Time-of-flight small-angle-neutron-scattering data reduction and analysis at LANSCE with program SMR

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ABSTRACT: A user-friendly, integrated system, SMR, for the display, reduction and analysis of data from time-of-flight small-angle neutron diffractometers is described. Its purpose is to provide facilities for data display and assessment and to provide these facilities in near real time. This allows the results of each scattering measurement to be available almost immediately, and enables the experimenter to use the results of a measurement as a basis for other measurements in the same instrument allocation.

Introduction

Neutron diffractometers at pulsed sources use time-of-flight (TOF) to calculate the magnitude of each neutron momentum, p. Due to the broad distribution of p from pulsed sources, a single measurement accesses a large domain of momentum transfer space, given as $Q = (2p/\hbar) \sin \theta$ ($\hbar$ is Planck's constant divided by 2π, and θ is half the scattering angle). This gives considerable advantage in data acquisition over similar instruments using monochromated neutron beams as a source.

In a small-angle TOF instrument with a two-dimensional position-sensitive detector, the data are taken as counts in three dimensional cells, $C_{i,j,n}$, where i and j refer to the x and y channels of the detector at which the scattering event is detected and n refers to the TOF channel. The number of data points is, thus, very large. For example, in the present configuration of the Low-Q Diffractometer (LQD) at the Los Alamos Neutron Scattering Center (LANSCE), there are 128 each of x and y channels and 147 TOF channels for a total of over 2.4×10^6 cells. The data must be remapped into physically meaningful one- or two-dimensional momentum transfer spaces as differential cross sections, $d\Sigma(Q)/d\Omega$ or $d\Sigma(\mathbf{Q})/d\Omega$, respectively. In this, the broad-band nature of the source introduces aspects of data reduction that must be considered carefully. These have been discussed in earlier papers [1-3], but are still an active area of research. It is likely that the reduction procedure will depend on the sample and the requirements of the analysis that will be used. By recording and storing all data for each measurement, we provide maximum flexibility for data reduction and analysis. Thus, as a consequence of the use of TOF measurement and the broad-band nature of the source, data reduction on TOF small-angle instruments is more complicated but has greater flexibility than on similar instruments that use monochromated neutron sources.

There are three primary functions that are supported in our system SMR (Show Me and Reduce). These are data display, reduction, and analysis all of which are required for the user to assess the data and draw some conclusions from it. Because of the large size of the data sets, a graphics display of data is essential. This should be interactive, allowing information to be returned to the program. Furthermore, our state of understanding the data reduction demands that the procedures should have flexibility built in to suit the needs of a particular measurement. Also, functions should be present that allow assessment of the data-reduction procedures.

Of major importance in the design of our system is that we have taken the point of view that near-real-time data display and reduction are an essential part of a neutron scattering experiment. Thus, facilities should be available during data acquisition, as well as after the measurement. This offers the possibility that the results of a measurement can be immediately available, allowing them to be used as a bases on which to plan the next measurement. The ability to assess the data quickly allows the well-prepared user to make optimal use of the current allocation and may save having to redo parts of an experiment at a later date. This is important at a scheduled user instrument because the user may have to wait several months for additional measurement time.

Therefore, the objectives for SMR are the following:

(1) Provide tools for assessment of TOF small-angle data as it is being acquired, which includes display of raw data and fast data reduction (not necessarily highly accurate in this mode).
(2) Provide data reduction to $d\Sigma(Q)/d\Omega$ and $d\Sigma(Q)/d\Omega$ in absolute units. In addition, tools should be provided to assess the efficacy of the data-reduction procedure itself. The program should thus be useable as a tool to research data reduction procedures.
(3) Provide basic data-manipulation functions and analysis procedures with appropriate interactive displays.
(4) All of this must be in the framework of a fast, user-friendly program that is easy to learn and use, and provides sufficient flexibility to meet the needs of all types of measurements. This implies that no knowledge of the data-acquisition-computer-operating system, beyond a list of simple operations, should be required, and that these operations should be readily available as menu options and/or commands.

We have found that these objectives are best met by an integrated system that automates most of the communications needed for the function of the different program parts, thus minimizing the amount of user interaction and input.

Organization

SMR must allow the user to retrieve and manipulate data from the instrument detectors in a manner that is transparent to the user. The different instrument detectors and the relationship with other parts of the data acquisition system are shown in Fig. 1. The LQD uses three detectors: the main, position-sensitive area detector; an upstream incident-beam monitor; and a downstream transmission monitor (currently under development).[4,5] The signals from the detectors are collected and processed by FASTBUS acquisition hardware and stored as histograms in the acquisition system BULKSTORE module. The FASTBUS crate is interfaced to a dedicated DEC µVAX workstation/GPX operating under VMS. A complete description of the data acquisition hardware and software is given elsewhere.[6]

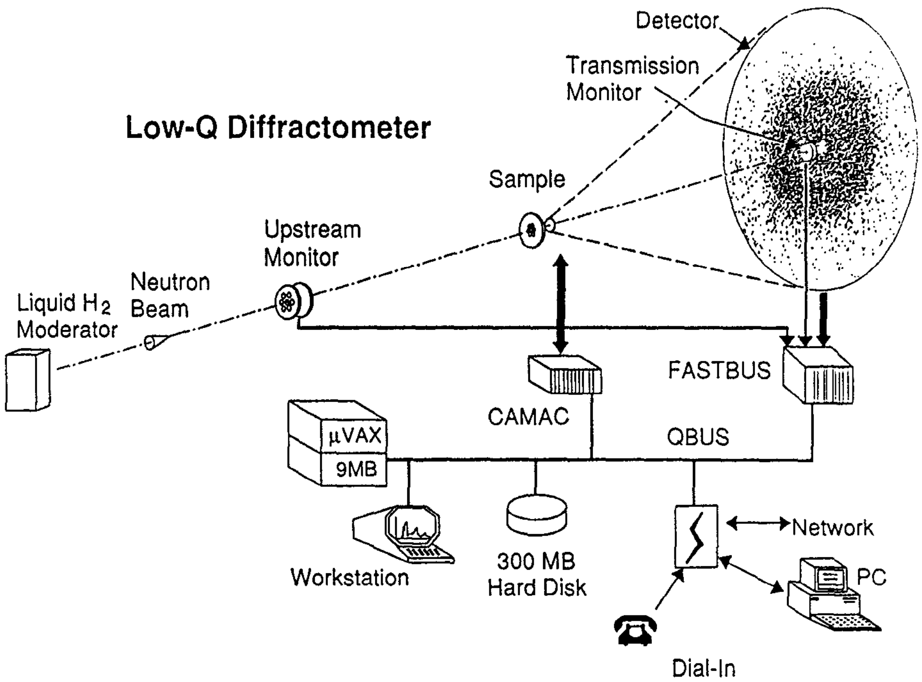

Fig. 1 The Low-Q Diffractometer at LANSCE and the integration of its components with the data acquisition system. The geometry of the LQD is shown with the positions of the different detectors and sensors. The upstream monitor is used to monitor the incident beam intensity just after the collimator entrance aperture. The sample position is located about 4 m downstream. A second transmission monitor is planned, which will be placed in the beam stop just in front of the main position-sensitive detector. Signals from the beam monitors and main detector are passed to the FASTBUS crate where they are mapped and stored in the bulkstore module. Sample environment information is passed to the CAMAC crate. The data in the CAMAC scalers and FASTBUS bulkstore are transferred to the dedicated µVAX via the QBUS. The µVAX, however, is not involved in the data acquisition per se, but in setting up the measurement and in data transfer. Communication with the data acquisition system is also through the µVAX. Data is passed between the computer and other devices by the QBUS.

SMR consists of a core of central tasks and a periphery of extensions and enhancements. The core of SMR is organized into four major subsystems as illustrated in Fig. 2. These are the user interface, the task management module, the task subsystem, and the data acquisition and instrument interface. The subsystems are further partitioned into modules and segments associated with specific tasks or program functions. This design is intended to ease the evolution of the system as functions are added, deleted, or redefined.

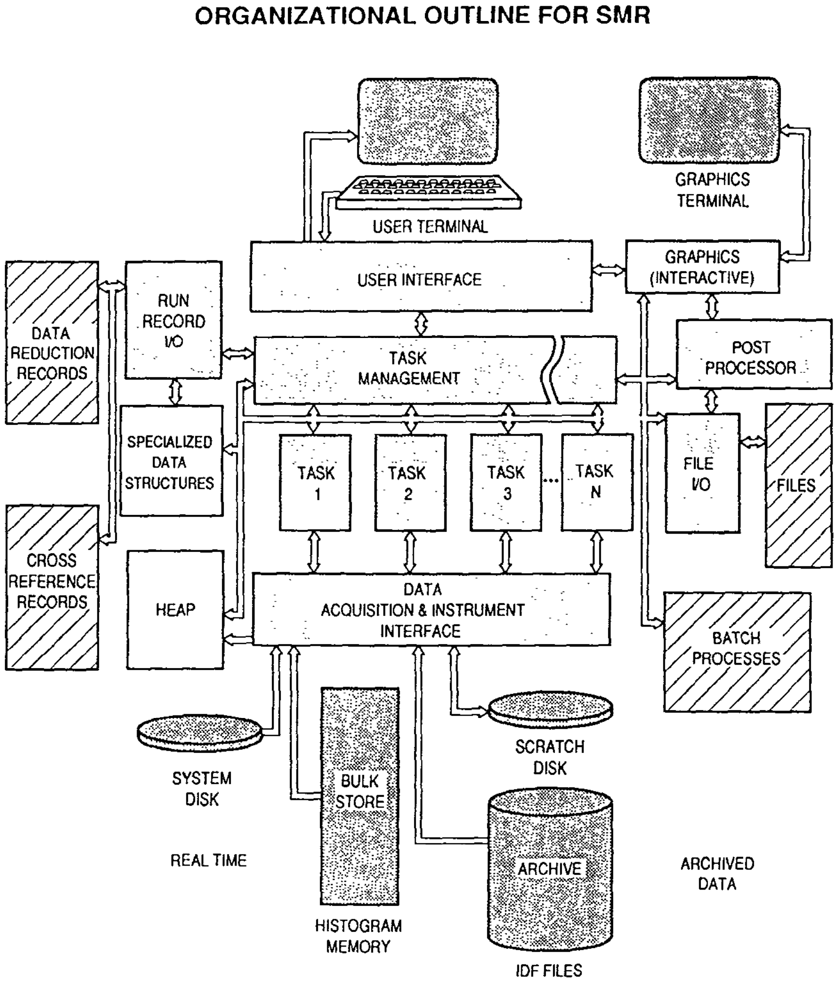

Fig. 2 The organization of SMR. Each of the major subsystems of SMR is illustrated by a light-shaded block. Files are represented by hatch blocks, physical devices by dark shading. Internal data structures are represented by open blocks. Tracks having arrows at both ends represent bidirectional information flow between the connected units and the different data structures, files, and devices. Single arrows indicate uni-directional flow.

The major peripheral subsystems are the interactive graphics, postprocessor and file I/O modules. All are organized with the same philosophy as the core subsystems. The postprocessor is an extension of SMR to provide flexible operations on reduced or raw data in analysis, normalization, scaling, background subtraction, averaging, and related functions. Its organization is like that of SMR (Fig. 2) except there is no instrument interface.

User Interface

User requests are communicated through the user interface. The various modules supporting different functions and options are organized as menus and submenus in a tree-like hierarchy. The branches of the tree correspond to the different program functions and their options. The user interface supports different interactive modes, depending on the type of terminal connected to the process. This interface includes a menu driver that can be used on DEC terminals or emulators and a command line interpreter for use on other terminals. Terminals are polled as to their capabilities and the appropriate part of the user interface is run. Future versions of the user interface will also use more advanced facilities that are under development for VAX workstations by the data acquisition section at LANSCE.[6]

Task management module

The requests generated by the user interface are organized by the task-management module. The task manager invokes the functions of SMR, after polling the control flags set up by the user interface, and passes control to the required functions that are organized into task modules (labeled in Fig. 2 as 1 through N). Appropriate data structures containing values obtained from the cross-reference records, data-reduction records, and the user interface are passed to the routines. The results of the computation are placed in data structures or passed by the task manager to the interactive graphics display facility or to file I/O routines, depending on user request. Control is then passed back to the user interface along with any other numerical results that should be reviewed by the user. Some of the calculations in data-reduction tasks require considerable computation times. Thus, there is an option for the task manager to pass these to detached processes run in batch mode (Fig. 2), returning control immediately to the user and informing him when the calculation is complete.

Task subsystem

The computational functions of SMR are set up in the different task modules of the system. Thus, functionality in SMR is easily altered by changing or adding modules. Raw data is obtained by these functions from the different bulk-storage devices through the data acquisition and instrument interface. Other preprocessed data and intermediate results are communicated between modules and between the main process and any tasks relegated to batch processes by way of file I/O procedures. The programs normally run in batch modes are non-interactive subsets of SMR.

All computations and tasks are supported internally by several data structures. The HEAP is a linked list of data structures.[6] A similar data structure containing information pertinent to the TOF measurement, instrument geometry, and detector configuration is maintained on the system disk during data acquisition[6], and a copy is stored as part of the archive file when the run is saved. The run information in the system or run HEAP is copied directly into the local HEAP and then used for data reduction, display, and analysis. Other data structures tailored to specific tasks and functions are also used, which include data for the interactive graphics facilities as well as parameters and cross references to files used in data reduction and analysis. The data in these structures are maintained in external data-reduction record files and in cross reference record files (Fig. 2) for later reference. These can be reviewed at any time. This recall is necessary as data reduction involves a number of options and values that may need to be changed if later assessment of the data reduction shows it to be faulty. The files are also used to communicate data-reduction information to batch processes.

Instrument and data acquisition interface

The modules of the instrument and data acquisition interface retrieve data from the different bulk storage and data acquisition devices. The bulkstore memory of the FASTBUS retain data currently being acquired. The system disk maintains run configuration information on the current run in the HEAP. Previously acquired data is stored in compressed form as an Instrument Data File (IDF) on the user disk or remotely on an archive disk. The modules of this interface determine the physical location of the requested data, retrieve the data, and pass it back to the calling routine. The interface searches the data archive using criteria supplied through the user interface, which may include run number, experimenter name, instrument name, experiment title and/or IDF file name. In this way the entire data archive, which consists of remotely mounted optical disks with a planned total storage capacity of 0.5 terabytes, is accessible for analysis or display in a manner transparent to the user. Accessed archived data are retrieved to a local scratch disk in global data areas to increase access speed. The basic-data retrieval functions are recovery of raw data for each time channel from the upstream monitor, the transmission monitor, and the main detector.

The peripheral subsystems: graphics, postprocessor and file I/O

The graphics output has several display options that support one- and two-dimensional displays. The current versions of the one-dimensional graphics and two-dimensional contour plotting routines use TEK4010/4016 graphics, which may be emulated on a wide variety of terminals. Two-dimensional color graphics is currently done by outputting to an IBM PC, which displays the data using programs developed by John Hayter of Oak Ridge National Laboratory. The graphics subsystem is in an early stage of development and will be expanded to accommodate other graphics systems and standards as determined by the LANSCE data acquisition section. User interaction with the graphics subsystem is used to pass information back to SMR for other data acquisition, reduction, and analysis tasks.

The interactive graphics is closely tied to the postprocessor of SMR, which contains the data analysis package. All sample-dependent data manipulation, e.g., scaling, is done in this part of SMR. Other tasks presently available in the postprocessor are regression analysis, free-formatted data manipulation (arithmetic operations on data sets and binary operations with data sets as arguments), and input and output in different file formats. This facility, which is also implemented in a stand-alone form, has organization like that of SMR. It is intended to give some flexibility in data treatment; it can be used to manipulate all SMR output, and is portable to VMS 4.6 and later versions.

The computational results (reduction or analysis) or raw data can be sent to an output file at the user's request. In addition, some procedures generate intermediate data files that may be found and used by subsequent tasks and detached processes. These output tasks are supported by the file I/O facility. We plan to support several file formats for user output to suit the needs of the experimenter. Our standard output file is block-formatted ASCII, including an abstract containing run identification, run-configuration information, and a running account of the various operations performed on the raw data sets, followed by labeled data blocks and the statistical (rms) precision of the data. The rms Q-precision of the differential cross section is included when appropriate. Descriptions of this format along with descriptions of subroutines available to read it are given in Appendix A.

Functions

Here we present a partial list of the various functions presently implemented in SMR, with an emphasis on those that allow assessment of raw and reduced data. As the number of data can be quite large, even in reduced form, there is a strong reliance on graphics.

Figure 3 illustrates the main menu and two submenus of the core user interphase of SMR, which give examples of some of the functions available. Selections are made by moving the cursor to a line by either typing the character indicated by **bold** (underscored in this rendition) on the menu or by using the cursor keys, arrows, return, tabs, spaces or backspace, then typing <ENTER>, <DO>, or <CTRL>-G. These illustrations are for a terminal supporting ANSI control sequences; otherwise (or if the "M" option (Fig. 3) is toggled), the same functions are achieved with a command line format (Fig. 4). The two submenus shown are for raw data **D**isplay and for data **R**eduction. In the particular example shown, an archived file has been accessed. This could also have been data in the FASTBUS bulkstore, and the same functions would have been available.

Raw-data display options currently available are, in order: a detector map for selected time slices projected onto either one or two dimensions; detector counts mapped into two-dimensional space defined by detector radius and time (R-T); and one-dimensional displays of the counts as a function of TOF channel for the integrated detector, upstream, or transmission monitors. Computation of the center of scattering intensity on the detector or entry of the beam center by the user is also available, as is a display of the contents of scalers.

The different data-reduction functions are also illustrated in Fig. 3. The first entry is the computation of the wavelength-dependent transmission coefficients of the sample. Next is the basic function of mapping the data into $d\Sigma(Q)/d\Omega$ and $d\Sigma(Q)/d\Omega$ spaces. These are output on an absolute scale (see below). The "quick and dirty" version of this is for quick reduction of data over a limited number of time channels (strictly for quick assessment of the data). The Q-lambda map is a normalized and scaled form of an R-T map and is used for assessment of the normalization and background subtraction of the reduced data. The Theta-T map is similar to the Q-lambda map except that the two-dimensional space is defined by the independent variable in Q, scattering angle, and TOF. The flux, as measured by the main detector and downstream (transmission) monitor, is also available. The two options for the beam

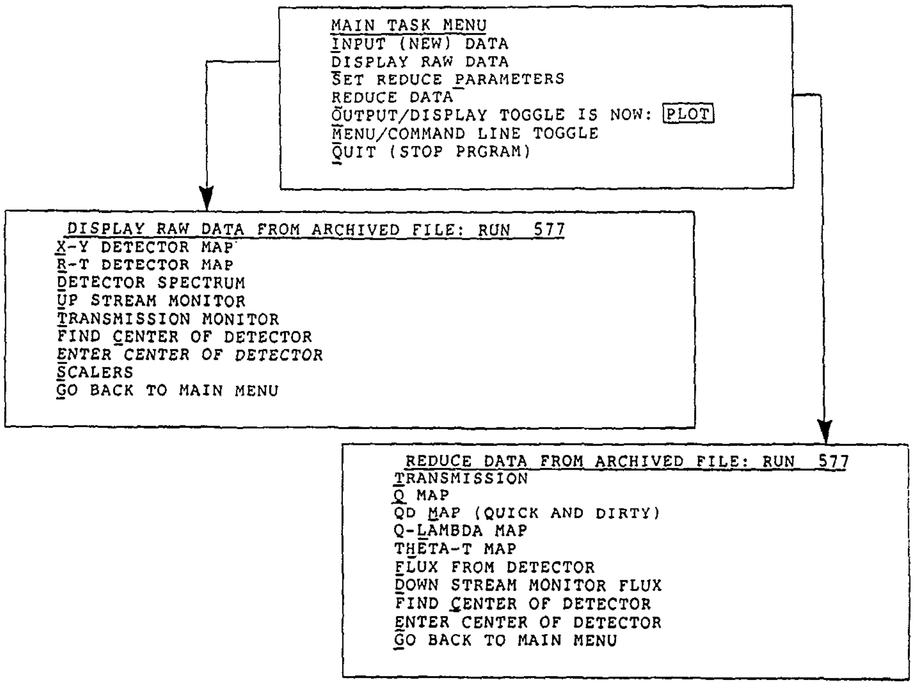

Fig. 3 An example from the main menu and two submenus of the SMR user interface. The main menu of the user interface is shown here, which illustrates the various options available to the user. Characters that appear in **bold** are underscored in this rendition. The data reduction and raw-data display submenus are also shown. The interaction with the menus is supported by a driver written in C.

BINNING PARAMETERS

COMMAND	PARAMETER	OPTION
-b	60	Number of (radial) Q-bins
-n	55	Number of radial detector bins used in detector and RT maps
-l	0.000 A	Lower limit for Q-map
-u	0.350 A	Upper limit for Q-map
-s	5 det ele	Smallest radius used on detector
-r	60 det ele	Largest radius used on detector
-m	0.00638	Instrument scaling constant
-bs	1.000	Fraction of background to be subtracted
-t	0.500	Position in the time channels from which the nominial value is taken.
-c	0.500	Position in the spatial channels from which the nominial value is taken.
-g		Go back (no further changes)
: -b 175 -s 10		

Fig. 4 The command line interpreter. An alternate interactive mode of the user interface is illustrated. This segment is from a facility for altering entries in the data-reduction options table for $d\Sigma(Q)/d\Omega$ and $d\Sigma(\mathbf{Q})/d\Omega$ maps. It illustrates the general form of this mode, in which a key followed by a parameter is entered into a command line. The display shows the options available, the parameter to be entered, if needed, and the default value, if any.

center are identical to those in the raw-data display menu and are needed to support the mapping functions of SMR.

Figure 4 is an example of the command line mode of the SMR user interface. In this case, the user has made a request to alter the values in the parameter table (a specialized data structure in Fig. 2) for the binning parameters for data reduction to a Q-map. The display for this mode includes a menu of the commands, the parameter to be entered and its default values (if applicable), and the resulting option invoked. A typical entry is shown, in which the number of Q-bins is changed to 175 and the smallest radius used on the detector is altered to be 10 detector elements. These become the new defaults for the duration of the computing session.

An example from the graphics and postprocessor user interface is shown in Fig. 5. This subsystem is used to manipulate and analyze output from the core functions of SMR in a flexible manner. It is also implemented as a stand-alone facility. Here the menu for file I/O, data manipulation, and analysis menus are shown, along with two submenus. On the left are the currently available analysis routines. On the right are the data manipulation routines. Here, three previously computed, background-subtracted $d\Sigma(Q)/d\Omega$ maps for measurements 263, 591 and 588 are being compared. One has been selected and its ordinate values are to be scaled by dividing by 10. Data arrays can be added to, subtracted from, multiplied or divided by each other in the postprocessor.

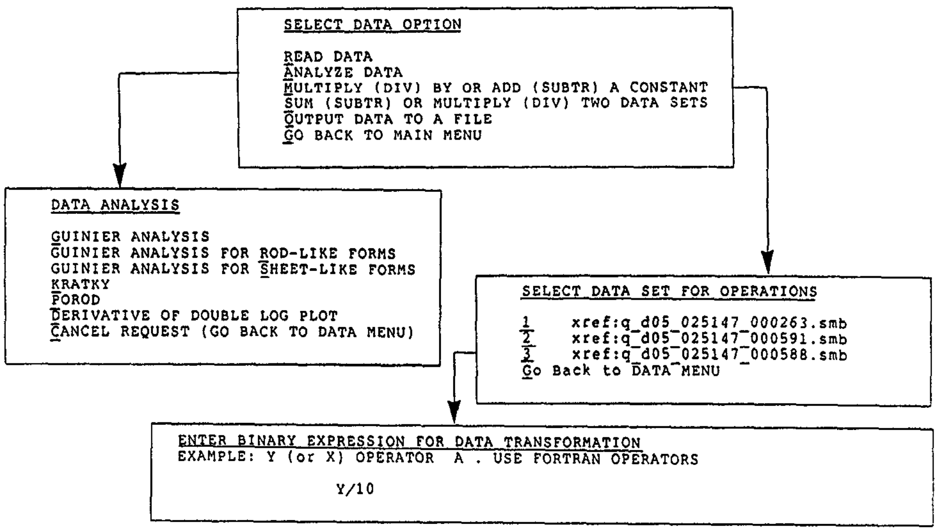

Fig. 5 An example from the postprocessor menu. The different options currently available in the postprocessor menu are illustrated, including data analysis and file-manipulation options.

Examples

The basic function of SMR is to provide the maps, $d\Sigma(Q)/d\Omega$ and $d\Sigma(Q)/d\Omega$. In this, the counts detected in each i, j[th] detector element in each n[th] time channel, C_{cn} , are placed into a bin, K, with a domain in Q (or Q) covering that of the i, j, n[th] cell. Each counts in cell is converted to an absolute differential cross section times the area density of scatterers by division with an appropriate normalization factor; thus, the map is given by the expression[1,3] :

$$N/A\ [d\Sigma/d\Omega]_K = \sum_{\{K\} \supseteq \{i,j,n\}} C_{i,j,n} \Big/ \sum_{\{K\} \supseteq \{i,j,n\}} \Delta\Omega_{i,j}\ I'_n\ \varepsilon_n\ \eta_{i,j}\ , \qquad (1)$$

where the differential cross section is in units of area and N/A is the number of scatters per unit area. Here $\Delta\Omega_{i,j}$ is the solid angle of the i, j[th] detector element, and $\eta_{i,j}$ is its counting efficiency; ε_n refers to the response of the detector to the neutrons in the n[th] time channel.(4) I'_n is the number of neutrons that passed through the sample neither scattered nor absorbed. Equation (1) is a statistically weighted average of the contributing cells, which optimizes the precision in Q and in differential cross section [1,3].

The measurement of $I'_n\varepsilon_n$ is critical to proper normalization of each cell. Errors in its determination can lead to distortions in the scattering curve. On the LQD, $I'_n\varepsilon_n$ is presently determined by making a separate measurement of the transmitted beam using a Cd mask as an attenuator, normalized to the upstream monitor. We are developing a transmission monitor in the beam stop to make this measurement concurrently with the scattering measurement.[4,5]

An example of the efficacy of the calculation represented in Eq. (1) is shown in Fig. 6 (from a display generated by the postprocessor), which compares data from a standard sample consisting of a mixture of deuterated and protonated polystyrene (PSD/PSH = 0.48[7]) measured on the LQD and the 30-m SANS at Oak Ridge National Laboratory. The shapes of the curves are, for all practical purposes, the same. Some differences are seen in the low-Q region, and this is likely to be the result of multiple scattering of the long wavelength neutrons which contribute to this part of the map. Inspection of the transmission coefficients at long wavelengths illustrates this (Fig. 7) and indicates a useful application of data reduction to transmission coefficients.

Displays available from SMR for $d\Sigma(Q)/d\Omega$ and $d\Sigma(Q)/d\Omega$ maps are shown in Figs. 8 and 9, which show data for polystyrene latex spheres in D_2O. The Guinier analysis given by the postprocessor (not shown) gives the radius of gyration as 143 Å, in good agreement with the known diameter of 380 Å for these particles. Figure 9 is a shaded monochrome rendition of the two-dimension color graphics display.

Figure 10 illustrates a diagnostic raw-data display, the R-T map. From this, some idea of the parts of the histogram that are contributing signal can be determined. An example of a normalized theta-lambda map is given in Fig. 11. The lines, which are contours of constant $d\Sigma(Q)/d\Omega$, will be straight on this double log display if the scattering is invariant at constant Q, which should be the case. Curvature in the

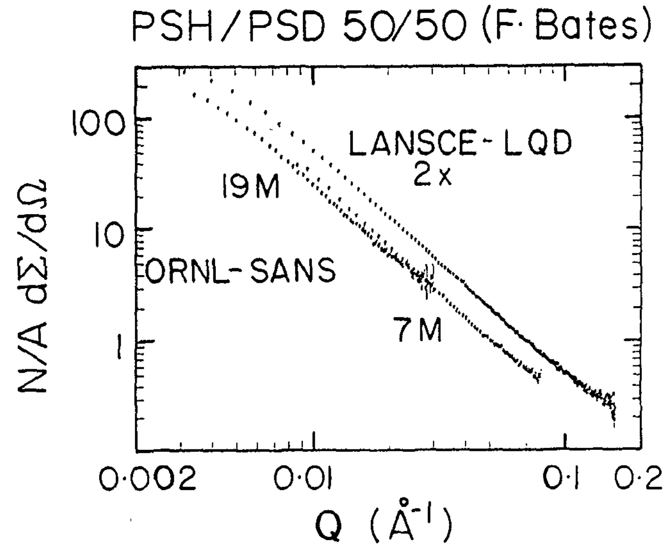

Fig. 6 A comparison of a map computed for a mixed perdeuterated/protonated polystyrene (PSD/PSH) sample and data taken for the same sample on the Oak Ridge SANS instrument. This figure is from a display generated by the postprocessor. Data taken on the ORNL 30-m SANS instrument at the 19-m and 7-m positions are indicated. Scattering computed from data taken on the LQD at LANSCE is scaled by a factor of two for clarity.

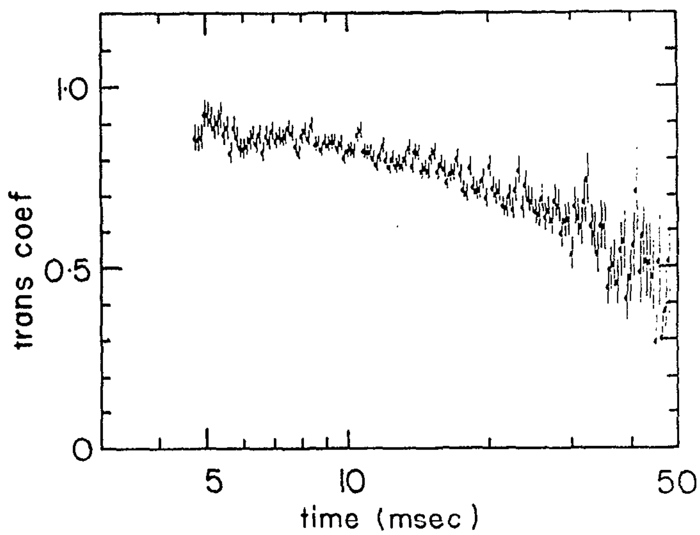

Fig. 7 Transmission of the PSD/PSH standard polystyrene sample. This is from the interactive graphics display generated by the transmission coefficient option of the reduce data submenu. Plotted are the transmission coefficients for each time-of-flight channel. These numbers are not used directly in computing Q-maps, but serve a function in assessing the possible presence of multiple scattering in the mapped data.

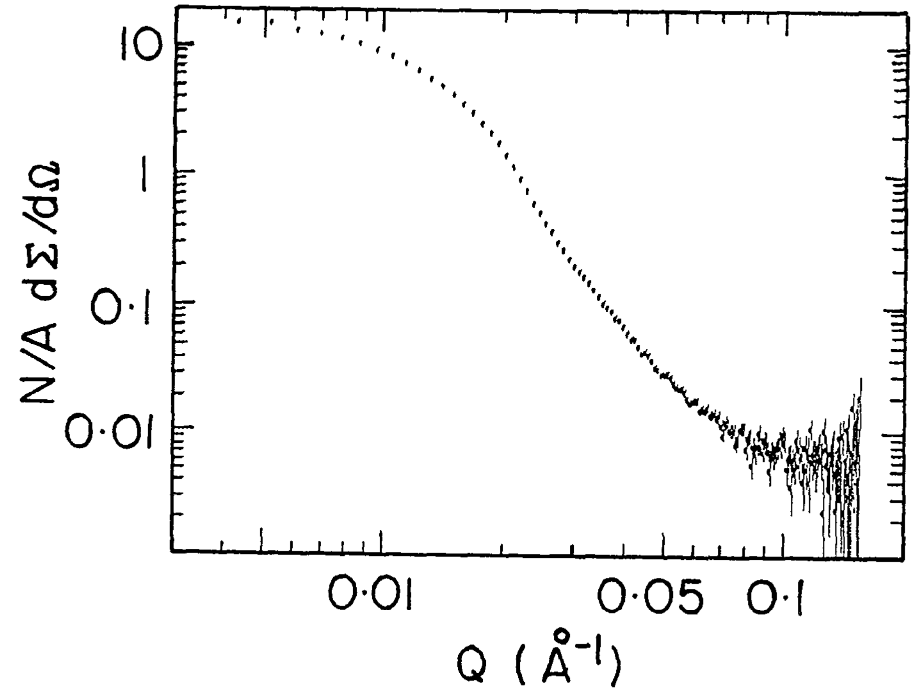

Fig. 8 An N/A $d\Sigma(Q)/d\Omega$ map of polystyrene latex spheres in D_2O. This is from the output generated by the Q-map option of the data reduction submenu using the one-dimensional output option. The test particles are spheres approximately 38 nm diameter.

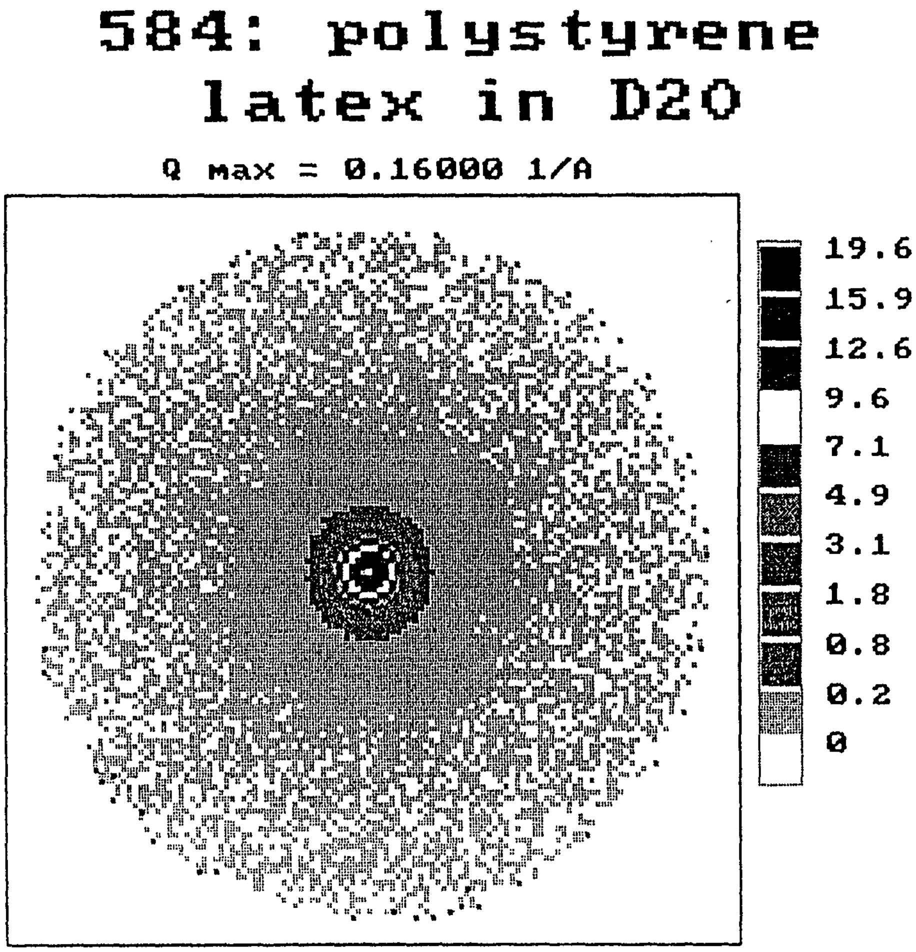

Fig. 9 An N/A $d\Sigma(Q)/d\Omega$ map of scattering from polystyrene latex spheres in D_2O. A monochrome reproduction of output generated by the Q-map option of the data reduction submenu using the two-dimensional color graphics option. Here, the values of N/A $d\Sigma/d\Omega$ are shown for each Q_y, Q_x cell. Values are indicated on the scale to the right. The values of the differential cross section increase monotonically toward the Q origin at the center.

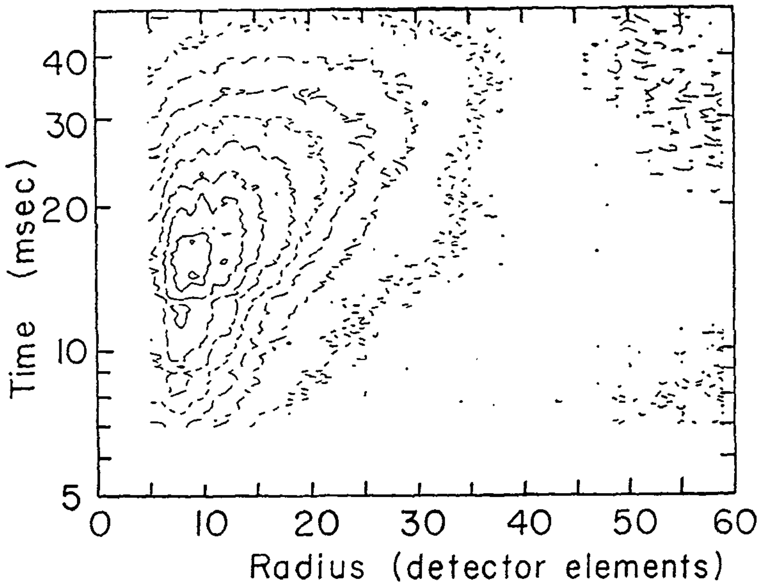

Fig. 10 A radius-TOF map of raw data taken from latex spheres in D_2O. This is from the output obtained from the R-T Map option of the Raw Data Display submenu using the contour map display option. In this, the counts in each radial-TOF cell are contoured at levels of 1% (_ _), 4% (___ ___), 9% (_ _ _), 16% (____ ____), 25% (_ _ _), 36% (_______), 49% (_____), 64% (_______), and 81% (_____) of the maximum value.

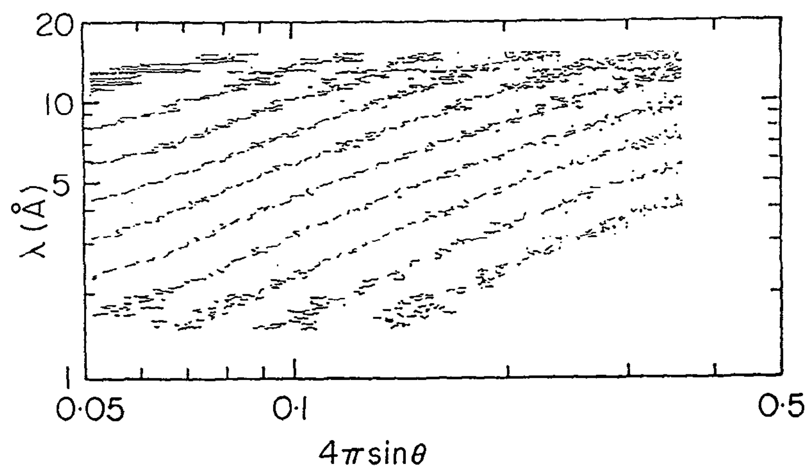

Fig. 11 A theta-wavelength map of data reduced from PSH/PSD. This is from output obtained from the Theta-Lambda option of the Reduce Data submenu using the contour display option. Here lines of constant N/A $d\Sigma(Q)/d\Omega$ are plotted for the wavelength and θ cells, using the same contouring intervals as in Fig 10. Wavelength is on a logarithmic scale, as is 4πsinθ.

lines is indicative of problems in normalization, background subtraction or instrumental effects, such as detector non-linearity or instrument resolution effects.[1-3] Sample dependent effects, such as multiple scattering[8] or inelastic effects[3], may also be seen from such plots.

Future directions

The basic features of SMR have now been outlined and future developments will involve the implementation of other facilities, particularly interactive graphics and data analysis. A major concern is improving the speed of the calculations. Presently, some of the maps require about 60 minutes of CPU time to calculate, necessitating that some tasks be relegated to batch processes. This clearly cannot be accepted given the objectives of SMR. Some improvements in speed can be obtained by more efficient code. However, acceptable computation times can only be obtained with hardware improvements such as attached processors. When such devices are available, it will be straightforward to alter the interface modules to use these, and near-real-time data assessment and analysis will then be possible.

References

1. Seeger, P.A., and Pynn, R., 1986, "Resolution of Pulsed-Source Small-Angle Neutron Scattering", Nucl. Instr. Meth., A245, 115-124.
2. Hjelm, R.P., Jr., 1987, "Resolution of Time-of-Flight Small-Angle Neutron Diffractometers", J. Appl. Cryst., 20, 273-279.
3. Hjelm, R.P., Jr., 1988, "The Resolution of TOF Low-Q Diffractometers: Instrumental, Data Acquisition and Reduction Factors", J. Appl. Cryst., 21, 618-628.
4. Seeger, P.A., 1988, "Neutron Detection Systems for Small-Angle Scattering", J. Appl. Cryst., 21, 613-617.
5. Seeger, P.A., Hjelm, R.P., Jr., and Nutter, M.J., 1989, "The Low-Q Diffractometer at the Los Alamos Neutron Scattering Center", Mol. Cryst. Liq. Cryst., (in press).
6. Nelson, R.O., Cort, G., Gjovig, A., Goldstone, J.A., McMillan, D.E., Ross, J., Seal, J., and Machen, D.R., 1987, "The Los Alamos Neutron Scattering Center Data Acquisition System", IEEE Trans. Nucl. Sci., NS-34, 1017-1032.
7. Wignall, G.D., and Bates, F.S., 1987, "Absolute Calibration of Small-Angle Neutron Scattering Data", J. Appl. Cryst., 20, 28-40.
8. Copley, J.R.D., 1988, "The Significance of Multiple Scattering in the Determination of Small-Angle Neutron Scattering Experiments", J. Appl. Cryst., 21, 639-644.

APPENDIX A:

Block-formatted ASCII files

Standard output data files from the LQD consist of a three-record abstract and a number of blocks of data, all in directly readable ASCII strings. A data block consists of a series of numbers that may include decimal points and/or exponent fields, which are separated by commas or blanks and terminated by '/' followed by a zero byte (ASCII <NUL>). For ease of printing, the string includes <CR><LF> sequences after every 126 or fewer characters, and the first character on the line is generally a blank. The subroutine REALOUT (ARRAY, NDATA, NUNIT) is provided to write these blocks. The string is designed to be read by a FORTRAN unformatted read statement, into a real array at least as long as the number of data. The array should be zeroed (or appropriately initialized) before the read statement, as null fields will not be modified during reading. The terminal zero byte has been included to assist parsing in other languages.

Abstract Record 1

Bytes 1- 4, File type (e.g., 'LOGT' or 'RT'). For 1-D spectra, the type generall specifies the inddependent variable.
Bytes 6-45, Title of run, usually terminated with '$'
Bytes 47-63, File ID; the instrument, date, and time at which data was saved, as assigned by the data-acquisition system; e.g., 'LQD_881002_183520'
Bytes 64-73, Integrated current (μA-h), real format (may be blank).

Abstract Record 2

This record is an ordered block (as defined above) of up to 100 parameters. Several parameters have been defined for use by various analysis programs (especially MPLOT and QBIN); these are as follows:

1. Number of channels in data blocks. This parameter is always required.
2. dt/t for the logarithmic time scale
3. Clock tick (μs); usually 0.1 μs
4. First time-channel boundary (μs)
5. Time delay of detector electronics (μs)
6. Source-to-sample distance (m)
7. Sample-to-detector distance (m)
8. Size of one detector element (mm)
9. X-position of beam center, in detector elements
10. Y-position of beam center, in detector elements
11. Power of units: 1 (default) for raw data, 0 for ratio
12. Number of bins that have been combined; usually 1
13. Number of bins per decade for uniform log scale
14. Incident energy for direct-geometry inelastic scattering (eV)
15. Final energy for inverse-geometry inelastic scattering (eV)
16. dQ/Q for Q bins below the switch point
17. Q at which bins switch from log to linear ($Å^{-1}$)

18. Width factor in Q-binning: radial bins wider than this factor times the Q-bin width are deleted.
19. Fraction of total neutrons kept during Q binning.

Abstract Record 3

This record is an algebraic expression of operations that have been performed on the data. Initially, it is a brief spectrum identifier enclosed in parentheses, with byte 1 blank. For instance, '(586, 25-147)' represents radially averaged detector time slices 25-147 of run 586, '(256,M1)' is the corresponding upstream monitor spectrum, and '(585, R=0-5)' is the sum of the central 5 radial zones of the detector for run 585, which was a transmission run. There must be no embedded blanks; the first blank after column 1 terminates the string. (The terminating blank may be followed by an ASCII <NUL>.) The string is divided into "lines" by a <CR><LF> after every 80 characters. Total length allowed is 720 characters (9 lines).

Byte 1 is blank if the term will not need parentheses added when another operation is appended,
is '+' if the last operation was + or -, and
is '*' if the last operation was * or /.

All data blocks following the abstract have keyword identifiers in the first record. If the first four characters aren't one of the standard identifiers listed below, the record is assumed to be the type identifier of a new abstract. A blank record should be used to separate data files within a file.

'POINTS' or 'BINS'

An optional block giving the values of the independent variable (POINTS) or of the boundaries of histogram bins (BINS). The number of points should equal the value given in the second abstract record; the number of bin boundaries is one greater than this number. This block may be omitted if the independent variable is the channel number, or if it is time of flight that may be computed from parameters 2-5 of the abstract. For two-dimensional data, the first block will refer to the X coordinate and the second (if any) to Y. The dimension of the second block is not included in the abstract.

'AREA'

An optional block of normalizing factors to be divided into the data. This is useful if the data are raw histogram counts. For two-dimensional data, the first block will refer to the X coordinate and the second to Y.

'RMSBIN'

An optional block giving the rms of the values of the independent variable, for instance, when finding an average of data within a bin. For two-dimensional data, the first AREA or RMSBINS block will refer to the X coordinate and the second to Y. Note that the read subroutines described below do not allow having both AREA and RMSBIN blocks associated with the same variable.

'DATA'

The dependent variable of a one-dimensional file (must not occur in a two-dimensional file). The number of data should agree with parameter 1 in the abstract.

'Y = nnn'

The identifier for this block has an '=' anywhere within the first four characters and an integer within characters 6 to 15. The integer is the row number in a two-dimensional array (i.e., the Y coordinate). The number of data in the block should agree with parameter 1 in the abstract (the X coordinate).

'STDDEV'

Standard deviations of the data. This block should immediately follow the 'DATA' or the 'Y= ' block to which it applies. May be omitted only if the data have Poisson statistics; i.e., for raw histograms or simple sums of channels.

Two standardized FORTRAN subroutines are available for reading these files, respectively, for one-dimensional and two-dimensional data. Both are written in Fortran 77 and should be highly transportable.

Subroutine READ_1D(IUNIT, TYPE, TITLE, FILEID, UAHR,
PARAMS, NP, HEADER, NH,
X, DX, Y, DY, IFLAG, IERROR)

Searches logical unit IUNIT for the next data file of type TYPE, or for any one-dimensional file if TYPE = ' '. Returns all abstract information and the arrays X, DX, Y, and DY. X is always converted to bin boundaries and DY defaults to SQRT(Y) if the STDDEV block was omitted. DX may be a normalizing factor (i.e., bin area) or the rms of points included in the bin (in which case IFLAG = 1).

Variables in calling sequence:

IUNIT	Integer	Input	Fortran unit number
TYPE	Char*4	In/Out	Type to search for, or type found
TITLE	Char*40	Output	Title from first record of abstract
FILEID	Char*17	Output	Instrument_Date_Time identifier
UAHR	Real	Output	Integrated beam current
PARAMS	Real(NP)	In/Out	Parameters in the abstract. May be preinitialized if missing from data file.
NP	Integer	Input	Maximum number of parameters to return
HEADER	Char(9)*80	Output	Character string describing operations previously performed on data

NH	Integer	Output	Number of characters in HEADER
X	Real(*)	Output	Bin boundaries (channels + 1)
DX	REAL(*)	Output	Normalizing function or rms of bins (see IFLAG)
Y	Real(*)	Output	Data values summed or averaged over bins
DY	Real(*)	Output	Standard deviations of Y
IFLAG	Integer	Output	0 if DX is normalization, 1 if rms, or -1 if neither
IERROR	Integer	Output	0 for successful read, -1 for end-of-file, or system-dependent message number.

Subroutine READ_2D(IUNIT, TYPE, TITLE, FILEID, UAHR, PARAMS, NP, HEADER, NH, X, DX, Y, DY, NY, Z, DZ, NXZ, IFLAG, IERROR)

Searches logical unit IUNIT for the next data file of type TYPE, or for any two-dimensional file if TYPE = ' '. Returns all abstract information, the one-dimensional arrays X, DX, Y, and DY, the two-dimensional arrays Z and DZ. X and Y are always converted to bin boundaries, and DX and DY may either be normalizing factors (i.e., bin areas) or the rms of the bins; IFLAG = 1 if DX is rms, 2 if DY is rms, or 3 if both, or defaults to -1 if no AREA or RMSBINS blocks were read.

Variables in calling sequence (see also READ_1D):

X	Real(*)	Output	Bin boundaries (channels + 1)
DX	Real(*)	Output	Normalizing function OR rms of bins
Y	Real(*)	Output	Bin boundaries (channels + 1)
DY	Real(*)	Output	Normalizing function OR rms of bins
NY	Integer	Input	Maximum value allowed for Y index
Z	Real(NXZ,*)	Output	2-D data array
DZ	Real(NXZ,*	)Output	Standard deviations of Z
NXZ	Integer	Input	First dimension of Z in calling program
IFLAG	Integer	Output	1 if DX is rms, 2 if DY is rms, 3 if both, 0 if neither; -1 if no blocks were read.
IERROR	Integer	Output	0 for successful read, -1 if end-of-file, or system-dependent error number

The following examples include a monitor spectrum, a portion of a two-dimensional (RT) data set, and a completely reduced I(Q) data set.

```
LOGT PS Spheres in D20$                    LQ0_881002_183520
 147,0.016,0.1,4766.4,3570.,4.522/
 (586,M1)
DATA
 39330,39577,39931,40154,42386,35093,43607,47696,48769,46142,53731,58027,64273,68768,64012,72744,88508,93455,98329,102528,
 99868,100849,95762,93260,94170,90028,89228,88547,86527,86744,82925,82224,82731,80713,74923,75558,72254,72749,70022,66343,
 66183,65638,63261,60258,57851,55409,52779,51917,48913,45940,42879,41453,38471,37038,34921,32556,31038,29203,27277,25627,
 24056,23515,22097,20390,19016,18146,17162,16163,15108,14568,13589,12519,12469,11358,10758,10121,9878,9326,8651,8254,7943,
 7335,6910,6815,6118,6091,5723,5206,4847,5023,4453,4358,4109,3945,3746,3532,3332,3142,2916,2909,2641,2383,2357,2074,1900,2017,
 1751,1629,1508,1402,1329,1220,1109,1061,928,984,954,773,767,685,668,596,555,454,527,472,466,432,405,401,569,493,498,467,433,
 477,307,237,218,195,228,171,173,244,211,201,187/

RT   PS Spheres in D20$                    LQ0_881002_183520
 55,0.016,0.1,4766.4,,8.56,4.16,4.00,63.80,65.46,1,1/
 (586,60-67)
BINS
 5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,
 48,49,50,51,52,53,54,55,56,57,58,59,60/
AREA
 36,41,45,55,61,64,72,78,89,87,97,107,111,117,118,130,137,141,147,151,164,167,170,178,186,198,195,200,212,219,225,223,239,245,
 247,253,256,274,269,280,286,292,305,297,312,318,329,332,327,342,352,357,363,363,380/
T=    60
 410,637,718,840,828,666,544,484,404,269,222,169,109,84,90,76,67,52,55,47,49,41,46,33,41,27,33,24,26,27,25,32,31,21,23,33,21,
 31,33,27,29,28,33,26,32,21,27,25,25,34,29,23,39,36,33/
T=    61
 463,644,711,792,791,661,603,475,395,290,254,162,121,125,97,77,61,53,59,43,54,41,50,52,45,38,44,36,27,33,19,30,24,28,32,20,22,
 35,35,26,28,34,25,27,26,32,20,27,26,35,22,24,25,31,39/
T=    62
 423,612,695,706,768,597,569,492,382,292,257,184,146,105,92,72,86,50,59,62,58,47,42,34,32,42,44,25,32,32,32,27,28,29,25,26,26,
 25,34,21,24,26,23,27,30,25,39,21,27,28,24,28,35,31,23/
T=    63
 413,580,656,787,708,651,564,505,408,253,204,201,148,142,85,100,74,44,68,38,46,44,33,39,33,29,35,28,22,27,34,29,17,20,32,25,
 31,26,26,25,24,21,43,22,16,21,30,32,23,24,28,28,24,42,35/
T=    64
 492,663,798,888,840,713,640,490,450,348,264,216,157,134,109,81,72,63,57,48,49,46,53,47,33,32,32,26,34,39,23,26,39,24,29,19,
 23,30,27,25,24,21,30,28,25,23,33,15,30,18,28,38,25,21,29/
T=    65
 563,716,873,959,961,817,743,636,538,412,327,250,189,133,118,93,88,76,69,66,58,42,43,42,55,35,34,32,32,23,21,28,38,24,27,27,
 25,31,30,20,24,24,29,22,22,39,29,32,31,27,31,35,32,31,20/
T=    66
 542,722,820,999,965,817,776,613,529,363,338,270,191,146,124,100,86,70,60,54,57,53,37,45,45,38,29,47,42,34,19,31,31,35,29,24,
 22,26,29,32,26,29,26,24,28,30,33,35,25,30,20,29,35,32,38/
T=    67
 537,744,878,1049,1043,835,734,650,597,447,375,298,203,166,136,106,88,75,82,66,64,55,32,46,41,49,31,39,36,34,33,32,24,27,26,
 29,22,24,28,31,34,22,25,27,19,31,27,33,26,29,23,23,32,28,35/
```

```
Q    PS Spheres in D2O, less background$      LQD_881002_183520
 175,0.016,0.1,4766.4,,8.56,4.16,4,64.38,65.32,0.001,1/
 .00638((((586,25-147)/(586,M1)-(266,25-147)/(266,M1))/((585,R=0-5)/(585,M1)-(26
6,R=0-5)/(266,M1)))-(((531,25-147)/(531,M1)-(266,25-147)/(266,M1))/((530,R=0-5)/
(530,M1)-(266,R=0-5)/(266,M1))))
POINTS
 .00436538,.00525528,.00614518,.00703507,.00792497,.00881487,.00970476,.0105947,.0114846,.0123745,.0132644,.0141542,.0150441,
 .015934,.0168239,.0177138,.0186037,.0194936,.0203835,.0212734,.0221633,.0230532,.0239431,.024833,.0257229,.0266128,.0275027,
 .0283926,.0292825,.0301724,.0310623,.0319522,.0328421,.033732,.0346219,.0355118,.0364017,.0372916,.0381815,.0390714,.0399612,
 .0408511,.041741,.0426309,.0435208,.0444107,.0453006,.0461905,.0470804,.0479703,.0488602,.0497501,.05064,.0515299,.0524198,
 .0533097,.0541996,.0550895,.0559794,.0568693,.0577592,.0586491,.059539,.0604289,.0613188,.0622087,.0630986,.0639885,.0648784,
 .0657682,.0666581,.067548,.0684379,.0693278,.0702177,.0711076,.0719975,.0728874,.0737773,.0746672,.0755571,.076447,.0773369,
 .0782268,.0791167,.0800066,.0808965,.0817864,.0826763,.0835662,.0844561,.085346,.0862359,.0871258,.0880157,.0889056,.0897955,
 .0906854,.0915753,.0924651,.093355,.0942449,.0951348,.0960247,.0969146,.0978045,.0986944,.0995843,.1004742,.1013641,.102254,
 .1031439,.1040338,.1049237,.1058136,.1067035,.1075934,.1084833,.1093732,.1102631,.111153,.1120429,.1129328,.1138227,.1147126,
 .1156025,.1164924,.1173823,.1182721,.119162,.1200519,.1209418,.1218317,.1227216,.1236115,.1245014,.1253913,.1262812,.1271711,
 .128061,.1289509,.1298408,.1307307,.1316206,.1325105,.1334004,.1342903,.1351802,.1360701,.13696,.1378499,.1387398,.1396297,
 .1405196,.1414095,.1422994,.1431893,.1440791,.144969,.1458589,.1467488,.1476387,.1485286,.1494185,.1503084,.1511983,.1520882,
 .1529781,.153868,.1547579,.1556478,.1565377,.1574276,.1583175,.1592074/
DATA
 15.80074,15.70131,14.03314,12.96971,12.01633,10.90885,9.68711,8.75951,7.62483,6.69195,5.7565,5.04184,4.27975,3.63639,
 3.059001,2.538635,2.137722,1.783712,1.453942,1.175721,.9619,.776271,.636827,.540689,.439162,.379775,.3173052,.2743633,
 .2390564,.2112663,.1905863,.1699791,.1552704,.138809,.1214706,.1087911,.1000655,.0932941,.0844305,.0795719,.0707361,.0630396,
 .0577417,.0560538,.0496642,.0442402,.0461346,.0431675,.0386537,.0343013,.0329244,.0302312,.0301376,.0306853,.0281162,
 .0257065,.0241313,.0236099,.0233133,.0218402,.0191624,.0182851,.0183507,.0186263,.0185539,.0156574,.0160597,.0154288,
 .0161062,.0140396,.0143537,.0146013,.0130907,.0140593,.011789,.0097659,.0125543,.011823,.010508,.0105019,.0105475,.0083308,
 .0090731,.0110781,.0110859,.0108139,.0076473,.0093324,.0096139,.0055737,.0080336,.0070772,.0079284,.0104317,.0080095,
 .0073824,.0090125,.0087587,.0073846,.0050881,.0073839,.006638,.0068199,.0072734,.0077057,.0089273,.007993,.0101284,.0089383,
 .0085859,.005316,.0064653,.0065707,.0037507,.006131,.0054479,.0066602,.00896,.0056243,.0077263,.0065532,.0041055,.0043105,
 .0080414,.0052919,.0077804,.0041736,.0112402,.0062016,.0070563,.0070565,.0053503,.0065116,.0075996,.0079357,.006434,.0064708,
 .0023693,.0110527,.0076639,.0059024,.0056123,.0037587,.0053503,.0073557,.0061682,.0081521,.0048909,.0025071,.0050546,
 .0059774,.0097345,.0049154,.003051,.0100641,.0019913,.0024025,.006469,-1.79600E-04,.0113137,.0048591,.0042823,.0024871,
 .007595,.0168763,.0073621,.010587,.0062251,.0130425,-.0022468,.0041678,.0205424,-.0074562,-.0129264,/
STDDEV
 .717393,.345432,.2101421,.1454645,.1084218,.0836344,.0666984,.0545952,.0449675,.037833,.0319837,.027756,.0240273,.0209081,
 .0182582,.0158739,.0139602,.0122865,.0106711,.00931563,.00818983,.00716184,.00635088,.00571524,.00506356,.00461366,.00416949,
 .00383574,.00355669,.00331412,.00311623,.00292196,.00277942,.00262959,.00245126,.00232701,.00221927,.00213281,.0020397,
 .00198352,.00187294,.00178925,.00171158,.00169016,.00161664,.00154567,.00156506,.00152939,.00147013,.00139441,.00139347,
 .00133801,.00134727,.00133559,.0013169,.00128089,.00125497,.00127077,.00125066,.0012423,.00121886,.00120157,.00119517,
 .00121128,.00120842,.00117917,.00119801,.0012098,.00118653,.00117883,.00118129,.0011879,.00118165,.00123311,.00118962,
 .00118007,.00120034,.00122497,.0012055,.00121189,.00123146,.00122012,.00121736,.0012676,.00128462,.00127746,.00123269,
 .00129147,.00126648,.00124511,.00129579,.00129783,.00130067,.00136043,.00130496,.00132162,.00132559,.0013478,.00135694,
 .00132136,.00135902,.00139566,.00140159,.00142109,.00143483,.00146811,.00146246,.00150942,.00148759,.00150284,.00148924,
 .0015071,.00151189,.00150778,.00154561,.00153916,.0015797,.00170547,.00160457,.00169956,.00163201,.0016256,.001657,.00175939,
 .00171204,.00182531,.00179535,.0018766,.00187524,.00192122,.00191439,.00188791,.00196929,.00202823,.00206691,.00201808,
 .0020899,.00202885,.00230308,.00217688,.00224597,.0022506,.0022238,.00235592,.00238541,.00255722,.0025574,.0025894,.00264652,
 .00270851,.00287466,.00297029,.0030018,.00308328,.00318072,.0033293,.0033508,.00361471,.00342613,.00360099,.00415799,
 .0040516,.00416767,.00464013,.00527943,.00499698,.00552287,.00512681,.00714689,.00665755,.00686036,.00967017,.00738286,
 .00997103,/
```