Using databases for improved instrument operations and administration at ISIS

K.M.Crennell

Rutherford Appleton Laboratory, ISIS Facility, Chilton, Didcot, Oxon, OX11 0QX UK

Abstract: As neutron scattering instruments become more complex, often with hundreds of detectors, it becomes increasingly important to monitor their performance effectively. A program, VUSLS, is described which uses interactive colour graphics to monitor operation of the SANDALS instrument at ISIS, and future plans outlined to use a database management system. The database system is currently used to manage the administration of the proposals for the use of ISIS Beam Time, including the names and addresses of our 4000 users, and automatic letter writing.

Introduction. The instrument SANDALS, is used for Small Angle Diffraction for Amorphous and Liquid Samples. It has an extensive low angle bank of zinc sulphide scintillator detectors typically 10mm wide and 200 mm tall. 360 are installed in the bank at 11 to 21 degrees scattering angle, and 120 in the 3 to 11 degree bank. Another 200 are to be installed towards the end of this year. Detectors are mounted two to a photomultiplier and arranged twenty to a module. An automated way of assessing detector performance is needed especially during commissioning. ISIS is a pulsed neutron source, counts are recorded at times up to 20000 microseconds after the passage of the main beam. In practise, few counts are seen at times of less than 200 microseconds, and there is more noise after 10000 microseconds, so counts for each detector are usually summed between these times.

The algorithm. We look at the data collected from a sample giving a uniform signal in all detectors. All detectors in a given module are adjusted to give a similar response, so their signals are averaged, and the ratio actual signal to average signal calculated for each detector. Any excessively noisy or low detectors are left out of the average, and out of any later data analysis. If more than half the detectors in a module are left out, the program asks the user for advice.

Program used An interactive colour graphics program, VUSLS, has been written in FORTRAN using the graphics package UNIRAS running on a VAX/VMS system with X-windows. The calculated ratio for each detector is displayed as a thick coloured line. The lines are drawn adjacent to one another to make the modules, with the detector numbers above. (See Figure 1) Average detectors are drawn in green, others are white, yellow, red or black. The scale in the upper part of Figure 1 shows the values of the ratios assigned to each colour. The number of detectors in each category is listed on the left of the scale. The user can change the values assigned to each colour interactively. This plot gives the user an instant appreciation of detector function, on a colour screen all the modules should be green, a few in other colours are easily seen. Notice that the very low signals occur in adjacent detectors, these probably have a defective photomultiplier.
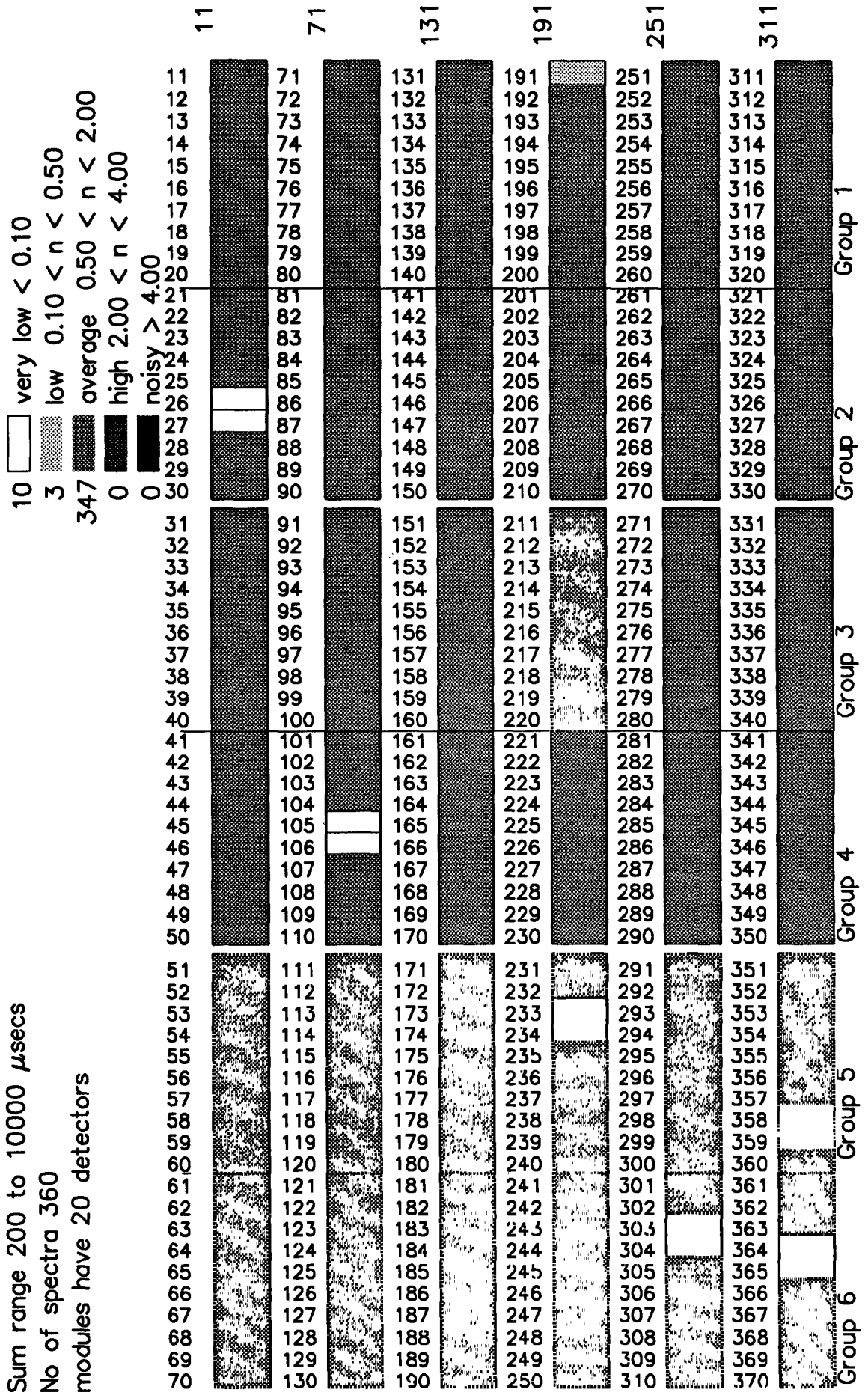
Figure 1   Default plot for one of the SANDALS detector banks

The detectors are arranged on a surface of constant resolution. They are used in groups whose signals are averaged together. The groups are shown by the lines crossing the modules in Figure 1 with their numbers at the bottom of the diagram.
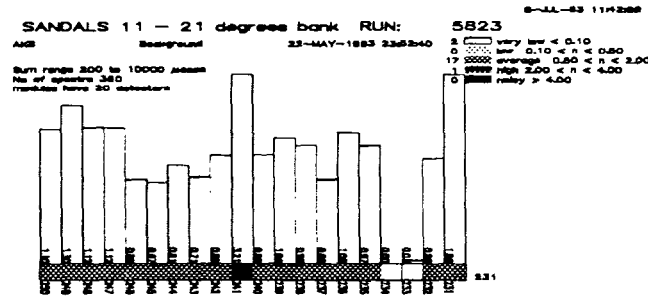

Figure 2   Greater detail in histogram for a single module

Another type of plot shows the counts as a histogram as well as the coloured lines, with a choice of either all the detectors in the chosen bank or a single module in greater detail. (see figure 2)

Further options allow sending the plot to hardcopy on laser or colour postscript printers, and the creation of a revised file which includes only the numbers of average detectors for use in subsequent data analysis. The revised file leaves blanks where detectors have been omitted so that it is easy for the user to see at a glance which detectors are missing.

```
9   451   452         454   455   456   457   458   459   460
8   461   462   463   464               467   468   469   470
written   18-MAY-93   11:42:50
   0 detectors not read from GROUPS90_det.DAT
  51 more detectors not average now file SLS5823.GRP
 490 spectra in 1160 time channels
summed between 200 and 10000 microseconds
```

Figure 3   Part of a revised file showing gaps for omitted detectors and the start of the history

The operating parameters of VUSLS are written at the end of the file for future reference. The user either starts with a default file with all good detectors, or can specify one made previously with VUSLS, so that they can accumulate a single file including only detectors known to be average for all the runs of their experiment.

Future Plans: There may be a variation in detector noise with time. Instead of summing counts for a detector, the count at each time recorded could be plotted as a coloured point on a line for each detector, with colour used to show the magnitude of the counts, as the lines are used in Figure 1. Detector lines would be plotted adjacent to one another to create a 2D 'image'.

Each time the program runs it could append a 'history' to a log file for the instrument manager, listing the non average detectors and the time of day. A further program could scan this daily and warn the manager of any new occurrences of nonaverage detectors. At this stage it might be worth storing the records in a database management system, at the moment, the overheads of this are too large.

The Administration System: As more instruments are built for use at ISIS, we receive more proposals, and find that we can give our world-wide users a faster, more accurate service using a database management system to store information relevant to their proposals for the use of ISIS beam time.
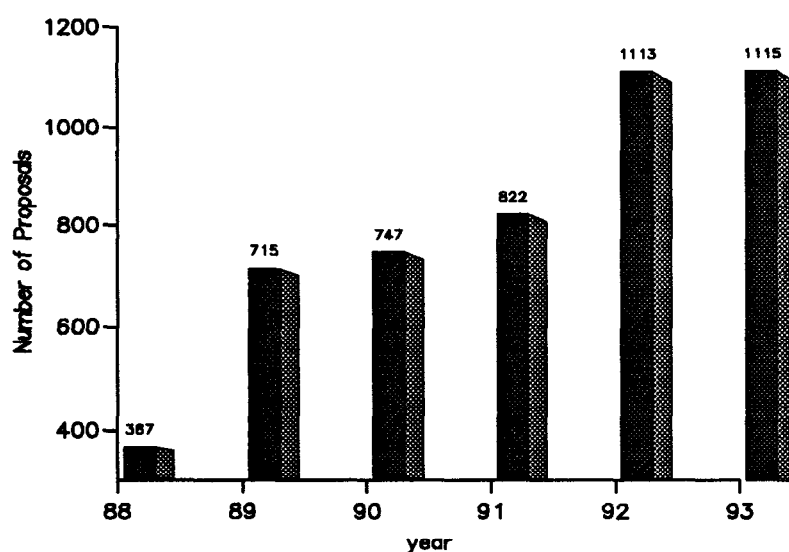
Growth in ISIS Proposals 1988–93

Figure 4 Histogram using information automatically extracted from the database

Figure 4 shows the growth in proposals submitted to ISIS over the last five years. Proposal submission rounds take place in April and October, at each one we now receive over 500 applications. On receipt, proposals are given a unique reference number which is stored with details of the experiment title, sample to be measured, instrument and sample environment needed and names and addresses of the proposer and collaborators. A relational database management system, S1032, is used, it runs on VAX/VMS on three of the workstations of our VAX cluster. Its query language can be used interactively for 'one off' queries or commands stored in a procedure file ready to make the reports we need regularly.

Figure 5 is a view of the system. The shaded area encloses the main datasets, which can be related to each other in a database as needed for production of reports. A selection panel meets in June and December to decide by peer review which proposals are awarded time. Their decisions and comments are recorded in the database, and information generated to print 'personalised' letters to each proposer giving them the results for all the proposals they submitted. Simple letters just adding name and address can use almost any 'mail merge' word processing system, we have found that only TeX can cope with more complex letters to a user who who submitted 10 proposals, some of which have been given time, some not, and any of which may have extra panel comments. We print about 300 letters for each proposals round.
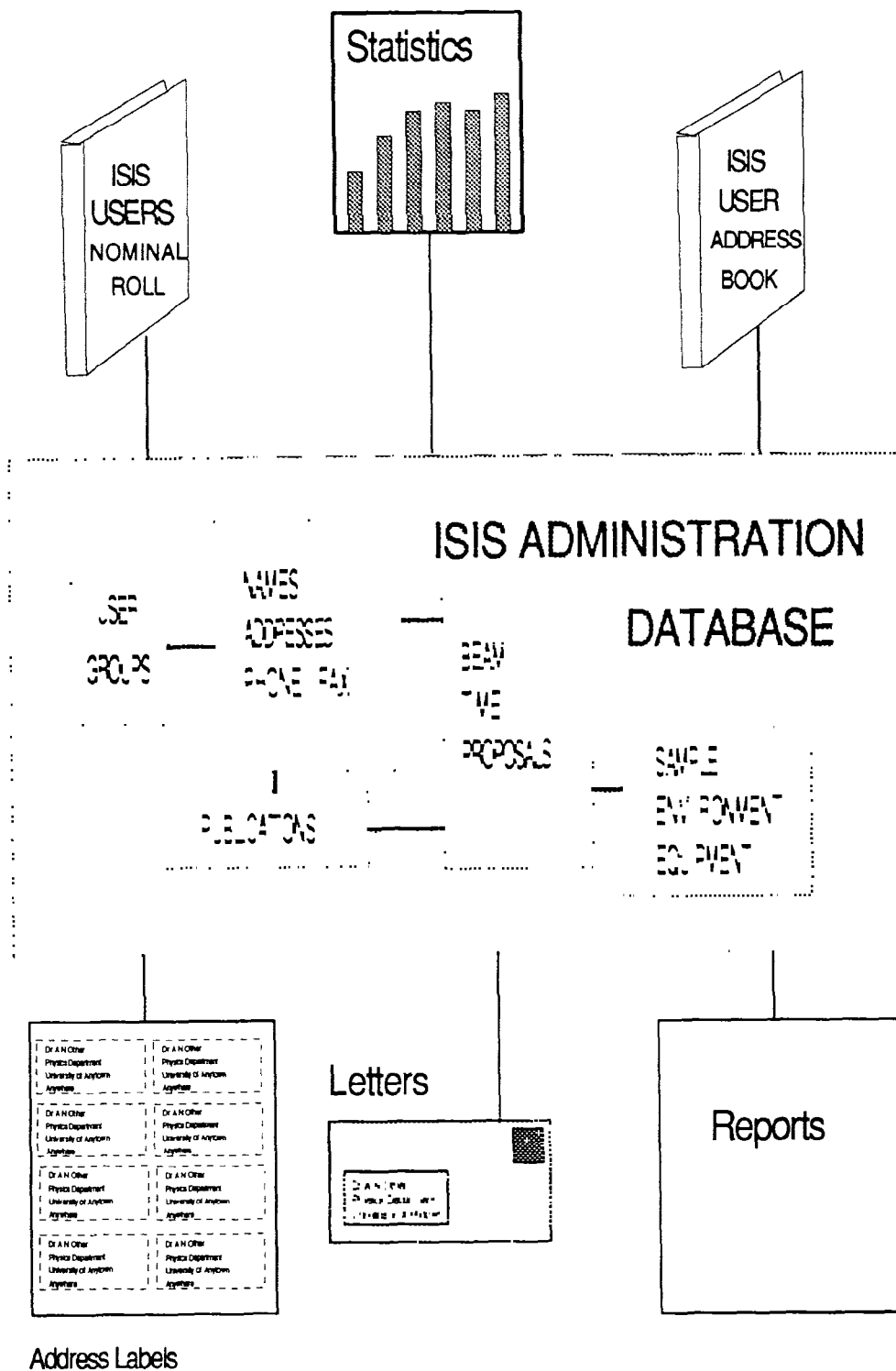
Figure 5   An overview of the ISIS Administration database

Most of the ISIS instruments are used for neutron scattering, a few for muons. Each instrument scientist schedules their own instrument manually and tells the operations manager what sample environment equipment is needed. He records the starting date for the experiment, resolves clashes of equipment and organises production of the 'scheduling letter' sent to the user, and the lists of equipment needed on each instrument by date. In future we hope to program the database to assist in the scheduling process. We also record the samples to be used, and whether they are hazardous, as each sample must be accompanied by a sheet of paper listing the hazards, handling precautions and first aid procedures.

Following completion of an experiment, the user sends us a report for publication in the ISIS Annual Report, and bibliographic references to published papers describing work done at ISIS. These are also stored in the database.

Statistics of ISIS usage are extracted from the database and read into spread sheet or graphics packages. Figure 4 was made using UNIGRAPH, it shows growth of number of proposals by year. Many other statistical plots are possible, we regularly make plots of usage by instrument, so have made a special procedure to do it quickly, more usually, the information is obtained interactively.

A list of UK users is printed annually in the 'ISIS Users Nominal Roll', which gives user addresses, phone and fax numbers. We have about 4000 names in our files, half of whom are UK residents; about 10% change their address during a year, so we are continually updating our files.

Over 50 procedures are in regular use producing our varied reports and we plan more to improve our instrument operations.

Future plans: Information from the printed proposals is currently typed into the database. We plan to accept 'electronic' proposals over the international computer networks in the near future, to improve the accuracy and reduce our typing and proof reading effort.

We are planning to integrate the system with that for issuing film badges for monitoring radiation exposure, and with a visitor registration scheme for greater laboratory security. The current forms management system will be replaced with a utility which uses 'OSF motif' window management system. We will then be able to store images in the database, possibly photographs of our equipment and users.

Raw data taken during an experiment is stored in an optical disk archive, using a 'home grown' cataloguing system. In future the location of these datasets may be stored in a database and linked to our possible instrument history records and our existing administration of the ISIS beam time proposals.