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Using VULOQ

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USING VULOQ

VULOQ is a data visualisation program which allows users to display neutron scattering data collected on the LOQ instrument at ISIS in a variety of graphical formats. The data can be viewed interactively on a terminal or output in a range of formats. VULOQ is particularly suited to colour terminals as the displays can be in full colour. A terminal with a windows-based environment is preferable as there are two windows : a terminal window from which selections are made and a graphics window.

Selections are made from menus according to on-screen instructions which should always be read carefully. To select a menu option type in the number and press <enter> or <return>. In this text command lines are denoted by dollar signs in the left margin and the user responses are shown in bold type. You should always press <return> after them. The program is not case sensitive.

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How to Run VULOQ

Before you can run VULOQ you must first log in to your ISIS VAXcluster account. If your login procedure does not execute the general login for LOQ users by default then you will need to invoke it by typing:

$ @LOQ$DISK:[LOQMGR]LOGIN_COMMON

If you are using a windows-based terminal or a PC running a terminal emulator then re-direct the screen output with the command

$ SET DISPLAY/CREATE/TRANSPORT=TCPIP/NODE= ###.###.##.##

where the hash marks constitute the computer's IP address (this will either be displayed on the computer or be available from local computer support).

Once the LOQ login has run, enter

$ VULOQ

A large dark window will appear which needs to be moved by pressing the left-hand mouse button whilst the cursor is in the title bar and dragging the window to the desired position before releasing the mouse button. The terminal window will contain a numbered top level menu (also see Appendix 1). Input focus must be regained in this window by clicking the left mouse button while the cursor is positioned in the window.

Summary of Menu Options

Option 1

allows the output device to be selected and only has real importance when generating hard copy as the correct terminal is usually automatically selected for you.

Option 2

is usually the first to be used on running VULOQ as it allows you to specify the data to be visualised.

Option 3

allows the type of plot to be selected. **Sub-option 1** generates an ordinary line graph of counts against X or Y position (column or row number) on the detector, specified as X15 for example. **Sub-options 2** and **3** give plots in 2 and 3 dimensions respectively. There are several ways in which the data can be presented and examples of these are given in Figures 1, 2 and 3 .

Option 4

displays the plot. This option must be entered before any changes will take effect and must always be entered to re-plot data after changing the output device to a printer. The image may take time to appear after **Option 4** has been selected especially if the data source is the DAE, or if you are using a terminal emulator on a PC rather than a VAX workstation.

Option 5

contains all the plotting options. These allow a variety of alterations to be made to the plot format and contour levels.

Option 6

allows time channel boundaries and times between readings from the DAE to be changed. It has no relevance with reduced data files.

Option 9

exits the program giving the opportunity to send the output to a printer.

Option 3: 1–Dimensional Plot (Graph)

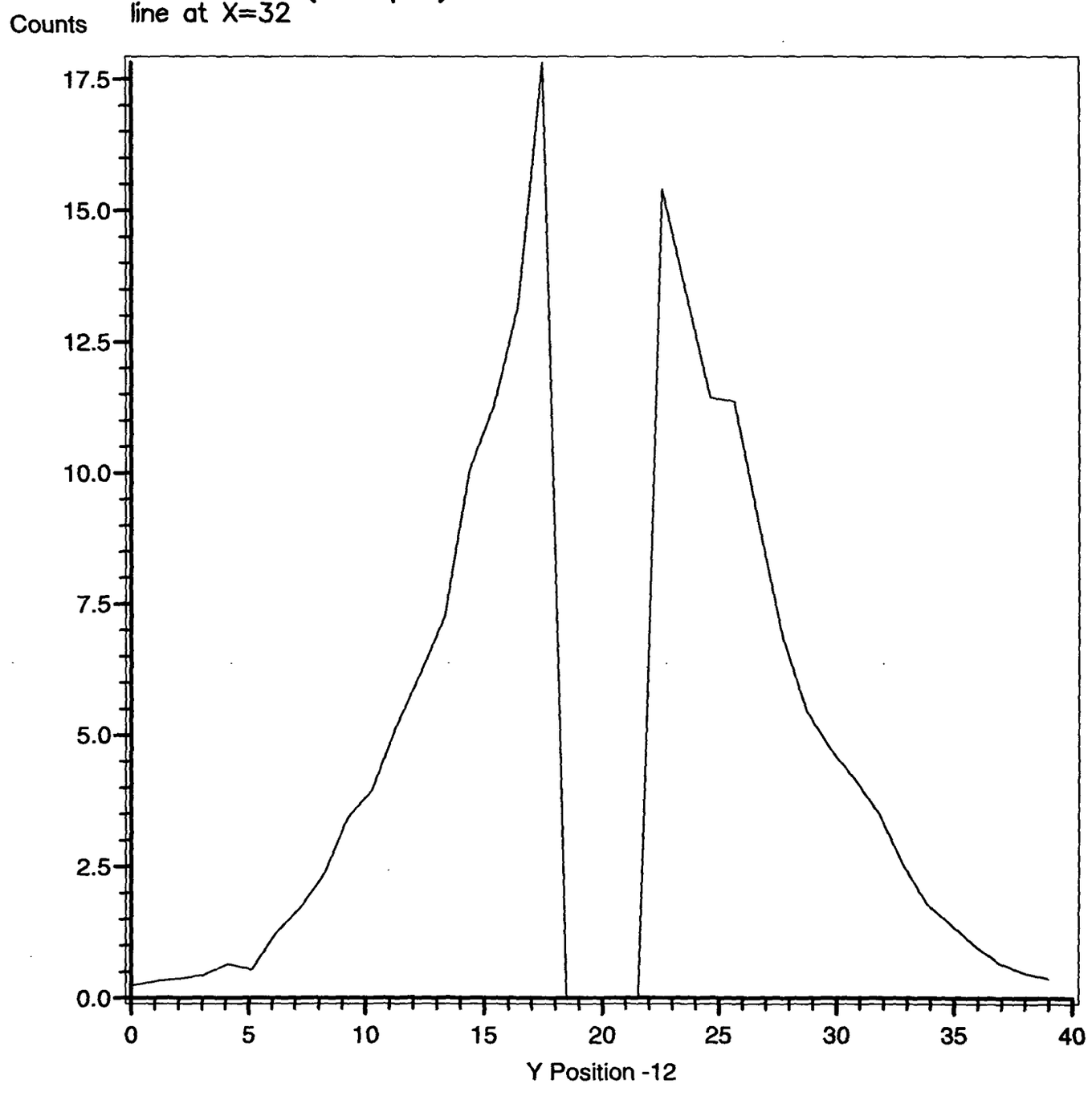


Figure 1

One-dimensional plot of the SANS by the <100> direction in a silicon crystal. The sub-title means that the graph shows the counts along column 32 (middle) of the detector.

Quick Guide to Plotting

(Also see Appendix 1 for a step-by-step illustration of the plotting and printing process)

Assuming that VULOQ correctly identifies your terminal type then the first menu selection is normally **2** so that the data file to be used can be specified. The DAE or CRPT can only be visualised when LOQ is running and you are running VULOQ on LOQ. Otherwise, **Sub-options 3** or **4** can be selected so that raw data or 2D reduced data from COLETTE can be plotted (see the guide to using COLETTE). For raw data a run number must be entered and for reduced data a file name is necessary.

You will then be asked whether you want to:

Change the contour levels to those for this dataset Y/N?

When entering VULOQ for the first time you must answer **Y**. If you enter **N** then the program will crash!

The default format is a colour two dimensional plot with exact colour pixels (and 12 logarithmic contour levels). To change plot type use menu **Option 3** .

To display the plot select menu **Option 4.**

If the two windows overlap then you may want to click the left mouse button when the cursor is in the graphics window so that the plot is not obscured. Note that when using an emulator terminal on a PC the plot may disappear when changing input focus between overlapping menu and display windows.

Plots can be detailed using menu **Option 5.** For example, it is possible to modify colour scales, contour levels, axes and sub-titles.

If you have chosen to display DAE data then you can change how often the display is updated using menu **Option 6.**

Some of the menu options are discussed in more detail below

Option 3: 2 Dimensional Plot Types

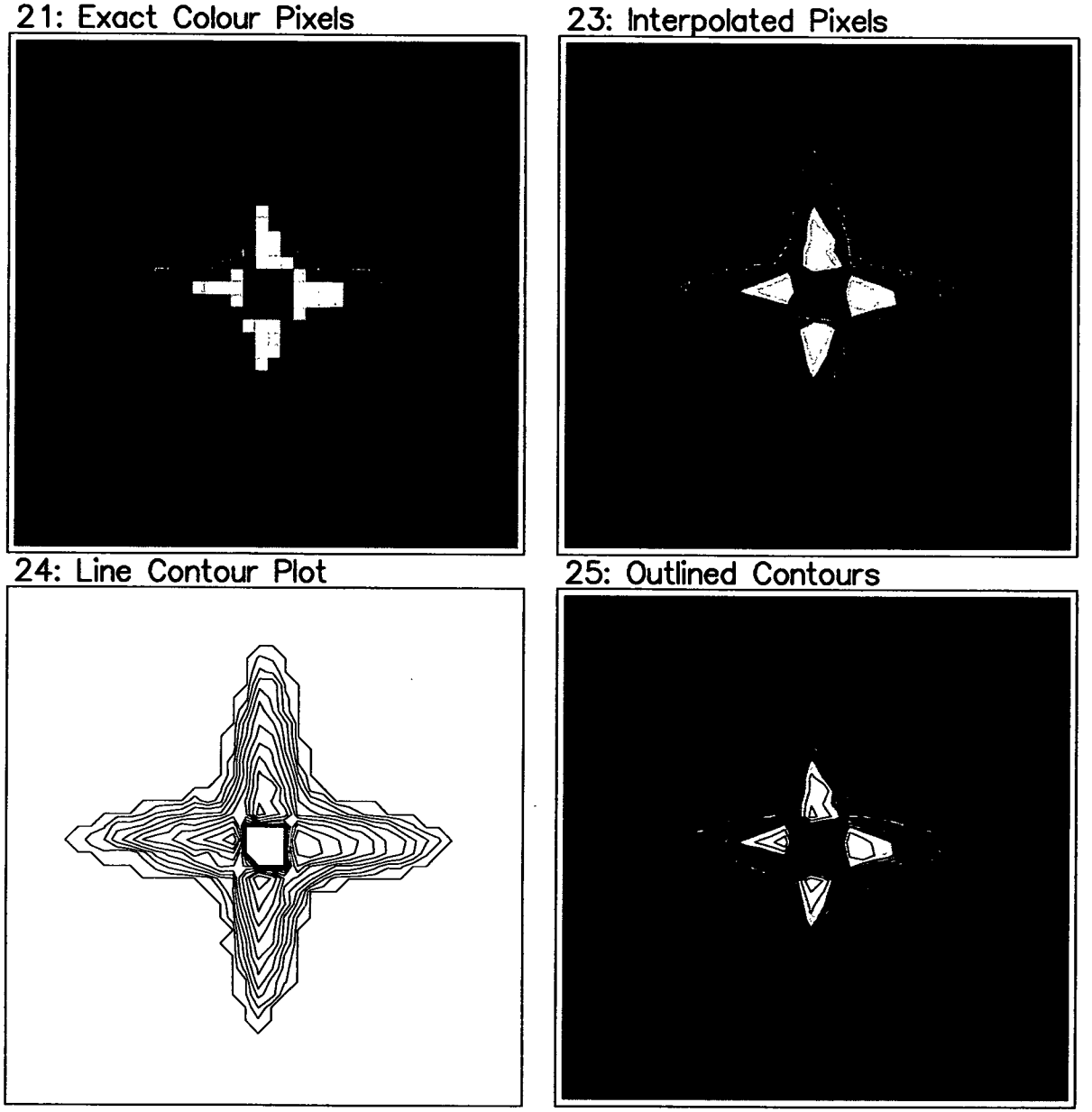


Figure 2

Two-dimensional plots of the same data as shown in figure 1.
The subtitles show the 2D sub-options available within option 3.

Option 2: Selecting a Data Source

1 DAE

For a regularly updated image of the current run select **Sub-option 1** for the DAE. The data will appear as four plots, each one showing a range of time channels. The title gives the time that the reading was taken and the time between readings from the DAE is also shown. The current time appears at intervals of 10 seconds in a box below the reading time. This option only works on LOQ.

VULOQ waits for the specified time interval before accessing the data acquisition electronics again and displaying the latest data. To change the frequency of image update or the time channel boundaries see the section on **Option 6**. The plot will take time to appear and the menu can then be brought back by regaining input focus, pressing any key and then pressing <return>.

2 CRPT

This will only give a plot (in the same format as for DAE data) if data has been copied to the CRPT. If no data has been copied to the CRPT then a warning is given that the maximum and minimum values in the dataset are equal and an opportunity to read data from another source is given. This option only works on LOQ.

To copy data to the CRPT use the operating system command

$ UPDATE

Note that you will have to exit VULOQ or use another LOQ terminal window to accomplish this.

3 RAW File

If raw data is selected using **Sub-option 3** then the run number must be entered.

4 2D Data File

Selecting **Sub-option 4** and entering a file name selects a COLETTE-format 2D reduced data file. A choice of plotting the data (0) or the errors (1) is then given.

Whenever you enter data from a new source you will be prompted to change the contour levels for that dataset. It is important that you do so when entering VULOQ for the first time as otherwise the program will crash!

Options 3&5: 3–Dimensional Plot Types & 3D Viewing Parameters

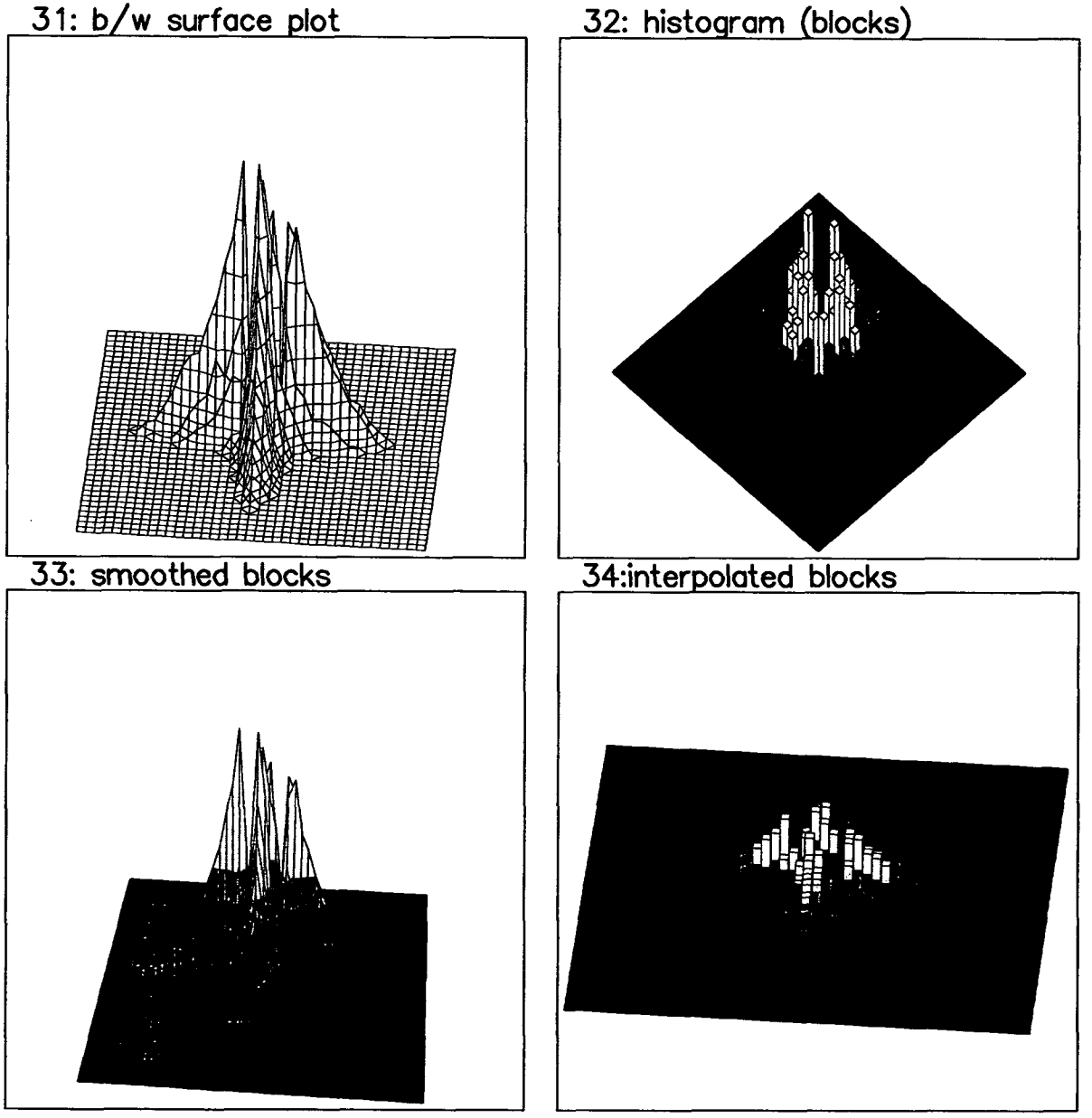


Figure 3

Three-dimensional plots of the same data as shown in the previous figures.
The subtitles show the 3D sub-options available within option 3.
Each plot also illustrates the effect of changing a 3D viewing parameter via sub-option 8 of menu option 5:
***31** has all the default parameters.*
***32** has been rotated about the X and Z axes by changing the theta and phi values to 60 and 45 degrees respectively.*
***33** has had the viewing distance changed from 100 to 5.*
***34** has had the ratio of the Z axis decreased from 1 to 0.2.*

Option 5: Plotting Options

1 Toggle Plotting of Contour Level Key

This alternately turns on or off the key showing the contour levels and their corresponding colours and is therefore only relevant to 2D and 3D plots.

2 Zoom In/Out on a Section of the Display

This allows you to zoom in and out of a particular area of a single full size plot according to the key shown in Table 1 below.

Table 1: Subdivision of the Display for Zooming

1 Top Left	**2** Top Centre	**3** Top Right
4 Left Centre	**5** Centre	**6** Right Centre
7 Bottom Left	**8** Bottom Centre	**9** Bottom Right

Sub-option 10 allows you to select some other plot area.To do this click the left mouse button when the cursor is at the bottom left-hand corner of the area you want to zoom in on. Next move the cursor to the top right-hand corner of the area you want to zoom in on and click the left mouse button again. Then regain input focus in the terminal window so that the enlarged plot area can be drawn. To regain the normal plot area select **0** to zoom out.

3 Change the Colour Scale

The colours of a display can be changed using the sub-menu which appears once this option is selected. Figure 4 shows some examples of the different colour scales. The default colour scale is blue to white (**Sub-option 1**)

4 Change the Type of Contour Mapping

Sub-option 1 controls the way in which the contour levels are calculated. There are a number of choices and these are explained in Appendix 2.

Sub-option 2 allows the number of contour levels to be selected. The maximum is 13.

Sub-options 3 and **4** only have noticeable effects on 2D black and white line contour plots:

Option 5: sub–option 3 Colour Scales

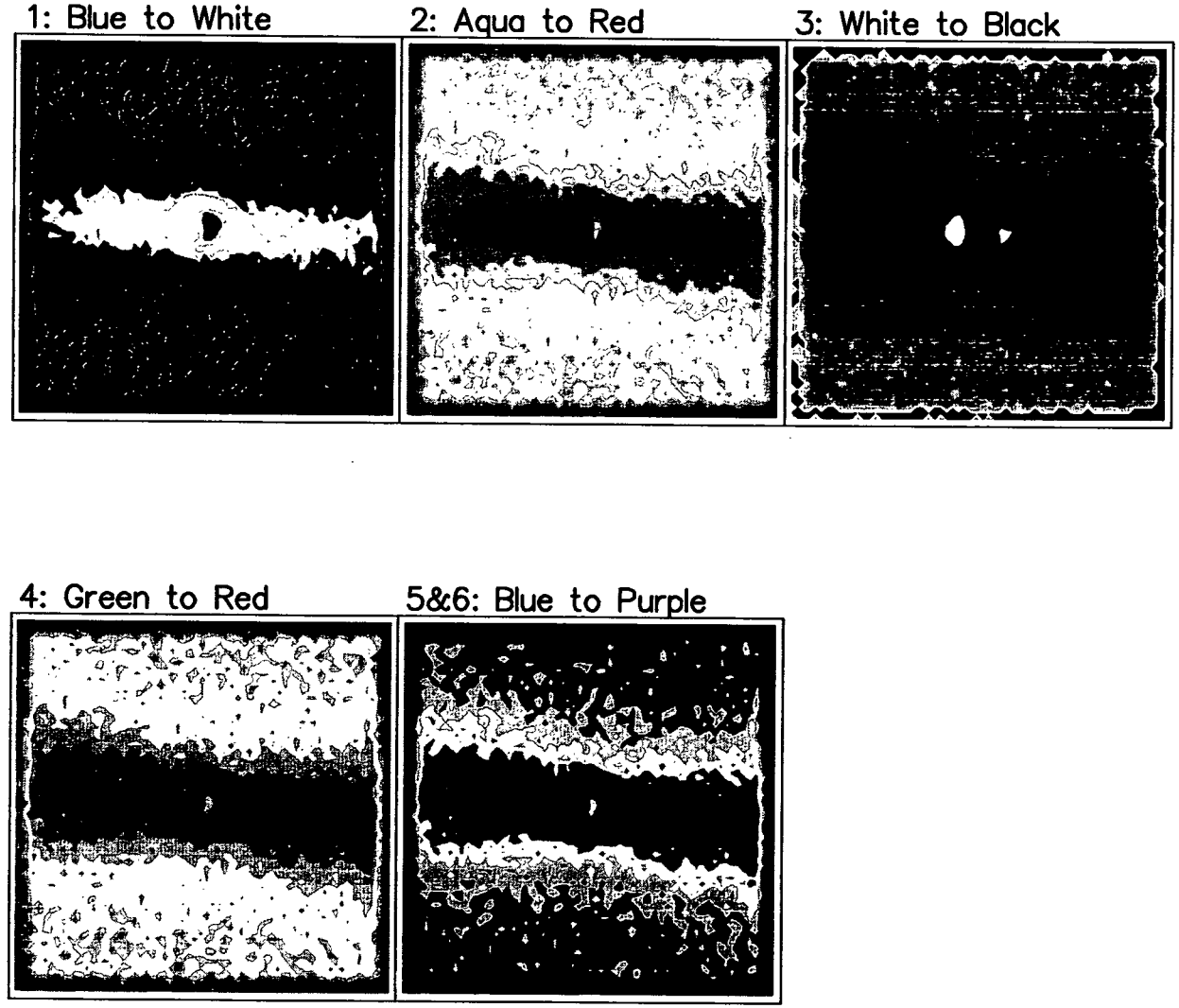


Figure 4

Two dimensional plots of the SANS from cellulose fibres showing all the colour scales available under sub-option 3 of menu option 5.

Sub-option 3 sets the minimum length of contour line to be plotted which must be greater than 4mm.

Only give the numerical value or the program will crash. The minimum line length can be increased to show only the major regions of a particular intensity.

Sub-option 4 allows the degree of smoothing applied to a 2D line contour plot to be specified.

5 Change the Contour Levels

This works on all 2D and 3D plots and allows you to specify maximum and minimum values to be plotted and to change any of the calculated contour levels.

The maximum and minimum values in the dataset are displayed and you can choose to change them. The contour levels are also listed and you can edit any of them by entering the contour level number and the desired boundary value as shown below. For example, entering

6, 24.25

will change contour level 6 to a value of 24.25.

6 Modify the Title or Subtitle

Some subtitles (such as run numbers for raw data and file titles for reduced data) will appear by default. These can be changed or removed using the sub-options here.

7 Modify Axes Plotting or Text

The axes and tick-marks can be switched on and off, and their units and titles modified using this option. Axis titles and units can be improved using subscripts, superscripts and special characters. To enter a subscript type

<

before the subscript text, and to enter a superscript type

>

before the superscript text.

To enter one of the special characters shown in Table 2 below type

^

and the relevant number code. For example to make Q(Ang-1) look like **Q ($Å^{-1}$)** enter the following:

Q (^29197^8175^8185)

Table 2: Special Characters

Symbol	Special Number(s)
Angstrom (Å)	29197, 30197, 33197, 36197
degrees (°)	218, 718, 1218, 2218, 3229, 3729
omega (ω)	1150, 2150
capital omega (Ω)	1050, 2050
theta (θ)	634, 2134
superscript -	2326, 2376, 8175
superscript 1	8185
superscript 2	8178
superscript 3	8179

8 Change 3D Viewing Parameters

This option changes the appearance of 3D plots.

1 Phi

rotates the plot about the Z (vertical) axis and can take values between + or -180 degrees.

2 Theta

rotates the plot about the X (horizontal) axis and can take values between 0 and 360 degrees.

3 Dist

acts like a magnification factor with smaller numbers making the plot appear farther away.

4 Zlen

acts like a scale factor taking values between 0 and 1. It controls the ratio of the length of the Z side to the lengths of the X and Y sides of the 3D box. This effectively changes the height of bars along the Z axis.

Examples of how these sub-options change the appearance of plots can be seen in Figure 3.

9 Set Number of Plots on Display

This is done by entering two numbers to specify the number of plots required in the X and Y directions. This means that several plots can be displayed simultaneously for comparison. For example Figure 2 was plotted by entering **2, 2.**

Any number of plots can be made on the screen but on small terminals detail is lost if more than 4 are used. A 1D plot cannot be entered as part of a *multi-plot* image.

Option 6: Changing Time Channels

1 Change Time Between Readings of the DAE

This option only takes effect when the data source is the DAE. It allows you to change the frequency with which the image is updated. Be careful not to specify too short a period as doing so will seriously slow LOQ down.

2 Change Time Channel Boundaries for Plots From DAE/CRPT

Changes are made by entering five channel boundary numbers between 3 and 102. This effectively changes the wavelengths of the scattered neutrons shown in each plot. The default time channel boundaries correspond to the neutron wavelengths: 2-4, 4-6, 6-8, and 8-10 Å. The wavelengths corresponding to various time channels are given in Table 3.

Table 3 : Neutron Wavelengths Corresponding to Time Channel Boundaries

Channel Boundaries	Neutron Time of Flight (μs)	Neutron Wavelength (Å)
34	7905.97803	2.02389
43	9873.48242	2.52756
50	11736.46680	3.00447
56	13610.70508	3.48427
62	15784.24512	4.04068
66	17422.85352	4.46016
71	19712.36133	5.04626
74	21228.05664	5.43427
75	21758.75781	5.57013
78	23431.80273	5.99842
81	25233.48828	6.45964
84	27173.70703	6.95633
87	29263.10938	7.49120
90	31513.16797	8.06721
92	33108.52344	8.47561
94	34784.64453	8.90469
97	37459.25781	9.58937
99	39355.63281	10.07484
101	41348.01172	10.58488
102	42381.41094	10.84950

3 Change Time Channel Boundaries for Summing From RAW files

The default is to sum over all the time channels or wavelengths but this can be changed by entering new summation boundaries. You are then asked if you want to change the contour levels for this new dataset. If you answer **Y** then the contour levels are automatically re-calculated.

Option 1 and Printing a Display

This option gives you the choice of output devices shown in the table in Appendix 1.

To print out a display you must select a printer as the output device by entering a number from **5** to **9** inclusive. Whilst at ISIS select devices **6, 7** or **8**. If you choose option **8** the image can still be sent (when you exit the program) to a black and white printer whereupon the coloured contour levels will be printed out in grey-scale. If the plot has a "black to white" colour scale (menu **Option 5, Sub-option 3**, selection **7**) then do not choose output device **8** or the program will crash!

When you select another output device, such as a printer, the display window and plot disappear. For this reason it is a good idea to make a note, *as you work* , of all the formatting steps which you have applied to obtain the desired image as the changes can no longer be seen in the display window.

At this stage it is very important to re-plot the data using menu **Option 4** otherwise an empty printer file will be created. Any special formatting or plot options such as colour scales must all be re-entered before re-plotting each plot of a *multi-plot* image otherwise it will be printed out with all the options and the sub-title of the previous plot.

Once you have entered all the formatting options and re-plotted the data you should enter menu **Option 9** to leave VULOQ.

You will then be asked whether you want to print to a black and white printer (see Appendix 1). If you answer **N** or press <return> then you will be asked if you want to print to a colour printer.

Whenever you answer **Y** you will be given a choice of printers at ISIS, each encoded by a letter according to their location; for example (D) for the printers located in the Data Assessment Centre (DAC). Once you have chosen where the image will print out by selecting the relevant letter you will be notified of which print queue the file has been sent to, for example:

$ print/queue=post$lsr0/form=post/notify sys$scratch:vuloq.post

where the underlined section denotes the exact printer selected (see Table 4). The computer will notify you when the task has been completed.

If you want to save the image file to your user disk space so that you can print it out again without having to go back into VULOQ then you can do so by issuing the following command:

$ copy scratch$disk:*[user-id]*vuloq.post user$disk:[user-id]new_file_name.*post*

inserting the relevant user identification and file name (shown in normal typeface above). The image files can be very large so take care to ensure that you only transfer essential files onto your user disk. Table 4 below shows the locations, queues and types of printer available at ISIS.

Table 4 ISIS Printer Queues

Printer Type	Printer Queue	Location
	post$lsr0	R3 Support Office
Black & White	post$lsr2	DAC
PostScript	post$lsr4	CRISP cabin
	post$lsr11	HET cabin
Colour PostScript	colour$ps	R3 Support Office
	post$ink2	DAC
	post$ink4	CRISP cabin
	colour$phaser0	R3 Reading Room

To print the PostScript file again from your ISIS account you can use:

*$ print/queue=*queue*/form=post/notify user$disk:[*user-id*]*new_file_name*.post*

Glossary

Abbreviation	Meaning
DAE	Data Acquisition Electronics
CRPT	Current Run Parameter Table. This is an area of the LOQ computer's memory containing data from the current run in the form of a raw data file.
COLETTE	LOQ Data Reduction Program

Appendix 1

This shows all the steps needed to create and print the basic two-dimensional image shown in figure 5. The title and sub-titles are those which are printed out by default. To change them see option 5 sub-option 6. All the commands and menu selections entered are shown in bold typeface below.

ISISE: > **set display/create/transport=tcpip/node=ndnt08**
ISISE: > **vuloq**

VULOQ Version 20 8 Sep 95
Choose one of the following output devices:

1 PC terminal(Emulator)
2 Terminal (Tek type)
3 Terminal (X-Window)
4 Workstation(X-Window)
5 Printer (Sixel, b/w)
6 Printer (PS, b/w)
7 Printer (EPS, b/w)
8 Printer (PS, colour)
9 Ink-Jet (PS, colour)
10 UNIRAS output segment
11 Another device

Enter zero (0) to keep the current selection
4

Initialising output device 4 please wait....

VULOQ TOP LEVEL MENU

1 Select output device...Workstation(X-Window)
2 Select data source.....NONE
DAE / CRPT; No file

3 Select type of plot....2D exact colour pixels
4 PLOT data
5 Plotting options
6 Change time channels

9 LEAVE VULOQ

2

VULOQ Possible INPUT DATA Sources

1 DAE (slow)
2 CRPT
3 LOQ RAW file
4 2D data file

Enter zero (0) to keep the current selection
4

Enter filename with type (Eg; MYDATA.LQA, STEVE.QXY, RKH.LQB)
eds_soap.lqa

This file contains both data and their errors. Which do you want to view:
Enter 0 for DATA or 1 for ERRORS
0

VULOQ TOP LEVEL MENU

4

VULOQ TOP LEVEL MENU

1

Choose one of the following output devices:
: 1 PC terminal(Emulator)
2 Terminal (Tek type)
3 Terminal (X-Window)
4 Workstation(X-Window)
5 Printer (Sixel, b/w)
6 Printer (PS, b/w)
7 Printer (EPS, b/w)
8 Printer (PS, colour)
9 Ink-Jet (PS, colour)
10 UNIRAS output segment
11 Another device

Enter zero (0) to keep the current selection
8

Initialising output device 8 please wait....

Screen display will be scaled to fit A4 page by default.
Change this [Y/N]?
N

VULOQ TOP LEVEL MENU

4

VULOQ TOP LEVEL MENU

9

Normal Exit from Program

You can print
• a POSTSCRIPT, ENCAPSULATED POSTSCRIPT or COLOUR POSTSCRIPT file (VULOQ.POST)

Print a BLACK/WHITE POSTSCRIPT file? [N]: **N**
Print a COLOUR POSTSCRIPT file? [N]: **Y**

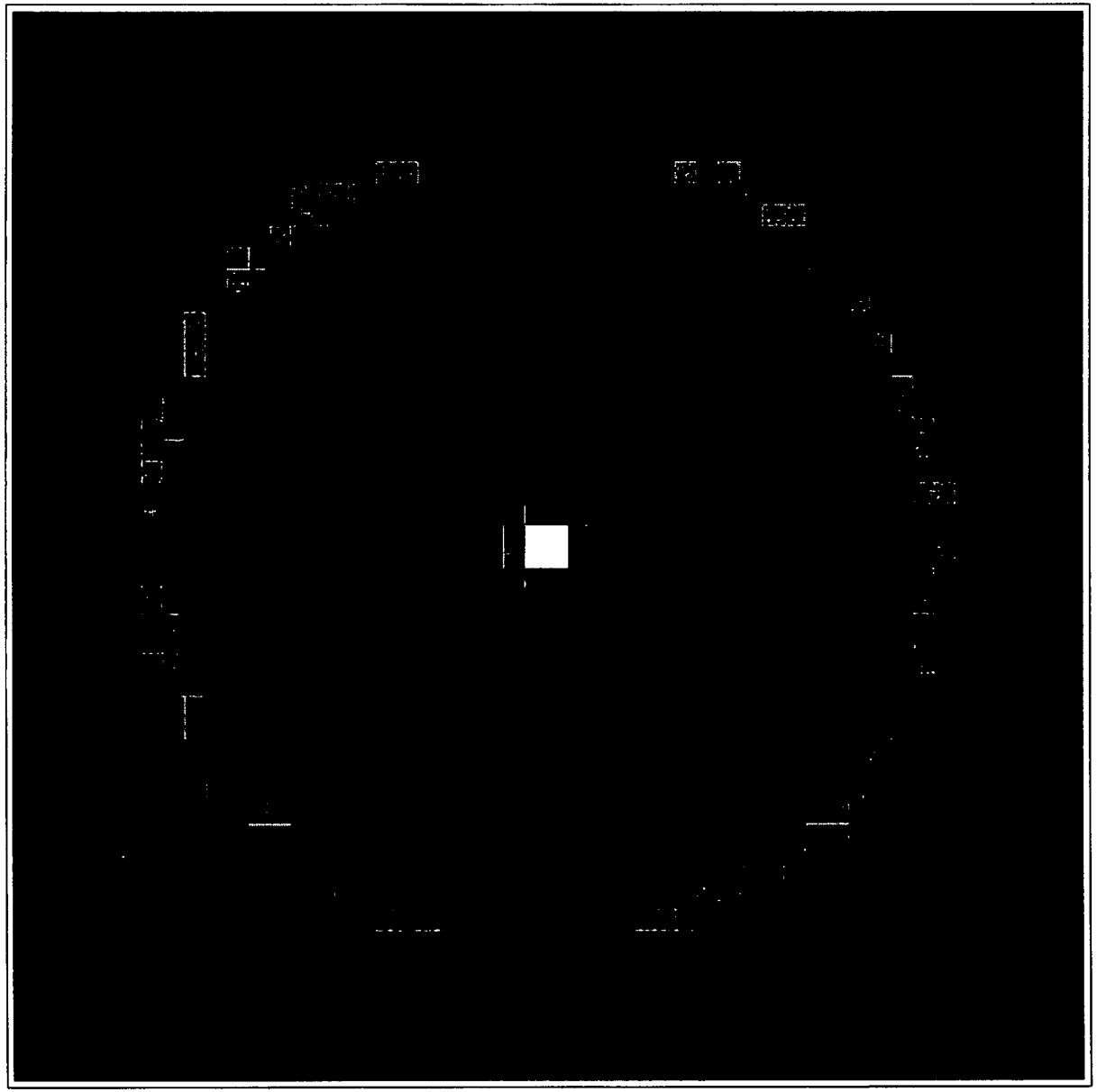
Which Colour PostScript printer? [R3 (S)upport, (R)eading Rm, (C)RISP, (D)AC]: **R**

$ print/queue=colour$phaser0/form=post/notify sys$scratch:vuloq.post

Job VULOQ (queue COLOUR$PHASER0, entry 331) started on COLOUR$PHASER0

$ set noverify

Thankyou for using VULOQ. Have a nice day!



Above	80.21
51.74 –	80.21
33.37 –	51.74
21.53 –	33.37
13.89 –	21.53
8.96 –	13.89
5.78 –	8.96
3.73 –	5.78
2.40 –	3.73
1.55 –	2.40
1.00 –	1.55
Below	1.00

Figure 5

Basic 2D Plot created using the steps shown in Appendix 1.

Appendix 2

The following formulae show how the types of contour mapping available through menu option **5 Sub-option 4** are calculated. Contour mappings **2,3** and **4** have no effect.

L=level number x_L=level value

max=maximum value in the dataset

min=minimum value in the dataset

N=total number of levels

1 sqrt 2:

$$x_{12} = \max$$

$$x_L = \frac{x_{L+1}}{\sqrt{2}}$$

5 sqrt 10:

$$x_{12} = \max$$

$$x_L = \frac{x_{L+1}}{\sqrt{10}}$$

6 Percent:

$$x_L = \min + \left[(\max - \min) \times \left(\frac{L^2}{100} \right) \right]$$

7 Log:

$$x_1 = \min \text{ or } x_1 = 1 \text{ if } \min < 0$$

$$x_L = x_{L-1} \times \left[\left(\frac{\max}{\min} \right)^{\left(\frac{1}{N-1} \right)} \right]$$

8 Y-squared:

$$x_1 = \frac{\max}{100}$$

$$x_L = L^2 \times x_1$$

9 Linear:

$$x_1 = \min$$

$$x_L = x_{L-1} + \left(\frac{\max - \min}{N} \right)$$