

Better visualisation of neutron scattering data using UNIRAS at ISIS

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Abstract: *The pulsed neutron source, ISIS, at the Rutherford Appleton laboratory in the UK is used for many experiments to determine the structure of materials. Data is often collected over a range of operating conditions to study phase changes in the material. Older instruments collected one dimensional data, some of the newer ones have area detectors which collect two dimensional data. The old data display programs dealt only with one dimensional data so new interactive graphics programs have been written using the UNIGRAPH package to display a series of one dimensional datasets as a two dimensional image which shows the phase changes much more clearly. Experiments are described on the use of an image processing library for the display of two dimensional neutron scattering data from the small angle scattering instrument, LOQ.*

Introduction: UNIRAS

UNIRAS(1) is a graphics system which consists of two main parts, a series of sub-routine libraries and several associated interactive programs to access them. It runs on a wide range of computers including VAX, IBM mainframes, and many types of workstation including Silicon Graphics and Sun. We use it on our VAX/VMS cluster, with colour displays on the neutron scattering instrument data collection workstations and on PC clones on scientists desks. The version we are running can display graphics in a single window of an X-windows terminal, more recent versions can display graphics in many windows, so we will be upgrading soon since we plan to standardise our workstations to use OSF-Motif X-windows, and often want to see several views of our data simultaneously.

The UK Science and Engineering Research Council and the University Funding Council collaborated on a joint purchase of UNIRAS for the UK academic community, which makes it cheaply available to any UK University. It is distributed by CHEST, the Combined Higher Education Software Team, based at the University of Bath.

UNIRAS routines can be called from user programs written in the programming languages Fortran77 or C. Four associated interactive programs access most of the routines in the libraries; we use one of them, UNIGRAPH, to prototype our visualisation ideas, before writing our own interactive graphics programs if necessary. UNIGRAPH has many menus to change the type of plot, has several colouring schemes, and a simple data manipulation language. It contains many different device drivers and has a way of saving the current plot to hardcopy, including the making of monochrome or colour PostScript files.

Visualisation of IRIS data:

(1) Spectroscopy of hexamethyl stannate.

IRIS is a time resolution quasielastic and inelastic scattering spectrometer(2,3) at the ISIS pulsed neutron source in Oxfordshire in the UK. In June 1992 it was being used by M.Prager and C.J.Carlile to study rotational tunnelling spectroscopy with neutrons(4) on a sample of hexamethyl distannate $(\text{CH}_3)_6\text{Sn}_2$ as a function of temperature between 5 and 15 degrees Kelvin. The data was normalised using the GENIE analysis and display program(5) and then written out at each temperature as a series of neutron intensities at a range of energy transfers.

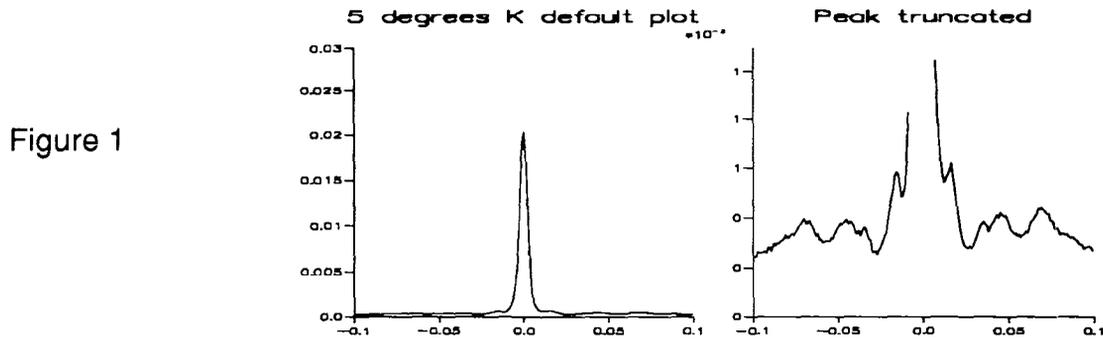


Figure 1

Figure 1 (left) shows the default plot for the lowest temperature made interactively using UNIGRAPH. Little detail can be seen due to the domination of the plot by the elastic peak, so data at the higher values was truncated and the data replotted as shown on the right hand side of Figure 1 where four peaks can be seen which were almost invisible before. When data is taken at a series of temperatures, it is often displayed as a series of plots displaced from one another vertically as shown in Figure 2, where different line types have been used for the different temperatures. To show all the plots on one graph, or 'multiplot', means they have to be plotted with a small scale, and although there is clearly some difference between the spectra represented by the lines at the extremes of the plot, it is hard to see exactly how they vary.

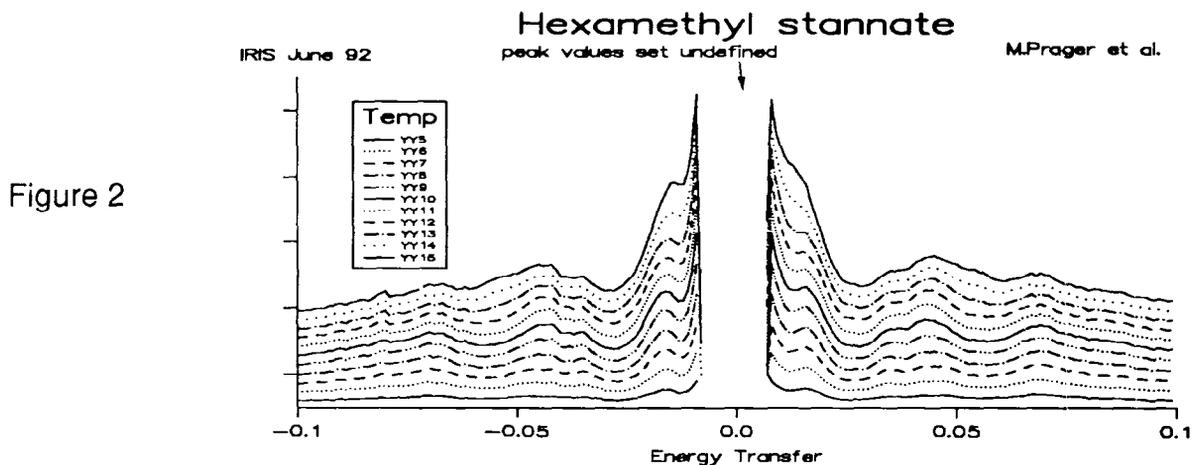


Figure 2

A new algorithm has been developed which considers each spectra as a slice through a three dimensional surface, with dimensions energy transfer, temperature, and intensity. The surface is made using the UNIGRAPH manipulation language to combine all the spectra into a two dimensional array, which is then displayed as an image, with spectral intensities represented as different colours or grey levels, as in Figure 3 which shows the same data as that of figure 2, but the transition at about 11 degrees Kelvin is much more obvious. This transition is thought to be due to changes in the tunnelling of the methyl groups.(4)

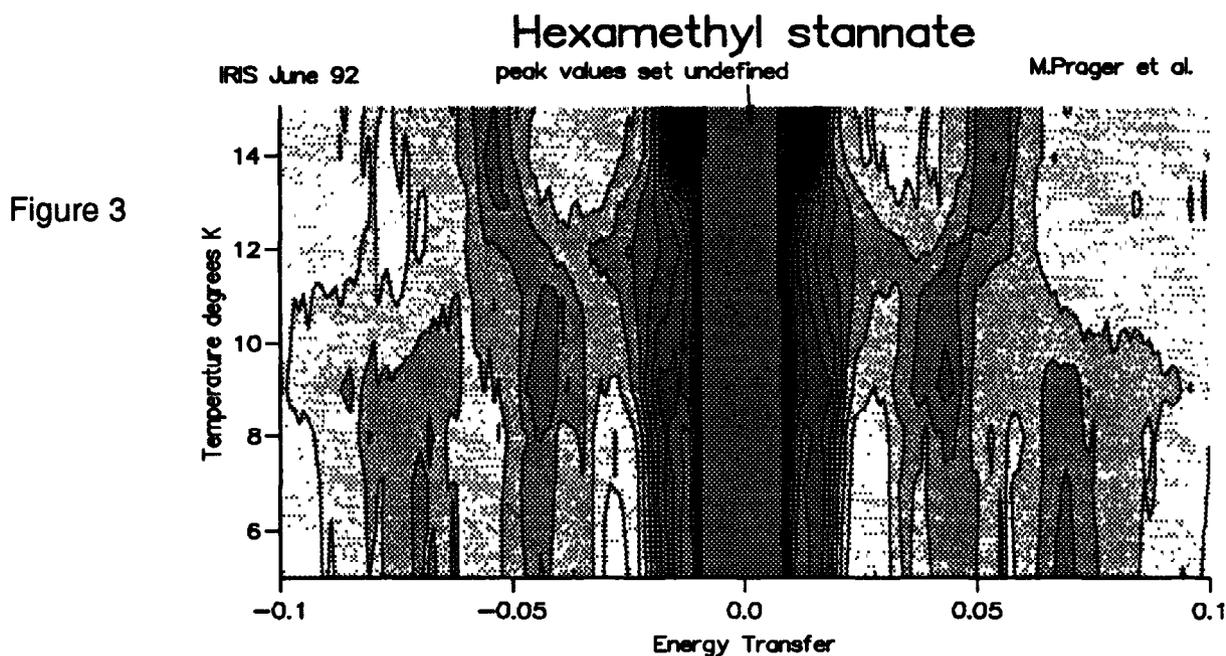


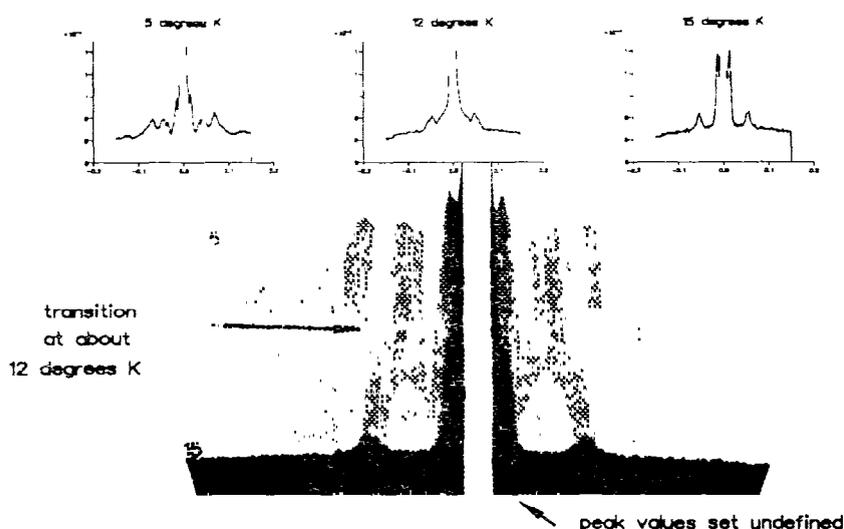
Figure 3

The individual datasets are read into UNIGRAPH using the command language, for example to read in a single dataset the commands are DATA IMPORT REPORT. They are given names, for example Y5, for the data taken at 5 degrees, Y6 for that at 6 degrees, and so on. These are combined together with a statement like:

Let "Y" "Y5//Y6" where the operator // means append dataset Y6 to Y5. When all the datasets have been accumulated together they can be converted to a two dimensional array by a statement like: Let "Y" "RESHAPE(Y,301,11,1)" where 301 is the number of entries in the X direction for each dataset, 11 the number of datasets in the Y direction, and there is only one set of values for the Z. There are many other commands in the UNIGRAPH data manipulation language; the main features it lacks are the ability to operate on a dataset and an associated error dataset in a single command, and to allow control to pass to a 'user' written routine during the data analysis.

The dataset Y can be shown as exact 'pixels', which may be necessary if measurements are to be made on the plot, but it is more difficult to see trends with that type of display. Figure 3 is a 2D contour plot, with some smoothing applied to the graphics before displaying it, and outlines added to emphasise the structure. The original data is not changed, only the graphical display is smoothed. Further interactive selections of subsets of the data can be made, for example the limits of X and Y can be changed to zoom into smaller regions of the data.

Figure 4

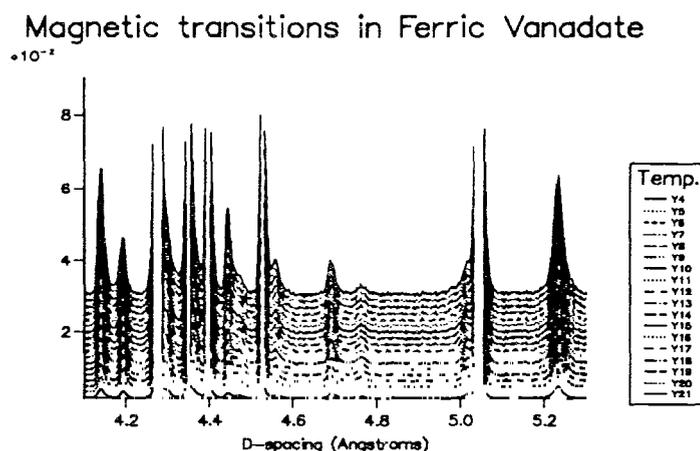


UNIGRAPH allows the superposition of several plots on the same page as shown in Figure 4, where a 3D view is shown in the centre, with 3 slices through the surface plotted at the top. The surface has been rotated relative to that of Figure 3 because it is easier to see the shape of the tunnelling peaks when viewed from the higher temperature end. These plots are normally seen in colour, where the surfaces of the peaks can be shown in a different colour. An interactive program is essential to make the optimum view by changing both the colourtable and the number of colours. We have only been using colour displays for a short time, and have found that although everyone agrees they can see the data well when displayed as grey scales, there is considerable disagreement about which colours should be used for an optimum display. We try to avoid combinations of red and green for the benefit of the colour blind.

(2)Magnetic crystal structure of ferric vanadate

This display algorithm can be used with any sets of data taken at regular intervals. Figure 5 shows a 'multiplot' of neutron scattering data taken on IRIS for the magnetic material ferric vanadate by J.B.Forsyth and C.J.Carlike in 1992. (6)

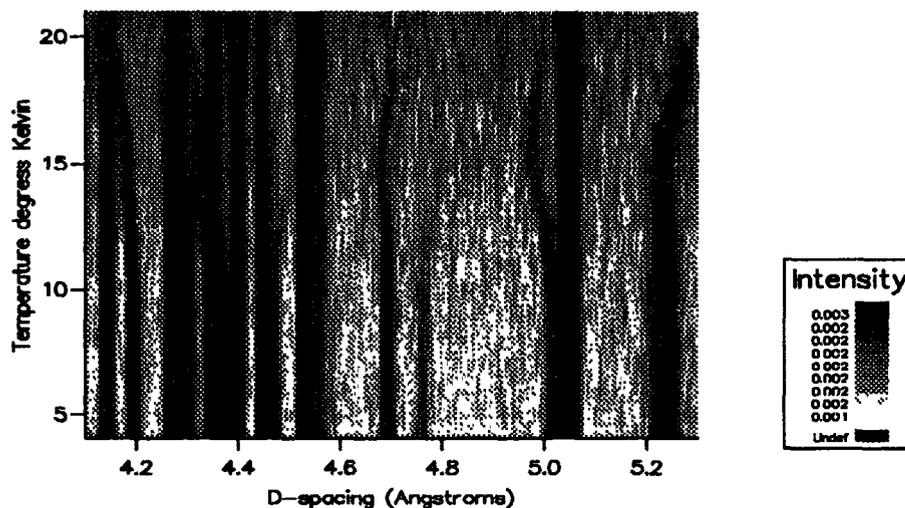
Figure 5



Neutrons scatter in two ways from this material; there is the usual Bragg diffraction from the structure, and additional scattering due to the interaction of the magnetic moment of the neutron with the magnetic structure of the material which is only seen at low temperatures, appearing as noise above 20 degrees K. The material undergoes two exothermic phase transitions at about 15 degrees K which involve an ordering of the electronic spins of the iron atoms.

Magnetic Transitions in Ferric vanadate

Figure 6



The Bragg peaks dominate this plot, so they have been truncated in order to see the detail in the magnetic diffraction lines which appear to change their position with temperature, as shown in Figure 6, a grey level 'image' plot with each line of data containing about 800 points. Between 5 and 10 degrees Kelvin the magnetic peaks show clearly as vertical lines, above that they curve dramatically. The two peaks at D spacings between 4.6 and 4.8 Angstroms curve in opposite directions as they decrease in intensity, indicating a complex ordering of the atomic moments in a helical geometry incommensurate with the atomic lattice. This can not be so clearly seen in Figure 5.

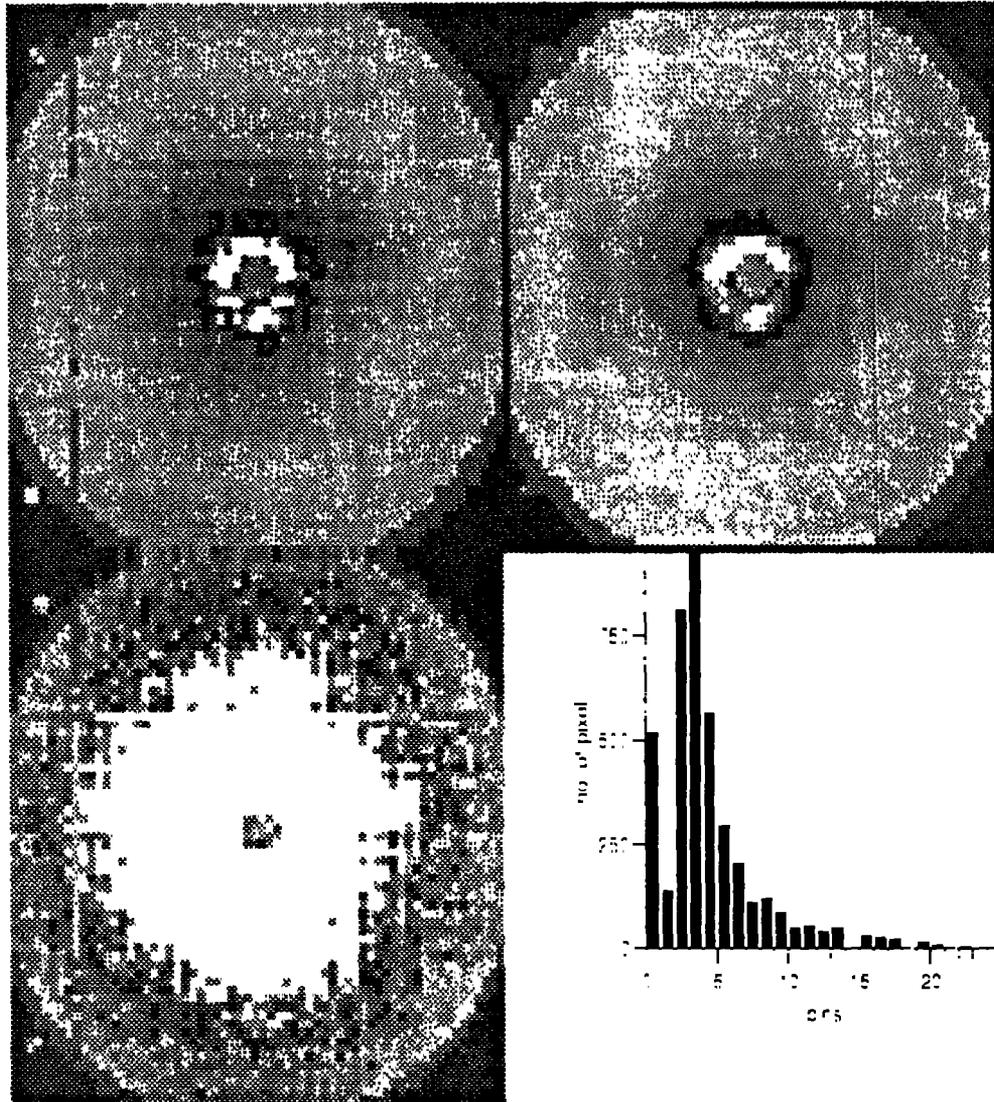
Display of LOQ Data.

In addition to using the interactive program UNIGRAPH, we have also used the UNIRAS subroutine libraries in a program, VULOQ(7), to display data from the LOQ instrument (2) which uses small angle diffraction to investigate the shape and size of large molecules. It has an area detector coded as 128 x 128 pixels, and so unlike IRIS, naturally collects data as a two dimensional array.

VULOQ can display 2 and 3D plots similar to those of Figures 3 and 4, another example is shown in upper left of Figure 7 which shows the data displayed as the exact pixels of an image. This was part of an experiment exploring the use of a conventional image processing library for improved data display. UNIRAS has many interpolation routines, but they need to be used with caution, an injudicious choice of parameters in interpolation routines can produce spurious artefacts not present in

the data. It may be that a simpler process from an image processing library has fewer problems. The plot at upper right of Figure 7 is the result of using a 3 x 3 median filter to smooth the data of upper left. This filter will reduce the image size by a row all the way round but should not introduce other spurious effects.

Figure 7



The histogram at lower right of Figure 7 shows the distribution of intensities in the image at upper left. A standard enhancement technique in image processing is to manipulate the intensities in the histogram, reducing the higher ones and increasing the lower ones, a process known as 'histogram equalisation'. As can be seen in Figure 7, lower left, it enhances image features. It might also improve the contrast in the 2D plots of Figures 3 and 6 to make the small signals more visible, but this has not yet been tried.

One problem with using conventional image processing routines on neutron scattering data is that many routines expect the intensities displayed in the image to have values less than 256, because that is the maximum intensity many optical cameras can record. Our intensities vary from many thousands to a few tens, and normalisation operations can result in negative values, so any image processing library used should not expect small positive numbers for intensities.

Conclusions:

Visualisation is a rapidly growing field (see Brodlie (7) for an overview). There may be techniques developed in other disciplines such as astronomy or medical image processing which could be applied to the display of neutron scattering data in future. There are also a growing number of image compression algorithms which might be investigated as a possible way to reduce the amount of data in our optical disk store.

Colour graphics is not just a gimmick for publicity purposes, it has a role to play in better understanding of the data because the human eye can readily distinguish fine changes in colour and so detect features in the data which might otherwise be missed. There are many high level graphics packages which could produce similar results, we use UNIRAS because it was made available to us cheaply, has many high level visualisation routines, many device drivers and can easily be built into our data analysis programs.

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