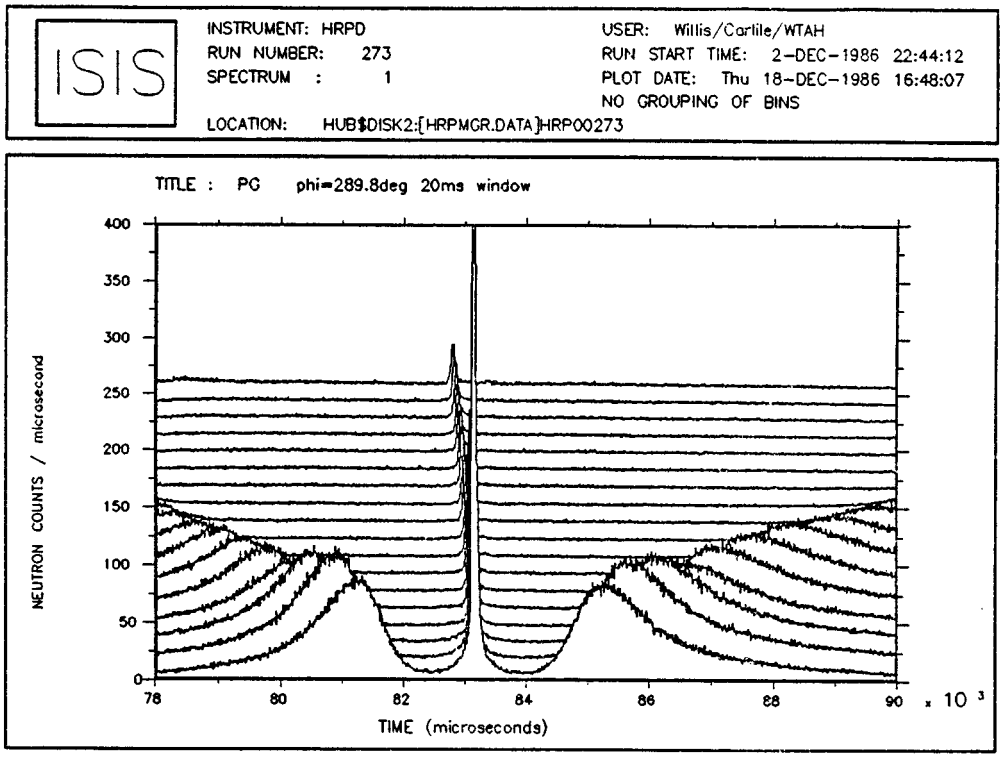
P U N C H

G E N I E M A N U A L

Version 2.3

"A LANGUAGE FOR SPECTRUM MANIPULATION AND DISPLAY"



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December 1986
RAL-86-102

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1 INTRODUCTION

1.1 OVERVIEW

GENIE is a data display and manipulation language that has been developed to satisfy the data-analysis requirements of both new user and expert for all the neutron-scattering instruments at the spallation neutron source, ISIS. This desire for commonality placed stringent demands on the design philosophy of GENIE with particular emphasis on flexibility and transparency of use.

In common with other experimental spectra, neutron scattering data-files take the form of series of spectra that may require modifications such as detector-efficiency corrections, background subtraction, normalisation or addition of spectra. The GENIE program allows the user to perform such manipulations and display or file the resulting spectra at any stage. GENIE contains the following major features:

- integrated GKS graphics
- interactive, command file or batch operation
- flow control
- FORTRAN-style algebraic manipulation of spectra
- correct propagation of data errors
- parameter substitution
- model fitting
- external user-definable functions

The GENIE program has been written for the VAX series of computers under the VMS operating system and assumes the user’s terminal to be a VT100 or VT200 series compatible terminal capable of emulating the Tektronix 4010 graphics.

1.2 USING GENIE

All of the GENIE KEYBOARD commands described below may be used ’directly’ at the terminal. In this case the program responds in the manner described and returns a >> prompt to the screen when completed.

In addition, GENIE KEYBOARD commands may be used from a **command file** containing a prepared list of commands. To initiate reading commands from a command file the @ instruction is used. Control is returned to the terminal when the end of the command file is reached.

When running from a command file the GENIE KEYBOARD commands may be augmented by the use of GENIE command language (GCL) commands.These commands are used for flow control, parameter I/O and parameter manipulation. KEYBOARD and GCL commands are indicated by the preceding symbol:

> , **!** or **$**

'**>**' precedes a GENIE KEYBOARD command, '**!**' precedes a comment and '**$**' precedes a GCL command. On the pages describing individual commands the prefix symbol is indicated.

All commands and command files may be aborted by pressing <CTRL Y>, that is by pressing Y while holding the CTRL key down.

1.3 GENIE DATA STRUCTURES

The program contains a number of general WORK-SPACES, a GRAPHICS WORK-SPACE and a number of BUFFERS. Each work-space contains data relating to a single spectrum. Essentially these are the x,y and error (e) values plus other parameters needed to interpret and manipulate the data.

At the beginning of the program the user defines the number (n) and length (l) of the work-spaces using the command

SET WORK n l

Users should note that this instruction alters the internal pointers to the workspace arrays and should only be used if the contents are no longer required.

The total length of the work-space arrays is at present 133000 words. **n** and **l** must be chosen to satisfy

(n + 1 + no_of_buffers) * l < 133000

The number of buffers is chosen automatically by the program depending upon the requested values for n and l. If it is less than 1 the program selects a lower number of workspaces.

1.4 GENIE DEFAULTS

Default files may be assigned to specific work-spaces (Wn) by the command

ASSIGN <file> Wn (n = 1, 2 , 3, ... , k)

Input to such work-spaces is assumed to be from their assigned default files unless otherwise stated.

A default file may be assigned to all work-spaces by the command

ASSIGN <file>

After this definition any reference to a spectrum is assumed to refer to this file unless otherwise specified.

The ASSIGN command supersedes any previous ASSIGN commands. Thus

```
ASSIGN  <f1>
ASSIGN  <f2>  w3
```

will leave <f2> assigned to w3 and <f1> to all other work-spaces.

A file definition is composed of 5 elements:

```
DISK  -  DIRECTORY  -  INSTRUMENT  -  RUN.NO  -  EXTENSION
```

Four of these (DISK, DIR, INST, EXT) may be given default values by the SET command.

Thus a <file> string may contain any combination of the five elements the user wishes to specify. Any missing elements are simply taken from the default settings.

eg

```
SET  DISK         DRB2:
SET  DIRECTORY    [MWJ]
SET  INSTRUMENT   SXD
SET  EXTENSION    SAV
```

In this case

```
ASSIGN  102  W1          assigns file DRB2:[MWJ]SXD00102.SAV TO W1
ASSIGN  [ADT]33.RAW  W4  assigns file DRB2:[ADT]SXD00033.RAW TO W4
```

The current defaults may be shown using the SHOW DEFAULT command.

It should be noted that on FEM computers

```
ASSIGN DAE
```

and

```
ASSIGN CRPT
```

are also permitted to allow direct access to FEM data.

1.5 GENIE SPECTRUM INPUT

There are several methods of getting spectrum data into genie to be manipulated or displayed.

'FORTRAN' style

The command:

Wn = <spectrum expression> (n = 1,2,3...g)

may be used to input an arithmetic combination of spectra into the work-space defined by the left hand side of the expression. For details see the 'Wn=' page in the command section.

DISPLAY command

DISPLAY AA(Sn)

loads the nth spectrum in the <file> designated by AA and displays this spectrum. ie is equivalent to:

```
Wg=AA(Sn)
D  {Wg}
```

READ command

The READ command enables the contents of a workspace that has been previously written to an INTERMEDIATE file to be copied back to a specific workspace.

eg.

READ Wn <file> m

Puts the mth spectrum from <file> into Wn.

LOAD command

The LOAD command enables the reading of any data file into a workspace. The user must provide a program to read the file and the data is then passed to GENIE using a standard routine. The command has the form

LOAD Wn <datafile> <program>

For full details see section 5.

1.6 SPECTRUM OUTPUT

The output of spectra data from GENIE is handled by the two commands.

WRITE command

The WRITE command enables the contents of a workspace to be stored on a disk file. Many spectra (workspaces) may be written to the same file. The files are written in a format given by the INTERMEDIATE FILE specification.

SHOW DATA command

The SHOW DATA command allows output of workspace data in an ASCII formatted file suitable for transport to other computer installations.

1.7 WORK-SPACE MANIPULATIONS

Arithmetic

W1 = (W1 + W2) / W3

See Wn= command section for details.

UNITS command

U/<unit> {Wn}

may be used to change the units of the x and y axes of the nth work-space. If the x-axis has the dimension D then the y values are automatically adjusted to have the dimension neutron.D^{-1}.

The work-space Wn may be omitted. In this case the last work-space loaded is assumed. If a display is being performed then the graphics work-space is transformed.

REBIN command

REBIN {Wn} X1 : X2 {Wm}

REBIN {Wn} X1 (&X) X2 {Wm}

REBIN {Wn} X1 [&X/X] X2 {Wm}

REBIN Wn Wm

may be used to reset the values used for the x-axis bin boundaries. See the REBIN command page for details.

User defined data manipulation

A user may define and execute data manipulations using the commands

FUNCTION Wn <program> Wm
TRANSFORM Wn <program> Wm

where <program> is a user-written program to perform an operation which calls standard routines to pass information to and from GENIE. For full details see sections 2 and 5.

1.8 GENIE DISPLAY

The command:

DISPLAY {Wn} {X1} {X2}

displays the nth work-space from x1 to x2. In addition to the basic display command the following may be used to modify the display:

ALTER
LIMIT
TOGGLE
ZOOM

Information may be obtained from the display using the commands:

CURSOR
FIND
KEEP
PEAK

1.9 GENIE COMMAND FILE CONTROL

GENIE can execute groups of commands in a command file by typing @<file>, where <file> is the name of the command file. To make command files more flexible, parameter manipulation and flow control commands have been added. Command files may also be called from within other command files and parameters passed between them. Full examples are given in section 4.

PARAMETERS : types

Parameters may be used within a command file. They are either INTEGER(*4), REAL (*4) or CHARACTER. In the case of INTEGER and REAL parameters the type is determined by their first letter.

A - H REAL

I - N INTEGER

O - Z REAL

CHARACTER parameters are defined by the statement in which they are assigned a value. This may be in either an INQUIRE or assignment statement.

PARAMETERS : values

Parameters may be set to specific values by the INQUIRE COMMAND or an assignment: eg.

```
$ INQUIRE NWORK 'type in the number of workspaces'
```

prompts the user with the string 'type in the number of workspaces' and the variable NWORK is given the entered value .

```
$ nwork= 5                (no space between nwork and =)
```

Is an assignment statement and sets the value of NWORK. Assignment statements currently support the same level of syntax as the Wn= command using + - / * () operators, plus the FORTRAN functions SIN, COS, TAN, ASIN, ACOS, ATAN, SIND, COSD, TAND, ASIND, ACOSD, ATAND, SQRT, LOG, EXP.

eg

```
$ lambda = 2 * d * sin( (omega - 0.25) / 2 )
```

FLOW CONTROL

The commands:

```
$ GOTO label ------->

$ label:  <---------
```

and

```
$ GOTO (L1, L2, L3) JJ ---->     (JJ is an integer parameter)

$ L1:  <-----------------           (for JJ=1)

$ L2:  <-----------------           (for JJ=2)

$ L3:  <-----------------           (for JJ=3)
```

enable single and multiple branching to be performed.

Loops are supported by the command:

```
$ DO J = J1, J2 {,J3}          (J3=1 if omitted)
    ...
$ END DO
```

PARAMETER substitution

Parameters enclosed in single quotes in either KEYBOARD or GCL commands will be substituted by their current values.

eg

```
$ DO J = 1, 10
> W'J' = S'J'
$ END DO
```

COMMENTS

Lines introduced by ! are regarded as comments and will be displayed at the terminal. Hence

```
$ A = 5
! The value of A is 'A'
```

will display

```
'The value of A is 5.0000'
```

on the terminal. Any text following a second ! will not be displayed.

PARAMETER PASSING

Parameters may be passed to other command files by adding them after the filename. eg. @FOCUS IRUNNO ISP NOSPEC These parameters appear in the called file as parameters with names P1 P2 and P3 respectively.

2 GENIE 'KEYBOARD' COMMANDS

This section of the GENIE manual gives a detailed description of all the GENIE commands and their associated options.

Conventions

All the command names are given in full with the shortest abbreviation boldened and capitalised.

Optional items are enclosed in curly brackets. Where a user supplied item is required a lowercase description of the type of item is given in angled brackets.

eg

ASSign **<**file**>** **{**Wn**}**

"file" is a user supplied item and "Wn" is an optional parameter

2.1 < C T R L Y >

<CTRL Y> may be used to abort any command or command file (<CTRL Y> means press Y while holding the CTRL key down).

Note that if <CTRL Y> is typed while GENIE is waiting for a keyboard command then GENIE is aborted and the user returned to the VAX operating system (indicated by a $ prompt). If this was not the intention then GENIE may be re-entered at the point that it was left by typing CONTINUE, provided no other command has been typed.

2.2 > @

@<filename> Directs all input to be read from the file <filename>. Commands may be preceded by a "**!**", "**$**" or "**>**".

An example of a command file is given below.

```
! This line is typed to the screen.
! Now set various defaults
$ INQUIRE nwork 'Give number of workspaces'
> SET WORK 'nwork' 10000
! User has 'nwork' workspaces
> SET INSTRUMENT HRP
> ASSIGN 35
```

On entering GENIE a DEFAULT command file is read to set up any instrument specific initial parameters. This file has the logical name GENIEINIT and can be assigned to an actual file in your VMS LOGIN.COM file.

eg

By putting the line

```
$ DEFINE GENIEINIT [WIFD.GENIE]HRPDGENIE.COM
```

in [WIFD]LOGIN.COM where HRPDGENIE.COM is the command file below

```
> SET DISK DRB2:
> SET DIR [HRPMGR.DATA]
> SET INST HRP
> SHOW DEF
> SET WORK 4 22000
> ASS 105
> T CH
> TIME :== J "SH TIME"
```

2.3 > s y n o n y m : = =

Short synonyms for long commands may be introduced by "**:==**" The commands can then be executed by typing the synonym.

For example:

```
>> TIME :== J "SHOW TIME"
>> TIME
31-DEC-1985 11:59:59
>> TIME
1-JAN-1986 00:00:01
```

2.4 > A B B R E V I A T E

ABBreviate <file> AA — designates the abbreviation AA (any two letter combination) to <file> . This enables AA to be used in place of the filename in the D and Wn= commands. <file> uses the current defaults described in default section.

2.5 > A L T E R

Alters parameters associated with graph plotting

Alter

Binning m {Wn} — Alters the bin grouping for a workspace to m. If Wn is omitted, the bin grouping for all workspaces is modified. The default bin grouping is 10.

Graticule { <nx> { <ny> }}

sets the graticule type for x and y.

<nx>, <ny> can take the values:
- 0 no graticules
- 1 graticules at major ticks only
- 2 graticules at major and minor ticks

Marker <n> — Sets the graphical marker to type <n>

n can have the values:
1 = dot, 2 = plus, 3 = star,
4 =circle, 5 = cross

Plot <left> <right> <bottom> <top>

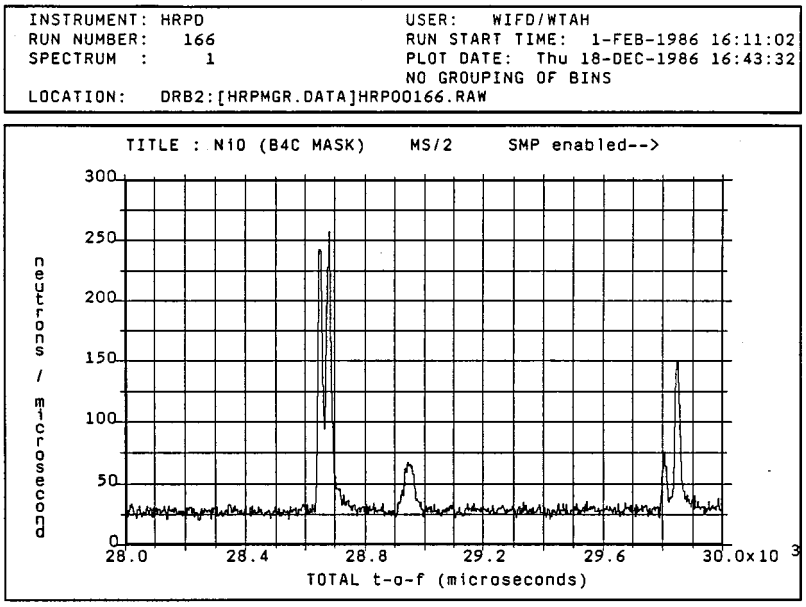
alters the fraction of the screen used for plotting. For example Alter Plot 0.5 1.0 0.5 1.0 uses the top right hand quadrant. The defaults are 0.0 1.0 0.0 1.0.

NOTE: This option can only be used when the header is switched off.

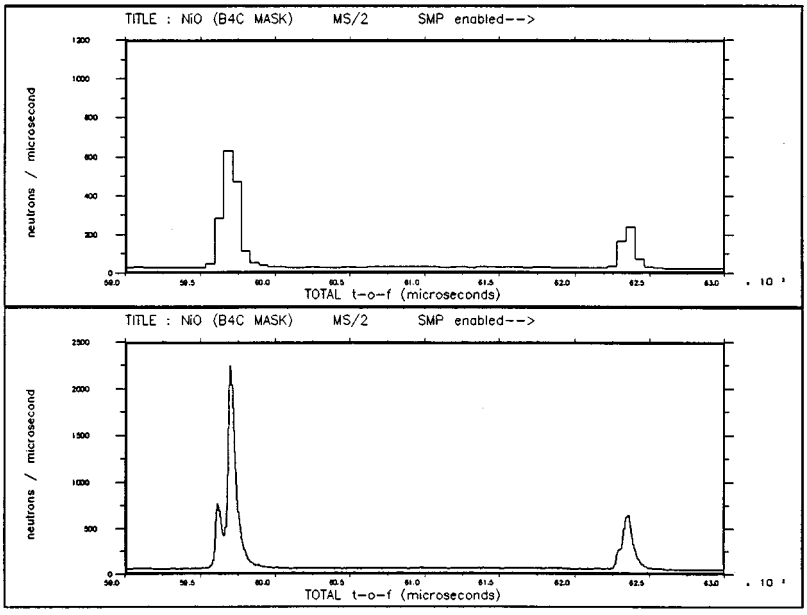
Resolution { <nx> { <ny> }}

speeds up plotting by degrading the screen resolution. nx,ny specify the number of pixels to gang together in each direction.

continued/



2.5.1 Display produced using Alter Graticule



2.5.2 Two displays together using the Alter Plot command

2.6 > A S S I G N

ASSign <file> {wn} makes <file> the default file for subsequent commands involving spectra. By specifying Wn, different default files may be associated with different workspaces.

On the HUB computer the item "<file>" may only be a file name (with defaults this usually reduces to a run number - see example).

On a FEM the identifiers "DAE" or "CRPT" may also be used.

Abbreviations (as set by the Abbreviation command) are not permitted in the <file> field - but the DISK/DIRECTORY/INSTRUMENT and EXTENSION defaults may be used.

eg

```
SET  DISK         DRB2:
SET  DIRECTORY    [MWJ]
SET  INSTRUMENT   SXD
SET  EXTENSION    SAV
```

In this case

```
ASSIGN  102  W1          assigns file DRB2:[MWJ]SXD00102.SAV TO W1
ASSIGN  [ADT]33.RAW  W4  assigns file DRB2:[ADT]SXD00033.RAW TO W4
```

The current defaults may be shown using the SHOW DEFAULT command.

2.7 > C U R S O R

Cursor — switches on the graphics cursor.

Command qualifiers:

/Vertical — switches on the graphics cursor and makes cursor added text vertical (the default).

/Horizontal — switches on the graphics cursor and make cursor added text horizontal.

When the cursor is in operation single character commands may be typed:

X — to display the X coordinate.

Y — to display the Y coordinate.

P — to display the X and Y coordinates.

B — displays the X and Y coordinates and will write to a file in CCSL format when a Keep/B command is issued.

C — displays the X coordinate and will write the X values to a file when a Keep/C command is issued. Keep/C writes all the x values to a file suitable for CELREF refinement.

E — exit from cursor.

T — to add extra text to the display at the cursor position. A line of text will be prompted for and takes the form:

<text> | <size>

where <size> is a real number giving the size of the characters as a fraction of the screen height. If <size> is omitted the default size of 0.0145 used.

L, **U** — defines the lower left hand corner of a box and is used with U. U defines the upper right hand corner of a box which is drawn once the U key has been pressed. Lines may be drawn as "thin" boxes.

2.8 > D I S P L A Y

Display

<Spectrum> { x1 { x2 { y1 { y2 }}}}

loads the spectrum specified into the graphics work-space. It then displays the graphics work-space from x1 to x2 with y limits y1 to y2.

Where <Spectrum> is any expression which defines a spectrum, currently these are.

AA(Sn) - the nth spectrum from the file with abbreviation AA.

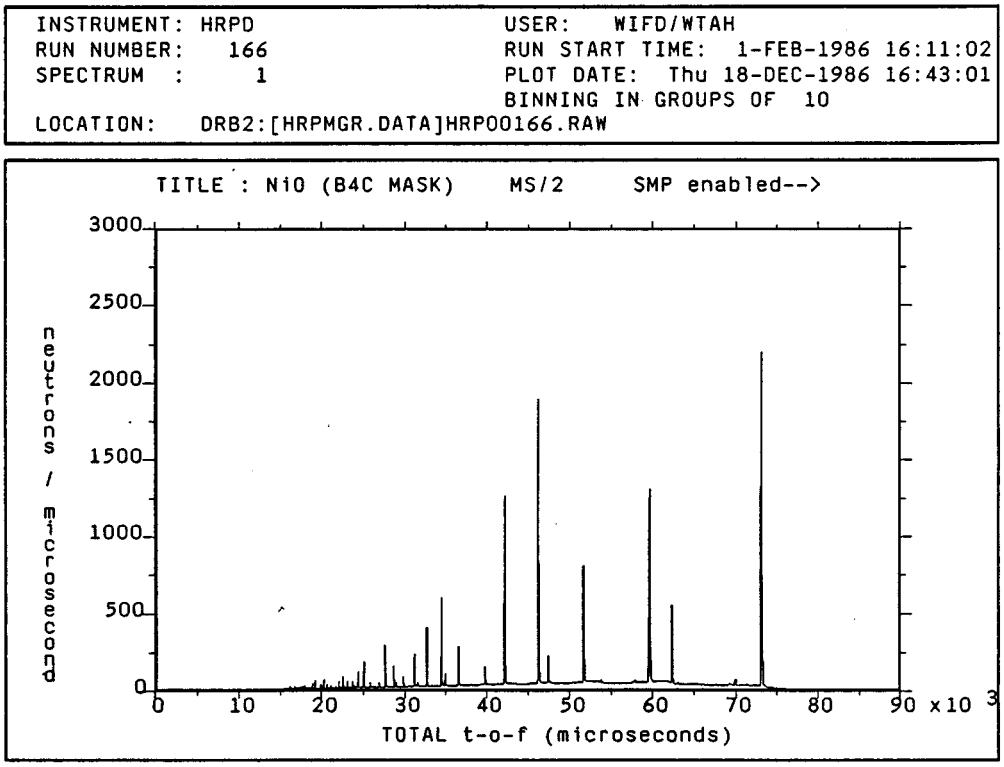
Sn - the nth spectrum from default file.

Wn - the contents of workspace n.

Command qualifiers:

/**M**arkers	Do the plot using markers
/**L**ine	Do the plot using a continuous line
/**E**rrors	Annotate points with error bars
/**H**istogram	Do the plot as a histogram

continued/



2.8.1 Typical output of the display command

2.9 > E X I T

Exit leaves the program

2.10 > F U N C T I O N

The function command provides a method of manipulating a workspace in a way not standard to GENIE. See section 5 for full details. It is restricted in that only the data points and errors may be manipulated, while the boundaries are fixed. A more general command is the TRANSFORM command. Several functions of general interest are available in GENIE_LIBRARY (see example)

Function Wn <prog_name> Wm

Runs the program <prog_name>.exe with Wn as input workspace and Wm as the output workspace. The x values in Wm are set equal to those in Wn. Note n may equal m.

eg

```
Function w1 GENIE_LIBRARY:MONCOR w2
```

performs a monitor correction on data in w1 and puts the corrected data in w2.

2.11 > H E L P

Help <topic> provides help information on the topic chosen.

eg

Help assign

2.12 > I N T E G R A T E

Integrate Wn <low_limit> <high_limit>

Performs a numerical integration of the workspace data by summing the bins. The result is displayed on the screen.

/**XMI**n = <low_limit> low limit for integration (default is minimum x-value in workspace)

/**XMA**x = <high_limit> high limit for integration (default is maximum x-value in workspace)

2.13 > J U M P

Jump "<command-line>" Jumps into VMS and executes the DCL <command-line> and then returns to GENIE.

eg

```
J "SHOW DEFAULT"
HUB$DISK0:[KJK.DOC]
```

2.14 > K E E P

Keep { <file> }

Command qualifiers:

/**H**ardcopy	Saves all plotting done since the last time the graphics screen was cleared. The plot is saved in a file suitable for output to the device specified in the Set Hardcopy command. The default is the LN03 laser printer. The filename will be the name of the chosen device prefixed by an "H". The default therefore will be a file "HLASER.DAT".
/**P**osition	writes the (x,y) positions already marked by the cursor to a file. Writes to DATA.POS if not specified.
/**X**_coordinate	writes the x positions marked by the cursor to a file. Writes to DATA.XXX if not specified.
/**Y**_coordinate	writes the y positions already marked by the cursor to a file. Writes to DATA.YYY if not specified.
/**B**ackground	write the positions marked by the cursor "B" command to a file. Writes to DATA.BAK if not specified. The data is formatted for input to CCSL.
/**C**ell	write the X positions marked by the cursor with the cursor C command to a file. Writes to DATA.BAK if not specified. The data is formatted for CELREF refinement.

2.15 > L I M I T S

The limit command sets new limits for the graph. They are retained until a new Limits, Display <spectrum>, or Zoom command is issued.

Note: a simple "Display" command does not reset the limits.

Limits

Command qualifiers:

/**X** X1 X2	Sets new x limits
/**Y** Y1 Y2	Sets new y limits
/**N**o_auto X1 X2 Y1 Y2	Sets both x and y limits
/**D**efault	Resets x and y limits to xmin, xmax, ymin and ymax respectively

2.16 > L O A D

The LOAD command provides a means of getting any data into GENIE using a user-written program. See section 5 for details. Some generally useful routines are kept in GENIE_LIBRARY (see example).

LOad Wn <datafile> <prog_name>

Loads Workspace Wn with data from <datafile> using the program <prog_name>.

eg

```
Load  w1  ISISBEAM.LOG  GENIE_SOURCES:VIEWISIS
```

loads data from an ISIS beam log file into w1 for viewing.

2.17 > MULTIPLOT

MUltiplot

```
    <spectra>  { Xmin { Xmax { b { Ydel { Ygap } } } } }
```

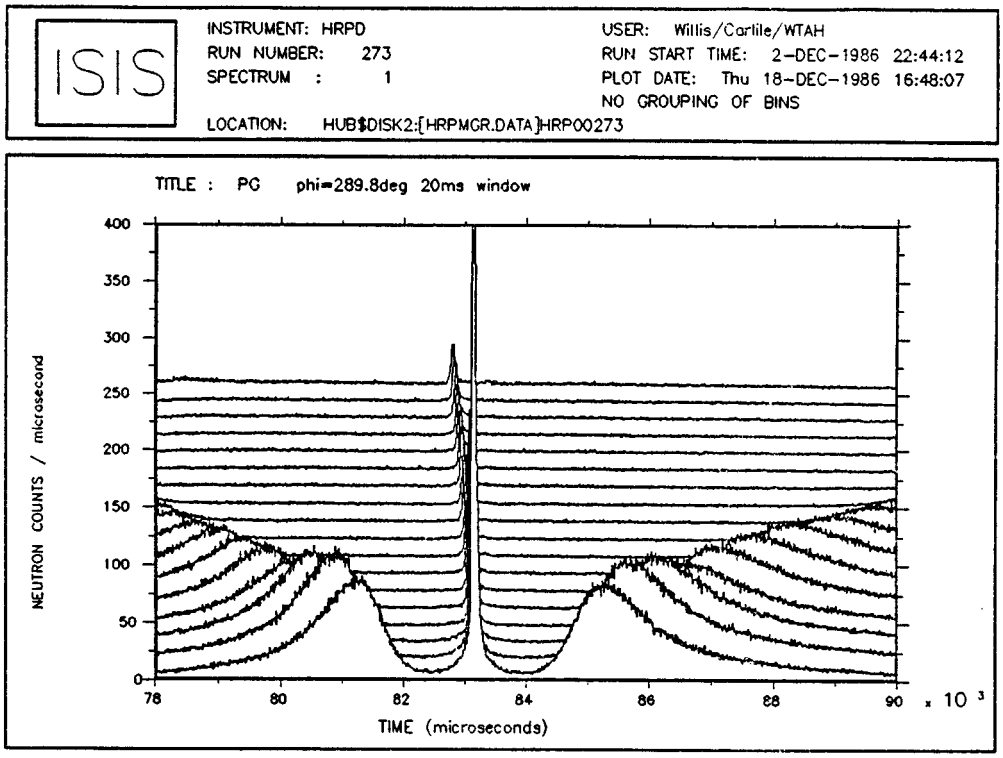
eg

```
        Multiplot  S1 + S2 + S3

        Multiplot  W1>W6  10000  15000  2  200  40

        Multiplot  AA( S20>S1 + S21>S40 )
```

Displays multiple spectra or workspaces data in a similar manner to the DISPLAY command. The first spectrum in the spectrum or workspace list is displayed normally. Each succeeding plot is displaced a distance Ydel on the scale. Ygap is the distance between the top of the last plot done and the top of the graph. The <spectra> are separated by the + symbol. If the > symbol is used each spectrum between the two is displayed.



2.17.1 Typical output from the MULTIPLOT command

2.18 > P E A K

This command must be used when a spectrum is currently displayed on the graphics screen.

PEak

{ Xmin Xmax } Xmin, Xmax limits may be set in the command line or selected on screen using the graphics cursor. A linear background is fitted and 0th, 1st and 2nd moments of the remainder are returned.

<prog_name> { Xmin Xmax }

Model-fitting may also be done using the peak command. A user written or standard supplied program may be used and returns parameters for a single peak.

Functions currently available are:
- Gauss (G)
- Kropff (ECG)
- ECL

These may be accessed using the logical name GENIE_LIBRARY.

eg

Peak GENIE_LIBRARY:gauss 20000 30000

Command qualifiers:

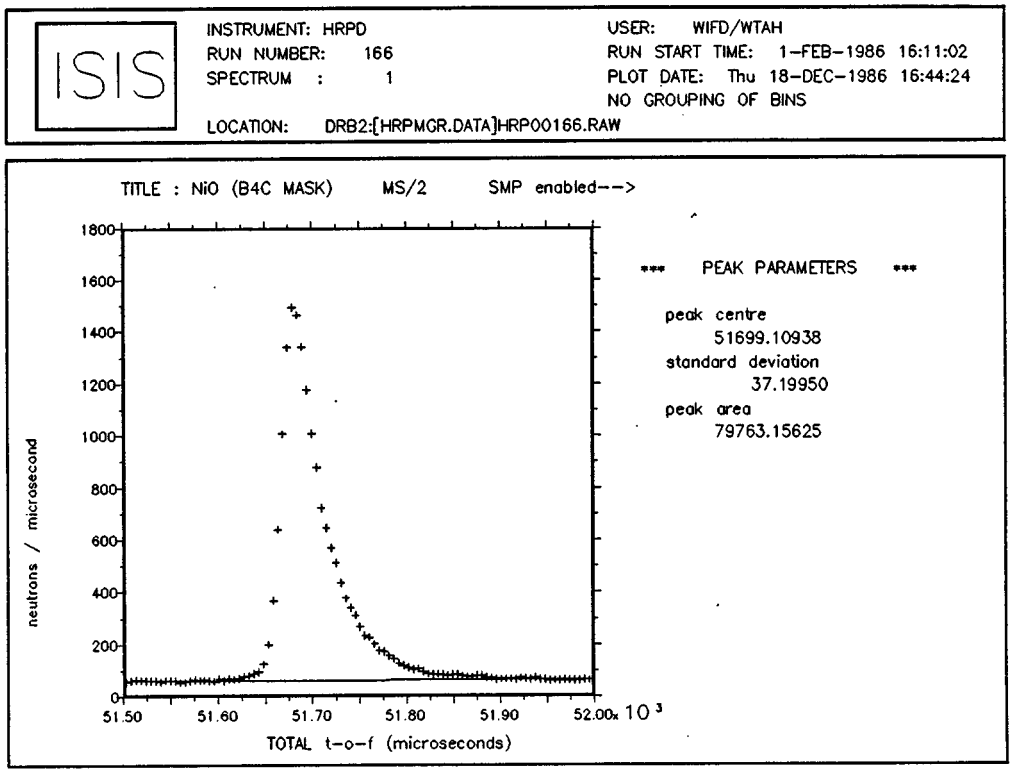
/NOWEIGHT uses unit weights (default = 1/y).

/NOCYCLES returns with the first guess of the parameters ('0th' cycle)

/NOGRAPH Inhibits graphics output.

/NOOUTPUT Inhibits alpha-screen output.

continued/



2.18.1 Typical output of the Peak command

2.19 > P L O T

PLOT will overplot an existing display leaving the axes intact.

Plot

<spectrum> <nbins> plots <spectrum> grouped in <nbins> bins over the current display.

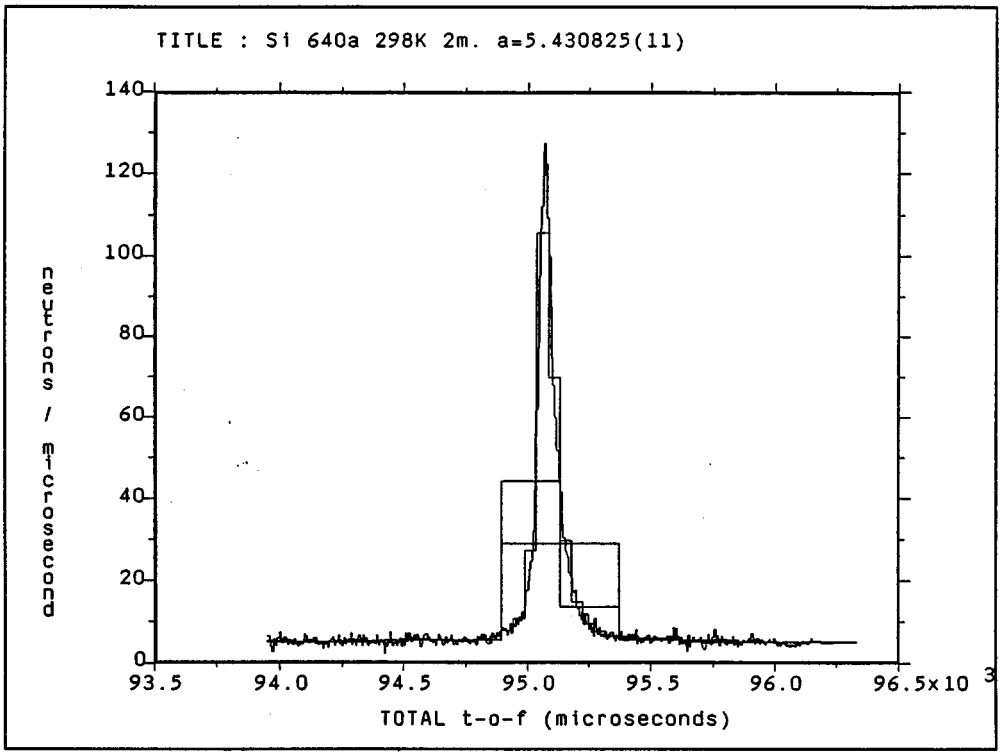
Command qualifiers:

/**H**istogram plots as a histogram (default)

/**L**ine plots with a line

/**M**arker plots with markers

/**E**rror plots with error bars



2.19.1 Example display using the Plot command

2.20 > R E A D

Only one file may be open for INPUT (reading) at any time.

Read

Wn m	Reads the entire contents of the mth block of the current file to the nth workspace. An error is returned if no file is open for input.
Wn <file> { m }	Closes any existing input file. Opens the file specified and reads the mth block to the nth workspace. If m is omitted the block number defaults to one.

Command qualifiers:

/**O**pen	Open input file.
/**C**lose	Close existing input file

2.21 > R E B I N

Enables the contents of a work-space or the graphics work-space to be ’rebinned’ on the x axis.

REBin

{Wn} X1 : X2 {Wn}	Redefines the x limits for the nth work-space to be X1 to X2. If no Wn is given the last Wn referred to is assumed. A "Display" command sets this to the graphics work-space.
{Wn} X1 (d1) X2 (d2) X3 (...	step from X1 to X2 in steps of d1, X2 to X3 in steps of d2 ...etc.
{Wn} X1 [d1] X2 [d2] X3 [...	step from X1 to X2 in steps of &X1/X1, X2 to X3 in steps of &X2/X2 ...etc. Where &X1, ..., &Xn are chosen such that dn = &Xn/Xn where &Xn is the bin width and Xn is the lower bin boundary.
Wn Wm	Rebins Wm using the x values from Wn.

eg

Rebin W1 10 (5) 10000	Rebins W1 into constant bin widths of 5 between 10 and 10000.
Rebin W1 1000 [0.001] 10000	Rebins W1 into logarithmically varying bins between 1000 and 10000. Bin boundaries occurring at 1000, 1001, 1002.001, ..., Xn + (dn * Xn)

Note:
The Rebin expressions using brackets may mix both [] and () bracket types.

2.22 > S E T

Set

DEVice <device> — selects the primary output device for GENIE. This command will be needed if a terminal other than a Perricom or Tektronix is used. Alternatively, a GENIE command file which is being used non-interactively can set the primary output device to be a hard-copy device such as the ZETA plotter or laser printer. Devices currently available are.

TEK	-	Tektronix 4010 or compatible
LASER	-	LN03 laser printer
ZETA	-	ZETA plotter
NDK	-	NDK Printstar (dot matrix)
SIG5684	-	Sigma 5684 terminal
SIG6160	-	SIGMEX 6160 terminal

Where a non-interactive device is selected, the output will be to an appropriately named file. eg LASER.DAT, ZETA.DAT, NDK.DAT.

DIRectory <dir> — sets the default directory (Note that [] means the current directory).

eg
```
Set directory [HETMGR.DATA]
```

DISk <disk> — sets the default disk.

eg
```
Set disk HUB$DISK1:
```

Extension <ext> — sets a default file extension.

eg
```
Set extension .RAW
```

Hardcopy <device> — Selects the device for which hardcopy journaling is enabled. See the Set Device command above for details of the <device> parameter. The default device is the LN03 laser printer. See also the **Keep/hardcopy** command.

continued/

Set (continued)

Instrument <name> — sets a default instrument name where <name> is the short form of the instrument name (ie HRP, LOQ, LAD, SXD, POL, EVS, IRS, CSP, HET, TFX, PRS).

eg
Set instrument POL

Parameters Wn L1 L2 2Θ Emode Efixed

sets the parameters listed for Wn
L1 - primary flight path
L2 - secondary flight path
2Θ - 2theta

Emode - 0 for elastic, 1 for direct geometry, 2 for indirect geometry. Efixed - fixed energy if Emode=1 or 2

Note: SET Parameters must be used before using the UNIT command.

Title Wn 'string' — resets the title for the nth workspace.

Work n l — sets n work-spaces of length l.

Ycode Wn -1 — sets the flag YCODE to -1. Must be used before a UNITS command if the Y values in Wn are ratios. (used as a work-around until YCODE set correctly by Wn=)

Emin n
Emax n — Set minimum and maximum energies for truncation on the UNIT command. As a default, energies below -1000 meV and above 5000 meV are truncated.

2.23 > S H O W

SHow

ABbreviations {SS} — shows all {or specific} abbreviations in use

ASsignments {n} — shows the assigned file for all {nth} work-spaces

DAta Wn — writes workspace data to a file in the format shown below, the default is to write the whole workspace.
Note: for histogram data the final values Y(N+k) and E(n+k) are never meaningful in the range specified.

Count	Wn	L1	L2	2Θ	EMODE	EFIXED
N	X(N)		Y(N)		E(N)	
N+1	X(N+1)		Y(N+1)		E(N+1)	
.....						
N+k	X(N+k)		Y(N+k)		E(N+k)	

/**XMI**n = <x-value> — Lowest X value to be output.

/**XMA**x = <x-value> — Highest X value to be output.

/**OUTPUT** = <file> — File to which the output is to be written, the default is FOR001.DAT. If the <file> parameter is given as TT, the output will be to the screen.

DEfault — shows default disk,directory, instrument and extension

Parameters Wn — shows parameters as given in SET PARAMETERS for workspace Wn.

Work — shows length and number of workspaces.

2.24 > S U B M I T

SUBmit

<file>	Submits a GENIE job to the batch queue with the command-file <file>.

Command qualifiers:

/**FAST**	Use FAST batch queue.
/**NONOTIFY**	Do not notify on completion.

2.25 > T O G G L E

This command causes the item specified (eg. HEADER) to be turned on or off - or the value to be reselected from a short, circular list.

Toggle

CHaracters	Select a hardware or software character font, the hardware fonts draw faster but with poorer quality.
CLear_screen	graphs over-print if this is switched off
Header	graphics header
LOGX	log x axes
LOGY	log y axes
R/X	rounding on x axes limits
R/Y	rounding on y axes limits
Tag	switches between 1,4 or 9 minor tags per major tag
Mode	switches between histogram and point-plot mode (ie. x values are taken to be centres of bins.)

2.26 > T R A N S F O R M

The transform command provides a method of manipulating a workspace in a way not standard to GENIE. See section 5 for full details. Some generally useful transforms are held in GENIE_LIBRARY (see example).

TRansform Wn <prog_name> Wm

Runs <prog_name>.exe with Wn as input and Wm as output. Note n can equal m.

eg

```
Transform  w1  GENIE_LIBRARY:TIM2TH  w1
```

replaces the data in w1 with the transformed data.

2.27 > T S H I F T

Shifts the time-scale of a workspace.

TShift <time> <Wn>	Adds <time> in microseconds to the x values in Wn. Note: If the x units are not time then the command will fail.

2.28 > U N I T

Modifies the units of the work-space specified. Note that in order for this command to succeed the SET PARameters command must have been used to set the geometry/energy parameters for the given workspace.

Unit

{Wn}	Change the units for workspace Wn

Command qualifiers:

ASSUMING ELASTIC SCATTERING

/C	channel no.
/D	d-spacing in A
/E	incident energy in meV
/LAM	wavelength in A
/Q	momentum transfer (A-1)
/SQ	Q**2 in A-2
/T	time in μs

ASSUMING INELASTIC SCATTERING

/LA1	wavelength for primary flight-path L1 in A
/W	energy transfer in meV

If Wn is not used then the last work-space referenced is assumed. If a DISPLAY is being performed then the graphics work-space is transformed.

2.29 $ < v a r i a b l e > =

NUMERIC ASSIGNMENTS

<variable> **=** <expression>

Sets <variable> to type NUMERIC VALUE and assigns it the value defined by the expression. The expression may include real or integer variables, constants, the symbols "()+-]" and the functions SIN, COS, TAN, ASIN, ACOS, ATAN, SIND, COSD, TAND, ASIND, ACOSD, ATAND, SQRT, LOG, EXP

eg

```
L2 = 3.87 * ( PAR2 - KG ) + SIND(60)
```

CHARACTER STRING ASSIGNMENTS

$ <variable> **=** **"** <string> **"** Sets <variable> to the type STRING and fills it with <string>.

eg

```
RUNNAME = "Calibration"
```

2.30 $ V n =

Allows a FORTRAN style assignment to special scalar parameters. Scalar parameters allow scalar variables to be passed to and from the FUNCTION, LOAD, PEAK and TRANSFORM commands. These parameters only take numeric values and should not be confused with the variables from the **<variable> =** command though they operate in a similar way.

Vn = <scalar expression> loads the <scalar expression> into the nth scalar parameter.

The rules for constructing a <scalar expression> are as follows.

- **Vm** refers to the mth scalar parameter
- integers/real numbers represent constants
- the symbols "**+**", "**-**", "*****", "**/**" take their usual meaning, but may only be used as binary operators.

eg

V1 = V2 + 20.0 * 'ival'

2.31 > W n =

Enables 'FORTRAN' style of input to work-spaces.

Wn = <spectrum expression> loads the <spectrum expression> into the nth work-space.

The rules for constructing a <spectrum expression> are as follows.

- **Wm** refers to the spectrum in the mth work-space
- **Sn** refers to the nth spectrum
- integers/real numbers represent constants
- the default file for the mth work-space is assumed in a **Wm =** command unless overridden by an abbreviated file specification.
- the symbols "**+**", "**-**", "*****", "**/**" take their usual meaning, but may only be used as binary operators.
- the symbol > means a repeated addition between spectra
- DD(.....) means that all spectra within the brackets will be read from file DD - set by the ABBreviate command.

eg

W1 = W2 + S4 adds 4th spectrum of default file to 2nd work-space and places the result in the first work-space.

W2 = (S1>S20) / S41 adds spectra 1+2+3...+20 and divides the result by spectrum 41 (all from default file).

W1 = 3.56 * AA(S6>S9) - S44

adds spectra 6,7,8,9 from file AA,and multiplies the result by 3.56. Spectrum 44 from the default file is subtracted from this result.

2.32 > W R I T E

Only one file may be open for output (writing) at any time.

Write

Wn	Writes the entire contents of the nth workspace to the next block of the currently open file. Error return if no file open for output.
Wn <file>	Closes any existing output file. Opens the file specified and writes the entire contents of the nth workspace to it.

Command qualifiers:

/**O**pen	Open new output file.
/**C**lose	Close existing output file.

2.33 > Z O O M

Zoom	returns to the graphics display with the cursor. Two keys (any character will do) are typed to define opposite corners of a box, this selects a portion of the plot area to be magnified.
/**E**rror	plots the new ('zoomed') graph with error bars.
/**M**arker	plots the new graph with markers.
/**L**ine	plots the new graph with a polyline.
/**H**istogram	plots the new graph with a histogram.

3 GENIE COMMAND LANGUAGE

Genie command language provides a simple FORTRAN like command language to allow automation of command sequences. The following commands only work within a GENIE command file although the command file may be run interactively or in batch.

3.1 $ D O

$ **DO** J = J1, J2 {, J3}

  ...

$ **END DO**

Executes a 'FORTRAN style' DO LOOP. J1 defines the starting value of J and J2 the ending value. J3 is an optional step parameter and defines the size of the steps between J1 and J2. If J3 is omitted the step value defaults to 1.

3.2 $ G O T O

$ **GOTO** LABEL

  ...

$ LABEL:

Executes an unconditional jump instruction to the label specified.

$ **GOTO** (LABEL1, LABEL2, LABEL3, ...) JJ
  ...
$ LABEL1:
  ...
$ LABEL2:
  ...
$ LABEL3:

Executes a conditional jump instruction to one of the labels specified. The nth label in the statement is used where n is determined from the value of JJ (ie if JJ = 2 LABEL2 is used.)

Note: A maximum of 20 labels are currently allowed on one $ GOTO

3.3 $ I N Q U I R E

$ INQUIRE <parameter> ’ <character_string> ’

Prompts the user with the character string and assigns the returned value to the variable <parameter>.

eg

```
$ INQUIRE  NWORK  ’Please type in the number of workspaces’
```

Prompts the user with the string "Please type in the number of workspaces" and the variable NWORK is set to the value the user types.

4 EXAMPLE COMMAND FILES

This section gives some examples of command files written in GCL.

4.1 HRPD detector focusing

The command file "FOCUS.COM" is used to prompt for 4 parameters including the sample position. According to which of the sample positions is chosen, 1 or 2, "FOCUS1.COM" or "FOCUS2.COM" is called.

command file FOCUS.COM

```
!     ***** SOFTWARE FOCUSING OF HRPD DIFFRACTION SPECTRA ******
!
!   This command file focuses NOSPEC spectra from run number IRUNNO.
!
$ INQUIRE IRUNNO "  Which run number do you wish to look at"
$ INQUIRE IPOS "  Is the sample at the 1m. or 2m. position (1/2)"
$ INQUIRE ISP "  Which spectrum do you wish to start with"
$ INQUIRE NOSPEC "  How many spectra do you wish to add together"
!
> @FOCUS'IPOS' IRUNNO ISP NOSPEC
```

command file FOCUS1.COM

```
$ IRUNNO= P1          ! Run number passed from FOCUS.COM
$ ISP= P2             ! Initial spectrum number
$ NOSPEC= P3          ! Number of spectra to be added together
> ABB 'IRUNNO' AA     ! Abbreviate data-file to AA for convenience
> W1= AA(S'ISP')      ! Fill workspace 1 with initial spectrum
$ ! Evaluate secondary flight path and two theta for each spectrum
$ PX= 1.09175
$ PY= 0.0775
$ XX= PX - 0.007*(ISP-1)
$ YY= PY + 0.015*(ISP-1)
$ PATH2= SQRT(XX*XX + YY*YY)
$ TTH= 180.0 - ATAND(YY/XX)
> SET PAR 1 95 'PATH2' 'TTH' 0 2
> U/D W1              ! Convert to d scale
$ NOSPEC= NOSPEC-1
$ DO I= 1,NOSPEC      ! Do loop beginning
$ ISP= ISP-1
> W2= AA(S'ISP')      ! Fill workspace 2 with next spectrum
$ ! Evaluate secondary flight path and two theta for each spectrum
$ XX= PX - 0.007*(ISP-1)
$ YY= PY + 0.015*(ISP-1)
$ PATH2= SQRT(XX*XX + YY*YY)
$ TTH= 180.0 - ATAND(YY/XX)
> SET PAR 2 95 'PATH2' 'TTH' 0 2
```

```
> U/D W2              ! Convert to d scale
> REB W1 W2           ! Make W2 bins commensurate with W1 bins
> W1= W1+W2           ! Add W2 to W1
$ END DO              ! End of Do loop
> W3= W1              ! Make W3 equivalent to W1
$ ! Find the middle spectrum and associated L2 and 2 theta
$ JSP= ISP + 0.5*NOSPEC
$ XX= PX - 0.007*(JSP-1)
$ YY= PY + 0.015*(JSP-1)
$ PATH2= SQRT(XX*XX + YY*YY)


$ TTH= 180.0 - ATAND(YY/XX)
> SET PAR 3 95.0 'PATH2' 'TTH' 0 2
> U/T W3              ! Convert W3 back to time-of-flight
> D W3                ! Display W3
```

command file FOCUS2.COM

```
$ IRUNNO= P1          ! Run number passed from FOCUS.COM
$ ISP= P2            ! Initial spectrum number
$ NOSPEC= P3         ! Number of spectra to be added together
> ABB 'IRUNNO' AA
> W1= AA(S'ISP')
$ PX= 2.09175
$ PY= 0.0775
$ XX= PX - 0.007*(ISP-1)
$ YY= PY + 0.015*(ISP-1)
$ PATH2= SQRT(XX*XX + YY*YY)
$ TTH= 180.0 - ATAND(YY/XX)
> SET PAR 1 96 'PATH2' 'TTH' 0 2
> U/D W1
$ NOSPEC= NOSPEC-1
$ DO I= 1,NOSPEC
$ ISP= ISP-1
> W2= AA(S'ISP')
$ XX= PX - 0.007*(ISP-1)
$ YY= PY + 0.015*(ISP-1)
$ PATH2= SQRT(XX*XX + YY*YY)
$ TTH= 180.0 - ATAND(YY/XX)
> SET PAR 2 96 'PATH2' 'TTH' 0 2
> U/D W2
> REB W1 W2
> W1= W1+W2
$ END DO
> W3= W1
$ JSP= ISP + 0.5*NOSPEC
$ XX= PX - 0.007*(JSP-1)
$ YY= PY + 0.015*(JSP-1)
$ PATH2= SQRT(XX*XX + YY*YY)
$ TTH= 180.0 - ATAND(YY/XX)
> SET PAR 3 96.0 'PATH2' 'TTH' 0 2
> U/T W3
> D W3
```

4.2 Multi-spectra plotting for HRPD

command file MULSP.COM

```
$ FIRST_OCTANT= "S20>S1"
$ SECOND_OCTANT= "S21>S40"
$ BOTH_OCTANTS= "'FIRST_OCTANT'+'SECOND_OCTANT'"
!
!                  ******************************
!                  **** MULTISPECTRA PLOTTING ****
!                  ******************************
!
$ INQUIRE TMIN "       Enter lower time limit"
$ INQUIRE TMAX "       Enter upper time limit"
!
!                  **** DETECTOR PLOT OPTIONS ****
!                      1          1st octant
!                      2          2nd octant
!                      3          both octants
!                  ******************************
!
$ INQUIRE IOPT "       Enter option"
!
!         Do you wish to use default multiplot values?
$ INQUIRE JOPT "         ( 1= defaults : 2= user-defined values)    "
$ GOTO (DEFAULTS,USER_DEFINED) JOPT
$ DEFAULTS:
$ JBIN= " "
$ YRISE= " "
$ YGAP= " "
$ GOTO START_PLOT
$ USER_DEFINED:
$ INQUIRE JBIN "       Enter bin grouping"
$ INQUIRE YRISE "       Enter y increment between plots"
$ INQUIRE YGAP "       Enter y gap at top of multi-plot"
$ START_PLOT:
$ GOTO (FIRST,SECOND,BOTH) IOPT
$ FIRST:
> MUL 'FIRST_OCTANT' 'TMIN' 'TMAX' 'JBIN' 'YRISE' 'YGAP'
$ GOTO END
$ SECOND:
> MUL 'SECOND_OCTANT' 'TMIN' 'TMAX' 'JBIN' 'YRISE' 'YGAP'
$ GOTO END
$ BOTH:
> MUL 'BOTH_OCTANTS' 'TMIN' 'TMAX' 'JBIN' 'YRISE' 'YGAP'
$ END:
!
!
```

5 ADDING EXTRA FACILITIES

Extra facilities can be added to GENIE by means of the LOAD, FUNCTION and TRANSFORM commands. The LOAD command is used to read files written in non-standard formats, while FUNCTION and TRANSFORM commands are used to manipulate a workspace. FUNCTION is restricted to manipulations only on the **y** and **e** values, while TRANSFORM allows manipulations of **y**, **e** and **x** values. The formats of these commands are given the keyboard commands section. This section describes how to create a new facility.

5.1 Including a new facility

Included in each command is a user-written program. This program takes the form below.

1. input data from GENIE and initialise some common blocks
2. perform a user-specific operation
3. output data to GENIE

Steps 1 and 3 are performed by standard subroutines. Step 2 must be provided as a program written by the user and must include the common blocks which pass the information to and from GENIE. The names are given in the table below. All files are in the area GENIE_SOURCES. To access the standard subroutines, the link command for the user written program must include a reference to the genie library.

ie

```
LINK <user program>, GENIE_LIB/LIB
```

A summary of the required routines and common blocks is given below with an example program.

Command	Input routine	Output routine	Common block file
LOAD	LOAD_IN	LOAD_OUT	LOADCOM.CMN
FUNCTION	FUNCTION_IN	FUNCTION_OUT	FUNCTCOM.CMN
TRANSFORM	TRANSFORM_IN	TRANSFORM_OUT	TRANSFORM.CMN

5.2 Example of a user-written program for use with the FUNCTION command

This program takes the square-root of a workspace. Negative values are set to zero.

```
      PROGRAM root

      include 'GENIE_SOURCES:functcom.cmn'
c
c
      call function_in
c
      do i=1,lpt
          if (yin(i).le.0.0) then
              yout(i)=0.0
          else
              yout(i)=sqrt(yin(i))
              eout(i)=0.5*ein(i)/yout(i)
          endif
      end do
c
      call function_out
      stop 'Square root completed'
      end
```

5.3 Common blocks

LOADCOM.CMN

```
c               Author:         W.I.F.David
c               Date:           12-JUNE-1985
c               Purpose:        Makes life easier for user in user
c                               program associated with LOAD command
c                               in GENIE: contains all the necessary
c                               parameters for data transfer.
c
c       mn              maximum possible number of points in array
c       L1 & L2         primary and secondary flight paths (metres)
c       xcode & ycode   code for unit contents of x and y arrays
c       ws_history      work space history
c       long_title      title
c       xcaption        x axis caption  (similarly ycaption for y axis)
c       infile          data file name
c       run_user        user name
c       start_time      start time of run
c       lpt             number of points in x,y,e arrays in data file
c       delta           stand-off time in microseconds
c       tthet & fi      two theta and azimuthal scattering angles
c       run_duration    real value corresponding to duration of run
c       no_spectrum     spectrum number
c       inst_name       instrument name
c       inst_code       instrument code
c       user_par        user-defined parameters
c       st_var          array of stored variables used in GENIE
      integer                 data_unit
      parameter               (mn=33000,data_unit=4)
      real                    L1,L2
      integer                 run_number,xcode,ycode
      character*200           ws_history
      character*80            long_title
      character*40            infile,xcaption,ycaption
      character*20            run_user,start_time
      character*8             inst_name
      common  /loader/        infile,lpt,x(mn),y(mn),e(mn),
     +                         xcaption,ycaption,long_title,
     +                         delta,inst_code,inst_name
     +                         xcode,ycode,L1,L2,tthet,
     +                         no_spectrum,run_number,run_user,
     +                         run_duration,start_time,fi,
     +                         user_par(30),st_var(20),ws_history
( see 5.4 for details of xcode and ycode )
```

FUNCTCOM.CMN

```
c.....................................................................
c               Author:         W.I.F.David
c               Date:           12-JUNE-1985
c               Purpose:        Makes life easier for user in user
c                               program associated with FUNCTION command
c                               in GENIE: contains all the necessary
c                               parameters for data transfer.
c
c       mn              maximum possible number of points in array
c
c.......................... INPUT PARAMETERS ..........................
c       L1 & L2         primary and secondary flight paths (metres)
c       xcode & ycode   code for unit contents of x and y arrays
c       in_history      input work space history
c       in_title        input title
c       xcaptin         x axis caption  (similarly ycaptin for y axis)
c       lpt             number of points in x,y,e arrays in data file
c       delta           stand-off time in microsecs of input workspace
c       tthet & fi      two theta and azimuthal scattering angles
c       inst_name       instrument name
c       inst_code       instrument code
c       user_par        user-defined parameters
c       st_var          array of stored variables used in GENIE
c
c.......................... OUTPUT PARAMETERS ..........................
c       xcode & ycode   code for unit contents of x and y arrays
c       out_history     output work space history
c       out_title       output title
c       xcaptout        x axis caption  (similarly ycaptout for y axis)
c       user_par        user-defined parameters
c       st_var          array of stored variables used in GENIE
c
c.....................................................................
      parameter               (mn=33000)
      real                    L1,L2
      integer                 xcode_in,ycode_in,xcode_out,ycode_out
      character*200           in_history,out_history
      character*80            in_title,out_title
      character*40            xcaptin,ycaptin,xcaptout,ycaptout
      character*8             inst_name
      common  /funct_in/      lpt,xin(mn),yin(mn),ein(mn),
     +                         xcaptin,ycaptin,in_title,
     +                         delta,inst_code,inst_name,
     +                         xcode_in,ycode_in,L1,L2,tthet,
     +                         no_spectrum,run_number,run_user,
     +                         run_duration,start_time,fi,
     +                         user_par(30),st_var(20),in_history
      common  /funct_out/     yout(mn),eout(mn),
     +                         xcaptout,ycaptout,out_title,
     +                         xcode_out,ycode_out,out_history
( see 5.4 for details of xcode and ycode )
```

TRANSCOM.CMN

```
c.....................................................................
c
c               Author:         W.I.F.David
c               Date:           11-JAN-1986
c               Purpose:        Makes life easier for user in user
c                               program associated with TRANSFORM command
c                               in GENIE: contains all the necessary
c                               parameters for data transfer.
c
c       mn              maximum possible number of points in array
c
c............................. PARAMETERS ..............................
c       L1 & L2         primary and secondary flight paths (metres)
c       xcode & ycode   code for unit contents of x and y arrays
c       in_history      input work space history
c       in_title        input title
c       xcaptin         x axis caption  (similarly ycaptin for y axis)
c       lpt             number of points in x,y,e arrays in data file
c       delta           stand-off time in microseconds of input workspace
c       tthet & fi      two theta and azimuthal scattering angles
c       inst_name       instrument name
c       inst_code       instrument code
c       user_par        user-defined parameters
c       st_var          array of stored variables used in GENIE
c.....................................................................
c
      parameter                 (mn=33000)
      real                      L1_in,L2_in,L1_out,L2_out
      integer                   xcode_in,ycode_in,xcode_out,ycode_out
      character*200             in_history,out_history
      character*80              in_title,out_title
      character*40              xcaptin,ycaptin,xcaptout,ycaptout
      character*20              start_time_in,start_time_out
      character*20              run_user_in,run_user_out
      character*8               inst_name_in,inst_name_out
      common  /trans_in/        lptin,xin(mn),yin(mn),ein(mn),
     +                          xcaptin,ycaptin,in_title,
     +                          delta_in,inst_code_in,inst_name_in,
     +                          xcode_in,ycode_in,L1_in,L2_in,tthet_in,
     +                          no_spectrum_in,run_number_in,run_user_in,
     +                          run_duration_in,start_time_in,fi_in,
     +                          user_par_in(30),st_var_in(20),in_history
      common  /trans_out/       lptout,xout(mn),yout(mn),eout(mn),
     +                          xcaptout,ycaptout,out_title,
     +                          delta_out,inst_code_out,inst_name_out,
     +                          xcode_out,ycode_out,L1_out,L2_out,tthet_out,
     +                          no_spectrum_out,run_number_out,run_user_out,
     +                          run_duration_out,start_time_out,fi_out,
     +                          user_par_out(30),st_var_out(20),out_history
```

(see 5.4 for details of xcode and ycode)

5.4 xcode and ycode

XCODE and YCODE are used to specify the current units for the workspace (as set by the Units command).

XCODE

1	CHANNEL NO.	ELASTIC
2	total time-of-flight (μS)	"
3	wavelength (Å)	"
4	d-spacing (Å)	"
5	energy (meV)	"
6	momentum transfer ($Å^{-1}$)	"
7	Q^2 in ($Å^{-2}$)	"
8	τ in μS/m	"
9	ΔE in meV (E1-E2)	INELASTIC

YCODE

1-9	as for xcode but the y units are in neutrons X^{-1} where X are the corresponding units along the x-axis
0	This occurs when the workspace contains a ratio making the y-axis dimensionless.

All the data read in from a .RAW file is in n/μs and therefore has XCODE = YCODE = 2.