NSE Data Reduction

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1 General Description

The objective of a Neutron Spin Echo experiment is the determination of the Intermediate Scattering Function, I(Q,t). This is the time correlation function of the scattering length density fluctuation (of wave vector Q) in the sample. However, during an experiment, what we measure is the polarization of the scattered neutron beam as a function of the phase current, at different Fourier times, at each pixel (size 1 cm²) of the 2D detector (32×32 pixels).



Fig. 1. Example of a Spin-Echo. The green line is the fit to equation 1. Note the N_{up} and N_{down} points at the end of the measurement. During a regular experiment only the points around the echo position (the absolute minimum of the curve) are measured.

The number of neutron counts at each position on the detector, N, as a function of the phase current, ϕ_c , can be fitted to a damped cosine function:

$$N = N_0 + A \exp\left[\frac{(\phi_c - \phi_0)^2}{2\sigma^2}\right] \cos\left[\frac{360}{T}(\phi_c - \phi_0)\right]$$
(1)

The amplitude A wholly contains the information regarding I(Q,t); however, a correct determination of A requires a careful determination of all the fitting parameters in Equation (1). The period of the cosine function, T, and the width of the Gaussian envelope, σ , depend only on the characteristics of the incoming beam (mean wavelength and wavelength spread). The average number of counts N_0 depends on many factors such as the counting time or the scattering power of your sample. The so called echo point ϕ_0 , depends on the field path experienced by the neutron.

The effect of the less-than-perfect efficiency of the flippers, the polarizer, and the analyzer is removed by measuring the count rates with the $\pi/2$ -flippers off and the π -flipper both off and on, giving the non spin flip, N_{up} , and spin flip counts, N_{down} , respectively. These are measured at the end of each echo scan at each Fourier time. The measured value of the polarization of the scattered beam at the echo point $\langle P_z \rangle_S$ is then given by:

$$\left\langle P_z \right\rangle_S = \frac{2A}{N_{up} - N_{down}}$$
 (2)

Inhomogeneities in the magnetic field may further reduce the polarization. As these inhomogeneities are not correlated with $S(Q,\omega)$ or $f(\lambda)$, their effect may be divided out by measuring the polarization from a purely elastic scatterer:

$$\left\langle P_z \right\rangle_E = \frac{2A^E}{N_{up}^E - N_{down}^E} \quad (3)$$

 $\langle P_z \rangle_E$ as a function of the Fourier time represents effectively the resolution of the instrument.

In order to ensure that the dynamic scattering from everything that is not the sample does not contribute to the final I(Q,t), a background measurement must be performed. The sample holder (including the pure solvent, if any) is measured under identical conditions to those of the sample.

The normalized intermediate scattering function at each position on the detector is then obtained by:

$$I = \left[\frac{2(A - TA^{bgr})}{(N_{up} - N_{down}) - T(1 - \phi_V)(N_{up}^{bgr} - N_{down}^{bgr})}\right] / \frac{2A^E}{N_{up}^E - N_{down}^E}$$
(4)

where *T* is the ratio of the transmissions of the sample and the background, and $(1-\phi_V)$ is the volume fraction of the solvent in the sample.



Fig. 2. Typical example of a measured echo. Note how only the section of the echo close to the echo point is measured.

The use of a 2D detector allows you to collect more data in the same amount of time. However, in analyzing your data you have to consider that the field path experienced by the neutrons collected in different parts of the detector will vary. Therefore, the echo points will be different. The usual procedure is to group the detector pixels in order to obtain a good signal to noise ratio (not forgetting to consider how strong is the Q dependence of the dynamics of your sample) and to analyze separately each of these 'super pixels'¹.

Therefore, the reduction procedure consists mainly of the following steps:

- 1) Fitting of the echo at each time and pixel according to equation (1).
- 2) Determination of the polarization of the scattered neutron beam using equation (2).
- 3) Correction for resolution and background effects using equation (4).

¹ In the following of this handout we will always refer to these 'super pixels' simply as pixel.

4) Grouping of different 'zones' of the detector into a limited number of Q arcs, to give the corresponding I(Q,t) functions (see fig. 3).



Fig. 3. Detector image. The detector is here divided in 7 arcs, delimited by the blue thick line. Each pixel of the detector has been grouped into a 2×2 'super' pixel (shown by the grid) in order to improve the signal to noise ratio. The green zones represent the part of the detector that is actually physically masked by the supports of the NSE. The cyan box indicates the currently selected pixel.

Whereas steps 2, 3, and 4 require only straightforward analytical data handling, the first fitting procedure is somewhat critical. As a matter of fact, the fitting to an oscillating function can be trapped in local minima, where the echo point is offset from the true echo phase current by ± 360 degrees (one oscillation of the cosine). Therefore, some user scrutiny is necessary during the reduction process in order to ensure the correct evaluation of I(Q,t). The user should make sure that the quality of each fit is satisfactory. Moreover, for obvious physical reasons, it is required that the ϕ_0 values obtained from the fit vary smoothly along the detector and as a function of the Fourier time.

Fortunately, the phase map (the value of the echo point phase current at each pixel on the detector at each Fourier time) does not depend on the scattering function. It should be nearly identical for any sample measured at the same instrument conditions. Therefore, the phase angle at the echo point is determined for the reference sample and exported for the fitting of the sample and background data.

2 NSE Data reduction in DAVE

The Neutron Spin Echo data reduction software in the Data Analysis and Visualization Environment (DAVE) reduces and analyzes data from the NG-5 Neutron Spin Echo instrument at the NIST Center for Neutron Research.

To get started, open DAVE and select "<u>Reduce NSE Data</u>" from the Data Reduction menu/tree. A window will pop-up, shown in Fig. 2. The window has several features:

- 1) A menu bar
- 2) A tab menu interface: DATA FILES; GENERAL; DATA SET; FITTING
- 3) A Detector Image
- 4) A help text line
- 5) A CD type menu for stepping through the Fourier times and
- 6) A Plot window.

You will see the detector image (top right) and the main plot (bottom right) displaying dummy data.



Plot Window

Fig. 4. NSE Data Reduction window in DAVE.

2.1 Load Data Files

From the file menu, select Open .echo file(s). A dialog window will open, which allows you to select the .echo files you want to reduce. You can browse through the directories and select as many files as the memory of your machine will allow. I recommend not opening more than a dozen or so files at a time to make organization more

clear. If all of the files open successfully, they will be displayed as data files in the directory tree under the " \underline{Data} files" tab, grouped according to their stated exchanged wave-vector, Q (see Fig. 5).

2.1.1 Echo files

The raw data collected by the NSE are saved in an ascii file named mxxxx.echo (xxxx is an automatically incremented 4-digit run number), usually rather big (~1.4 Mb). The echo file contains:

a) the description of the performed scan;

- b) for each Fourier time, the values of the currents set to the different coils and the corresponding physical parameters, e.g. Fourier time, Q,...
- c) for each phase point, the phase current, the counters and multimeter readings, and the neutron counts recorded on each detector pixel.

2.1.2 Echo file location

The echo files reside on the linux echo computer in the directory "/var/nse". In addition, they are mirrored to a central server, "Charlotte", in the "NSE Data/Current" folder. Charlotte is visible to Macs through Appleshare (connect as a guest), and to Windows through the Network Neighborhood (NCNR group, map the "NSE Data" folder as a network drive). This central server allows you to (within the building) work directly with data on Charlotte. You can see and reduce the data in the computer room or in the user office. Once your experiment is finished your data can be copied from Charlotte onto a Zip disk or CD and carried home. Data reduction can be completed (if necessary) at your home institution.

2.2 Select the file type

Select a file in the tree. Right-click on the selected file and a menu appears. The first submenu option, Select data set type allows you to choose the object type: untyped, resolution, sample, cell. The center of the file's icon indicates the type of file: red for resolution, green for sample, blue for cell, black for no type. The outside edge color of the icon refers to the file reduce status: red for not reduced, green for reduced.



Fig. 5. How to select the data file type.

2.3 Select the binning factor

In order to improve the signal to noise ratio it is advisable to group together different pixels on the detector. This can be done from the DATA SET tab (see section 3.3). 2×2 or 4×4 binning are most commonly suitable. In choosing the binning factor, remember that the NSE instrument has a quite large incoming wavelength spread and therefore not very good Q resolution; on the other hand the echo point varies along the detector. You can apply different binning factors to your samples, however, keep in mind that, later in the reduction process, to import the phases from your reference file, both the sample and the reference have to be analyzed with the same binning factor.

MSE Data Reduction m3859.echo: "1pp	o CP
File Plot Options Image Options Detector Options	Cal
DATA FILES GENERAL DATA SET FITTING	
Current Filename m3859.echo: ''1pp CPyC	
Binning/blocking Factor	
2 Apply Binning to all data	
Transmission	
1.00000	
Volume Fraction	
0.000000	
Apply Trans and volfrac	

Fig. 6. The binning factor.

2.3.1 Additional parameters in the DATA SET and GENERAL tabs

From the DATA SET tab you can also input the Transmission and Volume Fraction values for your sample. However, these quantities are not used until the final I(Q,t) is calculated. The program will ask anyway for these parameters before performing the final step of the reduction process.

From the GENERAL tab you can input the position of the beam center and the number of Q arcs in which your detector has to be divided. This will be the number of I(Q,t) functions you will end up with. Again, the statistical error of your final I(Q,t) point can be decreased using a reduced number of arcs and the Q resolution on NSE is not high; however, your sample might have a strong Q dependence of the intermediate scattering function. The beam center position and the number of Q arcs do not affect the reduction process until the final grouping into Q-arcs is performed; however, the image display of the different arcs will be affected.

2.4 Mask low quality pixels

Once the data set have been loaded, the Detector Image becomes able to show the integrated number of counts per echo scan at each pixel as a color coded image (the scale is shown on the left). The dark green areas cover the portion of the detector which is physically masked in the instrument. The blue thick lines mark the borders between the different Q arcs. The cyan rectangle highlights the pixel which is actually selected. The Main Plot Window is now able to show the measured echoes for the highlighted pixel. You can navigate around the detector image with the arrow keys when the mouse is in the image, or you can highlight a specific pixel by left clicking on it. You can also step through different Fourier times using the CD type menu bar or with the "Page Up" "Page Down" keys on your keyboard.

You will notice that some of the pixel have very bad counting statistics, and you may want to mask them before proceeding to the fitting of the echoes. The "m" key on your keyboard will mask/unmask the selected pixel. The "enter" key (always) and the right click button (except when the Detector Image is showing the Phase) will popup a menu that will allow you to a) apply the current mask to all Fourier times, b) apply masking of the highlighted pixel to all Fourier times; c) apply the current mask to the subsequent Fourier times, d) apply masking of the highlighted pixel to the subsequent Fourier times. The pixels masked by the user will get a light green color. You will be able to mask a pixel at any time during the reduction procedure.



Fig. 7. Masking of a low count pixel.

2.5 Mask low quality phase points

Sometimes, it may happen that the measurement gives obviously wrong results at some specific phase current value. This can be clearly seen from the main plot window showing I v. phase (I stands for intensity, neutron counts, and phase stands for phase current). This occurrence it may be related either to a change in the surrounding magnetic field (shown by the recorded magnetic fields at the sample position) or by an incorrect reset of the detector counts. You can mask/unmask that specific phase point by left clicking on the main plot window. The program will mask the point whose phase current is the closest to the phase current the mouse is pointing at. The masking will be effective for each pixel at that specific Fourier time.



Fig. 8. Masking of a bad phase point. Note that its color becomes cyan and the error bar is not displayed anymore.

2.5.1 The phase current expressed as a phase angle

During an echo scan the quantity that changes is the current going through the so called phase coil. In fact, in the live update program, for example, the phase points are plotted versus the value of this current. However, since the phase current is proportional to the precession angle of the neutron spin, this quantity can be expressed as an angle, as it is done in the NSE reduction program. A linear relation holds between the phase current values and the phase values expressed as an angle. However, the zero angle phase point (that should be the echo point) is only approximately pre-determined. As a matter of fact, this somewhat arbitrarily defined zero point is chosen in a way that the echo point for any pixel on the detector will fall inside the investigated window. The N_{up} and N_{down} counts are collected for a zero value of the phase current, as it can be seen from the live update, however, in the NSE reduction software, they are shown at high phase angle values only for clarity sake.



2.6 Reduce a Resolution Object

Select a resolution file in the tree, under the DATA FILES tab. Right-click on the selected object and when the menu appears select Fit Operations: Fit Echoes (Resolution).



Fig. 9. Fitting a resolution file.

This will bring up a progress bar and all of the echoes in the resolution file (corresponding to the different pixels) will be fit. Once it is done the file icon will have a green edge. Moreover, the detector image and the main plot window will display the results of the fitting. You can start the fitting procedure also from the FITTING tab clicking on the button Fit.

2.6.1 FITTING tab options

For the reduction of the resolution file, the default settings for the fitting procedures are "vary" for the Av, A, PH, and T parameters, and "fix" for the W parameter. In fact, the width of the Gaussian envelope has been determined previously by the instrument scientist. You should not change these settings, although, in special cases, you may do this. For example, if you have measured a complete Gaussian envelope with many phase current points you may want to determine the value of W. From the Method button you can choose among slightly different algorithms for the fitting of the echoes: arc, spiral, expand. The default value is arc.

2.7 Inspecting the fit results

After the fitting, the Detector Image is able to show the resulting fitting parameters: Av, Ph, T, W. It is also possible to inspect the signal (the polarization of the beam, calculated using equation 2) and the χ^2 of the fit. You can use any of these options to inspect thoroughly and efficiently the quality of the fit. To select the quantity to be shown on the detector image you can either use the Image option menu bar or the Detector Image popup menu that can be invoked by the 'enter' key (always) or by a right click (except when the Detector Image is showing the Phase) on the Detector Image window. The main plot window will now show, beside the measured echo point, the obtained fit as a thick red line.



Fig. 10. Different ways of selecting the quantities displayed in the Detector image and main plot windows.

2.7.1 The Error Bars Image

It may be interesting to inspect the error associated to each fitting parameter along the detector surface. To do so select Display Image Error bars from the Image Options menu, or with the right-click on the Detector Image. A new window will pop-up, showing a color-coded image of the absolute error of the quantity shown on the Detector Image. Of course, if the Detector Image is showing the raw counts on the detector, the error will be the square root of the counts.

Special care should be taken to ensure that the echo points found by the fitting procedure vary smoothly on the detector and with the Fourier time. To do this from the Image Options select Phase and in the main plot window choose Fit Phase v. Fourier Time. You can also toggle the Auxiliary Plot in order to be able to see at the same time the I v. phase and the Fit Phase v. Fourier Time plot. Remember, that the Auxiliary Plot does not allow any user interaction: you cannot mask phase points or refit data from the Auxiliary plot.

2.8 Refit pixels

During your inspection of the fit you may not be satisfied of the results of the fitting in few, many, or all the pixels. You have different options: you can refit a pixel in many ways.

2.8.1 ... from the FITTING tab

The Fit Pixel button on the FITTING tab will refit the pixel highlighted in the Detector Image using as starting parameters the values reported in the FITTING tab. You can input new starting parameters in the FITTING tab to obtain a more satisfactory fit. Type the desired fitting parameter value in and hit 'enter', the fitting function in the plot window will be updated as well, allowing you to have a feeling of the quality of your initial guess.

2.8.2 ... from the Detector Image (Phase map)

When you chose to have the detector image showing the echo Phase, a couple of sliders will pop-up.



Fig. 11. Sliders for choosing the starting phase and period values in the re-fit of a pixel echo.



Fig. 12. Re-fit of a bad pixel. Note the reduction of the χ^2 value.

Right clicking with your mouse on a pixel on the Detector Image window will refit the pixel using the values selected by the sliders as starting parameters for the phase and the period.

2.8.3 ... from the main plot window (Fit Phase v. Fourier Time)

One very useful tool is the plot of Fit Phase v. Fourier Time. If this plot is selected, then you can look at the fit phase curve, which should be smooth. If there are discontinuities, you can refit points by placing the mouse a) at the time to refit, b) vertically at the position of the phase value you would expect for a smooth curve, and c) by left clicking on that spot with the mouse. The pixel will be refit with the phase value at the mouse position as the starting value, and either T=360 or T = the value in the click-refit phase slider as the starting period. To see that the fit

worked correctly, you can also open an auxiliary window. The auxiliary window will show a plot that complements the main plot window.



Fig. 13. Re-fit of a bad pixel from the 'Fit Phase v. Fourier Time' plot window. Note the use of the auxiliary plot to check the quality of the fit.

2.8.4 ... from the fitting tab using the "smooth t" button

It is sometimes easier to use the "smooth t" button to redo the fits for all of the pixels at the current Fourier time. The smoothing routine starts at the center of the image and moves outward, keeping the phases within 180° of their neighbors as it moves out from the center. This is essentially the same routine that is applied in the "expand" method for fitting all of the data. If there is a bad fit at any pixel, the pixels farther from the center from it will be affected and will likely have the wrong phase as well.



Fig. 14. Re-fit of all the echoes at a Fourier Time using the 'smooth t'button.

2.8.5 ... from the fitting tab using the " \pm 360" buttons

If you believe that all of the phases are off by a period, you can use the "+360 refit" or "-360 refit" button to shift all of the phases in the Fourier time and redo the fits.

Inspect carefully your fits at each Fourier time. Remember that having good fits for your reference sample is crucial for a correct reduction of your data. If the statistical quality of one of the pixels is poor it might be better to mask that point instead of accepting a non-significant fit. If the signal from you reference sample is low, less than \sim 20 (it may happen on the edge of the detector, at high Fourier times), you are going to have big error bars for the corresponding point in the I(Q,t) of your sample; again it might be better to just mask the unsatisfactory points.

2.9 Reduce a sample or cell object

Once you have a completed the fitting of the resolution file, in the file tree, under the "Data Files" tab, select another data object with the same Q value. Again, you should inspect for pixels with bad counting statistics and for phase points with glitches. If any, mask them as you have learned to do for a resolution file.



Fig. 15. Fitting a sample or background (cell) file.

Right-click on the selected object and when the menu appears select Fit Operations: Import Phases (Sample, Cell). This will allow you to import the phases and the masking from the resolution object. You can perform the same operation from the "FITTING" tab, using the "IMPORT PHASES" button. Note that the resolution object must have the same binning as the current object in order to import its phases. After selecting import phases the following dialog appears.

🚳 SELECT PHASE SET 🛛 🛛 🔀	🚳 SELECT PHASE SET 🛛 🛛 🔀	🚳 SELECT PHASE SET 🛛 🔀
m3862.echo	m3062.echo	m3062.echo
phase Vary	phase vary	phase vary
period for	period fix	period fix
ОК	fit phase offset (constant phase) OK	Vary Ter UK
Cancel	Cancel	Cancel

Fig. 16. Options for the fitting of a sample or background (cell) file.

You can choose the filename of the data object with the phases and periods to import and decide whether to fix or vary these parameters during the fit process. Since the period and the echo phase point only depend on instrumental condition you should choose fix for both the parameters. However, in order to allow for a constant phase offset in your data, you may also select the "fit phase offset (constant phase)" option. When you choose this routine, the program will keep the phase as a free fitting parameter in the fitting of a four by four pixels area in the center of the detector at each Fourier time. The results obtained for these pixels will be compared with those obtained for the reference scan. The offset between the echo phase points found for the two measurements will be added to the echo phase points of the reference. It will be constant on the surface of the detector but it will vary with the Fourier time. The offset is kept as a fixed parameter in the fitting of all the other pixels. This procedure is not recommended for a cell object, when your counting statistics may be very poor. Once you made your selection, simply click "OK" to do the fits. When the fitting is complete, examine the results to see if individual pixels need to be refit or masked due to poor statistics.

2.10 Calculate I(Q,t)

Once you have fitted your sample, resolution and cell objects, you are ready to calculate I(Q,t). Note, by this point you should have entered the X and Y beam center values in the "GENERAL" tab. Select the data object you want to calculate I(Q,t) for and then right click on it. From the popup menu that will appear choose the option "Calculate I(Q,t)". You can also use the "Calculations" menu from the Menu bar.



Fig. 17. How to calculate I(Q,t).

A window appears which allows you to select the data objects for Sample, Resolution and cell (background). You can also set the number of Q arcs, the sample transmission, the sample volume fraction (e.g. 96% solvent means a volume fraction of 0.04), and the cell transmission value. Once everything is entered, hit the OK button. The results of the calculation will appear in a new window.

SELECT DATA FOR I(Q.1) C	slculation
Sample Choices m3860.echo	
Resolution Choices m3862.echo	*
Cell Choices m3884.echo	-
Number of Q Ascs 7	
Sample Trans 0.774	
Sample Volinac 0.072	
Cell Trans 0.873	
0K.	
Cancel	

Fig. 18. Files and parameters definition for the calculation of I(Q,t).

2.11 The I(Q,t) display

The I(Q,t) display window allows you a preliminary inspection of your results. You can resize the window, zoom in by either dragging the right mouse button on the plot or by entering values in the min and max fields, and unzoom by right-clicking in the plot. The legend can be dodged via the arrow keys and moved in the four corners of the screen using the "Page Up", "Page Down", "Home", and "End" keys. Since at times the plots get cluttered, you can step through the individual I(Q,t) curves via the "Step through curves" button.



Fig. 19. Display I(Q,t) window.

You can also perform a preliminary analysis of your data with an exponential or stretched exponential fit. Finally, from this window you can export your data in several different formats:

- 1) DAVE. The file saved using this format is binary can be loaded by other DAVE programs for visualization and analysis, in particular PAN (Peak Analalysis).
- 2) ASCII Files. Each I(Q,t) function will be saved on a different ascii file named IQT_q.qqqq.dat (where q.qqqq is the actual Q value). The files have one line column description and four (space separated, fixed size) columns: Q value, Fourier Time, I(Q,t), error bar. This is the format used by the IGOR NSE reduction program.
- 3) Ascii File. A single ASCII file with two header lines, indicating the arcs' Q values, and n_Q+1 (space separated, fixed size) columns (n_Q being the number of Q arcs). The format of the columns is: Fourier Time, I(Q₁,t), error bar, I(Q₁,t), error bar, ... The fit results are saved as well in a separate file with the info extension.
- 4) Separate 3 column ASCII files. Each I(Q,t) function will be saved on a different ascii file named IQT_q.qqqq.txt (where q.qqqq is the actual Q value). The files have eight lines of description and four (space separated, fixed size) columns: Q value, Fourier Time, I(Q,t), error bar.

2.12 Saving and restoring your session

At any moment during the reduction procedure you have the possibility to save your session. From the "File" menu in the menu bar just select "Save session". This will create a binary file with extension sav that can be loaded again using the "Restore session" command from the File menu. Remember that restoring a saved session will overwrite everything in the present session. When you "Quit" the NSE reduction program (again from the "File" menu) you will asked to save your session.

You can also choose to save only the selected object. Do this either through the File menu or from the "Data Files" tab popup menu. When you restore an object it will be added to the present session. The option restore an object allows you to load a saved session as well, however, only the first file will be loaded and added to the objects already present.

3 Additional operations

There are additional operations that you might or might not need during the reduction of your data.

3.1 Remove a Fourier time

For many possible reason you may choose to remove the data corresponding to one or more Fourier time. You can do this right-clicking the object you want to remove the Fourier time from. From the popup menu choose Remove Fourier times. A new interactive window will pop out. Select the undesired Fourier time and hit the button "Remove T". A new object will be created which is missing the indicated Fourier time. Although the run number will be the same as the original file you will recognize it by the labeling that appear when you point on an object.



Fig. 20. Removing a Fourier Time.

3.2 Merge object

Sometimes you may have performed different runs of the same sample at different Fourier times. For example, this could happen if you had to interrupt a run. In this case you want to merge the two runs in one object. You could ask your local contact to do this by working on the original echo files; however the reduction program allows you to do that in DAVE. Right-click on the object you want to merge with another object. From the popup menu choose "Merge". A new interactive window will pop out. From the drop down menu choose the run number of the object you want to merge. A new object will be created containing the data corresponding to the Fourier times from both the runs.



Fig. 21. Merging two files.

3.3 AutomaskSomething

This is another feature that it can help you for the reduction of your data. Instead of looking one by one for unsatisfactory pixels you can just ask the program to look for them and mask them out. The problem is how to define a reliable procedure to identify pixels that are not satisfactory. Here are few possible choices:

- Set a minimum value for total scattering intensity.
- Set a minimum value for the average intensity fit parameter.

- Set a minimum value for the signal (resolution only).
- Set a maximum value for the error bar associated to any of the obtained fitting parameters.



Fig. 21a. Automask Something: After selecting the option from the menu bar (a) a new window will pop-up (b). Select the quantity you want to base your filtering on (c) and then choose between the options 'greater than' or 'less than' (d). Finally, put in the threshold value (e).

Selecting the AutomaskSomething command will pop up a new window. From there you can select the quantity, you want to use for your filtering. The total echo counts and the fitting variables, with their relative error bars, are available to be chosen. Then you can choose to mask all the pixels with the selected quantity being greater or smaller than a threshold value you have chosen.