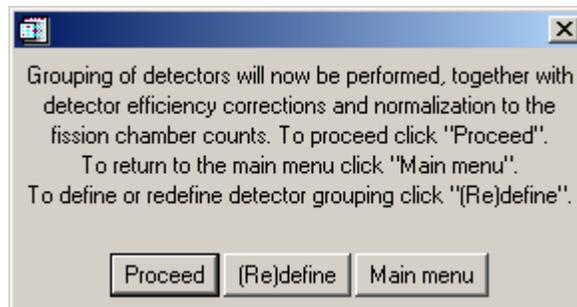
Similarly we must decide whether or not to correct for variations in detector efficiency, and if so how. As we have a vanadium data file we click “Compute”.

■ Grouping detectors

The next window (not shown) asks whether you want to group the detectors. Since you do, click “Grouping”. The following widget will appear.



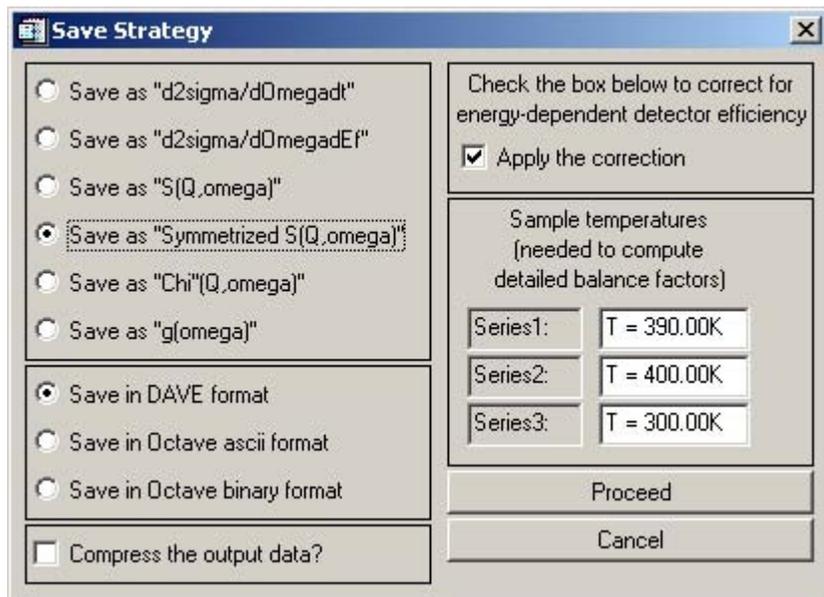
If you make any changes you will need to click “Assign detectors to groups” to implement the changes. You may wish to save the grouping information for later use. When you are satisfied with the detector grouping click “Proceed”.



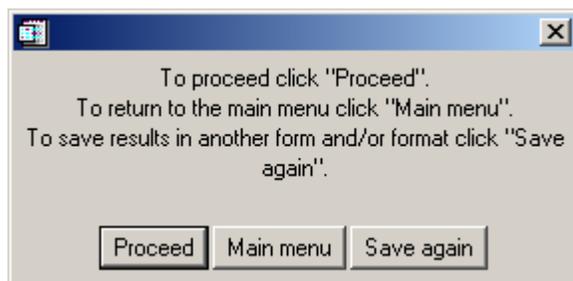
At this point you can redefine the grouping, proceed or return to the Main menu. If you click “Proceed” the program will perform a number of operations on the data: beam

closed background subtraction, detector grouping, beam monitor normalization, detector efficiency corrections, and corrections using empty can and cadmium runs (if supplied). The results for each sample condition will be saved to disk in the DAVE format (with names containing the string “cor.dave”). This may take some time.

■ Deciding the form of the output



The “save strategy” widget allows you to choose the form in which to save the reduced data. In this example the “Symmetrized S(Q,omega)” format was chosen. Note the checked box indicating that the data will be corrected for the energy dependence of the detector efficiencies. When you click “Proceed” the necessary data conversions are performed and the results are saved to disk in the DAVE format (with names containing the appropriate string, in this case “SSQW.dave”).



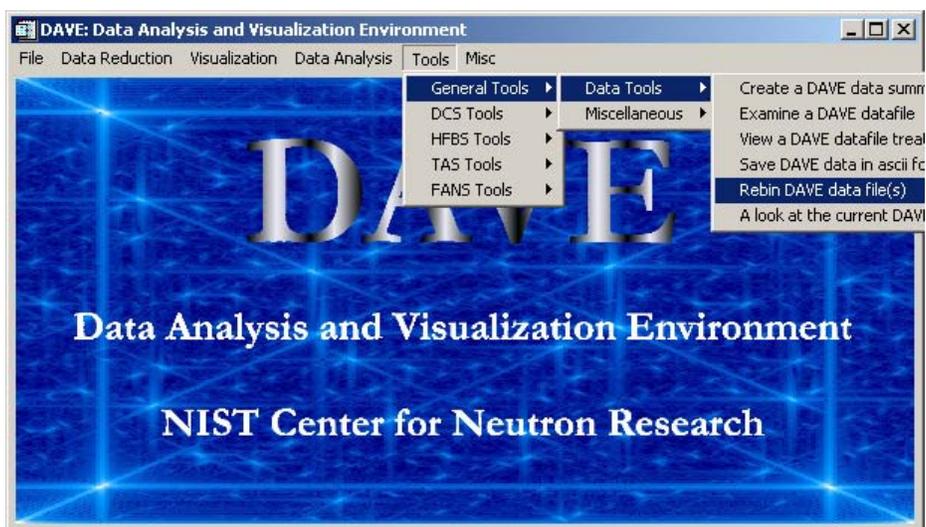
When this dialog appears you may click “Save again” if you want to save the data in another format, e.g. S(Q,ω) itself. In that case you will be presented with the “Save strategy” widget once again. If you click “Proceed” you will be asked whether or not to delete certain files and you will then be returned to the Main menu.

At this point the data reduction is complete and data files containing the symmetrized scattering function S(Q,ω) are in your working directory.

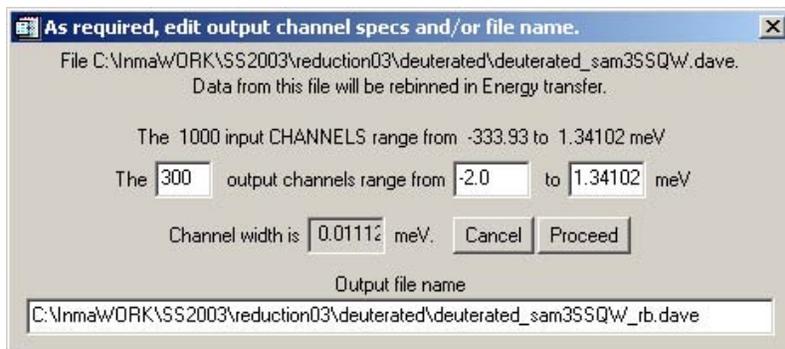
Rebinning the DAVE files

Before proceeding to the data analysis we need to rebin the $S(Q, \omega)$ data files. We do this for two reasons. First of all, we are interested in a very small range of energies either side of the elastic line and there is no need to retain the complete energy range (which extends to > 300 meV in neutron energy gain). The other reason has to do with the energy channels being unequally spaced. This can make Fourier transforms more difficult, and much slower, than if the energy channels have identical widths. Furthermore equal width energy channels are necessary if you wish to include the instrumental resolution function in the data analysis using the “PAN” utility (see below).

- To rebin, click on Tools→General Tools→Data Tools→Rebin dave data file(s)



You will be asked to select the DAVE file(s) that you want to rebin. In this particular example we have chosen the file “deuterated_sam3SSQW.dave”. First you are asked if you wish to rebin in Energy transfer. Click “Yes”. Next you are asked if you wish to rebin in Q. Click “No”.



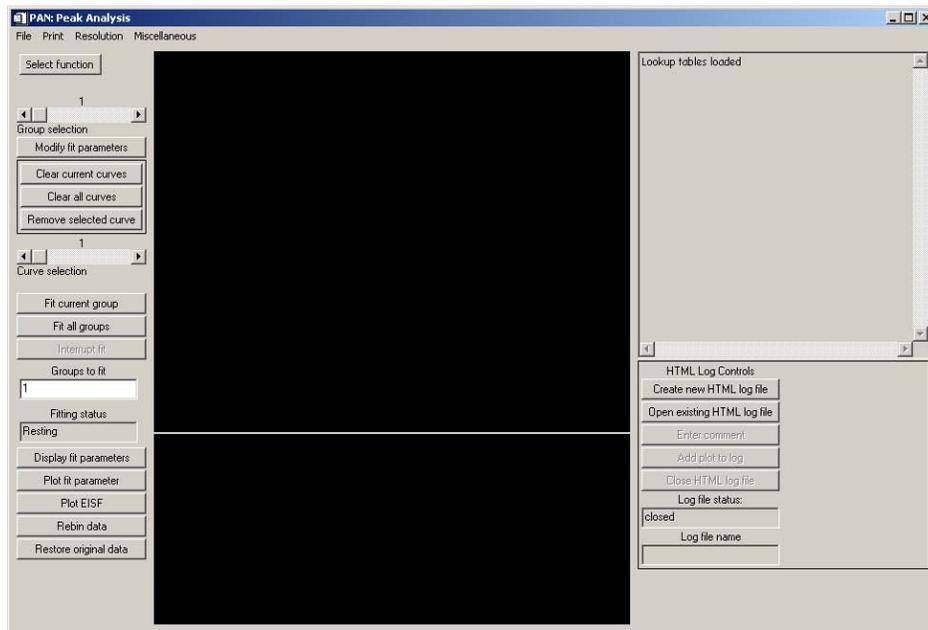
- You are now asked how you want to rebin the energy channels. It is generally a good idea to have very roughly the same number of channels within the chosen energy

range before and after rebinning. In this example we chose 300 output channels between -2.0 meV and 1.34102 meV, giving a channel width of 0.01112 meV. The default output file name, displayed at the bottom of the window, may also be edited. Once you are satisfied, click “Proceed” and the rebinned data file will be created.

Fitting model functions to the data

To determine the EISF we must determine the relative integrated intensities of the elastic and quasielastic contributions to $S(Q, \omega)$. To get these quantities we will use the program PAN, which is part of DAVE. We will provide a detailed example that shows how to use PAN to fit the DCS reduced data files. For more information about PAN the reader can view the PAN manual at <http://www.ncnr.nist.gov/dave>.

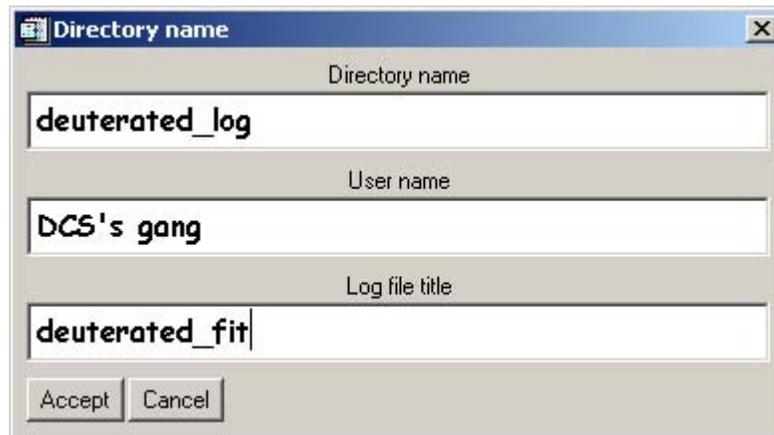
- Start PAN by selecting Data Analysis \rightarrow PAN (Peak Analysis)



- To load the file to be analyzed, select File \rightarrow Load DAVE file. The data will appear in the upper window of the widget. By default you will see the first group. If you want to see the other groups use the “Group selection” scroll bar.

- To save information related to the current session you may wish to create an html file by clicking “Create new HTML log file” (at bottom right).

Edit the entries and click “Accept”.



Directory name

deuterated_log

User name

DCS's gang

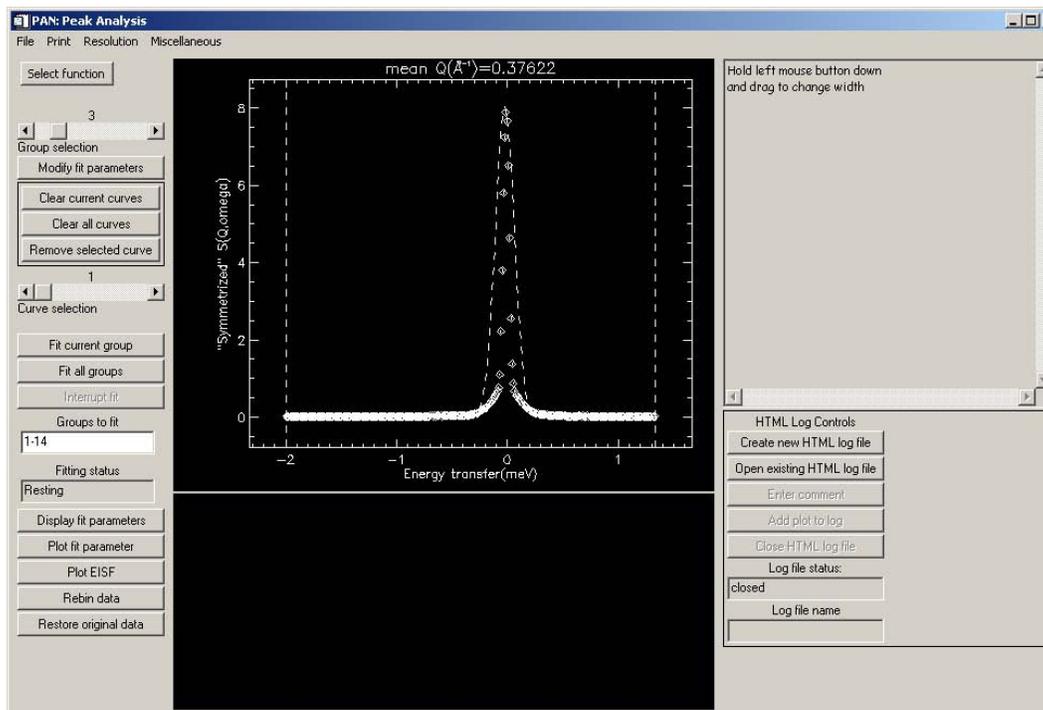
Log file title

deuterated_fit

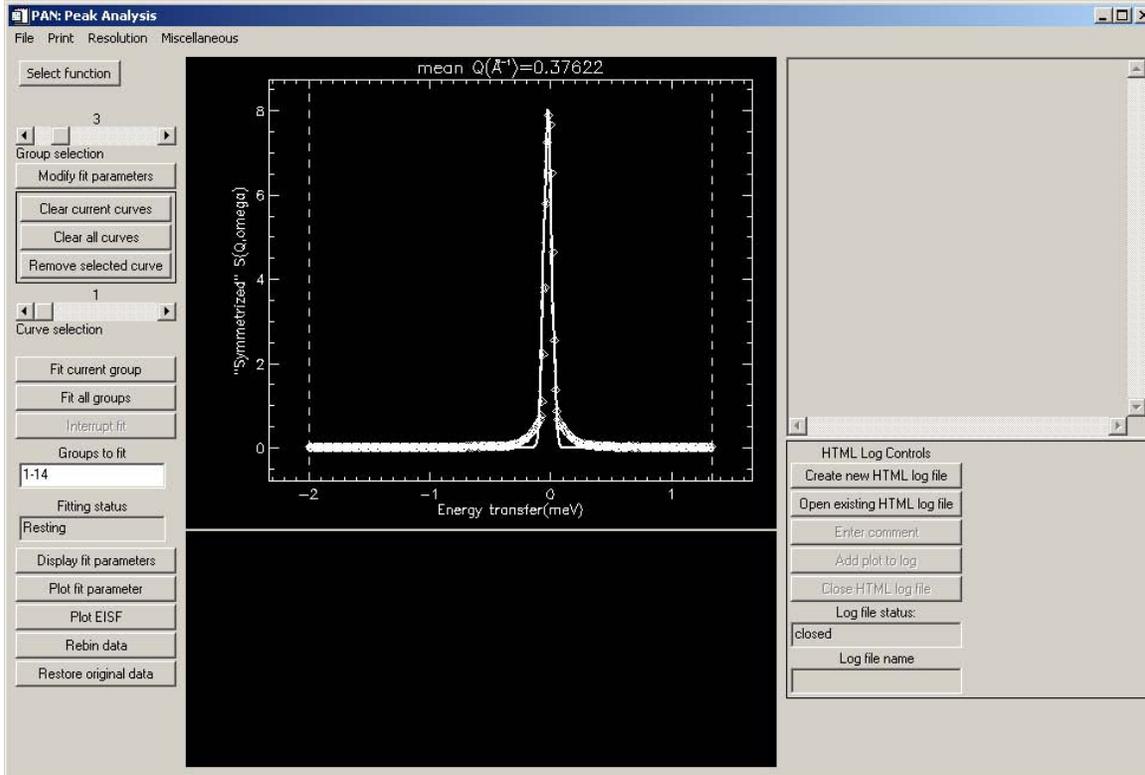
Accept Cancel

A new file called “index.html” will be created in the newly created directory “deuterated_log” (which is a subdirectory of your working directory). Once it has been created you can click “Enter comment” in order to place some text in the file. You can also click “Add plot to log” and the graph on the screen will be added to the log file. Once you are finished with PAN, you should click “Close HTML log file” to close the file. You can always reopen it if you wish, by clicking “Open existing HTML log file”

■ A reasonable model to fit the experimental data uses a Gaussian function to fit the resolution-broadened elastic peak and a Lorentzian for the quasielastic scattering. To create an initial Gaussian click “Select function” and then select “gaussian”. The text box at top right will tell you what to do next; it will read as follows: “Hold left mouse button down and drag function centroid”. In this way you can vary both the centroid and the amplitude of the Gaussian.



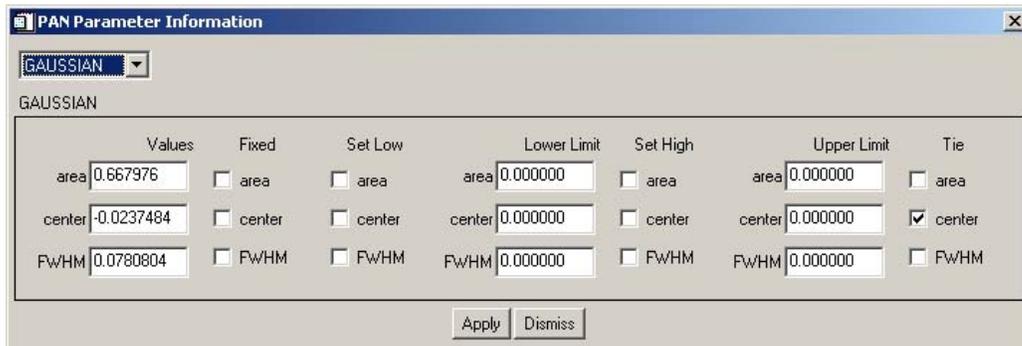
When you release the left mouse button, the following message will appear: “Hold left mouse button down and drag to change width”.



This time, on releasing the button, a Gaussian based on your choices of centroid, amplitude and width is displayed as a solid line. You can use the same procedure to add a Lorentzian function. If you want the residuals to be plotted click the left mouse button after defining the functions.

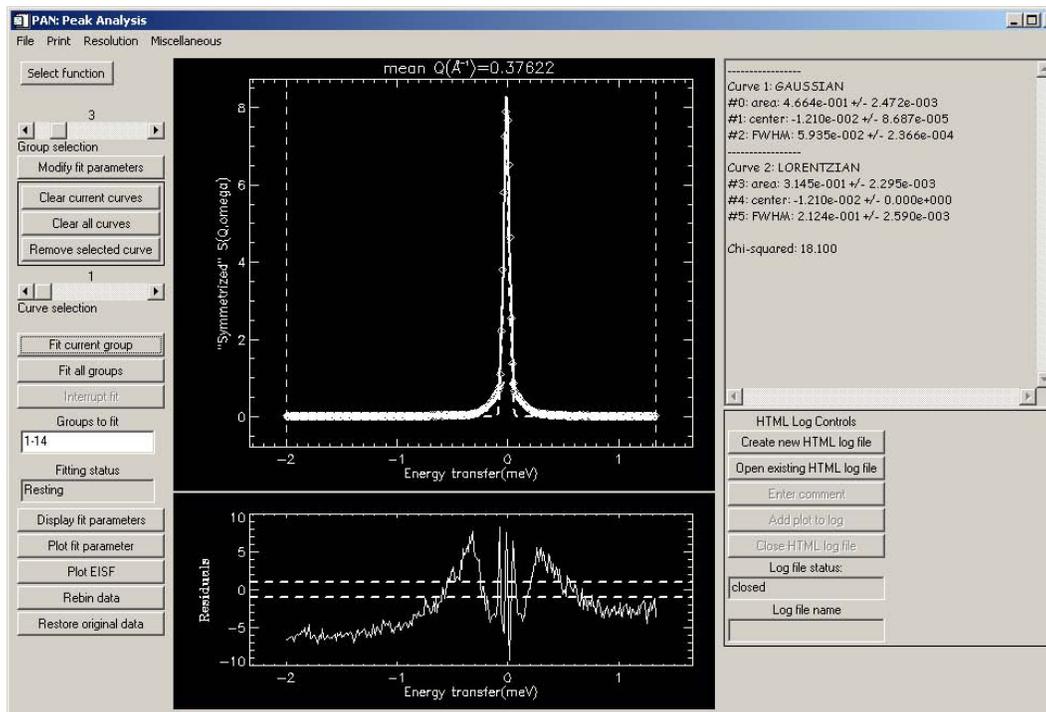
As a general rule, click the right mouse button to autoscale any plot.

Before attempting to fit this group you should constrain the fit by forcing the centers of the Gaussian and the Lorentzian to be the same. To apply constraints, or to change the values of the parameters, click “Modify fit parameters”.

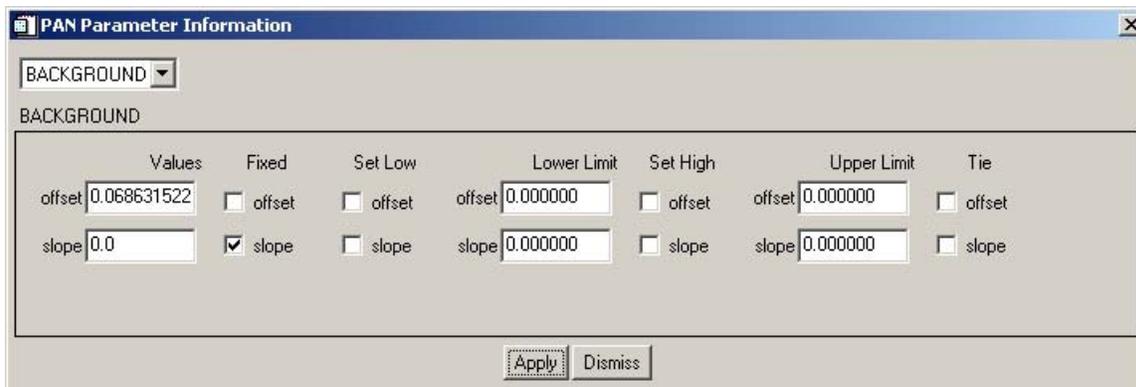


Displayed is parameter information for the first curve that you chose to fit the data. By default there are no conditions on the refinement, so you should check appropriate boxes, enter values as needed, and then click “Apply”. In the present example we wish to “tie” the centers of the Gaussian and Lorentzian curves. To do so we must check the “Tie center” boxes for both curves. Finally click the “Dismiss” button.

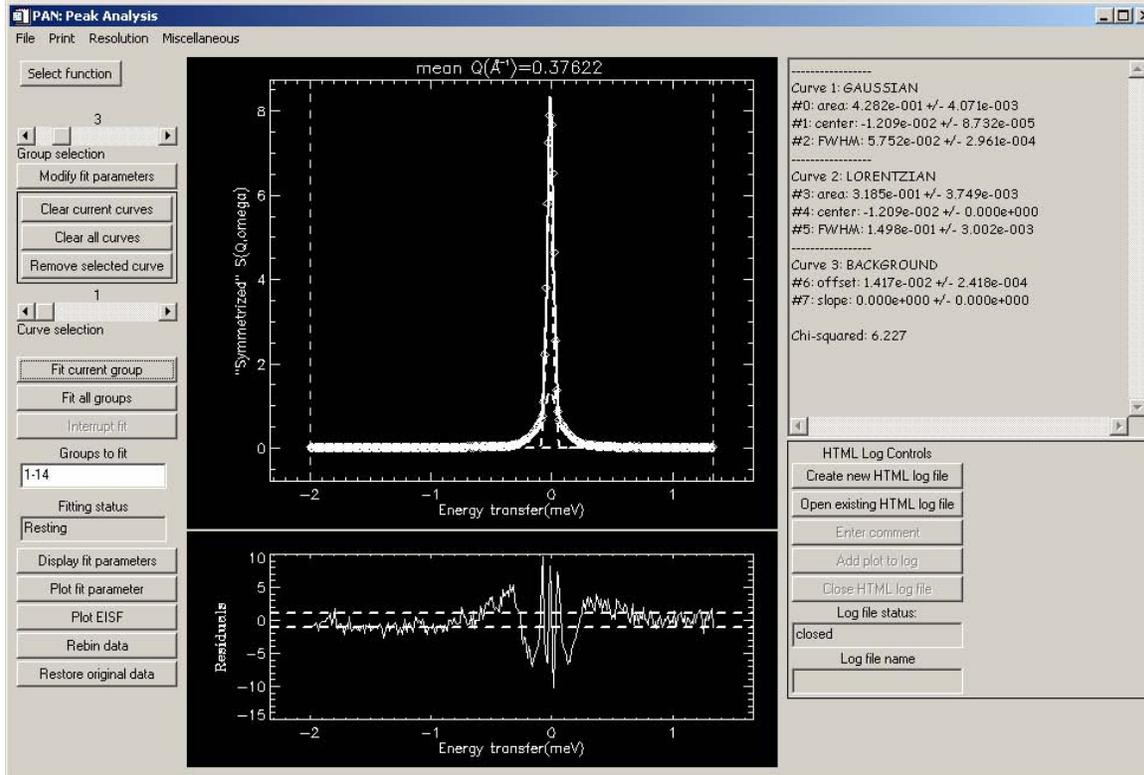
■ Click “Fit the current group”



In order to evaluate the fit you should examine the residuals in the lower plot window and the fitted parameters in the upper right text area. Looking at the residuals in the present example you will see that there are two problems. First, there is an overall offset in the y direction. Second, the experimental data are not fully described by the combination of a Gaussian and Lorentzian. The first problem should be resolved by adding a background to the fit. Click “Select function”, select “background” and follow the instructions to characterize the function. It is good practice to start with the background flat (i.e. zero slope). Click “Modify fit parameters”, select “BACKGROUND”, and check the “Fixed” box for the slope (whose default value is 0.0).



Click “Fit current group” again and see the improvement.



Given the fit parameters and the residuals, it is necessary to decide whether or not the fit is acceptable. There is no general formula for this decision. In the present case, given that we have not taken into account the instrumental resolution function, we can reasonably argue that the fit is acceptable.

Once we're happy with the fit to a single group, we can click the button “Fit all groups”. Fitting will occur for all of the groups specified in the box labeled “Groups to fit”. You can change the groups to be fitted. This is sometimes imperative, e.g. if the detector mask was defined such that one or more of the groups contains no data, in which case PAN cannot fit these groups. In this case the “Fitting status” box will read “Fit cancelled”.

Having clicked “Fit all groups” you can watch as the program fits the selected groups using the chosen model including constraints. At this stage you should check the fits to make sure that everything is OK.

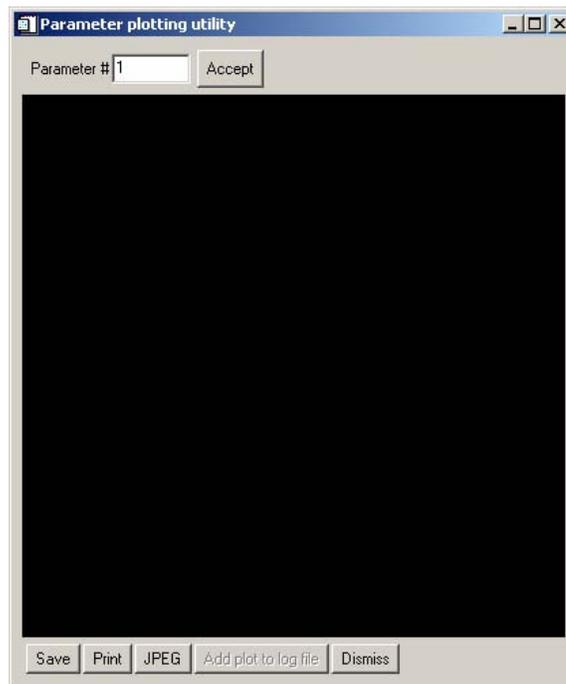
You can save the fitted data by clicking “File → Save fit parameters as text”. A text file will be created with the fit information. The following screen shot shows an example of such a file.

```
deuterated.fit - WordPad
File Edit View Insert Format Help
#####
Group: 1
#####
Curve 1: GAUSSIAN
#0: area: 1.490e+000 +/- 3.586e-002
#1: center: -1.184e-002 +/- 5.827e-004
#2: FWHM: 5.748e-002 +/- 1.282e-003
-----
Curve 2: LORENTZIAN
#3: area: 2.706e+000 +/- 6.514e-002
#4: center: -1.184e-002 +/- 0.000e+000
#5: FWHM: 5.820e-001 +/- 2.379e-002
-----
Curve 3: BACKGROUND
#6: offset: 1.951e-002 +/- 1.142e-002
#7: slope: 0.000e+000 +/- 0.000e+000

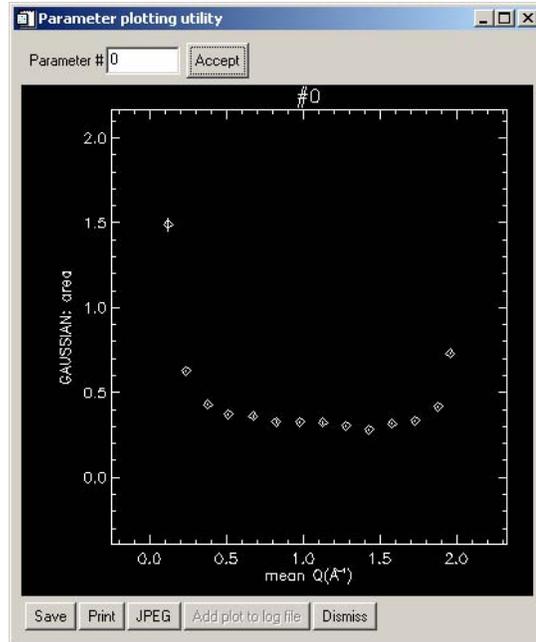
Chi-squared: 0.875
#####
Group: 2
#####
Curve 1: GAUSSIAN
#0: area: 6.262e-001 +/- 4.008e-002
```

Note that this file does not contain information about the constraints that you imposed.

■ A very useful tool within PAN allows you to plot the fit parameters as functions of Q and to save them in three-column text files. Click the button “Plot fit parameter” and the following screen will appear.

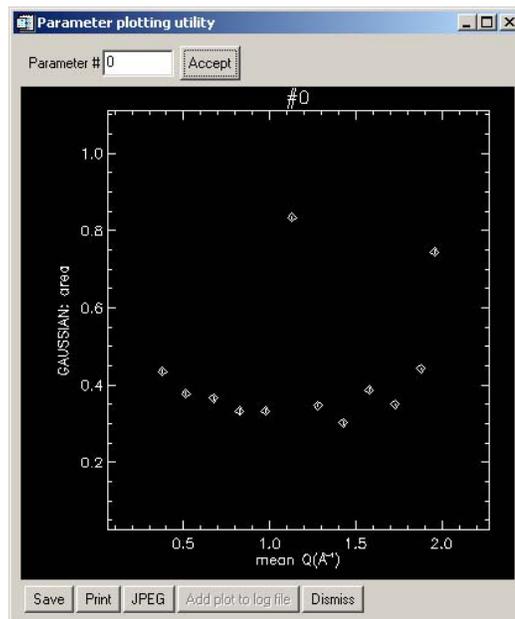


You can now examine any fitting parameter by entering its number. If you do not remember which is which, take a look at the text box on the right hand side of the main PAN widget.



In this example parameter #0 is the area of the Gaussian. For the first group, and perhaps the second group also, the parameter does not behave as expected. It is quite often the case that DCS data at low angles is problematic, so it is prudent to ignore these groups.

The example below (using different input data) illustrates a situation where a single group is clearly suspect, suggesting that something went wrong during data reduction.



These examples are intended to show that there is no way to do the data analysis without a certain amount of critical human intervention. It is important to check each fit, having in mind some idea of the expected behavior of the various fit parameters.

■ Within the application “Plot fit parameter” clicking “Save” will create a three-column text file containing Q, Parameter(Q), Error_Parameter(Q). An example follows.

```

AreaG.txt - Notepad
File Edit Format Help
# mean Q(13!sA!r!u!9 %!3!n!E-1!N) GAUSSIAN: area Error
0.118550      1.4899157      0.035856972
0.235795      0.62619898     0.0040079714
0.376218      0.42821930     0.0040711854
0.513126      0.37128243     0.0038005932
0.674625      0.35932549     0.0048570965
0.823851      0.32709957     0.0060900922
0.976357      0.32652417     0.0050481186
1.12889       0.32184995     0.0070761349
1.27890       0.30290061     0.0044743913
1.42887       0.28181024     0.0048791296
1.57799       0.31429279     0.0038804216
1.72812       0.33468799     0.0029891068
1.87967       0.41534489     0.0020040440
1.95852       0.73104866     0.0048359324
  
```

Getting the EISF from the fit

Given the fits to the protonated and deuterated samples, we wish to obtain an experimental EISF. One possibility is to use the following expression:

$$\text{EISF} = \frac{G_p}{G_p + L_p - w \cdot L_d}$$

where G_p and L_p are the areas of the Gaussian and Lorentzian functions that fit the protonated sample scattering function, L_d is the corresponding area of the Lorentzian

function for the deuterated sample, and $w = m_p / m_d$, m_p and m_d being the masses of the protonated and deuterated samples respectively.

Since there are relatively few groups, you can do this type of calculation using Excel, paper and pencil, or whatever method takes your fancy. The following table shows an example calculation.

Protonated 410K					Deuterated 400K		
Q	Gp	eGp	Lp	eLp	Ld	eLd	EISF
0.119	1.283	0.030	2.826	0.061	2.711	0.064	0.535
0.236	1.617	0.005	0.453	0.004	0.386	0.004	0.886
0.376	1.806	0.003	0.477	0.003	0.316	0.003	0.867
0.513	1.535	0.004	0.565	0.003	0.313	0.003	0.807
0.675	1.345	0.005	0.678	0.004	0.296	0.004	0.733
0.824	1.190	0.005	0.758	0.005	0.298	0.004	0.676
0.976	1.041	0.005	0.806	0.005	0.295	0.003	0.627
1.129	0.930	0.009	0.805	0.008	0.291	0.005	0.600
1.279	0.851	0.005	0.758	0.005	0.301	0.003	0.600
1.429	0.836	0.005	0.696	0.005	0.295	0.004	0.621
1.578	0.836	0.004	0.594	0.004	0.270	0.003	0.664
1.728	0.832	0.003	0.543	0.003	0.263	0.002	0.688
1.880	0.760	0.003	0.471	0.002	0.268	0.002	0.716
1.959	0.841	0.006	0.464	0.005	0.254	0.004	0.735
EISF=Gp/(Gp+Lp-w*L_d)					w=m_h/m_p=3.6/5.7		

Note that errors are not calculated.

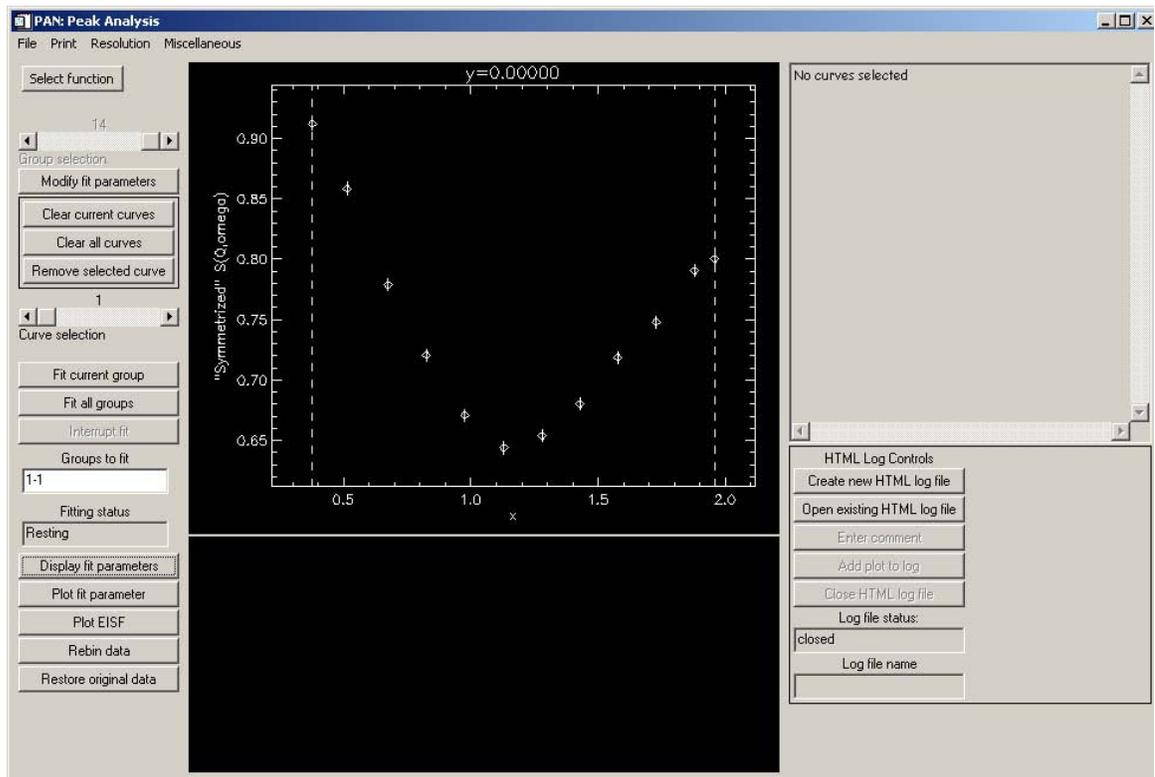
■ Once you have generated your experimental EISF, you can create a three-column text file and then use PAN to fit the EISF to a model such as one of the models described in the Summer School handout. Here is an example of an experimental EISF text file, called “410K-EISF.txt”:

```

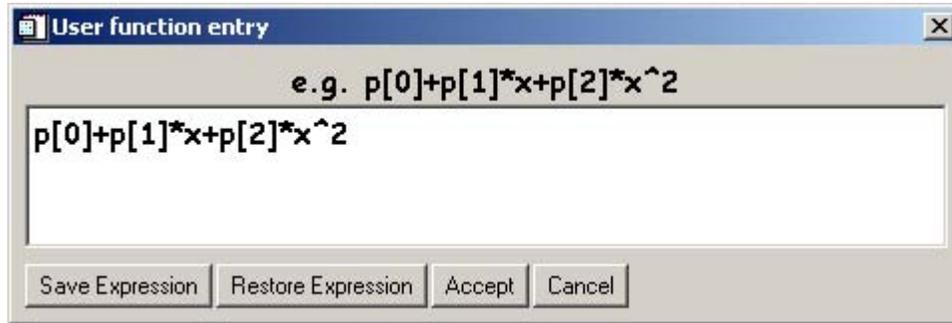
410K-EISF.txt - Notepad
File Edit Format Help
# mean Q(1315A1r1u19 %131n1E-11N) LORENTZIAN: area Error
0.376218 0.912186257 0.005
0.513126 0.858558058 0.005
0.674625 0.778845159 0.005
0.823851 0.720735567 0.005
0.976357 0.670732387 0.005
1.12889 0.643845986 0.005
1.2789 0.653886362 0.005
1.42887 0.680011161 0.005
1.57799 0.718775341 0.005
1.72812 0.747863048 0.005
1.87967 0.790612514 0.005
1.95852 0.800421436 0.005]

```

■ You can load this type of file within PAN, selecting “File → ASCII files → Load three col ascii data”.



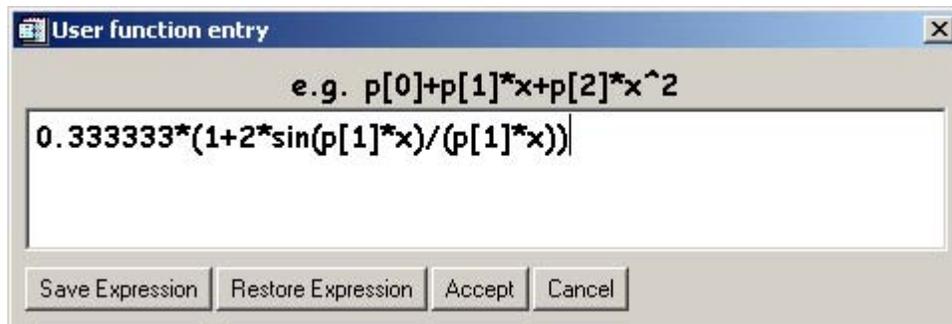
■ To fit the EISF you have to define a user function. Click the “Select function “ button and select “userfunction”.



The default expression, shown above, should be replaced with something more appropriate. As an example, the user function for a model where a proton is jumping among three equivalent sites equally spaced on a circle is as follows:

$$0.333333*(1+2*\sin(p[1]*x)/(p[1]*x))$$

where $p[1]$ is the parameter r , which is the distance between any two sites.



Note that you can save the expression and later restore it.

Now that your function is defined, the refinement may be performed in the same fashion as before. With luck you will be able to interpret the values of the fit parameters in terms of the model.

Good luck!