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SUSIE
A PROGRAM FOR ANALYSIS OF 1 DIMENSIONAL SPECTRA
VERSION: 20 Feb. 1981

Martin Neiman

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SUSIE

A PROGRAM FOR ANALYSIS OF 1 DIMENSIONAL SPECTRA

VERSION: 20 FEB 1981

Martin Neiman

Nuclear Science Division
Lawrence Berkeley Laboratory
University of California
Berkeley, CA 94720

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INTRODUCTION

Susie is a program for analysis of 1 dimensional spectra. It uses a disk for spectrum storage, only keeping one spectrum (the current spectrum) in core at a time. This enables Susie to manipulate 20 spectra, numbered from 1 to 20. All commands operate upon the current spectrum. There are commands to fit peaks and otherwise manipulate the data in the spectra as well as commands to move spectra both to and from the disk and to and from magnetic tape.

Following this introduction there is a list of commands, followed by a more detailed description of each individual command. Finally there is a section with some practical information and an example of a brief session using Susie.

In this manual I have used the following notational conventions:

1) Parentheses indicate optional parameters.
2) Underlining means that the text string, rather than a numeric value, is wanted.

All text strings may be abbreviated by using only the first four letters.

LIST OF COMMANDS

ADD	SPECTRUM, FIRST SPECTRUM (,LAST SPECTRUM) REAL NUMBER
CHANGE	OLD, NEW
COMPRESS	CHANNELS
DIVIDE	SPECTRUM, SPECTRUM NUMBER REAL NUMBER
EXIT	
EXPAND	(LOW, HIGH)
FIT	(FUNCTION)
GET	SPECTRUM NUMBER
INPUT	(AXC)
LABEL	
LIN	(ALL)
LOG	NUMBER OF CYCLES) (,ALL)
MAKE	FUNCTION,A1,A2
MAP	(FIRST, LAST)
MARK	(CHANNEL)
MOMENTS	(LOW, HIGH)
MULTIPLY	SPECTRUM, SPECTRUM NUMBER REAL NUMBER
OLD	SPECTRUM NUMBER (,NUMBER OF CHANNELS) ALL (,NUMBER OF CHANNELS)
PLOT	(FLATBED)
PRINT	(LOW, HIGH)
READ	SPECTRUM NUMBER, TAPE FILE (, RELATIVE NUMBER IN FILE) (, SKIP, NUMBER OF CHANNELS)
RESTORE	(ALL)
SAVE	SPECTRUM NUMBER

SCALE	(FULL SCALE)
SET	CHANNEL, CONTENTS
SHIFT	CHANNELS
SIZE	NUMBER OF CHANNELS (, ALL)
SMOOTH	
SUBTRACT	SPECTRUM, SPECTRUM NUMBER REAL NUMBER
SUM	(LOW, HIGH)
TAPE	UNIT (NEWTAPE)
WRITE	(FIRST SPECTRUM) (, LAST SPECTRUM)
ZERO	(LOW, HIGH)

ADD SPECTRUM F (L) or

ADD R

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

EXAMPLES

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

CHANGE OLD NEW

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

EXAMPLE

CHAN 100 47

COMPRESS C

Compress will take the current spectrum and compress it by adding C channels together. If C is a real number small rounding errors may result.

EXAMPLE

```
COMP    10
COMP    1.03
```

DIVIDE SPECTRUM S or
DIVIDE R

The first form will divide the current spectrum by spectrum number S. Zero channels in spectrum S are treated as follows: If the corresponding channel in the current 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 spectrum, channel by channel, by the real number R. The result is rounded to an integer.

EXAMPLES

```
DIVI   SPEC  14
DIVIDE 28.3
```

EXIT

This command is used to terminate the program.

EXPAND (LOW HIGH)

This command is used to select an interval of the current 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 apear and is used to inicate the desired interval.

EXAMPLES

```
EXPA    123  550
EXPAND
```

FIT (FUNC)

where FUNC may have the value: PEAKS, EXPONENTIAL, or LINE.

This command is used to fit a function to an interval of the current spectrum.

If FUNC = PEAKS (or is absent), the function is a linear background plus 1 to 3 Gaussian peaks (all of the same width).

The function used is

$$Y(x) = A_1 + A_2x + A_4e^{-\frac{1}{2}\left(\frac{x-A_5}{A_3}\right)^2} + A_6e^{-\frac{1}{2}\left(\frac{x-A_7}{A_3}\right)^2} + \ldots$$

First the interval to be fit is indicated, using the cursor. Then the peak positions are indicated with the cursor. One indicates that the cursor is in the desired position by hitting a key on the Tektronix keyboard. If a space is used, the cursor will remain on the screen so that additional peaks can be indicated. Any key other than a space will initiate the fitting.

If FUNC = EXPONENTIAL the function used is

$$Y(x) = A_1e^{A_2x}$$

The interval to be fit is indicated using the cursor.

If FUNC = LINE the function used is

$$Y(x) = A_1x + A_2$$

The interval to be fit is indicated using the cursor.

EXAMPLES

```
FIT
FIT     PEAK
FIT     EXPO
FIT     LINE
```

GET S

This command will get spectrum S from the disk, display it, and make it the current spectrum.

EXAMPLE

```
GET     12
```

INPUT (AXC)

If one has a time-consuming or repetitious series of 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. Input allows Susie to switch its input file between the console and disk partition AXC. Input alone will switch the input to the console. If the optional parameter AXC is present, input will be taken from disk partition AXC. In the latter case the user must provide a list of commands on this partition. This list should terminate with either an input or exit command.

To produce the command list, one can use the editor to make a file on the source library (USL) and then use the macro $MTXT FILE,AXC which will move the text (in noncompressed form) to AXC.

EXAMPLES

```
INPUT
INPUT   AXC
```

LABEL

This command will request a 32 character label. The label will be displayed on the screen and be printed out when a spectrum is printed or plotted.

LIN (ALL)

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

EXAMPLES

```
LIN
LIN     ALL
```

LOG (N) (ALL)

This command will change the display of the current spectrum to semi-log. If the optional parameter N is given, the 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 spectra, when displayed, will be semi-log.

EXAMPLES

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

MAKE FUNC A_1 A_2

Where FUNC may have the value: EXPONENTIAL, LINEAR.

This command will produce a spectrum containing a calculated function. Only the interval of the spectrum displayed will contain the function, the remainder being set to zero. If FUNC = EXPONENTIAL the function used is

COUNTS(CH) = A_1*EXP(A_2*CH)

If FUNC = LINEAR the function used is

COUNTS(CH) = A_1*CH + A_2

EXAMPLES

```
MAKE    EXPO  0.1  0.04
MAKE    LINE  4.0  9.0
```

MAP (FIRST, LAST)

This command will print a map of the input 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.

MARK (C)

This command is used to mark a channel in the current spectrum. If the optional parameter C is given, that channel will be marked on the display. If no channel is given, the cursor will appear and is used to indicate the channel desired, and the number and contents of the channel are printed. 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.

EXAMPLES

```
MARK    307
MARK
```

MOMENTS (LOW HIGH)

This command will define an interval of the current 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: $\mu_2 = \langle x^2 \rangle - \langle x \rangle^2$

$$\mu_3 = \langle x^3 \rangle - 3\langle x^2 \rangle\langle x \rangle + 2\langle x \rangle^3$$

EXAMPLES

```
MOME    100  400
MOMENTS
```

MULTIPLY SPECTRUM S or
MULTIPLY R

The first form will multiply the current spectrum by spectrum number S. The second form will multiply the current spectrum, channel by channel, by the real constant R. The result is rounded to an integer.

EXAMPLES

```
MULT    SPEC  9
MULT    14.42
```

OLD SPEC (NUMBER OF CHANNELS)
ALL (NUMBER OF CHANNELS)

The spectra in Susie are stored on the upper disk (on partition RSW). This command tells Susie to use the data on the disk as spectra. The first form of the command defines spectrum SPEC as existing on the disk. The second form defines all spectra as existing. If the optional parameter NUMBER OF CHANNELS is given, the spectra are defined to have that length; otherwise, the spectra are assumed to be the maximum size (defined when Susie is called).

EXAMPLES

```
OLD     ALL
OLD     3  1024
```

PLOT (FLATBED)

This command will make a plot of the current spectrum. Full scale, LIN/LOG mode, and the interval of the spectrum plotted will be the same as seen on the display. If the optional parameter FLATBED is given, the plot will be an exact duplicate of the screen plotted on the Tektronix flatbed plotter. Otherwise, the plot will appear on the Versatec printer. There will be short tic marks every 10 channels and longer tic marks every 100 channels.

EXAMPLES

```
PLOT
PLOT    FLAT
```

PRINT (LOW, HIGH)

This command will print a listing of the current spectrum on the line printer. If the optional parameters LOW and HIGH are given, only the interval from low to high will be printed.

EXAMPLES

```
PRINT
PRINT   400  800
```

READ S F (N) (SKIP, C)

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

If the optional parameters SKIP and C are present, the first C channels of the spectrum will be skipped before starting to read.

EXAMPLES

```
READ    1  1
READ    3  47  4
READ    12  9  SKIP  100
READ    20  3  2  SKIP  512
```

RESTORE (ALL)

This command will restore the display of the current spectrum, so that the entire spectrum is displayed. If the optional parameter ALL is given all spectra will be restored (when they are displayed).

EXAMPLES

```
REST
REST    ALL
```

SAVE S

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

EXAMPLE

```
SAVE    20
```

SCALE (F)

This command is used to change the full scale of the display of the current spectrum. If the optional parameter F is given the full scale is set to F; otherwise, the cursor appears and is used to indicate the full scale desired.

EXAMPLES

```
SCALE
SCAL    2500
```

SET C K

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

EXAMPLE

```
SET     510  23492
```

SHIFT CHANNELS

Shifts the current spectrum by CHANNELS. The channels shifted out are lost, and zeros are shifted in. If channels > 0 the spectrum is shifted to the right; if channels < 0 the shift is to the left.

EXAMPLES

```
SHIFT   3
SHIF    -5
```

SIZE N (ALL)

Size will change the size of the current spectrum to N channels. If the optional parameter ALL is given, all spectra will be changed to N channels.

EXAMPLES

```
SIZE    512
SIZE    1024  ALL
```

SMOOTH

This command will smooth the current spectrum using a 3 channel interval. The formula used is:

$$Y'(CH) = \tfrac{1}{4}Y(CH-1) + \tfrac{1}{2}Y(CH) + \tfrac{1}{4}Y(CH+1).$$

SUBTRACT SPECTRUM S or
SUBTRACT R

The first form will subtract spectrum number S from the current spectrum. The second form will add real constant R, channel by channel, to the current spectrum. The result is rounded to an integer.

EXAMPLES

```
SUBT    SPEC  1
SUBT    100
```

SUM (LOW HIGH)

This command will define an interval of the current 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.

EXAMPLES

```
SUM     100  450
SUM
```

TAPE UNIT (NEWTAPE)

This command defines the tape station used. The allowable values for UNIT are 1, 2, 9 indicating MT1, MT2, MT9 respectively. If the optional parameter NEWTAPE is given, the tape is assumed to be a new tape meaning that spectra will be written directly at the beginning of the tape.

EXAMPLES

```
TAPE    2
TAPE    1  NEWT
```

WRITE (F) (L)

This command is used to write spectra on tape. If no parameters are given, the current spectrum is written. If the optional parameter F is given alone, spectrum number F will be made the current spectrum (but not displayed) and written on tape. If both F and L are specified, spectra numbers F through L will be written. Each spectrum will be written on its own file. A title (maximum 32 characters) will be requested.

EXAMPLES

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

ZERO LOW HIGH

Sets the contents of all channels in the inclusive interval from LOW to HIGH to zero.

EXAMPLE

```
ZERO    1000  1023
```

PRACTICAL INFORMATION

Susie uses both the teletype console and the Tektronix display, so both tasks B and C will be removed by Susie. To execute the program one must give the command /SUSIE/EXE,,TU to the operator communication task (OC). 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 lose track of the tape position. One can reinitialize the file counting by using the tape command.

```
XSUSIE/EXE,,TU

SUSIE      VERSION: 20 FEB. 1981
MAXIMUM  20 SPECTRA OF 4096 CHANNELS
COMMAND=
TAPE 1
COMMAND=
MAP
COMMAND=
READ 1 2
CALIBRATION N-SOURCE                    6. PARAMETER #  6
COMMAND=
READ 2 4 SKIP 20
CALIB OF SUM N-SOURCE GAIN NORM    6. PARAMETER #  6
COMMAND=
LABEL
LABEL=
THIS IS A DEMONSTRATION.
COMMAND=
ADD SPEC 1
COMMAND=
SAVE 3
COMMAND=
LOG 3
COMMAND=
PLOT
COMMAND=
EXPA
COMMAND=
FIT
CHI SQUARE=    8.213                FWHM=  12.805
POSITION=    117.3 +-   0.06        HEIGHT=    3191.9 +=   33.2
AREA=      43507.5 +- 1314.4
POSITION=     99.0 +-   0.05        HEIGHT=    5894.2 +=   51.0
AREA=      80342.6 +- 1594.8
POSITION=     84.2 +-   0.17        HEIGHT=    2246.6 +=   56.9
AREA=      30622.5 +- 1597.0
COMMAND=
FIT EXPO
CHI SQUARE=    1.094
A1=434345.375 +- 56937.016     A2=     -0.035 +-      0.001
COMMAND=
GET 1
COMMAND=
SUM 210 265
LOW= 210 HIGH= 265   SUM=        4074
COMMAND=
MARK 300
COMMAND=
SMOOTH
COMMAND=
EXIT
```

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LAWRENCE BERKELEY LABORATORY
UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA 94720