Lawrence Berkeley Laboratory
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SUSIE REFERENCE MANUAL

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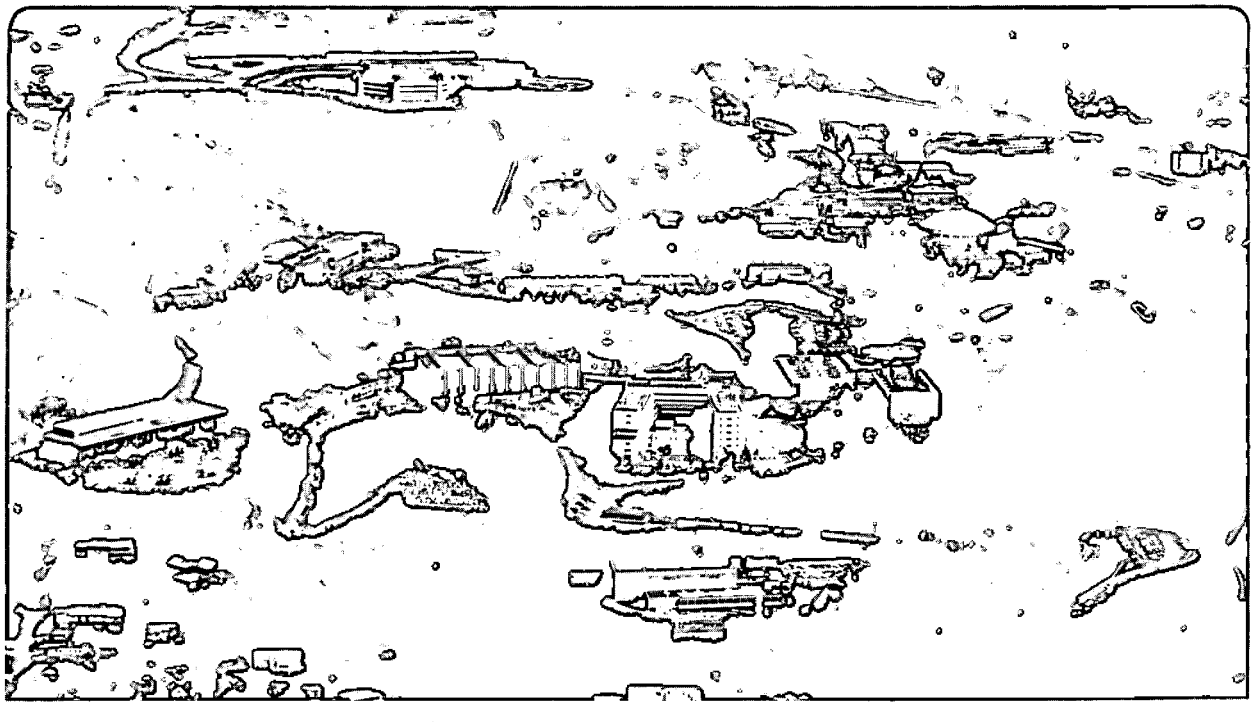

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SUSIE Reference Manual

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1. INTRODUCTION

SUSIE is a program for interactive analysis of one and two dimensional spectra. It runs on the Modcomp Classic computers, and uses the Tektronix 4014 with a high-speed DMA interface and a LBL designed supplemental control panel. The original Modcomp version was written by M. Neiman (LBL PUB-3014, FEB. 1981). The current version is the result of a number of major revisions and extensions, the most significant being the addition of 2-D spectra, and the ability to access spectra which are created by the EVA event sorting program.

All spectra are stored on the disk, keeping only one 1-D spectrum (the current spectrum) in memory at a time. The user may select either the large (300 mb) or the small (DIABLO) disc for spectrum storage. If the small disc is selected, there will be space for 30 1-D spectra and no 2-D spectra will be allowed. If the large disc is selected, there will be space for 500 1-D spectra and 64 2-D spectra. The disc space used by SUSIE is not shared by any other program, making it easy to resume an interrupted analysis session.

All 1-D commands operate upon the **current** spectrum, that is, the spectrum currently displayed on the screen. There are commands to fit peaks and otherwise manipulate the data in the spectra, commands to move spectra between disc and magnetic tape, commands for plotting on the Versate or Tektronix plotter, and commands to project 1-D spectra from a 2-D spectrum in various ways. Several interactive displays are available for both single and two dimensional spectra.

2-D spectra may be read from SUSIE's disc area, from the disc space used by EVA, and directly from the Dataram memory. All 2-D commands require the spectrum name or number(s) to be supplied as part of the command.

The GET, LABEL, READ, WRITE, and LOAD commands will handle both 1-D and 2-D spectra.

When a 2-D spectrum is displayed (GET command) it is first read from the disc into a 256 by 256 word array, adding channels together as necessary to make it fit. The display (scatter plot, projections, and isometric view) is then created from this array. This is necessary to allow dynamic projections to be made in a reasonably short time. When a projection or window is requested (PROJ or W2D commands) data is re-read from the disc in order to get full resolution.

Following this introduction there is a list of commands, followed by a more detailed description of each individual command.

In this manual the following notational conventions are used:

- Brackets "[ ]" indicate optional parameters.
- Parameters which are text strings rather than numeric values are shown in *ITALICS*.
- NUMBER means a number with a decimal point, such as 3.14, is required.
- INTEGER means a number with no decimal point.
- CONSTANT means that either a NUMBER or an INTEGER is allowed.

1.1. RECENT CHANGES

- MIN command. Calculates the average of the minimum value of each channel over a range of spectra.
- DEF command. Defines the size and location of 2-D spectra in the Dataram memory.
- FLAT command. Directs plot output to either the Versatec or the Tektronix flatbed plotter.
- MAKE command. The option LAST was added to create a spectrum from the parameters of the last (most recent) fitting operation.
- SUP command. Superimposes any 1-D spectrum over the spectrum currently being displayed.

2. GENERAL INFORMATION

2.1. STARTING THE PROGRAM

SUSIE uses both the DECwriter console and the Tektronix display. To prevent interference, any tasks which use either of these devices should be removed before starting SUSIE. To excecute the program type CTRL-C on the DECWRITER, then type:

```
/SUSIE/EXE,,TT
```

SUSIE begins by announcing its version number. The disc partitions used are controlled by program option bit 3 which is set in the task's resources and will not normally need to be altered by the user.

If option bit 3 is off, two partitions on the large disc will be used to store the spectra. The partition "SU4" holds 500 1-D spectra, each consisting of 4096 channels with 32 bits per channel. The partition "SU3" holds up to 64 2-D spectra, the actual number of spectra depends on the size of the spectra stored. The current amount of space available is about 5000 tracks, which is equivalent to 40,960,000 16 bit

channels, or 20,480,000 32 bit channels.

If option bit 3 is on, partition "RSW" on the upper DIABLO disc will be used to store the spectra. This disc has space for only 30 1-D spectra, and no 2-D spectra.

2.2. TAPE FILES

SUSIE keeps track of the files on tape by counting the file marks; therefore, if the tape goes off line it is possible that SUSIE will loose track of the tape position. The TAPE command can be used at any time to rewind the tape and reinitialize file counting.

2.3. ESCAPE TOGGLE

The switch marked "ENTER OPTION" on the 4014 keyboard is used to return control to the main command routine. It can be used to prematurely terminate the GET, LOAD or SHOW commands, and is the only way to return from the K or K2 command.

2.4. CHANNEL NUMBERING

The convention used in SUSIE is that the first channel of a spectrum is channel 0, so the channels of a 1024 channel spectrum are numbered 0-1023.

The maximum size of any 1-D spectrum is 4096 channels, with 32 bits per channel. Each 1-D spectrum is allocated this amount of space, regardless of actual size.

2-D spectra are allocated only the space actually required, and may use either 16 or 32 bits per channel.

When a spectrum is read from tape, the number of channels is established, and the first and last channel pointers are set to display the whole spectrum. The first and last channels displayed may be changed by the EXPAND and RESTORE commands. The total number of channels may be reset by the SIZE command.

The maximum number of channels in a 2-D spectrum is 4096 x 4096.

2.5. SPECTRUM NUMBERING

1-D spectra are numbered from 1 to 30 (small disc) or from 1 to 500 (large disc). 2-D spectra stored on the large disc are numbered from 501 to 564. 2-D spectra in the Dataram memory are numbered from 990 to 999.

2.6. I/O TIMES FOR 2-D SPECTRA

2-D spectra which occupy large amounts of disc space will require correspondingly large amounts of time for input and ouput operations. A full-track disc buffering package is used which provides access times of approximately 80 microseconds per data point. The time to read a 1000 by 1000 spectrum from disc is about 80 seconds, the time to read a 4000 by 4000 spectrum is about 21 minutes.

2.7. COMMAND INPUT

All commands and text strings may be abbreviated by using only the first THRee letters.

The delimiter between parameters can be either a space or a comma.

3. SUMMARY OF COMMANDS

ADD	[*SPEC*, FIRST_SPECTRUM [, LAST_SPECTRUM]] [CONSTANT]
AUTO	[ON] [OFF]
A2C	SPEC1, CONSTANT, SPEC2
A2S	SPEC1, SPEC2, SPEC3
B2D	DEST, SRC1,S RC2
BYE	
C	ANY REMARK
CALibrate	[AAA.A, BBB.B] [*SPEC*,N1,N2] [*FROM*,N] [*PRO*][?]
CHAnge	OLD, NEW
CNP	
COMpress	CONSTANT
CONnect	LOW, HIGH
C2D	SPEC1, SPEC2, XFACTOR, YFACTOR [,WPC]
COR	SRC, DEST
CP	[NEW]
DCP	N
DEF	SPEC, OFFSET, NX [,NY]
DEL	SPEC
DIR	
DISplay	[S1, S2, S3...]
DIVide	[*SPEC*, SPECTRUM_NUMBER] [CONSTANT]
D2C	SPEC1, CONSTANT, SPEC2
D2D	
D2S	SPEC1, SPEC2, SPEC3
DO	*FILE_NAME*
EXIt	
EXPand	[LOW, HIGH]
FIT	[*FUNCTION*] [W/N] [EXP]
FLAT	[ON] [OFF]
FWHM	CONSTANT
GET	SPECTRUM_NUMBER
INItialize	DISC
INTegrate	FIRST_CHANNEL, LAST_CHANNEL
K	[SPECTRUM_NUMBER]
K2	[SPECTRUM_NUMBER]
LABel	[-N] [, FIRST_SPECTRUM] [, LAST_SPECTRUM]
LINear	[*ALL*]
LOAd	[FIRST_SPECTRUM, COUNT, FILE_NO, SPEC_NO_IN_FILE]
LOG	[NUMBER_OF_CYCLES] [, *ALL*]
MAKe	[FUNCTION, C1, C2] [LAST]

MAP	[FIRST_FILE, LAST_FILE]
MARk	[CHANNEL]
MIN	FIRST_SPEC, LAST_SPEC, FIRST_CHAN, LAST_CHAN, N
MOMents	[LOW_CHANNEL, HIGH_CHANNEL]
MULtiply	[*SPEC*, SPECTRUM_NUMBER] [CONSTANT]
M2C	SPEC1, CONSTANT, SPEC2
M2S	SPEC1, SPEC2, SPEC3
PLOt	[STEPS_PER_CHANNEL]
PL2	SPECTRUM_NUMBER [, STEPS_PER_CHANNEL] [,*FLATBED*]
POWer	CONSTANT
PRG	SRC, DEST, N, AXIS, L, NCHAN [,WIDTH]
PRInt	[LOW, HIGH] [NUMBER OF_CHANNELS]
PROject	SPEC, *AXIS*, [, FIRST_CHANNEL, LAST_CHANNEL] [CHANNELS]
RCP	
REAd	SPECTRUM_NUMBER, TAPE_FILE [, RELATIVE_NUMBER_IN_FILE]
REStore	SPECTRUM_NUMBER [, *ALL*]
SAVe	SPECTRUM_NUMBER
SCAle	[FULL_SCALE] [, AUTO]
S	[FULL_SCALE] [, AUTO]
SET	CHANNEL, CONTENTS
SHIft	CHANNELS
SHOw	[FIRST_SPECTRUM] [, LAST_SPECTRUM]
SIZe	NUMBER OF_CHANNELS [,FIRST_SPECTRUM, LAST_SPECTRUM]
SMOoth	[SPEC1 [, SPEC2]]
SUBtract	[*SPEC*, SPECTRUM_NUMBER] [CONSTANT]
SUP	SPECTRUM_NUMBER
SUM	[LOW, HIGH] [ALL]
S2C	SPEC1, CONSTANT, SPEC2
S2S	SPEC1, SPEC2, SPEC3
TAPe	UNIT [, *NEWTAPE*]
TRAnspose	SPEC1, SPEC2
USE	EVA_SPECTRUM_AREA
USL	USL_FILE_NAME
VPG	FIRST,LAST
VPLot	PAGES
W2D	SPEC1, SPEC2, XMIN, XMAX, YMIN, YMAX
WRIte	[FIRST_SPECTRUM] [, LAST_SPECTRUM]
ZERo	[LOW, HIGH]

4. COMMAND DESCRIPTIONS

4.1. ADD CONSTANT TO 1-D SPECTRUM

ADD *SPEC*, F[L]
ADD C

The first form will add 1-D spectrum number F to the current 1-D spectrum. If the optional paramenter L is given, all 1-D spectra from F to L will be added to the current spectrum. The second form will add the constant C, channel by channel, to the current 1-D spectrum. The channel contents are integers, so the sum is rounded to an integer.

```
ADD     SPEC, 3
ADD     SPEC, 5, 9
ADD     7.0
```

4.2. ADD CONSTANT TO 2-D SPECTRUM

A2C SPEC1, CONSTANT, SPEC2

The value of CONSTANT will be added to each channel of the 2-D spectrum SPEC1 and the result will be stored in SPEC2. SPEC1 and SPEC2 may be the same 2-D spectrum.

```
A2C 201, 100, 209
```

4.3. ADD TWO 2-D SPECTRA TOGETHER

A2S SPEC1, SPEC2, SPEC3

Each channel of SPEC1 is added to the corresponding channel of SPEC2, the result is stored in SPEC3. SPEC1 and SPEC3 may be the same 2-D spectrum. SPEC1 and SPEC2 must have the same dimensions.

```
A2S 201, 202, 209
```

4.4. AUTOMATIC SCALING OF 1-D SPECTRA

AUTO [ON] [OFF]

This command sets the automatic scaling mode on or off. When AUTOSCALE is ON (default), the full scale value of a 1-D spectrum is automatically set to 1.1 times the highest value in the currently displayed part of the spectrum. When AUTOSCALE is OFF, the full scale value is changed only by the SCALE command.

4.5. BUILD 2-D SPECTRUM

B2D DEST,S1,S2

This command creates a 2-D spectrum DEST from the product of the two 1-D spectra S1 and S2.

```
B2D     201,9,10
```

4.6. BYE

BYE

When this command is issued, SUSIE terminates immediately. All spectra are left on disc, and will be recovered automatically when SUSIE is restarted. This command is the same as the EXIT command.

4.7. TYPE A COMMENT

C Any one line remark

This command accepts whatever is typed, then draws a line of asterisks.

4.8. CALIBRATE 1-D SPECTRUM

CAL
CAL C1, C2
CAL *SPEC*, N1 [,N2]
CAL *FROM*, N
CAL *PRO*
CAL ?

If no options are present, the current set of calibration points (see CP command) are fitted to a straight line and the slope and offset of the current 1-D spectrum are set to C1 and C2 from the equation:

$$ENERGY = C1 * CHANNEL + C2$$

If the options consist of two real numbers C1 and C2, then the slope and offset of the current 1-D spectrum are set to C1 and C2.

If the SPEC option is present, the calibration constants of the current 1-D spectrum (set by a previous CAL command) are copied to 1-D spectrum N1, or to 1-D spectra N1 through N2.

If the FROM option is present, the calibration constants of the 1-D spectrum N are copied to the current spectrum.

If the PRO option is present, the calibration coefficients of the current spectrum are saved for later use by the PRO command.

If the ? option is present, the current calibration values are typed.

```
CAL .191, 3.22
CAL SPEC, 11
CAL FROM,21
```

4.9. CHANGE CHANNEL CONTENTS

CHANGE OLD, NEW

Change will scan the current 1-D spectrum, channel by channel. If any channels are found which contain OLD counts, the contents of that channel is changed to NEW.

```
CHA 100, 47
```

4.10. CLIP NEGATIVE POINTS

CNP

This command will set all channels of the current spectrum which contain a negative value to zero. The number of counts thus removed are reported as "counts added".

4.11. COMPRESS A 1-D SPECTRUM

COMPRESS C

Compress will take the current 1-D spectrum and compress it by adding C channels together. If C is less than one the 1-D spectrum will be edxpanded instead of compressed. If C is a non-integer small rounding errors may result.

The energy calibration factor (if any) will be recalculated.

```
COMP 10
COM 1.03
COM 0.97
```

4.12. COMPRESS A 2-D SPECTRUM

C2D SPEC1,SPEC2,XCF,YCF [,WPC]

SPEC1 is copied to SPEC2 with the X and Y axes compressed by adding XCF channels together in the X direction and adding YCF channels together in the Y direction. XCF and YCF must be positive integers.

The WPC parameter specifies the words per channel of the destination spectrum. The value of WPC must be 1 or 2. If WPC is missing, the destination will have the same words per channel as the source.

```
C2D 201,209,2,3
C2D 204,211,2,1,2
```

4.13. CONNECT POINTS IN 1-D SPECTRUM

CON FIRST,LAST

The channels between FIRST and LAST are set to values which will, when plotted, draw a straight line between FIRST and LAST.

4.14. CREATE CORRELATED SPECTRUM

COR SPEC1,SPEC2

A correlated 2-D spectrum SPEC2 is created from SPEC1.

COR 201,202

4.15. CALIBRATION PEAK DEFINITION

CP
CP *NEW*

This command expects the user to define one or more calibration peaks in the current 1-D spectrum using the cursor on the CRT. For each peak the user is asked to "MARK PEAK CENTER" and to "MARK PEAK LIMITS". The cursor is positioned with the thumbwheel and the spacebar is used to indicate when the cursor position is to be read. When a peak has been designated, it is fitted to a gaussian and the fitted function is drawn on the screen. The user is then asked if the peak is OK. If the reply given is "Y" the channel of the peak is saved in the next available slot of the calibrating peak table. If the reply is anything else the peak is ignored. The user is then asked to mark another peak.

When all desired peaks have been designated, the user types some character other than the spacebar. The program then prints the channel number of each peak and asks the user to enter the associated energy.

If the option NEW is present, the calibration peak table is initialized, i.e. the first peak entered will go to slot one of the table.

Note that this command DOES NOT actually calibrate any spectrum, it simply sets up the calibration table. To calibrate a spectrum, you must use some form of the CAL command.

4.16. DEFINE CALIBRATION POINTS

DCP N

Defines N calibration points. The user is prompted for channel and energy of each point. The data entered goes into the same calibration point table used by the CP and CAL commands.

4.17. DEFINE DATARAM SPECTRUM

DEF SPEC,OFFSET,NX[,NY]

This command must be used before any command can access a spectrum in the Dataram memory.

SPEC is the spectrum number, must be from 990 to 999.

OFFSET is the address in the Dataram memory of the first word of the spectrum.

NX is the number of X channels in the spectrum, NY is the number of Y channels. If NY is missing, the value of NX will be used.

4.18. DELETE A 2-D SPECTRUM

DEL N

Delete the 2-D spectrum N, if it exists. The number of tracks recovered is printed on the Decwriter.

4.19. DISPLAY A GROUP OF 1-D SPECTRA

DIS [S1,S2,...,S8]

This command displays the requested 1-D spectra simultaneously on the CRT screen. Up to ten 1-D spectra may be displayed at once. If no 1-D spectrum numbers are present, the list of 1-D spectra from the previous DIS command is used.

Also see the SHOW command.

DIS
DIS 1,2,3,7,21,22

4.20. PRINT SPECTRUM DIRECTORY

DIR

This command prints a 4 page report on the Versatec showing the names of the 1-D and 2-D spectra currently on the disc.

4.21. DIVIDE 1-D SPECTRUM

DIVIDE *SPEC*, S
DIVIDE C

The first form will divide the current 1-D spectrum by 1-D spectrum number S.

Zero channels in 1-D spectrum S are treated as follows: If the corresponding channel in the current 1-D spectrum contains a zero, the result is set to 1; otherwise, the result is set to the arbitrary value 10,000.

The second form will divide the current 1-D spectrum, channel by channel, by the constant C. The result is rounded to an integer. C must be greater than 0.5 .

```
DIV       SPEC  14
DIVIDE    28.3
```

4.22. DIVIDE 2-D SPEC BY CONSTANT

D2C SPEC1,CONSTANT,SPEC2

Each channel of the 2-D spectrum SPEC1 will be divided by CONSTANT and the result will be stored in SPEC2. SPEC1 and SPEC2 may be the same 2-D spectrum.

```
D2C 201,100,209
D2C 201,1.03,209
```

4.23. DISPLAY DIRECTORY OF 2-D SPECTRA

D2D

A directory of the 2-D spectra currently in SUSIE'S disc space is displayed on the Tektronix screen. This display shows the number of tracks used by each spectrum, and the label field of each spectrum descriptor.

4.24. DIVIDE 2-D SPECTRUM

D2S SPEC1,SPEC2,SPEC3

Each channel of SPEC1 is divided by the corresponding channel of SPEC2, the result is stored in SPEC3. SPEC1 and SPEC3 may be the same 2-D spectrum. SPEC1 and SPEC2 must have the same dimensions.

```
D2S 201,202,209
```

4.25. DO COMMANDS FROM USL

DO *NAME*

If one has a time-consuming or repetitious series of 1-D spectrum manipulations to peform, it can be convenient to prepare all the commands at once using the editor [SED] and then merely point SUSIE to the command list. This command executes a set of SUSIE commands found on the file NAME in the current USL file (default is RSL). When the last command in the file has been executed, control is returned to the keyboard. The assignment of the USL file may be changed with the USL command.

```
DO  CMDLIST
```

4.26. EXIT

EXIT

When this command is issued, SUSIE terminates immediately. All spectra are left on disc, and will be recovered automatically when SUSIE is restarted. This command is identical to the BYE command.

4.27. EXPAND 1-D SPECTRUM

EXPAND [LOW HIGH]

This command is used to select an interval of the current 1-D spectrum and expand it so that it fills the entire width of the display screen. If the optional parameters LOW and HIGH are given, the interval from LOW to HIGH will be displayed. If they are absent, a cursor will appear and is used to indicate the desired interval.

```
EXP          123 550
EXPAND
```

4.28. FIT FUNCTION TO CURRENT SPECTRUM

FIT [FUNC] [W/N] [EXP]

FUNC may have the value: **PEAK, TAIL, EXP**onential, or **LINE.** This command is used to fit a function to an interval of the current 1-D spectrum.

If the 2nd parameter is W (or is missing) all points are weighted by 1/Y. If the 2nd parameter is any other character, the weighting factor is set to 1.0 for all points.

The third parameter is the value of EXP used in the TAIL fit only (Default = 3.0).

The region to be fitted is designated with the thumbwheel cursor on the Tektronix keyboard. After moving the vertical cursor bar to the desired location, one of the following keys must be used:

L Defines the limits of the region to be used. The upper and lower limits are both designated by the "L" key, and either the lower or upper limit can be entered first.

E Defines the limits of a region to be excluded from the fit. Any number of regions may be excluded.

P Defines the approximate center of each peak to be fitted.

F Tells the program to begin the fitting calculation.

Q Use this key if you want to quit without fitting.

If FUNC = *PEA* (or is missing), the function is a linear background plus 1 to 3 Gaussian peaks, all of the same width. The function used is:

$$y[x] = A_1 + A_2 x + A_4 e^{\frac{1}{2}\left[\frac{x-A_5}{A_3}\right]^2} + A_6 e^{\frac{1}{2}\left[\frac{x-A_7}{A_3}\right]^2} + \cdots$$

The initial value of the A_3 parameter can be set with the FWHM command.

When the least-squares fit is completed, a table showing the center, height, and area of each peak is printed. The height and area are measured *above* the background, i.e. adding a constant to the spectrum does not change the height or area. If the iterative fitting routine is unable to achieve a fit, the comment "NO CONVERGENCE" is printed.

If FUNC = EXP, the function used is:

$$y[x] = A_1 e^{A_2 x}$$

If FUNC = TAIL, the function used is:

$$y[x] = A_1 x^{EXP} e^{\frac{X}{A_2}}$$

If FUNC = LINE, the function used is:

$$y[x] = A_1 x + A_2$$

4.29. SET FLATBED MODE ON OR OFF

FLAT [ON] [OFF]

This command directs all output which normally goes to the Tektronix 4014 screen to go to the flatbed plotter instead. The plotter must be ready (pen and paper loaded) before "FLAT ON" is issued. To return displays to the screen, the command "FLAT OFF" must be issued.

4.30. SET INITIAL FWHM PARAMETER

FWHM CONSTANT

This command is used to initialize the value of the full width, half maximum parameter used by the gaussian peak fitting routine. The default value of this parameter is 2.0.

FWHM 5.7

4.31. GET SPECTRUM AND DISPLAY

GET S

This command will get spectrum S from the disk, and display it. S can be either a spectrum number, or the name of a spectrum in the EVA space on the disc.

If S is a 1-D spectrum it will be made the current spectrum.

If S is a 2-D spectrum, it will be displayed with 256 by 256 resolution with dynamic X and Y projections. The Z (intensity) axis is used to show the number of counts in each channel. The Z threshold may be adjusted to emphasize the area of interest. The X and Y cursors may be used to define a "window" which is then magnified to fill the whole display area. The restore key is used to remove a window which has been defined. To leave this display, momentarily press the EXIT key.

GET 12

4.32. INITIALIZE

INI *DIS*

This command will set the 2-D disc area to empty. This may be necessary to recover space used by 2-D spectra previously placed on the disc. The purpose of the argument DIS is to reduce the chance of the 2-D space being accidentally cleared.

Individual 2-D spectra may be deleted by using the DEL command.

INI DIS

4.33. INTEGRATE 1-D SPECTRUM

INTEGRATE FIRST,LAST

The channels of the current 1-D spectrum from FIRST to LAST are integrated. Beginning with the channel designated by FIRST, each channel is set to the integral of the previous channels. Integration may be done in either direction.

4.34. K (INTERACTIVE CENTROIDS)

K [SPECTRUM NUMBER]

This command sends control to an interactive display which uses the keyboard toggle switches to move two cursors across the display. If the optional SPECTRUM NUMBER is present, a "GET SPECTRUM NUMBER" is performed before going to the interactive subroutine.

A continuous display of the channel and counts corresponding to each cursor is presented, along with the SUM of all channels between the cursors, the CENTROID, and VARIANCE of the area between the cursors.

If the MARK switch is depressed, the MOMENTS of the area currently between the cursors are printed on the DECwriter.

The cursors are moved individually left and right by the two outermost "POSITION CURSORS" switches. The "BOTH CURSORS" switch is used to move both cursors at the same time.

The "PRIOR" and "NEXT" switches select the next higher or lower numbered spectrum, keeping the same cursor position and expansion factor.

The "PRIOR BLOCK" and "NEXT BLOCK" switches select the next higher or lower block of channels in the same spectrum.

The "EXPAND/RESTORE" switch may be used to change the X-axis scaling. Raising the switch expands the X-axis so that the channels between the cursors fill the screen. Lowering the switch restores the scale to whatever it was when this display was entered.

The "AUTO SCALE" switch is used to reset the vertical scale to 1.1 times the highest channel currently visible on the screen.

The "LOG-LIN" switch is used to change the vertical axis from linear to logarithmic or from log to linear.

To return control to the DECWRITER, *momentarily* depress the "EXIT" switch.

4.35. K2 (PEAK MARKING)

K2 [SPECTRUM NUMBER]

This command sends control to an interactive display which uses the keyboard and toggle switches to select a number of peaks. If the optional SPECTRUM NUMBER is present, a "GET SPECTRUM NUMBER" is performed before going to the interactive subroutine.

The purpose of this display is to create a list of selected peaks. This list is used by the VPLOT command to print the channel or energy of each peak in the graph of the spectrum.

The method used is to define a line of one or more straight segments which cross the peaks to be selected.

To define the line, *momentarily* depress the key labeled "DEFINE LINE". The 4014 crosshair cursor will appear. Position the crosshair at the left-most point of the line and type a space. Move the crosshair right to the next point and type a space. Repeat, always moving to the right, until you have reached the last point on the line. On the last point press the X key instead of the space. You can display the line by pressing the "SHOW LINE" key. If the line is unsatisfactory the "DEFINE LINE" sequence may be repeated.

When a satisfactory line is found, *momentarily* press the "FIND PEAKS" key. The number of peaks found will be displayed on the screen.

To make a plot, first leave this display by depressing the "EXIT" key, then use the VPL command.

The "SUBTRACT BACKGROUND" key can be used to suppress the background level of the spectrum, this may make it easier to define the line which crosses the desired peaks.

4.36. DEFINE SPECTRUM LABELS

LABEL [-N] [SPEC 1] [SPEC 2]

This command is used to change any of the four 32-byte labels that are associated with each spectrum. N is the label number (1-4). If -N is missing, label number 1 will be changed.

If SPEC 2 is missing, only SPEC 1 will be relabeled. If SPEC 1 is missing, only the label of the current 1-D spectrum will be changed.

The command will request a 32 character label which will be applied to the designated spectra.

The four labels are displayed on the screen and are printed when a 1-D spectrum is printed or plotted.

The NSD standard tape header format allows only the 32 bytes of LABEL 1 and the first 24 bytes of LABEL 2 to be written on tape.

4.37. LINEAR DISPLAY MODE

LINEAR [*ALL*]

This command will change the display of the current 1-D spectrum from logarithmic to linear on the Y axis. If the optional parameter ALL is given, all 1-D spectra, when they are displayed, will be in linear form.

```
LINEAR
LIN   ALL
```

4.38. LOAD SPECTRA FROM TAPE

LOAD [SPEC],[N],[F],[S]

This command will load N 1-D spectra from the tape, beginning with file F on the tape. The spectra will be stored on the disc begining with spectrum number SPEC. The S'th spectrum from each file is the one which will be read. The default for all four parameters is 1.

SPEC can be either 1-D or 2-D but must agree with the spectrum type found on the tape.

```
LOAD      1,10
LOA 1,10,20
LOA 10,5,20,2
```

4.39. LOGARITHMIC DISPLAY MODE

LOG [N] [*ALL*]

This command will change the Y-axis display of the current 1-D spectrum to logarighmic. If the optional parameter N is given, the 1-D spectrum will be displayed with N cycles. N may assume values from 2 to 9. If N is omitted [or zero] the number of cycles will automatically adjust. If the optional parameter ALL is given, all 1-D spectra, when displayed, will be logarithmic.

```
LOG 3
LOG 4,ALL
```

4.40. MAKE A 1-D SPECTRUM

MAKE FUNC A B

Where FUNC may have the value: LASt, EXPonential, LINear, or POWer.

This command will produce a 1-D spectrum containing a calculated function y= F(x), where x is the channel number, and y is the number of counts in that channel.

If the function is LAST, the function and the coefficients from the last invocation of the FIT command will be used.

If FUNC = EXP the function used is:

$$y = Ae^{Bx}$$

If FUNC = LIN the function used is:

$$y = Ax+B$$

If FUNC = POW the function used is:

$$y = Ax^{B}$$

```
MAKE    LAST
MAKE    EXPO 0.1 0.04
MAKE    LINE 4.0 9.0
MAKE    POW  4,1.03
```

4.41. PRINT MAP OF A SPECTRUM TAPE

MAP [FIRST, LAST]

This command will print a map of the input 1-D spectrum tape on the line printer. The map will show the contents and titles of all files. If the optional parameters FIRST and LAST are given, only the interval from FIRST to LAST will be printed.

4.42. MARK A CHANNEL

MARK [C]

This command is used to mark a channel in the current 1-D spectrum. If the optional parameter C is given, that channel will be marked on the display with a vertical line. If no channel is given, the operator must position the cursor to the desired channel, and type any character. The channel number and its contents will be printed on the DECwriter.

If the cursor position is indicated by typing a space, the cursor will return and another channel can be marked. Any character other than a space will terminate the command.

```
MARK      307
MARK
```

4.43. FIND AVERAGE MINIMUM

MIN FIRST,LAST,FCH,LCH,N

This command creates a spectrum in which each channel contains the average of the smallest values found in a group of consecutive 1-D spectra.

FIRST is the first spectrum in the group, LAST is the last spectrum in the group.
FCH and LCH are the first and last channels to be averaged. Channels outside of this range are set to zero.
N is the number of samples to be averaged. For example, the group could contain 10 spectra, but if N was set to 5, the resulting value for each channel would be the average of the 5 smallest values found in the group of 10.

4.44. CALCULATE MOMENTS

MOMENTS [LOW,HIGH]

This command will define an interval of the current 1-D spectrum and calculate the first three moments of the distribution of counts in that interval. If LOW and HIGH are given, they are used to define the interval; otherwise, the cursor appears and must be used. The moments are defined as follows:

CENTROID:

$$\mu 1 = \langle x \rangle$$

VARIANCE:

$$\mu 2 = \langle x^2 \rangle - \langle x \rangle^2$$

THIRD MOMENT:

$$\mu 3 = \langle x^3 \rangle - 3\langle x^2 \rangle \langle x \rangle + 2\langle x \rangle^3$$

```
MOM       100 400
MOMENTS
```

4.45. MULTIPLY 1-D SPECTRA

MULTIPLY *SPEC,S*
MULTIPLY C

The first form will multiply the current 1-D spectrum by 1-D spectrum number S.

The second form will multiply the current 1-D spectrum, channel by channel, by the constant C. The result is rounded to an integer.

```
MULT      SPE 9
MUL  14.42
```

4.46. MULTIPLY 2-D SPEC BY CONSTANT

M2C SPEC1,CONSTANT,SPEC2

Each channel of the 2-D spectrum SPEC1 will be multiplied by CONSTANT and the result will be stored in SPEC2. SPEC1 and SPEC2 may be the same 2-D spectrum.

```
M2C 201,100,209
M2C 201,1.34,209
```

4.47. MULTIPLY 2-D SPEC BY ANOTHER

M2S SPEC1,SPEC2,SPEC3

Each channel of SPEC1 is multiplied by the corresponding channel of SPEC2, the result is stored in SPEC3. SPEC1 and SPEC3 may be the same 2-D spectrum. SPEC1 and SPEC2 must have the same dimensions.

```
M2S 201,202,209
```

4.48. PLOT ON VERSATEC

PLOT [STEPS PER CHANNEL]

This command will make a plot of the current 1-D spectrum on the Versatec printer. Full scale, LIN/LOG mode, and the interval of the 1-D spectrum plotted will be the same as seen on the display. There will be short tic marks every 10 channels and longer tic marks every 100 channels.

If the parameter STEPS PER CHANNEL is missing, the plot will be automatically sized to two pages on the Versatec if possible. The limits on the scaling of the x-axis are from 1 to 25 steps/channel. One step is 0.01 inch.

Also see the VPLOT command.

```
PLOT
PLO  5
```

4.49. PLOT TWO SPECTRA

PL2 SPEC [STEPS PER CHANNEL]

This command will plot the current spectrum and spectrum SPEC on the Versatec simultaneously. The current spectrum will appear as a solid line, spectrum SPEC will appear as a dotted line. The mode of the plot (log or linear), full scale, and number of channels will be the same as if the current spectrum was plotted by itself.

The STEPS PER CHANNEL parameter has the same meaning as in the PLOT command.

```
PL2  11
PL2  11,5
```

4.50. RAISE SPECTRUM TO A POWER

POWER C1

This command will raise the contents of each channel in the current 1-D spectrum the the C1 power. C1 may be greater or less than one.

```
POWER    2
POW      .5
```

4.51. PRINT SPECTRUM

PRINT [LOW, HIGH] [N]

This command will print a listing on the line printer showing the number of counts in each channel of the current 1-D spectrum. It the optional parameters LOW and HIGH are given, only the interval from low to high will be printed.

If the single parameter N is given, the first N channels will be printed.

4.52. MAKE PROJECTION OF 2-D SPECTRUM

PRO SPEC *AXIS* [L,H] [,W] [,N]

This command makes a 1-D projection from a 2-D spectrum. SPEC is the 2-D spectrum number, AXIS defines the type of projection, which must be X, Y, D, or P.

X = Project onto the X axis. If L and H are missing, the last position of the 2-D spectrum's horizontal cursors will be used. From 1 to 6 sets of [L,H] values may be specified.

Y = Project onto the Y axis. If L and H are missing, the last position of the 2-D spectrum's vertical cursors will be used. From 1 to 6 sets of [L,H] values may be specified.

D = Make projection perpindicular to the diagonal of the spectrum, containing the number of channels specified by the W parameter. If W is missing, the projection will contain the maximum possible number of channels.

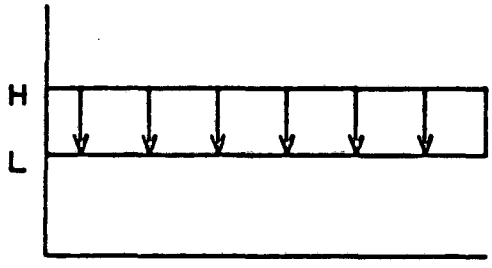
P = Make projection parallel to the diagonal.

In all cases the projected spectrum becomes the current spectrum, and can be saved and manipulated like any other 1-D spectrum.

The parameters L, H, W, and N are defined in the following diagrams.

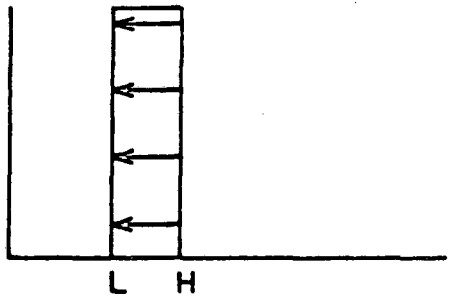
"X" PROJECTION

PRO 201, X, L, H



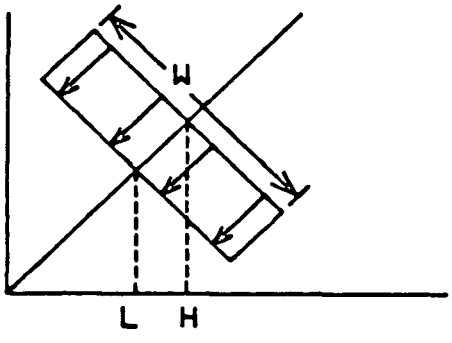
"Y" PROJECTION

PRO 201, Y, L, H



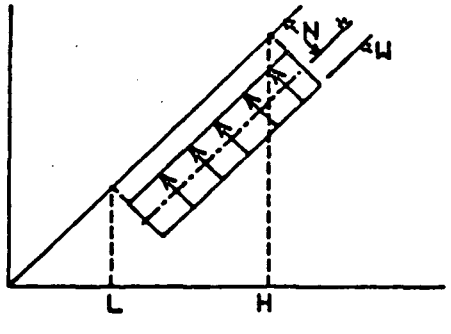
"D" PROJECTION

PRO 201, D, L, H, W



"P" PROJECTION

PRO 201, P, L, H, N, W



4.53. PROJECT GROUP OF 1-D SPECTRA

PRG SRC,DEST,N,AXIS,L,NUMCHAN [,W]

This command is similar to the PRO command, but it creates a group of consecutively numbered 1-D spectra instead of just one. SRC is the 2-D source spectrum, DEST is the first 1-D destination spectrum. N is the number of 1-D projections to create. AXIS is the X, Y, or D projection type, as in the PRO command. L is the first channel of SRC to use, NUMCHAN is the number of channels of SRC used in each projection. W is the maximum number of channels in each projection (D projections only).

4.54. RESET CALIBRATION PEAKS

RCP

This command prints the current table of calibration peaks to allow the user to change energy values. After each peak is printed, the user may type a new energy value. A carriage return may be typed if no change in the energy is desired.

4.55. READ SPECTRUM FROM TAPE

READ S F [N]

This command is used to read one spectrum from tape. It will read one spectrum from file F, and place it on disk as spectrum number S. If it is a 1-D spectrum it will be made the current spectrum. If there is more than one spectrum in file F, the Nth spectrum is read. If N is omitted, N = 1 is assumed.

```
READ        10,2,2
READ        201,47
```

4.56. RESTORE SPECTRUM SIZE

RESTORE SPEC
RESTORE [*ALL*]

This command restores the maximum and minimum channel numbers to the full size of the spectrum.

If no parameter is given it will restore the display of the current 1-D spectrum, so that the entire 1-D spectrum is displayed.

If the optional parameter ALL is given, all 1-D spectra will be restored (when they are displayed).

If SPEC is given, it will restore only the spectrum SPEC, which may be either 1-D or 2-D.

```
RESTORE
RES ALL
REST        207
```

4.57. SAVE 1-D SPECTRUM

SAVE S

This command saves the current 1-D spectrum on disk as 1-D spectrum number S.

```
SAVE        20
```

4.58. SET FULL SCALE VALUE

SCALE [F] *[AUTO]*
S

This command is used to change the full scale value used when displaying the current 1-D spectrum. If the optional parameter F is given, full scale is set to F; if the option parameter AUTO is present, full scale is set to 1.1 times the largest channel; otherwise, the cursor appears and is used to indicate the full scale desired.

The single-letter command "S" is the same as "SCALE AUTO".

```
SCALE
SCA     2500
SCA     AUTO
```

4.59. SET CHANNEL CONTENTS

SET C K

This command is used to change the contents of one channel in the current 1-D spectrum. It will take channel number C and insert K counts in it.

```
SET   510,23492
```

4.60. SHIFT SPECTRUM LEFT OR RIGHT

SHIFT CHANNELS

Shifts the current 1-D spectrum by CHANNELS. The channels shifted out are lost, and zeros are shifted in. If channels > 0 the 1-D spectrum is shifted to the right; if channels < 0 the shift is to the left. The offset calibration factor (if any) is adjusted to compensate for the shift.

```
SHIFT      3
SHI -5
```

4.61. DISPLAY A GROUP OF 1-D SPECTRA

SHOW FIRST, LAST

This command will display on the screen the 1-D spectra from FIRST to LAST, inclusive.

```
SHOW       1 5
SHO 11,18
```

4.62. SET SPECTRUM SIZE

SIZE N, [*FIRSTSP, LASTSP*]

Size will change the size of the current 1-D spectrum to N channels. If the optional parameter *FIRSTSP, LASTSP* is given, the size of all 1-D spectra from *FIRSTSP, LASTSP* will be changed to N channels.

```
SIZE 512
SIZ  1024,100,149
```

4.63. DATA SMOOTHING

```
SMOOTH
SMOOTH      SPEC
SMOOTH      SPEC1,SPEC2
```

The first form of this command will smooth the current 1-D spectrum using a 3 channel interval. The second form will replace the spectrum SPEC with a smoothed version. The third form will create or replace SPEC2 with a smoothed copy of SPEC1.

The formula used for 1D spectra is:

$$y'[x] = \frac{y[x-1]}{4} + \frac{y[x]}{2} + \frac{y[x+1]}{4}$$

where x is the channel number.

When a 2-D spectrum is smoothed, each point is created by taking 1/2 of the value of the point plus 1/8 of the value of each of the 4 adjacent points.

4.64. SUBTRACT FROM 1-D SPECTRUM

```
SUBTRACT    SPEC, S
SUBTRACT    C
```

The first form will subtract 1-D spectrum number S from the current 1-D spectrum. The second form will subtract the constant C, channel by channel, from the current 1-D spectrum. The result is rounded to an integer.

```
SUBT        SPEC 1
SUB  100
```

4.65. SUBTRACT CONSTANT FROM 2-D SPEC

S2C SPEC1,CONSTANT,SPEC2

CONSTANT will be subtracted from each channel of the 2-D spectrum SPEC1, and the result will be stored in SPEC2. SPEC1 and SPEC2 may be the same 2-D spectrum.

```
S2C  201,100,209
```

4.66. SUBTRACT 2-D SPEC FROM ANOTHER

S2S SPEC1,SPEC2,SPEC3

Each channel of SPEC2 is subtracted from the corresponding channel of SPEC1, the result is stored in SPEC3. SPEC1 and SPEC3 may be the same 2-D spectrum. SPEC1 and SPEC2 must have the same dimensions.

S2S 201,202,209

4.67. SUM CHANNELS IN 1-D SPECTRUM

SUM [LOW HIGH] [ALL]

This command will define an interval of the current 1-D spectrum and sum the counts in the interval. If the optional parameters LOW and HIGH are given, they are used to define the interval; otherwise, the cursor appears and must be used. The interval includes the end points.

SUM 100 450
SUM

4.68. SUPERIMPOSE OTHER SPECTRUM

SUP SPEC

This command draws the spectrum SPEC over the current spectrum on the Tektronix screen. Only the data is drawn (no text or axis), and the channel range and full scale of the current spectrum are used.

4.69. DEFINE TAPE UNIT

TAPE UNIT [*NEW*]

This command defines the tape station currently in use, for both input and output. Whenever this command is issued, the selected tape is rewound. The allowable values for UNIT are 1,2,6,7,9 indicating MT1, MT2, HT6, HT7, and MT9 respectively. If the optional parameter NEW is given, the tape will be treated as a new tape, and the next WRITE command will start writing at the beginning of the tape.

TAPE 2
TAP 1 NEW

4.70. TRANSPOSE 2-D SPECTRUM

TRANSPOSE SPEC1,SPEC2

This command creates the 2-D spectrum SPEC2 which is the transpose (rows and columns interchanged) of the 2-D spectrum SPEC1. SPEC1 and SPEC2 may not be the same spectrum.

TRA 201,207

4.71. DEFINE EVA SPECTRUM AREA

USE N

This command defines which of the EVA5 spectrum partitions will be used when accessing spectra. The parameter N is the partition number (1-8).

USE 7

4.72. DEFINE USL FOR COMMAND LIST

USL name

This command is used to change the location for command lists used by the DO command. The default location is the partition RSL. Any File Manager file name or partition name may be used.

USL MSL
USL USL:ADOBE

4.73. PLOT GRAPH IN VERSAPLOT FORMAT

VPLOT [N] [,SPEC]

This command creates a graph of the current spectrum using the VERSAPLOT subroutine package. This format has fully labeled axes in both X and Y, and will show either channel number or energy on the X axis.

If the second parameter SPEC is present, the spectrum SPEC is superimposed over the current spectrum.

If the K2 display has been used to identify peaks, the channel or energy of each selected peak will be drawn on the graph.

The parameter N is the length of the desired plot, in pages.

4.74. PLOT A GROUP OF 1-D SPECTRA

VPG FIRST,LAST

This command will plot a group of 1-D spectra, from FIRST to LAST, on the versatec, using the versaplot format.

4.75. COPY WINDOW FROM 2-D SPECTRUM

W2D S1,S2,FIRSTX,LASTX,FIRSTY,LASTY

This command creates a 2-D spectrum from a section of the 2-D spectrum S1. The new spectrum will consist of the area bounded by FIRSTX, LASTX, FIRSTY, and LASTY. The channels of S2 will be numbered from 0 to (LASTX-FIRSTX) and 0 to (LASTY-FIRSTY).

```
W2D         201,207,1,100,10,101
```

4.76. WRITE SPECTRA TO TAPE

WRITE [F] [L]

This command is used to write spectra on tape. If no parameters are given, the current 1-D spectrum is written. If the optional parameter F is given alone, spectrum number F will be written on tape.

If both F and L are specified, spectra number F through L will be written. Each 1-D spectrum will be written on its own file.

Spectra F through L must all be either 1-D or 2-D.

```
WRITE
WRI 3
WRIT        5 14
```

4.77. ZERO SPECTRUM CHANNELS

ZERO LOW HIGH

Modifies the current 1-D spectrum by setting the contents of all channels in the inclusive interval from LOW to HIGH to zero.

```
ZERO    1000 1023
```

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