

# NSE Data Reduction

- 1 General Description
- 2 Tutorial guide through the reduction process
  - 2.1 Load Data Files
    - 2.1.1 [echo files](#)
    - 2.1.2 [echo file location](#)
  - 2.2 Select the file type
  - 2.3 Select the binning factor
    - 2.3.1 Additional [DATA SET](#) and [GENERAL](#) tabs parameters
  - 2.4 Mask low quality pixels
  - 2.5 Mask low quality phase points
    - 2.5.1 [Phase current and phase angle](#)
  - 2.6 Reduce a Resolution Object
    - 2.6.1 [Fitting tab options](#)
  - 2.7 Inspecting the fit results
    - 2.7.1 [Display Image Error Bars](#)
  - 2.8 Re-fit pixels
    - 2.8.1 ... from the Fitting tab
    - 2.8.2 ... from the detector image (Phase map)
    - 2.8.3 ... from the main plot window (Fit phase vs Fourier time)
    - 2.8.4 ... from the fitting tab using the “smooth t” button
    - 2.8.5 ...from the fitting tab using the “ $\pm 360$ ” buttons
  - 2.9 Reduce a sample or cell object
  - 2.10 Calculate  $I(Q,t)$
  - 2.11 The  $I(Q,t)$  display
  - 2.12 Saving your session
- 3 Additional object operations
  - 3.1 Removing Fourier Times
  - 3.2 Merging objects
- 4 NSE reduction command and operations

## 4.1 The menu bar

### 4.1.1 File Menu

- 4.1.1.1 Open .echo File(s)
- 4.1.1.2 Save Session
- 4.1.1.3 Restore Session
- 4.1.1.4 Save Object
- 4.1.1.5 Restore Object
- 4.1.1.6 Import Parameters File
- 4.1.1.7 Export Parameters File
- 4.1.1.8 Quit

### 4.1.2 Plot Options Menu

- 4.1.2.1 I v. Phase
- 4.1.2.2 Fit Phase v. Fourier Time
- 4.1.2.3 Fit Amplitude v. Fourier Time
- 4.1.2.4 Signal v. Fourier Time
- 4.1.2.5 B\_x v. Phase
- 4.1.2.6 B\_y v. Phase
- 4.1.2.7 B\_z v. Phase
- 4.1.2.8 All v. Phase
- 4.1.2.9 Contour Echo
- 4.1.2.10 Toggle Up/Down Display
- 4.1.2.11 Toggle Auxiliary Plot

### 4.1.3 Image Options Menu

- 4.1.3.1  $S(Q(x,y),t=0)$
- 4.1.3.2 Signal
- 4.1.3.3 Av-Average
- 4.1.3.4 A-Amplitude
- 4.1.3.5 PH-Phase
- 4.1.3.6 W-Echo Gaussian Width
- 4.1.3.7 T-Period
- 4.1.3.8 CHISQ

- 4.1.3.9 Display Image Error Bars
  - 4.1.4 Detector Options Menu
  - 4.1.5 Calculations Menu
    - 4.1.5.1 Calculate  $I(Q,t)$
    - 4.1.5.2 AutomaskSomething
    - 4.1.5.3 AutographNSE
    - 4.1.5.4 Calculate Average Width
  - 4.1.6 Printing Menu
    - 4.1.6.1 Print Image
    - 4.1.6.2 Print Plot
    - 4.1.6.3 Print Auxiliary Plot
- 4.2 The DATA FILES tab
  - 4.2.1 Select Data Set Type
  - 4.2.2 Object Operations
  - 4.2.3 Remove Fourier Times
  - 4.2.4 Fit Operations
  - 4.2.5 Calculate  $I(Q,t)$
- 4.3 The GENERAL tab
- 4.4 The DATA SET tab
- 4.5 The FITTING tab
- 4.6 The detector image
- 4.7 The Fourier time CD type interactive menu
- 4.8 The main plot window

## 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  $1 \text{ cm}^2$ ) of the 2D detector ( $32 \times 32$  pixels).

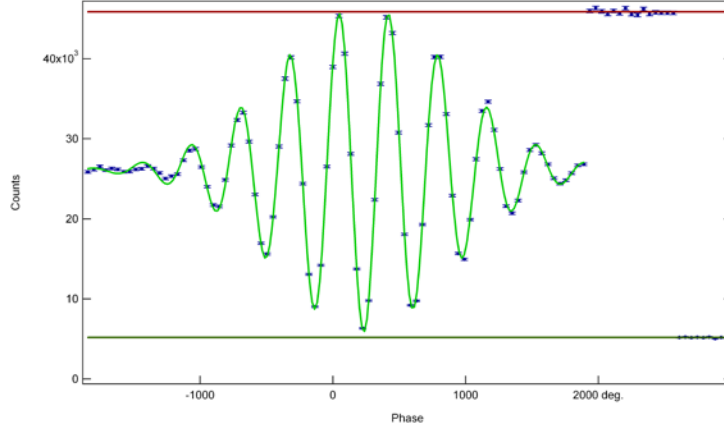


Fig. 1. Example of a Spin-Echo. The green line is the fit to equation 1. Note the  $N_{up}$  and  $N_{down}$  points at the end of the measurement. During a regular experiment only the points around the echo position (the absolute minimum of the curve) are measured.

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

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

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,  $\sigma$ , 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  $\phi_0$ , 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  $\pi$ -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:

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

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:

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

$\langle P_z \rangle_E$  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:

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

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.

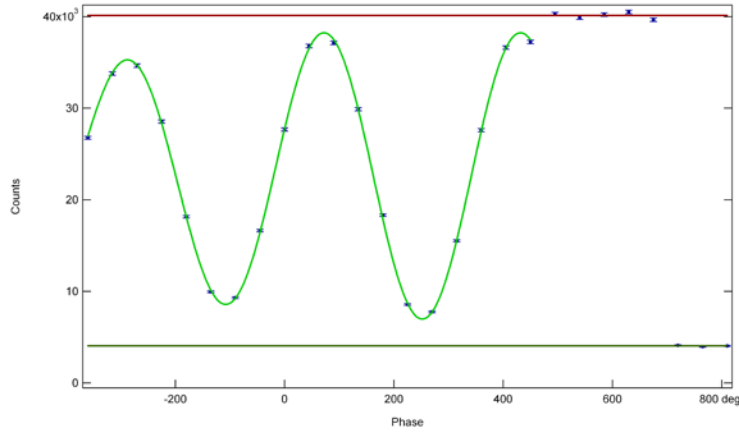


Fig. 2. Typical example of a measured echo. Note how only the section of the echo close to the echo point is measured.

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’<sup>1</sup>.

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).

<sup>1</sup> 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).

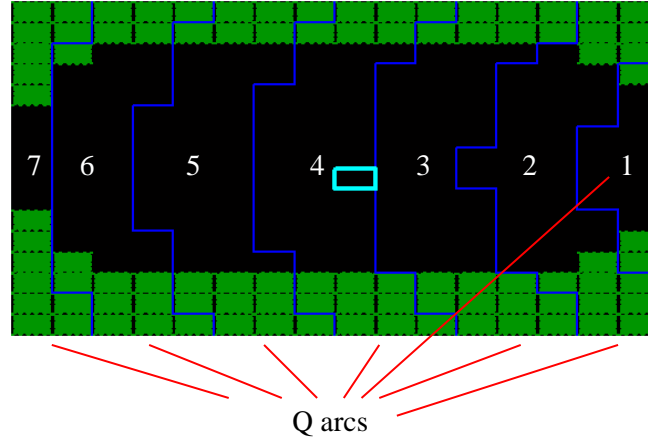


Fig. 3. Detector image. The detector is here divided in 7 arcs, delimited by the blue thick line. Each pixel of the detector has been grouped into a  $2 \times 2$  ‘super’ pixel (shown by the grid) in order to improve the signal to noise ratio. The green zones represent the part of the detector that 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  $\pm 360$  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  $\phi_0$  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 “Reduce NSE Data” 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.

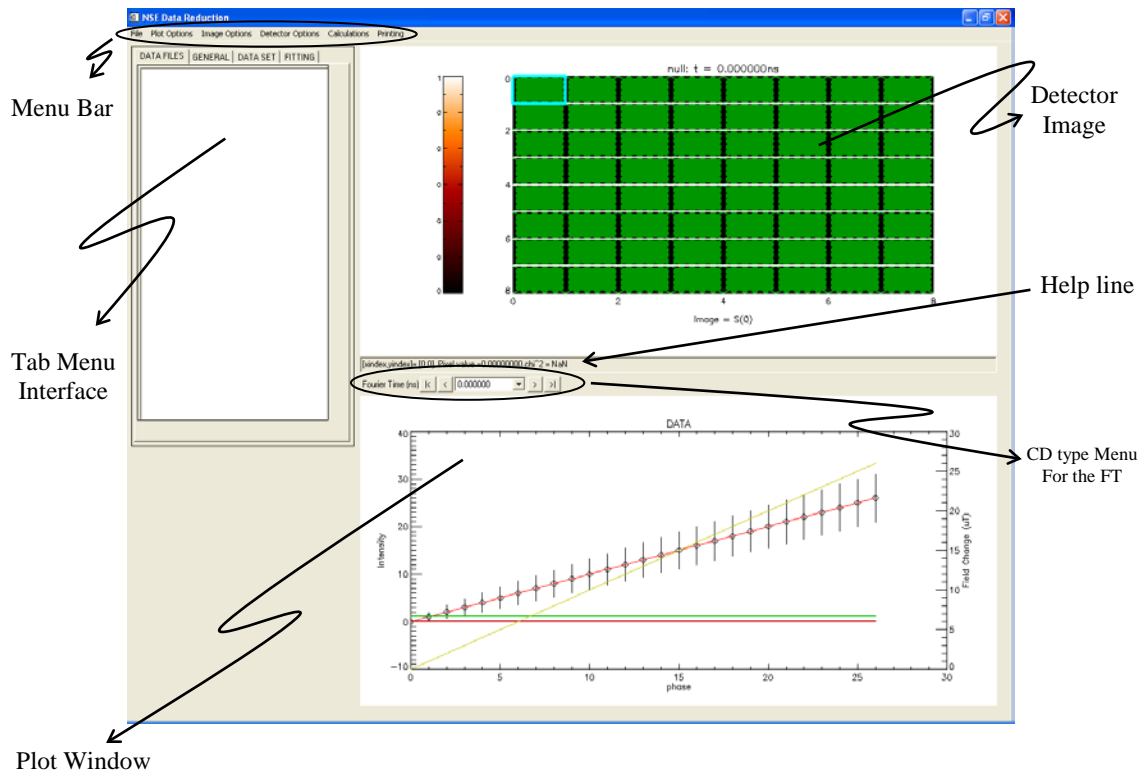


Fig. 4. NSE Data Reduction window in DAVE.

### 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 “[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.

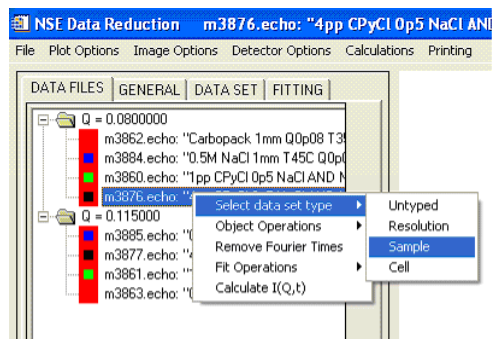


Fig. 5. How to select the data file type.

## 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.

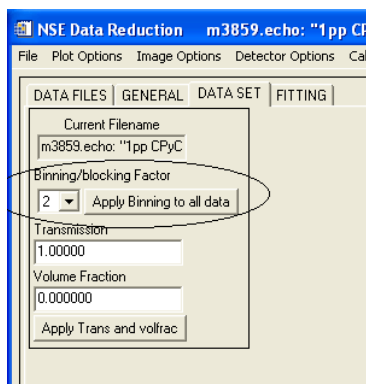


Fig. 6. The binning factor.

### 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.

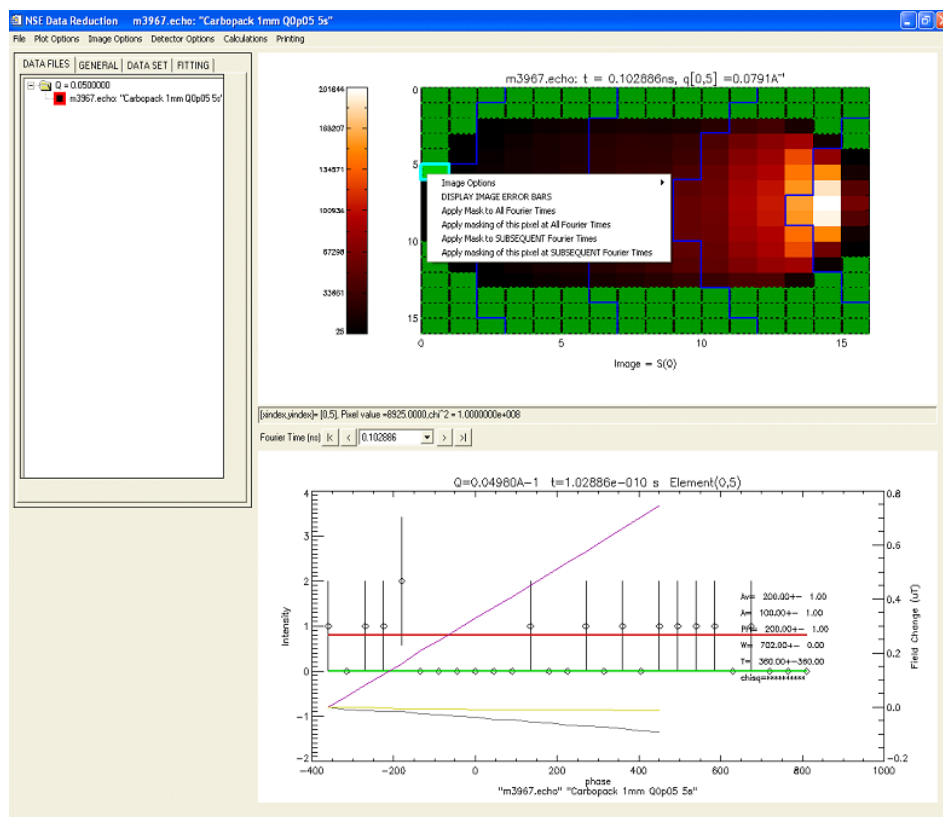


Fig. 7. Masking of a low count pixel.

## 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.

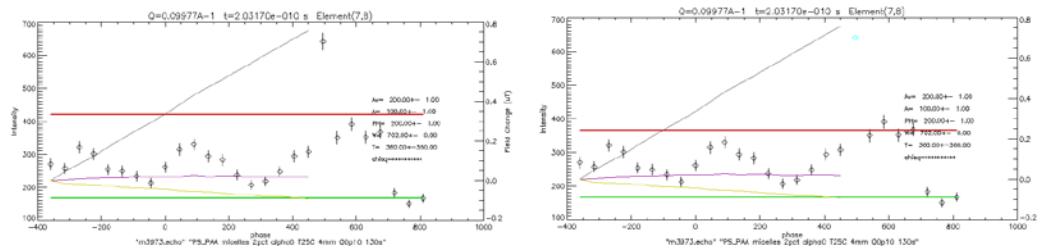


Fig. 8. Masking of a bad phase point. Note that its color becomes cyan and the error bar is not displayed anymore.

### 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.

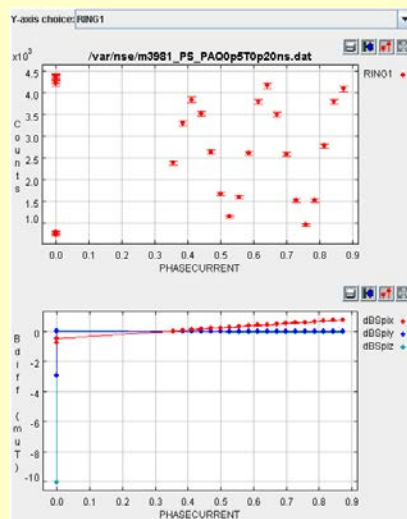


Fig. 8a. Live update window. Note how the echo scan is plotted versus the phase current. Also note that the  $N_{up}$  and  $N_{down}$  points are all taken for a zero value of the phase current.

### 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)**.

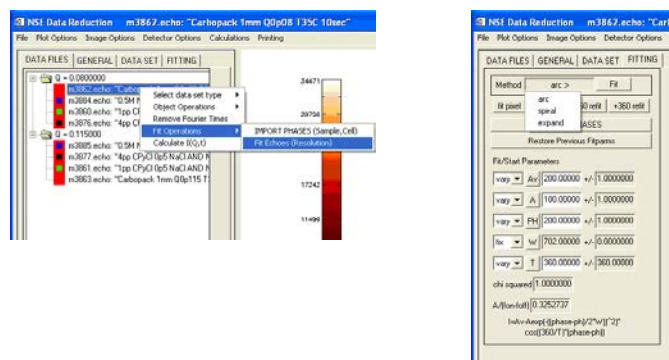


Fig. 9. Fitting a resolution file.

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  $A_v$ ,  $A$ ,  $PH$ , 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:  $A_v$ ,  $Ph$ ,  $T$ ,  $W$ . It is also possible to inspect the signal (the polarization of the beam, calculated using equation 2) and the  $\chi^2$  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.

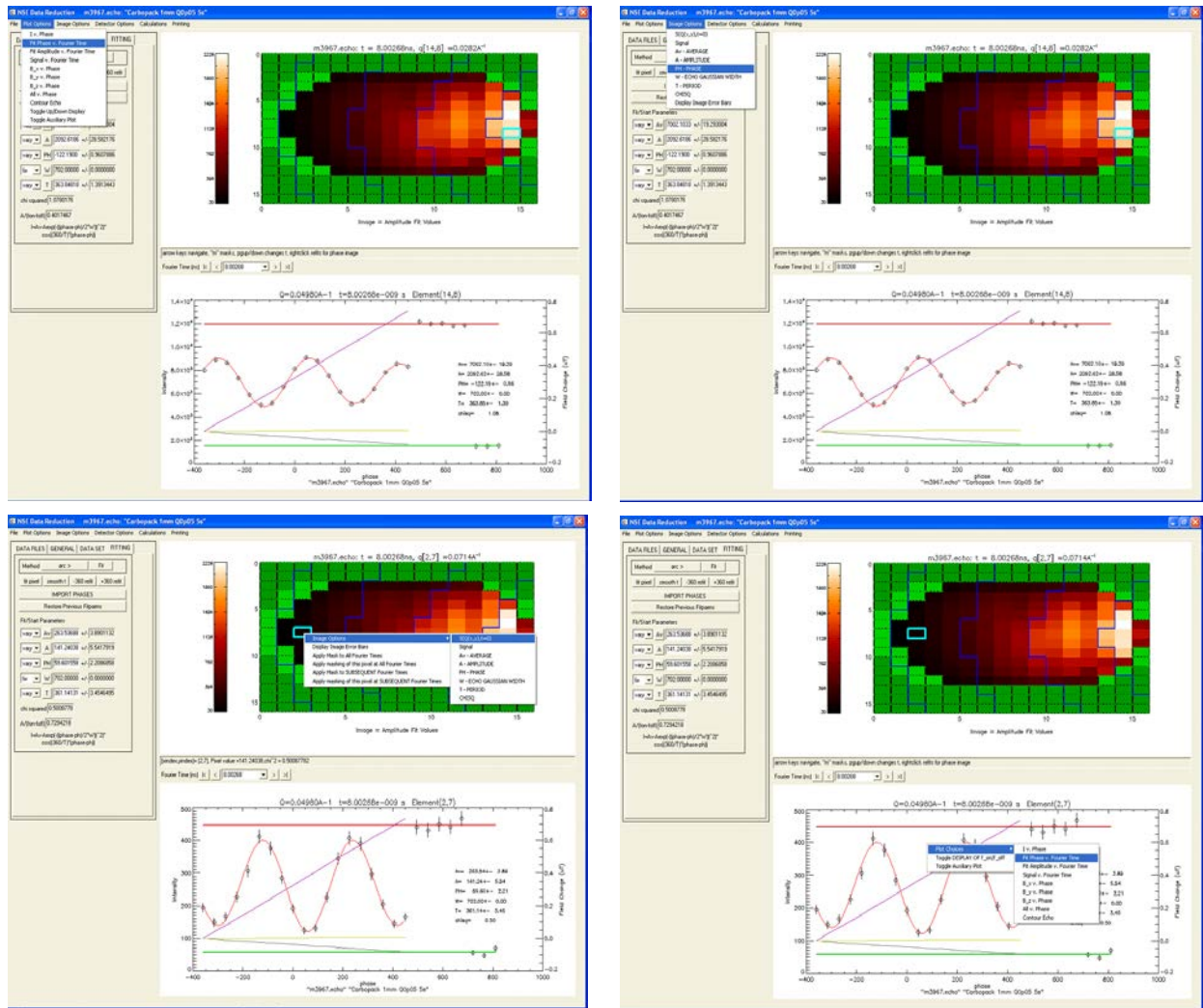


Fig. 10. Different ways of selecting the quantities displayed in the Detector image and main plot windows.

### 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.

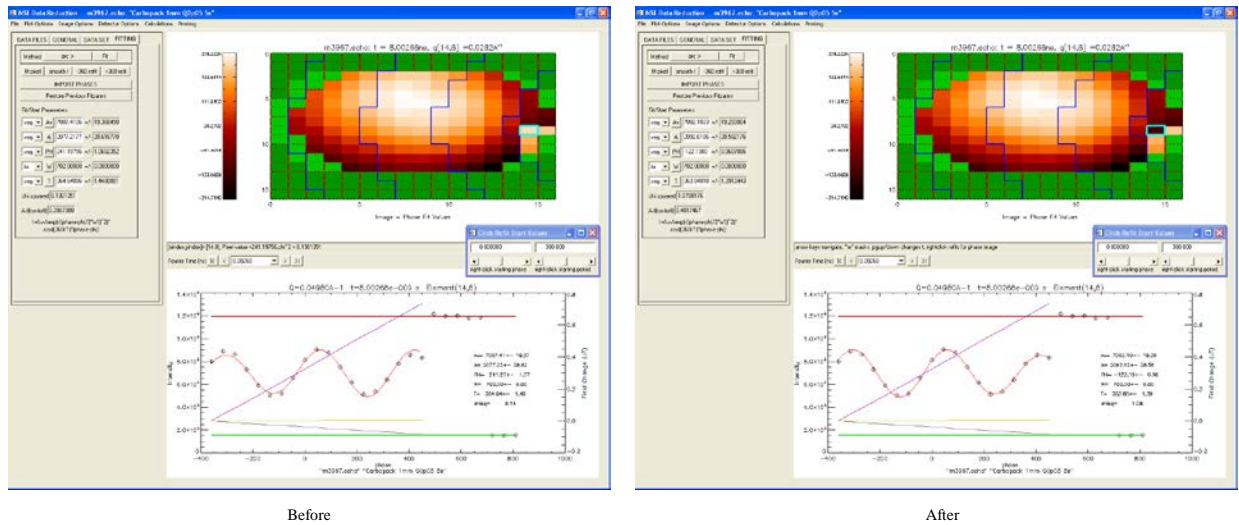


Fig. 12. Re-fit of a bad pixel. Note the reduction of the  $\chi^2$  value.

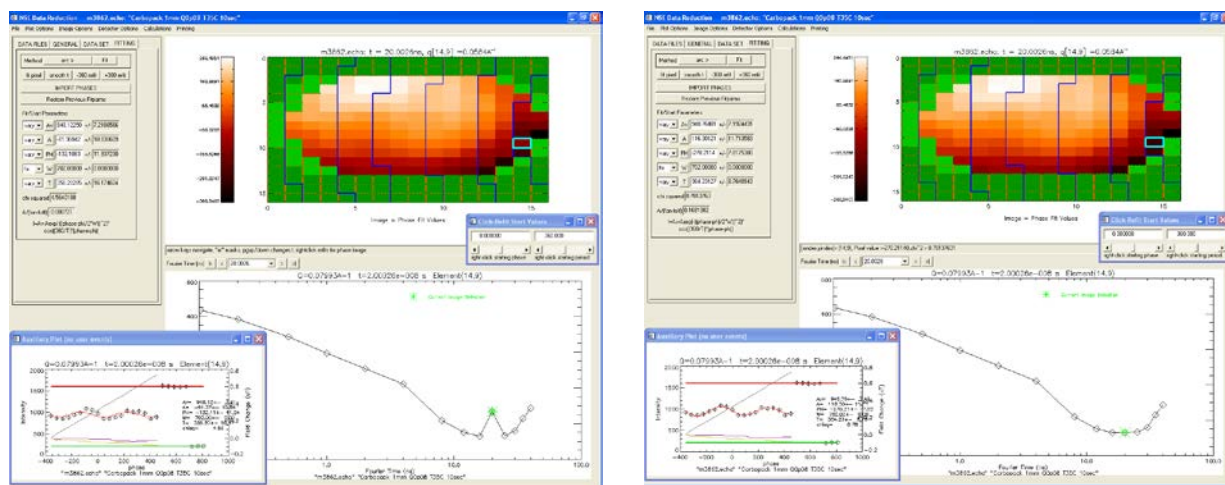
Right clicking with your mouse on a pixel on the **Detector Image** window will refit the pixel using the values selected by the sliders as starting parameters for the phase and the period.

### 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



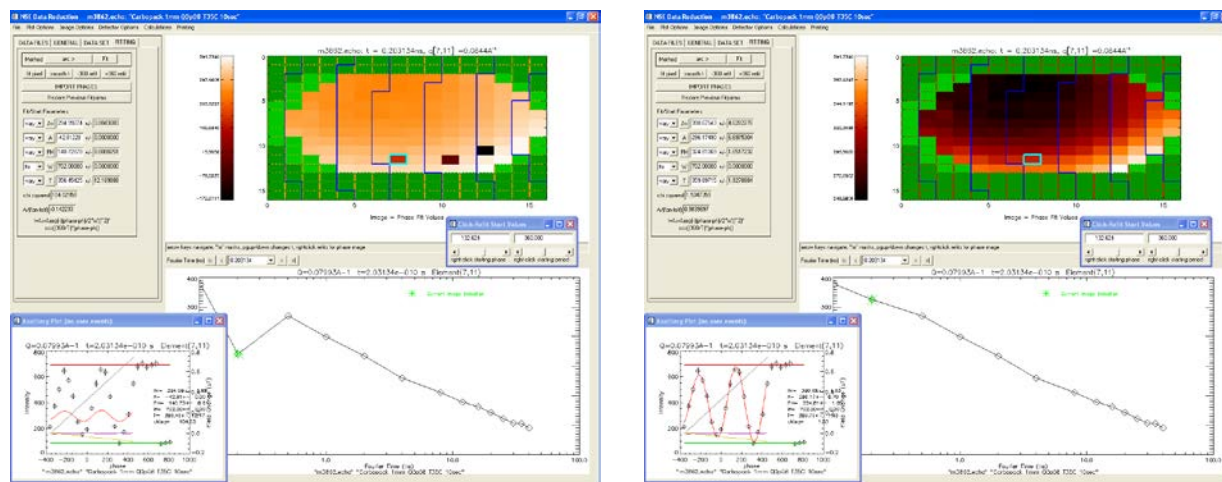
worked correctly, you can also open an auxiliary window. The auxiliary window will show a plot that complements the main plot window.



Before  
 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.



Before  
 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 “±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 ~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.

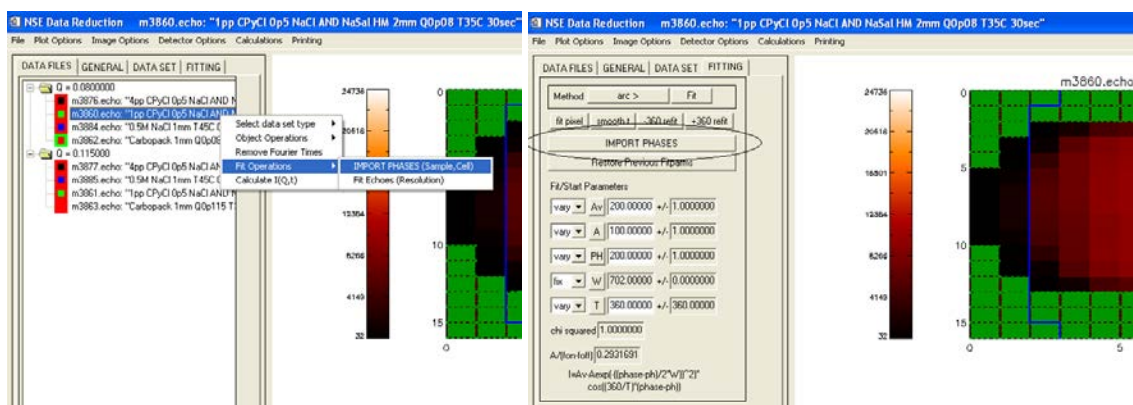


Fig. 15. Fitting a sample or background (cell) file.

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.



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 (you can always do so, pixel by pixel, using the [Fitting Tab](#)) 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.

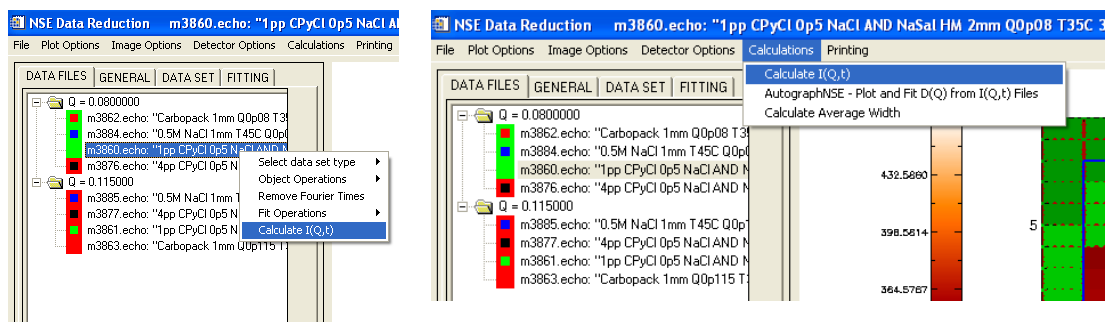


Fig. 17. How to calculate  $I(Q,t)$ .

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.



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.

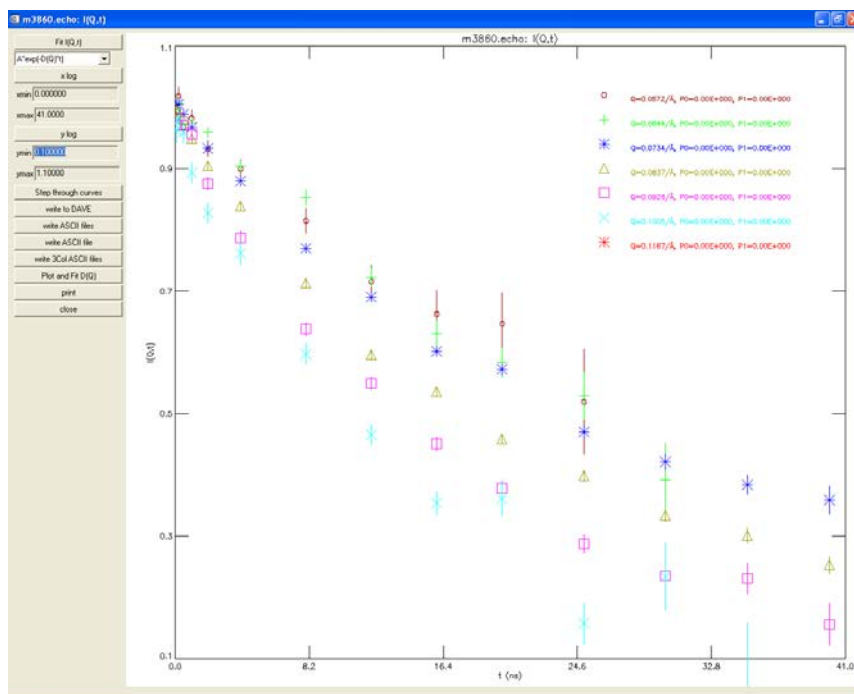


Fig. 19. Display  $I(Q,t)$  window.

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 Analysis).
- 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,  $I(Q_1,t)$ , error bar,  $I(Q_1,t)$ , 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 be 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.

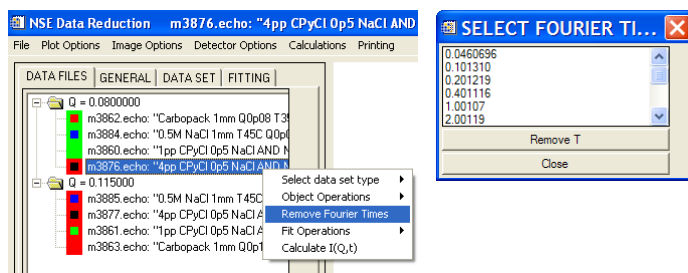


Fig. 20. Removing a Fourier Time.

#### 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.

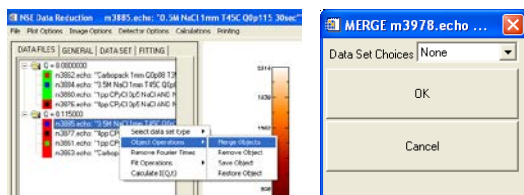


Fig. 21. Merging two files.

#### 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.

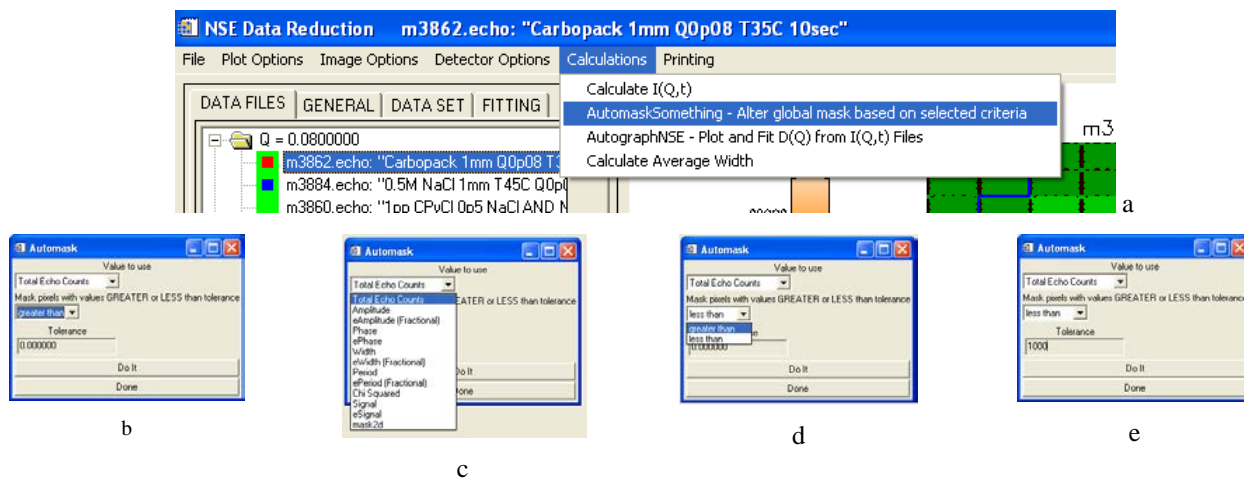


Fig. 21a. Automask Something: After selecting the option from the menu bar (a) a new window will pop-up (b). Select the quantity you want to base your filtering on (c) and then choose between the options 'greater than' or 'less than' (d). Finally, put in the threshold value (e).

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.

## 4 NSE reduction program command and operations

In this section, we systematically describe the different commands and operations of the NSE reduction program.

### 4.1 Menu Bar

The Menu Bar mainly manages the read/write files operations (printing included), the selection of the detector image and main plot window display, and the I(Q,t) calculation and analysis programs.

#### 4.1.1 File Menu

The File menu handles the options for interacting with files.

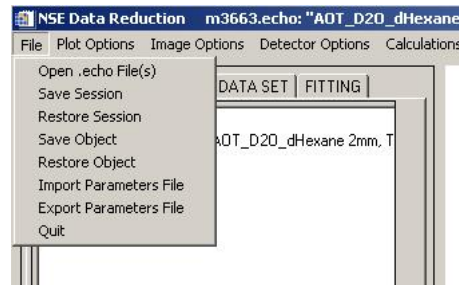


Fig. 22. The Menu bar: File.

##### 4.1.1.1 Open .echo File(s)

Open one or more .echo files to begin reduction.

##### 4.1.1.2 Save Session

Save the current state of the Reduction program. The result will be a binary .sav file.

##### 4.1.1.3 Restore Session

Restore the state of the program from either a .xml file or a .sav file. The .xml files will be supported for users who have already saved in this format, but new .xml files will not be created. Note that this operation closes all data sets in the current session before reading in the saved session.

##### 4.1.1.4 Save Object

Save a single data set/object. This will be saved in the .sav format. This .sav file can be read in using Restore Object or Restore session.

##### 4.1.1.5 Restore Object

Restore a single object from a .sav or .xml file without deleting any current objects. If multiple objects exist in the file, only the first will be read.

##### 4.1.1.6 Import Parameters File

Import a file containing parameters for the session, such as beam center and Gaussian Width. The file must have a .nse extension and have the format reported in Fig. 23.

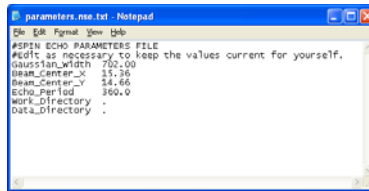


Fig.23. Example of a parameter file.

#### 4.1.1.7 Export Parameters File

Export a file containing parameters for the session. The file will have a .nse extension.

#### 4.1.1.8 Quit

Quit the application. The user will be prompted to save the work.

#### 4.1.2 Plot Options Menu

These options apply to the main plot window. These are the possible data and options for what can be plotted in the plot window.

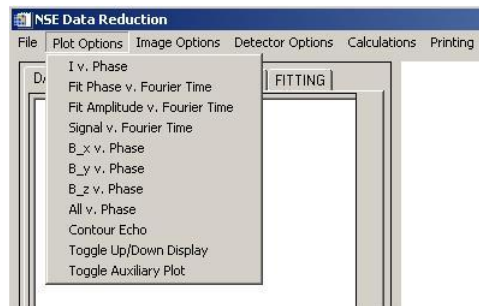


Fig. 22. The Menu bar: Plot Options.

##### 4.1.2.1 I v. Phase

Plot the intensity as a function of the phase current.

##### 4.1.2.2 Fit Phase v. Fourier Time

Plot the Phase (PH) fit parameter as a function of Fourier time.

##### 4.1.2.3 Fit Amplitude v. Fourier Time

Plot the Amplitude (A) fit parameter as a function of Fourier time.

##### 4.1.2.4 Signal v. Fourier Time

Plot the Signal ( $2A/(N_{up} - N_{down})$ ) as a function of Fourier time.

##### 4.1.2.5 B\_x v. Phase

Plot, beside the intensity as a function of phase, the change (with respect to the first phase point) in the x (along the beam direction) component of the magnetic field, B. The scale is reported on the right vertical axis.

##### 4.1.2.6 B\_y v. Phase

Plot, beside the intensity as a function of phase, the change (with respect to the first phase point) in the y (horizontal, perpendicular to the beam direction) component of the magnetic field, B. The scale is reported on the right vertical axis.

#### 4.1.2.7 B<sub>z</sub> v. Phase

Plot, beside the intensity as a function of phase, the change (with respect to the first phase point) in the z (vertical) component of the magnetic field, B. The scale is reported on the right vertical axis.

#### 4.1.2.8 All v. Phase

Plot, beside the intensity as a function of phase, the change (with respect to the first phase point) of the three components of the magnetic field, B, at the sample (x: black; y: violet; z: yellow). The scale is reported on the right vertical axis.

#### 4.1.2.9 Contour Echo

Create a contour plot of the echoes as a function of time.

#### 4.1.2.10 Toggle Up/Down Display

Toggle the display of  $N_{up}$ ,  $N_{down}$  points on the plot.

#### 4.1.2.11 Toggle Auxiliary Plot

Toggle an auxiliary plot on/off. The auxiliary plot complements the plot in the plot window, and it is displayed in its own resizable window.

### 4.1.3 Image Options Menu

These options apply to the detector image display.

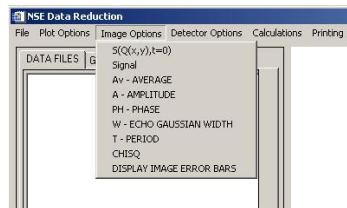


Fig. 23. The Menu bar: Image Options.

#### 4.1.3.1 $S(Q(x,y),t=0)$

Display an image of the sum of all counts for the echoes. This image is equivalent to a not normalized image of  $S(Q,t=0)$ .

#### 4.1.3.2 Signal

Display the signal ( $2A/(N_{up}-N_{down})$ ).

#### 4.1.3.3 Av – Average

Display the average count number, **Av**, fit parameter over the image.

#### 4.1.3.4 A – Amplitude

Display the amplitude of the echo, **A**, fit parameter.

#### 4.1.3.5 PH – Phase



Display the Phase, **PH**, fit parameter. Selecting this a new window will pop-up with two interactive sliders. Right-clicking on a pixel of the image will re-fit the echo using as starting parameters for **PH** and **T** the values reported on the sliders.

#### 4.1.3.6 W – Echo Gaussian Width

Display width of the echo envelope, **W**, fit parameter. This parameter is usually fixed to a constant predetermined value.

#### 4.1.3.7 T – Period

Display period of the echo, **T**; fit parameter.

#### 4.1.3.8 CHISQ

Display  $\chi^2$  for the echo fits at each pixel. This is very useful for quickly inspecting the quality of your fits.

#### 4.1.3.9 Display Image Error Bars

Pops-up a new window displaying the error bars for the current image in a separate resizable window.

### 4.1.4 Detector Options Menu

These options apply to the detector being used. Currently only the 32x32 detector is supported.

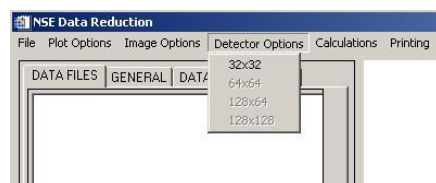


Fig. 24. The Menu bar: Detector Options.

### 4.1.5 Calculations Menu

The Calculations menu handles the programs for calculating and analyzing  $I(Q,t)$ .

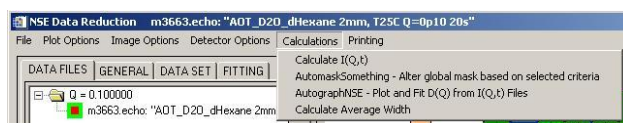


Fig. 25. The Menu bar: Calculations.

#### 4.1.5.1 Calculate $I(Q,t)$

Starts the program to calculate the  $I(Q,t)$  functions for the fully reduced data.

#### 4.1.5.2 AutomaskSomething

Pops-up an interactive window for masking data based on criteria like: Variable/Fitting Parameter greater/less than a user defined value.

#### 4.1.5.3 AutographNSE

Analyze the  $I(Q,t)$  data written to 4-column ASCII files. This will raise a dialog to analyze  $D(Q)$  based on the  $I(Q,t)$  data read from files.

#### 4.1.5.4 Calculate Average Width

Calculate the average width of the fit echoes. This is useful for setting the width following a full scan of the echoes following changes in the instrument configuration.

#### 4.1.6 Printing Menu

Manages the printing options.

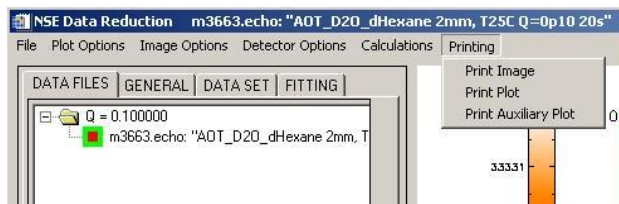


Fig. 26. The Menu bar: Printing.

##### 4.1.6.1 Print Image

Prints the detector image.

##### 4.1.6.2 Print Plot

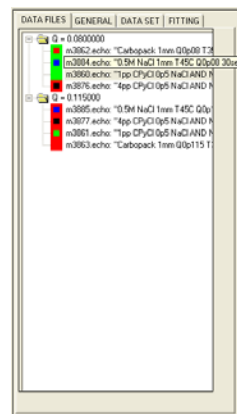
Prints the content of the main plot window.

##### 4.1.6.3 Print Auxiliary Plot

Prints the content of the auxiliary plot window, if it is available.

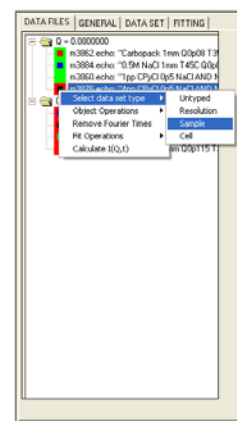
#### 4.2 DATA FILES tab

The data files tab is an interactive window which organizes the data sets into a tree structure based on their mean Q value. Pointing on any data set in the tree structure will make an additional information label appear. Each data set can be selected. The currently selected set will be displayed in the detector image and plot window. Right-clicking on any of the data sets will bring up a context menu that allows you to perform the main operations of the reducing procedure.



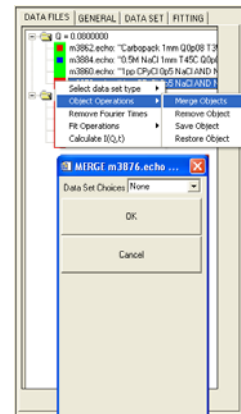
##### 4.2.1 Select Data Set Type

It allows you to determine the type of the data set: **Untyped**; **Resolution**; **Sample**; **Cell**. These set the object type. The type is indicated by the color of the icon corresponding to the data set (black: **untyped**; red: **resolution**; green: **sample**; blue: **cell**). If the data set have been reduced the outer part of the icon will be displayed in green, otherwise it is displayed as red.



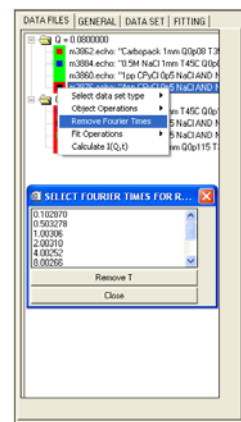
### 4.2.2 Object Operations

This menu will allow you to manage the data set. These allow you to remove a data set from the NSE reduction program memory (**Remove object**), save it (with the results of its analysis) to an XML file (**Save Object**), restore a data set (with the analysis) from an XML file (**Restore Object**), or merge two data sets together (**Merge Objects**).



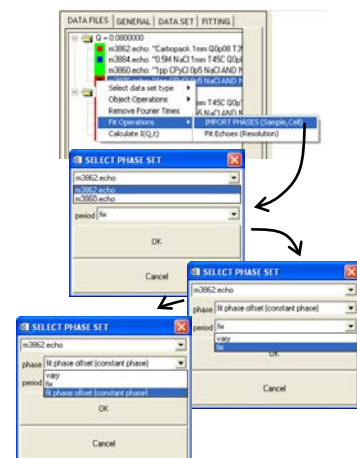
### 4.2.3 Remove Fourier Times

This allows you to remove Fourier times from the currently selected object. It pops up a list menu which allows you to select Fourier times for removal. If a Fourier time is removed, the newly created object will be the selected object. There must always be at least 2 Fourier times available in each file.



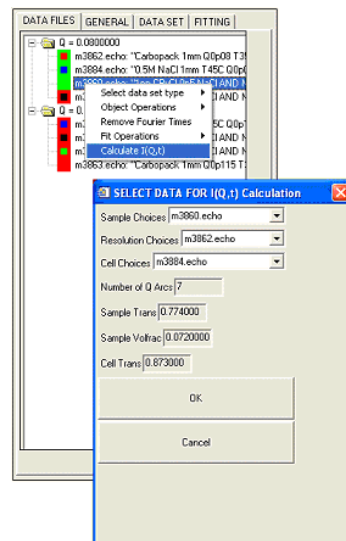
### 4.2.4 Fit Operations

Use this submenu to start the fitting procedure of your data. You can choose to either let the phase and the period be free fitting parameters (**Fit Echoes**) or to import (**Import Phases**) their values from a reference, already analyzed, data set (typically the resolution). Use **Fit Echoes** to analyze your resolution sample. The **Import Phases** command will pop-up a new window which allows you to choose the reference file, and the method of fitting to employ. You can either fix or let vary the period. You can either fix or let vary the phase, and also allow for a constant phase offset only dependent on the Fourier time not changing from pixel to pixel.



#### 4.2.6 Calculate I(Q,t)

This pops up a menu so you can calculate I(Q,t). If you did not enter the transmissions and volume fraction values under **DATA SET** tab, don't worry! The I(Q,t) dialog will prompt you for the required parameters. You will be able to select the data sets for the resolution, the actual sample and the background among the files with common Q, using drop-down menus. It is also possible to not use any resolution file (resolution =1) or background, which is useful for a preliminary investigation. (Note: to use ONLY the resolution file, you would select the data set type of the resolution file to be 'sample' before beginning the I(Q,t) calculation, and then proceed as with the sample-only calculation. Return the type to resolution when you are ready to perform other calculations.) You will be asked for the number of Q arcs you want once again. Remember that you must select a file in the **DATA FILES** tab in order to calculate I(Q,t).

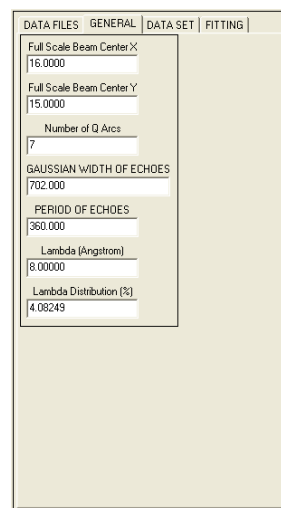


#### 4.3 GENERAL tab

From the GENERAL Tab you can vary the value of parameters common to your set of measurements:

- The x and y positions of the beam center
- The number of Q arcs
- The Gaussian Width of the Echoes
- The Period of the Echoes
- The incoming wavelength
- The incoming wavelength distribution

The Gaussian width of the echoes is determined by the characteristics of the incoming beam and should not be changed, although using the **GENERAL** tab you can change it for all your data sets. You are allowed to change this parameter for a specific data set using the **FITTING** tab. Since the period is usually let vary in the fit, the value reported in the GENERAL tab is just the starting point for the fit of all your data.



#### 4.4 DATA SET tab

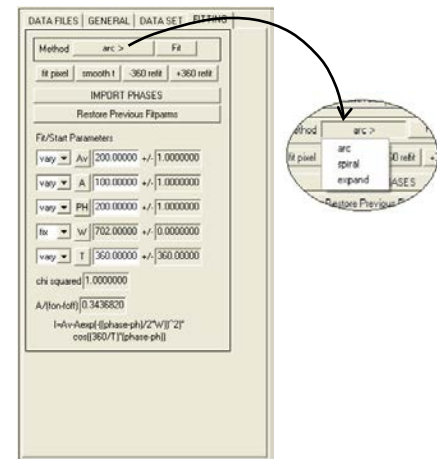
The **DATA SET** tab allows you to change the parameters specific to each sample. It shows:

- A non-editable text with the currently selected filename and file description (**Current Filename**).
- A dropdown menu for selecting the **Binning/blocking factor**, with a button to apply that factor to all available data sets.
- A text field to enter the **Transmission** value (valid for sample, cell and untyped data sets only).
- A text field to enter the **Volume Fraction** of the sample.
- A button to **Apply the Transmission and Volume Fraction** values to the data set.



#### 4.5 FITTING tab

The fitting tab controls the fitting activities for the selected data set. You can use a dropdown button menu to choose among three available fit methods (**Method arc/ spiral/expand**). The **Fit** button starts the fitting of all the pixels at all the Fourier times using the starting point and the options stated in the **Fit/Start Parameters** interactive table. Using this table you can choose to fix or vary any of the fitting parameters. The meaning of the abbreviations for the parameters is explained by the information labels that appear when holding the mouse over them. In the lower section of the window the fitting function is reported as well.

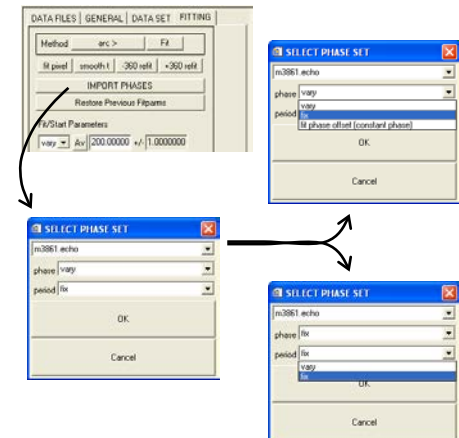


The **fit pixel** button fits the currently selected pixel using the starting point and the options stated in the **Fit/Start Parameters** interactive table.

The **smooth t** button fits all of the pixels in the current Fourier time, starting at the central pixel and moving outward from there. It compares the phase of each pixel to the results found for the closer pixel toward the center.

The **±360 refit** buttons fit the pixels of the current Fourier time starting from the current results, except for the phase, to which 360° are added/subtracted.

The **IMPORT PHASES** button import phases and periods from another suitable data object as the starting point for fitting for each echo. After pressing this button a new window opens which allows you to select from a list the data set from whom the phases and periods can be imported. You can also decide whether you want to fix the phase and/or period values to those of the presumed resolution object during the fit process. You can also choose to allow



for a constant phase offset in your data using the “fit phase offset (constant phase)” option. When you use 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, constant on the surface of the detector but varying with the Fourier time, and kept as fix parameter in the fitting of all the other pixels.

The **Restore Previous Fitparms** will allow you to undo the last fit operation you have performed. This way, it is easy to remediate to mistaken actions or to check the effect of the **smooth t**,  **$\pm 360$  refit**, ... commands.

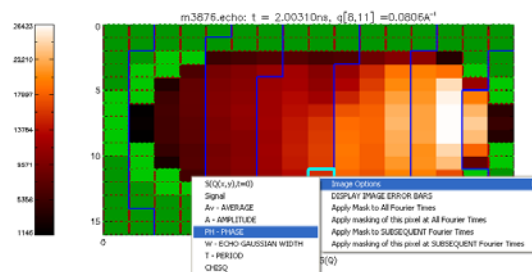
The **Fit/Start parameters** panel reports the value of the 5 fitting parameters: **Av** (Average), **A** (Amplitude), **PH** (Phase), **W** (sigma), and **T** (period). Any of these parameters can be either a free fitting parameter or fixed. The default configuration for a reference run is with only **W** fixed. Using the **Import Phase** option to fit your data, the period and the phase may be fixed as well. You can change the fix/vary status of the parameters at any time to fit a single pixel or the whole detector image at each Fourier time. You can also use **Fit/Start parameters** to have a better estimate of your starting parameters: input your estimate guess of each parameter, the fitting plot will update every time you hit the return key.

In the Fitting tab it is also reported the  $\chi^2$  of the fit, as well as the **signal**,  $A/(f_{on}-f_{off})$ .

Finally, the fitting function, equivalent to equation 1, is reported in terms of **Av**, **A**, **PH**, **W**, and **T**.

#### 4.6 The detector image

On the top-right quadrant of the NSE reduction software window you will find the detector image. This is a color scale picture of the detector divided in already binned pixels. On the left the color scale is displayed. Just above the picture you will find the name of the corresponding data set, Fourier time, and the Q value of the highlighted pixel (this is indicated by a light cyan box).



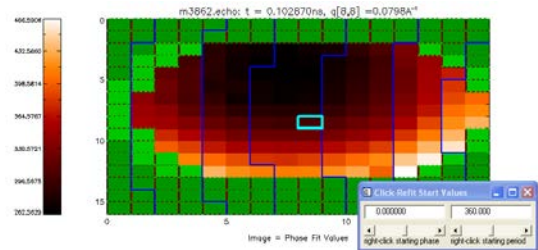
The dark green pixels mark zone of the detector which are physically masked and, therefore, are automatically masked. The light green color indicates pixels that you have masked. The blue continuous lines indicate the Q-arc boundaries. You can select any pixel by clicking on it or by moving with the arrow keys when the mouse is on the image.

The image itself is useful to have a clear display of the value of different quantities pixel by pixel. Before the echoes have been fitted the only available choice is the recorded intensity,  $S(Q(x,y),t=0)$ , calculate as the mean value of the echo counts. After the fitting you the detector image can show: the value of the five fitting parameters, the average count number, **Av**, the amplitude of the echo, **A**, the Phase, **PH**, the width of the echo envelope, **W**, the

period of the echo, **T**; the value of the **signal**,  $2A/(f_{on}-f_{off})$ ; and the  $\chi^2$  of the fit. You can change the displayed quantity either using the Image Options menu from the menu bar or right-clicking on the image. Except when the detector image is showing the phase, a new menu will pop-up having the same functionalities as Image Options menu bar.

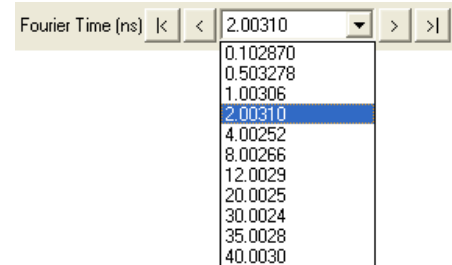
Right-clicking on the image will also give you the possibility to apply the current detector mask to all the Fourier times (**Apply Mask to All Fourier Times**), apply the masking of the selected pixel to all the Fourier times (**Apply Masking of This Pixel at All Fourier Times**), to apply the current detector mask to the SUBSEQUENT Fourier times (**Apply Mask to SUBSEQUENT Fourier Times**), or to apply the masking of the selected pixel to the SUBSEQUENT Fourier times (**Apply Masking of This Pixel at SUBSEQUENT Fourier Times**).

When the detector image displays the fitting parameter PH, a double slider window will pop-up. Now, you can also use the detector image to execute the fitting of the echo for a selected pixel, by right-clicking. The sliders control the initial values of the parameters PH and T, when the fit current pixel command is issued by right-clicking on one pixel of the detector image. You can either type in the desired starting values, use the arrow buttons, or the bar on the slider.



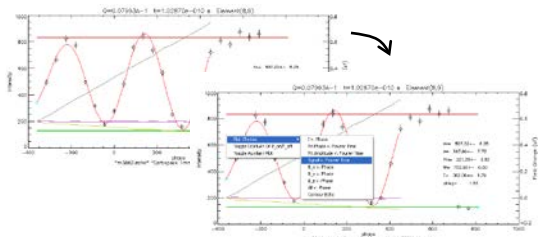
#### 4.7 Fourier time CD type menu

In order to scan through the different Fourier times you will have to use this menu. You can move one Fourier time higher or lower using the buttons **>** and **<**, or just go to the lowest or maximum Fourier time using the buttons **|<** and **|>**. You can also go directly to a specific Fourier time using the drop-down menu reporting the value of the actual Fourier time. If a file has not been properly loaded, because it was not finished or the file is corrupted, you will find a series of 0.0000 Fourier time at the end of the menu. These are obviously unreal data and should be discarded using the **Remove Fourier Times** option.



#### 4.8 The Plot Window

The plot window occupies the lower right quadrant of the NSE reduction program window. Its default configuration is to show the echo detected in the pixel selected in the **Detector Image** window as a function of the phase current.

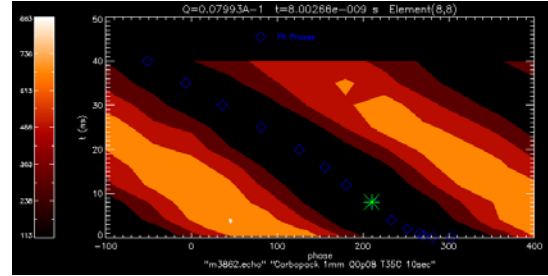


On top of the plot the Q value corresponding to the center of the detector is reported together with the Fourier time and the indexes of the currently selected pixel. The thick red and green lines represent the average value of the  $N_{up}$  ( $f_{on}$ ) and  $N_{down}$  ( $f_{off}$ ) counts respectively. The thin black, blue and yellow lines are the variation of the magnetic field at the pi flipper position with respect to their values at the first echo point. The right axis scale refers to the



magnetic fields values. Once the echo has been fitted the window will report the fit function (red) and the results for the fitting parameters together with their errors and the value of the  $\chi^2$ . Right-clicking on the window a new menu will pop-up, having the same functionalities of the **Plot Options Menu**, that allows you to change the quantities displayed on the main plot window and to open up an auxiliary plot (**Toggle Auxiliary Plot**). Therefore, for the currently selected pixel, the main plot window can display the echo as a function of the phase current (**I v. Phase**), the fitted phase as a function of the Fourier time (**Fit Phase v. Fourier Time**), the fitted amplitude as a function of the Fourier time (**Fit Amplitude v. Fourier Time**), the signal (defined as  $2A/(f_{on}-f_{off})$ ) as a function of the Fourier time (**Signal v. Fourier Time**). You can also choose whether to have the  $N_{up}$ ,  $N_{down}$  points shown or not (**Toggle Up/Down Display**), and either none or anyone (**B\_x v. Phase**, **B\_y v. Phase**, **B\_z v. Phase**) or all (**All v. Phase**) of the three components of the magnetic field detected at the pi flipper position displayed on the plot.

The main plot window can also show a color coded image of the echo recorded at the selected pixel as a function of both the phase current and the Fourier time (**Contour Echo**). The fitted echo point is displayed by a blue diamond.



When the **Main Plot Window** shows the fitted phase as a function of Fourier time, you can refit the echo 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.