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The MODES User Guide v3

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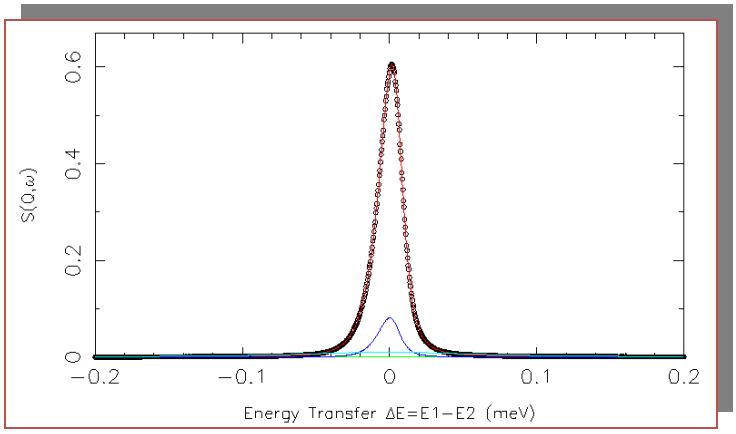

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February 2010

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Contents

1. Introduction

MODES3 is the latest version of MODES, the Graphical User Interface for the old IDA (Iris Data Analysis) package. It is based on OpenGenie with the GUI windows from Tcl/Tk. The original IDA had a GUI interface (GUIDE) which submitted old Genie-like programs and stand-alone FORTRAN programs for batch processing and graphics was provided interactively by old Genie routines.

The aim of the new package is to provide an integrated ('one-stop') interface. Much of the data manipulation is performed using OpenGenie routines with Genie Command Language (GCL). However, more complex and involved calculations are easier and more efficiently performed in FORTRAN. Thus, FORTRAN modules are called by GCL and have been converted to OpenGenie Modules. The basic operation consists of a selection of GCL commands (referred to as the Ida Command Language, ICL). In the line-mode option, there are question and answer routines in GCL which provide parameters for the ICL commands. In the Tcl/Tk mode, menus and graphics are provided and GUIs are used to provide the parameters for the ICL commands.

The package contains the many commonly used functions for the analysis of quasielastic neutron data and should provide the tools necessary for the new users to this technique and become a workhorse for the regular user. For the more experienced user, there is the option of incorporate their own .GCL or .ICL routines (which will be converted to run on as GCL scripts).

The information in this document has been organized as follows: the first section gives an overview of the theory behind converting raw output from the quasielastic spectrometers to physical and accurate quantities using MODES. In the next section, after a description of how to initialize the program, each item on the menu and its functions are described in detail. Installation instructions can be found in the appendix.

2. General overview

Data handling of Quasielastic Neutron Scattering (QENS) data from instruments such as IRIS and OSIRIS can be divided into two sections: **Reduction** and **Analysis**.

Reduction involves taking the raw data in time-of-flight and converting it into an instrument independent scientific function such as S(Q,w) which depends only on the dynamics of the sample measured. The operations include:

- Converting from time-of-flight to energy transfer (or other unit such as d-spacing)
- Summing of spectra into groups and converting from detector angle to Q value
- Correcting for container scattering (if necessary)
- Correcting for absorption (from sample and container) and multiple scattering. In the package the data after these processes are saved in 'Intermediate file' format. Subsequent analysis involves operations on Intermediate files which in general are smaller than the original raw files.

Analysis will be taken to refer to science based interpretation of the reduced data. In

quasielastic scattering this is dominated by methods for measuring the peak shapes and widths, and relating these to some theoretical model for the dynamics. This can take the form of:

- Fitting quasielastic peaks using a convolution method
- Calculating peak parameters using Bayesian techniques
- Performing transformations from S(Q,w) to I(Q,t)
- Fitting peak widths using jump diffusion models
- Fitting I(Q,t) to models

In the package all these operations are controlled from the main OpenGenie window.

MODES comprises the OpenGenie program package and the MODES package itself. The programs run on several computer operating systems: VMS, UNIX and MS Windows. MODES3 is available for users to use on their home institute computers. Details of the installation procedures are given in Appendix A

3. MODES overview

3.1 Calibration

This procedure determines the instrument parameters required, such as flight paths, scattering angles and detector efficiencies. The flight paths and scattering angles on IRIS and OSIRIS are fixed and have been determined by the instrument scientists. Detector efficiencies are measured using a vanadium standard by instrument scientists at the beginning of each cycle or by the user as part of the experiment. This vanadium run also serves to determine the energy resolution and provide an absolute cross-section calibration. One or two ranges can be specified and would normally correspond to a region around zero energy transfer about the width of the resolution (elastic component), and a region out in the wings at high energy transfer (background).

For the 1 region option, examples include the elastic component alone or the full time range, corresponding to an integral over all energies within the observable window.
For the 2 region option, there are a further 2 options:
a) the integrated elastic component is the elastic region sum minus the background region sum. This is the option used for the vanadium calibration
b) the background region divided by the elastic region. This is useful for checking on the stability of the detectors.

On the instrument control computers there is a file called *detector.dat* in the instrument tables directory which contains a table of angles and detector efficiency for each detector/spectrum. This is kept up-to-date by the instrument scientists. The Instrument Control Program (ICP) which runs the data acquisition reads this file and writes the values to the header block of the *.RAW* file.

The purpose of calibration program CALIB is two-fold: firstly, to provide a correct version of the

detector angles in the user's area; secondly, to store the vanadium intensities, if the user wishes to normalise the data. The default copy of this data file called *IRIS_detector.calib* or *OSIRIS_detector.calib* is edited and written into the user's area.

3.2 Conversion to I(Q,ω)

The procedures ICON *&* IONIAN use the parameters from 3.1 to convert the *.RAW* data into I(Q,ω), or strictly speaking I(2θ,ω). The *RAW* file will normally contain the standard values of 2θ, but the user can chose whether to update the detector efficiency or if the spectra need to be normalised to the vanadium. The user may also choose how to combine spectra into a smaller number of groups. This procedure is carried out for all runs in the experiment.

Since IRIS can use the Graphite and Mica analysers simultaneously, the program will have to be run twice for any run if both analysers are to be used and the output file names (extensions) differentiate between the two types of analysers.

Both programs read the monitor spectrum, correct for efficiency & convert to wavelength. For each spectrum or group of spectra, the spectra are read, converted to wavelength, normalised to the corrected monitor spectrum and converted to energy transfer. The data is then converted to I(Q,ω).

3.3 Diffraction

IRIS and OSIRIS can also be used for diffraction experiments - either dedicated solely to diffraction or for using the diffraction detectors in parallel with quasielastic scattering. In this case the detector angles and efficiencies are fixed and the calibration is not necessary. Instead of calculating I(Q,ω) the reduction routine converts the raw data into d-spacing. There is a bank of detectors with each detector at a different scattering angle (which then give different d-spacings for the same time of flight) and several runs may be carried out at different wavelength bands in order to extend the d-spacing range. There is therefore a routine to merge several data-sets into one spectrum spanning the whole d-spacing range.

3.4 Corrections

A complete set of runs will normally contain, in addition to the samples and vanadium, the background (instrument empty), empty sample environment equipment (eg cryostat, furnace) and empty containers. The first, and most important, set of corrections is that for absorption (self-scattering and neutron absorption). This usually incorporates the container correction. If necessary, multiple scattering corrections may then be applied, but the calculation requires some knowledge of the inelastic scattering and is therefore an iterative procedure.

3.4.1 Absorption

The main correction to be applied to neutron scattering data is that for absorption both in the sample and its container, when present. For flat plate geometry, the corrections can be analytical and have been discussed for example by Carlile [1]. The situation for cylindrical geometry is more complex and requires numerical integration. These techniques are well known and used in liquid and amorphous diffraction, and are described in the ATLAS manual [2]. The routines used here have been developed from the corrections programs in the ATLAS suite and take into account the wavelength variation of both the absorption and the scattering cross-sections for the inelastic flight paths.

The absorption corrections use the formulism of Paalman and Pings and involve the attenuation factors $A_{i,j}$ where i refers to scattering and j attenuation. For example, $A_{s,sc}$ is the attenuation factor for scattering in the sample and attenuation in the sample plus container. If the scattering cross sections for sample and container are Σ_s and Σ_c respectively, then the measured scattering from the empty container is $I_c = \Sigma_c A_{c,c}$ and that from the sample plus container is $I_{sc} = \Sigma_s A_{s,sc} + \Sigma_c A_{c,sc}$. Thus $\Sigma_s = (I_{sc} - I_c A_{c,sc}/A_{c,c})/A_{s,sc}$. In the package, the program *Acorn* calculates the attenuation coefficients $A_{i,j}$ and the routine *Analyse* uses them to calculate Σs which we identify with S(Q,ω).

3.4.2 Multiple scattering

Multiple scattering is calculated using the Monte Carlo program MINUS derived from DISCUS by M W Johnson [3]. The program requires a sample S(Q,ω) and can handle both plate and cylindrical geometries. The S(Q,ω) can either be calculated using a suitable model, such as a set of Lorentzians with specified Q dependence of the widths, or a tabulated set of data.

The following parameters are required:

- Number of neutrons for calculation (default=1000); larger values give better statistics
- 2 integers to start the random number generator. Need not be changed but if the statistical accuracy needs to be checked several runs should be performed with differing random numbers.
- Number of multiple scattering events, up to 5 for each neutron. Single scattering is 1. The relative intensities of the various orders of multiple scattering could first be checked with low statistics and better statistics obtained with fewer scattering events. In most cases 3 ought to be sufficient.
- Sample geometry: infinite plate, finite plate or cylinder
- Sample thickness, width & height (in cm) for plate or sample radius & height (in cm) for cylinder
- Angle of plate sample to beam (perpendicular is zero)
- Incident or analysing wavelength is obtained from the *ICON* file
- Sample temperature (K)
- Sample number density (atoms/Å^3)
- Absorption cross section (barns)
- Bound scattering cross-section (barns)

The Q-ω grid and the S(Q,ω) are defined by:

- Number of Q points & increment ($Å^{-1}$)
- Number of ω points & increment (μeV)
- Option for scattering cross section in file or constant
- If constant, scattering cross section (barns)
- Form of S(Q,ω) input
  - input file
  - calculate n peaks from diffusion constants (cm^2s^{-1})
  - calculate n peaks with width as a 5 order polynomial in Q (ie up to Q^4)

The number of angles and their values are obtained from the *ICON* file.

The line-printer output (LPT) gives the input parameters, the table of S(Q, ω) values and the width parameters. For each angle, there is a table giving, for each energy, the following:

J_1^*	single scattering assuming no absorption & no other scattering
J_1	first scattering
J_2-J_5	2nd to 5th scattering, range as specified
Total	Total scattering J_t =sum all J_n
Mult	Multiple scattering J_{ms} =sum J_n from 2 to 5
R1	ratio J_1/J_t
$R1^*$	ratio J_1^*/J_t

R_1 is the normal output, this is the multiple scattering only; R_1^* can be used to correct for multiple scattering, attenuation due to re-scattering and absorption all at once. The value of R_1 (or R_1^*) is averaged over the positive & negative energy values and is printed. This is also the form of the data in the *.ANS* file.
The use of multiple scattering corrections is not straightforward and will depend on the method of data interpretation employed.

The two cases that have been used most frequently are:

1) Corrections to the Elastic Incoherent Structure Factor (EISF). In this case only the fraction of the scattering that is multiple scattering is used - that is, the total scattering is reduced by the multiple scattering fraction.
2) Fitting of peak shapes. In this case, the shape of the multiple scattering with energy transfer is important. The multiple scattering can change the shape of the sample S(Q,ω) and therefore must be applied before the resolution broadening is applied.

3.5 Convolution peak fitting

3.5.1 Theory

The measured data I(Q,ω) is proportional to the convolution of the scattering law S(Q,ω) with the resolution function R(Q, ω) of the spectrometer via $I(Q,\omega) = S(Q, \omega) \otimes R(Q, \omega)$. The traditional method of analysis has been to fit the measured I(Q, ω) with an appropriate set of functions related to the form of S(Q,ω) predicted by theory.

- In quasielastic scattering the simplest form is when both the S(Q,ω) and the R(Q,ω) have the form of a Lorentzian - a situation which is almost correct for reactor based back-scattering spectrometers such as IN10 & IN16 at ILL. The convolution of two Lorentzians is itself a Lorentzian so that the spectrum of the measured and resolution data can both just be fitted with Lorentzians. The broadening of the sample spectrum is then just the difference of the two widths.
- The next easiest case is when both S(Q,ω) and R(Q,ω) have a simple functional form and the convolution is also a function containing the parameters of the S(Q,ω) and R(Q, ω) functions. The convoluted function may then be fitted to the data to provide the parameters. An example would be the case where the S(Q,ω) is a Lorentzian and the R(Q, ω) is a Gaussian.
- For diffraction, the shape of the peak in time is a convolution of a Gaussian with a decaying exponential and this function can be used to fit the Bragg peaks.
- The final case is where R(Q,ω) does not have a simple function form so that the measured data has to be convoluted numerically with the S(Q,ω) function to provide an estimate of the sample scattering. The result is least-squares fitted to the measured data to provide values for the parameters in the S(Q,ω) function.

This latter form of peak fitting is provided by SWIFT. It employs a least-squares algorithm which requires the derivatives of the fitting function with respect to its parameters in order to be faster and more efficient than those algorithms which calculate the derivatives numerically. To do this the assumption is made that the derivative of a convolution is equal to the convolution of the derivative-as the derivative and the convolution are performed over different variables (function parameters and energy transfer respectively) this should be correct. A flat background is subtracted from the resolution data before the convolution is performed.

Four types of sample function are available for S(Q, ω) :

- Quasielastic - this is the most common case and applies to both translational (diffusion) and rotational modes, both of which have the form of a Lorentzian. The fitted function is a set of Lorentzians centred at the origin in energy transfer.
- Elastic -comprising a central elastic peak together with a set of quasi-elastic Lorentzians also centred at the origin. The elastic peak is taken to be the un-broadened resolution function.
- Shift - a central Lorentzian with pairs of energy shifted Lorentzians. This was originally used for crystal field splitting data but more recently has been applied to quantum tunnelling peaks. The fitting function assumes that the peaks are symmetric about the origin in energy transfer both in position and width. The widths of the central and side peaks may be different.
- Polymer - a single quasi-elastic peak with 3 different forms of shape. The theory behind this is described elsewhere [4,5]. Briefly, polymer theory predicts 3 forms of the I(Q,t) in the form of $\exp(-at^{2/b})$ where b can be 2, 3 or 4. The Full Width Half-Maximum (FWHM) then has a Q-dependence (power law) of the form Q^b. The I(Q,t) has been numerically Fourier transformed into I(Q,ω) and the I(Q,ω) have been fitted with functions of the form of a modified Lorentzian. These latter functions are used in the energy fitting

procedures.

3.5.2 Hints on running

When running the program:

- the program was originally written for a symmetric energy window, that is Emin=-Emax . Using an asymmetric window appears to work but is to be treated with caution.
- the energy increment should not be less than the energy bin in the input data otherwise the result may be unreliable due to the method of rebinning the data. Using 100 points (provided the previous comment applies) provides good results.
- the background and origin parameters can start at zero.
- the elastic peak height is the fraction of the measured resolution peak.
- the quasielastic peak height is the real peak height , which can be read directly off a plot. This can be the starting parameter if the broadening is greater than the resolution width. If the broadening (function width) of the peak is less than the resolution the start parameter should be the measured sample height multiplied by the ratio of resolution width to estimated broadening. For example, if the broadening is a quarter of the resolution, then multiply the height by 4. This is to take into account the reduction in height on convoluting when the area remains constant.
- the parameter width is the HWHM of the scattering function. The printed output will show this and also give the FWHM.
- when fitting more than 1 peak it is best to start off fitting 1 peak in order to obtain estimates for peak heights and background and origin. When increasing the number of peaks it may be useful to constrain some of the parameters in order to obtain a fit and these parameters can then be used as starting parameters for a full parameter fit.
- when fixing parameters, the routine asks how many to fix. The background and origin are the first to fix.

3.5.3 Multiple scattering version

This version uses the MS corrections previously calculated by the program MINUS and stored in the *.ANS* file. The calculated sample function is corrected for MS and then fitted to the experimental data.

A full analysis should be an iterative process with steps as follows:

1) use SWIFT without MS corrections to obtain first estimates for widths, which are then used to generate S(Q,ω) in MINUS
2) use SWIFT with MS corrections to obtain a new set of widths and use them to calculate S(Q,ω) again in another run of MINUS
3) repeat step 2 until widths do not change within the errors on the widths

3.6 Transform to I(Q,t)

3.6.1 Theory

The measured spectrum I(Q,ω) is proportional to the four dimensional convolution of the scattering law S(Q, ω) with the resolution function R(Q, ω) of the spectrometer via I(Q,ω) = S(Q,ω) ⊗ R(Q,ω), so S(Q,ω) can be obtained, in principle, by a deconvolution in Q and ω. The method employed here is based on the Fourier Transform (FT) technique [6,7]. On Fourier transforming the equation becomes I(Q,t) = S(Q,t) x R(Q,t) where the convolution in ω -space is replaced by a simple multiplication in t-space. The intermediate scattering law I(Q,t) is then obtained by simple division and the scattering law S(Q,ω) itself can be obtained by back transformation. The latter however is full of pitfalls for the unwary. The advantage of this technique over that of a fitting procedure such as SWIFT is that a functional form for I(Q,t) does not have to be assumed. On IRIS the resolution function is close to a Lorentzian and the scattering law is often in the form of one or more Lorentzians. The FT of a Lorentzian is a decaying exponential, exp(-αt) , so that plots of ln I(Q,t) against t would be straight lines thus making interpretation easier.

In general, the origin in energy for the sample run and the resolution run need not necessarily be the same or indeed be exactly zero in the conversion of the *RAW* data from time-of-flight to energy transfer. This will depend, for example, on the sample and vanadium shapes and positions and whether the analyser temperature has changed between the runs. The procedure takes this into account automatically, without using an arbitrary fitting procedure, in the following way. From the general properties of the FT, the transform of an offset Lorentzian has the form $(\cos \omega_0 t + i \sin \omega_0 t) \exp(-\Gamma t)$, thus taking the modulus produces the exponential $\exp(-\Gamma t)$ which is the required function. If this is carried out for both sample and resolution, the difference in the energy origin is automatically removed. The results of this procedure should however be treated with some caution when applied to more complicated spectra in which it is possible for I(Q,t) to become negative, for example, when inelastic side peaks are comparable in height to the elastic peak.

The interpretation of the data must also take into account the propagation of statistical errors (counting statistics) in the measured data as discussed by Wild et al [8]. If the count in channel k is X_k , then $X_k = \langle X_k \rangle + \Delta X_k$ where $\langle X_k \rangle$ is the mean value and ΔX_k the error. The standard deviation for channel k is $\sigma_k^2 = \langle \Delta X_k \rangle^2$ which is assumed to be given by $\sigma_k = \langle X_k \rangle$. The FT of X_k is defined by $X_j = \langle X_j \rangle + \Delta X_j$ and the real and imaginary parts denoted by X_j^I and X_j^I respectively. The standard deviations on X_j are then given by $\sigma^2(X_j^R) = 1/2\ X_0^R + 1/2\ X_{2j}^R$ and $\sigma^2(X_j^I) = 1/2\ X_0^I - 1/2\ X_{2j}^I$.
Note that $\sigma^2(X_0^R) = X_0^R$ and from the properties of FT $X_0^R = X_k$. Thus the standard deviation of the first coefficient of the FT is the square root of the integrated intensity of the spectrum. In practice, apart from the first few coefficients, the error is nearly constant and close to X_0^R. A further point to note is that the errors make the imaginary part of I(Q,t) non-zero and that, although these will be distributed about zero, on taking the modulus of I(Q,t), they become positive at all times and are distributed about a non-zero positive value. When I(Q,t) is plotted on a log-scale the size of the error bars increases with time (coefficient) and for the resolution

will reach a point where the error on a coefficient is comparable to its value. This region must therefore be treated with caution. For a true deconvolution by back transforming, the data would be truncated to remove this poor region before back transforming. If the truncation is severe the back transform may contain added ripples, so an automatic back transform is not provided.

3.6.2 Hints on use

When running the program:

- the program was original written for a symmetric energy window, that is Emin=-Emax. It will accept an asymmetric window and appears to work in this mode, but caution is recommended.
- the energy increment should not be less than the energy bin in the input data otherwise the result may be unreliable due to the method of rebinning the data. Using 100 points (provided the first point applies) provides good results.

A discussion of the analysis has been present in [9]. Some examples of usage are:

1) quasielastic peaks - a single Lorentzian would produce a straight line in the plot of *ln* I(Q,t) versus t . Deviations from a straight line would indicate that either there are more than one Lorentzians or that the shape is not a Lorentzian. In the former case it is often difficult to establish any quantitative conclusions as to the number of peaks or their relative gradients.
2) inelastic peaks - a pair of broadened peaks transforms into a damped cosine function. The central elastic peak would add a constant. This is the case where the I(Q,t) could become negative and taking the modulus makes the shape less easy to recognise.
3) non-Lorentzian shape - this could be either a stretched exponential form $\exp-\alpha t^{\beta}$, where β can range from 0 to 1, or not of standard function form. The former case has been discussed by Arrighi et al [10].
4) EISF - the transform provides an immediate estimate of the EISF without any arbitrary fitting procedure. From the properties of FT, the elastic peak (δ-function) transforms to a constant and the first time coefficient (t=0) is the integrated count, so the ratio of I(Q,t) at long time to zero time is the EISF provided that I(Q,t) has become constant at long time. However, bear in mind that due to taking the modulus the long time limit will be scattered around a positive non-zero value rather than zero itself, when the elastic component is zero.

3.7 Bayesian analysis

3.7.1 Introduction

An alternative and better method of data analysis to model fitting is the use of Bayesian methods which involve the direct use of probability theory [11]. This technique has now been applied to quasielastic scattering [12] to determine the number and widths of Lorentzian peaks and to tunnelling [13] to determine the number and positions of side peaks. A more recent development for quasielastic scattering is the determination of the exponent β in a stretched

exponential.

3.7.2 ResMem

This program creates a smooth, finely-interpolated, file for the resolution function from coarse and noisy data. Smoothness is imposed through an invariant Gaussian interpolant whose width can be optimised. A linear background may be subtracted. The x-binning (energy transfer) must be constant.

The User does not normally need to run this program. The appropriate resolution files have already been created by the instrument scientists.

3.7.3 ResNorm

This program creates a group 'normalisation' file by taking a resolution file as defined in section 11.3 and fitting it to all the groups in the resolution data file which has the same grouping as the sample data of interest. The routine varies the width of the resolution file to give a 'stretch-factor' and the area provides an intensity normalisation factor.

The output is written to an ASCII file with the name *FOR007.DAT* in the following format:

- data-file
- resolution file
- amplitude stretch-factor Q-value X_{min}^2
- repeat for each group

3.7.4 Quasi_Lines

The model that is being fitted is that of a δ-function (elastic component) of amplitude A(0) and Lorentzians of amplitude A(j) and HWHM W(j) where j=1,2,3. The whole function is then convolved with the resolution function. The δ-function and Lorentzians are intrinsically normalised to unity so that the amplitudes represent their integrated areas.

For a Lorentzian, the Fourier transform does the conversion: $1/(x^2+\sigma^2) \Leftrightarrow \exp[-2\pi(\sigma k)]$.
If x is identified with energy E and 2πk with t/ħ where t is time then: $1/[E^2+(\hbar/\tau)^2] \Leftrightarrow \exp[-t/\tau]$ and σ is identified with $\hbar/\tau$.

The program estimates the quasielastic components of each of the groups of spectra and requires the resolution file (*.RES* file) and optionally the normalisation file created by ResNorm. A summary of the fitted parameters for one and two Lorentzians per group is written to files with the following structure for each spectrum:

<Q> A(max) W(max)
a(0)
a(1) w(1)
a(2) w(2)

var[a(0)a(0)]
var[a(0)a(1)] var[a(1)a(1)]
var[a(0)w(1)] var[a(1)w(1)] var[w(1)w(1)]
var[a(0)a(2)] var[a(1)a(2)] var[w(1)a(2)] var[a(2)a(2)]
var[a(0)w(2)] var[a(1)w(2)] var[w(1)w(2)] var[a(2)w(2)] var[w(2)w(2)]

Here A(max) and W(max) are the scale-factors by which the a and w parameters need to be multiplied to obtain the amplitudes A(j) and HWHMs W(j); var is the variance. Routines are provided for converting these to the simpler width versus Q form.

3.7.5 Stretched_Quasi

This variation replaces the choice of several Lorentzians with a single function with the shape of a stretched exponential: $\phi_\beta(x) \Leftrightarrow \exp[-2\pi(\sigma k)^\beta]$.

This, in the energy to time FT transformation, is $\phi_\beta(E) \Leftrightarrow \exp[-(t/\tau)^\beta]$.
So σ is identified with $(2\pi)^\beta \hbar/\tau$.

The model that is fitted is that of an elastic component and the stretched exponential and the program gives the best estimate for the β parameter and the width for each group of spectra.

3.7.6 Jump fits

One of the models used to interpret diffusion is that of jump diffusion in which it is assumed that an atom remains at a given site for a time τ and then moves rapidly, that is, in a time negligible compared to τ; hence 'jump'.

In the Chudley-Elliott form the jump takes place to a new site at a point distance L from the original site. The fitted function is of the form $\Delta E = A*(1 - \sin(QK)/QK)$ where ΔE is the FWHM of the Lorentzian. The fit parameters are then: A is h/πt; K is L.

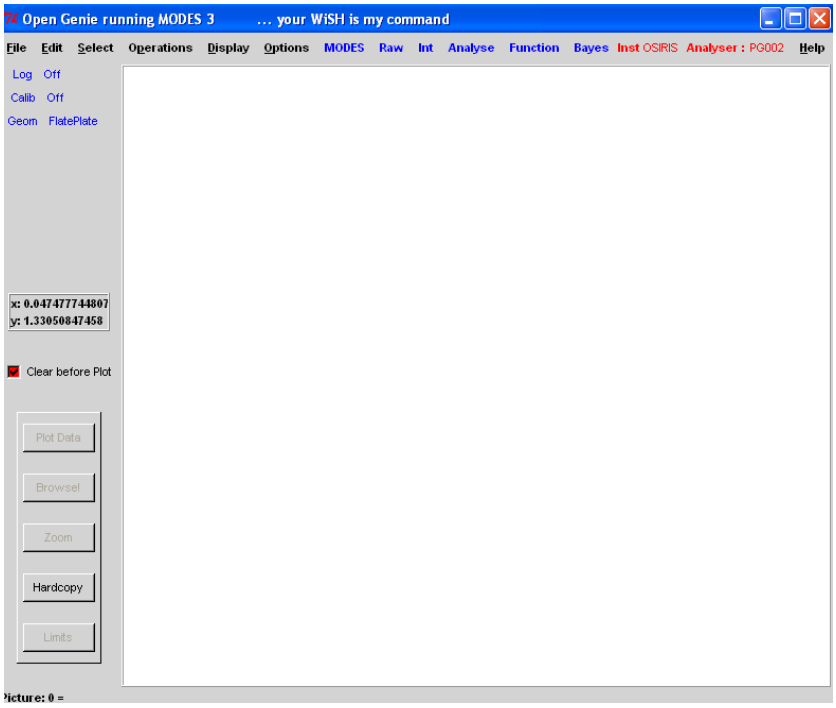
In the Singwi-Sjölander form the fitted function is $\Delta E = A*(- \exp(-r^2Q^2))$.

4. Getting started

With MODES3 installed (see Appendix A for installations instructions) click on the icon on your desktop to start the program and choose IRIS (1) of OSIRIS (2). The main MODES window will appear as shown below. This is a modified version of the Open Genie Tcl/Tk window. Menus in black are OpenGenie while those in blue are MODES commands. Note that some of OpenGenie menus have extra Modes commands.

Many of the commands especially in Modes will create new windows. These will contain some of the following Tcl/Tk elements:

- Text message
- Input box (for text or numbers) – input MUST be terminated with a Return or Tab. In many cases this changes the focus to the next appropriate input box.
- Radio button (round) – to provide a choice of options
- Button (rectangular) – to invoke an action. These are colour coded: Red – dangerous operation; Green - normal operation; Blue - plot commands; Yellow - browse function
- Menu button – rectangular with a drop-down menu of commands
  Combo box – input box with a drop-down menu
- NoteBook – this is a pane with overlayed pages; the page required is selected by clicking on the appropriate Tab at the top of the pane



Many routines make use of the Browse window which opens when the yellow 'Browse' button is clicked. The main pane of the window then shows a list of files with the specified extension that exist in the working area. Click on the required file and its name then appears in the box at the bottom of the window. Click on 'Select' and the window will close and in the main window the name of the selected file will appear in the appropriate box.

In order to make the package more user-friendly the following features have been implemented:

- Within a window all the command buttons except the first one will be disabled on start-up and will appear with just the text in light grey. If the command invoked by a button is successful, then the next button(s) will be enabled and will change to its appropriate colour. If there is an error, a message will appear and the subsequent buttons will remain disabled.
- When plotting a workspace array the routine checks if the input value is valid
- Many routines check on the consistency of the data by checking on parameters in the intermediate file header. The following checks are carried out:
  - analyser in file is consistent with analyser defined for program
  - when manipulating more than one file (eg. analyse), the reflections must be consistent

5. Toolbar

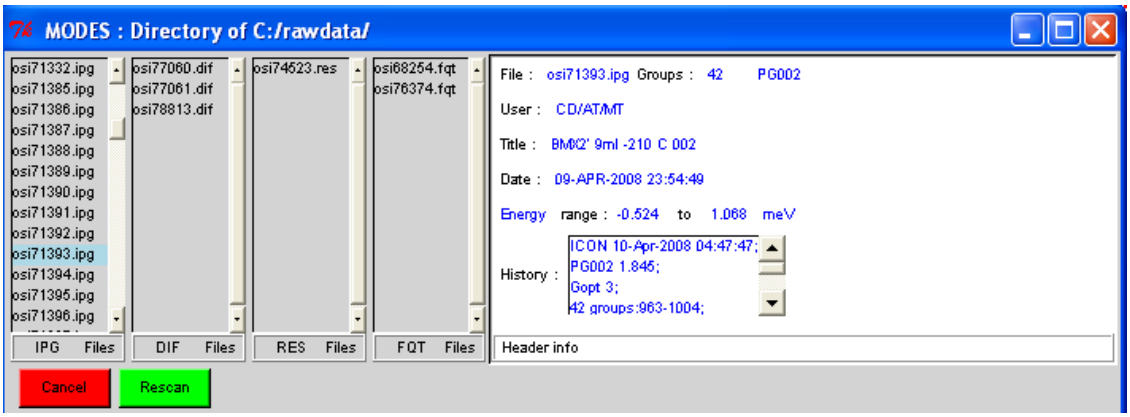
This section describes the commands that appear across the top of the window. Those in black are standard OpenGenie commands and are described in the manual. Those in blue are Modes commands and are described here. There are extra choices on the OpenGenie commands File, Display & Select and the additions are also described here.

5.1 File

The commands above the separator line are OpenGenie commands and the ones below are MODES commands.

5.1.1 Directory

This command opens a new window showing files in the working area. There are 5 panes showing those with extensions .IPG, .DIF, .RES and .FQT, plus the last pane containing the file header information. The display does not update automatically; to update click on Rescan.



5.1.2 Read Int

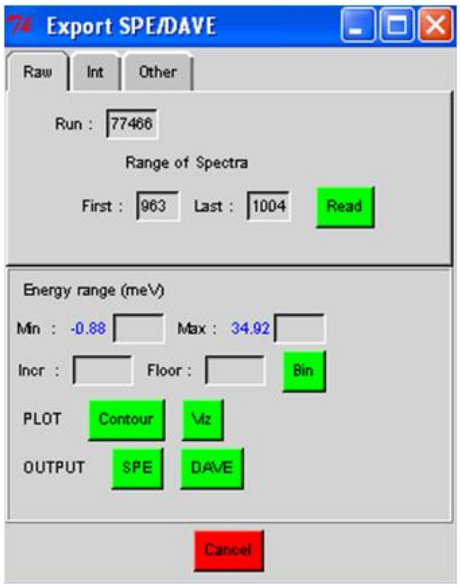
Read data from file into workspaces. There are 2 options: 1 block (enter workspace name eg. w) or all blocks.

5.1.3 Write Int

Write data from workspaces to file. There are 2 options: 1 block or all blocks.

5.1.4 Export

Export data from .RAW or MODES-treated files (eg .IPG) to formats readable by other Data Analysis Programs such as MSLICE or DAVE. Data can be cropped in x-axis and binning modified.



5.1.5 Import

Import data from other Data Analysis Programs such as MSLICE or DAVE.

5.1.6 Exit

This exits Modes and OpenGenie. A warning window will appear for confirmation.

5.2 MODES

The commands here define various general parameters for use in the program. They can be altered at any time. The default values given below are those set on start up. The values chosen here will affect the way other routines are performed.

5.2.1 Raw

This will change the location (ie disk & directory) for the raw data files.

5.2.2 Work

This will change the location (ie disk & directory) for intermediate data – that is the area where all the calculations will be performed. It does not need to be the area from which the program is started, although the user must have access rights to that area. The type of file - extension and format (Genie .ipg or Nexus) – can also be defined.

5.2.3 Analyser

This defines the analyser crystal and reflection. IRIS has Graphite and Mica; OSIRIS only has graphite. Default: PG002.

5.2.4 Calib

This defines whether the detector efficiencies in the files *IRIS_detector.calib or OSIRIS_detector.calib* [previously *detector.calib*] are to be used by ICON & IONIAN. Default: not used.

5.2.5 Geom

This defines the shape of the sample - flat plate or cylinder and is only needed if absorption and/or multiple scattering corrections are to be carried out. Default: flat plate.

5.2.6 Log output

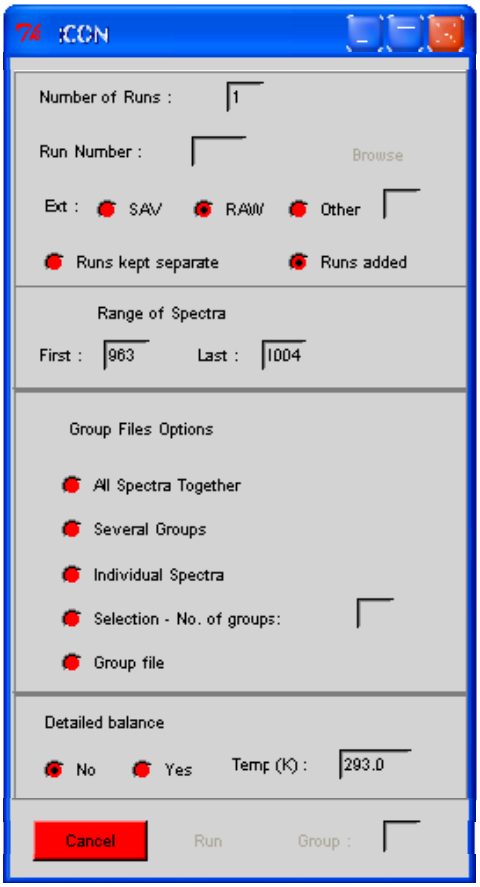
If set to 'ON', this option creates a file with the name <program name>_<date>_<time>.log, which contains some of the information that is in the header file (as it appears in 'Directory' – section 5.1.1), together with the ICL commands used.

5.3 Raw

The routines described in this section are the operations performed on the raw data.

5.3.1 Icon

This combines spectra into groups and converts from time-of-flight to energy transfer. An intermediate file is NOT created – this version is best used for checking data during the run.
The program requires the files *IRIS_detector.calib* or *OSIRIS_detector.calib* in order to read the angles.

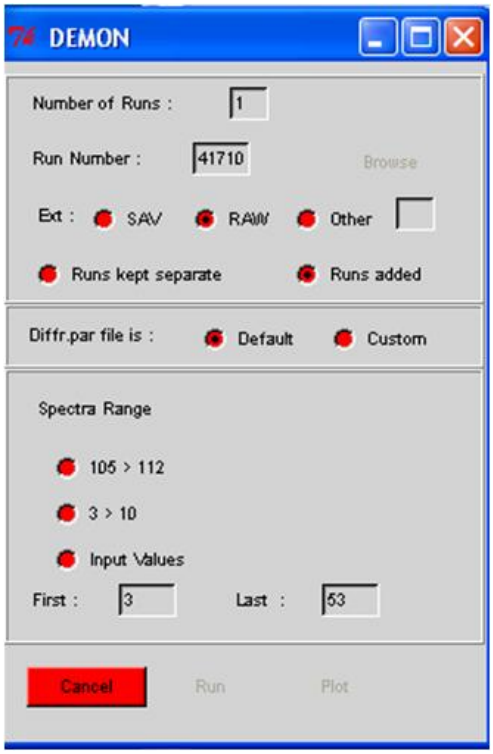


- Frame 1:
  - Insert number of runs. If there is more than 1 run, pressing Return will open a new window to either use 'Calculate' to set a sequence of run numbers or input each Run Number in 'Selection'.
  - Select extension: *.SAV, .RAW*, or Other, and enter into 'Other' box.
  - If more than 1 run has been selected, choose whether the runs are kept separate (ie. a file for each run) or added (ie. only 1 file created)
- Frame 2: Insert range of spectra. Default values given are those for the analyser selected.
- Frame 3: Select grouping scheme - creates files with *.grp* extension.
  - If 'All Spectra Together' is chosen, all spectra will be added together; *pg1op1.grp* created.
  - If 'Several Groups' is chosen, a new window appears to define the selection; enter the number of spectra per group (constant) or the number of groups (variable); *pg1op2.grp* created.
  - 'Individual Spectra' is chosen for no grouping; pg1op3.grp created.
  - 'Selection' can be used to make groups of non-consecutive spectra; *pg1op4.grp* created.
  - If 'Group file' is chosen, a new window appears with a list of *.grp* files, click on the one required, its name appears in the box, click on Select. The format of a user-created *.grp* file is:

#groups	5		
2	first spectra #	last spectra #	[first gp]
.	.	.	.
.	.	.	.
.	.	.	.
2	.	.	[last gp]

    This method is recommended when restarting MODES to maintain consistency. During a session MODES remembers the options and groups from previous usage.
- Frame 4: allows for detailed balance corrections at the sample temperature.
- Click on Run
- Each group can then be plotted: change group number, and Return or click on Group button.

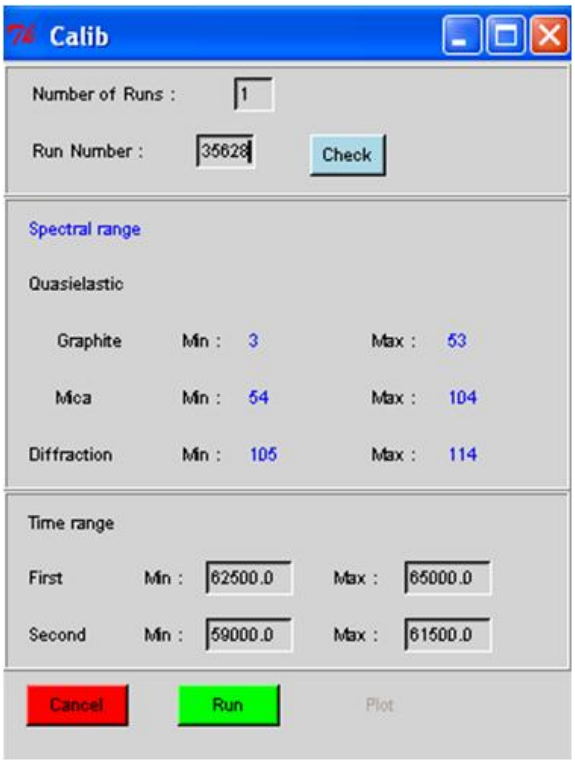
5.3.2 Demon



This combines all the diffraction spectra into 1 group and converts from time-of-flight to d-spacing in Å. An intermediate file is NOT created – this version is best used for checking data during the run. The program requires the file *IRIS_detector.calib* or *OSIRIS_detectors.calib* in order to read the angles and a *diffr.par* to define the time-of-flight to d-spacing correspondence. This parameter file would have been provided by the instrument scientist but the option is given to input a custom file.

- Frame 1: Same as in ICON.
- Frame 2: Use 'Default' or 'Custom' diffraction parameter file.
- Frame 3: Define range of spectra for diffraction detectors – on IRIS 105>114 is the range for the quasielastic setup and 3>12 is the range for the diffraction setup
- Click on Run
- Plot if required

5.3.3 Calib



This routine reads the raw file of a vanadium run and calculates the area of the elastic peak for each spectrum. When run, the default *IRIS_detector.calib or OSIRIS_detector.calib* is then edited and the new version created in the working area [In the past it used *detector.calib*].

- Frame 1: Insert number of runs and run number; if more than one is chosen, a new window will appear to enter individual run numbers. Press 'Check' to plot.
- Frame 2: Gives detector numbers for PG, Mica and diffraction.
- Frame 3: Define time ranges of spectra. First range defines the elastic peak; second range defines the background.
- Click on Run
- Plot, if required, to see the results

5.3.4 Slice

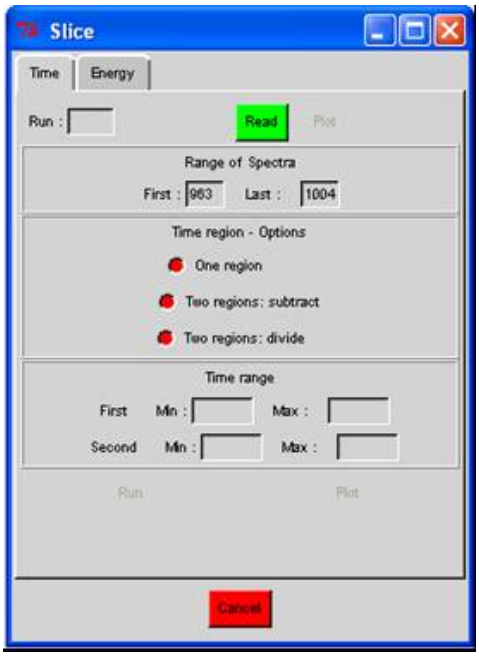
These routines perform integrations over a specified time-of-flight or energy range for each spectrum. Its most frequent use would be to calculate 'elastic window' scans. The window is a NoteBook, 'Time' or 'Energy' can be chosen by clicking on the appropriate Tab. The 'Energy' option is primarily used for analysing data to give the mean-squared-deviation (MSD) and will treat a series of *.RAW* files.

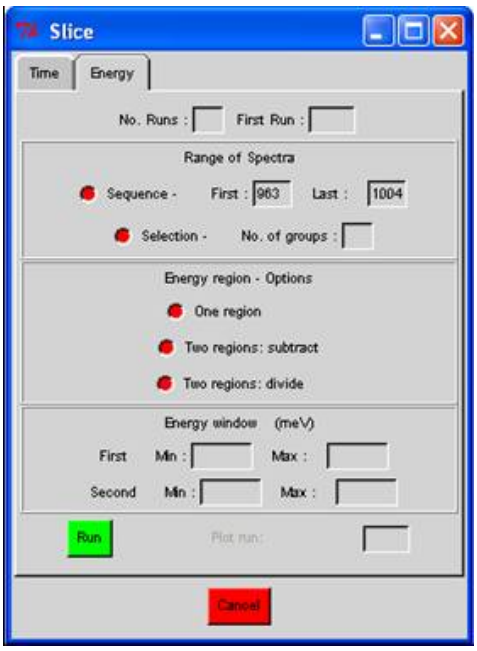
For 'Time' option:

- Frame 1: Insert run number& Read. Plot displays first spectrum to show time range
- Frame 2: Select range of spectra
- Frame 3: Define time range option
- Frame 4: Define time ranges. The second range details only appear when the 'Two regions' option is selected.
- Run
- Plot if required

For 'Energy' option:

- Frame 1: Insert number of runs. Insert the number for the first run, the program then loops over all the consecutive runs starting with that run
- Frame 2: Select range of spectra, under either 'Sequence' or 'Selection'
- Frame 3: Define energy range option
- Frame 4: Define energy ranges (in meV). The second range details only appear when the 'Two regions' option is selected.
- Run
- Plot if required. Insert the run sequence number, then Tab/Return or click on 'Plot' button





5.4 Int

The routines described in this section are the operations performed on the intermediate format data.

5.4.1 Ionian

This is the same as ICON (section 5.3.1) but files *.IPG* and *.GRP* are created in the working area.

5.4.2 Dorian

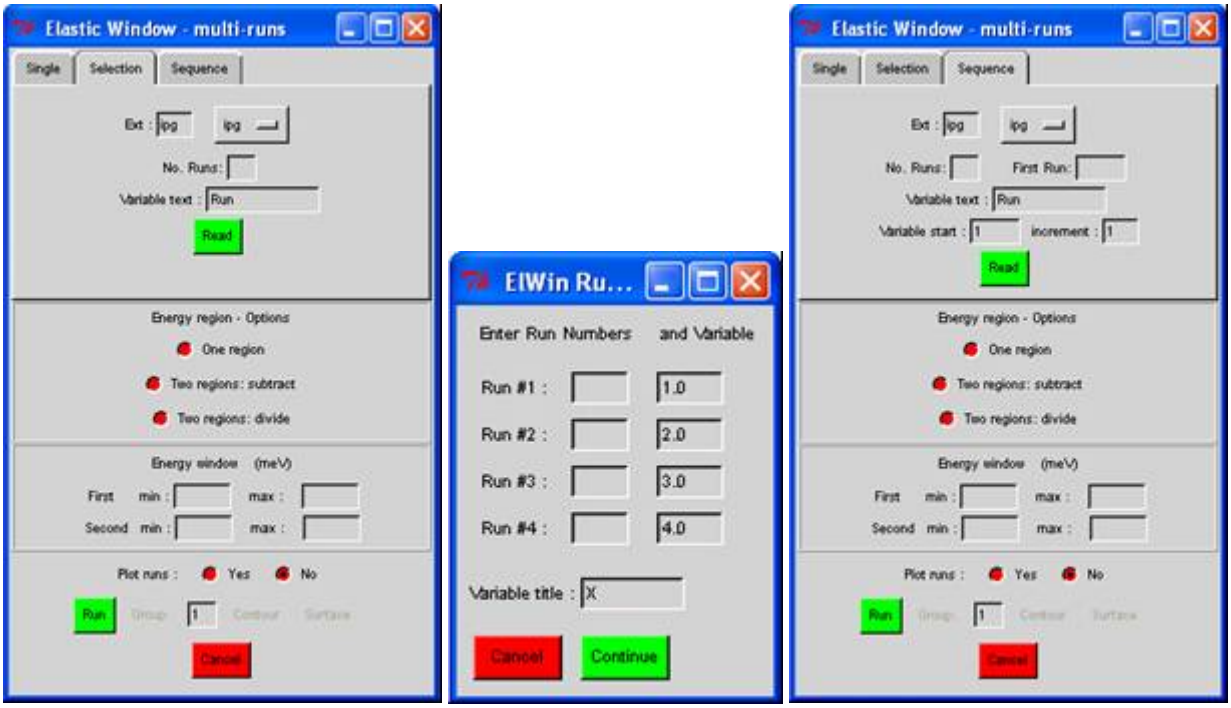
This is the same as Demon (section 5.3.2) but a file *.DIF* is created in the working area.

5.4.3 ElWin

This performs 'elastic window' scans by summing over the specified energy range.

Perform the following operations:

- Frame 1: is a NoteBook with tabs – click on Tab
  - Single: specified groups from a single intermediate file
    - Insert run number, or press 'Browse' to choose an *.IPG* file from a new window
    - 'Read' data
  - Selection: specified groups from a selection of intermediate files
    - Enter extension or choose from drop down menu
    - Enter number of runs and press enter/tab – new window will appear
    - Enter individual run numbers, the variable title, the value of the variable, and the variable name
    - 'Continue' and 'Read' the data
  - Sequence: specified groups from a sequence of intermediate files
    - Enter extension or choose from drop down menu
    - Enter number of runs and number of first run
    - Enter variable text, the first value of the variable and the increment
    - 'Read' the data
- Frame 2: select energy option (eg. one region for energy range of elastic line)
- Frame 3: insert minimum and maximum energies for the integration
- Frame 4: plotting runs
  - To plot integrated counts versus Q or Q^2, select 'Yes'. A new window appears when 'Run' is pressed; choose either Q or Q^2; choose 'Next' to proceed to next run, or 'Cancel' for the program to integrate the counts but not plot.
  - To plot integrated counts versus run number (variable), select 'No'. Use the 'Group' button to plot integrated counts of each group (Q) as a function of variable (run).

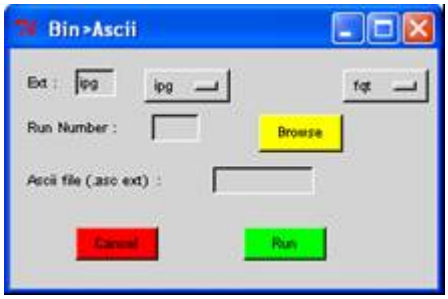


The program creates two ASCII files of the result by run number: a file *.ELQ* of intensity and errors as a function of Q, and a file *.MSD* of intensity and errors as a function of Q^2. The latter file is then the input into program MSD fit (section 5.7.5). In addition, when running the 'Yes' option in Frame 4, an extra file *.ELQ* is created where all Q, run variable and integrated counts are stored.

5.4.4 S(Q,w)

Similar to ICON but allows rebinning of data in Q and E. Creates *.SPE* files that can be read by MSLICE and *.SQE* files which contain S(Q,w) data. Contains the options CONTOUR (section 5.9.1) and VIZ (section 5.9.2).

5.4.5 Bin>Ascii



This routine is used to convert binary files into ASCII versions.

- Choose the extension of the binary file from drop-down menus (graphite intermediate files, mica intermediate files and data analysis files).
- Insert run number or 'Browse'
- Insert filename (automatically gives an extension *.ASC*)
- 'Run'
- The *.asc* file created will have some header information plus three columns [Energy (meV),

S(Q,w) and error in S(Q,w)]. Data for each group is given one after the other.

5.4.6 Ascii>Bin

This routine is used to convert ASCII files into binary files. The input format should be three columns corresponding to Energy (meV), S(Q,w) and error in S(Q,w). Only one Q can be read.

5.5 Diff

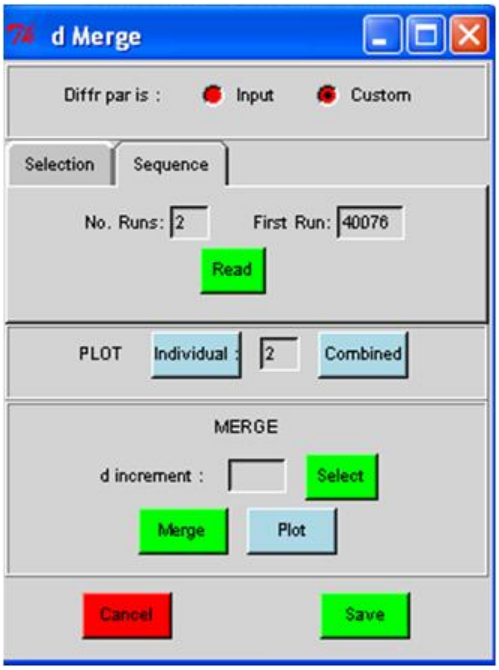
5.5.1 dVan

This is DORIAN for vanadium standard and creates a *.DVN* file in the working area.

5.5.2 dNorm

This normalizes diffraction data (*.DIF*) by the measured vanadium standard (*.DVN*). Creates a *.DIN* file in the working area.

5.5.3 dMerge



This merges the data from several *.DIF* diffraction files into one spectrum.

• Frame 1: Use 'Input' (default) or 'Custom' diffraction parameter file.
• Frame 2: Select range of spectra, under either 'Selection' (Return to enter Run Number) or 'Sequence'. Then Read.
• Frame 3: Plot 'Individual' run or 'Combine' the runs.
• Frame 4: Defines Merge parameters: d-increment - common for all spectra; 'Select' opens a new window to define the d-range for each spectrum - min & max values calculated from the data are shown; 'Merge' performs merge; 'Plot' shows merged spectrum
• 'Save' writes merged spectrum to file with extension .DIM

5.5.4 dCor

Performs absorption corrections (section 5.6.2).

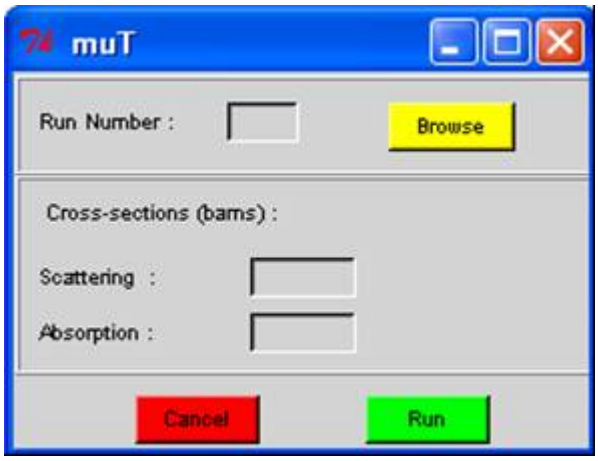
5.5.5 dAna

Performs multiple scattering and container corrections for diffraction data (section 5.6.4)

5.6 Analyse

The routines in this section are used to calculate the absorption and multiple scattering and use them on sample and container data.

5.6.1 Mut

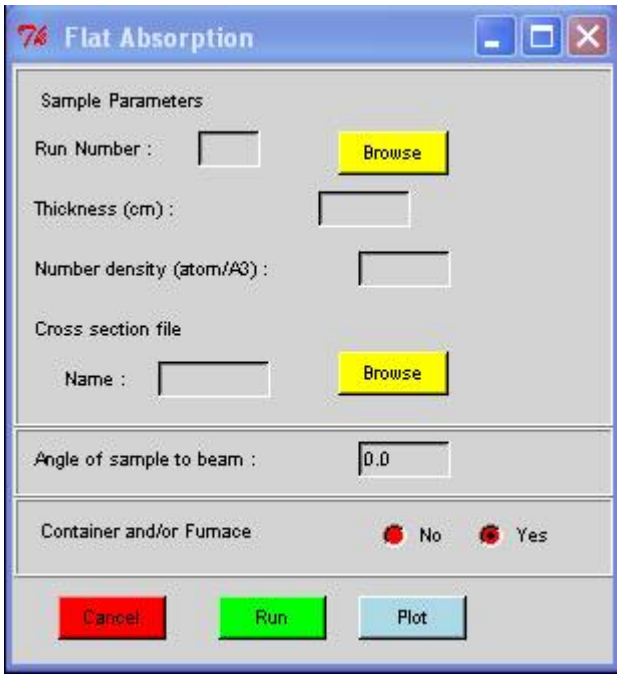


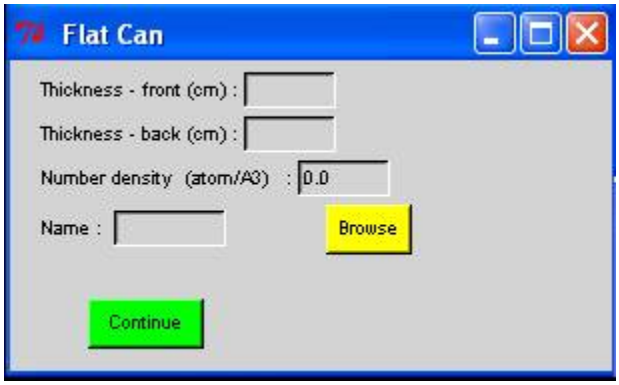
This creates a cross-section file with extension *.MUT*. Perform the following operations:

• Frame 1: Insert run number or 'Browse' & Select
• Frame 2: Insert scattering & absorption cross-sections. 'Run' to create file and display graph.

5.6.2 Acorn

This calculates the absorption corrections. A different layout of window appears for each type of sample geometry (flat or cylinder) depending on which sample geometry has been chosen in the MODES options. There MUST be a *.MUT* file for each sample (and container) used.





For <u>flat plate</u> geometry, perform the following operations:

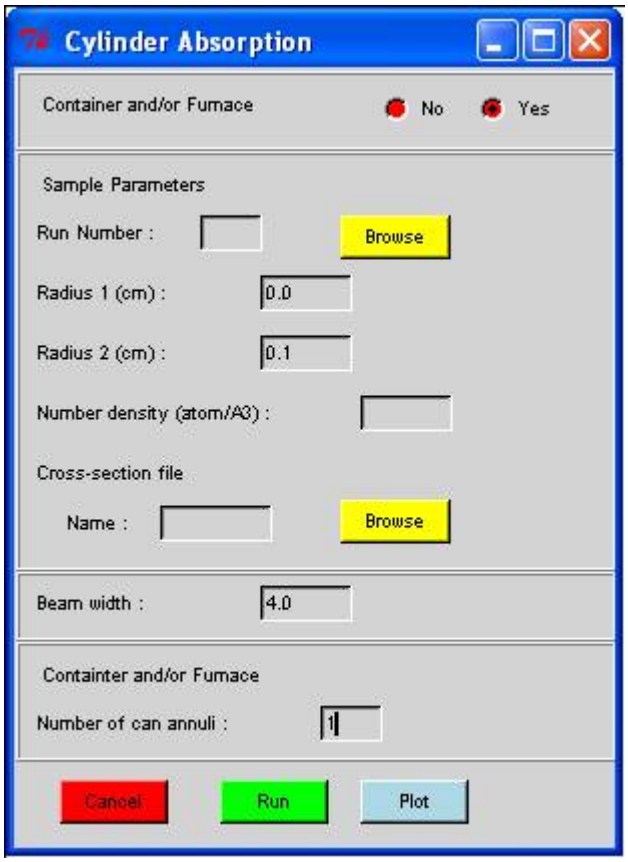
• Frame 1:
- Insert sample run number or 'Browse' & Select
- Insert sample thickness & number density

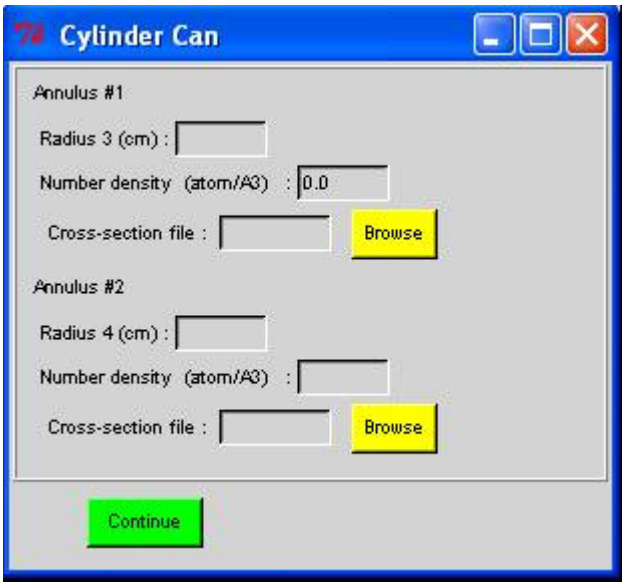
- Insert name of *.MUT* file or 'Browse' & Select

• Frame 2: Insert angle of sample to beam

• Frame 3: Select container 'No' or 'Yes'. If 'Yes', a new window will appear for the can parameters:

- Insert thickness of front and back
- Insert number density
- Insert name of *.MUT* file or 'Browse' & Select





For cylindrical geometry, perform the following operations:

• Frame 1: Select container option 'No'/'Yes'

• Frame 2:

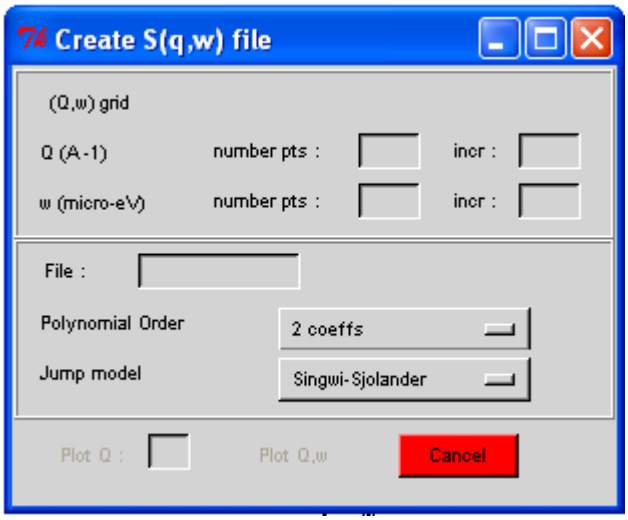
- Insert sample run number or 'Browse' & Select
- Insert sample inner radius, outer radius & number density (if sample is a solid cylinder, r1=0, r2=outer radius)
- Insert name of *.MUT* file or 'Browse' & Select

• Frame 3: Insert beam width

• Frame 4: For annular geometry. Insert number of annuli. For standard IRIS/OSIRIS cells, insert '1'. Values of r1, r2 and r3 will be inner sample radius, outer sample radius and (outer sample radius+2xcan wall thickness), respectively. If your container has more than one annulus, for each annulus insert radius, number density and name of *.MUT* file or 'Browse' & Select and

'Continue'.
• 'Run' and 'Plot' the results, if required

5.6.3 Create S(Q,w) file



This creates an S(Q,w) file to be used as input in the multiple scattering correction program MINUS (section 3.4.2).

• Frame 1: Define the (Q,w) grid size
• Frame 2: Set an output file name, including the extension. Create S(Q,w) file based on one of two options: Polynomial or a Jump Model. Choose model option and a new window will appear to input parameter values. In all cases the model will be used to calculate the half-width w_0 such that S(Q,w) is then calculated as $S(Q,w)=Peakheight*w_0/(w_0^2+w^2)$.

The input for the polynomial function has a maximum of 5 parameters (c1 to c5), so that the half-width is: $w_0=c_1+c_2Q+ c_3Q^2+ c_4Q^3+ c_5Q^4$.

Two Jump Models are available:

a) Chudley-Elliott: Input parameters A and K such that $w_0=A*[1.0-\sin(QK)/QK]$
b) Singwi-Sjolander: Input parameters A and R2 such that $w_0=A*[1.0-\exp(-R^2Q^2)]$

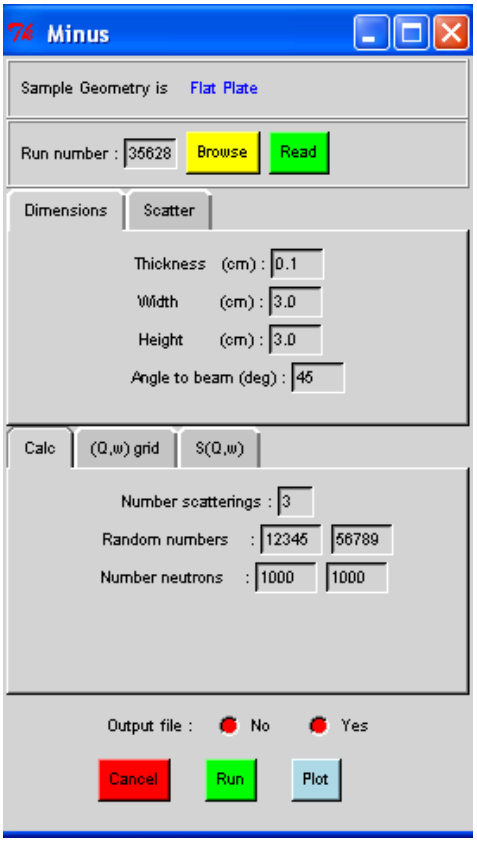
5.6.4 Minus

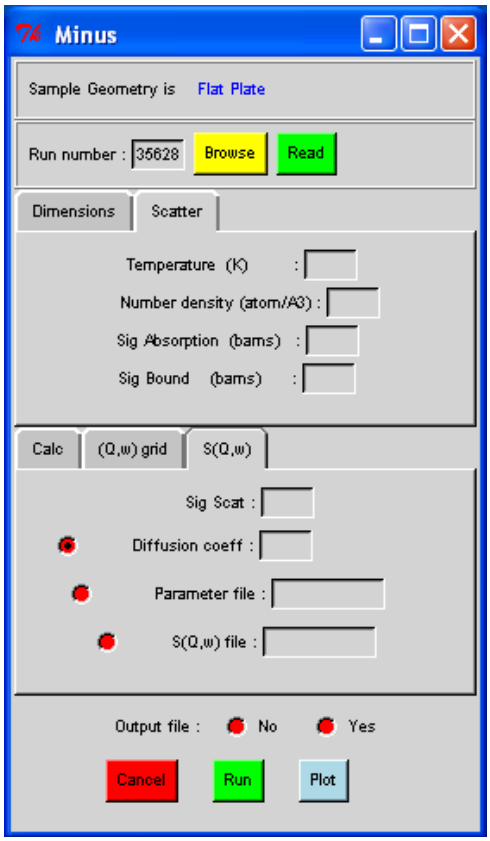
This calculates the multiple scattering corrections based on Monte Carlo calculations (section 3.4.2).

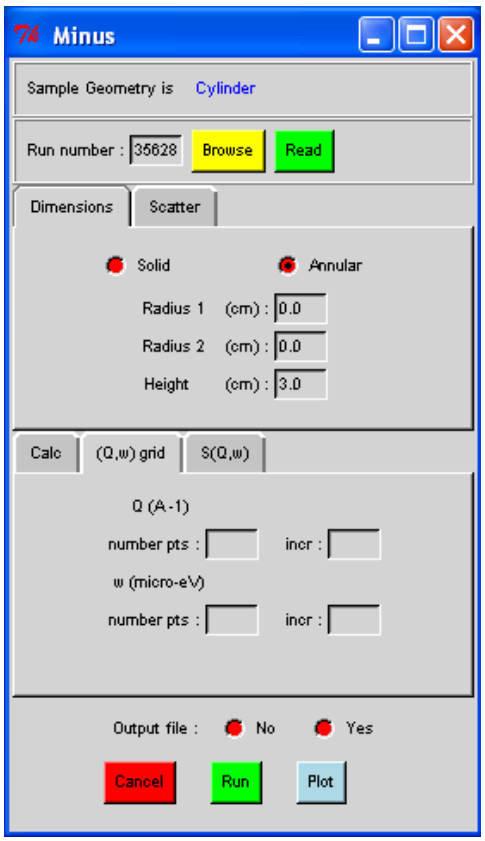
• Top Frame: Indicates which sample geometry has been chosen in MODES options.
• Frame 1: Insert sample run number or 'Browse' & Select, then 'Read'
• Frame 2: Is a Notebook with tabs – Click on tab
  - Dimensions: are those for the sample
    * For flat plate, insert thickness, width, height and angle to beam
    * For cylinder, insert radius 1 (outer diameter of the sample) and height
    * For annular, insert radius 1 and 2 (inner and outer sample diameters, respectively), and height
  - Scatter: insert temperature of run & number density, cross-sections for absorption and bound scattering for sample
• Frame 3: Is a Notebook with tabs – Click on tab
  - Calc: parameters for Monte Carlo routine

    * Insert number of scatterings (for single scattering, 1)
    * Insert random number starting values –values to start random number generator
    * Insert number of neutrons for the simulation
- (Q,w) grid: same as in section 5.5.3
- S(Q,w): similar to that in section 5.5.3. Here you can insert scattering cross-section and choose the form of S(Q,w)
    * Input diffusion coefficient in units of 10^{-5} cm^2/s
    * Enter a parameter file containing diffusion coefficients for polynomial function (section 5.5.3)
    * Input S(Q,w) file name created in section 5.5.3

• Frame 4: Choose whether you want an output file
• 'Run' to start calculation and 'Plot' to see the results.



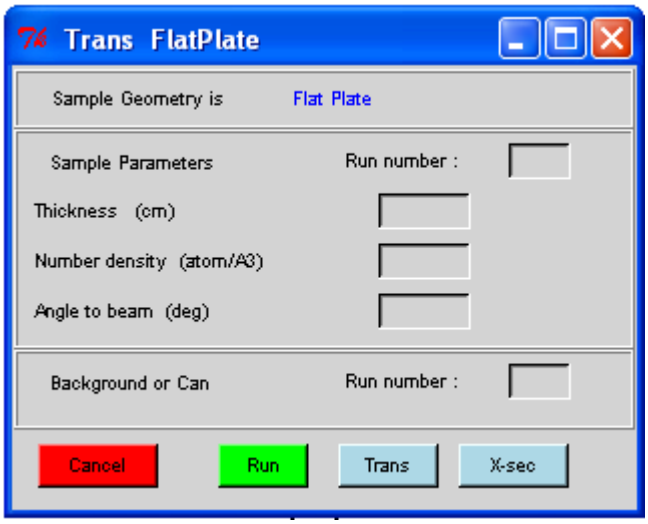




5.6.5 Trans

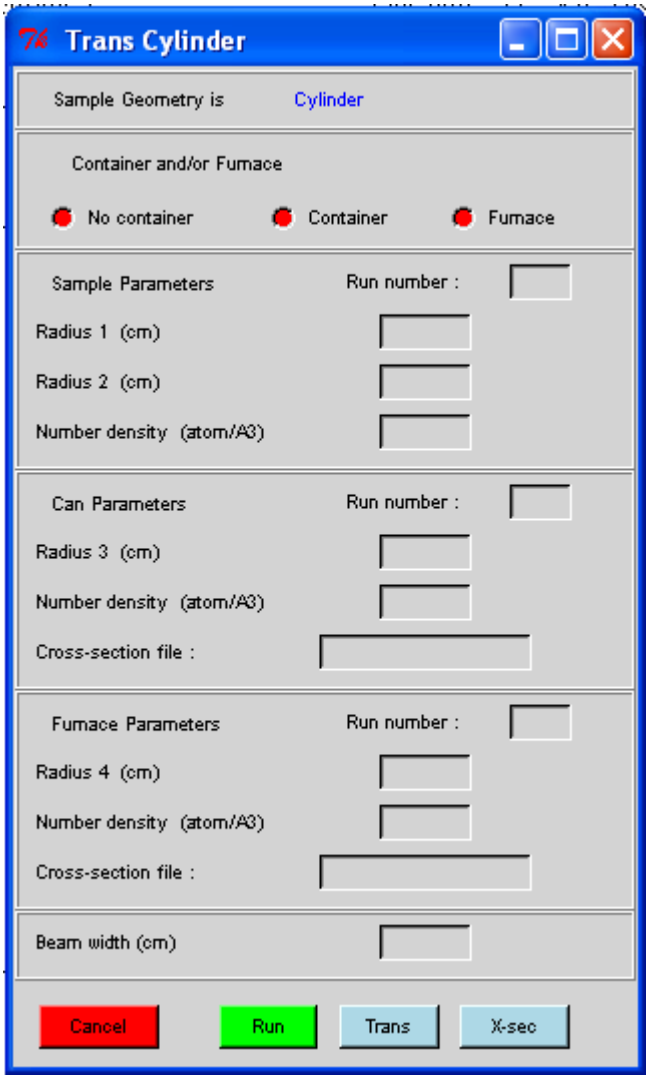
This calculates the transmission and cross-sections using the monitor spectra. Top Frame indicates which sample geometry has been chosen in MODES options.

For flat geometry, perform the following operations:



• Frame 1: insert sample run number, sample thickness, number density and angle of can to beam.
• Frame 2: Insert background or empty can run number.
• 'Run' to perform calculations
• Use 'trans' to plot transmission
• Use 'x-sec' to plot calculated cross-sections

For cylindrical geometry, perform the following operations:



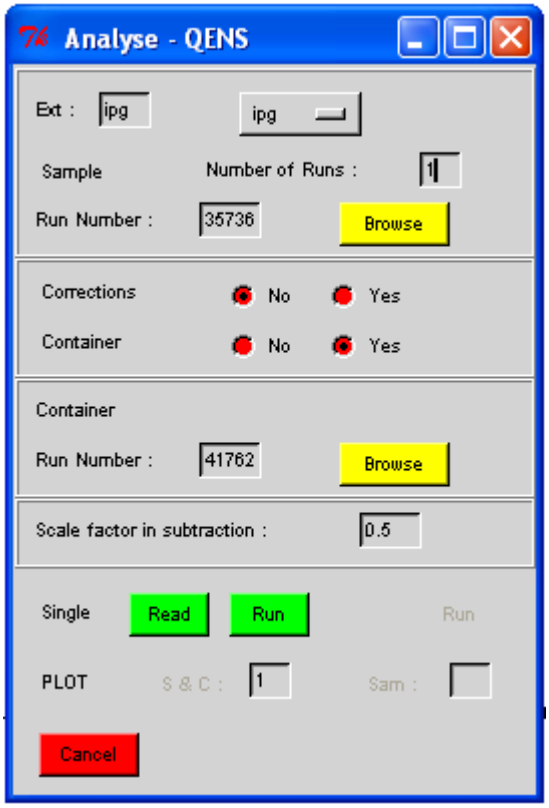
• Frame 1: Choose contained and/or furnace option.
• Frame 2: Insert sample run number, radii 1 and 2 and number density.
• Frame 3: If no container, insert background run number; if container insert empty can run number, can radius, number density and *.MUT* file.
• Frame 4: Will appear if a furnace is selected. Insert sample run number, furnace radius, number density and *.MUT* file.
• Frame 5: Insert beam width
• 'Run' to perform calculations
• Use 'trans' to plot transmission
• Use 'x-sec' to plot calculated cross-sections

5.6.6 Analyse

This routine subtracts the container from the samples and performs absorptions corrections if required. With the corrections option off, it can be used to compare 2 sample runs.

• Frame 1: Insert number of runs, sample run number or 'Browse' & Select.
• Frame 2: Switch 'Corrections' to On/Off and switch 'Container' to On/Off.

• Frame 3: Insert Container run number or 'Browse' & Select.
• Frame 4: Inset scaling factor for the subtraction (default 1).
• 'Read' and 'Run' to subtract the data.
• Plot options:
  - 'S & C' to plot sample & container together
  - 'S' to plot subtracted



For simple subtraction (ie. no corrections), an *.IBG* file is created from *.IPG* or *.IBM* from *.IMI*. For corrected data, an *.IAG* file is created from *.IPG* or *.IAM* from *.IMI*.

5.7 Function

These are a set of routines for performing various functions, such as fitting data.

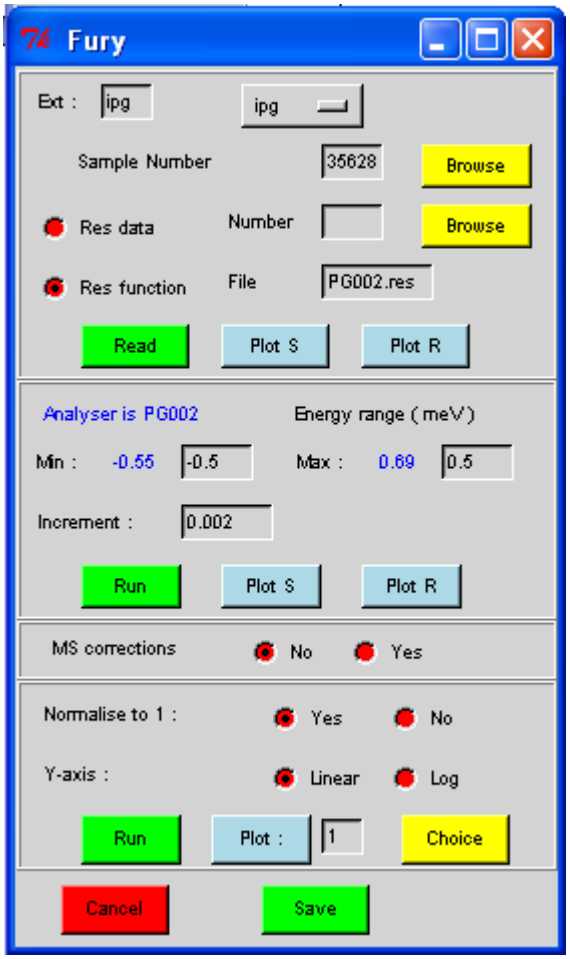
5.7.1 Fury

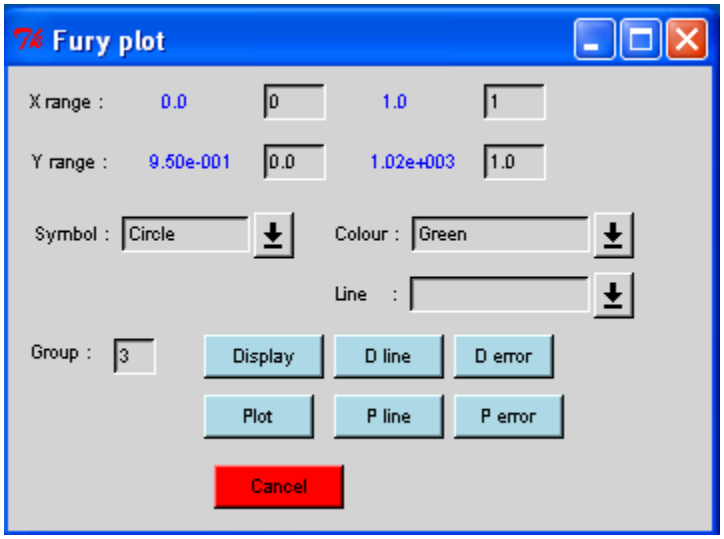
This converts the S(Q,ω) to I(Q,t) using a Fast Fourier Transform routine. Perform the following operations:

• Frame 1: Choose sample and resolution runs:
  - Choose the file extension from the drop-down menu
  - Insert sample run number or 'Browse' & Select
  - Insert resolution run number or use provided one [*PG002.res*]
  - 'Read' then 'Plot' Sample ('S') and/or Resolution ('R') to check energy range of the first group
• Frame 2: The analyser chosen in MODES options is shown.
  - Choose energy range and increment step for Fourier Transform
  - 'Run' to rebin energy then 'Plot' Sample ('S') and/or Resolution ('R') to check energy range of the first group
• Frame 3: Choose whether to apply MS corrections.
• Frame 4:
  - Choose whether to normalise to 1
  - Choose type of scale for the y-axis
  - 'Run' to perform FFT
  - Insert group number and 'Plot', or 'Choice' for multiple plots. A new window will appear:
    * Insert X range (after using 'Plot') in nanoseconds
    * Insert Y range
    * Choose Symbol, Colour & Line from drop-down menus

* Insert group number and ‘Display’ (& Plot line and P error if required)
* To add further groups, change group number, and change the Symbol and/or Colour and/or Line, then ‘Plot’ to add data set to graph.
* N.B. ‘Display’ will always clear the graph of all data sets before plotting the desired one, whereas ‘Plot’ will plot the desired data set on top of the ones already plotted.

• ‘Save’ as *.FQT* file.

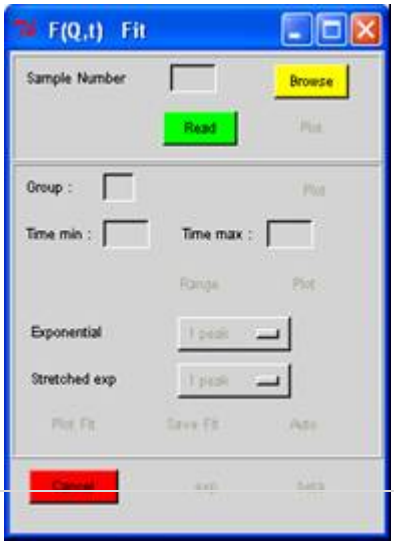


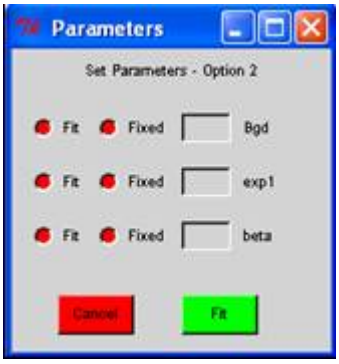


5.7.2 Fqt Fit

This fits the I(q,t) with a specified function.

• Frame 1:
- Insert run number or ‘Browse’ & Select
- ‘Read’ to read all the groups
- ‘Plot’ to see the first group and



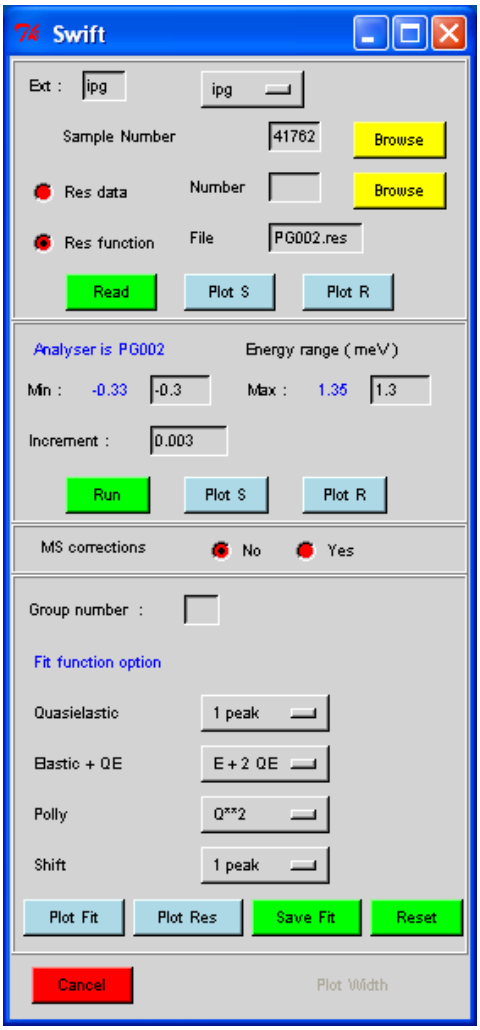


check on time range (in nanoseconds)

- Frame 2:
  - Insert Group number and 'Plot'
  - Insert time range & click on 'Range' to rebin
  - 'Plot' if required
  - Choose the type of fit from the appropriate drop-down menu:
    * Exponential function requires 2 parameters, exp1 [ns^{-1}] and Bgd [value between 0 and 1], for the form I(Q,t)/I(Q,0)=exp(exp1*t)+Bgd
    * Stretched exp requires 3 parameters, exp1[ns^{-1}], Bgd and beta [values between 0 and 1], for the form I(Q,t)/I(Q,0)=exp(-exp1*t)$^{\beta}$+Bgd

A second window titled Parameters also opens upon opening the F(Q,t) Fit window, and is also opened when either of the drop down menus are clicked:

- Insert starting value & choose whether the parameter is to be fitted or stays fixed
- Click on 'Fit' to close the parameter window and start the fitting procedure
- 'Plot fit' to see the fit
- 'Save fit' to save results, if required
- 'Auto' to automatically fit all Groups
- 'Exp' plots the saved values of exp1 as a function of Q
- 'Beta' plots the saved values of beta as a function of Q for the stretched exponential function.



5.7.3 Swift

This performs a convolution fit, that is, it convolves a specified function with the measured
resolution data and fits the result to the measured sample data. Four options are available:

1. A set of quasielastic peaks
2. An elastic peak with quasielastic peaks
3. Polymer shapes
4. An elastic peak with a set of inelastic peaks

Perform the following operations:

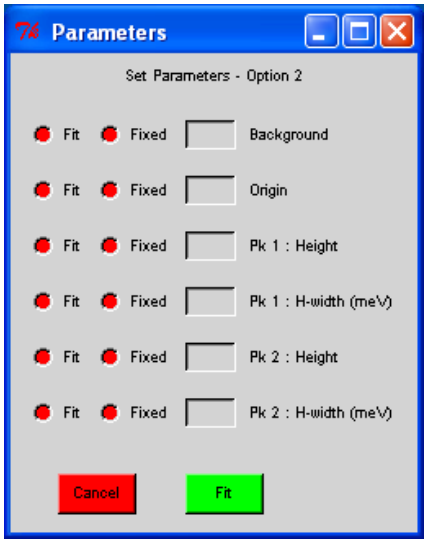
- Frame 1:
  - Choose the file extension from the drop-down menu
  - Insert sample run number or 'Browse'
  - Insert resolution run number or 'Browse', or enter resolution file name
  - 'Read' to read all groups into workspaces
  - 'Plot' S(ample) and 'Plot R(es)' to plot first group of each file
- Frame 2:
  - The analyser chosen in MODES options is shown

- Define energy range and increment for fit
- Run to rebin data to new energy range
- Plot S(ample) and Plot R(es) to plot first group of each file

• Frame 3:
- Choose Group number
- Choose type of fit function & number of peaks from drop-down menu
- 'Plot Fit' displays the fit, 'Plot Res' displays the residuals
- 'Save Fit' stores parameters in file and 'Reset' zeroes stored parameters
- 'Plot width' plots stored fitted half-widths

A new window will appear to set starting fit parameters for each option. These can be set to remain fixed or to be fitted. Use 'Fit' to close the window and start the fitting procedure.

Option 1:
- Background
- Origin
- Elastic height
- Height and half-width (meV) for each Lorentzian



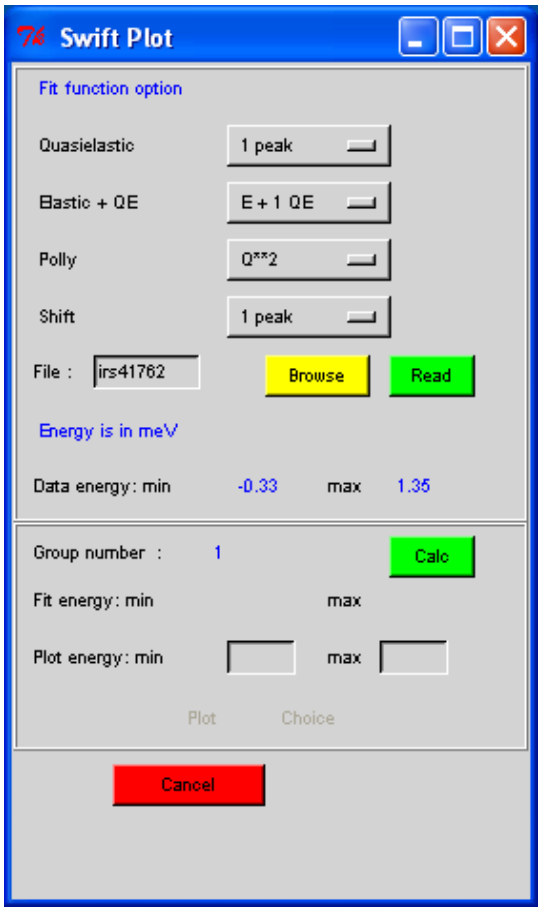
Option 2:
- Background
- Origin
- Elastic height
- Height and half-width (meV) for each Lorentzian

Option 3:
- Background
- Origin
- Height and half-width (meV) for each Lorentzian

Option 4:
- Background
- Origin
- Height and half-width (meV) for the elastic peak
- Height and half-width (meV) for the inelastic peak

After the first fit, when the parameter window opens it will show the fitted values of the previous fit. So if a set of groups is to be fitted when a good first fit is obtained these values may be used as starting values for the next group. Alternatively, for a given group the fitted values for 1 peak may be used as starting values for a 2 peak fit. To fit each group individually enter the Group number. To start the fit for all groups, click 'Auto'.

5.7.4 Swift Plot



This allows you to plot saved fit parameters from SWIFT.

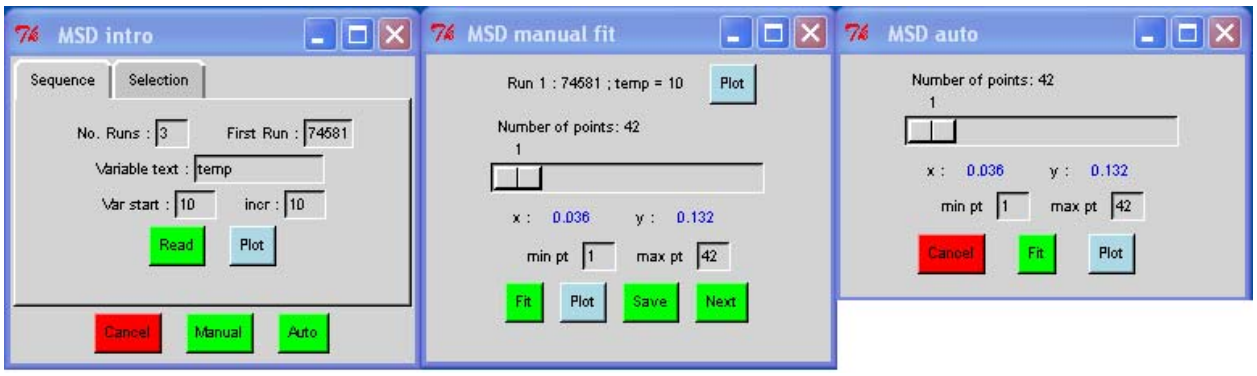
- Frame 1:
  - Choose the fit function (section 5.7.3)
  - Insert sample run number or 'Browse'
  - 'Read' to read all groups into workspaces
  - Energy range is given for the data
- Frame 2:
  - Enter the group number and 'Calc'
  - Choose energy range for display and 'Plot'.
  - Use 'Choice' to choose colour, symbol and line type for the plot (similar to that in section 5.7.1).

5.7.5 Msd Fit

This routine fits a straight line to data in order to calculate the mean-squared-displacement (msd). The input files have the extension *.MSD* which were created by the program ELWIN (section 5.4.3).

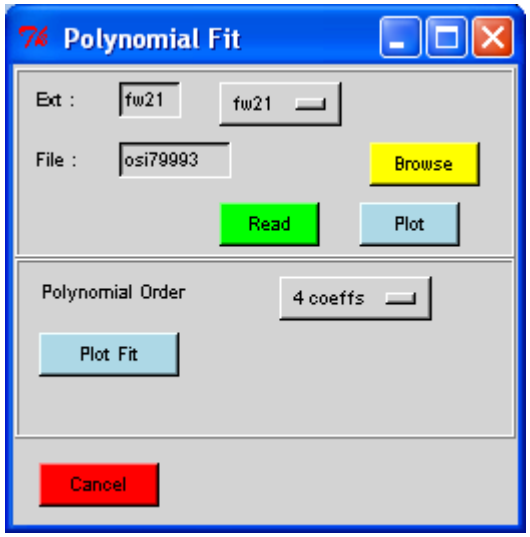
In the first window, insert the number of run numbers, the first run number, the variable (eg. Temperature), the variable start value and the increment, 'Read', and 'Plot'. The plot will be Ln (Intensity) vs. Q^2. The data will be fitted with a straight line, where the gradient is the msd. There are then 2 options (new windows will appear):

- 'Manual': allows you to fit each run and each group (point) individually
  - Use the scroll bar to see the values of 'x' and 'y' for each point (group)
  - Choose the fit range with 'min pt' and 'max pt' numbers.
  - Click 'Fit' to start fitting.
  - 'Save' the fit parameters for the run. Output file with extension *.LINE_LOG*
  - Click 'Next' to fit the next run



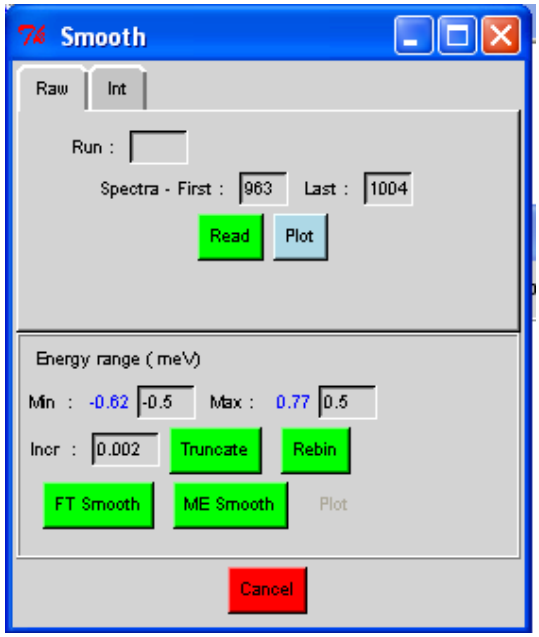
• 'Auto': will fit all runs in one go
  - Use the scroll bar to see the values of 'x' and 'y' for each point (group)
  - Choose the fit range with 'min pt' and 'max pt' numbers.
  - Click 'Fit' to start fitting.
  - 'Plot' msd as a function of the variable (eg. Temperature). An output file is automatically created with the msd data with extension *.MST*

5.7.6 Poly Fit



This routine fits polynomials up to the 5th order to full-width at half-maximum values obtained using the BAYES program (section 5.8). The input files have extension .FW<n><m>. To fit, choose the extension from the drop-down menu, enter file number or 'Browse', 'Read' and 'Plot'. Choose the nth order polynomial for the fit and when a new window appears, enter initial guesses for the coefficients, and choose fixed or fit. Then 'Plot Fit'. The fit values will be store in the output file with extension *.POLY_LOG*.

5.7.7 Smooth



This routine performs a smoothing operation on a spectrum via one of 2 techniques:

1) FFT Smooth: transform, apply the Weiner filter to truncate the noisy high x-values and back transform

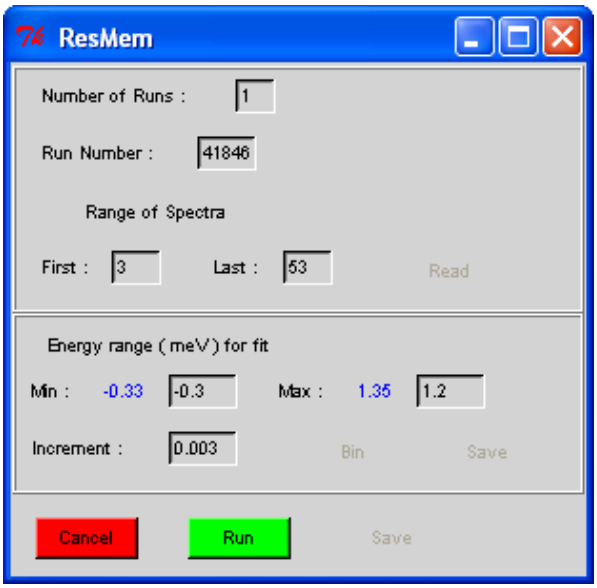
2) Maximum Entropy (ME) Smooth: uses same concept as in ResMem (section 3.7.2)

5.8 Bayes

This section contains a set of programs performing analysis using Bayesian methods. Several of the routines use a 'Res file'; this contains a smooth curve representing the resolution function if the instrument.

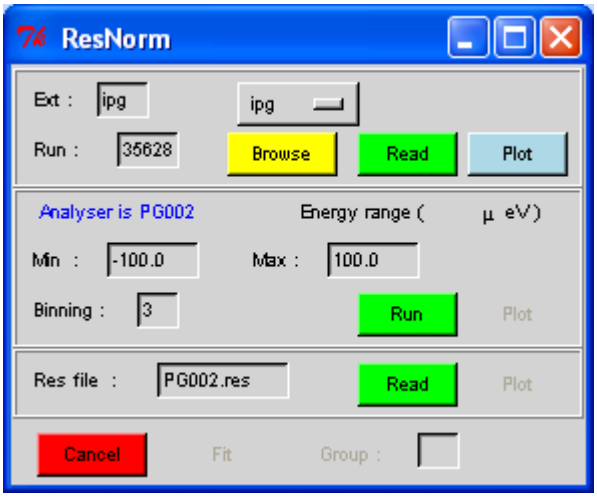
5.8.1 ResMem

This routine creates a *PG002.RES* file from chosen vanadium run. It also outputs a *.VAN* file.



- Frame 1:
  - Insert number of runs
  - Insert sample run numbers
  - Insert range of spectra
- Frame 2:
  - Choose energy range for the fit (meV)
  - Choose increment for 'Bin'
  - 'Save' the rebinned data as a *.VAN* file.
- 'Run' and 'Save' creates the file *<analyser>.RES* where *<analyser>* is eg. PG002 as defined in MODES setup.

5.8.2 ResNorm



This routine fits the 'Res file' to the measured resolution data and creates a *.RES* file containing the stretch factor for the width and the integrated intensity. Perform the following operations:

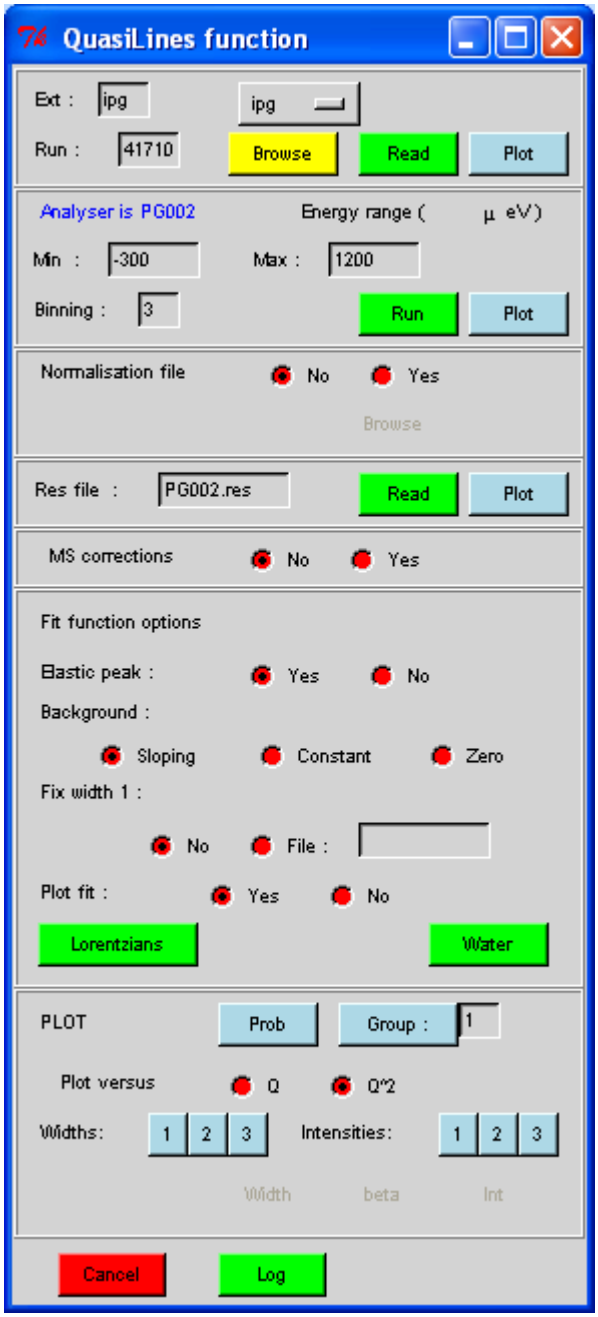
- Frame 1:
  - Choose the file extension from the drop-down menu
  - Insert run number or 'Browse'
  - 'Read' and 'Plot' the first group
- Frame 2: shows the analyser selected in the MODES option.
  - Choose energy range for the fit (meV)
  - Define energy range and binning
  - 'Run' to rebin
  - 'Plot' first group (if required)
- Frame 3: shows appropriate *.RES* file the analyser selected. 'Read' file and 'Plot' (if required)
- Fit and 'Plot' group

A file with the name *run_name.RES* is created.

5.8.3 QL function

This runs the QuasilLines program using the 'Res file' function for resolution and the *.RES* file created by ResNorm, if required. Perform the following operations:

- Frame 1:
  - Choose the file extension from the drop-down menu
  - Insert run number or 'Browse'
  - 'Read' and 'Plot' the first group



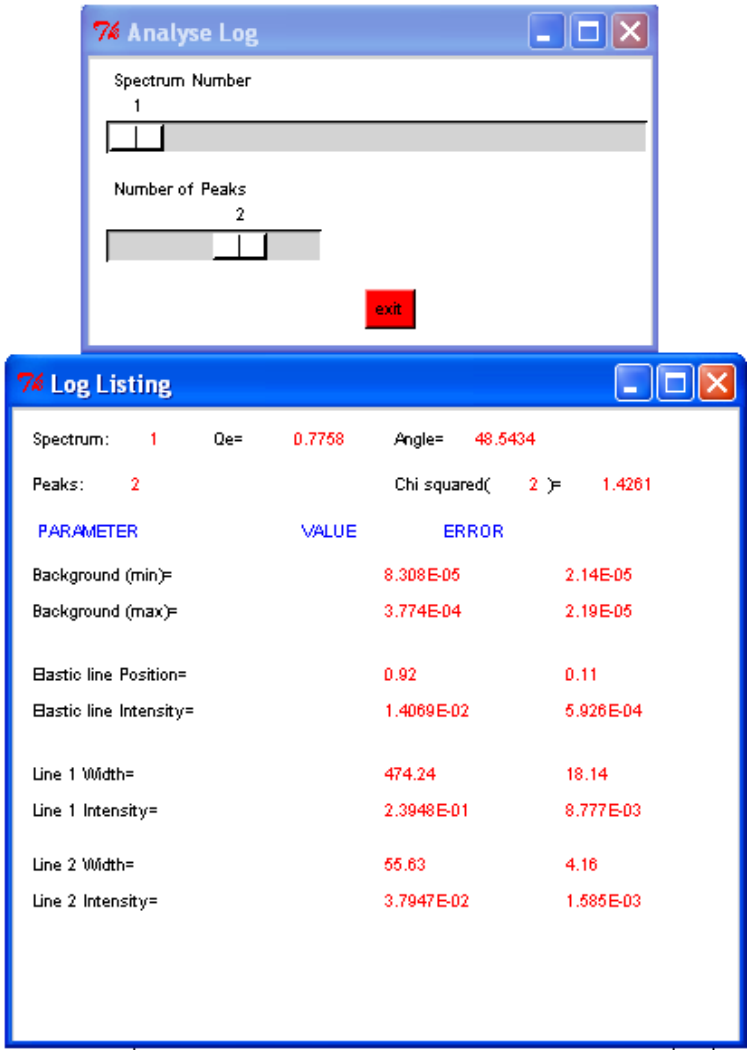
- Frame 2: shows the analyser selected in the MODES option.
  - Choose energy range for the fit (meV)
  - Define energy range and binning
  - 'Run' to rebin
  - 'Plot' first group (if required)
- Frame 3: choose whether to use a Normalisation file. If yes, insert *.RES* file name or 'Browse'.
- Frame 4: shows *.RES* file appropriate for selected analyser. 'Read' file and 'Plot' (if required)
- Frame 5: choose to apply multiple scattering corrections (requires a *.MSC* file from MINUS)
- Frame 6: choose fit parameters - options are:
  - Elastic peak: 'Yes' or 'No' to fit the peak
  - Background: 'sloping' (linear), 'constant' (flat) or 'zero'
  - Fix width 1: 'No' or 'File' to fix one of the three quasielastic peaks with widths as defined in a text file (including extension) with 2-column format, i.e. <width> <error in width> (use one line per group).
  - Plot fit : 'Yes' to show plots for each group or 'No'
  - The start fit with:
    * Lorentzians: elastic peak & up to 3 quasielastic peaks
    * Water: elastic peak & 3 linked quasielastic peaks

    If the Plot option is 'On' then after each fit a window appears to allow plotting of the fitted data and/or the residuals; Lorentzians – elastic only (0) or with peaks (1,2,3); Water – elastic only (0) or with peaks (2). 'Next' moves on to the next group and 'Cancel' switches off the plotting option and the fitting continues for all groups.
- Frame 7: selection of Plot options
  - 'Prob' for probability of each Lorentzian as a function of group. Plotted as Log[no. of quasi-elastic lines]- the less negative the value, the better the fit (the top curve is the best). This is very useful to decide how many Lorentzians are appropriate to fit the data.
  - 'Group' for fit for chosen group
  - Choose whether the x-axis is to be Q or Q^2
  - Plot 'Widths' & 'Intensities' for 1, 2 or 3 peaks

• The Log button opens 2 windows that give a summary of the fitted parameters. Use the sliders to choose the spectrum number and the number of peaks fitted. For each spectrum, the parameters, their errors and the Chi-squared value are given.

The program creates files with extensions for:

Lorentzians: *.Q2lpt* is the full printout of the fitting procedure, *.QL1* the fit parameters for 1 peak, *.QL2* for 2 peaks and *.QL3* for 3 peaks. If the results are plotted, then the routine uses the Conv>width routines (section 5.8.4) to create ASCII files of the fitted parameters. These have extensions as follows: the widths are *.FWnm* where *n* is the number of peaks fitted and *m* the peak number, the peak amplitudes are *.AMnm* using the same nomenclature for *n* and *m* and where *m*=0 is the elastic peak, and the calculated Elastic Incoherent Structure Factors are *.EIn*



Water: *.QWlpt* is the full printout of the fitting procedure, *.QLW* the fit parameters. If the results are plotted, then the routine uses the Conv>width routines (section 5.8.4) to create ASCII files of the fitted parameters. These have extensions as follows: the widths are *.WAT1* and *.WAT2*, and the amplitude as *.WATnm* where *n* is the number of peaks fitted and *m* the peak number.

5.8.4 Str Function

This is similar to QL function (section 5.8.3), but allows the data to be fit to a Stretched Exponential function. The frames are the same except for:

• Frame 6: does not have the option to input a Width file
• Frame 6a: enter the size of the search grid for the stretched exponential parameters Beta (stretching exponent) and Sigma (width/2). To start click 'Search': the program will test fits

with different combinations of beta and sigma. A new window will appear with option for plotting the results:

- 'Contour' and 'Viz' to plot grid showing the correlation between the beta and sigma parameters
- 'Beta' plots the distribution of beta parameters that fit the data.
- 'Sigma' plots the distribution of sigma parameters that fit the data.

• Frame 7: same as in section 5.8.3, but now Plot 'Width' & 'Beta' & 'Int'. In stretched exponential model the fit is with either an elastic peak only (0) or with a quasielastic peak with stretched form (1).

The program creates files with extensions: *.QSElpt* is the full printout of the fitting procedure, and *.QSE* for the fit parameters. Creates also *.SE0* (elastic intensity), *.SE1* (width), *.SE2* (beta) and *.SE3* (peak intensity).

5.8.5 QL data

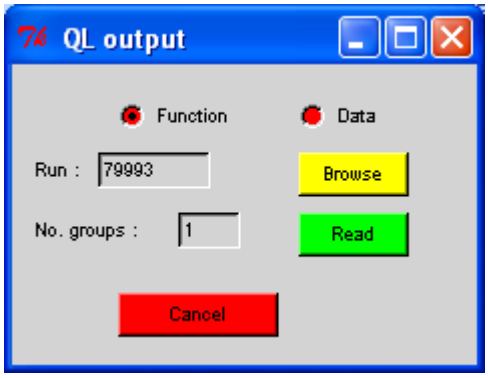
This is similar to QL function (section 5.8.3), but allows the data to be fitted using a measured resolution data. The frames are the same except for:

• Frame 3: is not needed (so is not there)
• Frame 4: enter the measured resolution file. Insert run number or 'Browse'. Choose energy range and binning. Click 'Range' and 'Plot' group 1 (if required).

The program creates files with extensions: *.QRlpt* is the full printout of the fitting procedure, *.QL1* the fit parameters for 1 peak, *.QL2* for 2 peaks and *.QL3* for 3 peaks. If the results are plotted, then the routine uses the Conv>width routines (section 5.8.4) to create ASCII files of the fitted parameters. These have extensions as follows: the widths are *.FWnm* where *n* is the number of peaks fitted and *m* the peak number, the peak amplitudes are *.AMnm* using the same nomenclature for *n* and *m* and where *m*=0 is the elastic peak, and the calculated Elastic Incoherent Structure Factors are *.EIn*

5.8.6 LPT Output

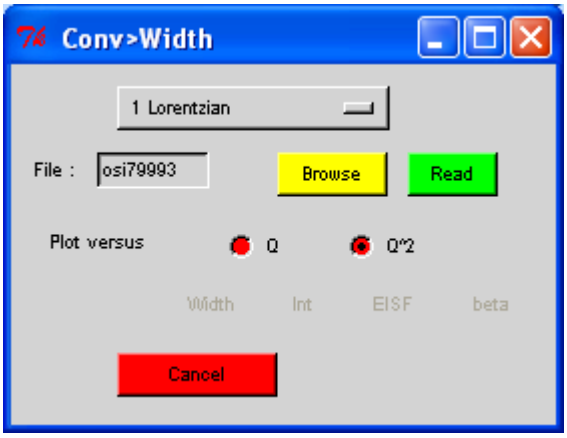
This routine reads *.Q2lpt* data (select 'Function') and opens 2 windows that give a summary of the fitted parameters. Use the sliders to choose the spectrum number and the number of peaks fitted. For each spectrum, the parameters, their errors and the Chi-squared value are given. It also reads *.QRLPT* (select 'Data') files for when using measured resolution data.



5.8.7 Conv>Width

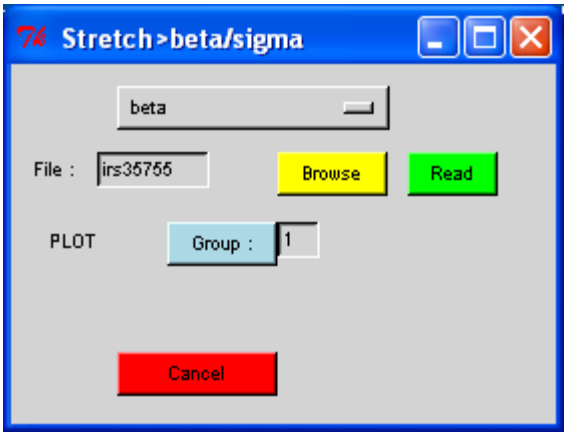
This routine converts fit parameters in the *.Q** files (depending on the model) to ASCII files. The widths and amplitudes (intensities) can then be plotted. Perform the following operations:

• Choose an option from drop-down menu: choice of 1, 2, or 3 Lorenztian peaks, water, or stretched exponential.
• Insert file name or 'Browse' and 'Read'
• Choose whether to plot Q or Q^2 In x-axis
• Plot 'Width', 'Intensity', 'EISF' or 'beta'



5.8.8 Stretched> beta/sigma

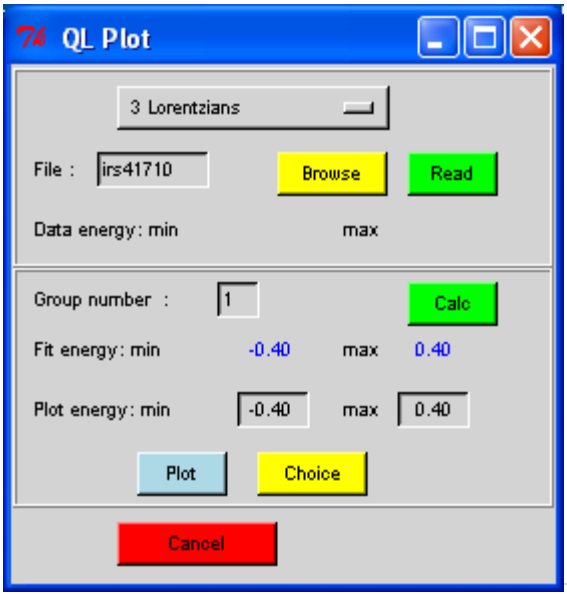
This routine converts fit parameters from the STR FUNCTION search (beta *.QSB* and sigma *.QSS*) to ASCII files. They can be plotted by first 'Reading' the data and then 'Plotting' the group.

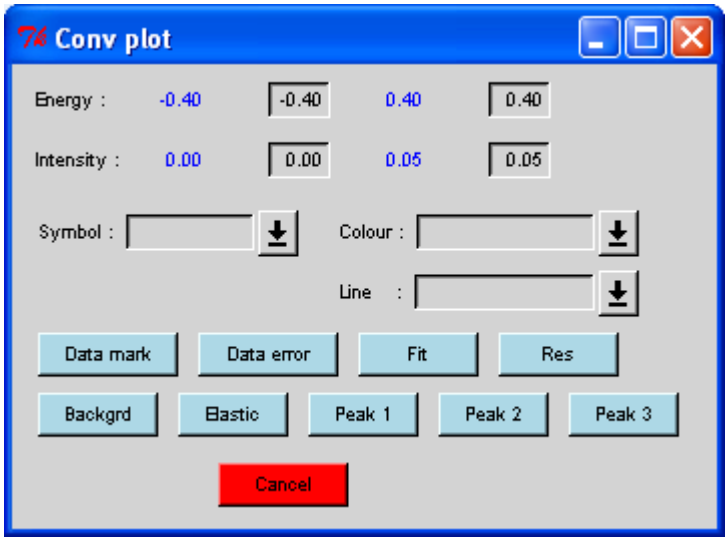


5.8.9 QL Plot

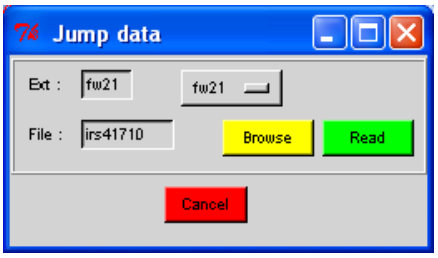
This routine plots the fits saved in *.QL** files. Perform the following operations:

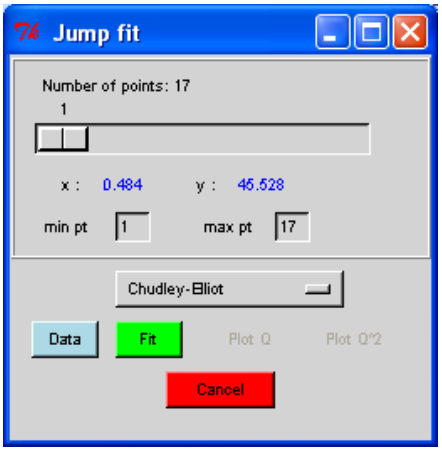
• Frame 1:
  - Choose the number of Lorentzians used in the fit from the drop-down menu
  - Insert run number or 'Browse' and 'Read'.
  - Energy range of data will be displayed
• Frame 2:
  - Choose group number to display and press 'Calc'.
  - Energy range used for fit will be displayed
  - Choose energy range for plot and 'Plot'. Data plus all fit curves will be plotted.
  - Press 'choice' to change axis ranges, colour and type of fit curves. A new window will appear.





5.8.10 Jump fit



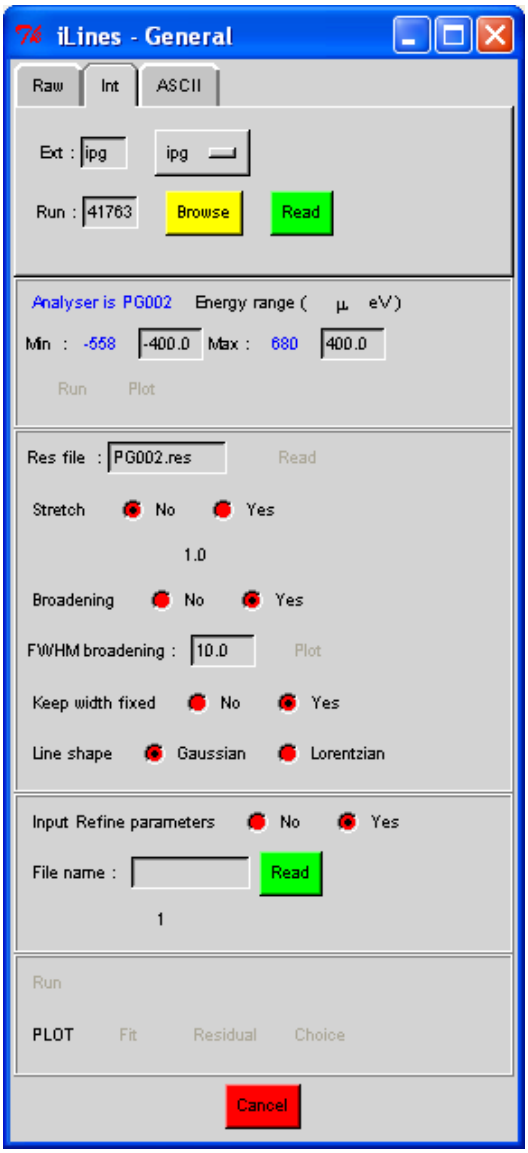


Two forms of jump motion can be fitted (section 3.7.2): the Chudley-Elliott model or the Singwi-Sjolander model. Perform the following operations:

- Choose an option from drop-down menu
- Insert file name or 'Browse' and 'Read'

A new window will open to choose the model:

- Use scroll bar to see x- and y-values of each point
- Choose fit range for groups (points)
- Choose a model from the drop-down menu
- Plot data with 'Data' and 'Fit'
- 'Plot' result as a function of Q or Q^2



5.8.11 iLines

This routine fits for *.RAW, .IPG* and *.ASCII* files where data contains inelastic peaks. There are 2 options 'General' for inelastic peaks not necessarily symmetrical, 'Symmetric' for similar peaks on each side of the elastic peak (eg. Tunnelling). Perform the following operations:

- Frame 1: Choose the input file from the tabs. In each case enter run number or 'Browse' and 'Read'
- Frame 2: shows the analyser selected in the MODES option and the input energy range. Choose the energy range for fitting, Run and Plot (if required).
- Frame 3: shows *.RES* file appropriate for selected analyser. 'Read' file.
  - 'Stretch' allows you to stretch the width of the resolution file. The default is 1.0. This will perform an operation that is similar that in QL when using the normalisation file created by RESNORM which finds the most appropriate stretch factor.
  - 'Broadening' of elastic peak/inelastic peaks. If 'Yes' then enter value of FWHM and 'Plot' (if required)
  - 'Keep width fixed': if 'Yes', choose 'Gaussian' or 'Lorentzian'
- Frame 4: input parameters for the refinement. If 'No' then specify number of inelastic peaks to fit. If 'Yes' enter ascii filename and 'Read'. The format of the ascii

file should be first line with background at lowest & highest energy; then 1 line for each peak with parameters peak centre position & height.
• Frame 5: ‘Run’ and ‘Plot’

In Symmetric: as above except in Frame 4 where you should specified number of pairs of peaks.

5.9 Display

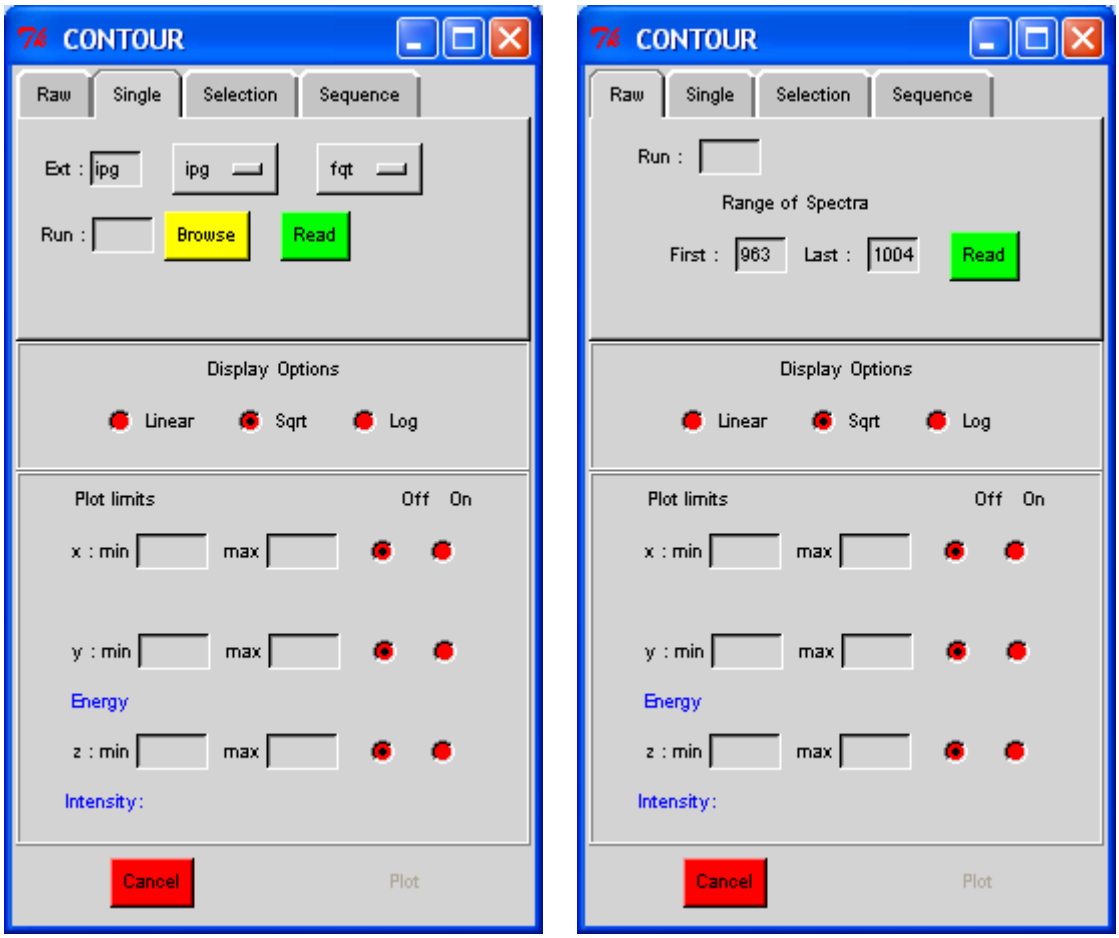
The commands above the separator line are OpenGenie commands and the following are MODES commands.

5.9.1 Contour

This routine provides a colour contour plot. Perform the following operations:
Frame 1: is a NoteBook with Tabs to give choice of input

- Raw: specified spectra from raw data file
  - Insert run number
  - Choose spectral range
  - ‘Read’ to read data
- Single: specified groups from a single intermediate file
  - Insert run number or Browse (extension is chosen using drop down menus)
  - ‘Read’ to read data
- Selection: specified single group from a selection of Intermediate files
  - Choose extension from drop down menu
  - Insert number of runs & a new window will appear
  - Input run numbers and a variable for each (e.g. temp)
  - Input a title for the variable & ‘Continue’
  - Insert Group number & ‘Read’ to read data
- Sequence: specified group from a selection of Intermediate files, in sequence
  - Choose extension from drop down menu
  - Insert number of runs and the number of the first run
  - Input group number and press calculate
  - ‘Read’ to read data

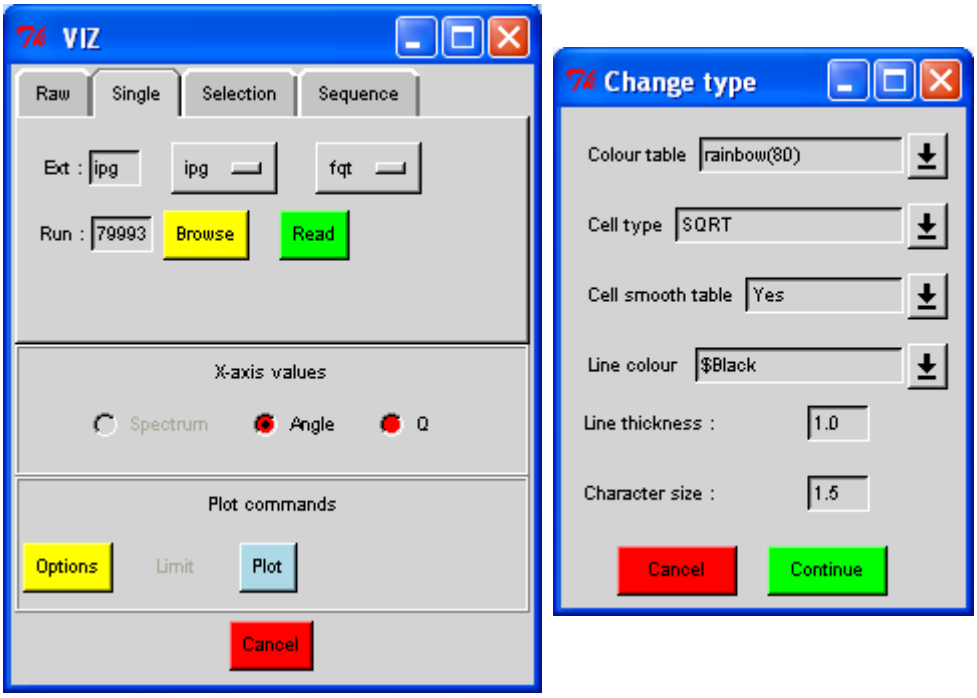
• Frame 2: select option for intensity scaling. The sequence from Linear to Log enhances the low count regions.
• Frame 3: choose limits & switch On/Off.
• ‘Plot’ to plot graph.



5.9.2 Viz

This routine provides a colour contour plot and then, by using the cursor, plots of cuts in the horizontal and vertical direction are produced. The cursor can be moved to a different point and new cuts plotted. Perform the following operations:

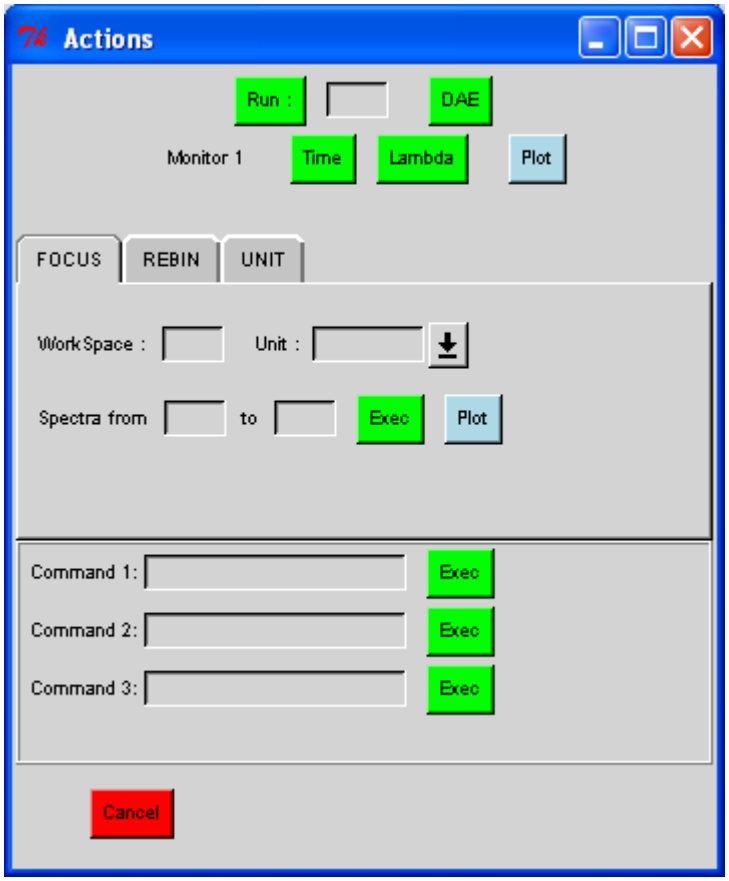
- Frame 1: is a NoteBook with Tabs to give choice of input (same as in CONTOUR, section 5.9.1)
- Frame 2: Select option for x-axis – 'spectrum number', 'angle' or 'Q value'.
- Frame 3: 'Plot' to plot graph.
  - Click on position shown by cursors in contour plot to display slices
  - Click middle mouse button (scroll wheel) to remove cursors before Cancel; other routines cannot be run until cursors have been cancelled.- 'Options' will open a new window and allow changes in colours, smoothing etc…

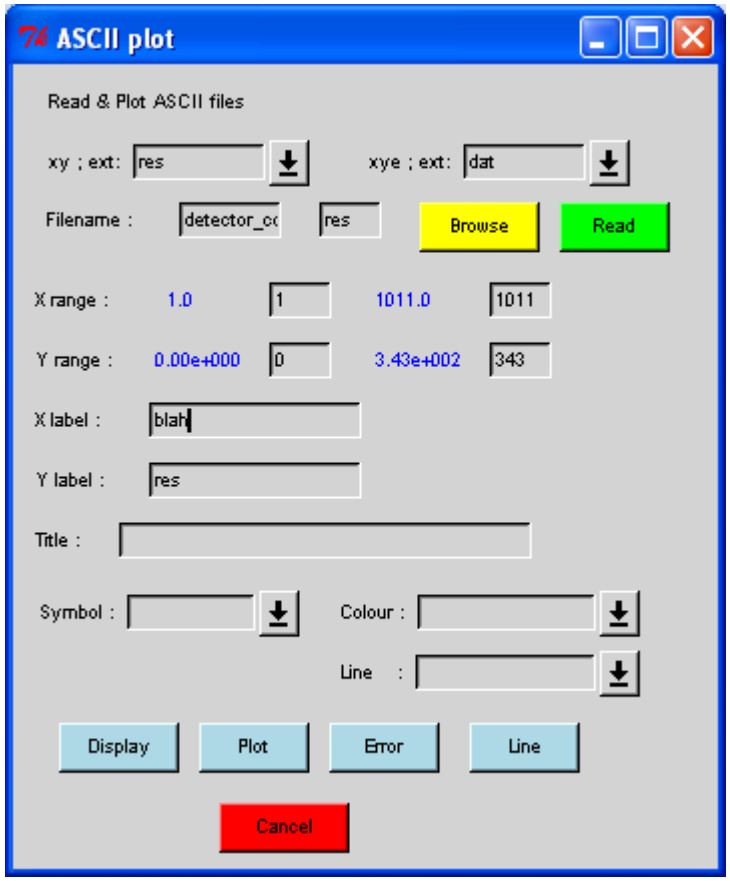


5.9.3 Actions…

This window provides a selection of commands for displaying data. It is of most use during an experiment to check on progress of a run. Perform the following operations:

- Frame 1: is for monitor 1 spectrum
  - Insert run number & click 'Run' for Raw data
  - Click on 'DAE' for current data in the DAE
  - To plot the spectrum in time-of-flight click on 'Time' & 'Plot'
  - To plot the spectrum in wavelength click on 'Lambda' & 'Plot'
- Frame 2: is a NoteBook with Tabs for workspace manipulation
  - Focus: sums the specified range of spectra
    - Insert name of workspace & choose unit from drop-down menu
    - Insert range of spectra & 'Exec' to run & 'Plot'
  - Rebin: rebins the specified workspace; the value shown is that previously defined
    - Insert name of workspace & choose unit from drop-down menu
    - Specify the range: 'From' is minimum, 'to' is maximum, 'by' is increment.
    - 'Truncate': increment is not required; the range becomes maximum to minimum.
    - 'Linear': the increment specified is the linear step.
    - 'Log': the increment specified is the logarithmic step
    - 'Plot' the result
- Frame 3: is for up to 3 OpenGenie commands. Type the command in the box & click on 'Exec' to run.





5.9.5 ASCII…

This window is for plotting data which are in ASCII files. It is of most use in plotting the results from QL FUNCTION and QL DATA fits. Perform the following operations:

• Choose the type of ASCII file (x,y) or (x,y,error) and the extension
• Insert the run number or 'Browse', then 'Read'
• Insert required X & Y range for plotting
• Insert required X & Y labels and main 'Title'
• Choose Symbol, Colour and Line type from drop-down menus (make sure you select each of them before the next step)
• 'Display' for first plot. Display always clears the screen for a new plot and the X- and Y-ranges will be fixed for overplotting.
• 'Error' to add error bars
• 'Line' to add a line
• In order to do multiple plots: change filename, 'Read', change Symbol and/or Colour and 'Plot' and 'Error' or 'Line' if required.
• After the 'Read' command the maximum & minimum values of x and y as calculated from the data are displayed in blue.

5.10 Select

5.10.1 Select limits

Allows you to set the limits on the x- and y-axes of the active plot.

5.10.2 Select picture

Allows you to re-plot any graph previously plotted within a session.

References

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Further reading

- Information on Open Genie can be found at http://www.opengenie.org/Main_Page
- IRIS User Guide can be found at http://www.isis.stfc.ac.uk/instruments/iris/documents/iris-user-guide-20014931.pdf
- OSIRIS User Guide can be found at http://www.isis.stfc.ac.uk/instruments/osiris/documents/osiris-user-guide6672.pdf
- Manual for IDA, the original data analysis program for IRIS data (M Telling and W S Howells, RAL Report RAL-TR2000-004 (2000))

Appendix A: Installation Instructions for MODES3

1. Installation/Startup on a PC

1.1. OpenGenie install from the ISIS website http://www.opengenie.org/Main_Page

1.2. Getting MODES files and quick installation

To install MODES on your computer you need to:

- Download the pre-zipped folder Modes3-Windows.zip from the ISIS anonymous ftp site *ftp.nd.rl.ac.uk/pub/ida* and place this file in your desired location on your computer, e.g., C:\
- Unzip Modes3-Windows.zip. On most PC's, this task can be achieved by right-clicking on Modes3-Windows.zip and selecting *WINZIP → Extract to here.* This operation should generate a Modes3 folder containing all requisite files and directories. We recommend placing the Modes3 folder at the top level of your drive (i.e., C:\Modes3).
- Proceed to section 1.4 of this Appendix.

1.3. Manual installation of PC folders/directories

If a pre-zipped version of MODES is not available, the following zip files are needed and can be copied by ftp from the ISIS anonymous ftp site *ftp.nd.rl.ac.uk/pub/ida/Modes3-Windows*:

modes_gcl.zip contains gcl code files
modes_lib.zip contains files for Library
modes_main contains main Modes files
modes_so contains compiled modules extension SO
modes_tables contains various settings files
modes_tcl contains tcl code files

Create the following tree structure on disk *C:*

```
Modes3 >    Lib
            Main > Gcl
                   Mod
                   Tcl
            Tables
```

Copy contents of Modes_gcl.zip to Main/Gcl
Modes_lib.zip to Lib
Modes_main to Main

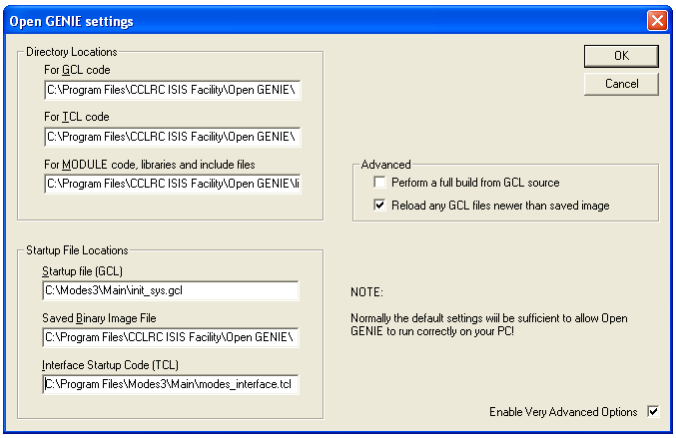
Modes_so to Main/Mod
Modes_tables to Tables
Modes_tcl to Main/Tcl

The folders can be anywhere as long as there is a tree-structure Modes3 etc
eg C:\Program files\Modes3 or G:\My Programs\Modes3
The Open Genie program files are in
C:\Program files\CCLRC ISIS Facility\Open Genie

1.4. Genie settings

Run the program Open Genie settings and set the following:

- The top box of settings - *Directory Locations* do not need changing
  Click on tick box next to *Enable Very Advanced Options* to allow changes to
- The bottom box of settings - *Startup File Locations*
  Set startup locations to point to your Modes3 folder eg.
  Startup file (GCL) C:\Modes3\Main\init_sys.gcl (for ISIS instruments)
  Or C:\Modes3\Main\init_sys_forte.gcl (for non-ISIS instruments)
- Saved Binary Image File keep as default
- Interface Startup Code (TCL) C:\Program Files\Modes3\Main\modes_interface.tcl
  The locations could also be C:\Modes3\ or G:\My Programs\Modes3
  Or \\olympic\babylon5\Public\IRIS_analysis\Modes3\etc
- The file init_sys.gcl in the folder Modes3\Main needs to be edited. In the section for WINNT, the variable System.root needs to be changed to point to the appropriate Modes3 folder. Note: in this file there is also a variable System.home which is the folder containing the file MODES_user.gcl. This allows the latter file to be in a different location to the program – necessary, for example, when the program is on the central disk.



1.5. Installing OpenGenie modules

Modules in MODES are Fortran routines which are called from the OpenGenie command language (GCL) and have to be compiled & linked by OpenGenie to create object files with extension SO. If your PC does not have a Fortran compiler then you will have to obtain the SO file from ISIS. These are already in the file modes_so.zip.

NB. If MODES does not run properly at the end of this installation, it might be due to incorrect compilation of the Fortran routines by Microsoft. If this is the case, download the modes_mod.zip file from our ftp site, which contains all Fortran modules and the filelink_all.gcl. This file can be used to compile the Fortran modules. To run, double-click on the file. A new window will appear running OpenGenie on 'command line' mode. There will be diagnostic information for each module and then to end the program and close the window type Exit<return>.

1.6. Startup

OpenGenie has its own menu in the main Programs menu. There are 3 programs:

- Open Genie settings: used to setup Modes (section 3 above)
- Open Genie (line mode)
- Open Genie (Tcl mode): the version for running Modes3

On installing OpenGenie a shortcut will be created called OpenGenie - this will start the program in the line mode option. To run Modes3, a new shortcut needs to be created for the Tcl version: - in the shortcut creator Browse to the OpenGenie program folder (eg C:\Program Files\CCLRC ISIS Facility\Open GENIE) and select the program tkgenie32.exe; then in the target input box add the options '-k –l' at the end (eg "C:\Program Files\CCLRC ISIS Facility\Open GENIE\tkgenie32.exe" -k –l) and optionally change the short cut name (in the General tab) to eg Modes3.

When starting MODES, there will be a question in the startup Genie window asking for the instrument and stating 1=IRIS, 2=OSIRIS. BUT if you start using the Start Program menu it will just prompt with 'Instrument?'

2. Installation/Startup on Linux/Mac

This is broadly similar to the PC setup. The Linux distributions are available in both 32bit and 64bit formats.

Install OpenGenie from its website (http://www.opengenie.org/Main_Page).

Download MODES3 from the directory Modes3-Linux (*ftp.nd.rl.ac.uk/pub/ida/Modes3-Linux*) and create files in the same tree format (see section 1.3). Use the appropriate SO files – 32 or 64.

Linux does not have a Geniesettings program so instead you should create a command script file to run. For example, to run the Tcl/Tk option for IRIS, create a file itkgen (say) with:

```
#!/bin/csh
setenv HOME_DIR <home path>
setenv MODES_ROOT <root path>
setenv GENIE_PROG "MODES"
setenv GENIE_USER_INSTR "IRIS"
setenv GENIE_GCL_INIT "${MODES_ROOT}/ Main/init_sys.gcl"
setenv GENIE_TCL_INIT "${MODES_ROOT}/ Main/modes_interface.tcl"
setenv GENIE_USER_MODES_DIR "${MODES_ROOT}/ Main/"
setenv GENIE_USER_LIBRARY_DIR "${MODES_ROOT}/ Main/Mod/"
setenv GENIE_USER_OGLIB_DIR "${MODES_ROOT}/ Lib/"
setenv GENIE_USER_TABLES_DIR "${MODES_ROOT}/ Tables/IRIS/"
setenv MODES_HELP "${MODES_ROOT}/ Lib"
setenv GENIE_BGD "white"
genie -k -l
```

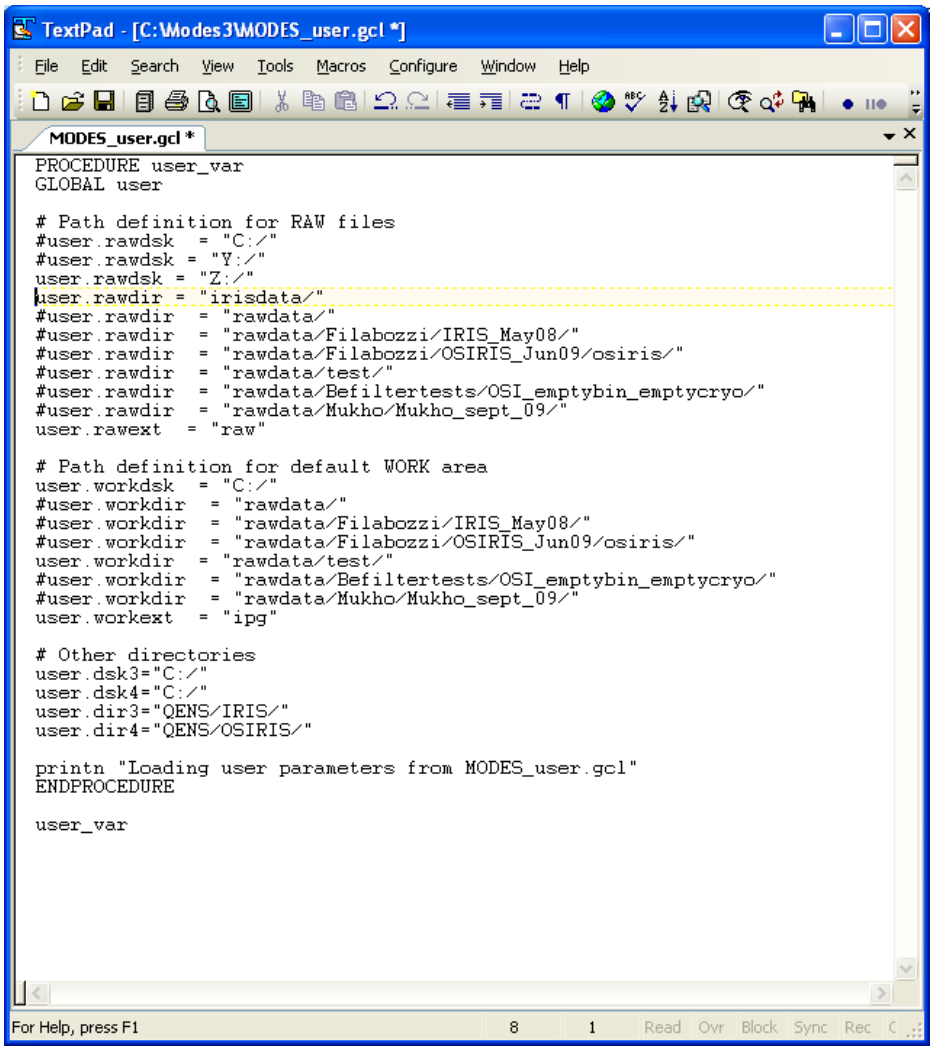
where <root path> is the directory for the program and <home path> the directory for MODES_user.gcl. The program is then started with the command "./itkgen".

Change the instrument with GENIE_USER_INSTR and for the command line version use genie –l.

5. Work area

This is the folder/directory where the created files are stored. It is usually on the C: disk, or if using XP/Vista it might have to be C:\Documents and Settings\<user>\My Documents. Many folders may be created. The folder Modes3 contains 2 files – MODES_user.gcl & FORTE_user.gcl to define these folders/directories. For MODES3 edit the file MODES_user.gcl so that user.rawdsk, user.rawdir define where the RAW files are and user.workdsk, user.workdir define where you create all the other files. 2 extra folders can be defined as user.dir3 & user.dir4

NB. The folder containing MODES_user.gcl must be the same as that defined in init_sys.gcl as System.home.

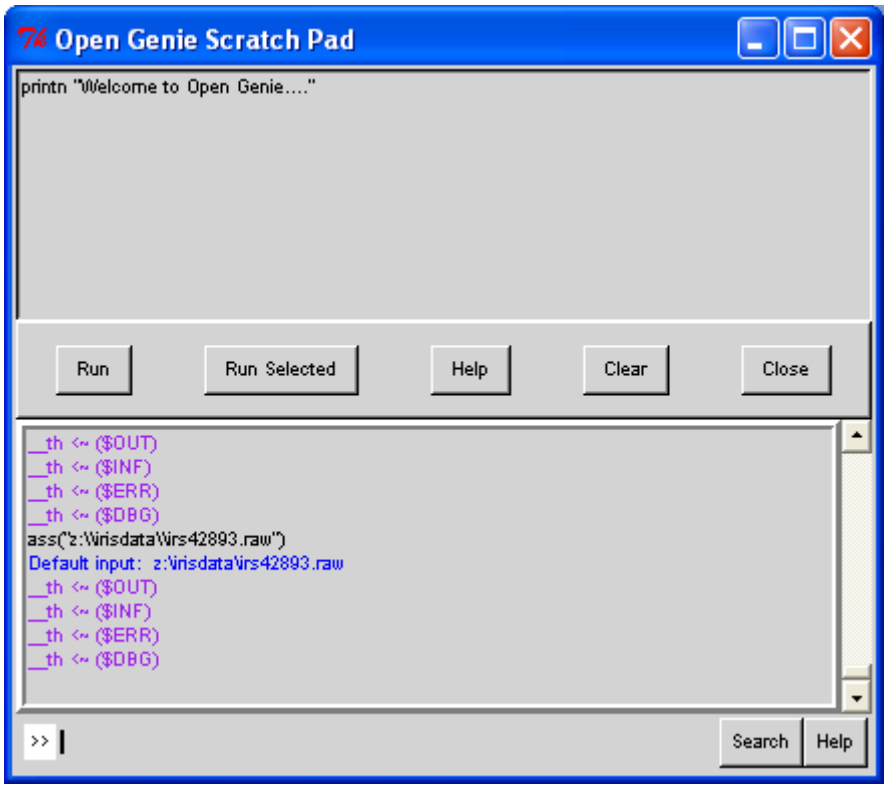


MODES_user.gcl can be opened using any text editor. In the example given above, the raw data (with extension .raw) is read from the "Z:\irisdata\" directory and the reduced files will be stored in the working directory "C:\rawdata\test\". The user may store a number of directories and edit the file by commenting out (adding a '#' at the beginning of the relevant line) the directories not being used.

NB. Note the use of "/" rather than "\" in the syntax of the file.

Appendix B: Frequently used GCL commands

It is useful in many occasions to use the command line to perform certain action in Open Genie such as displaying or over plotting a number of data sets. For this the Open Genie Scratch Pad can be used. This can be found in the 'File' menu, as 'Open Genie Console'.



Alternatively, the Actions GUI (5.9.3) may be used with the Genie commands inserted into the 'Command' box and Executed.

Here are some common examples of Open Genie commands:

COMMAND	DEFINITION
pwd	shows path to working directory
sh/def	shows path definitions
ass("c:\\irisdata\\irs42893.raw")	reads the raw data from the given path
d s(10)	displays spectrum '10'
w=s(1)	saves raw data in spectrum 1 into the workspace 'w'
d w	displays data in workspace 'w'
u/lam s(1)	changes the x-units of spectrum 1 to wavelength
u/t s(1)	changes the x-units of spectrum 1 to time

integrate(s(2))	integrates counts in spectrum 2
w_int=integrate(w[1],xmin,xmax)	integrates data in workspace ‘w[1]’ between xmin and xmax and saves in new workspace ‘w_int’
w_rebin=rebin:lin(w,0.0,0.01,1.0)	perform a linear rebinning of the x-axis of workspace ‘w’ between 0 and 1, with a bin size of 0.01, and save the rebinned data in a new workspace ‘w_rebin’
writexye s(100) “data.txt”	writes data in spectrum 100 into the ascii file ‘data.txt’ in 3-columns, x, y and error
writexye w “data.txt”	writes data in workspace ‘w’ into the ascii file ‘data.txt’ in 3-columns, x, y and error
d w10_T1	displays data in workspace ‘w10_T1’ (for example containing data for 10^{th} detector at 1^{st} measured Temp)
d w10_T1 -0.5 0.5 0 0.1	constrains the display of data in workspace ‘w10_T1’ to an range in x of -0.5 to 0.5, and in y of 0 to 0.1
a/pc $black; d w10_T1	displays data in workspace ‘w10_T1’ in black [a/pc = alter plot colour]
a/pc $green; p w10_T2	plots data in workspace ‘w10_T2’ in green over that already displayed with ‘d w10_T1’
t/logy	toggles to log-scale on y-axis
d/m w d/l w d/e w	displays data in workspace ‘w’ with markers displays data in workspace ‘w’ with lines displays data in workspace ‘w’ with errors
a/b 5	alters binning to every 5
c/h	shows cursor (press ‘ctrl+x’ to show x-value, or ‘ctrl+y’ to show y-value; press ‘e’ to exit)

Appendix C: Summary of input/output files for programs

PROGRAM	INPUT files	OUTPUT files
ACORN	.MUT, .IPG or .IMI	.ABS
ANA	.DIF or .DIN	
ANALYSE	.IPG or .IMI	.IBG or .IAG or .IBM or .IAM
CALIB	IRIS_detector.calib or OSIRIS_detector.calib	IRIS_detector.calib or OSIRIS_detector.calib, .DET
CONV>WIDTH	.Q*	.FW<n><m>, .AM<n><m>, .EI<m> or .WAT1, .WAT2 .WAT<n><m>, or .SE0, .SE1, .SE2, .SE3
DEMON DORIAN	.RAW or .SAV or .s<m>	.DIF
DMERGE	.DIF, diffr.par	.DIM
DNORM	.DVN	.DIN
DVAN	.RAW or .SAV or .s<m>	.DVN
ELWIN	.IPG or .IAG or .IBG or .IMI or .IAM or .IBM	.ELQ, .ELF, .MSD
EXPORT	.RAW or .IPG or .IAG or .IBG or .IMI or .IAM or .IBM	.SPE or .DASC
FQT FIT	.FQT	.FQT_F<n><m>
FURY	.RES, .IPG or .IAG or .IBG or .IMI or .IAM or .IBM	.FQT
ICON IONIAN	.RAW or .SAV or .s<m>	.IPG or .IMI, .GRP
ILINES	.RAW or .IPG or .IAG or .IBG or .IMI or .IAM or .IBM or .ASC, .RES	.ILLPT or .ISLPT
JUMP FIT	.FW<n><m>	.CEFIT, .CELPT or .SSFIT, .SSLPT
LPT OUTPUT	.Q*LPT	N/A
MINUS	.IPG or .IMI	.MSLPT, .MSC
MSD FIT	.MSD	.MST, .LINE_LOG
MUT	.IPG or .DIF	.MUT
POLY FIT	.FW<n><m>	.POLY_LOG
QL FUNCTION QL DATA	.RES, .IPG or .IAG or .IBG or .IMI or .IAM or .IBM	.Q2LPT, .QL1, .QL2, .QL3, .FW<n><m>, .AM<n><m>,

		.EI<m> or .QWLPT, .QLW, .WAT1, .WAT2, .WAT<n><m>,
QL PLOT	.QL*	N/A
RESMEM	.RAW or .SAV or .s<m>	.VAN, <analyser>.RES
RESNORM	<analyser>.RES, .IPG or .IAG or .IBG or .IMI or .IAM or .IBM	.RES
S(Q,w)	.RAW or .SAV or .s<m>	.SQE, .SPE
STR FUNCTION	.RES, .IPG or .IAG or .IBG or .IMI or .IAM or .IBM	.QSELPT, .QSE, .SE1, .SE2, .SE3, .QSB, .QSS, .EI<m>
STRETCHED>BETA/SIGMA	.QSB, .QSS	N/A
SWIFT	.RES, .IPG or .IAG or .IBG or .IMI or .IAM or .IBM	.Q<n>_<m> or E<n>_<m> or P<n>_<m> or S<n>_<m>
TRANS		.TRM

Appendix D: IDA Command Language (ICL) Glossary

1. ICON

1.1 aco – defines the analyser

aco *energy first-spectrum last-spectrum analyser-code*

where *energy* = analyser energy
first-spectrum = first spectrum to be grouped
last-spectrum = last spectrum to be grouped
analyser-code = code for reflection
analyser-code = 1 for PG002; =2 for PG004;
= 3 for MI002; =4 for MI004; =5 for MI006

(eg for PG002 the default values are 1.8450 3 53 1)

1.2 map – defines the grouping

map *group-option number-groups number-spectra*

where *group-option* = coding for type of grouping
number-groups = number of groups
number-spectra = number of spectra in group

1.3 grps_out – creates output file of grouping scheme (optional)

the filename format is "PG" or "MI", *analyser-code*, "OP" & *group-option* with extension ".grp"

1.4 grps_in – reads in the grouping scheme. Can be used instead of *map*.

grps_in *filename*

where *filename* is the name of the file & it assumes the extension is ".grp"

1.5 det-bal – sets of the detailed balance correction

det_bal *option temp*

where *option* = 0 for off, = 1 for on
temp = temperature in K (when on)

1.6 ic_first – runs icon for 1 run number (this can be repeated to create individual output files for each run number specified)

ic_first *runnumber*

where *runnumber* = run number

1.7 to add runs into one output file (the output file will have the run number of the first run)

ic_first *runnumber* – for first run
ic_loop *runnumber* - for each subsequent run to add
ic_ave *number-runs*

where *number-runs* = total number of runs

1.8 write_int - creates an output file (if required)

the extension will be ".ipg" or "imi" according to *analyser-code*

2. DEMON

2.1 dif – defines the spectral range

dif *first-spectrum last-spectrum*

where *energy* = analyser energy

first-spectrum = first spectrum to be grouped

last-spectrum = last spectrum to be grouped

(default for QENS mode on IRIS is 105 112)

2.2 demon_first – runs demon for 1 run number (this can be repeated to create individual output files for each run number specified)

dem_first *runnumber*

where *runnumber* = run number

2.3 to add runs into one output file (the output file will have the run number of the first run)

dem_first *runnumber* – for first run

dem_loop *runnumber* - for each subsequent run to add

dem_ave *number-runs*

where *number-runs* = total number of runs

2.4 demon_int int - creates an output file (if required)

the extension will be ".dif"

3. ANALYSE

3.1 sandc – reads data for sample & container

sandc *sample-run can-run*

where *sample-run* = runnumber for sample

can-run = runnumber for container

3.2 for subtraction with no corrections:

subtr *factor*

where *factor* is the scaling factor for the container, so that S=S-factor*C;

default = 1.0

3.3 for subtraction with corrections:

corr *can-option factor*

where *can-option* =1 for no can; =2 with can

factor is the scaling factor so that S =S-factor*correction*C;

default = 1.0

3.4 write_int - creates an output file (if required)

set/extension *outExt*

where *outExt* is the extension for the output file

the convention is :

for graphite with input ".ipg", output is ".ibg" for subtr or ".iag" for corr

for mica with input ".imi", output is ".ibm" for subtr or ".iam" for corr

4. dMerge

4.1 read_diffm – reads in input files

read_diffm *runnumber run-sequence number-runs*

where *runnumber* = runnumber

run-sequence = sequence number

number-runs = number of runs

this command is repeated *number-runs* times with *run-sequence* increasing from 1 to *number-runs*

4.2 dm_ran – defines the d-range to be used for each run

dm_ran *runnumber run-sequence d-min d-max*

where *runnumber* = runnumber

run-sequence = sequence number

d-min = minimum d for that run

d-max = maximum d for that run

runnumber & *run-sequence* are the same as those in 4.1

4.3 dm_start – defines the increment in d-spacing & starts the merging

dm_start *d-increment*

where *d-increment* = increment in d-spacing, same for all runs

4.4 dm_save int - creates an output file (if required)

extension is ".dim"

5. Fury

5.1 sw_read – reads the sample & resolution data

sw_read *sample-run res-runn*

where *sample-run* = sample runnumber

res-runn = resolution runnumber

5.2 fugue – starts the transforming

fugue *e-min e-inc e-max unit-option ms-option*

where *e-min* = minimum energy

e-inc = energy increment

e-max = maximum energy

unit-option =1 to normalise to unity, =0 not normalised

ms-option = 1 for MS corrections, =0 no corrections

5.3 fury_int - creates an output file (if required)

set/extension "fqt"

6. Export

6.1 read_int – reads data

read_int *runnumber*

where *runnumber* = runnumber

6.2 export-bin – defines energy range

export_bin *emin emax einc*

where *emin* = minimum energy

emax = maximum energy

einc = energy increment

6.3 for SPE format output

export_file 1 *runnumber*

where *runnumber* = runnumber

6.4 for DAVE format ouput

export_file 2 *runnumber floor*

where *runnumber* = runnumber

floor = minimum value for data (default 0.0)