CLRC

Technical Report
RAL-TR-96-006

IDA – Iris Data Analysis

W S Howells

January 1996

COUNCIL FOR THE CENTRAL LABORATORY OF THE RESEARCH COUNCILS

Enquiries about copyright, reproduction and requests for additional copies of this report should be addressed to:

The Central Laboratory of the Research Councils
Library and Information Services
Rutherford Appleton Laboratory
Chilton
Didcot
Oxfordshire
OX11 0QX
Tel: 01235 445384 Fax: 01235 446403
E-mail library@rl.ac.uk

ISSN 1358-6254

IDA

IRIS DATA ANALYSIS

W S Howells

ISIS Facility
Rutherford Appleton Laboratory
Chilton
Didcot
OX11 0QX

January 1996

CONTENTS

1 INTRODUCTION

IDA (IRIS Data Analysis) is a suite of programs for the analysis of data obtained on the IRIS spectrometer at ISIS. As the title suggests the package was conceived for the IRIS spectrometer however, with minor modifications, it can be adapted for data on other ISIS instruments and even for instruments on other neutron sources. As such it can then be considered as a package for the analysis of quasielastic neutron scattering, where the term can also mean inelastic scattering at small energy transfers. It is an integrated package in which the programs fit into a logical scheme and it has been made as user-friendly as possible.

The analysis of scattering data can be divided into two sections : data treatment and data interpretation. In data treatment the raw data is converted into a form which is independent of the instrument parameters and the neutron scattering process. In other words, it is reduced to the scattering function $S(Q,\omega)$ which depends only on the dynamics of the sample measured. In this treatment the data is corrected for absorption, container scattering, multiple scattering and normalised to an absolute scale of intensity.

The next process is then one of data interpretation and in quasielastic scattering this is dominated by methods of measuring the peak shapes and widths and relating these to some theoretical model for the dynamics.

Many of the routines in the package have been in existance for decades. Most of those in the treatment section had origins in packages at the ILL which have been adapted and improved for use at ISIS. Similarly, the fitting routines are updated versions. However, there are many new routines and ideas, especially the techniques of Bayesian analysis and the package will be continuously upgraded and modified as new methods become available.

2 COMPUTER OVERVIEW

The programs were developed on DEC computers using the VMS operating system and can now run under both the VMS and Alpha (AXP) operating systems. They make extensive use of system routines. Many of the programs involve the use of the ISIS data manipulation program Genie. It is assumed that the user is familiar both with DEC computers and Genie.

2.1 Setup

At ISIS the progams are stored in two areas : iris$disk:[irsmgr.progs], which has the logical name ida_vms, for the VMS routines and iris$disk:[irsmgr.alpha], which has the logical name ida_alpha, for the Alpha routines. There is a command file ida_vms:ida_logs.com which sets up all the logical names and should be called in the user's login.com file. When this setup command file is called it determines which operating system is being used and assigns the logical name i_p to either ida_vms or ida_alpha as appropriate. All further routines then use the programs resident in i_p. The setup file will also contain other definitions such as the Genie initialisation file for IRIS.

The Fortran & other sources are in the area iris$disk:[irsmgr.sources]

These two program areas are only fully accessible with iris_manager rights and are thus restricted to Instrument Scientists.

Routines are usually developed elsewhere and working versions are copied into these areas. The user only has read & execute rights.

The logical name iris_data refers to the following areas :
iris$disk:[irsmgr.data] , iris$disk0:[irsmgr.data] & scratch$disk:[irsmgr.data]
and is setup by the system so that when using Genie the commands

set disk iris_data <Return>
set dir <Return>

will always give access to the RAW files. The logical name inst_abrv_name is the abbreviated name of the instrument and is also setup by the system; for IRIS it is IRS. This is used by many of the routines using Batch processing.

At ISIS the user should have in his/her login.com file a call to execute the ida_logs setup procedure. For non-RAL use, the user should have a login.com or other command file to define the logical names ida_vms or ida_alpha, iris_data & inst_abrv_name and it should also call ida_logs.com.

Some of the programs also require files situated in the area iris$disk:[irismgr.tables] which has the logical name norm_par & par_iris. The logical name norm_par is used by other program packages (eg ATLAS) and the logical name genieinit initialises Genie. These assignments need to change according to the instrument so the user must have a method for making these changes. A scheme has been worked out to do this and suitable command files are available in iris$disk:[irsmgr.setup].

In normal use the user will always access RAW files from iris_data. All the routines in this package create files either in the user's current directory or on scratch-disk for temporary files. The user's scratch area has the logical name sys$scratch corresponding to scratch$disk:[<username>].

2.2 Restoring of archived data sets

The command *RESTIRIS* will setup a batch job to restore a selection of files with extensions RAW, SAV or LOG. The files will be created in scratch$disk:[irsmgr.data] and is therefore accessible using iris_data. RESTIRIS is a synonym for *@i_p:restiris* and is defined in the ida_logs command file.
The spawned routine chooses the catalague name according to the run_number. This will be changed by an Instrument Scientist after each cycle.

2.3 Batch jobs

When running under batch, the command files will prompt for the name of the batch queue to be used. The default value is usually the generic name sys$batch. When this is selected, the operating system will submit the job to any of the VMS computers on the Local Area Network (DECNET). Alternatively, a specific computer may be selected. The generic name of the Alpha batch queue is alpha$batch.

2.4 Genie

The package makes extensive use of the Genie program and the Genie file structure type. Many of the Genie routines can be run either interactively or in batch. The latter is recommended for time consuming and routine operations.

The raw data is in the standard format for files with extension RAW or SAV. Subsequently created files are all in Intermediate file format and interact with Genie via the REad and WRite commands.

All these files are in binary form. Routines are available to convert into ASCII format if required.

2.5 Export

The suite of programs may be exported to any user provided the correct operating system and version is installed on the computer together with a version of Genie. The package is in the area iris$disk:[irsmgr.export] as Backup files. There are 3 files ida_exe.bck for the .EXE files, ida_com.bck for the command .COM files and ida_tab.bck for the files resident in norm_par such as the .RES, .CALIB, .FP and .DAT files. The files may be obtained either using anonymous ftp or the World Wide Web.

2.6 Other instruments

The package can also be used on data from other instruments, including those from other neutron sources. For non-ISIS instruments data, in ASCII form may be converted into Genie Intermediate files which can then be easily used by the rest of the program suite. This has been successfully done with data from LLB (Mibemol), ILL (IN5) and IPNS (QENS). Further details may be obtained from an Instrument Scientist.

3 OUTLINE OF PROGRAMS

The suite of programs consists of :

1	Calibrate	I,B	- calibrate detector efficiency
2	ICON	I,B	- convert data into I(Q,ω)
3	DEMON	I,B	- diffraction data
4	ACORN	G,B	- correct for background, can & absorption
5	IMPS	B	- correct for multiple scattering
6	SWIFT	G	- convolution fitting
7	FURY	G	- Fourier transforms
8	Utilities	G	- various routines for use in Genie
9	RESNORM	I,B	- resolution normalisation
10	IRIS_LINES	I	- Bayesian analysis of tunnelling lines
11	QUASI_LINES	I,B	- Bayesian analysis of quasi-elastic peaks
12	Plot Routines	I	- various forms of hard-copy graphics

The G denotes that the routine is a Genie command and can be run interactively.
The B denotes that a batch job can or must be run.
The I denotes a stand-alone program run interactively.
For batch running, user-friendly Command files with menus will be used.

Programs create files using the Genie *WRite* command with successive blocks containing groups of spectra. In this suite of programs the filenames follow the general form IRS<runnumber>.ext, eg IRS01234.IPG, where each routine creates a different extension.
All programs are capable of reading these files - the extension always has to be defined.
In this way the path of analysis for any sample/run can easily be followed.

The data analysis can be divided into two sections: data reduction and data interpretation.
In the former the raw data (in counts per channel) is converted into the scattering law $S(Q,\omega)$.
This removes all the parameters specific to the instrument and can also apply corrections for absorption and multiple scattering.
The interpretation seeks to understand the science by way of mathematical models, often determined by theory.

The various steps required are as follows :

3.1 Calibration

This procedure determines the instrument parameters required, such as flight paths, scattering angles and detector efficiencies. The flight paths and scattering angles on IRIS are fixed and have been determined by the Instrument Scientists. Detector efficiencies are measured with a standard vanadium by Instrument Scientists at the beginning of each cycle or by the user as part of the experiment. This vanadium run also serves to determine the energy resolution and provide an absolute cross-section calibration.

3.2 Conversion to I(Q,ω)

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

3.3 Corrections

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

3.4 Interpretation

The form this takes will depend on the dynamics of the samples being investigated. The more traditional technique has been the fitting of peaks to the spectra. This can involve either a set a quasielastic peaks or a set of inelastic peaks (or a combination of both), sometimes also with an elastic component. In the fitting procedure a set of functions representing the sample scattering are folded with the resolution function and least-squares fitted to the measured sample spectra.

An alternative technique is to convert the S(Q,ω) to the intermediate function I(Q,t) using a Fourier transformation. The resolution is also taken into account. This method is useful when the form of the scattering function is unknown or not of a standard form or when a theory gives I(Q,t)

A more recent technique has been to use Bayesian statistical methods instead of curve fitting.

As another aid to interpretation various forms of graphics may also be employed , for example the conversion of the I(2θ,ω) into a true I(Q,ω).

3.5 Diffraction

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

Data interpretation is then carried out using standard diffraction routine.

4 CALIBRATION

CALIBRATE is a special setup for running the Fingerprint program, FING. FING is a Genie look-alike program similar to ICON (see 5.2 below). FING sums the counts between specified time-of-flight limits for each spectrum and writes the result to a Genie Intermediate file as integrated count per spectrum.

One or two ranges can be specified and would normally correspond to a region around zero energy transfer about the width of the resolution (elastic component) and a region out in the wings - high enegy transfer (background).
For the 1 region option, examples are : the elastic component alone ; or the full time range, corresponding to an integral over all energies within the observable window.
For the 2 region option, there are a further 2 options :
a) the integrated elastic component is the elastic region sum minus the background region sum. This is the option used for the vanadium calibration
b) the background region divided by the elastic region. This is useful for checking on the stability of the detectors.

On the IRIS FEM there is a file called detector.dat in the irsmgr.tables area which contains a table of angles and detector efficiency for each detector/spectrum. This is kept up-to-date by the Instrument Scientist. The Instrument Control Program which runs the data acquisition reads this file and writes the values to the header block of the .RAW file. If this file is correct when an experiment is started then the calibration routine is not required.

The purpose of CALIBRATION is to provide a correct version in the user's area. There is a copy of this file in the norm_par area called detector.calib and an option in FING edits this file and creates a corrected version in the user's area. The default file for pre-1994 experiments is detector_old_94.calib.

The files defining the time regions and group structure are also in norm_par with the name fp**.cal where ** can be g2 and g4 for Graphite 002 or 004 respectively and m4 for Mica 004. For pre-1994 the names are fp**_old.cal.

The format of the files is :

line 1 : code for operation
line 2 : start and end values of up to 2 time regions
line 3: number of spectrum groups
line 4 onwards : first and last spectrum in group (1 line for each group as defined on line 3)

For example	Graphite spectra are	3 to 53
	Mica spectra are	54 to 104
	Diffraction spectra are	105 to 114

The following commands are available :

GRoup
This specifies the name of the fp*.cal file to be used

RUn
This command defines the run number to be used. The program uses routines which calculate dead time corrections, this option can be switched off with the qualifier /NODEAD. This is the preferred option.

BEgin
This starts the calculation. The file containing the results is automatically created with the extension .DET.

OUT <filename>
Initiates editing of the detector file with name <filename>. The output file is called detector.calib in the current area.

The commands RUn, BEg (and Out) may be repeated.

The following Genie commands are also available :

SET disk , dir and inst
EXIT HELP JUMP SHOW
TOGGLE has been modified to remove options associated with plotting.

Interactive use :- use the command *CALIB*

It will use the Genie initialising command file so that, for example, the default area for data is iris_data.

A typical set of commands would be :

```
GR fpg2.cal
RU/NODE 1234
BE
OUT norm_par:detector.calib
```

Batch use :- Option 1 on the IDA Menu (see section 13.1)

5 ICON - calculate I(Q,ω)

There are two versions of an ICON type program: the first is a new version of the original routine ICON used in Genie and the second is a stand-alone Genie type program. These programs are used for the full data analysis. A simplified version of the Genie ICON, replacing the original ICON, should be used for examining data on the FEM during the experiment.

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

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

5.1 Genie version

The input required is :

1 data type : DAE or RAW file
2 if RAW file, run number
3 the analyser & its order of reflection
the routines then display the range of spectra available and asks for
4 first & last spectra to be analysed
the spectra can be grouped or kept individual, so the routine asks for
5 type of grouping, choice is :

- all spectra in range added together into one group
- grouped spectrum
- all spectra in range as single spectrum in group

6 if the second option, there are two methods of grouping

- constant number of spectra per group - input number of spectra per group
- variable number of spectra per group - input first & last spectrum per group

The data will be in Genie WorkSpaces beginning at W5 - in ascending order of spectrum number. The data is not automatically written a to file when run interactively - this can be done using the Genie *WRite* command if required. When run under batch, files are produced containing the groups/spectra in ascending order of spectrum number. The files also contain information on angles, analysers & analysing energy.

For Graphite the extension is IPG whilst for Mica it is IMI.

Interactive use :- within Genie use the command
@l_p:icon & follow instructions.

5.2 Stand-alone version

The new ICON program is a Genie look-alike program without the ability to plot. The command structure looks the same, but many of the *FUnction* routines used in the Genie command file ICON have been incorporated into subroutines within the ICON program. The program should thus run faster because of the reduction in FUnction calls.

Many of the instrument parameters are taken from the header block of the RAW file - their values are read from the detector.dat file on the IRIS FEM area [irsmgr.tables] when the run is started. This includes the detector angles. The system has been in operation since January 1993, runs prior to this date will have incorrect values. In 1994, the mapping between detector number and spectrum number was changed to be more logical.

The output files are in Genie Intermediate File format with extension IPG for graphite and IMI for mica, the diffraction data has the extension DIF.

The structure of the file for spectrum grouping is as follows:

- line 1: number of groups
- then a line for each group definition containing :
  - number of parameters on line, then first and last spectrum for each sub-group eg
    - 2 6 12 would be groups 6 to 12
    - 4 6 8 10 12 would be groups 6 to 8 and 10 to 12
    - for single spectra the first parameter must be negative followed by the numbers of all the individual spectra

The following commands are available :

SET Analyser <code> <efix>

The <code> defines the analyser as before ie 1 is PG(002) 2 is PG(004) 3 is Mica(006) etc, but now there is the extra code d for diffraction.

set & analyser can be abbreviated to s & a respectively.

Examples: *set a 1 or s a d.*

Diffraction spectra will be either 108 to 117 (as used in quasielastic mode) or 5 to 16 (when setup especially for diffraction only).

<efix> is the analyser energy and when this parameter is included the default value in the program can be changed. This is useful when the temperature of the analyser changes during an experiment, thus changing the energy.

CALibrate

This command instructs the program to read the detector information from the file detector.calib in the user's current area as produced by the Calibration program and previous values are overwritten. This option, which can be abbreviated to CAL, should be used for old data and when the header block in the RAW file is likely to be incorrect.

EFFiciency

This command controls the options for calculating the efficiency of the monitor and detectors and can be abbreviated to EFF. On its own, the command switches on the correction for both monitor and detectors. There are three qualifiers : /N switches off both corrections, /M switches the monitor only on, /S switches the detectors only on. The parameters for calculating the efficiency are in the header block for new data or in the file detector.calib for old data.

For the detectors, the efficiency takes into account the analyser 'efficiency' and no wavelength dependence - so spectra/groups will be normalised to each other.

GRoups

This defines the way in which the spectra are added into groups. The command can be abbreviated to GR and can take several forms :

GR <file> reads a file which defines the group structure, if the file name is omitted then a name is prompted.

GR/T enables interactive typing in of the groups, the program prompts for : number of groups, then for each group the number of spectra and their values

(not yet the same format as the file structure above).

RUN

This command defines the run numbers to be used - it can take up to 8 run numbers on a line and these will be added together, unlike the old ICON Genie command where each run produces a separate file.

In its simplest form the command would be *RUN 1234.*

If more than 8 runs are needed then other RUN commands can be used but with the qualifier /CONTinue. Dead time corrections are automatically calculated, this can be switched off with the qualifier /NODEAD - recommended as standard at present.

If the run number is set to zero than the program will read the data from the CRPT - this will only work when running the program on the IRIS FEM computer and after an UPDATE command has been executed. The file created will have the runname IRS0000.

BEgin

This is the final command to start the calculations. When finished, a new run can be defined with RUN and the BEgin command repeated.

The following Genie commands are also available :

EXIT HELP JUMP

SET with Disk & Directory SHOW

TOGGLE has been modified to remove options associated with plotting

Interactive use :- use the command *IKON* which is equivalent to the command *run l_p:ICON_4_1_2_sys* . The numbers in the program name refer to the version number and will change as new versions are produced while *sys* refers to the opeating

system VMS or AXP. IKON is defined in the ida_log setup command so should be the correct version. It will use the Genie initialising command file so that, for example, the default area for data is iris_data.

A typical set of commands would be :

```
SET a 1
CAL
GR PG1OP20.grp
RUN/NODE 1234
BEG
```

Batch use :- Option 2 on the IDA menu (see section 13.2)

6 ACORN - Absorption CORrectioNs

6.1 Theory

The main correction to be applied to neutron scattering data is that for absorption both in the sample and its container, when present. For flat plate geometry the corrections are analytical and have been discussed for example by Carlile [1]. The situation for cylindrical geometry is more complex and requires numerical integration. These techniques are well known, and used, in liquid and amorphous diffraction and are described in the ATLAS manual [2]. Two sorts of programs are provided : a quick version with some simplifying assumptions, and a more accurate set which can take into account the wavelength variation of both the absorption and the scattering cross-sections.

6.2 Simple and quick programs

The absorption corrections can be carried out for plate geometry using the Genie function ABS_PLATE or cylindrical geometry using ABS_CYL.
The input run data for PLATE geometry will contain the scattering angle and the routine will ask for the following :

Analyser type - Graphite or Mica
for Graphite the input file will have extension IPG
for Mica it is IMI
For the sample, the run number then -
angle between beam & sample
density in g/cc
thickness in cm
molecular weight
total (ie incoherent + coherent) scattering cross section in barns
absorption cross section at 1.8Å in barns
If background subtraction is required
the background run number
If container subtraction is required, the container run number, then -
density
thickness (both walls)
total cross section
absorption cross section

The routine then loops through each group of spectra in the input data file.
The output files will be called IAG if input is IPG or IAM if input is IMI.

Interactive use :- within Genie use the command
@i_p:abs_plate & follow instructions.

Batch use :- Option 3 on the IDA menu (see Section 13.4)

For CYLINDRICAL geometry the input data is the same as Plate except for sample thickness which becomes sample radius.

Interactive use :- within Genie use the command
@l_p:abs_cyl & follow instructions.

Batch use :- Option 3 on the IDA menu (see Section 13.4)

6.3 New programs

These have been developed from the corrections programs in the ATLAS suite. The input data is similar to that of section 6.2 with the addition of files containing the wavelength dependent cross-sections for the sample (and container). These files usually have the extension .MUT. There are now two programs :

- ACORN provides the input for the corrections programs, which are run in Batch mode and create files containing the corrections. It can also create a .MUT file from input cross-sections.
- ANALYSE is a Genie command file which reads these corrections files and applies them to the IPG type data files

ACORN is a stand-alone program similar to ICON. On starting, the directory and disk must be defined with the SET command. The extension of the input data files must also be defined with the SET EXT command - the extension is typically IPG.

A MUT file is necessary for the sample and container, when present.
The first command is
RUN <runnumber> the program then replies with information of the form :
nrm> USER$DISK:IRS10154.IAG has 12 spectra of 1939 points
assign> analyser energy 1.85900
assign> output wavelengths from 5.500 to 8.000

the MUT file is then created with the command
MUT the program then asks
mut> scattering cross-section ? this is in barns
mut> absorption cross-section (1.8 A) ? also in barns
the program replies with
mut> creating cross-section file IRS10154.MUT
mut> elastic wavelength 6.6329
These 2 commands can be repeated for as many runnumbers as neccessary.

The next command is BEgin and the program asks
> C(ylinder) or F(lat) Geometry ? [C]
> V(anadium) or S(ample) ?
> Container and/or Furnace (Y or N) ? [N]

the program asks for the dimensions of the sample :

for plate geometry
sam> FLAT geometry
sam> thickness of sample (cm) ?

for cylindrical geometry
sam> CYLINDRICAL geometry
sam> height (cm) ? [6.00]
sam> radius 1 (cm) ? [0.00] for a solid sample the default value is 0 otherwise the value is the inner radius
sam> radius 2 (cm) ? this is the outer radius

next comes details of the sample :
sam> number density (atom/A3) ?
the program then reads the appropriate MUT file
sam> reading cross section data file IRS10154.MUT
sam> number wavelengths in c/s file = 6
the absorption cross section in the MUT file is then the default value of the next question
sam> absorption cross section (@1.8A) [1.0000]?

if a container has been specified then the following questions are asked :
for plate geometry
can> FLAT geometry
can> how many layers ? [1] this gives option for multiple cans
can> thickness - front (cm) ?
can> thickness - back [<default>] ? the default will be the front value input

for cylindrical geometry
can> CYLINDRICAL geometry
can> how many annuli ? [1]
can> radius 3 (cm) ? this is the outer radius of the container, it is assumed that the inner radius of the container is the outer radius of the sample

this is followed by data about the container material :
can> number density (mol/A3) ?
can> file name for cross section data ?
sam> absorption cross section (@1.8A) [1.0000]?

finally come details of the instrument :
for the plate option
beam> angle beam to sample [0.0] ? this is the angle between the normal to the plate face and the beam , so the default (0.0) is plate perpendicular to beam

beam> incident beam width (cm) ?
beam> incident beam height (cm) ? [4.00]
beam> spectrum 1 at angle : 30. this is repeated for each spectrum
out> step size (cm) ? [0.02]
out> filename : IRS10154.AIN

the job is submitted to a batch queue with
submit> batch queue ? [SYS$BATCH]
submit> job with name ABS10154.COM

The data is then corrected using Genie.

ANALYSE is a Genie command file which is run with the command
@l_p:analyse
the routine has the following dialogue :
Options are 1 = Sample only
2 = Sample & can
Type option
Input data : IPG (1) or IMI (2)
Sample run number
If there is a can then
Can run number

The batch version :

after typing in the run number the routine checks if the absorption data file <runnumer>.ABS exists, if it does not then an error message is displayed :
Absorption file <filename> does not exist
You MUST run the ACORN program first

Input data : IPG (1) or IMI (2) [default 1] ?

7 IMPS - MultiPle Scattering

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

Two versions are available :
MINUS, which reads an ICON file to obtain the scattering angles
MINIM, which requires interactive input of the scattering angles.

The following parameters are required :
- the instrument (eg IRS) has already been defined
- run number (any number for MINIM)
- extension of ICON file (for MINUS only)
- title : to describe the run
- number of neutrons for calculation (default=1000)
  larger values give better statistics
- 2 integers to start the random number generator
- number of multiple scattering events , up to 5 for each neutron
- sample geometry : infinite plate, finite plate or cylinder
- sample thickness, width & height (in cm) for plate
  or sample radius & height (in cm) for cylinder
- angle of plate sample to beam (perpendicular is zero)
- incident or analysing wavelength ; this is input for MINIM, but MINUS reads it from the ICON file.
- sample temperature (K)
- sample number density (atoms/Å^3)
- absorption cross section (barns)
- bound scattering cross section (barns)

The Q-ω grid for the S(Q,ω) is defined by :
- number of Q points & increment (Å^{-1})
- number of ω points & increment (µeV)
- option for scattering cross section in file or constant
- if constant, scattering cross section (barns)
- option for output into files : runnumber.ANS is a data file for reading into Genie & runnumber.LPT is printer output of the calculation.
  0=no, 1=correction is R_1, 2=correction is R_1^*
  positive values give reduced LPT output,
  negative values give full LPT output
- option for S(Q,ω)
  0= input file
  n=calculate n peaks from diffusion constants
  -n=calculate n peaks with width as a 5 order polynomial in Q (ie up to Q^4)

- if positive n diffusion coefficients (cm^2s^{-1})

or if negative n 5 polynomial parameters

For MINUS, the program reads the angles from the specified ICON file; for MINIM, the scattering angles must be input :

- number of angles
- their 2θ values

A command file runnumber.minb_com (MINUS) or .mimb_com (MINIM) is created and is submitted to the specified batch queue. The log files have extensions minb_log & mimb_log. It may be more appropriate to run MINIM to establish the correct parameters and get a feel for the problem before running a full MINUS job.

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

J_1^*	single scattering assuming no absorption & no other scattering
J_1	first scattering
J_2-J_5	2nd to 5th scattering, range as specified
Total	Total scattering J_t =sum all J_n
Mult	Multiple scattering J_{ms} =sum J_n from 2 to 5
R_1	ratio J_1/J_t
R_1^*	ratio J_1^*/J_t

R_1 is the normal output, this is the multiple scattering only; R_1^* can be used to correct for multiple scattering, attenuation due to re-scattering and absorption all at once.
The value of R_1 (or R_1^*) is averaged over the positive & negative energy values and is printed. This is also the form of the data in the ANS file.

Both versions of the program run in batch use :- see Section13.5.

There are two Genie *FUNction* programs to read in the results from the ANS file :

MS_read asks for the name of the ANS file (assumes the ANS extension) and reads the results for the first angle. It displays this angle and the scattering angle in the WorkSpace and asks if the data is to be kept or whether to continue to the next angle in the file. The User can then move through the ANS file to the required angle.
The ANS file contains the corrections at the positive energy transfers specified during the running of Minus so the routine interpolates the correction to the energy values in the WorkSpace.

MS_cor is a version of MS_read for automatic looping over all angles. The name of the ANS file is taken from the WorkSpace and the angle in the file is compared with the scattering angle in the WorkSpace. It goes through all angles in ANS until it finds the correct angle; if correct angle does not exist it exits with an error message.

The use of multiple scattering corrections is not straightforward and will depend on the method of data interpretation employed.

Two cases have been used so far :

1. corrections to the Elastic Incoherent Structure Factor (EISF). In this case only the fraction of the scattering that is multiple scattering is used - that is, the total scattering is reduced by the multiple scattering fraction.

2. fitting of peak shapes. In this case, the shape of the multiple scattering with energy transfer is important. The multiple scattering can change the shape of the sample $S(Q,\omega)$ and therefore must be applied before the resolution broadening is applied - see program SWIMS (section 8.4).

8 SWIFT - Convolution Peak Fitting

8.1 Theory

The measured data I(Q,ω) is proportional to the convolution of the scattering law S(Q,ω) with the resolution function R(Q,ω) of the spectrometer via

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

The traditional method of analysis has been to fit the measured I(Q,ω) with an appropriate set of functions related to the form of S(Q,ω) predicted by theory.

In quasielastic scattering the simplest form is when both the S(Q,ω) and the R(Q,ω) have the form of a Lorentzian $L(\omega) = a\omega^2/(\omega^2+\Gamma^2)$ - a situation which is almost correct for the IN10 spectrometer at ILL. The convoluton of two Lorentzians is itself a Lorentzian so that the spectrum of the measured and resolution data can both just be fitted with Lorentzians. The broadening of the sample spectrum is then just the difference of the two widths.

The next easiest case is when both S(Q,ω) and R(Q,ω) have a simple functional form and the convolution is also a function containing the parameters of the S(Q,ω) and R(Q,ω) functions. The convoluted function may then be fitted to the data to provide the parameters. An example would be the case where the S(Q,ω) is a Lorentzian and the R(Q,ω) is a Gaussian. For diffraction, the shape of the peak in time is a convolution of a Guassian with a decaying exponential and this function can be used to fit the Bragg peaks.

The final case is where R(Q,ω) does not have a simple function form so that the measured data has to be convoluted numerically with the S(Q,ω) function to provide an estimate of the sample scattering. The result is least-squares fitted to the measured data to provide values for the parameters in the S(Q,ω) function.

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

A flat background is subtracted from the resolution data before the convolution is performed.

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

- Quasielastic - this is the most common case and applies to both translational (diffusion) and rotational modes, both of which have the form of a Lorentzian. The fitted function is a set of Loretzians 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 [4.5]. 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,ω) and the I(Q,ω) have been fitted with functions of the form of a modified Lorentzian. These latter functions are used in the energy fitting procedures.**

8.2 Program

The routine is started with the Genie command *swift* (if this has been defined as *l_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 eg at IPG or IAG stage
4 *group number* - ie 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 which will ask the following questions, default values are enclosed in []:

1 *shapes are : Elastic , Quasi, Shift or Polly [Q]*
type E, Q, S or P
2 *how may peaks ?[1]*
3 *input starting values of parameters*
background (P1) & origin (P2)
4.1 for Q(uasi) : *quasi-el peak <n> : height P(3) & h-width P(4)*
and repeated for each peak
4.2 for E(lastic) : *elastic peak height (P3)*
quasi-el peak <n> ; height P(4) & h-width P(5)
and repeated for each quasi-elastic peak
4.3 for 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 (ie the area). Then for each

quasielastic 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.

8.3 Hints on use

When running the program :

- 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.
- the energy increment should not be less than the energy bin in the input data otherwise the result may be unreliable due to the method of rebinning the data. Using 100 points (provided the previous comment applies) provides good results.
- the background and origin parameters can start at zero.
- the elastic peak height is the fraction of the measured resolution peak.
- the quasielastic peak height is the real peak height , which can be read directly off a plot. This can be the starting parameter if the broadening is greater than the resolution width. If the broadening (function width) of the peak is less than the resolution the start parameter should be the measured sample height multiplied by the ratio of resolution width to estimated broadening. For example, if the broadening is a quarter of the resolution then multiply the height by 4. This is to take into account the reduction in height on convoluting when the area remains constant.
- the parameter width is the half-width half maximum of the scattering function. The printed output will show this and also give the full-width half maximum.
- when fitting more than 1 peak it is best to start off fitting 1 peak in order to

obtain estimates for peak heights and background and origin. When increasing the number of peaks it may be useful to constrain some of the parameters in order to obtain a fit and these parameters can then be used as starting parameters for a full parameter fit.

- when fixing parameters, the routine 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).

8.4 Mutiple scattering version

Version SWIMS uses the MS corrections previously calculated by the Program MINUS and stored in the ANS file. The program uses the filename specified for the sample for the ANS file and checks the angle as in the Genie function MS_cor. The calculated sample function is corrected for MS and then fitted to the experimental data.

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

1. use SWIFT to obtain first estimates for widths, which are then used to generate $S(Q,\omega)$ in MINUS
2. use SWIMS to obtain a new set of widths and use them to calculate $S(Q,\omega)$ again in another run of MINUS
3. repeat 2 until widths do not change within the errors on the widths

8.5 Sloping background

Version SLOPE is similar to SWIFT except that instead of a flat background it is a sloping one. So instead of the one background parameter there are two - the gradient and the intercept.

8.6 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.

9 FURY - FFT Deconvolution

9.1 Theory

The measured spectrum I(Q,ω) is proportional to the four dimensional convolution of the scattering law S(Q,ω) with the resolution function R(Q,ω) of the spectrometer via

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

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

$$L(\omega) = a\,\omega^2/(\omega^2 + \Gamma^2)$$

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 $L(\omega - \omega_0)$ has the form (cos ω_0t + i sin ω_0t) 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 $\sigma_k^2=\langle\Delta X_k\rangle^2$ 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 $\sigma^2(X_j^I)=1/2\,X_0^R - 1/2\,X_{2j}^R$
Note that $\sigma^2(X_0^R)=X_0^R$ and from the properties of FT $X_0^R=\sum X_k$. 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 therefore be treated with caution.

For a true deconvolution by back transforming, the data would be truncated to remove this poor region before back transforming. If the truncation is severe the back transform may contain added ripples, so an automatic back transform is not provided.

9.2 Hints on use

When running the program :

- 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.
- the energy increment should not be less than the energy bin in the input data otherwise the result may be unreliable due to the method of rebinning the data. Using 100 points (provided the first point applies) provides good results.

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

1. quasielastic peaks - a single Lorentzian would produce a straight line in the plot of 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.

2. inelastic peaks - a pair of broadened peaks transforms into a damped cosine function. The central elastic peak would add a constant. This is the case where the I(Q,t) could become negative and taking the modulus makes the shape less easy to recognise.

3. non-Lorentzian shape - this could be either a stretched exponential form $\exp\text{-}\alpha t^{\beta}$, where β can range from 0 to 1, or not of standard function form. The former case has been discussed by Arrighi et al [10].

4. EISF - the transform provides an immediate estimate of the EISF without any arbitrary fitting procedure. From the properties of FT, the elastic peak (δ-function) transforms to a constant and the first time 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, bear in mind that due to taking the modulus the long time limit will be scattered around a positive non-zero value rather than zero itself, when the elastic component is zero.

9.3 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 logy*.

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.

9.4 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.

9.5 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 11, instead of the measured data. The routine is called i_p:q_fury and instead of asking for the resolution runnumber asks for the analyser code.

10 Utilities

10.1 Reading files

The Genie command file i_p:irsgrps will read all the groups in an intermediate file into Workspaces starting from W1. It asks for the run number and the file extension. The files must be in the current area (disk and directory).

A second version i_p:irsgroups is a version of irgrps which also asks for the area where the files can be found (disk and directory). This is uesful when the files are not in the current directory.

A third version i_p:irscrpt reads a file which has been created from the CRPT data and therefore assumes that the file name is IRS00000.ext.

10.2 Converting from Binary to ASCII

There are two versions :

For a single workspace use the Genie *FUnction* command W2A eg *FUn Wn i_p:w2a Wn.* The filename for output will be prompted.

For large IPG style files use the stand alone program i_p:IGB2A

10.3 Subtraction

The Genie command file i_p:subtract will subtract a background or container file from the sample file. No corrections are performed. The results are in the workspaces W21 onwards.

10.4 Absorption corrections

The absorption corrections of section 6 may be carried out interactively using the Genie functions i_p:abs_plate for flat plate geometry or i_p:abs_cyl for cylindrical geometry. The input is the same as that described in section 6.

10.5 Merging diffraction data

A set of diffraction data with different d-spacing ranges may be merged into one pattern using the Genie command file i_p:splice . It is assumed that there are several files containing sections in d-spacing which have overlaps. There are small regions at each end of the spectra which are unreliable and these should be omitted in the merging. By displaying in Genie each spectrum, a range in d-spacing is chosen for each spectrum such that the overlapping regions in d-spacing agree in intensity.

The routine requires the following information :

Type output file name (with ext) this is the final result
Delta_d constant (0) or Delta_d/d constant (1)
Delta_d (or /d) for the final merged file
Type minimum d value for merged file

Type maximum d value for merged file defines the ouput values for d-spacing
How many files do you want to merge together
For each file you will be asked the lower
and upper bounds on d to be combined
then for each file
File name (+ext)- assumes files are in current area
Type LOWER d value for this group
Type UPPER d value for this group

10.6 Fitting data

In Genie the *PEAK* command can be used for fitting a function shape to the spectrum. The following shapes are available : Gaussian, Lorentzian & a Gaussian convoluted with an exponential (sometimes referred to as the Kropf function)

There is also a Genie FUNction program i_p:fit_lor to fit a Lorentzian.

10.7 Reading ASCII data

This can be done using 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 points followed by
the x, y and e values as one set per line

10.8 Smoothing

These are Genie Function programs to carry out smoothing using the Fast Fourier Technique with a Weiner filter to determine the cut-off statistically.

i_p:smoo_0_vms performs a smoothing

i_p:smoo_1_vms performs a smoothing and gives the first derivative

10.9 Symmetric S(Q,ω)

In some cases the symmetric S(Q,ω) is the more appropriate function to use.
This is defined as

$$\tilde{S}(Q,\omega) = exp(-\hbar\omega\beta/2)S(Q,\omega)$$

where $\beta=1/k_BT$. The Genie FUNction program to perform this is i_p:symm and it will ask for the temperature (in K). The changes will be most marked when the temperature is low and ω is large.

10.10 Transmission cross-sections

These routines calculate the total cross-section as a function of wavelength using the data from the transmission monitor. The flat plate version is i_p:tfr and the cylindrical version is i_p:tcr.
They begin with
Sample run number ?
Background run number ?
this is the background if the sample has no container *or* the container if there is one
the data is then rebinned in wavelength according to
Default REBIN 3.0 (0.5) 7.0
Options 0 = Keep 1 = Change
if the change option is selected then asks
Minimum lambda ?
Lambda increment ?
Maximum lambda ?

the cross-section is then calculated with the following parameters
for flat plate geometry
transflat> sample thickness (cm) ?
*transflat> sample no. density (per A**3) ?*
for cylindrical geometry
transcyl> beam width (cm)?
transcyl> beam width (cm)?
transcyl> 1st radius (cm) ? [0.0] the default refers to a solid sample
transcyl> 2nd radius (cm) ? outer radius of sample
transcyl> 3rd radius (cm) ? [0.0] the default refers to no container
otherwise it is the outer radius of the container, the outer radius of the sample is taken to be the inner radius of the container
*transcyl> sample no. density (per A**3) ?*
if there is a container this question is repeated for the container

then there are further options :
Options 0 = Exit 1 = Output
2 = Rebin & Calc 3 = Calc only
Type option

Option 0 exits immediately; Option1 provides an ASCII file ouput and a file name is requested; Option 2 repeats the rebinning and cross-section calculation; Option 3 repeats the cross-section calculation. The output file will have a nmae of the form IRS01234.MUT. The result may then be displayed if required.

10.11 CROSS-section

This is a stand-alone program to calculate the various cross-sections for a sample using the cross-sections for the elements and isotopes compiled by Sears.

The program is started with the command *CROSS*
and has the following dialogue :
Give 1 for natural elements or 2 for isotopes >
Default cross-section data file is g_f:sears91.dat
Type CR to accept, or give alternative file spec. >
If default is selected
File g_f:sears91.dat read successfully
Number of entries in file = 97

A working example for D_2O would be :
How many elements in the sample?2
For each element in turn give chemical symbol and x where
x = number of atoms of element in one scattering unit
(x need not be an integer)

Element 1 > D 2
Element 2 > O 1
*Give density in gcm**-3, 0 if not known or*
a negative value if in atoms per cubic Angstrom > 1.

The cross-sections values from the file are
Units: b in fm, sigma in barns, A in amu (12C)
PRIMARY DATA...

Z	A	Symbol	b_bar	sig_scatt	sig_abs
1	2.016000	D	6.67100	7.64000	0.00052
8	15.999400	O	5.80300	4.23200	0.00019

The results are displayed on the screen before it asks
Give name only for output XSECT file > d2o
which produces an ASCII file of the results

The results are presented in two forms :

- values per scattering unit - in our example it is for the D_2O molecule
- values per atom - this is the average per atom

11 Bayesian analysis

11.1 Introduction

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

11.2 Plotting

The programs in this section use the plotting package PGPLOT. Interaction with this package is performed interactively via a set of questions which appear in all programs. The first two questions concern the character size and line-width for the graphs. The defaults are sensible for plotting on the screen, but they may need to be increased for publishable quality hard copy output. At various points there will be a prompt for a graphics device. Typing a question mark (?) will list the possible options , but useful ones are : /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 /PS for a postscript file called PGPLOT.PS which can later be sent to a postscript printer for a hard copy. In some programs the Null option is the default.

11.3 Data format

Most of the programs are able to read data in Genie Intermediate file format, eg IPG files), but a few require the data to be in ASCII format and the conversion from binary to ASCII can be performed using either the Genie function W2A or the program IBG2A (see section 12).

The programs also require a resolution function and this file, normally named with the extension RES, is in ASCII and consists of two columms : energy (in μeV) and amplitude. The function should be on a grid which is fine enough to allow linear interpolation between the points and must be in constant energy bins. It is probably advisable to use the smooth and interpolated output from a smoothing routine rather than the raw resolution data themselves. Versions of the programs which use the raw resolution data do however exist and can be used when a suitable smooth form is unavailable.

11.4 ResMem

This program creates a smooth, finely-interpolated, file for the resolution function from coarse and noisy data. Smoothness is imposed through an invariant Guassian interpolant whose width can be optimised. A linear background may be subtracted. The input file is an ASCII file, with four header-lines, as created by the Genie function W2A.
The x-binning (energy transfer) must be constant.

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

Interactive use :- use the command *run i_p:resmem*

11.5 ResNorm

This program creates a group 'normalisation' file by taking a resolution file as defined in section 11.3 and fitting it to all the groups in the resolution data file which has the same grouping as the sample data of interest. The routine varies the width of the resolution file to give a 'stretch-factor' and the area provides an intensity normalisation factor.
The output is written to an ASCII file with the name FOR007.DAT in the following format :

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

After running the program, it is recommended that the file FOR007.DAT be renamed, for example, to IRS<runnumber>.RES.

Interactive use :- use the command *run i_p:resnorm.*
Batch use :- see section 13

11.6 IRIS_Lines

This program estimates tunnelling lines for a single spectrum or group and requires the resolution file (.RES file) and optionally the normalisation file created by ResNorm. The input file must be in ASCII format. The summary file of the results is FOR051.DAT. Hard-copy graphics output can also be generated.

Interactive use :- use the command *run i_p:iris_lines.*

11.7 Quasi_Lines

This program estimates the quasielastic components of a single spectrum or group and requires the resolution file (.RES file) and optionally the normalisation file created by ResNorm. The input file must be in ASCII format. The summary file of the results is FOR052.DAT. Hard-copy graphics output can also be generated.

Interactive use :- use the command *Q0* which is equivalent to the comand *run i_p:quasi_0_sys* where *sys* refers to the operating system *VMS or AXP.*

11.8 Quasi_Lines_2D

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

The program estimates the quasielastic components of a series of groups of spectra and requires the resolution file (.RES file) and optionally the normalisation file created by ResNorm. The input file must be an intermediate Genie binary file. The summary file of the results is FOR053.DAT.

A summary of the fitted parameters for one and two Lorentzians per group is written to files FOR001.DAT & FOR002.DAT respectively. The structure of these files, for each spectrum, is :

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

Here A(max) and W(max) are the scale-factors by which the a and w parameters need to be multiplied to obtain the amplitudes A(j) and HWHMs W(j); var is the variance.

Hard-copy graphics output can also be generated.

Other variants of the program are :

Quasi_1 which asks for a single group in a file of many groups
Quasi_20 which assumes there is no elastic peak
Quasi_2FB which assumes that the background is a flat constant

then there is an equivalent set in which the resolution data is a measured data file

Quasi_1R
Quasi_20R
Quasi_2R

Interactive use :- use one of the commands

Q1 equivalent to *run i_p:quasi_1_sys*
Q1R equivalent to *run i_p:quasi_1R_sys*
Q2 equivalent to *run i_p:quasi_2_sys*
Q2R equivalent to *run i_p:quasi_2R_sys*
Q20 equivalent to *run i_p:quasi_20_sys*
Q20R equivalent to *run i_p:quasi_20R_sys*
Q2FB equivalent to *run i_p:quasi_2FB_sys*

Batch use :- quasi_lines_2d may be run in batch see Section 13.7.

11.9 Quasi_strexp

A further variation replaces the choice of several Lorentzians with a single function with the shape of a stretched exponential where I(Q,t) is proportional to $\exp(-\alpha t^{2/\beta})$ see section 8.1. The program then estimates the best value for β.

Interactive use ;- use the command

QSE equivalent to *run i_p:quasi_strexp_sys*

11.10 C2FWHM

This program reads the results file (either FOR001.DAT or FOR002.DAT) from a Quasi_lines program and produces an ASCII file of the format

Q FWHM(μeV) error on FWHM.

The results can then be used in subsequent programs such as the plotting routine SUPLOT (see section 12) or CEPOLY.

The program asks :

INPUT> filename ? the reply would be FOR00n.DAT or alternative name

it then prints out the file header information and the number of Lorentzians

OUTPUT>filename ? this is the name you wish to give the new file

11.11 CEPOLY

This performs a fitting of the Chudley-Elliott function on the output from Quasi_lines and then fits a series of polynomials to the deviation between experimental and fitted data. The CE function is of the simple, one jump, form

$$\Delta E = h/\pi\tau \ (1 - \sin(QL)/QL)$$

where ΔE is the FWHM of the Lorentzian, τ is the characteristic jump time, L is the jump distance and h is Planck's constant.

The program uses the usual PGPLOT commands and starts with

INPUT> filename ? this is the data of Q versus ΔE as produced by C2FWHM

DATIN> scaling const for error-bars? (def=1.0)

PLOT> ymax? this is for the input data

PLOT>ymax? this is for the data with a lower graph of deviations from CE fit

the program then fits the extra polynomials

PLOT> probability of polynomial order gives indication of goodness of fit

SHOW-FIT> which order (CE=-1)

then it prints the fit parameters

Coeff A is $h/\pi t$

Coeff K is L and finally

write fit to a file? filename this will be the fitted curve.

12 PLOTTING ROUTINES

12.1 PLOT2D

Displays data as a function of scattering angles and energy transfer. The input data is in the form of an intermediate Genie binary file and the 'normalisation' file is recommended.

Interactive use :- use the command *run i_p:plot2d*

12.2 PLOTQE

Displays data as a function of Q-vector and energy transfer. The input data is in the form of an intermediate Genie binary file and the 'normalisation' file is recommended.

Interactive use :- use the command *run i_p:plotqe*

12.3 QEOUT

as PLOTQE but outputs result as binary file

12.4 SUPERPLOT

there are two versions of this program which produces graphs using the PGPLOT package.
For black & white displays, use the command
SUPLOT which is equivalent to *run i_p:superplot*
For colour displays, use the command
SUPLOTC which is equivalent to *run i_p:superplotc*

13 BATCH PROCESSING

Many of the routines, especially those that take a long time to run, can be run in Batch mode. There is a top level menu facility which is intiated with the SYSTEM command *IDA* (defined in ida_logs.com). The first display gives the default instrument, as defined by the logical name instr_abrv_name - this should be IRS.

The menu then displays the following options :

1 Calibrate
2 ICON
3 DEMON
4 ACORN
5 IMPS
6 ResNorm
7 Quasi_Lines
0 Exit

For option 1 (old version), 2 & 3 the structure of the questions follows as closely as possible that in the corresponding Genie command file. A Genie batch job will be submitted.

WARNING : Genie must not be run more than once at the same time from the same directory (the Genie *FUnction* commands will interact with each other !!). Therefore do not run more than one batch job at the same time and do not run Genie interactively if a batch job is running. This problem can be overcome by working from several directories.

If the user is logged in there will be a message on the terminal stating that the job has completed. Two files are created : IRS<runnumber>.????_com in the user's current directory is the command file & .????_log in the user's scratch_area is the batch log file, where ???? denotes the program. If problems are encountered these files can be read to find out the cause.

The routines will ask for a Batch queue - the default will be SYS$BATCH - the operating system will send the job to one of a selection of computers on the DECNET cluster . To run on an Alpha batch queue, use the logical name ALPHA$BATCH.

Programs requiring RAW data usually use the logical name iris_data, these routines will print out the directories covered by iris_data and ask if the data is in one of these areas. Under normal circumstance the answer will be the default Yes. This applies to data before archiving and data restored from Archive with RESTIRIS.

13.1 Calib

The routine asks the following questions :

1 *Analysers are : 1=pg002 2=pg004 3=mi004 4=mi004 5=mi006*
or type 0 if you want to input a file name
Analyser code (default=1 pg002) ?
The codes specified are to be used for new format data, for old pre-1994 data the input file is required

1.1 if code= 0 the routine asks

FP file name (eg norm_par:fpg2_old.cal)?

2 *Run number*

3 *Default calibration file to edit is norm_par:detector.calib*
New file name (Return to keep default)
For pre-1994 data, a new file is required eg norm_par:detector_old_94.calib

13.2 ICON

The batch job uses the new ICON and is created by the command file l_p:icon_b. A command file with extension ICON_com is created and the log file with extension ICON_log is created in sys$scratch. If the calibration file detector.calib does not exist in the current area then the latest version is automatically copied to the area.

The old version can be used by running the command file l_p:ic_b. The questions follow those of Genie function ICON(IofQW), described in section 4. There is an extra question asking if the data is in the area defined by iris_data and question 1 is omitted. The batch files have extensions IQWb_com & _log.

The command file asks the following questions:

1 *Do you want to add runs into a single file [M]*
or several runs into individual files [S default]
The M option only takes up to 8 runs at present - if more are needed contact the Instrument Scientist.

2 *Change the relative efficiency detector table [N] ?*
reply Y if you wish to read the detector.calib file. It must be in the current directory. If the file does not exist the routine will exit after printing an error message.

3 *How many sample runs [1] ?*

4 *Run number ?* repeated for the value given in previous question

5 *Which analyser reflection*
1) PG002 2) PG004 3) MI004 4) MI006 5) MI006
Enter option 1 to 5

6 *Change the analyser energy [N] ?*
Only needed if the default value is incorrect (eg due to temperature changes)

6.1 If the answer is Y
Default analyser energy is ...
New analyser energy ?

7 *?? Choose from spectrum <first> to <last> (default values)*
First spectrum :
Last spectrum :
where ?? is PG or MI to signify which analyser has been chosen
and <first> & <last> are the default values chosen according to the run number and analyser

8 *Use groups file* : 0
Add all spectra together : 1
Add spectra into several groups : 2
Individual spectra : 3
Enter option 0/1/2/3:

8.1 If answer 0 asks: *Groups filename (assumes GRP extension)*

8.2 If answer 2 asks: *Constant (0) or Variable (1) number of spectra per group*

8.2.1 If 0 asks: *How many spectra per group*

8.2.2 If 1 asks: *How many groups :*

then for each group

Group <n> : Default first spectrum is <first>

First spectrum :

Last spectrum :

The default first spectrum for Group 1 is the First spectrum defined in question 7 and thereafter the previous Last spectrum plus one.

The routine creates a groups file with extension .GRP with a file name like PG2OP20 where to first 2 characters are the analyser (PG or MI), the next character is the analyser reflection (the answer to question 5), the OP (meaning OPtion) followed by the answer to question 8. Option 2 is either 20 or 21. This file can then be reused using Option 0 in question 8. thus ensuring that all runs have the same grouping. Alternatively having created one file , it can be used as a template to create a more specialised version.

13.3 DEMON

Questions 1 to 4 as in ICON then

5 *Which spectra range ?*

1) 108 117 2) 6 15 (runs < 8776)

3) 105 114 4) 3 12 (runs > 8776)

5) input values

Enter option 1 to 5

5.1 If option is 5 asks : *First spectrum Last spectrum*

The routine creates a Groups file with the name DIFF.GRP.

13.4 ACORN

The routine first asks :

S(ubtraction) or C(orrection) ?

The reply S will carry out the procedure described in Section 10.3

The reply C will prompt the question :

O(ld) or N(ew) version ?

For the Old version -

The routine first asks if the sample geometry is plate (answer P) or cylinder (C). The batch job is created by a command file i_p:ap_b (for plate) or i_p:ac_b (for cylinder). The questions are those of Genie function ABS_PLATE except that instead of asking if background or container subtraction is required it asks for the appropriate run number and a RETURN signifies NO. The batch files have extensions AFb_com & _log.

For the New version -

the first question is :
Options are 1 = Sample only
2 = Sample and container
Type option ;
Sample runnumber
Container runnumber (if required)
The routine then checks if the sample .ABS file exists. If it does not then the error message is printed :
Absorption file <filename> does not exist
You MUST run the ACORN program first

If the file exists, the routine continues with :
Input data : IPG (1) or IMI (2) [default 1] ?

13.6 IMPS

The routine first asks for the type of angle input : answer S (specify angles) or I (IofQW file). The batch job is created by the command files i_p:minus_b & minim_b.

13.7 ResNorm

The batch job is created by the command file i_p:res_b. The routine asks for the following information :

1 *Resolution run number*
2 *File extension (default IPG)*
3 *Default batch queue is .....*
Batch queue ?
4 *Minimum energy (ueV)*
5 *Maximum energy (ueV)*
6 *Resolution file (default =norm_par:pg002.res)*

The routine then prints out :
Job is run by file IRS<runnumbr>.resb_COM
Log of job is in file sys$scratch:IRS<runnumber.resb_LOG
Normalisation file will be IRS<runnumber>.RES

The batch job is created by a command file with the extension RESb_com and the log file has the extension RESb_log. The output file FOR007.DAT is automatically given the name IRS<runnumber>.RES.

13.8 Quasi_Lines

The batch job is created by the command file i_p:qe2_b. The routine asks for the following information :

1 *Sample run number*
2 *File extension (default IPG)*

3 *Resolution run number*

4 *File extension (default RES).*
This is the ouput file from ResNorm, if it does not exist the routine prints
**** The Normalisation file does not exist ****
**** RESNORM must be run - then try again* *** and exits.

5 *Default Batch queue is ....*
Batch queue?

6 *Minimum energy (ueV)*

7 *Maximum energy (ueV)*

8 *Resolution file (default =norm_par:pg002.res)*

9 The graphical output produced is then listed
Log prob - plot to Postscript file
Width - 3 plots to Postscript file
EISF - NO plots
Amplitude - NO plot

The routine then prints out :
Job is run by file IRS<runnumber>.qe2b_COM
Log of job is in file sys$scratch:IRS<runnumber>.qe2b_LOG

The batch job is created by a command file with the extension QE2b_com and the log file has the extension QE2b_log.
The output files from Fortran streams 1 & 2 (FOR001 & FOR002.DAT) are automatically given the names IRS<runnumber>.QL1 & QL2, while stream 53 is named IRS<runnumber> .QLPT.

Postscript files are created for the following plots : log prob, width of 1 peak, width of peak 1 of 2, width of peak 2 of 2. Files are NOT created for the EISF plots. The files have the name PGPLOT.PS;n where n is the version number - in this case it would be, say, 1 to 5. To plot these files use the command
*PRINT /QUE=POST$LSRm PGPLOT.PS;** where m denotes the required printer.
If these files need to be kept they should be renamed, as subsequent use of programs using PGPLOT routines will create more files of the same name.

14 References

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

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

3 M W Johnson, AERE Report R7682 (1974)

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

5 J S Higgins, G Allen, R E Ghosh, W S Howells & B Farnoux, Chem Phys Lett **49** 197 (1977)

6 D C Champeney, Fourier Transforms & their physical 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)

11 D S Sivia, Physica B **202** 332 (1994)

12 D S Sivia, C J Carlile, W S Howells & S Konig, Physica **B 182** 341 (1992)

13 D S Sivia, C J Carlile, J Chem Phys **96** 170 (1992)

Acknowledgements

It is a pleasure to thank all who have contributed, in their various ways, to the production of this package and manual. In particular, Devinder Sivia for writing all the Bayesian analysis programs, and Colin Carlile and Mark Adams, as Instrument Scientists for IRIS, for suggestions and comments. Thanks also to the Users for, unknowingly at times, testing the programs, and for suggesting additions, changes and improvements in the user-friendliness of the programs.