GUIDE

IRIS DATA ANALYSIS

1st Edition

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January 2000

PREFACE

This report provides a single, comprehensive point of reference to the suite of software available for the analysis of neutron scattering data collected on the IRIS spectrometer at the ISIS facility, UK. It supersedes “IDA – Iris Data Analysis, W.S.Howells, 1996, RAL-TR-96-006” and incorporates “IGIS – A Graphical User Interface, W.S.Howells et al, 1997, RAL-TR-97-074”. Historically, many of the programs used for Iris Data Analysis (IDA) have existed for decades. In fact, many evolved from packages originally used at the Institut Laue Langevin (ILL), Grenoble, France, having been adapted, and improved, for use at ISIS. However, as new routines and ideas are developed, such as the technique of Bayesian analysis, so the IDA package, and therefore this manual, will be updated and modified.

ACKNOWLEGEMENTS

It is a pleasure to acknowledge all those who have contributed, in their various ways, to the production of the GUIDE package and this subsequent manual. In particular, Dr. Devinder Sivia for writing all the Bayesian analysis routines, Tony Csoka and past and present members of the Crystal Analyser Group at the ISIS facility, UK, for fruitful discussion and comment. Thanks is also expressed to the IRIS Users for, unknowingly at times, testing the programs and suggesting additions and changes that have helped maintain the User-friendliness of this suite of data analysis software.

CONTENTS

I. INTRODUCTION

IDA (IRIS Data Analysis) is a suite of programs for the analysis of data collected using the IRIS spectrometer at ISIS. This manual supersedes "IDA – Iris Data Analysis, W.S.Howells, 1996, RAL-TR-96-006" and incorporates "IGIS – A Graphical User Interface, W.S.Howells et al, 1997, RAL-TR-97-074" so that the User has a single, comprehensive point of reference to the suite of software available for analysis of IRIS data. It is assumed that the reader is familiar with the general IRIS instrument User guide – "The IRIS User-Guide – M.A.Adams – 1997- RAL-TR-97-052" - copies of which may be obtained from the Instrument Scientist. In addition, since the IDA suite makes extensive use of the data visualisation package Genie to view the results of data analysis, it is also assumed that the reader is familiar with the Genie package. For more information see 'Rutherford Appleton Report: RAL 86102 "Punch GENIE manual. Version 2.3. A language for spectrum manipulation and display", DAVID W.I.F', a copy of which should be available in the instrument cabin.

As the title suggests the IDA package was conceived for use alongside the IRIS spectrometer. However, with minor modifications, it may be adapted to analyse data collected on other ISIS instruments and even for instruments at other neutron facilities. Consequently, IDA may be considered a package for the analysis of quasi-elastic neutron scattering / inelastic scattering at small energy transfers. It is an integrated package in which the programs fit into a logical scheme and has been made as user-friendly as possible. The analysis of neutron scattering data can be divided into two sections:

i) *Data Treatment:*

Raw data is converted to a form independent of the instrument parameters and the neutron scattering process i.e. it is reduced to the scattering function $S(Q,\omega)$ dependant only on the dynamics of the sample measured. The data is corrected for absorption, container scattering etc. and normalised to an absolute scale of intensity.

ii) *Data Interpretation:*

For quasi-elastic scattering, data interpretation is dominated by the determination of peak heights and widths. The results may then be compared and contrasted to theoretical models describing the possible dynamics processes within a material.

Historically, many of the programs used for IDA have existed for decades. In fact, many evolved from packages originally used at the Institut Laue Langevin (ILL), Grenoble, France, having been adapted, and improved, for use at ISIS. However, as routines and ideas are developed , such as the technique of Bayesian analysis, so the IDA package, and hence this manual, will be updated. and modified.

II. COMPUTER OVERVIEW

The programs were developed on DEC computers and are run on workstations running the Alpha (AXP) operating system. To access all IRIS specific data analysis software, the User should modify his / her *login.com* file to include:

```
$ IRIS :== @IRIS$DISK:[IRSMGR.PROGS]USER_LOGIN.COM
$ IRIS
$ IF f$mode().nes."BATCH" then goto cont
$ EXIT
$ CONT
```

The login.com file should then be re-run by typing @login. In brief, the command file iris$disk:[irsmgr.progs]:user_login.com runs ida_log.com which in turn assigns logical names for all directories containing IRIS specific data analysis software – a full list of logical names along with their definition is given on the next page. The setup file also initialises Genie for use with both the IDA package and IRIS data. The User has only read and execute rights to all programs.

Logical Name:		*Location:*
IRIS_DATA	=	IRIS$DISK1:[IRSMGR.RESTORE] SCRATCH$DISK:[IRSMGR.DATA] SCRATCH$DISK:[IRSMGR.RESTORE] IRIS$DISK:[IRSMGR.DATA] IRIS$DISK0:[IRSMGR.DATA]
IDA_ALPHA	=	IRIS$DISK1:[IRSMGR.ALPHA]
IDA_GEN	=	IRIS$DISK:[IRSMGR.PROGS]
NORM_PAR / PAR_IRS	=	IRIS$DISK:[IRSMGR.TABLES]
I_D	=	IRIS$DISK0:[IRSMGR.DATA]
I_G	=	IRIS$DISK:[IRSMGR.GENIE]
I_P	=	IDA_GEN IDA_ALPHA
GENIEINIT	=	IDA_GEN:IRIS_INIT.COM
IRS	=	INST_ABRV_NAME

2.1. RESTORING ARCHIVED DATA SETS

The Raw data collected during an experiment on IRIS is stored in directory iris$disk0:[irsmgr.data] However, at regular intervals this data is deleted, after first being copied to the ISIS central data archive. Should a required data sets not be listed in iris$disk0:[irsmgr.data] it will need to be restored from the central data archive. To restore archived IRIS data type RESTIRIS, press <RTN>, and follow the prompts. All un-archived files are restored to scratch$disk:[irsmgr.data].

2.2. BATCH JOBS AND QUEUES

Data processing may be performed using any User specified computer, the computer used not necessarily being the one on which the User is working. The data is queued (in what is referred to as a Batch Queue) for processing where it remains until the processor is free to attend to it. Submitting data to a Batch Queue is known as submitting a Job. Suitable Batch Queues for IRIS data analysis are *iris$batch* and *alpha$batch*.

III. GUIDE – THE IDA GRAPHICAL USER INTERFACE

3.1. INTRODUCTION

GUIDE (**G**raphic **U**ser Interface for **I**RIS **D**ata **E**valuation) is a User friendly window driven means of launching the suite of IDA programs. The programs use the Tcl/Tk computer language with further extensions from Tix. For information on these languages the User should refer to the appropriate manuals [1]. Use of the window interface requires a fast computer and it is recommended that this package should only be run on an Alpha computer.

3.2. DISPLAY SETTINGS

To display Tcl/Tk graphics, and hence use GUIDE, the computer on which the User is working must be running an X-server. All computers at ISIS have either on board X-server capabilities (i.e. are UNIX or VMS Workstation) or run X-server emulators (programs such as eXcursion or eXceed). However, should you be logging into ISIS from remote using a PC that is not running emulation software then either a) install one of the above packages or b) log into ISIS from a UNIX or VMS Workstation (if available)

When logging into ISIS from remote, the ISIS computer must be told where to display subsequent graphics windows. Follow the following procedure:

i) Telnet to ISISA (isisa.nd.rl.ac.uk). Log in using your ISIS username and password.

ii) If logging into ISIS from a PC then start the PC X-server program.

iii) In the telnet window type:

SET DISPLAY/CREATE/NODE='my_ip_address'/TRANS=TCPIP

iv) If you wish to create a DEC terminal (DECterm) then type:

CREATE/TERM/DETACH

Should an error message appear to say that the 'display cannot open' then…

- *For VMS:*

In 'session manager', select 'Security...' under the 'Options' menu - this will open a dialog box with your current security settings. To allow access from any host via tcp/ip enter * in the Node and Username fields, and TCPIP in the Transport field. Click OK and then select "Save Session Manager" under the "Options" menu.

- *For UNIX*:

From a terminal on your local machine type: xhost +

- *eXcursion*

Open the control panel, click on the 'Access' tab and ensure that the 'Enable Access Control' in unchecked.

- *eXceed*

In the eXceed folder double-click on the Xconfig icon. Open the 'Security' option and select the "Disabled" radio button in the "Host Access Control List" box.

3.3. DATA INPUT

A typical GUIDE window, the Start-Up window (section 4.1), is shown below to illustrate the three methods of either entering data (run numbers etc) or selecting different options.

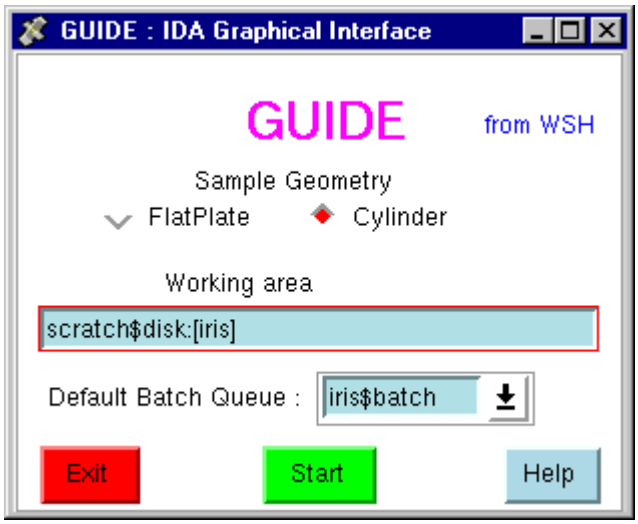

Figure 1: *A typical GUIDE data input window.*

Options and data are selected / entered using the mouse and keyboard respectively. For example, in the Start-Up window above, the User's Working Area (i.e. the area to which files created during the data analysis procedure are to be written) is entered manually via the keyboard in the Working Area input field. In contrast, the geometry of the sample can used during an experiment is specified by clicking on the 'diamond shaped' or 'radio' (see below) button associated with either Flat Plate or Cylinder. There are four types of button:

i) *Main Button* - Large with text label. Used to initiate one of three specific commands / operations:

- Help - Blue. A new window appears containing text describing the operations performed from the window containing the button.

- Run / Continue - Green. The first initiates the task described in the window while the second is usually used when the window is no longer needed. In both cases the window is closed.

- Stop / Cancel - Red. When used the operations defined in the window are not carried out and the window is closed.

ii) *Radio Button* - Refers to a series of white diamond shape buttons that turn red when active. Each button has an associated text label. To change an option, click on the new corresponding diamond.

iii) *Check Button* - This has a square shape and is a straight forward on / off button

iv) *Drop Down Menu* - These buttons are usually within the main part of the window and incorporate a drop-down menu. Clicking on the button brings up the menu and the option can then be chosen using the mouse.

3.4. INPUT FIELDS

Values (run numbers etc.) are typed into specific input fields, or boxes, that have a descriptive label. To activate a certain input field the mouse pointer must be positioned inside the box and clicked. The value may then be entered.

*An input value **MUST** be terminated either with the Return <RTN> or <Tab> key*

In most cases the input cursor then moves to the next appropriate input box or, if it is the last box in the window, carries out the command defined by the Run (green) button. A variable retains its value until changed. If it is used in several programs, then once defined will become the default for subsequent programs.

3.5. WINDOWS

These appear at various stages of operation and may be iconised if required. There are two main types…

i) *Program Menu windows* - specific to a program or option and only appear for that option and are closed when finished.

ii) *Message windows* - shows text messages. Window is closed when no longer required.

IV. GETTING STARTED

4.1. THE START-UP WINDOW

GUIDE is started by typing ‘Guide’ and pressing <RTN>. Before data analysis can commence certain fields must be defined, namely the sample geometry, the User’s working area and the Batch Queue to be used. Such information is entered in the GUIDE Start-Up window shown below.

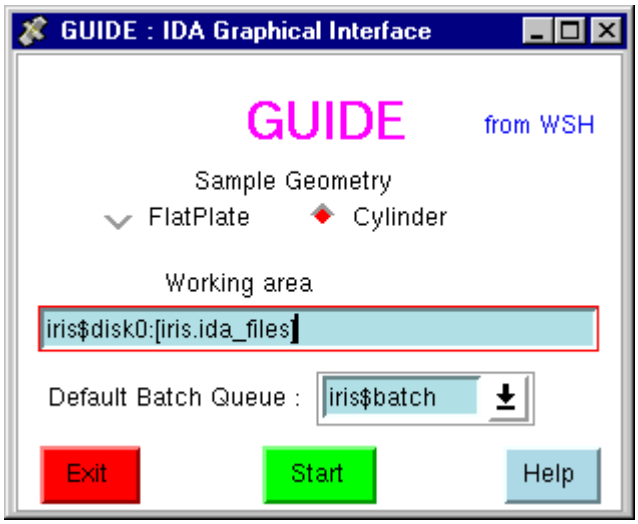

Figure 2: *The GUIDE Start-Up window*

Sample Geometry - Radio buttons are used to specify the geometry of the sample can used (Cylinder or Flat Plate). Once checked, the specified geometry will remain the default for all subsequent programs and until it is changed.

The Working Area **-** Defines the disk and directory in which the files to be used (other than Raw files) are stored and where the new files (except Log files) will be created. The default value is the directory from which GUIDE has been launched.

Default Batch Queue – The Batch Queue defined in the Start Up window will remain the default option for all subsequent data analysis programs.

- POINTS TO NOTE

i) The Working Area may be changed at any time during a GUIDE session.

ii) Log files are written to scratch areas. For example, if the working area is user$disk:[user] the log file will be written to scratch$disk:[user]. The log file should be the first point of reference should the User encounter problems with a particular IDA program – use the TYPE command to view the .LOG file.

- POSSIBLE ERROR MESSAGES

Possible Error Message	Probable Cause
Error: couldn't change working directory to "": invalid argument	Check spelling of directory assigned to Working Area. Check directory exists.

Upon pressing the Start button, two new windows appear…

4.2. THE FILE-LIST WINDOW

The File-List window, shown in Figure 3, consists of five panes listing GUIDE specific files found in the User's Working Area and scratch$disk directory. To update the lists click on the Rescan button. A file is selected by clicking on it – the name of the file appearing in the Selection box. A file can be sent to a printer by clicking on the Print button – the printer to be used can be entered manually, or selected by using the pull down menu in the Printer Queue field.

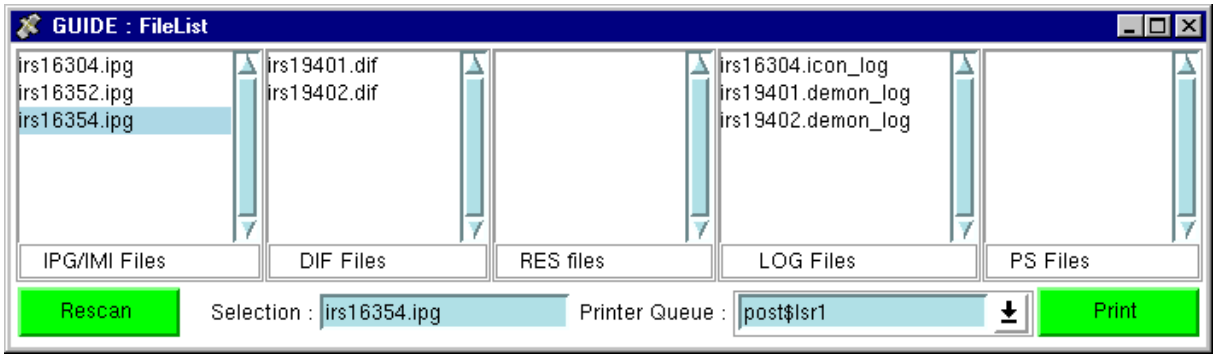

Figure 3: *The File-List window.*

- POINTS TO NOTE

i) Only log files (.LOG) and Postscript files (.PS) should be sent to a printer – all other types are BINARY files!

- POSSIBLE ERROR MESSAGES

Possible Error Messages	Probable Cause
Error: error running command: VMS error	Check filename entered in Selection field and check printer name entered in Printer Queue Field

4.3. THE GUIDE OPTIONS WINDOW

The main GUIDE Options window lists all available IRIS specific data analysis packages. Details about the various options are given below while the packages themselves are described in Section 5. However, it should be noted that the input required by some subsequent analysis programs is dependant upon the options selected in the GUIDE options window itself.

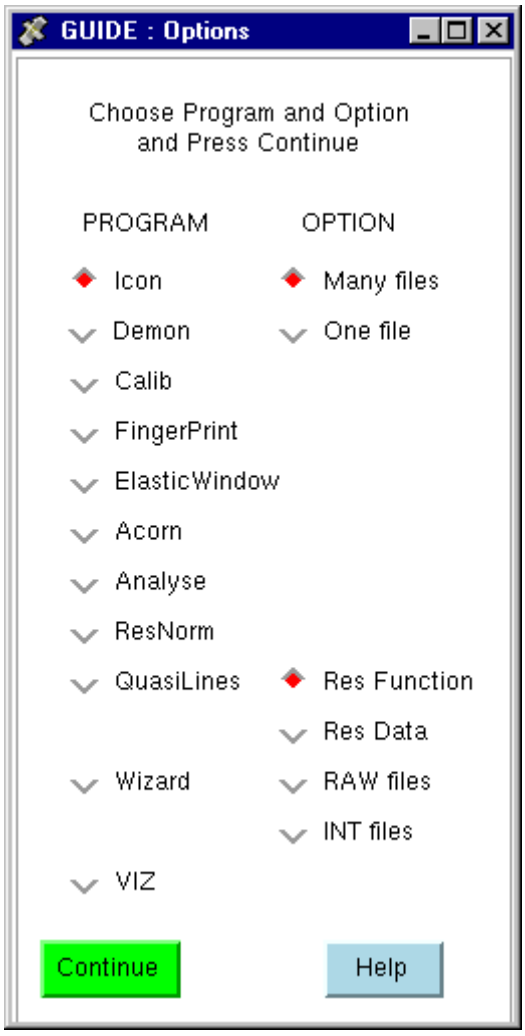

Figure 4: *The main GUIDE options window.*

Program – To launch a program click on the appropriate radio button and then Continue. The GUIDE window for the specified program will then appear. The suite of data analysis programs consists of:

1	CALIB	- calibrate detector efficiency (5.1)
2	ICON	- convert data into I(Q,ω) (5.2)
3	DEMON	- for diffraction data (5.5)
4	ACORN	- absorption & bckgnd correction (5.3.1)
5	ANALYSE	- absorption & bckgnd correction (5.3.2)
6	ELASTIC WINDOW	- Integration of elastic line (5.4)
7	WIZARD	- Creates .VIZ file for use in VIZ (5.7.1)
8	VIZ	- Plots Q vs E (or t.o.f) vs Intensity (5.7.2)

Many Files – The User will enter several run numbers and subsequent analysis programs will treat each one individually i.e. individual output files are written for each data set.

One File - For analysis where several runs require combining into a single file. This option is most apparent when an overnight run has been broken into discrete segments (time / μamps) to avoid 'spoiled' data due to sample environment failure.

Raw Files and *INT Files* - Sets the file type on which data analysis is to be performed. For raw data select RAW Files while for Genie Intermediate Files Format (.IPG and .IMI) files select INT Files. However, the data file type to be used is usually determined by the type of analysis being performed. For example, ICON will only use Raw data.

RES Function and *RES Data* - Determine whether the instrument resolution, to which experimental data will be compared, should itself be experimental i.e. data collected from a vanadium standard during the experiment.

5. DATA REDUCTION

As previously mentioned, the data analysis may be considered a two stage process i.e. data reduction and data interpretation. For the former, addressed in this section, the raw data (in counts per channel) is converted to the scattering law, $S(Q,\omega)$. The reduction procedure removes all instrument specific parameters and can also be used to apply corrections for neutron absorption and instrument background effects. In contrast, data interpretation seeks to understand the science by way of mathematical models, often determined by theory.

NOTE: *At present the GUIDE package is **NOT** suitable for **pre-1994** data. Should the User wish to analyse pre-1994 data then consult the Instrument scientist.*

Each of the data reduction packages listed in (4.3) will be detailed individually and in the order in which one would expect to perform a typical data reduction procedure.

So that the User may familiarise him / herself with the GUIDE package, and perform each step detailed in forthcoming sections, the data files used to illustrate the analysis packages have been copied to *iris$disk0:[iris.ida_files]*. In addition, and for the purpose of comparison, the output files generated by each analysis routine are also to be found in the said directory. The data itself – files IRS16304.RAW (vanadium resolution measurement), IRS16354.RAW (data from an empty sample can) and IRS16352.RAW (experimental data collected from Poly(propylene glycol) with a monomer unit of [OCH(CH3)CH2]) (PPG7) under 2kBar of pressure at 360K) – constitutes part of an on going and in-depth quasi-elastic neutron scattering study of

dynamics in PPG by Dr Dennis Engberg and Charbel Tengroth (Chalmers, Sweden), and their experimental team – the data having kindly been donated for inclusion in this manual by Dr. Engberg. For more information about the study of dynamics in polymer electrolytes the User should refer to [2] and references therein. For reference, the PPG sample (1mm thick) was mounted in a standard cylindrical IRIS aluminium sample holder. The vanadium measurement, collected for resolution and detector efficiency determination, was collected using a cylindrical vanadium standard. These geometries were therefore selected in the GUIDE Start up window.

The various steps required are as follows…

5.1. CALIB – DETECTOR CALIBRATION

To remove instrument specific parameters from a data set four basic variables should be known i) the primary neutron flight-path from moderator to sample detector, ii) the angle of a detector relative to the incident neutron beam iii) the neutron flight-path from sample to detector and iii) the detector efficiency. These values have been determined and are tabulated in norm_par:detector.dat. However, while flight paths and scattering angles rarely change, detector efficiencies may vary slightly from cycle to cycle.

Relative detector efficiencies may be determined using the incoherent scattering from a vanadium standard – this measurement being made either during the User's experiment or by the Instrument Scientists at the beginning of a cycle. Calibration manipulates the vanadium standard measurement to determine the relative efficiency of each detector. It then writes the results to a copy of detector.calib in the User's area for use with subsequent analysis programs. To launch Calib from the GUIDE options window click on the Calib radio-button. The following window will appear:

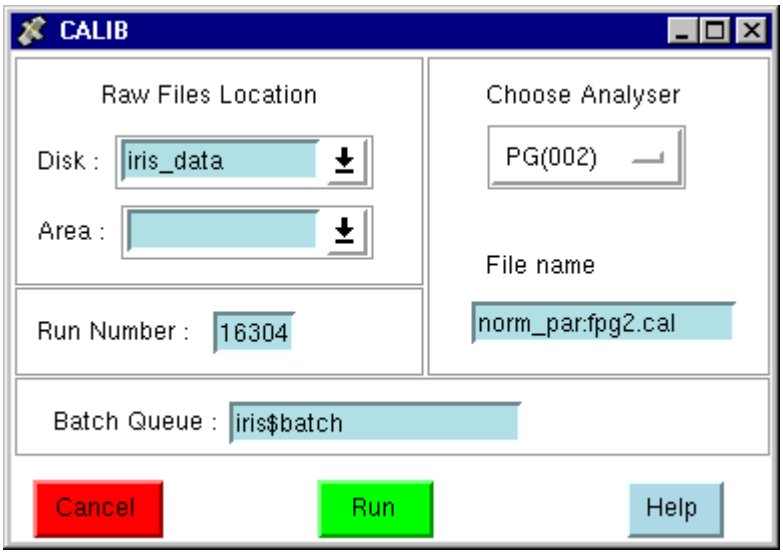

Figure 5: *The Calib data input window*

Raw Files Location - The location of RAW files defaults to iris_data. Should the requested run number not be found in iris_data then there will be an error message. The User should copy the files to scratch$disk:[irsmgr.data].

Choose Analyser - The analyser is chosen via a button with a drop-down menu and the entry in the File Name box defaults to that required for use with the chosen analyser and reflection. In brief, this file, fp**.cal (where ** represents either g2 or g4 for Graphite 002 or 004 or m4, m2 or m6 for Mica 002, 004 and 006) defines a region in time of flight over which integration of the raw resolution data will occur.

Run Number - Enter the run number of the file containing the resolution data and terminate the entry using the <TAB> or <RTN> key.

Batch Queue - If the batch queue is changed, terminating that entry initiates the batch job as if the Run button had been pressed.

When the job as been submitted a message window appears giving the filename, and location, of the command file being run and the LOG file being written. Click Continue to close the window.

Figure 6: *A typical job submission message window*

- OUTPUT FILES

Once the job has finished the User should find that a copy of Detector.Calib, containing updated detector efficiency values, has been copied to his/her working area. The column of interest is 'ut2' since this assigns an efficiency value to each detector. The Detector.Calib file generated using resolution measurement IRS16304.RAW can be viewed in *iris$disk0:[iris.ida_files]* the first few lines of which are printed below.

NOTE: It is worth typing this file to check the contents of column ut2. Should column ut2 consist of nothing but zeros then re-run Calib

Number of detectors, Number of user table parameters/detector

115 4

Det no.	Delta	Len2	Code	2theta	ut1	ut2	ut3	ut4
1	0.0	-0.37	1	180.0	2.0	0.2075	784	4.0
2	0.0	2.12	1	0.001	2.0	0.2075	784	4.0
3	0.0	1.4700	1	25.75	3.0	0.338	0.0	4.0
4	0.0	1.4700	1	28.50	3.0	0.675	0.0	4.0
5	0.0	1.4700	1	31.25	3.0	0.706	0.0	4.0
↓	↓	↓	↓	↓		↓	↓	↓
114	0.0	0.8510	1	172.41	1.0	0.5	10.0	4.0

File 'Detector.Calib' created by Calib using the vanadium resolution measurement IRS16304.RAW

- POINTS TO NOTE

i) Should a Job be terminated with an error status then check the .LOG files for clues as to the most probable cause.

- POSSIBLE ERROR MESSAGES

Possible Error Messages	Probable Cause
IDA could not find your RAW file in any of the default disk areas	Check the requested files are located in either iris$disk0:[irsmgr.data] or scratch$disk:[irsmgr.data]
Error: error running command: VMS	Check name in Batch Queue field.

- THE OUTPUT FROM CALIB CAN BE USED IN…

i) ICON – to convert the RAW data into I(Q,ω) (5.2)

ii) Wizard – to create a .VIZ file for use in program VIZ (5.7.1)

5. 2. ICON – CONVERSION TO I(Q,ω)

To launch ICON click on the corresponding radio button in the GUIDE Options window.

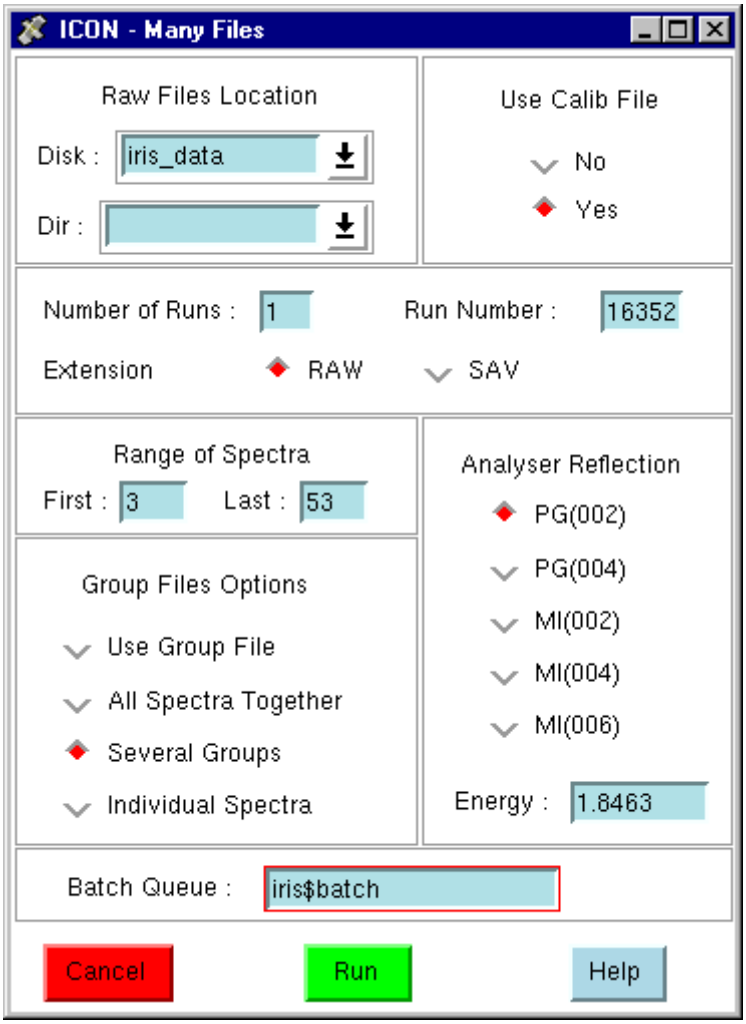

Figure 7: *The ICON data input window*

The ICON procedure converts RAW data into I(Q,ω), or strictly speaking I(2θ,ω). The program reads the monitor spectrum, corrects for detector efficiency and converts 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). Note: The banner at the top of the main ICON window highlights whether the file option 'Many Files' or 'One File' was selected in the Main GUIDE Options window.

Raw Files Location - The location of the RAW data files defaults to iris_data. However, this location may be changed manually if necessary.

Use Calib File - Select the YES radio button to apply the calibration file generated using the program Calibration (section 5.1.1) to the data.

Number of Runs – Should the number of runs be set to 1 the input caret moves to the Run Number input box. However, if the number of runs is greater than 1 a new window appears with an entry box for each run and the caret moves to the next box upon terminating the entry to a box. When a run number is input, the appropriate range of spectra appears in Range of Spectra boxes. In addition, radio buttons are provided to specify the extension of the data file(s) to be used (i.e. .RAW or .SAV).

Analyser Reflections - Radio buttons specify the analyser type / reflection used and energy. The analysing energy may be altered if required.

Group File Options – Details how the 51-graphite / mica spectra are to be grouped together. Four options are presented:

i) *Use Group File* - A new window appears to allow the User to input a .GRP grouping filename. See *Several Groups*

ii) *All Spectra Together* - No further action. The number of spectra to be grouped together is limited by the values entered into the Range of Spectra input boxes.

iii) *Several Groups* -A new window appears with radio buttons to choose either Constant or Variable grouping. When one is clicked the text for the other turns grey. The active entry box requires input. On pressing Continue, a grouping (.GRP) file is written to the User's working area containing details of the grouping options entered in the Several Groups window. Should subsequent data sets require similar grouping then the corresponding .GRP file may be selected in "Use Group File". The selected grouping remains default until changed.

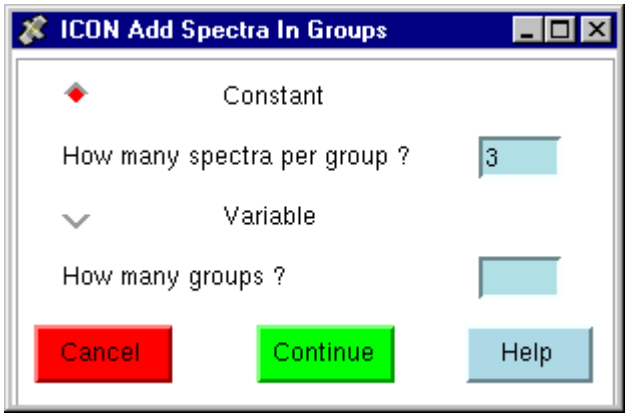

Figure 8: *The 'Several Groups' option window*

iv) *Individual Spectra* - No further action required. The number of individual spectra is limited by the values entered in to the Range of Spectra input boxes.

v) *Batch Queue* - If the batch queue is changed, terminating that entry initiates the batch job as if the RUN button had been pressed.

When the job as been submitted a message window (Figure 6) appears giving the filename, and location, of the command file being run and the LOG file being written. Click Continue to close the window. Once defined the values entered for 'number of runs' and 'run number', together with all the other options selected, become the default settings for the next time ICON is run.

- OUTPUT FILES

The User should find either an IPG or IMI file has been written to his/her working directory – the extension used depending upon the analyser used to collect the data. To view the contents of an IPG or IMI file see Section 6.1.

- POSSIBLE ERROR MESSAGES

Possible Error Messages	Probable Cause
IDA could not find your RAW file in any of the default disk areas	Check files are in iris$disk0:[irsmgr.data] or scratch$disk:[irsmgr.data]
Error: error running command: VMS error	Check name entered in Batch Queue field.
File PG1.GRP does not exist	Check the .GRP file to be used exists
Error: Bad Window Path Name	Entry terminated with <TAB>. Use <RTN> key or green Continue button
Job ICON_17888 (queue IRIS$BATCH, entry 375) terminated with error status	Check Detector.Calib file exists and is located in User's working directory
Group options not defined	Click on a radio button under Group File Options

- POINT TO NOTE

i) It is possible to collect data using both the Graphite 002 and Mica 006 reflections simultaneously when IRIS is operating in PG002, 50Hz mode. Should both data sets require analysis, however, ICON will need to be run twice - use the same run number but change Analysing Reflection. The extension of the ICON output file, IPG or IMI, differentiates between data collected using the Graphite and Mica analyser respectively.

- THE OUTPUT FROM ICON CAN BE USED IN…

- ResNorm – Resolution normalisation (5.6)
- Acorn - absorption corrections are applied to data (5.3.1)
- Elastic Window – Fixed limit integration of elastic line (5.4)
- Genie - view IPG / IMI file (I(Q,ω) vs). Black and white plots (6.1)
- PG Plotting Routines - view IPG/IMI (Q vs ΔE). Output data. Colour plots (6.2)

5.3. ACORN AND ANALYSE – ABSORPTION CORRECTIONS

A complete set of data will normally contain, in addition to the sample and vanadium resolution measurements, some estimate of the instrument 'background', be it from an empty instrument, empty sample environment equipment (e.g. cryostat, furnace) or an empty sample container. However, the first, and most important, set of corrections are those for absorption (self-scattering and neutron absorption). For flat plate geometry the corrections are analytical and have been discussed, for example, by Carlile [3]. The situation for cylindrical geometry is more complex and requires numerical integration. However, these techniques are well

known, used in liquid and amorphous diffraction and take into account the wavelength variation of both the absorption and the scattering cross-sections.

Absorption correction using the IDA package is a two-stage process requiring GUIDE programs Acorn and Analyse with Acorn being run first. These programs having been developed from the corrections programs in the ATLAS [4] suite. In brief:

- *Acorn* - launches a GUIDE window to allow data necessary for the absorption correction calculations to be input. The package generates files, with the extension .MUT and .ABS, containing wavelength dependent cross-sections for the sample (and container)

- *Analyse* - reads the correction files and applies them to the Intermediate File format (IPG / IMI) type sample data files created using ICON.

5.3.1. ACORN

To launch Acorn click on the corresponding radio button in the GUIDE Options window. Acorn starts off with a Prelude window:

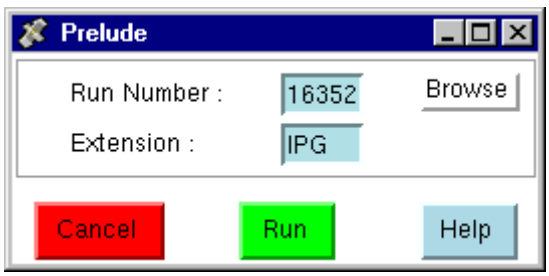

Figure 9: *The Acorn 'Prelude' window*

Run Number - The run number - which can be input either by typing in the entry box or found using the Browse button

Extension - The file extension defaults to IPG but can be changed for IMI files.

Clicking the Run button launches that main Acorn window (Figure 10).

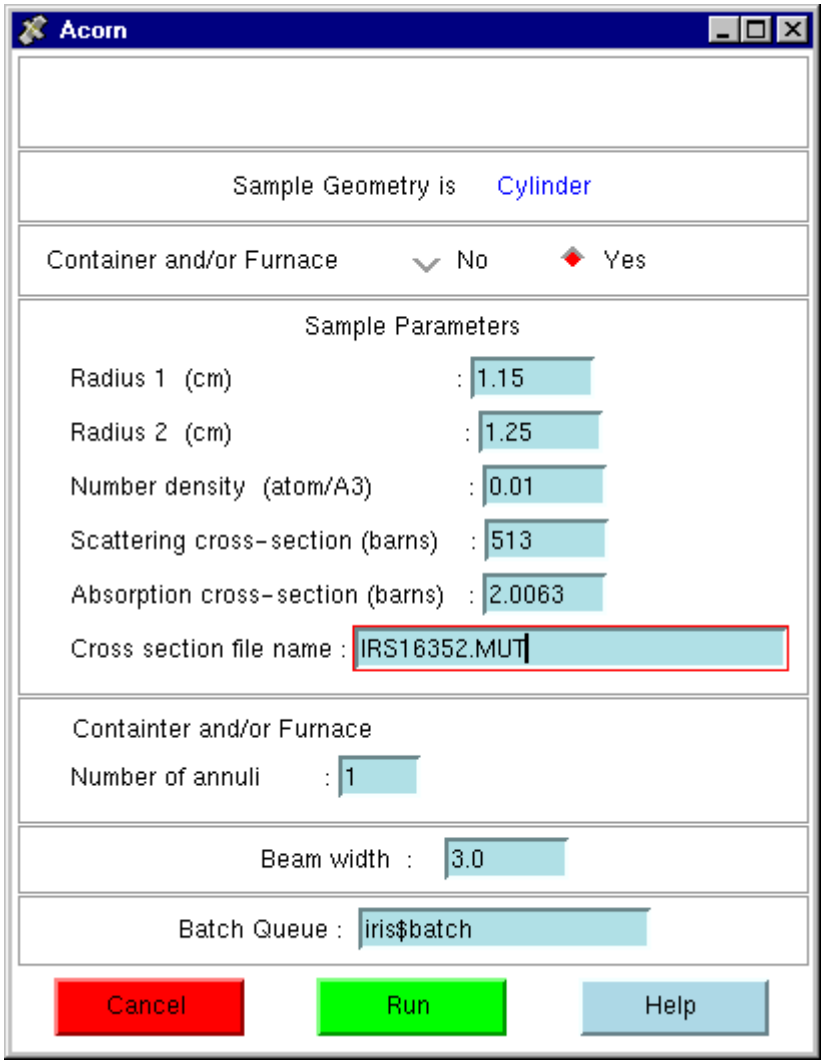

Figure 10: *The Acorn data input window*

The parameters required depend upon whether the Flat Plate or Cylinder sample can geometry radio button was selected in the GUIDE Start UP window. The window for a cylindrical sample can is shown below. However, should Flat Plate have been selected then i) Radius will be replaced by sample Thickness (cm) and ii) Beam Width will be replaced by Angle of Sample to Incident Beam.

If Acorn is being run for the first time then the top frame (above Sample Geometry) will be blank. If not, then the message 'Data From File' will appear in blue. In this case, the values asked for are read in from an .AIN, this file being created after Acorn has been run for the first time.

Sample – Highlights the sample geometry selected in the Options window.

Container and/or Furnace – Select whether beam attenuation / absorption effects due to sample environment equipment should be corrected for. If NO then the input field below Cross Section Filename remains blank. However, if such corrections are required this field asks for either the number of layers that make up a Flat Plate Can or the number of annuli of a cylindrical canister.

Radius 1 / Radius 2 - For solid cylindrical samples the default value is 0. However, should the sample be annular then the values required are the inner and outer radii of the sample respectively. For example, the PPG sample was mounted by spreading a thin layer (0.5 mm thick to avoid potentially problematic multiple scattering effects) between two sheets of thin Al foil. The resulting polymer 'sandwich' was then moulded into a hollow cylinder and slid inside a standard IRIS aluminium cylindrical sample can. Should the sample have been mounted in a Flat Plate can the thickness of the sample will be required.

Number Density – Enter the Number Density, or scattering unit per angstrom cubed (atom / A^3). For example, considering PPG, the basic repeat unit, or monomer consists of 1 oxygen, 6 hydrogen and 3 carbon atoms. The Number density is simply the Bulk Polymer Density multiplied by Avagadro's Number ($Na=6*10^{23}$) and divided by the Molar mass of monomer i.e.

Density of PPG is approximately $1000kg / m^3$

Formula for PPG monomer is [OCH(CH3)CH2] giving a molar mass of…

$6*1 + 3*12 + 1*16 = 58$

Therefore the Number Density (PPG) ~ 1e-2 atoms / $angstrom^3$.

If the above parameters are not readily to hand, the User can determine the Number Density by noting the mass of the sample can before and after loading a sample, along with the cell dimensions. Consider a sample of Al_2O_3 with:

Mass of can + sample: 31.63 g

Mass of empty can: 19.98 g

Mass of sample: 11.65 g

Diameter of sample can: 0.952 cm

Height of sample (h): 5.5 cm

Element	*Atomic Weight*	*XS (Barns)*	*XA (Barns)*
Al	27	1.503	0.2310
O	16	4.232	0.0002

where XS is the total (i.e. incoherent and coherent) scattering cross section per atom and XA is the absorption cross section per atom in barns. Both values are for neutrons of velocity of $2200ms^{-1}$ (1.8 Angstrom). XS and XA for most elements and isotopes can be found in the article '*V.F.Sears "Neutron Scattering Lengths" Neutron News 1992* ***3*** *26*' or at *http://www.isis.rl.ac.uk/ISISPublic/ISISlibrary.htm*

i) First calculate the mass of one Al_2O_3 scattering unit in kilograms:

$$M = (26.982 \times 2 + 15.999 \times 3) / (6.022 \times 10^{23}) = 1.694 \times 10^{-25} \text{ Kg}$$

ii) Next calculate the sample volume:

$$V = \pi r2h = 3.141 \times 0.4762 \times 5.5 = 3.914 * 10^{-6} \text{ m}^3$$

iii) Finally calculate the number of scattering units / m^3:

N / V = (weight of sample) / (mass of scattering unit x volume)

= 11.65 / (1.694x10-22 x 3.914) = 1.757×10^{28} m^{-3}

= 0.0176 scattering units / $Å^3$

Number of Annuli - If the option to correct for absorption effects due to the sample can (see Container and / or Furnace) has not been chosen the text in this box will be left blank. Otherwise the number of layers of the flat plate sample can, or annuli of the cylindrical sample cell, must be entered. Terminating the entry launches the Container window below

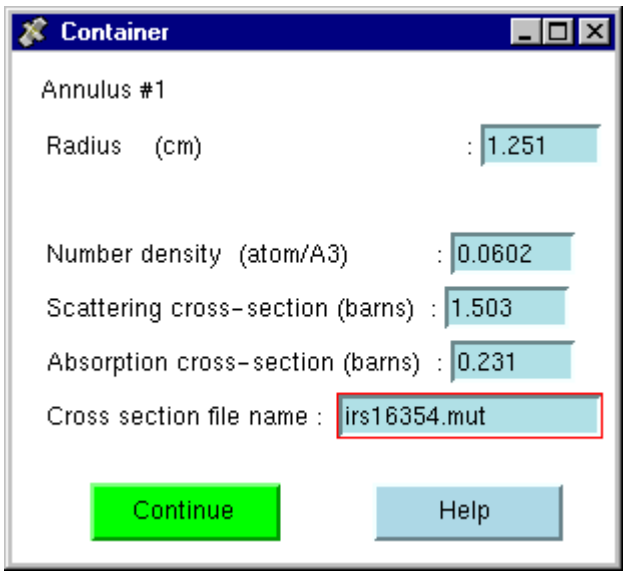

Figure 11: *The Acorn 'Sample Container' data input window*

The majority of sample cans on IRIS are made of aluminium – if you are unsure ask the Instrument Scientist. For reference, aluminium has a Face Center Cubic crystal structure with a lattice constant of 4.0495 Å and a density of 2700Kgm^{-3}. The total scattering and absorption cross sections for aluminium are given above.

Beam Width (cm) – Information requested here will depend on the sample geometry. For Flat Plate, enter the angle of the sample can to the beam as detailed in Figure 12 below. For a Cylinder enter the beam width (For IRIS the beam is 3cm high by 2 cm wide).

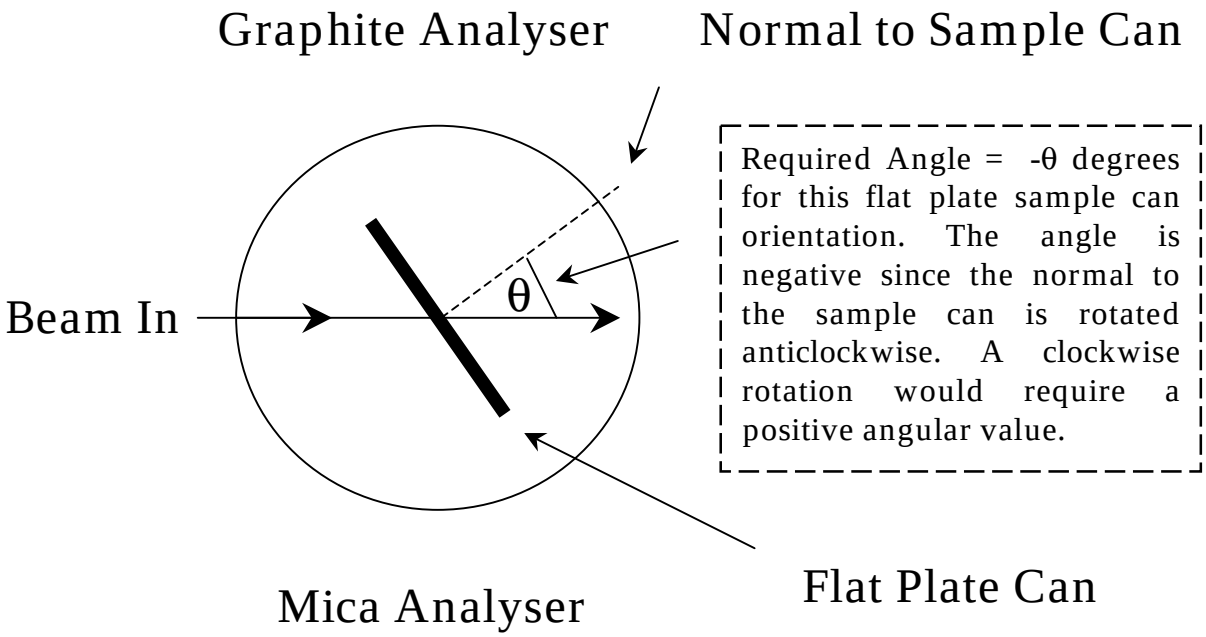

Figure 12: *Nomenclature for the angle of a Flat Plate sample can relative to the incident beam as requested by Acorn*

Batch Queue - If the batch queue is changed, terminating that entry initiates the batch job as if the RUN button had been pressed.

- OUTPUT FILES

Once the job has finished the User should find a MUT, an ABS and an AIN file has been written to his/her working directory.

- POSSIBLE ERROR MESSAGES

Possible Error Messages	Probable Cause
File: IRS*****.IPG/IMI does not exist	Check requested files are in User's working directory. Check spelling
Error: error running command: VMS	Check name in Batch Queue field.
Error: Can't Read "Get Files": No such variable	Re-enter filename manually and terminate entry with <RTN> key.
Error: Bad Window Path Name	Entry terminated with <TAB>. Use <RTN> key or green Continue button

- THE OUTPUT FROM ACORN CAN BE USED IN…

i) Analyse – Application of absorption corrections to data (section 5.3.2)

5.3.2. ANALYSE

Analyse must be run after Acorn and begins with the following introductory 'Introit' window.

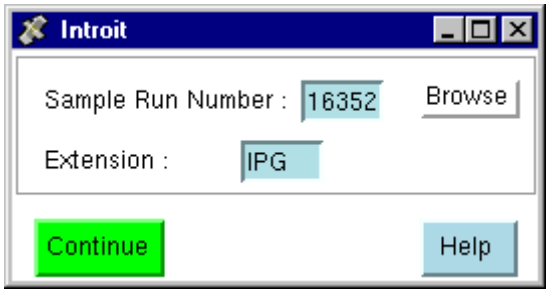

Figure 13: *The Analyse 'Introit' window*

Sample Run Number – Run number to which corrections are to be applied.

Extension - Defaults to IPG but can be changed for IMI files

The routine then checks for an ANAB_DAT file (create after Analyse has been run for the first time) before closing and opening the main Analyse window. Should no ANAB_DAT file exists the top frame will be blank. Alternatively, the message 'Data from File' is displayed in blue. In the latter case the values in the subsequent frames will be those read in from the said file.

Corrections – Determines whether sample dependent absorption corrections are to be applied to the measured sample data set.

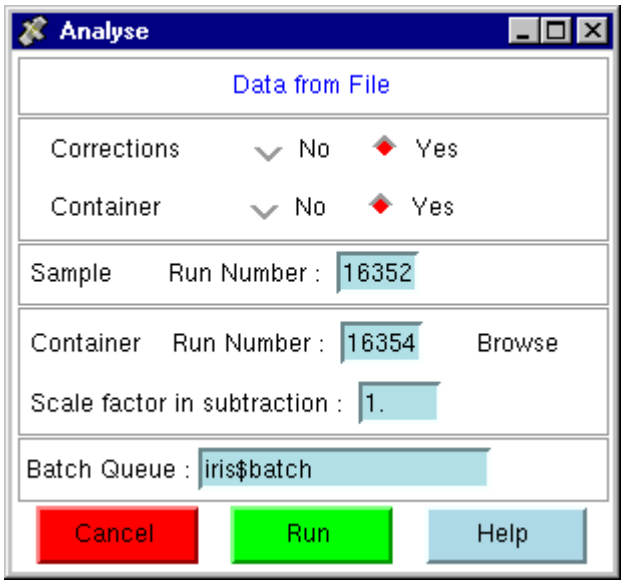

Figure 14: *The Analyse data input window*

Container – Determines whether absorption corrections due to sample can are to be applied in addition to subtraction of the empty cell measurement from the sample data set. If NO container corrections are to be applied then the field below SAMPLE will be blank. However, should YES be selected then the sample container run number can be input (either by typing in the entry box or found using the Browse button) together with a subtraction Scale factor (default = 1).

Sample – Enter the required Run number if input field is blank. In practice choosing the correct run number in the Analyse Introit window should ensure that this input field is filled.

Batch Queue – If the batch queue is changed, terminating that entry initiates the batch job as if the Run button had been pressed.

Container Run No – see Container above.

Scale Factor - The 'scale factor' should be set to 1. However, should the absorption corrections not be entirely correct (i.e. the density / volume / cross-sections / sizes are not accurately known) then this factor can be use to scale the subtraction of the background measurement to maintain a meaningful .IAG file data set.

The Analyse routine then loops through each group of spectra in the input data file correcting the data as instructed

- ## OUTPUT FILES

Once the job has finished the User should find an .IAG (for PG analyser data / IPG file) or an .IAM (if the MICA analyser were used) has been written to his / her working directory. In addition, the file .ANAB_DAT, containing information (sample / container runs etc) about the correction procedure will have been written.

- ## POINTS TO NOTE

i) Using the BROWSE option to select the run number in the Introit window can be temperamental. Should this not work then simply enter the desired run number manually and click on Continue.

- POSSIBLE ERROR MESSAGES

Possible Error Messages	Probable Cause
File: IRS*****.IPG / IMI does not exist	Check requested files are in Users working directory. Check spelling of extension
Error: error running command: VMS error	Check name entered in Batch Queue field.
Error: Can't Read "Get Files": No such variable	If this occurs in main ACORN window then re-enter file name manually and terminate entry with <RTN> key.
Error: Bad Window Path Name	Entry terminated with <TAB>. Use <RTN> key or green Continue button

- THE OUTPUT FROM ANALYSE CAN BE USED IN…

- Genie - view IPG / IMI file (I(Q,ω) vs). Black and white plots (6.1)
- PG Plotting Routines - view IPG / IMI (Q vs ΔE). Output data. Colour plots (6.2)

5.4. ELASTIC WINDOW (ELWIN)

Elastic Window is a stand alone analysis tool that allows the User to monitor broadening of the elastic line as a function of Q or, for example, temperature at a specific Q value. In brief, the program works by integrating the data collected in each detector over a fixed User defined energy range and writing the results to an ELQ or ELR file.

Consider a PG002 vanadium resolution measurement collected at room temperature and corrected for detector efficiency using the calibration file Detector.Calib in ICON. Assuming fixed limits of integration, the integrated area returned from all 50 spectra in the IPG file should be constant. Hence, program Elastic Window can be used as a quick test to ensure that the corrections are being applied before full data analysis commences. The result of using Elastic Window on the vanadium resolution file IRS16304.RAW for both efficiency corrected and uncorrected data is illustrated below.

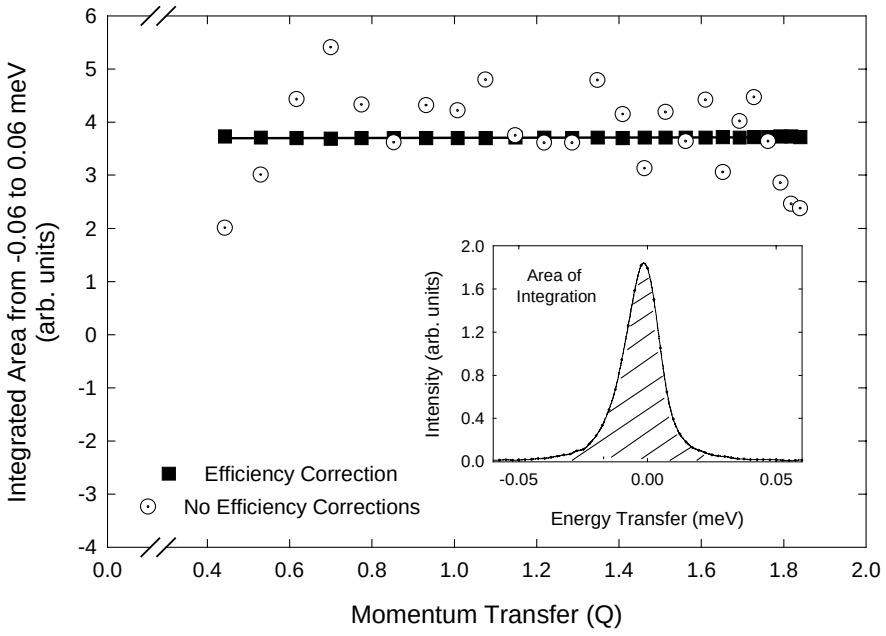

Figure 15: *The effect of using program Elastic Window on vanadium resolution spectra corrected (■) and uncorrected (○) for detector efficiency*

Alternatively, Elastic Window may be used to help determine transition temperatures. By monitoring the result returned from fixed limit integration of certain spectra, or more correctly at a certain Q value, as a function of temperature a tentative transition temperature may be ascertained from where the integrated area starts to decrease, as illustrated below.

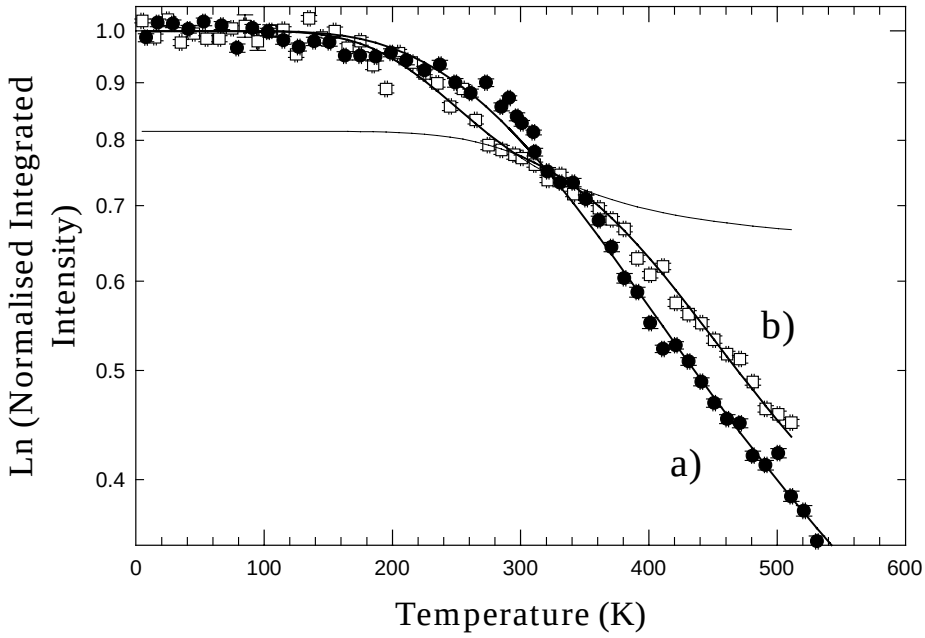

Figure 16: *Plot of elastic scattering intensity vs. temperature for fully hydrogenated (a) and deuterated (b) PEG:aCD (D.G.Bucknall and H.W.Beckham, ISIS Annual Report 1999)*

To launch Elastic Window click the corresponding radio button in the GUIDE Options window. The main Elwin window is shown in Figure 17 and defaults to 'Single Run' mode of operation.

- Single Run mode:

Single Run – This option should be chosen should the variation of the elastic line as a function of scattering angle / Q be required. The output file has extension .ELQ. The following input fields required entry when running Elwin in Single Run mode:

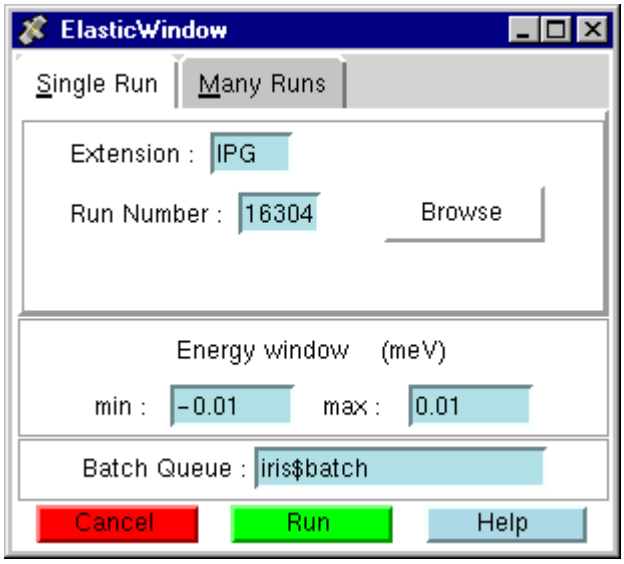

Figure 17: *The Elwin data input window (Single Run)*

Run Number – Enter the run number of the data file to be used either manually or using the Browse option. If the file number is entered manually then terminate the entry using the <TAB> or <Return> key.

Ext - Defines the extension of the Intermediate file be used. Default is IPG.

Energy Window – Enter energy limits for integration.

Batch Queue - If the batch queue is changed, terminating that entry initiates the batch job as if the Run button had been pressed.

- Many Runs mode:

Many Runs – Click on this tab if, for example, the variation of elastic line as a function of temperature, but at a specified Q, is required. The output file has extension .ELR. The following window will appear…

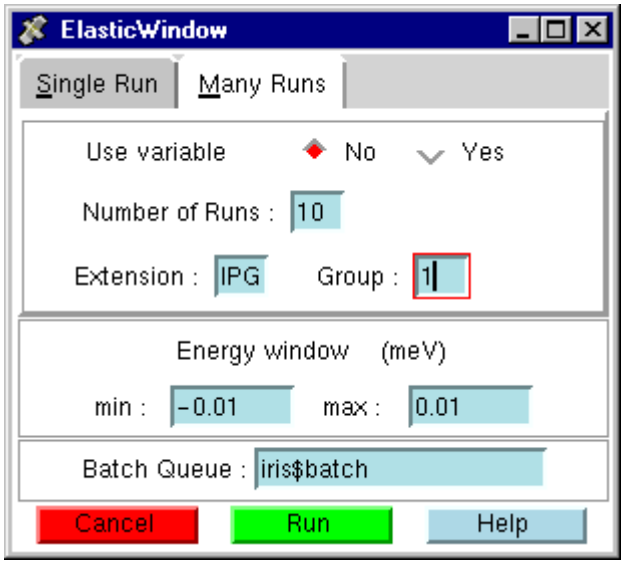

Figure 18: *The Elwin data input window (Many Runs)*

Number of Runs – The Number of Runs must be greater than one. Upon entry a new window can appears to allow input of all the run numbers to be used and the value of the variable. If the Variable option is not chosen then the Variable input boxes will be grey.

Extension - defines extension of the Intermediate file created using ICON to be used. The default is IPG.

Group – defines which angle / Q is to be. Relates to grouping options used to create IPG / IMI files in ICON.

Energy Window – Enter energy limits for integration.

Batch Queue - If the batch queue is changed, terminating that entry initiates the batch job as if the Run button had been pressed.

- OUTPUT FILES

Once the job has finished the User should find a three column .ELR or .ELQ ASCII file has been written to his/her working directory – the extension dependant upon whether the Single run or Many run option had been chosen. The file format is:

Run No *Integrated Area* *Error* - for an ELR file

Q value *Integrated Area* *Error* - for an ELQ file.

- POSSIBLE ERROR MESSAGES

Possible Error Messages	Probable Cause
IDA could not find your RAW file in any of the default disk areas	Check requested files are located in iris$disk0:[irsmgr.data] or scratch$disk:[irsmgr.data]
Error: error running command: VMS error	Check name entered in Batch Queue field. Check limits in Energy Window
File IRS*****.IPG/IMI does not exist	Check name entered in Run Number field
Error: cant read '***': no such variable	Check file extension, number of runs. Terminate entry with <RTN> key.

- THE OUTPUT FROM ELWIN CAN BE USED IN…

i) Genie – To view the contents of an ELR/ELQ file. Black and white plots (6.1)

5.5. DEMON – ANALYSIS OF NEUTRON DIFFRACTION DATA

As well as being a high-resolution quasi-elastic spectrometer IRIS also possesses long d-spacing neutron diffraction capabilities. The instrument can therefore be used solely as a neutron diffractometer or alternatively for quasi-elastic neutron scattering studies with the diffraction detectors being run in parallel to monitor structural phase transitions etc.

On IRIS, neutron diffraction data is collected using 10 He^3 gas-tube detectors oriented at $2\theta=170$ degrees. Detector calibration is unnecessary since the efficiency of a He^3 gas-tube may be determined theoretically. However, since each detector subtends a slightly different scattering angle from the sample position, the d-spacing range collected by each tube varies slightly for the same time of flight. The purpose of Demon is to correct the RAW diffraction data for monitor and detector efficiency, normalised to monitor counts and merged the spectra collected in each detector together to produce a single spectrum. Data interpretation is then carried out using standard diffraction routine i.e. Rietveld analysis.

To launch Demon from the GUIDE options window click on the corresponding radio button. The Demon window is shown in Figure 19 and requires entry in the following input fields:

Raw Files Location - The location of Raw files defaults to iris_data. Should the requested run number not be found in iris_data then there will be an error message. The files should be copied to scratch$disk:[irsmgr.data]

Spectra Range - The range of spectra containing the neutron diffraction data may be set either manually or using the radio button provided. Should IRIS have been used solely as a diffractometer then the diffraction data is written to spectra 3-12. However, when both diffraction and analyser detectors are in use spectra 105 to 114 contain the diffraction data. If the field next to the Spectra Range radio buttons is

blank, enter the run number of the data file to be used and press <RTN>. When using the Input Values option to enter spectra manually remember to terminate the entries put into the boxes using the <RTN> key.

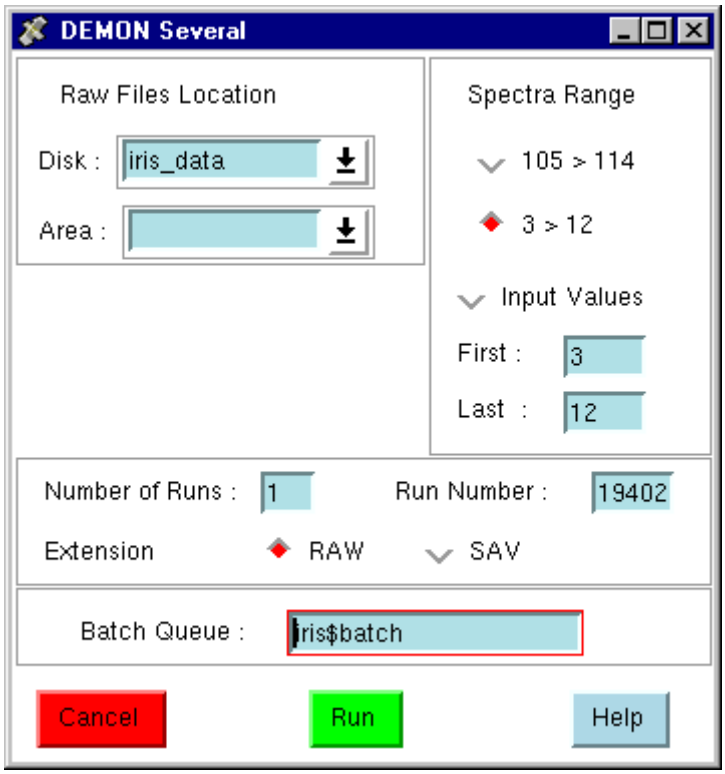

Figure 19: *The Demon data input window*

Number of Runs - Should the number of runs be set to 1 the input caret moves to the Run Number input box. However, if the number of runs is greater than 1 a new window appears with an entry box for each run - the caret will move to the next box upon terminating the entry. When a run number is input, the appropriate range of spectra appears in Range of Spectra boxes.

Extension - Specify the extension of the raw data file to be used (RAW / SAV).

Batch Queue - If the batch queue is changed, terminating that entry initiates the batch job as if the Run button had been pressed.

When the job as been submitted a message window appears giving the filename, and location, of the command file being run and the LOG file being written. Click Continue to close the window. All values entered, and options selected, in the Demon window become the default values the next time Demon is run.

Once the job has finished the User should find a .DIF file written to his/her working directory. To view the contents of .DIF file see section 6.1

- POSSIBLE ERROR MESSAGES

Possible Error Messages	Probable Cause
IDA could not find your RAW file in any of the default disk areas	Check the requested files are located in either iris$disk0:[irsmgr.data] or scratch$disk:[irsmgr.data]
Error: error running command: VMS error	Check name entered in Batch Queue field.

So that the User may familiarise his/herself with Demon, files IRS19401.RAW and IRS19402.RAW have been copied to directory iris$disk0:[iris.ida_files] and may be used for practice running the program. The two data sets constitute a complete silicon calibration spectrum (file IRS19402.RAW containing Si diffraction data from 0.5 to 2.8 Å while file IRS19401.RAW contains data from 2.0 to 4.0 Å). After correcting the spectra using Demon, the Genie program 'Merge' (6.1) may be used to combine the two resulting .DIF files and produce a single spectrum suitable for Rietveld analysis (see

http://www.isis.rl.ac.uk/crystallography). The result of such analysis on the two data files detailed above is shown below in Figure 20. The solid line through the data is the result of multi-phase Rietveld refinement. The additional peaks are due to the presence of vanadium and aluminium in the beam; the former arising from the vanadium can used to mount the Si sample and the latter from the Al windows on the IRIS sample bin.

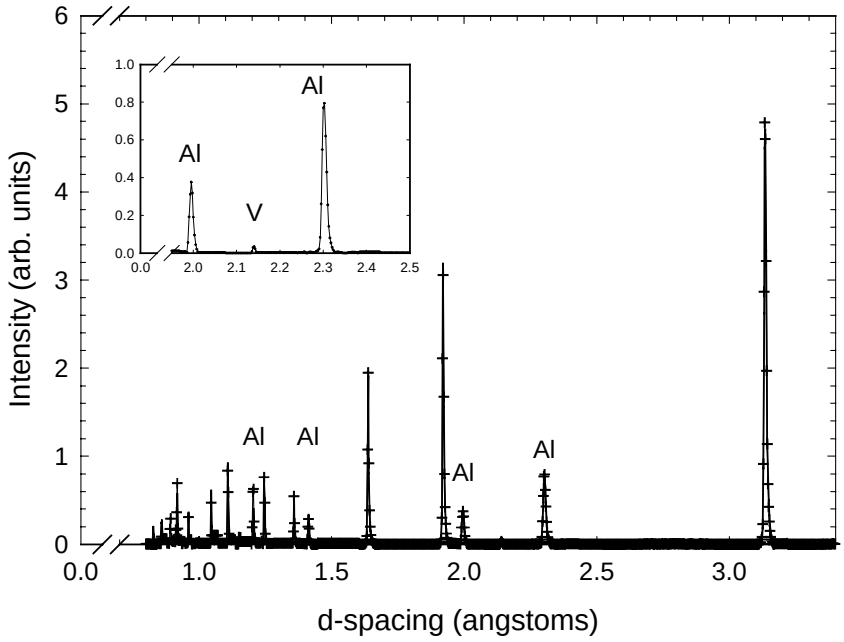

Figure 20: *The result of correcting diffraction data files IRS19401.RAW and IRS19402.RAW using Demon and combining the resulting .DIF files using the Genie program 'Merge'. The solid line is the result of a performing a multi-phase Rietveld refinement on the final merged data set (Al = Aluminium, V = Vanadium).*

- THE OUTPUT FROM DEMON CAN BE USED IN…

i) Genie – To view corrected diffraction data. To merge together several (6.1)

5.6. RESNORM – RESOLUTION NORMALISATION

In brief, ResNorm works by least squares fitting a smooth, finely-interpolated resolution function data set (pg002.res, mi004.res etc) to each spectrum in an experimental (e.g. vanadium) resolution IPG or IMI data file. The routine varies the width of the peak defined by the .res data file until it 'maps' the experimental data. A 'stretch-factor' is then ascertained, as is the more important spectrum intensity normalisation factor determined by integrating the broadened data set over fixed User defined energy limits.

The output file created by ResNorm is used in conjunction with the PG Plot graphics packages detailed in section (6.2). However, the program itself need ONLY be run if the file Detector.Calib was *NOT* used during the creation of the IPG/IMI files by ICON - the ICON procedure converting Raw data into $I(Q,\omega)$, or strictly speaking $I(2\theta,\omega)$. If not, then the spectral intensities in the subsequent IPG file(s) will not have been normalised and the PG Plot Graphic routine will not display a true intensity map. In this case, the output file from ResNorm should be read into the PG Plot package, when prompted for, to correct the spectral intensities.

At present, ResNorm is mostly redundant since in the majority of cases the Detector.Calib file is applied to the Raw data. However, it will, in the future, provide a necessary preface to the Data Interpretation program Quasi-Lines (in development) and hence it's inclusion in this manual.

To launch ResNorm, click on the 'ResNorm' radio button, the following input window will appear (Figure 21).

Resolution Run Number - can be input either by typing in the entry box or found using the Browse button. The default extension is IPG but will change should the a mica analyser resolution file be selected in the Choose Analyser field

Energy - defines the energy range over which the resolution file (pg002.res, mi004.res etc) will be fit to the resolution data.

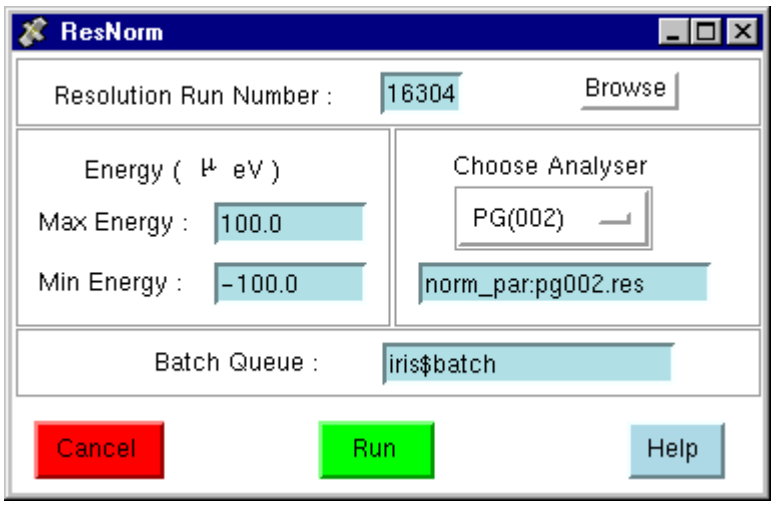

Figure 21: *The ResNorm data input window*

Analyser - chosen via a button with a drop-down menu. For data collected prior to June 1999, one should use resolution files: norm_par:pg002_old.res and norm_par:pg004_old.res for data collected using the PG analyser

Batch Queue - If the batch queue is changed, terminating that entry initiates the batch job as if the Run button had been pressed.

When the job as been submitted a message window appears giving the filename, and location, of the command file being run and the LOG file being written. Click Continue to close the window.

- OUTPUT FILES

Once the job has finished the User should find a four column IRS*****.RES ASCII file (where ***** is the run number of the experimental resolution data set) has been written to his / her working directory. The file format of the file is:

Amplitude *Stretch-factor* *Q-value* *Chi squared* (χ_{min}^{2})

The chi squared values denoting the "goodness" of fit of the smooth, finely interpolated, resolution file to each group in the experimental data set.

- POSSIBLE ERROR MESSAGES

Possible Error Messages	Probable Cause
File ****.IPG / IMI does not exist	Ensure requested IPG / IMI file is in the User's working directory
File ****.IPG / IMI does not exist	Ensure analysing reflection selected under 'Choose Analyser' reflects the use of either an IPG or IMI file.
Error: error running command: VMS error	Check name entered in Batch Queue field.

- THE OUTPUT FROM RESNORM CAN BE USED IN…

- PG Plot Visualisation routines – Plot2D and QEOut (6.2)

5.7. WIZARD AND VIZ

VIZ provides the User an easy means of examining large quantities of data – e.g. the variation of intensity as a function of scattering angle / Q as a function of energy - in order to see, if you like, 'what is going on'. VIZ was originally written by Dennis Mikkelson (University of Wisconsin, Stout) for use at IPNS, Argonne National Laboratory. An early version is described in the proceedings of WONSDA-2. The package has been adapted to run at ISIS. To do so a bridging routine (WIZARD) is required to convert the ISIS binary data files into ASCII.

5.7.1. WIZARD

WIZARD converts data in binary form, such as .RAW or Intermediate Format files (e.g. IPG) into ASCII files suitable for VIZ. To launch WIZARD from the GUIDE options window check on the WIZARD radio-button.

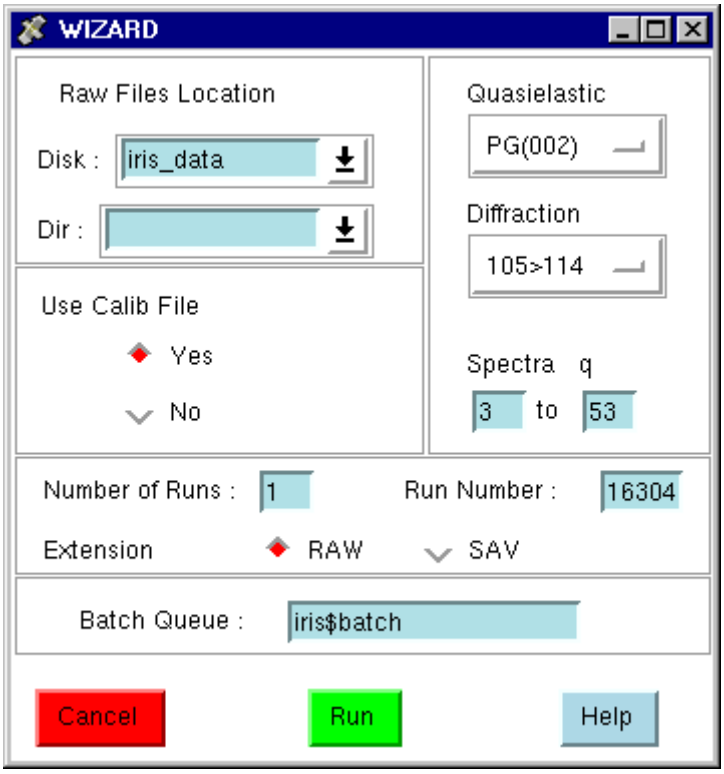

Figure 22: *The Wizard data input window*

Raw Files Location - The location of RAW files defaults to iris_data. Should the requested run number not be found in iris_data then there will be an error message. The User should copy the files to scratch$disk:[irsmgr.data].

Use Calib File - Select the YES radio button to apply Detector.Calib (generated using the program Calibration, section 5.1.1) to the data. Like Elastic Window, VIZ provides a simple method of testing that calibration corrections are being applied.

Quasi-elastic / Diffraction – For quasi-elastic scattering experiments the analyser reflection used is chosen via drop down menus. Alternatively, spectra containing neutron diffraction data may be set either manually or using the radio button provided. Should IRIS have been used solely as a diffractometer then diffraction data is written to spectra 3-12. However, when both diffraction and analyser detectors are in use spectra 105 to 114 contain the raw data

Run Number - Enter the run number of the file containing the resolution data. Terminate the entry using the <TAB> or <RTN> key. Default file extension is IPG.

Batch Queue - If the batch queue is changed, terminating that entry initiates the batch job as if the Run button had been pressed.

When the job as been submitted a message window appears giving the filename, and location, of the command file being run and the LOG file being written.

Once the job has finished the User should find that a .VIZ (for quasi-elastic neutron scattering measurements) or a .DIZ (for diffraction data) file has been written to his/her working area.

- POSSIBLE ERROR MESSAGES

Possible Error Messages	Probable Cause
IDA could not find your RAW file in any of the default disk areas	Check the requested files are located in either iris$disk0:[irsmgr.data] or scratch$disk:[irsmgr.data]
Error: error running command: VMS error	Check name entered in Batch Queue field.
File Detector.Calib file does not exist	Check that the file Detector.Calib file is in the User's working directory

- THE OUTPUT FROM WIZARD CAN BE USED IN…

i) VIZ – To allow complex (Q vs ΔE vs Intensity) data sets to be viewed (5.7)

5.7.2. VIZ

To launch VIZ from the GUIDE options window click on the VIZ radio-button. A VIZ window displaying the vanadium resolution file IRS16304.RAW, corrected using Detector.Calib, is shown below. Note: while VIZ is running other GUIDE options are disabled until the VIZ window is closed.

The main section of the VIZ window displays all the data in a loaded data file as a large colour contour plot. Clicking the mouse on the main image activates a set of cross-wires. By using the mouse to move the cross-wires over the image, horizontal and vertical cuts through the main plot are instantly displayed below and

beside the main image. Information about the data at the cursor position, such as angle, wavelength, etc, is also given.

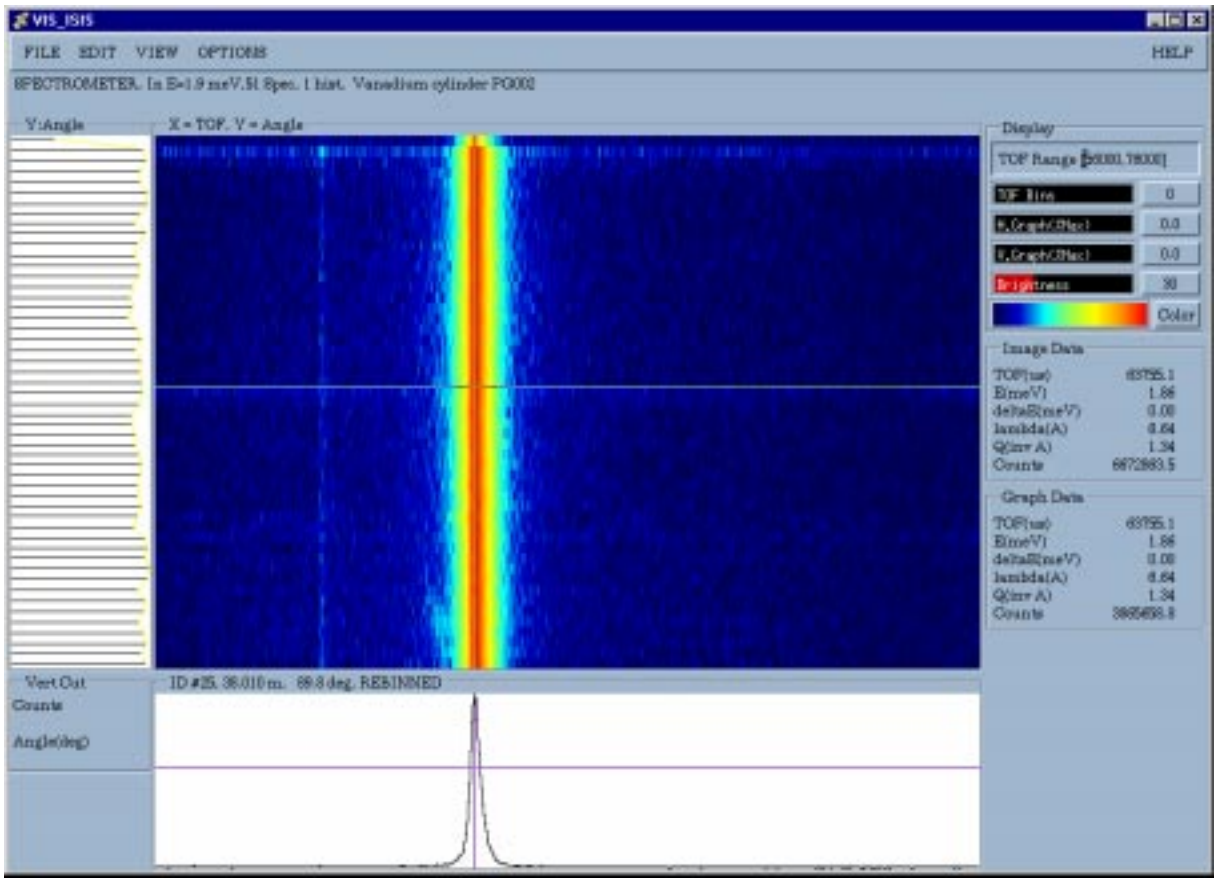

Figure 23: *The Viz display window*

While most of the options in VIZ are self-explanatory, it is worth describing the more useful features. Drop-down menus are linked to the commands across the top bar and perform the following:

i) *Options available under 'FILE'*

QUIT - exit from the program. All GUIDE options are reactivated.

LOAD DATA FILE - activates a pop-up menu detailing the directory structure of the Users working directory. The disk and directory in which data files are to be found may be changed manually using the Filter box or, alternatively, by simply clicking on the appropriate name. Clicking on the Filter button will refresh the display

PRINT - activates a pop-up menu to provide a graphical output of either the main image or the Horizontal/Vertical side graph. The print options define whether the required graphic is to be written as a postscript file, sent directly to the printer or previewed in a separate PGPLOT window.

ii) *Options available under 'EDIT'*

IMAGE - removes from the display the spectrum directly under the crosswire.

HOR. GRAPH – When activated, the plot in the horizontal graph turns blue. Instead of being over written when the cursor next moves, the plot remains such that spectra at different cursor positions, or more correctly, Q can be are over laid and compared with the static image. Once activated, additional options are also presented to clear a saved plot.

iii) *Options available under 'VIEW'*

IMAGE X AXIS - enables the units of the x-axis to be changed. The choice depends on the type of measurement e.g. diffraction or inelastic. Choices not available will be in grey and disabled.

IMAGE Y AXIS - enables the units of the y-axis to be changed. ID refers to the spectrum number.

HOR. GRAPH DATA - gives the User the choice to view either RAW or re-binned data

VERT. GRAPH Y AXIS - gives the User the choice to view the data in terms of either ID (spectrum number) / angle or momentum transfer (Q).

NEXT HISTOGRAM - not applicable to IRIS data.

iv) *Options available under 'OPTIONS'*

PRINT LEGEND – invokes a drop down menu which defines where the legend should be printed.

v) *Options available under 'DISPLAY'*

Located towards the top right corner of the screen, the DISPLAY options allow parameters such as contrast, brightness etc, associated with the main display, to be altered. The top field of the DISPLAY box details a) the units of the x-axis and b) the plot limits. The latter can be edited manually and, once terminated, the display is refreshed.

TOF BINS - To change this value click on the right hand button displaying the current bin number. This activates a new window in which a slider control is used to change the number of bin used to display the data.

H.Graph (%Max) / Y.Graph (%Max) - Alters the y-scale of the Horiz and Vert graphs respectively. Clicking on the right hand button, showing the current % of max height, activates a new window with a slider to change the value.

Brightness - Changes the brightness of the main display. Clicking on the right hand button, showing the current brightness value, activates a new window. A slider control is used to alter the brightness value. This is a trial-&-error process - basically it varies the colour scale such that low or high values can be enhanced. For example, low intensity features at the base of the main elastic line may be highlighted.

Colour Spectrum – a drop-down menu gives the colour types available. The recommended colour map is Rainbow.

Image Data box – lists the values of the various parameters (Q, Energy Transfer, Time of Flight) corresponding the centre of the cross-wires in the main graph.

Graph Data Box – as above but lists the values of the various parameters corresponding to the centre of the cross-wires in the horizontal graph. The cross-wires in the horizontal graph move independently to those in the main graph.

Vert Cut Box - bottom left corner, gives the values of the various parameters listed corresponding the centre of the cross-wires in the vertical graph. The cross-wires in the vertical graph move independently to those in the main graph.

6. DATA VISUALISATION

6.1. GENIE II

At present, the graphical interface to view the IDA package makes extensive use of the Genie II program and general Genie file structures. It should be noted, however, that since the IRIS data analysis suite is continually evolving, there is concerted effort to move all visualisation packages over to the newly developed Genie III platform, more commonly referred to as OpenGenie (*http://www.isis.rl.ac.uk/OpenGENIE*). At time of writing this conversion was incomplete and therefore the Genie II methods of data visualisation are addressed. However, when the new packages are fully functional the entries in this section will be updated.

The raw data collected on IRIS is in the standard format for files with extension .RAW or .SAV. However, subsequent files created during the GUIDE analysis procedure are written in Intermediate file format and interact with Genie via the REad and WRite commands. It is assumed that the reader if familiar with the Genie package. For more information see '*Rutherford Appleton Report: RAL 86102 "Punch GENIE manual. Version 2.3. A language for spectrum manipulation and display", DAVID WIF'* – a copy of which should be available in the instrument cabin.

To launch Genie, type GENIE at the command prompt in an active DECTERM window. The following options should appear in the Genie window. Typing the keyword links to specific Genie visualisation routines:

>> Type GENIE for a list of general Genie routines

>> Type INELASTIC for Inelastic Scattering specific analysis programs

>> Type DIFFRACTION for a list of Diffraction specific data analysis programs

Most of the programs listed under each of the above keywords are self-explanatory, simply follow the command prompts. However, a brief description is given where necessary.

- GENIE

Upon typing GENIE, the following general Genie programs may be accessed:

```
>>      GENERAL GENIE ROUTINES
>>
>>      TP - Plots Sample Environment  temperature file
>>      TPC - Plots current Sample Environment temperature file
>>      LASER - Allows you to make plots of GENIE data
>>      WI ( Write IDA) – IDA data in Genie workspaces written to BINARY files
>>      WIA (Write IDA ASCII) - IDA data in Genie workspaces written to ASCII files
>>      IRSGRPS - Reads in IDA output files (IPG / IMI / DIF...) from User specified area
```

- TP and TPC – TPC exactly same as TP (detailed below) but accesses DAE directly.

```
>>      Temperature log file plotting routine (TP)
>>
>>      Please enter the run number for which you want a temp plot:  19751
>>
>>      load w1 iris_data:irs19751.log i_p:load_log.exe

>>      Give start date / time: 11-AUG-1999 03:24:29
>>      Give finish date / time : 11-AUG-1999 08:32:18
>>      Give Se block name : TEMP
>>      Please give units (K or C): K

>>      Which log column do you want, 2 or 3 (Def 3)? 3

>>      d  w1
```

- IRSGRPS is a standalone Genie visualisation program to read in and display Intermediate File Format files created using the GUIDE package, be they IPG, IMI, IAG, DIF etc. The program asks for the run number(s) and the file extension.

  The location of the file(s) to be viewed may be entered manually else the current area (i.e. disk and directory from which genie was launched) is assumed.

- WIA and WI – two command files used to convert IDA generated Intermediate File Format files (IPG, IMI, IAG, DIF etc read into Genie using IRSGRPS) to ASCII and BINARY format respectively and write the results to .DAT files. To load subsequent ASCII files into Genie use the Genie *LOAD* command which has the general form:

  LOAD Wn <datafile> <program>.

  The data in <datafile> is read into workspace Wn using the program <prognam>. The following programs are available:

i_p:lo_res	reads a RES file
i_p:lo_xye	reads a data set as an ASCII file in the format: Line 1 containing the number data points followed by a list of x, y and e values.

- INELASTIC

  Upon typing INELASTIC, the following programs may be accessed:

>> INELASTIC / QUASI-ELASTIC SPECIFIC PROGRAMS

>>

>> SWIFT (see Appendix I)

>> FURY (see Appendix II)

>> OFFSET - Displays time-shifted spectra

>> GAUS - Multiple gaussian fitting routine

>> OI (offset ida) - Reads in and offsets IDA data

>> SPURION - Program to check for spurious features

>> ELF - Lorentzian fitting program for tunnelling data

>> GEC - Fits a gaussian with an exponential decay to data

>> ICON - Normalises data to the monitor and converts it to S(Q,w)

However, it should be noted that the majority of these Genie programs available for inelastic/quasi-elastic analysis have been superseded and modified for use in the GUIDE package. For comprehensive data analysis the versions in the GUIDE package should be used. However, programs such as ICON are useful tools for a quick 'look-see' to examine trends in data sets while running an experiment. In addition, programs Swift and Fury, yet to have a GUI interface, are outlined in Appendix I and II respectively.

- DIFFRACTION

Upon typing DIFFRACTION the following programs may be accessed:

>> DIFFRACTION SPECIFIC PROGRAMS

>>

>> ADD - Analyses diffraction data properly.

>> DAEUPD - Update diffraction pattern every minute.

>> ADDDAE - View diffraction data in DAE. No corrections made.

>> MERGE - Merge N workspaces containing different d-spacing diffraction data

- ADD, ADDDAE and DAEUPD – command files used to view neutron diffraction data. Should full data analysis be required then one should refer to Demon (Section 5.5). However, the above packages provide a quick and easy method of looking at the diffraction data being collected. In brief, ADDDAE and DAEUPD are very much 'look see' tools which allow the evolution of a diffraction pattern to be monitored as a function of time. In contrast, ADD performs full detector efficiency and monitor corrections. Obviously, the latter can only be used once a measurement is complete. All three packages ask for the operating mode of the spectrometer (i.e. operating solely as a diffractometer or as an inelastic instrument with diffraction capabilities). However, while ADD and ADDDAE continue by asking whether or not to exclude data collected in certain detectors from the final diffraction pattern, DAEUPD requires the time interval (mins) between successive DAE readings, and hence updates of the displayed diffraction pattern, to be set.

- MERGE - A set of diffraction measurements, each detailing different d-spacing ranges, may be merged to create one continuous diffraction pattern suitable for Rietveld refinement.

6.2. PG PLOT

The programs detailed in this section utilise the plotting package PGPLOT to enable creation of publication quality colour graph postscript files. Interaction with each package is via a set of standard questions common to all programs. The first three of these questions concern the character size and line-width of the graph to be generated. While the default values suggested are suitable for plotting to the screen, they may need to be refined for publishable quality hard copy output.

To view a graph the programs will prompt for a suitable graphics device. Typing '?' will list the possibilities, however, useful options include : /R for a Pericom-type terminal (with graphics capability), /VT for an ordinary workstation, /XW for a X-windows workstation, /N for a null device (no plotting) and /CPS for a postscript file called PGPLOT.PS which can later be sent to a postscript printer for a colour hard copy. In some programs the Null option is the default. The programs read Genie Intermediate file format data files (e.g. IPG/IMI/IAG files etc) and request a resolution measurement. However, the latter, generated using the program ResNorm (section 5.6), need ONLY needs to be read in should the calibration file, Detector.Calib, have not been applied to the Raw data during creation of the IPG/IMI file(s).

- PLOTTING ROUTINES

i) PLOT2D

Displays data as a function of scattering angle and energy transfer. Input data should be in Intermediate Genie File format (i.e. IPG, IMI etc). To run Plot2D type 'Plot2D' followed by return.

ii) PLOTQE

Displays data as a function of Q-vector and energy transfer. Input data should be in Intermediate Genie File format (i.e. IPG, IMI etc). To run PlotQE type 'PlotQE' followed by return.

iii) QEOUT

Similar program to PlotQE. Displays data as a function of Q-vector and energy transfer with the option to output the displayed data to a binary file. Input data should be in Intermediate Genie File format (i.e. IPG, IMI etc). To run QEout type ‘QEout’ followed by return.

By way of an example, the input variables requested by PlotQE and QEOut to produce a colour image, along with suitable values for each, are detailed below. The result , illustrating data file IRS16352.IAG found in isis$disk0:[iris.ida_files] (the culmination of all data reduction processes outlined in this manual) is presented in Figure 24.

Program PlotQE
****

$ PLOTQE

PLOT> Character Size ? (def=1.5) : 1.5
PLOT> Line-widths ? (def=1) : 1.5
INPUT> Filename ? (interm. GENIE format) : IRS16352.IAG

> Read in a detector-normalisation file? Y / N (def=N) : N

Emin & Emax = -5.637E-01 5.717E-01
Qmin & Qmax = 4.304E-01 1.973E+00

SELECT> Emin, Emax, Qmin & Qmax for plot ? : -0.563 , 0.5717, 0.4304, 1.973
SELECT> Nx & Ny for plot ? : 100,100

Smooth> FWHM(x) & FWHM(y) ? (pixels) : 3, 2

(1) Surface

(2) Colour: Grey-Scale

(3) Colour: Heat

(4) Colour: Rainbow Spectrum

(5) Colour: BGYRW

(6) COLOUR: Serpent

(7) Colour: Read in from file

PLOTQE> Type ? : 5

Minimum value = -1.3683477E-08

Maximum value = 0.2397484

>> Ymin & Ymax for plot ? (def=-1.368E-08, 2.397E-01) : RTN

>> Contrast factor ? (def=1.0) : 0.8

Graphics device/type (? to see list, default /NULL): /XW

> Write out a Q-E binary file ? Y/N (def=N) : Y

OUTPUT> Filename ? : TEST.DAT

> View the current region again ? Y/N (def=Y) : N

> View another Q-E region ? Y/N (def=Y) : N

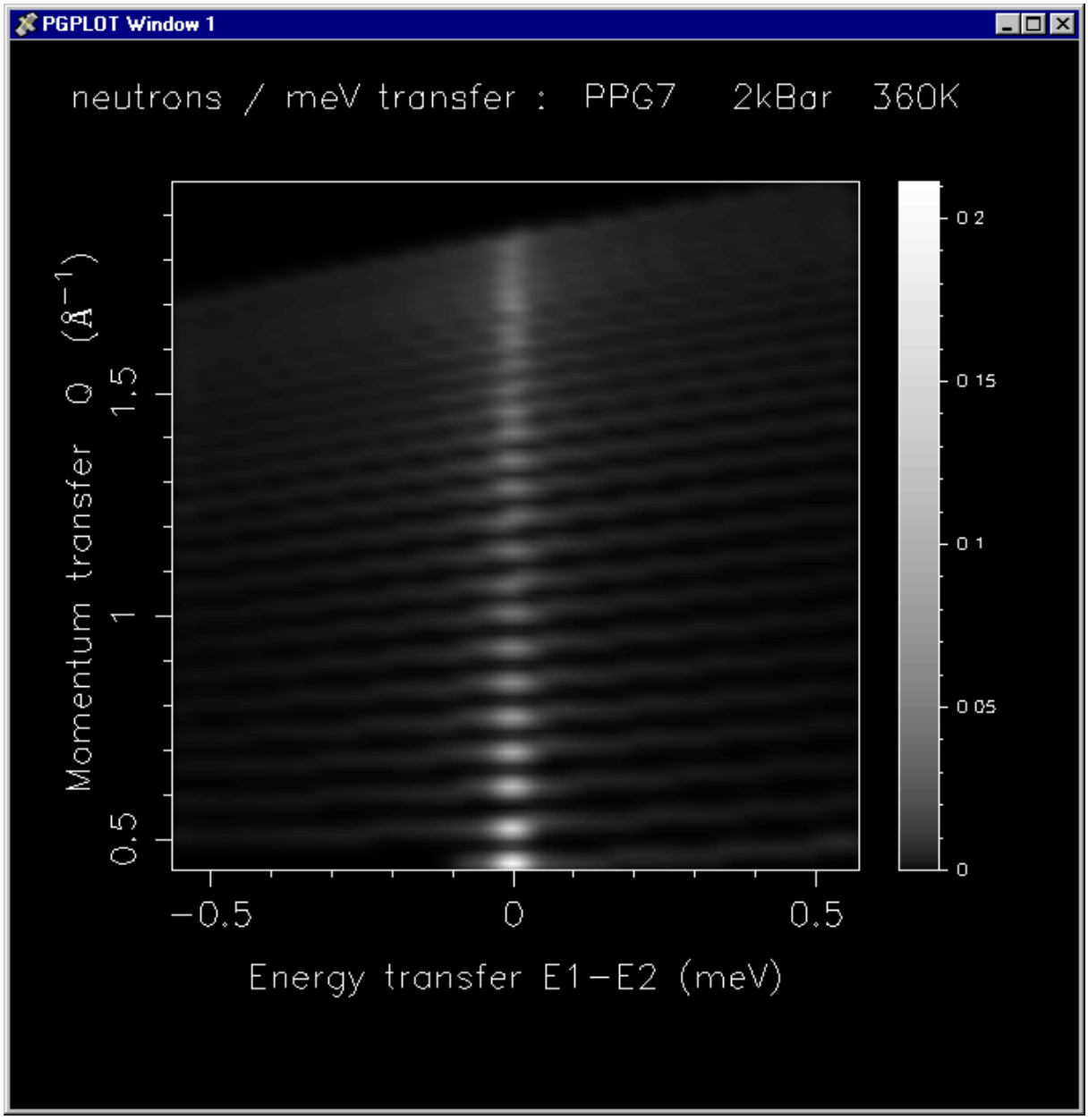

Figure 24: *File IRS16352.IAG as displayed by plotting program PlotQE*

VII. REFERENCES

1) B B Welch, Practical programming in TCL and TK. 3rd ed. Upper Saddle River, N.J. : Prentice Hall, 1999

2) M Bee, 'Quasi-elastic neutron scattering. Principles and applications in solid state chemistry, biology and materials science'. Adam Hilger 1988

3) C J Carlile, Rutherford Laboratory report, RL-74-103 (1974)

4) A K Soper, W S Howells & A C Hannon, RAL Report RAL-89-046 (1989)

5) J S Higgins, R E Ghosh, W S Howells & G Allen, JCS Faraday II **73** 40 (1977)

6) D C Champeney, Fourier Transforms & their applications (Academic Press)

7) E Oran Brigham, The Fast Fourier Transform (Prentice Hall)

8) U P Wild, R Holzwarth & H P Good, Rev Sci Instr **48** 1621 (1977)

9) A Heidemann, W S Howells & G Jenkin, Neutron Spin Echo, Lecture Notes in Physics **128**, Ed F Mezei, (Springer verlag) 1980

10) V Arrighi, J S Higgins, A C Burgess & W S Howells, Macromolecules **28** 2745 (1995)

APPENDIX I. SWIFT

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 quasi-elastic 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 the IN10 spectrometer at ILL. The convolution of two Lorentzians is itself a Lorentzian so that the spectrum of the measured and resolution data can simply both 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. SWIFT provides this latter form of peak fitting. It employs a least-squares algorithm that

requires the derivatives of the fitting function with respect to its parameters in order to be faster and more efficient than those algorithms that 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 $S(Q,\omega)$:

- 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 unbroadened 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 [5]. Briefly, polymer theory predicts 3 forms of the I(Q,t) in the form of $\exp(-\alpha t^{2/\beta})$ where β can be 2, 3 or 4. The Full Width Half-maximum then has a Q-dependence (power law) of the form Q^{β}. The I(Q,t) has been numerically Fourier transformed into $I(Q,\omega)$ and the $I(Q,\omega)$ have been fitted with

functions of the form of a modified Lorentzian. These latter functions are used in the energy fitting procedures.

The routine is started with the Genie command *swift* (if this has been defined as *i_p:swift*) which will ask for :

1 Sample run number

2 Resolution run number

3 *File extension* - the same for both sample and resolution. This means that a fit can be performed at any stage of the data analysis e.g. at IPG or IAG stage

4 *Group number* - i.e. group number in file

5 *Energy limit (meV)* - note that Genie only works in meV and not in μeV

6 *Energy increment (meV)*

The routine then calls the SWIFT routine that will ask the following questions, default values are enclosed in []:

1 Shapes are : *Elastic , Quasi, Shift or Poly [Q] type E, Q, S or P*

2 How may peaks ?[1]

3 Input starting values of parameters background (P1) & origin (P2)

*4.1 F*or Q(uasi) : *quasi-el peak <n> : height P(3) & h-width P(4). R*epeated for each peak

*4.2 F*or E(lastic) : *elastic peak height (P3) quasi-el peak <n> ; height P(4) & h-width P(5)*

*4.3 F*or S(hift) : *central peak height P(3) & h-width P(4), side peak <n> ; shift P(5), height P(6) & h-width P(7)* and repeat for each pair of side peaks

4.4 For P(olymer) : *power law ? [2], polymer peak height P(3) & h-width P(4)*

5 Fix any parameters (Y/N) ? Default=N

5.1 If answer is Y, *input <n> values of IFIT* , where <n> is the number of parameters. IFIT=1 to fit that parameter or 0 to keep it constant.

For the broadened peaks, the width is the half-width at half-maximum and the height is that of the measured sample (not the height of the function). For the elastic peak the height parameter is the fraction of the resolution peak height. The fitted parameters and their errors are then printed - if a parameter is fixed the error is quoted as zero. Then a selection of areas is printed : *peak count* is just the sum over the whole energy range and *summed* is the peak count multiplied by the energy increment (i.e. the area). Then for each quasi-elastic peak the full width half maximum and the integrated area. The latter should be the summed peak area, but depends on the width of the peak relative to the energy window - if the peak extends beyond the window, the integrated area will be greater than the summed one. For the elastic peak, again the summed and integrated areas are given.

The fitting routine then returns to Genie to plot the data and the fitted curve. The routine asks if a new set of limits for the plot are required, then if hardcopy is required and if a new plot is required. Then it asks if a new fit is required and finally if a new group is required.

W1 will contain the input resolution and W2 the input sample data. A *Function* routine calculates a flat background for the resolution, subtracts it and puts the result in W3. The result is also written to a temporary file which is read by the fitting routine and deleted. W4 will contain the fitted curve and W2 & W4 will be plotted.

The fitted parameters are written to a file with a name of the form IRS<runnumber>.g<nn>_<type> where <nn > is the group number and <type> is the peak type option defined above eg IRS01234.g01_Q.

The individual *Functions* can be used, but the resolution background subtraction must be carried out before each fit in order to create a scratch file containing the resolution data. Good quality plots of the fitted data, in which each component of the fit is displayed, can be obtained by using the Genie command *i_p:pg_sw*. The routine uses the fit parameters in the file created by SWIFT and the

PGPLOT plotting package. The questions follow those of SWIFT with an extra one asking if the plot is to be on the screen or a Postscript file. With the latter the file created can then be submitted to a Postscript printer queue.

- HINTS ON USE

When running the program :

i) The program was originally written for a symmetric energy window, that is E_{min}=-E_{max} . An asymmetric version is available *i_p:aswift* which appears to work but is to be treated with caution.

ii) 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.

iii) The background and origin parameters can start at zero.

iv) The elastic peak height is the fraction of the measured resolution peak.

v) 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.

vi) The parameter width is the half-width half maximum of the scattering function. The printed output will show this and also give the full-width half maximum.

vii) 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.

viii) When fixing parameters, the routine prints out the total number of parameters and asks how many to fix. The IFIT parameters are then typed in with 1 to fit and 0 to fix. The background and origin are the first to fix, so for a 2 peak elastic option the IFIT values could be 0 0 1 1 1 (values separated by spaces).

• SLOPING BACKGROUND

Version SLOPE is similar to SWIFT except that instead of a flat background a two parameter (gradient and intercept) sloping background is applied.

• QUICK VERSION

There is a quick version of SWIFT which uses for the resolution the function provided as a RES file, as defined in section 11, instead of the measured data. The routine is called i_p:q_swift and instead of asking for the resolution runnumner it asks for the analyser code. This routine is useful during the experiment when there may not be a suitable resolution file available.

APPENDIX II. FURY – FFT DECONVOLUTION

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,

$$I(Q,\omega) = S(Q,\omega) \otimes R(Q,\omega)$$

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,

$$I(Q,t) = R(Q,t) \times S(Q,t)$$

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,

$$L(\omega) = \alpha\omega^2 \Big/ (\omega^2 + \Gamma^2)$$

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 ω_0t + i sin ωt) exp(-Γt) , thus taking the modulus produces the exponential exp(-Γt) 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 $\sigma_\kappa^2=\langle\Delta\Xi_\kappa\rangle^2$ which is assumed to be given by $\sigma_k^2=\langle X_k\rangle$. 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^R 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

$$\sigma^2(X_j^I) = 1/2X_0^R - 1/2X_{2j}^R$$

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 coefficents, 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 coefficent is comparable to its value. This region must be treated with caution. For 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.

- HINTS ON USE

When running the program :

i) The program was original written for a symmetric energy window, that is E_{min}=-E_{max}. It will now accept an asymmetric window and appears to work in this mode, but caution is recommended.

ii) 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.

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

- Quasielastic peaks - a single Lorentzian would produce a straight line in the plot of lnI(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.

- 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.

- Non-Lorentzian shape - this could be either a stretched exponential form $\exp -\alpha\tau^{\beta}$, 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].

- 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 coefficent (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, note 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.

• THE PROGRAM

This routine carries out a deconvolution using a Fast Fourier Transformation procedure. The resolution curve has a flat background subtracted as in SWIFT, but no temporary file is created. Both the sample and the resolution are transformed from I(Q,ω) into I(Q,t) and the sample is divided by the resolution. A flat background is subtracted from the reolution before the FT otherwise it would appear as a δ-function at the origin in the I(Q,t).

The routine is started with the Genie command *FURY* (if it has been defined as *@i_p:fury*) which will ask :

1 sample run number

2 resolution run number

3 file extension

4 group number

5 maximum energy (meV) - note Genie only works in meV and not in μeV

6 minimum energy (meV)

7 energy increment (meV)

The routine then returns to Genie to plot the I(Q,t). Then it asks if a new set of limits for the plot are required, if hardcopy is required and if a new plot is required. Then it asks if a new group is required. Remember that the Genie command to change the y scale from linear to log scale is *toggle log y*. The input I(Q,ω) will be in W1 & W2 for sample & resolution respectively. The data is Fourier transformed using the Genie *TRAnsform* command with the routine i_p:ftr_vms or i_p:ftr_axp. The transformed I(Q,t) will be in W3 & W4 while the deconvoluted I(Q,t) will be in W5. When looping over groups the deconvoluted data will be copied from W5 to W(10+n) where n is the group number.

• BACK TRANSFORMING

A back transform to I(Q,ω) can be carried out as follows: truncate the I(Q,t) to remove the noisy data at long times by using the REBIN command in the form *reb 0:tmax,* then perform the back transform with the command *tr w<n> i_p:ftr_vms w<m>* where W<n> indicates the workspace for the I(Q,t) as defined above eg W5 and the W<m> the workspace for the backtransformed I(Q,ω). This may be compared with the original I(Q,ω) in w1.

- QUICK VERSION

There is also a quick version of FURY which for the resolution uses the function provided in a RES file, as defined in section (5.6), instead of the measured data. The routine is called i_p:q_fury and instead of asking for the resolution run number asks for the analyser code.