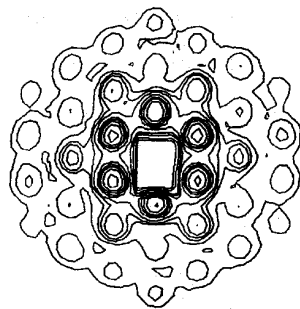


A Computing Guide for Small-Angle Scattering Experiments

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Preface to the Fifth Edition

The programs here have evolved as a set of tools to treat the large range of scientific problems, different instrument configurations and increasing volumes of data produced in SANS measurements at the ILL. This note is intended to help users find a way of objectively combining component spectra to derive useful information in a stylised and reliable fashion. These programs permit examination of the separate contributions at most stages through treatment since they are stored in a common format. This greatly helps disentangling the source of problems, either with the instrument, or a specific sample or background.

The preceding editions of this manual contained an initial foreword written by Gernot Kostorz with exhortations on performing proper measurements before attempting data reduction and analysis. This was expanded with help from members of the Large Scale Structures group at the ILL to offer a more detailed guide to performing reliable measurements. The echo of the original remains here: it is the task of the experimenter to produce good data with adequate statistical reliability. The stage of checking the correct functioning of the instrument will always be a prerequisite for reproducible measurements. A tradition has built up of each user performing basic calibration measurements matching the instrument configuration. The archive of data has been transcribed to match current data standards, so data from early days can be inspected and treated with current programs, again made possible because of the completeness of most measurements following this tradition. Measurement procedures and treatment have changed little; skilled sample conception and preparation remain the keys to successful results.

New additions presented here include the easy integration of data reformatting programs for regrouped data. The examples implemented here produce XML data files which can be directly read by Microsoft Excel 2003. Developments to the fitfun data fitting package, and a new GUI Clickfit now allow users to treat sequences of data; a second variant allows simultaneous fitting of several datasets. Both have relevance to current practice of exploring constraint space (temperature, shear rate etc.) and deuterium substitution experiments.

To help the occasional or first-time user we have included a worked example of a simple measurement; we have also included some references which describe calibration techniques and other practical aspects.

The programs here serve the primary role of data reduction; no attempts are made at resolution or multiple scattering corrections which are typically sample, instrument configuration, and scattering kernel dependent, and beyond general treatment.

Whilst networked computers (changing to Linux from SGI) are used for much data treatment at the ILL, the emphasis is now on the simple deployment of all programs on PCs. Much development effort since the last edition has been in producing a Windows environment within which existing programs run comfortably, and new programs are easily introduced. The graphical tool *prop* fulfils these needs. The PC distribution includes the basic libraries built with the GNU/MinGW open source compilers, and users are encouraged to add to the

program set themselves. Externally most programs resemble those described previously, but now include many modifications which, for example, take into account the different detectors past and present. Web technology for downloading data can use browsers (see IDA at <http://barns.ill.fr>) In addition there are basic facilities for treating SANS data and visualization with a browser, though downloading data and local treatment offers much richer scope

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November 2006

Acknowledgements

We wish to thank the many scientists within ILL and visiting users, past and present, who have offered comments on the programs and the manuals. The examples are drawn from the archives from experiments performed by Ibel, Kistorz, Clark, Kalus, Timmins, Ottewill, Lindner and their co-workers.

The PGPLOT graphical library from Tim Pearson (California Institute of Technology) has formed the basis for all graphics. The Windows display driver GRWND.EXE from Tsuguhiro Tamaribuchi has added a notable comfort and utility to PC graphics.

Further information can be found from the home-page of the ILL <http://www.ill.fr> and from the Large Scale Structures' group page:URL http://www.ill.fr/lss/lss_data_treatment/LSS_treatment.html

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Whilst a great effort has been made with help from many collaborating scientists to check the operation of programs described in this guide, users may encounter unforeseen problems with their own specific sequence of operations. or data. Please report any anomalous behaviour, preferably with example data and output, to Ron Ghosh, ron@ill.fr.

Illustrations	Scattering Experiments
Cover	Contrast illustrations
Frontispiece	Charge stabilised polystyrene latex, Ottewill et al, 1989
Page 55	Spherical viruses, Timmins et al, 1987
Page 83	Micelle systems static, and under shear, Kalus et al, 1988, Ni-Al alloys, Kistorz et al 1975, Annealing Ni-Al Super-alloys, coalescence of γ domains, Leberman, Bellet et al.
Tailpiece	Oriented Retinal Rods, Charbre et al, 1975 Origins of Spolly: Ghosh, Goeltz, Higgins and Kistorz, 1974

Introduction

1

This set of programs has been implemented at the ILL to cover most needs for standard data display and reduction necessary for the efficient use of the small angle spectrometers D11 and D22, D17 in SANS mode, and the diffractometer D16 used in a similar mode.

The programs will perform calculations on data from the whole detector, or on pre-grouped radial intensity functions. The uniformity of the data formats throughout the treatment, and at the final stage enables the data to be listed on the printers, plotted and transferred by network at any stage to external institutions for further analysis.

All raw and treated data are stored as ASCII (text) files. This simplifies interchange between systems, and allows simple inspection using standard text editors when all else fails. Graphics output is in PostScript format, again ASCII text, offering portability. On PCs the graphics can be printed directly to standard Windows printers.

Data for the current cycle and the preceding cycle are stored directly on the ILL data-server. The permanent archive from 1974 is all held on disk in compressed form. When accessed by the programs here, the data are automatically uncompressed. before treatment. Utility programs *dzarch*, *zcat*, *uncompress*, and *gunzip* can be used to decompress the data files.

During the treatment individual cells or regions of the detector can be systematically eliminated by invoking one or several masks which are superposed to define the required cells. Spurious data allocated to addresses corresponding to inactive corners of the detectors are always eliminated from the principal regrouping calculations.

To avoid repetitive questions each time programs are run a number of environment variables hold information concerning location of raw data, local printer, and display attributes. The user may decide to modify these by hand. The login procedure for the short-term visitors on the instruments automatically defines equivalent environments on the different computer systems. Individuals using other accounts will find information on environment settings in chapter 5.

To provide a Windows environment on PCs with similar environment features and less hostile than the Unix terminal/command line interface a utility, *prop*, described in Appendix 4, simplifies access to programs and viewing results.

Treatment of Small Angle Scattering Data

2

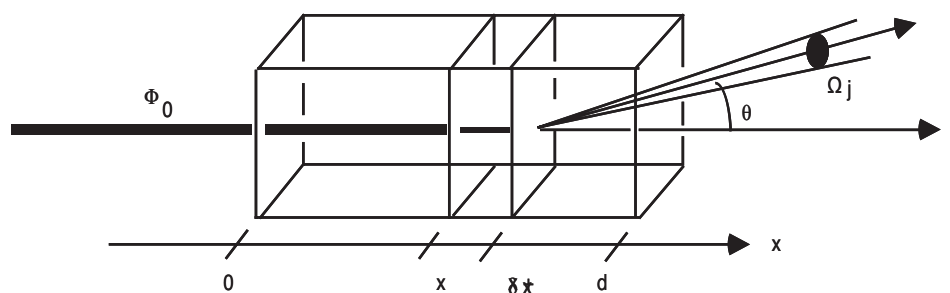
This introduction describes the formalism for correcting the neutron intensity, I , scattered by the sample to account for background, detector response and geometry to obtain the differential cross-section $d\sigma/d\Omega$. The coherent component of this, $d\sigma_c/d\Omega$, contains the information on the structure of the sample.

The problems of resolution and multiple scattering are strictly sample dependent and will not be discussed here.

2.1 Small angle scattering by an isolated sample

The incident beam traversing the sample is attenuated by absorption and scattering within the sample, and the scattered neutrons are likewise attenuated on passing through the remainder of the sample before the flight path to the detector. Hence the measured intensity must be corrected to account for this loss.

Incident flux	$\Phi_0 \text{ n cm}^{-2} \text{ sec}^{-1}$
Area of sample	$A \text{ cm}^2$
Solid angle subtended by detector cell j	$\Omega_j \text{ ster.}$
Efficiency of detector cell j	E_j
Number density of sample	$\rho \text{ atoms cm}^{-3}$
Coherent differential cross-section	$\frac{d\sigma_c}{d\Omega}$
Incoherent differential cross-section	$\frac{d\sigma_i}{d\Omega}$
Linear attenuation coefficient	$\mu \text{ cm}^{-1}$



Intensity measured in cell j

$$I_j(\theta) = \int_0^d \Phi_j \Omega_j E_j e^{-\mu x} A \rho e^{-\mu(d-x) \cos \theta} \left\{ \frac{d\sigma_i}{d\Omega} + \frac{d\sigma_c}{d\Omega} \right\} dx \quad (2.1)$$

Since the scattering considered here is always at small angles the cosine term may be taken as unity.

$$I_j(\theta) = \Phi_0 \Omega_j E_j A \rho d e^{-\mu d} \left\{ \frac{d\sigma_i}{d\Omega} + \frac{d\sigma_c}{d\Omega} \right\} \quad (2.2)$$

In reality this measured intensity actually contains contributions from doubly and other multiply scattered neutrons where the proportions will vary depending on each sample, the volume, and the relative absorption and scattering cross-sections. In this expression it is assumed that the first scattering process is dominant. The sample transmission is given by:

$$\frac{I}{I_0} = e^{-\mu d} = T \quad (2.3)$$

The sample characteristics terms $A \rho d$ are combined to give N , the total number of scattering centres.

$$I_j(\theta) = \Phi_0 \Omega_j E_j T N \left\{ \frac{d\sigma_i}{d\Omega} + \frac{d\sigma_c}{d\Omega} \right\} \quad (2.4)$$

Multiple scattering leads to systematic effects in the scattered intensity. For two cases this may be assessed.

(a) When absorption by the sample is the principle mechanism for attenuation the multiple scattering is small and may be ignored.

(b) When incoherent scattering predominates (as in the case of hydrogen containing substances), multiple scattering processes are mainly incoherent-incoherent, and hence isotropic. Thus :

$$I_j^{\text{coh}}(\theta) = \Phi_0 \Omega_j E_j T N \frac{d\sigma_c}{d\Omega} \quad (2.5)$$

The intensity not transmitted directly is to be found scattered equally over 4π steradians:

$$I_j^{\text{incoh}}(\theta) \approx \Phi_0 \Omega_j E_j (1 - T) \frac{A}{4\pi} \quad (2.6)$$

Hence the total intensity measured by the detector is:

$$I_j(\theta) \approx \Phi_0 \Omega_j E_j \left\{ T N \frac{d\sigma_c}{d\Omega} + (1 - T) \frac{A}{4\pi} \right\} \quad (2.7)$$

If all instrumental resolution effects (finite wavelength spread, finite detector pixel size, etc) are ignored then for incident neutron wavelength λ Å,

$$I(Q) = I(\theta) \quad \text{where } Q = (4\pi/\lambda) \sin(\theta/2) \quad (2.8)$$

It is conventional to present data as $I(Q)$ versus Q , the wavevector transfer, since this allows data measured with different instruments and configurations to be merged easily.

Macroscopic cross-section

This is the cross-section per unit volume of material, which consequently has dimensions cm^{-1} . The total cross-section, denoted by Σ_t is the sum of the scattering cross-section and the absorption cross-section, and for the transmitted beam is equal to μ , the coefficient of linear attenuation.

The coherent differential cross-section contains the information on the spatial correlations in the sample:

$$I^{\text{coh}}(Q) = \Phi \Omega E T d \left(\frac{d\Sigma^{\text{coh}}(Q)}{d\Omega} \right) \quad (2.9)$$

2.2 Absolute intensity calibration using vanadium

In the case of vanadium $d\Sigma/d\Omega = \Sigma_i/4\pi$ since the incoherent scattering predominates over the coherent, and the Debye-Waller factor is very small at or below room temperature; the resultant scattering is isotropic. For a sample thickness d_v :

$$I_j(Q) = \Phi_0 \Omega_j E_j T d_v \Sigma_i/4\pi \quad (2.10)$$

It is necessary to include the correction for loss of neutrons by absorption in the sample. The absorption cross-section for vanadium is 0.371 cm^{-1} at 1.8 Å , and is a linear function of wavelength. The attenuation factor is hence $\exp(-0.206\lambda d_v)$

$$I_j(Q) = \Phi_0 \Omega_j E_j (\exp(-0.206\lambda d_v)) d_v \Sigma_i/4\pi \quad (2.11)$$

Thus a measure of $I_j(Q)$ gives the product of $\Omega_j E_j$, namely the correction factor which must be applied to compensate the measured intensity of any sample to account for the detector surface being planar rather than spherical, and for the counter detection efficiency. The angle a given cell subtends at the sample is independent of the arm offset position on D16 or D17 since the arm rotates about the sample axis. The detector carriage on D22 allows the detector to be both displaced laterally and rotated about a vertical axis, presenting the same geometry, though this mode is rarely used.

This formalism is correct providing the vanadium intensity is measured for the same cell or group of cells as the sample intensity measurements, thus corrections made on a cell-by-cell basis are identical to the corrections made on the sums of intensities from the same set of cells.

secondary standards

If only relative cross-section results are required then any sample which has a uniform cross-section in the Q range accessible by the detector will suffice; thus often a water sample with a thickness of 1 mm may be employed. Comparisons

with vanadium spectra under similar conditions enable absolute cross-sections to be derived using this secondary standard.

It is possible to prepare standard coherent scattering samples where $d\Sigma^{\text{coh}}(0)/d\Omega$ can be calculated and then compared with extrapolated measurements. This value is then used to renormalise a flat spectrum. Ideally such standards should have similar correlations to the sample under investigation and be measured with the same instrument configuration. Then the Q dependence can also serve as a cross-check on resolution effects.

Other calibration methods

Direct measurement of detector efficiency

The cross-section is the ratio of the scattered flux to the incident flux. Using sets of calibrated attenuators to protect the detector from the full incident beam intensity, it is possible to measure the absolute efficiency of the detector at the wavelength used. This can serve as a cross-check in the case of the large multi-detectors in use at ILL, where it is impractical to scan the whole surface through the main beam routinely.

2.3 Treatment of sample holder

Unlike the ideal cases illustrated above the neutron beam passes through a window before and after the sample, and each window gives rise to some intensity scattered at small angles. Scattering and absorption in the sample holder windows may be accounted for by measuring this signal when the holder is empty, together with a transmission measurement. When the sample+holder are measured the signal component from the first window is diminished due to the sample attenuation, as is the beam intensity incident on the second. The intensity arising from the sample alone is thus:

$$I_S = I_{S+SB} - \frac{T_{S+SB}}{T_{SB}} \cdot I_{SB} \quad (2.12)$$

where the suffix S refers to the sample, and SB refers to the holder.

2.4 Treatment of background

So far the signal has been accepted as originating from the beam which has passed through the beam flux monitor, and has been scattered by the sample and its holder. Two types of background are usually present and especially for weak scattering samples must be measured carefully and subtracted to obtain the true intensity.

(a) Beam Independent

During all measurements the detector records neutrons not originating in the incident beam and not having passed through the sample. In addition electronic noise contributes a small background. The sum may be assessed by replacing the sample by cadmium and measuring the residual signal. Boron Carbide or ${}^9\text{LiF}$, used separately or in combination, are often preferred since they avoid the production of a capture γ background to which some detectors are sensitive.

(b) Beam Dependent

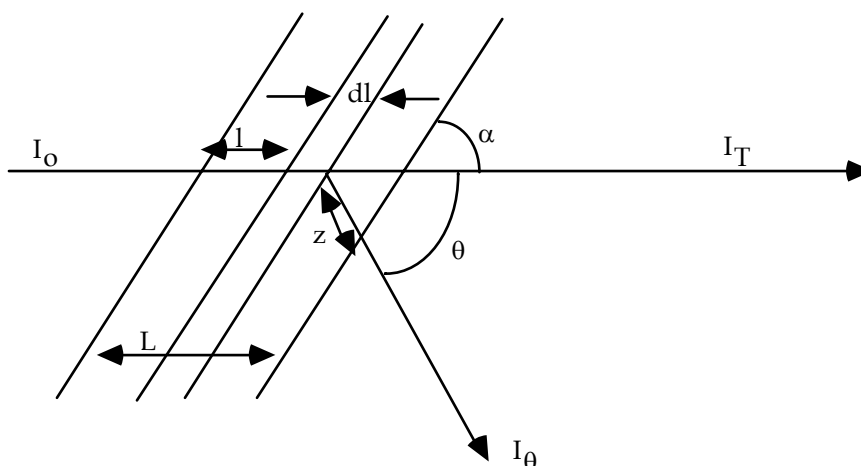
This can arise from air scattering and the wings of the neutron beam profile due to faulty collimation, and is detected during the preparations for the experiment when the spectrum from the diaphragms only, with no sample or holders present, is measured. The residue is treated as a part of the sample holder spectrum.

2.5 Validity at larger scattering angles

Instruments and programs have been constructed with small-angle scattering in mind. To measure out to higher Q values it is hence preferable to use shorter wavelengths rather than very short sample to detector distances, where the geometry of the sample and normalisation pose problems. The example presented here gives some guidance on effects to be expected.

These programs may be used for data acquired at angles in the range 0-30 degrees with acceptable precision providing the transmission of the sample is greater than 80%. The main problems arise from the variable path taken through the sample, and suitable calibrations for the detector. Both can be resolved by performing the calibration runs with an isotropically scattering sample which has approximately the same transmission as the sample. In fact the longer sample path traversed at higher angles for both the sample and the reference only modify the intensities as a second order effect (ignoring multiple scattering etc.) since there is a balance between the attenuation factor and the increased amount of potential scattering material in the beam (for a single detector no correction is required if the planar sample is half-angled with the detector movement).

For the off-axis multi-detector instruments it is useful to perform only one detector efficiency calibration experiment rather than at each of the possible offset positions. In this case the mean intensity which is usually measured at small angles for the reference must be modified by an angle dependent factor F_θ .



$$I_\theta = I_0 \int_0^L \exp(-\rho\sigma l) \cdot \rho \frac{d\sigma}{d\Omega} dl \cdot \exp(-\rho\sigma z) \quad (2.13)$$

$$\text{where } \frac{z}{\sin \alpha} = \frac{L - l}{\sin(\pi - (\alpha + \theta))}$$

if $s = \rho L \sigma$ and noting $\frac{I_T}{I_0} = e^{-s}$

$$I_\theta = I_0 \rho L \frac{d\sigma}{d\Omega} F_\theta \quad (2.14)$$

$$F_\theta = \frac{\exp(-s(\sin \alpha / \sin(\alpha + \theta))) - \exp(-s)}{s(1 - \sin \alpha / \sin(\alpha + \theta))} \quad (2.15)$$

if $p = \frac{\sin \alpha}{\sin(\alpha + \theta)}$ and s is small

$$F_\theta = \left\{ \frac{(1 - ps + p^2 s^2 / 2) - (1 - s + s^2 / 2)}{s(1 - p)} \right\} \quad (2.16)$$

$$I_\theta = I_0 \rho L \frac{d\sigma}{d\Omega} \left\{ 1 - \frac{s}{2} \left(1 + \frac{\sin \alpha}{\sin(\alpha + \theta)} \right) \right\} \quad (2.17)$$

Again this is valid only for samples with a transmission of greater than 80%. This reference spectrum must then be regrouped with the same parameters as the sample to associate the appropriate sets of cells. The value of this correction for a sample scattering 20%, normal to the beam, measured at 30 degrees is about 0.5%.

The calculation above assumes that the scattered beam is attenuated by the total cross-section σ_T in the same way as the transmitted beam. This corresponds to absorption processes σ_A and scattering processes. For a mainly incoherent scatterer, neutrons are scattered approximately isotropically and thus may still enter the detector. It is only necessary to account for scattered neutrons lost by absorption (S. J. Cocking, 1967).

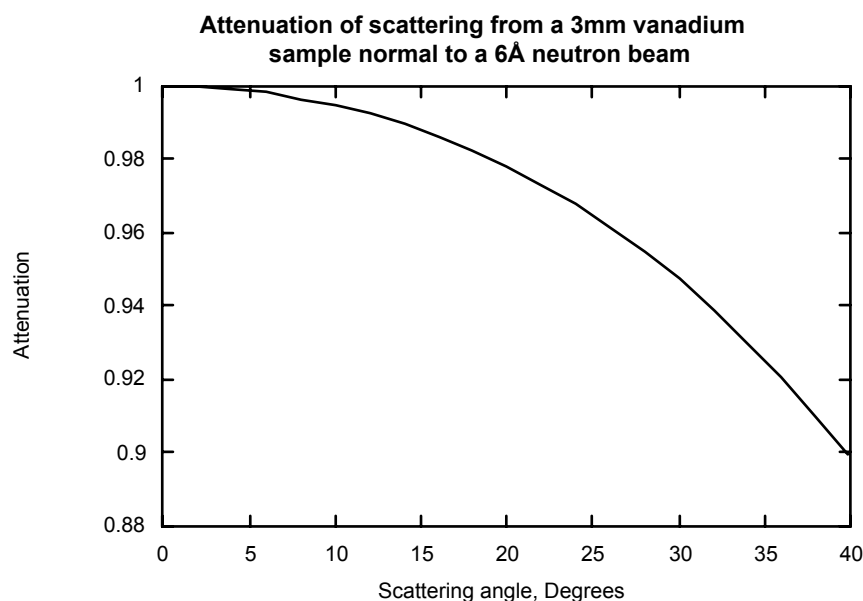
$$F_\theta = \left\{ 1 - \frac{\sigma_A}{2} \left(\frac{\sigma_T}{\sigma_A} + \frac{\sin \alpha}{\sin(\alpha + \theta)} \right) \right\} \quad (2.18)$$

The next section shows that this is true for scattering from hard materials like vanadium, but is more difficult to quantify for soft matter where inelastically scattered neutrons are only detected with a low probability.

The vanadium samples used have transmissions of less than 50% and the exponential terms in F_θ must be calculated explicitly.

The result is still only weakly angularly dependent as shown by the curve calculated for a 3 mm vanadium sample normal to a 6Å beam which has a transmission of 50% and is shown on the next page.

A recent review of the practical consequences of measurements out to angles beyond 10° is given by Brûlet et al. (2007).



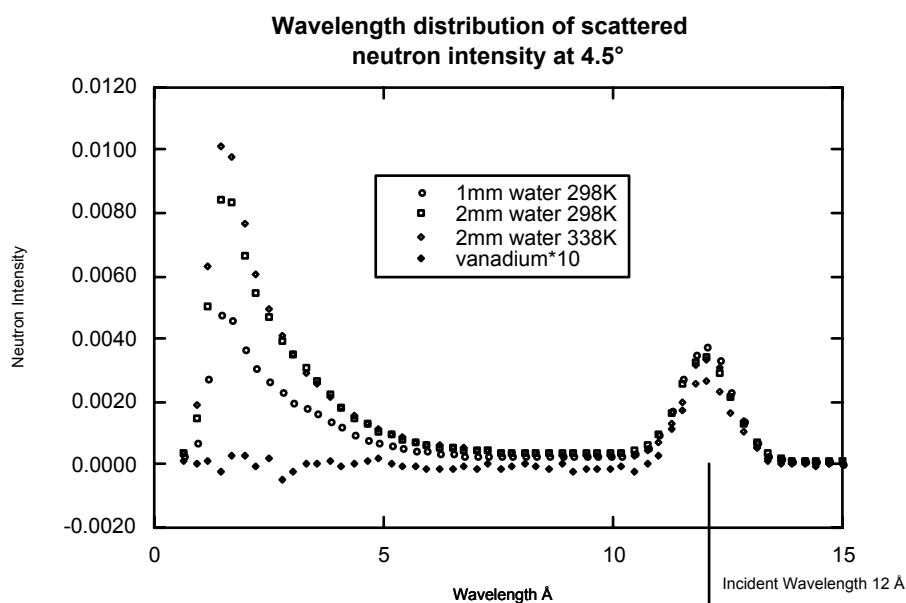
2.4 Validity for real samples in the real world

The formalism presented above represents a single scattering event. Most experimenters wishing to maximise their use of available instrument time appreciate that placing a greater mass of sample in the beam leads to a larger signal, up until the stage where the beam passing through the sample itself is attenuated by scattering. Often samples scattering up to 50% of the beam are used. The mean free path of the neutron in these cases is less than the dimensions of the sample and some broadening effects are observable due to multiple small angle scattering, for which some corrections have been proposed by Schelten and Schmatz (1980).

The second assumption is that the scattering process is elastic, i.e. no energy (wavelength) change occurs during the scattering process.

By introducing a chopper to pulse the neutron beam before the sample on D17 it was possible to wavelength-analyse the neutrons received by the detector (Ghosh and Rennie, 1990). The results for a vanadium and three water samples are shown following. The detector efficiency as a function of wavelength λ is $[1-\exp(-\alpha\lambda)]$. For early 1cm pixel LETI BF₃ 2D multi-detectors α had a value of about 0.123, for more recent detectors, e.g. D22 ³He, α is 0.338. The efficiency corrected distributions are shown here.

As expected vanadium, a hard metal, has few low energy modes which the cold neutron can de-excite (high Debye temperature) and there is little change in the mean scattered neutron wavelength. These measurements were made at long wavelengths and it was necessary to use a thinner vanadium sample because of absorption problems. Thus the effective thickness of the vanadium was 10% of the 1mm water sample. In the case of water the elastic scattering at 12Å diminishes with increasing thickness, and sample temperature.



In more recent measurements, (Ghosh and Rennie, 1999), with better wavelength resolution, the scattering between 1 and 5 Å can be separated into a distinctive librational mode at 1.1 Å, and a broad Maxwellian envelope around 2.5 Å.

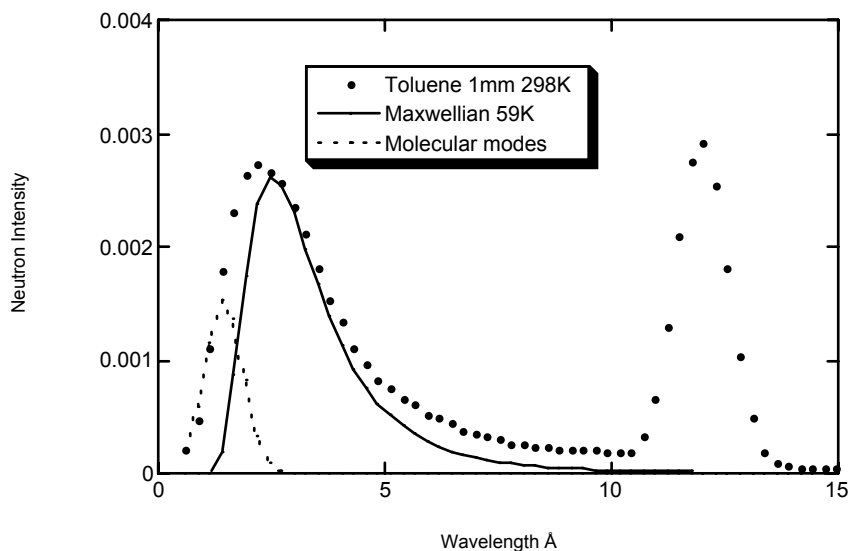
This is simply a consequence of the neutron being *thermalised* on its passage through the thick sample and container windows. The characteristic temperature of the 12Å neutrons is 7K. Water, with its librational mode of high amplitude, has actually long been used to thermalise fast neutrons. Because of this mode the envelope of the inelastic scattering deviates further from a Maxwellian, compared to simpler liquids like toluene.

The linear attenuation coefficient μ in eq. 2.3 is equal to the total cross-section $N\sigma_t$. For 8Å neutrons about 52% of the beam is lost by scattering and absorption after passing through 1mm of water at 25°C. This corresponds to a total cross-section of 7.4 cm⁻¹ (220 barns/molecule) where absorption losses are less than 1%. Assuming the neutrons are uniformly scattered over 4π steradians, the level SANS spectrum which is measured should correspond to the differential cross-section of 0.59cm⁻¹sterad⁻¹. The transmission measurement is instrument independent.

*Use of transmission data
in water calibration
measurements*

Using the wavelength distribution measured in the time of flight experiments and the approximate detector efficiency value, α , for the BF₃ detector of D11 it can be shown that approximately 40% of 8Å incident neutrons scattered by the water are counted. For the D22 ³He detector the figure is about 67%, the major increase arising from the much higher efficiency at shorter wavelengths. The count rate per unit solid angle for the new detector, hence the effective water cross-section is thus twice that of the earlier detector. Fortuitously the count rate per pixel in similar configurations remains similar due to the smaller cell area (0.56cm²) for D22 as compared to 1cm² for D11. Note the effective differential cross-section of water is only related to the measured transmission once the detector efficiency as a function of wavelength is taken into account. Only in the case of vanadium, where there is high absorption is it necessary to correct the scattered incoherent intensity for sample transmission (eq. 2.18).

Wavelength distribution of scattered neutron intensity at 4.5°

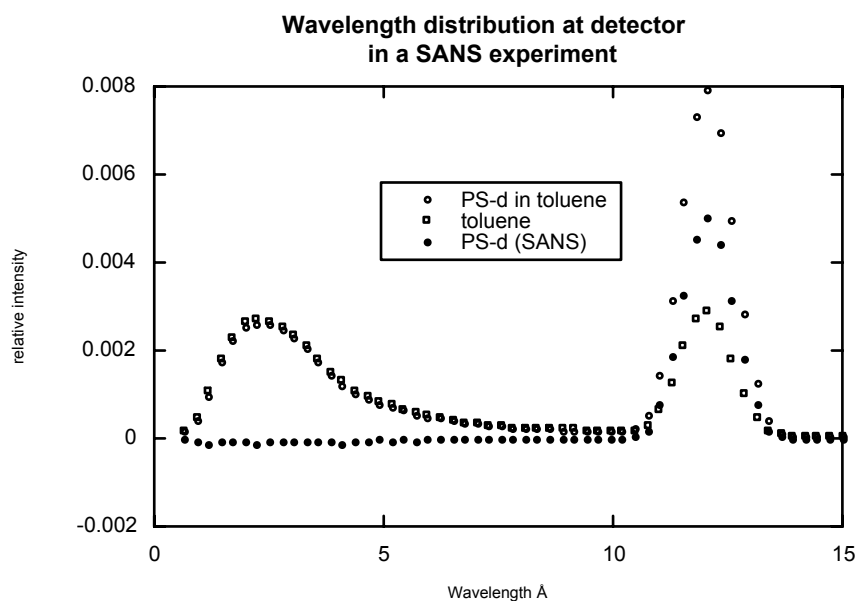


The envelope of inelastic scattering at shorter wavelengths for 1mm of toluene at 25C can be simply represented by a gas of neutrons having Maxwellian energy distribution with a characteristic temperature about 60K. At greater thicknesses this characteristic temperature increases as more complete thermalisation of the 12Å incident neutrons takes place. Thermally excited low energy internal molecular vibrational modes also transfer energy to the cold neutrons, and are represented here at shorter wavelengths by a Gaussian envelope roughly the resolution width of the instrument. The two fitted components summed together match most of the measured inelastic intensity curve.

Wavelength analysis of a SANS measurement

The same experimental setup was used to analyse the SANS signal in the case of a well characterised sample of polystyrene-d in toluene C_7H_8 . Like water, toluene has a large incoherent scattering cross-section, and being a liquid, has many low frequency diffusive motions which can transfer energy to the incoming cold neutrons.

The diagram following shows the measured spectrum of the solution, and then the SANS signal after subtracting off the solvent using the simple formalism presented in this chapter. The result shows convincingly that much of the background solvent scattering is in fact inelastic, but that it may be accurately removed if the correct transmission factors are employed.



A more general corollary to be drawn from these measurements is that the dynamics of the pure solvent and the solvent in solution must be essentially identical. Secondly, heating a sample changes the internal dynamics; to account for this it is necessary to measure the transmission of the sample at each temperature. It is also necessary to control the temperature of samples and reference standards.

The measured scattering from soft-matter samples depends somewhat on the incident wavelength. Because detectors have individual efficiencies which vary as a function of the wavelength, empirical functions to rescale cross-sections to so-called standard water samples are only approximate and have to be determined for each instrument.

The results presented here have been corrected for this efficiency factor. For the D17 detector the nominal efficiency at 4Å is about 20% of that at 12Å. There is hence, in general, some innate discrimination with these older detector systems against counting inelastically scattered events.

Wavelength dependence of detector normalisation

Whilst absolute calibrations are occasionally made today with good quality vanadium single crystals, more often secondary standards such as water are employed. Although detectors are very stable, current practice is to measure calibrants for each set of measurements. This complete set of data contains information on the configuration actually used, and which cannot necessarily be exactly re-established on a later occasion, for example after the detector amplifiers have been adjusted.

For this reason use of a *coherent* scatterer to establish an absolute value for the sample cross-section scale using $d\Sigma^{\text{coh}}(0)/d\Omega$ will give a true value for that wavelength, provided, as shown above, that conventional corrections are applied and this can be used to define an effective cross-section for a level water spectrum.

Interpretation of SANS data

3

3.1 The measured intensity and the scattering cross-section

The aim of this short section is to summarise the principal mechanisms contributing to the observed SANS cross-section. We wish to determine the spatial distribution of the scattering centres in the sample. This is often simply a means to a final end intention to measure another property, for example nucleation and growth during phase transitions where the SANS is used as a metric for the number and size of growth sites. Simple modelling can obviate the need to invert the data, which are inevitably measured within a restricted real space resolution range. SANS has been used in studies ranging widely, from magnetic flux lattice lines through to triangulation of proteins in cell nucleus constituents; often the terminology used is different in each field. Some of these variants are presented here. There are few recent reviews on the subject of data analysis, but some are given in the references appendix.

Squires (1978) gives a derivation of the scattering cross-section for neutrons in the static approximation for an assembly of nuclei at sites $\mathbf{R}_i, \mathbf{R}_j$ with scattering length b_i and b_j as

$$I(Q) = \langle \sum b_i b_j \exp(i \mathbf{Q} \cdot (\mathbf{R}_i - \mathbf{R}_j)) \rangle \quad (3.1)$$

where the wave-vector transfer $Q = (4\pi/\lambda) \sin(\theta/2) \text{ \AA}^{-1}$ for neutrons with an incident wavelength of λ Angstroms scattered through an angle θ , and averages over all orientations have been made. The cross-section is consequently a sum of terms and cross-terms. To extract a specific component requires several reliable measurements to eliminate the unwanted parts.

When $i \neq j$, i.e. the scattering arises from two different nuclei, then interference can occur, and the scattered intensity is dependent on the magnitude of the scattering lengths b_i and b_j and their distance apart. b varies from element to element and between isotopes with no obvious correlation with atomic number z . This is in strong contrast with X-ray cross-sections which increase monotonically with z^2 .

Table 1. Coherent and incoherent scattering lengths of common nuclei

Nucleus	b_{coherent} fm	$b_{\text{incoherent}}$ fm
H	-3.742	25.217
D	6.674	4.033
C	6.648	
O	5.805	
N	9.36	
S	2.847	0
^{35}Cl	11.66	6.0
^{37}Cl	3.08	.02

from Sears (1984)

If the nuclei have spin, then there is a possibility of losing coherence between incident and scattered neutron waves when the spin state of the neutron is changed. The detailed spatial information is then lost. The first term of the cross-section shown below in equation 3.2 has the structural information from the coherent cross-section, arising from the square of the difference in the scattering lengths. The second term corresponds to the term $i=j$, and depends on the difference in the squares of the scattering lengths; this part of the cross-section is uniform with no structural information.

$$\frac{d\Sigma}{d\Omega} = n \frac{d\sigma_c}{d\Omega} + n(\overline{b^2} - \overline{b}^2) \quad (3.2)$$

There is a large difference in the scattering amplitude of the proton spin $\pm 1/2$ depending whether this is parallel or antiparallel to the neutron spin $\pm 1/2$. This gives rise to the very large incoherent cross-section since there is a high probability of spin-flip scattering at either site. In magnetic systems the direction of magnetisation in the sample is defined by an external field, and the measured cross-section is anisotropic. The magnetism due to the electrons contributes a large scattering effect, adding to or subtracting from the nuclear cross-section.

In the context of SANS, the cross-section is usually presented in terms of the scattering cross-section per unit volume of sample, and consequently is given in units of cm^{-1} .

In typical SANS experiments the distance scale probed is greater than interatomic distances, and the coherent cross-section can be expressed as an integral

$$I(Q) = (\overline{b} - \overline{b})^2 \int F(R) \exp(iQ \cdot R) dR \quad (3.3)$$

where \overline{b} is the average scattering length. This shows the dependence of the scattering on the autocorrelation function $F(R)$ of the scattering centres expressing the probability of scattering at two points separated by distance r . (Formally this adds a contribution to $I(0)$, though since this is indistinguishable from the transmitted beam, the notion of $I(Q)$ as the measured differential cross-section remains correct.)

The difference $(b - \overline{b})^2$ is referred to as the contrast of the scatterer with respect to a reference medium, solvent or matrix. SANS experiments are insensitive to the atomic scale and a marked simplification in interpretation can be easily achieved by considering the cross-section as a measurement of the scattering density correlation function of the scattering centres. The scattering density ρ is the mean coherent scattering density per unit volume of a solvent, solute or void volume often expressed in units of 10^{-6}\AA^{-2} . Some typical systems are shown in the following table; a most important factor is the negative scattering length of hydrogen compared to deuterium and the ability to mix hydrogenous and deuterated solvents to create a medium with a controllable scattering density either to match or contrast with solutes.

Table 2. Example scattering length densities

	$\rho_{\text{coh}} \times 10^{-6} \text{\AA}^{-2}$
H ₂ O	-0.56
D ₂ O	6.35
CHCl ₃	2.35
CDCl ₃	3.10
Polystyrene(H)	1.4
Polystyrene(D)	6.3
Protein(H)*	1.9-3
Protein(D)*	6-7

In the case of proteins, and other systems with labile protons, some exchange equilibration with the solvent protons/deuterons occur, hence the scattering density depends on the H/D ratio of the solvent, the first figure given is in pure H₂O, then D₂O.

Expressing (3.3) now in terms of scattering density

$$I(Q) = (\rho - \bar{\rho})^2 \int P(R) \exp(iQ \cdot R) dR \quad (3.4)$$

$P(R)$ is the equivalent of the crystallographers' Patterson function describing the density-density auto-correlation function of the system.

Examining equation 3.1 these summations can be grouped into N assemblies of atoms (macromolecules, particles, voids, etc.) and $N(N-1)$ pairs of such assemblies. The cross-section observed is due to the sum of a single assembly $P_A(R)$, and that of all assemblies present, modulated by their inter-centre distance $P_C(R)$

$$I(Q) \propto (\rho - \bar{\rho})^2 \left(N \int P_A(R) \exp(iQR) dR + N(N-1) \int P_A(R) P_C(R) \exp(iQR) dR \right) \quad (3.5)$$

Performing the Fourier transforms give the intra-assembly form factor, usually denoted by $P(Q)$ a molecular form-factor, and the inter-assembly form factor or structure factor usually denoted by $S(Q)$. Note: in the literature of scattering from polymers the term 'structure factor' is often used indiscriminately for the total scattering, the scattering from individual molecules, or the scattering arising from the interference scattering from components of the sample. Hayter and Penfold (1983) showed that where there is little orientational correlation, for example between charged, nearly spherical globular micelles, and little polydispersity, the averaging required in equation 3.1 can be performed separately and the convolution term in 3.5 may be approximated by the product of $P(Q)$ and $S(Q)$.

$$I(Q) \propto N^2 (\rho - \bar{\rho})^2 P(Q) \cdot S(Q) \quad (3.6)$$

N is assumed to be large, simplifying the equation; note that $P(Q) \cdot S(Q)$ has the dimensionality of $1/N$.

For dilute solutions, $N^2 \ll N$, the first term in (3.5) is dominant, and hence the scattering intensity is then peaked at $Q=0$. At higher concentrations the second term becomes very much larger and $I(0)$ is a value reflecting the compressibility of

the system, with a peak in $I(Q)$ at non-zero values of Q . Because $I(Q)$ is a product of $P(Q)$ and $S(Q)$ this peak should not simply be interpreted as a characteristic inverse distance in the sample.

The single particle correlation function $P_A(R)$ can be calculated for a number of simple shapes. For a sphere, radius R_s ,

$$I(Q) = N(\rho - \bar{\rho})^2 \left[\frac{3(\sin QR_s - QR_s \cos QR_s)}{(QR_s)^3} \right]^2 \quad (3.7)$$

The scattering from other simple shapes has been calculated in the approximation of random orientations by Guinier and Fournet, (1955).

Limiting values at low and high Q

3.2 The Guinier Radius and the Porod Equation

Guinier showed in 1938 that in general terms the scattering curve could be characterised by a single metric, the radius of gyration R_G of the assembly and that approaching $Q=0$ the form of the curve was closely approximated by

$$I(Q) = N(\rho - \bar{\rho})^2 \exp(-Q^2 R_G^2 / 3) \quad (3.8)$$

For the scattered intensity, the scattering density, rather than the mass, is used as weighting in the moment of inertia. This approximation holds irrespective of the size and shape of the assembly for values of $QR_G \ll 1$ though it is most appropriate for compact particles. Note this Guinier radius must not be confused with, say, the radius of a sphere since in this case $R_G^2 = 3R_s^2/5$. Other approximations for different characteristic distances are applicable for particles showing very large anisometry e.g. long fibres or lamellar sheets

The intensity extrapolated to forward scattering gives the scattering per particle, and hence the molecular weight in the case of macromolecules (Jacrot and Zaccai, 1981).

Porod in 1955 showed that at large Q the final slope of the scattering intensity was proportional to Q^4 for systems where there was a well defined interface between the two phases.

$$I(Q) = N_p (\rho - \bar{\rho})^2 A_p Q^4 / 8\pi^3 \quad (3.9)$$

where A_p is the surface area of the particle or void region

3.3 Intermediate Q ranges

The variation of $I(Q)$ with Q can be compared with models which show different dependences on Q . For a rigid rod $I(Q) \propto Q^{-5/3}$; for a polymer with excluded volume $I(Q) \propto Q^{-1}$; for a polymer behaving as a Gaussian coil $I(Q) \propto Q^{-2}$; (Cotton, 1991).

3.4 Contrast Variation

Much of the utility of the SANS technique has resulted from ingenious use of H/D contrast variation. In complex biological systems, for example 50S ribosomal subunits from *E. coli*, synthesis of sets of assemblies with different pairs of D marked proteins have been analysed by transformation back to pair distribution functions (Glatter(1991), May(1991)); at small radii this distribution function shows peaks due to the intra-protein correlations, at larger radii there is a peak due to the inter-protein correlations. The remaining protonated proteins in the ribosome are masked by being matched to the solvent. In polymer systems there is now considerable experience in making and marking polymers to measure specific conformation effects (Williams,1991; Higgins and Benoît,1996).

All the above models are valid for dilute systems where there are essentially no interparticle interactions.

3.5 Interacting systems, the random phase approximation

The dependence of the neutron differential cross-section on scattering density correlations offers a direct method of measuring thermodynamic properties of condensed matter. The value of $I^{\text{coh}}(0)$ is inversely proportional to the isothermal compressibility which can be expressed in terms of the chemical potential μ , the partial molar free energies of constituents with volume fraction ϕ as $\partial\mu/\partial\phi$. For ideal solutions, $I^{\text{coh}}(0)$ has a maximum value, and this diminishes towards zero for strong interactions; the behaviour of $I(Q)$ is hence strongly dependent on the strength of interactions. For two polymers A and B, with form factors $P_A(Q, N_A)$ and $P_B(Q, N_B)$, with volume fractions ϕ_A and ϕ_B then (Doi, 1996)

$$P(Q) = \left[\frac{1}{\phi_A P_A(Q, N_A)} + \frac{1}{\phi_B P_B(Q, N_B)} - 2\chi \right]^{-1} \quad (3.10)$$

where χ is the Flory-Huggins interaction parameter. In blends of hydrogenated and deuterated polymers, interactions (except for long polymers) are small and χ is effectively zero. Here model particle form factors, e.g. the Debye function for random coils, can fit well the measured cross-section curve $d\Sigma(Q)/d\Omega$:

$$\frac{d\Sigma(Q)}{d\Omega} \left(\frac{1}{K} \right) = \left[\frac{1}{\phi_A P_A(Q, N_A)} + \frac{1}{\phi_B P_B(Q, N_B)} - 2\chi \right]^{-1} \quad (3.11)$$

where K is an experimental constant described in section 3.8. For solutions $N_B=1$; here P_B is 1. The interactions in concentrated solutions can thus be measured

$$P(Q) = \left[\frac{1}{\phi_A P_A(Q, N_A)} + \frac{1}{(1-\phi_A)} - 2\chi \right]^{-1} \quad (3.12)$$

Thus both in melts and concentrated solutions phase behaviour can be studied as a function of composition, concentration, temperature etc.

At higher concentrations contrast variation also offers a powerful tool to elicit particle form factors by cancellation of terms containing the inter-particle form factor using measurements of mixtures of deuterated and undeuterated polymers

of the same type in the melt. Many more specialised measurements on polymers are described by Higgins and Benoît(1996).

A number of systems, such as charged micelles interact strongly. Treatment of these systems has involved modelling the inter-particle structure factor $S(Q)$ (Hayter and Penfold, 1983).

*Absolute intensity
calculations*

3.6 Example calculations of experimental intensity in SANS measurements

Calculation of the absolute intensity can often provide an important check on the validity of models and sometimes is a prerequisite in the interpretation of SANS data. The following examples show how this can be done for some simple physical systems. The calculation is shown in detail as it is often difficult to relate physical units to the quantities measured. The estimates below assume that the differential scattering cross-section is to be calculated in units of inverse length (this arises as a scattering cross-section per unit volume of sample). The theory behind these calculations for dilute samples can be found in various text books (e.g. Higgins and Benoît, (1996), chapter 5) but all the formulae are based on the simple estimate of $d\Sigma(Q=0)/d\Omega$ being a number density of scattering objects multiplied by their coherent scattering cross-section (or volume multiplied by scattering length density all squared). If the procedures outlined in the use of programs such as *spolly* are followed results should be obtained on an absolute scale and compared with these calculations. Simple examples of colloids and polymers are presented but the calculations can equally be applied to biological materials or inclusions or structures in inorganic and metallic materials.

3.7 Absolute Intensity of Polystyrene Latex in Water (H₂O)

The intensity for non-interacting particles can be calculated from the following general formula and the known physical constants and properties of the dispersion.

$$d\Sigma(Q)/d\Omega = n V^2 (\rho_p - \rho_s)^2 P(Q) \quad (3.13)$$

where, for a sphere radius R_s

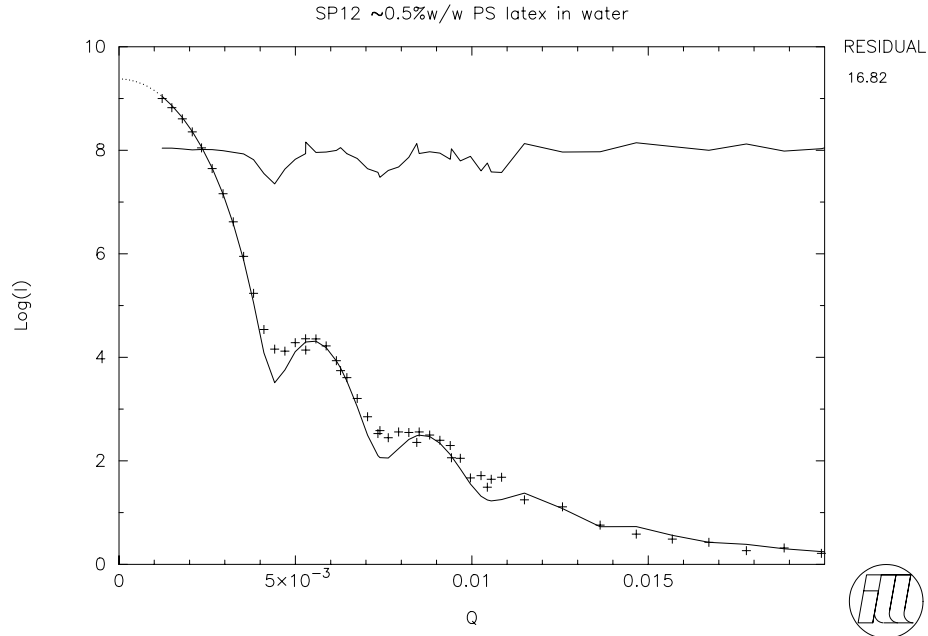
$$P(Q) = [(3 (\sin(QR_s) - QR_s \cos(QR_s)))/(QR_s)^3]^2 \quad (3.14)$$

Q is the amplitude of the scattering vector, V is the the volume of the particle (which equals $4\pi R_s^3/3$) and n the number density of particles. $P(Q)$ is a normalised form factor for uniform spheres which has a value of 1 at Q equal to zero. The quantities ρ_p and ρ_s are the scattering length densities of the particles and the dispersion medium respectively.

The chemical formula of polystyrene is $-(CH_2-CH(C_6H_5))_n-$ or $-(C_8H_8)_n-$ and the coherent scattering length per monomer is therefore (see Table I) $23.3 \times 10^{-5} \text{ \AA}$ (or $2.33 \times 10^{-12} \text{ cm}$). The mass, m , of a monomer is 104 g mol^{-1} and so the volume of a monomer v_{mon} can be calculated from the known density, ρ_m , of bulk polystyrene (1.06 g cm^{-3}) as:

$$v_{\text{mon}} = m / \rho_m N_{\text{AV}} \quad (3.15)$$

where N_{AV} is Avogadro's constant ($6.02 \times 10^{23} \text{ mol}^{-1}$). This gives a volume per monomer of 163 \AA^3 or $1.63 \times 10^{-22} \text{ cm}^3$. The scattering length density of polystyrene



The data are shown for the latex SP12 obtained from different measurements which have been combined (smorger) and fitted (rfit) with a simple sphere model, including resolution effects. The data have been normalised against water and cover more than four orders of magnitude. The final background level at large Q is approaching the value of 1, corresponding to the water medium.

is therefore $1.43 \times 10^{-6} \text{ \AA}^{-2}$ or $1.43 \times 10^{10} \text{ cm}^{-2}$. Similarly water has a molecular volume of 30 \AA^3 and thus a scattering length density of $-0.56 \times 10^{-6} \text{ \AA}^{-2}$ or $-0.56 \times 10^{10} \text{ cm}^{-2}$.

If the weight fraction w of the dispersion is known (in this example 0.5% w/w , found by drying to constant weight) and the particle radius is known from fits to scattering data or other measurements, it is possible to calculate the absolute intensity. For the latex SP12, the diameter is 2080 \AA and the radius R is 1040 \AA . This gives the particle volume V as $4.71 \times 10^9 \text{ \AA}^3$ or $4.71 \times 10^{-15} \text{ cm}^3$. The weight fraction can be converted to the number density, n as

$$n = w / \rho_m V \quad (3.16)$$

If we take the density of the dispersion to be unity this gives $n = 1.06 \times 10^{12} \text{ cm}^{-3}$. Substituting for n , ρ_p , ρ_w and V in Eq. 1 gives $d\Sigma(Q=0)/d\Omega$ as $1 \times 10^{12} \times 2.22 \times 10^{-29} \times 3.96 \times 10^{20}$ or $9.32 \times 10^3 \text{ cm}^{-1}$ ($\log_e 9320 = 9.14$, see figure above). This compares with the scattering of H_2O which would give rise to an incoherent background with a signal that is about 1 cm^{-1} (this varies with wavelength of the incident beam). The intensity at the position of the first maximum in the scattering function away from $Q=0$ is however about two decades smaller than that extrapolated to Q

equal zero. The large size of this particle means that a high intensity is measured even without recourse to special isotopic labels at low volume fractions.

3.8 Polymers in Solution or as Melts

The intensity is again

$$d\Sigma(Q)/d\Omega = n V^2 (\rho_p - \rho_s)^2 P(Q) \quad (3.17)$$

The scattering can be expressed as a product of the form factor which is often taken to be the Debye expression for a Gaussian segment density distribution and a contrast term. $P(Q)$ has the form

$$P(QR_g) = 2 (x - 1 + \exp(-x)) / x^2 \quad (3.18)$$

where x is the dimensionless variable $(QR_g)^2$. Note that this is expressed in terms of a radius of gyration rather than a simple radius.

V is the volume actually filled by a polymer molecule which will be much less than the volume permeated by the random configuration and n is the number density of polymer molecules. V can be expressed as

$$V = M / \rho_m N_A = N m / \rho_m N_A \quad (3.19)$$

For polymers in solution or as melts it is usual to formulate the expression of the absolute scattered intensity in terms of the molecular mass, M_w or degree of polymerisation of the polymer, N . These are related to the molecular mass, m of a monomeric repeat unit by

$$M_w = N m \quad (3.20)$$

The number density of molecules in a solution, n is related to these quantities by

$$n = c N_A / N m \quad (3.21)$$

where c is the concentration in mass per unit volume. Substituting in (3.17) we obtain

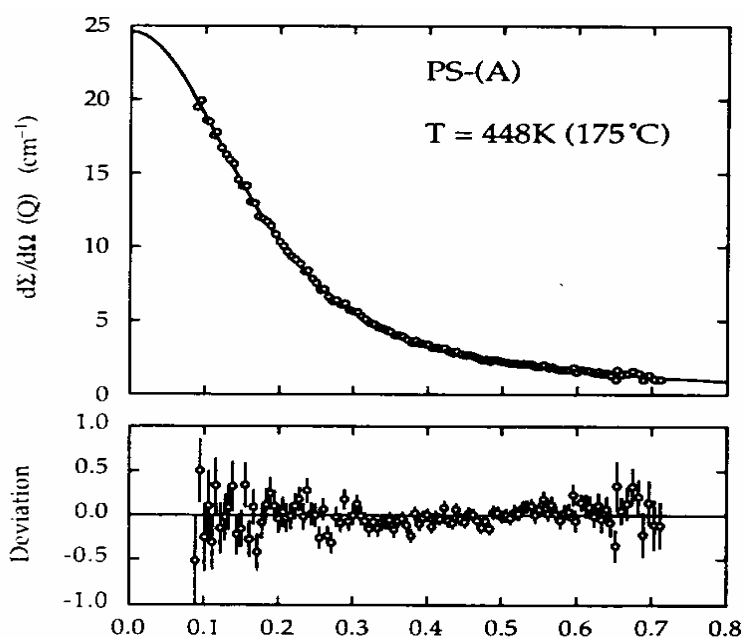
$$\begin{aligned} d\Sigma(Q=0)/d\Omega &= \{c N_A / N m\} (N m / \rho_m N_A)^2 (\rho_p - \rho_s)^2 \\ &= \{c N m / N_A \rho_m^2\} (\rho_p - \rho_s)^2 \end{aligned} \quad (3.22)$$

Taking values for polystyrene $-(C_8H_8)_n$ in deuterated toluene (C_7D_8) with a density of 0.94 g cm^{-3} the scattering length densities are $1.43 \times 10^{10} \text{ cm}^{-2}$ and $5.66 \times 10^{10} \text{ cm}^{-2}$ respectively. A solution of polymer with molecular mass, M of 80000 g mol^{-1} prepared at a concentration c , 0.015 g cm^{-3} in deuterated toluene will therefore have a scattering cross section at $Q = 0$ of

$$\begin{aligned} d\Sigma(Q=0)/d\Omega &= (0.015 \cdot 8 \times 10^4 / 6.02 \times 10^{23} \cdot 1.06^2) (1.43 - 5.66)^2 \times 10^{20} \\ &= 3.2 \text{ cm}^{-1} \end{aligned}$$

Similar calculations can be performed for polymer melts and in some cases the concentrations may be much higher as the random arrangement of molecules allows the single chain form factor to be measured even in systems with a high

concentration of labels provided there is no physical interaction causing preferential mixing or demixing. For deuterated polystyrene ($M=122000 \text{ g mol}^{-1}$) blended at 5.5% w/w in protonated polystyrene, the scattering length densities are 6.30×10^{10} and $1.43 \times 10^{10} \text{ cm}^{-2}$ respectively which gives $d\Sigma(Q=0)/d\Omega = 23.5 \text{ cm}^{-1}$. Use of the simple model to fit and extrapolate measured data to $Q=0$ is shown in the figure below.



3.9 Commentary

The calculated absolute intensity may not be exactly matched to the measured values for a variety of reasons. Experimental errors may arise in both the neutron measurements and in the determination of parameters concerning the sample. Absolute precision is often 10% or worse but relative changes within a series of samples measured under identical conditions will usually be measured to much higher accuracy.

If small signals are to be measured a limiting factor may well be the determination of background which may be dominated by incoherent scattering from the sample.

The simple theory outlined above has also ignored interactions which for colloids may cause large perturbations and even peaks that correspond to inter-particle structure. Even for polymers the interactions in solution may give rise to significant virial terms that alter the results and require measurements with extrapolations to zero concentration.

Basic procedure for measuring and analysing data

4

*See Appendix 5 for a
summary Check List*

This section offers advice on obtaining data with a certain quality to yield a reproducible corrected cross-section. It is not intended to be a comprehensive guide to performing experiments, merely highlighting some simple precautions to be taken. Wignall and Bates (1987) review SANS calibration methods.

High count rates imply accurate results (and statistical precision better than 1% is easily achieved), however there is no satisfactory formalism for estimating counting losses with the present electronics and multi-wire detectors. Mis-coding can be identified in part with the D11 and D17 detectors by examining contents of inactive cells in the corners. At count rates above 25kHz non-linear effects can be detected. Experimenters wishing to extract coherent scattering on top of high backgrounds should be aware of this, especially when rescaling data with markedly different count rates.

The simple pin-hole geometry minimises the number of instrument variables, but again, to exploit the precision of the data, the measurement sequence of sets should be performed with the instrument in one configuration. Thus, when possible, a set of transmissions should be measured with the attenuator in place, and then this should be removed and the set of SANS measurements made. The accuracy of the final results depends as much on the quality of the samples as on skilled use of the instruments.

4.1 Setting up the instrument

4.1.1. Wavelength and sample to detector distance

The spectrometers have a large accessible range of momentum transfer Q . It is nearly always possible to choose values of the configurations of wavelength, collimation, and sample to detector distance to ensure that the diffuse scattering under study impinges on the detector outside the central region where spatial resolution effects are most important. It is possible to merge routinely data measured under different configurations when it is necessary to extend the Q range beyond that of a single spectrum; it is necessary that the full set of sample and calibration spectra and transmissions are measured for each instrument setting.

When wishing to extend the Q range of the instruments it is preferable to make all measurements at the same wavelength, and vary the sample-detector distance. Then absorption and hence sample transmission effects remain identical.

To obtain a beam of monochromatic neutrons from a continuous (reactor) source a mechanical velocity selector is usually used. Geometrically this consists of a cylindrical drum with a set of helical slots along the axis. As the assembly rotates

only the neutrons within a range of velocities can travel through the helical path adjacent to the axis of rotation.

For a neutron mass m , Planck's constant h , the wavelength λ transmitted by a helical-slot velocity selector with length L and overall pitch angle ϕ and rotational frequency ω is

$$\lambda = \frac{h \phi}{m L \omega} \qquad \frac{d\lambda}{\lambda} = \left(2\alpha + \frac{d}{R}\right) \frac{1}{\phi} \quad (4.1)$$

where the slot has a radius R , width d , and the incoming beam has a divergence 2α . Typical dimensions are L , R and d 50, 50 and 1 cm. The pitch angle is only a few degrees. Any misalignment of the selector directly affects the effective ϕ and the selectors must be replaced very carefully if previous wavelength calibrations are to be used. It is possible to increase the flux, at the expense of resolution by changing the alignment, inevitably modifying the constant which links rotational speed with wavelength.

4.1.2 Wavelength check using Silver Behenate

This compound has a $d(001)$ lattice spacing of 58.38 \AA , i.e. $Q(001) = 0.1076 \text{ \AA}^{-1}$ (Huang et al, 1993). The diffraction from a powder specimen offers a simple method for systematically checking the wavelength at each measurement session, especially on instruments where the detector can be set quickly to a distance to bring this $Q(001)$ value into range. The wavelength spread is probably best measured independently by time of flight analysis using a chopper.

4.1.3. Guides in the incident beam

The intensity of the incident beam on the sample is not a simple function of the length of the set of guides in use, and their transmission is also a function of wavelength. For very precise work, at several detector positions, it is preferable to use a single long setting for this incident collimation matching the longest sample-detector distance. Though the mis-match leads to an obvious loss of potential intensity for the short sample-detector distance measurements, merging data is simplified.

4.1.4. Diaphragm

Placed just in front of the sample position this serves to define the beam incident on the samples. To enable precise comparisons it must remain completely static throughout the sequence of measurements since the beam is not completely uniform spatially in wavelength or intensity. The aperture should be smaller than the sample.

4.1.5. Beam stop alignment

While the beam stop protects the detector from damage due to the intense direct beam, the consequent high count rates due to beam stop misalignment entrain unacceptable counting losses and incorrect address encoding. The choice of size depends on the collimation, the aperture, and the sample-detector distance (but see section 4.6 on masking during data treatment). Providing the main beam is not actually on the detector the exact position is not important, though to simplify monitoring of experiments it is useful if it can be moved and replaced reproducibly. It is usually aligned to the nearest mm by measuring the strong

forward scattering from a scatterer such as PTFE, and centering the area masked by the beam stop. The image of the sample diaphragm alone, with an attenuated beam, gives an idea of the geometrical beam spread.

4.1.6. Sample holder

The sample should be larger than the incident beam. Note that the exit from the holder should not obscure scattering at high angles. When this is inevitable (as in use of thick cells, or magnet pole-pieces, or other cadmium shielded components blocking the exit path) a separate calibration measurement using a sample with uniform scattering should be performed in the same geometry.

4.1.7. Preliminary check of empty sample holder

A short measurement allows verification, that there are no stray reflections or scattering. The design of the holder should avoid walls parallel to the beam axis. This is often a major problem with optical grade quartz cells..

4.1.8. Measurement of cadmium or B₄C in the sample position

This offers a check for general background levels and beam independent electronic noise, as well as ensuring that all is correctly aligned. Except when very low scattering samples are to be measured the duration of this measurement can be a few minutes simply to look for problems. In general this component of background is small and can be ignored in the treatment. However, if this background is comparable to the scattering being measured, the duration of this run must be similar to that of the sample.

4.1.9. Determination of the beam centre

Several methods may be used including recording a spectrum of the attenuated incident beam passing through the sample diaphragm or the symmetric scattering from a very strong forward scatterer. At certain settings the silver behenate powder spectrum can also be used. Visual inspection of the raw counts data allows the centre to be set within 0.5 cells, adequate for data analysis. Examining the transmitted beam also offers a useful check that this region of the detector can be used reliably for subsequent transmission measurements.

It is useful to review all spectra quickly using xplots to check for anomalous effects

Selecting and examining a window on the detector using windet can reveal potential problems, as in the windet example

4.2 Detector calibration

As described in section 2.2 measurement of the uniform scattering from an incoherent scatterer serves to place the measured spectra on an absolute scale, correcting for detector efficiency and solid angle subtended by the detector elements. This requires that the calibration is repeated if the instrument configuration is modified.

It is useful to perform a simple analysis on the calibration measurements at the time of measurement, regrouping the data, and subtracting the holder etc. Plotting out these results identifies potential analysis problems at an early stage.

4.2.1. Vanadium

The incoherent scattering from a single crystal with etched faces, and known history has served as a primary standard. Vanadium plate may have density fluctuations and interstitial hydrogen present resulting from rolling and annealing in a reducing atmosphere. This gives it an abnormally high cross section which is

more wavelength dependent than pure vanadium. The scattering from a 3 mm thick sample is approximately 30%, giving a spectrum in a reasonable time.

4.2.2. Water

This remains the preferred secondary standard because of the high scattering cross-section and proven reproducibility. The principal disadvantage of its use lies in the temperature and wavelength dependence of the scattering of the 1 mm thick standard sample. Use for absolute calibration depends on an empirical formula originally relating observed scattering to the vanadium standard, though now it may refer to known coherent standards. The effects are especially notable at long wavelengths and are due to inelastic scattering by the water and consequently the dependence of specific detector sensitivity as a function of energy. Using the 1 mm sample the transmission is typically about 50%; for most practical purposes the deviation from a flat spectrum (as compared to vanadium) is very small (Sequeira et al, 1995).

4.3 Systematic cross section measurements

For every sample or calibration measurement the following sets of spectra must be obtained in sequence to ensure identical conditions.

Transmissions

Empty holder

Empty sample container

Filled sample container

Scattering

Empty holder (an optional check)

Empty sample container

Filled sample container

Cell reproducibility can be checked and a typical cell used for the empty cell measurements.

4.3.1. Transmissions

The attenuator is used to protect the detector from the direct beam when performing transmission measurements on the multi-detector. In some cases these function by scattering; in other cases a micro-perforated absorber is used. (where scattering attenuators are implemented it is normal to see a slight increase in the monitored beam intensity due to back-scattered neutrons). The beam stop is then displaced from its protecting position in front of the detector. The transmission is estimated as the ratio of the intensities of the beam transmitted through sample or cell with respect to that through the empty holder. Normally simple summation over the central area suffices to obtain this intensity (ignoring small background); when there is very strong small angle scattering there are increased problems in assessing the transmitted beam due to the high background. The incident beam is not uniform, and to obtain reliable results the correct repositioning of the

attenuator should be checked. The *windet* and *colrow* program examples show that a critically located row or column of mis-counting detector cells might have a profound effect on the reliability of transmission measurements.

4.3.2. Accuracy of transmission measurements

These measurements are equal in importance to the scattering spectrum measurements. Sufficient time must be allowed to obtain statistically meaningful results. Note that even with integrated total counts of 20000 there remains a mean error of 1% in transmission values. This may be of importance when attempts are subsequently made to subtract high flat incoherent backgrounds to extract the small residual coherent scattering component.

The water transmission is normally very reproducible.

THE TRANSMISSION MEASUREMENTS FOR THE WHOLE SEQUENCE OF SAMPLES SHOULD BE PERFORMED UNDER CONDITIONS OF IDENTICAL GEOMETRY.

Sequences of transmission measurements performed at different times should contain at least one common sample.

The programs *windet* and *detec* print and sum specific windows within the spectrum. It is useful to assess the transmissions of all the samples and holders at the stage of the measurements since the printouts give a clear indication of both the states of the instrument and the samples.

In general, except for solids with high Debye temperatures measured at low temperatures, all transmissions measured with long wavelength neutrons are temperature dependent. This requires that additional measurements of transmissions should be made when the temperature of the sample is to be varied.

4.3.3. Small-angle scattering measurements

It is recommended practice to divide long measurements (60 minutes or more) into two or more separate measurements. The program *rundex* can list summaries of results sorted by sets of samples, which helps intercomparisons. This allows the instrumental reproducibility to be checked, noting especially the water calibration. The latter should be performed at the start and at the end of the measurement period.

The optimum sample thickness is dependent on the ratio of coherent to incoherent (and hence background) scattering. At large sample-detector distances the small solid angle subtended by the detector minimises the effect of the incoherent scattering. In general it is not necessary to consider absorption processes in deciding thickness except when strong absorbers are present and long wavelengths are in use. The maximum acceptable detector count rate imposes further limitations. The finite dead time shows up in a non-linear response for strong coherent scatterers.

THE SAMPLE THICKNESS AND COMPOSITION MUST BE UNIFORM AND KNOWN TO THE SAME ACCURACY AS THE INTENSITIES MEASURED IN THE SAMPLE SPECTRA AND TRANSMISSIONS!

4.4 Summary of measurement procedure and data reduction to absolute cross section

After aligning the beam stop, sample holder, and performing all preliminary checks...

1. Measure C the electronic and ambient background using cadmium or other absorber to stop the beam at the sample position.
2. Measure VB the vanadium or water sample holder and transmission T_{VB}
3. Measure V the vanadium or water in its sample holder and transmission T_{V+VB}
4. Measure SB the sample holder and transmission T_{SB}
5. Measure S the sample and transmission T_{S+SB}

All the above are normalised for the same incident flux by dividing by the monitor counts.

Calculate the detector corrections using:

$$V_f = V - C - \frac{T_{V+VB}}{T_{VB}} \cdot (VB - C) \quad (4.2)$$

Subtract the sample holder from the sample using

$$S' = S - C - \frac{T_{S+SB}}{T_{SB}} \cdot (SB - C) \quad (4.3)$$

Normalise the sample signal with the vanadium, and include the self shielding due to the bulk macroscopic cross sections of the sample and vanadium, and their respective holders; the N_V/N_S factor ratios the cross-section between the number of sample entities and vanadium atoms present.

$$\frac{d\sigma}{d\Omega} = S_f = \frac{S'}{V_f} \cdot \frac{T_{V+VB}}{T_{S+SB}} \cdot \frac{N_V}{N_S} \cdot \frac{d\sigma_v}{d\Omega} \quad (4.4)$$

This is the procedure performed by the programs *spolly* and *anpoly*.

When the samples consist of mixtures of non-interacting components it is sometimes useful to place each spectrum on an absolute scale by this normalisation before attempting subtractions to yield the spectrum due to an individual component. Because the full history of each treated spectrum is not checked, the error calculations take no account of correlated errors, e.g. having pre-normalised each component separately with the same vanadium.

In complex analyses the errors shown should be assessed by noting additionally the scatter of points in the resulting spectra.

From the equation 4.4 it is clear that the result will be in the same units as the reference spectrum. Often metallurgists will use a differential cross-section in barns per unit solid angle. In biological and polymer science where solutions are often compared normal practice is to give the cross-section in cm^2 per unit volume,

which results in the cross-sections being quoted in units of cm^{-1} . The incoherent cross-section of a 1mm thick sample of water measured at 10\AA is often taken as about 1 cm^{-1} . Since water is usually necessarily present in biological samples the coherent cross-section can be easily judged as measurable knowing it is on top of a certain uniform signal of water/heavy-water mixture. It is relatively straightforward to measure coherent cross-sections as small as 0.05cm^{-1} .

4.5

Radial averaging

4.5.1. Definition of beam centre X0, Y0, DETECTOR-0

D11

DETECTOR-0 (given in degrees) is always zero: X0 and Y0 may be assessed by examining the scattering from a symmetrically scattering sample e.g. PTFE, or allowing the attenuated beam through the diaphragm to be used for the experiments and examining the multidetector spectrum (e.g., *detec*, *windet*, *colrow*).

D22, D17, D16

- (a) Detector in the position normal to the incident beam, coder reading zero: as above, DETECTOR-0 is 0; X0 and Y0 are determined as above.
- (b) Detector angle offset, DETECTOR-0 is set to the coder value
 - X0 is set to the value of X0 measured as in (a)
 - Y0 is set to the value of Y0 measured as in (a).

When ISUM (see section 3) is calculated only those cells actually within the bounds of the detector are used, and the result is normalised to the intensity per cell.

units for X0 and Y0

In all the following programs X0 and Y0 are entered as the cell addresses within the ranges 0-15, 0-63, or 0-127.

This ensures that the values correspond with the live-displays on the instruments, and with listing programs. The values are converted and stored in cm by the programs. In the case of the 4K spectra for D11 and D17 there is exact correspondence between the two since the cell spacing is 1 cm.

4.5.2. Allocation of cells in regrouping programs

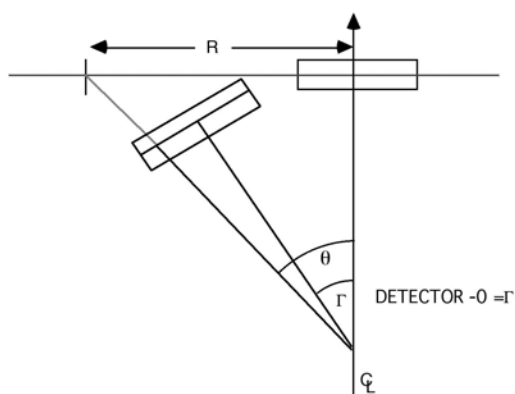
The user gives a radial step length (in cm) for the regrouping. This is transformed into a fixed step in Q, the momentum transfer, namely dQ . The Q value for

each cell j is calculated, q_j , and the smallest and largest values determined. Using the step dQ the measurable Q range is divided into these equal steps.

$$\text{and } Q_n - dQ/2 \leq q_j < Q_n + dQ/2$$

then the cell counts are allocated to this nominal value Q_n .

After performing this examination (omitting masked cells where necessary) for all cells the average Q_n for each step is calculated (and it is this value which is subsequently printed and stored). For convenience a reference "radius" is recalculated from the Q values and corresponds to the radius R in the diagram beneath. In the case of the detector not being perpendicular to the incident beam there is clearly no exact correlation with the physical cone of scattering at the detector.



For small offset angles and when the detector is normal to the centre line of the beam the physical distance is a useful concept.

Once the values of q_j have been calculated and allocated all the counts are associated with the Q value corresponding to the cell centre. This is justifiable within the inherent resolution limits of the detector, and the incident beam monochromation.

An alternative stratagem adopted in *red16* is to attribute pixel contents proportionately between the nearest angle bin, precalculated on a regular mesh since the detector is often step-scanned. Comparison with *rnd16* shows a negligibly small effect due to the linear interpolation if the detector is functioning correctly.

Extending the Q range of a measurement

The most common problems which arise are the matching of data measured with different instrument configurations, usually employed to extend the Q range, and to minimise resolution effects, and then to place the data on an absolute scale. We wholeheartedly recommend this latter exercise, which engenders a feel for the sensitivity and reality of the results. The aim of this short section is to offer advice on these two aspects of data correction.

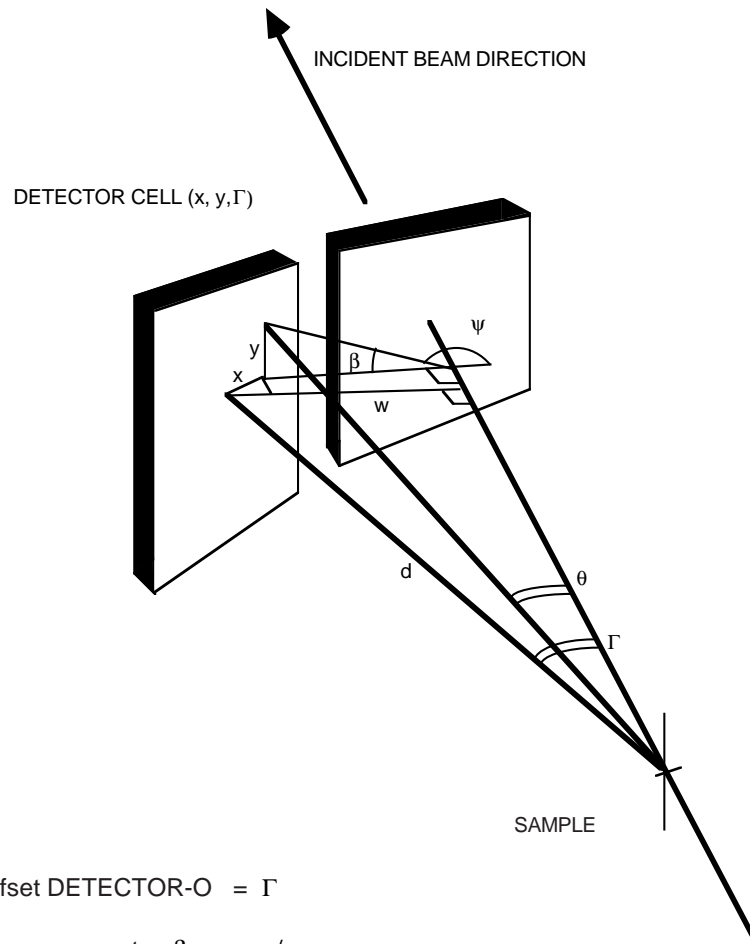
We have shown that the spatial information about the sample is contained in the coherent elastic small angle scattering signal. The measured intensity is reduced by absorption effects within the sample, which are assessed by the transmission measurements at the same incident wavelength. These effects are wavelength dependent.

The simplest way to extend the Q range covered by the instrument, and hence to be recommended, is to use the same incident wavelength, but with several sample to detector distances (with appropriate collimation changes). Any change in the guides for the incident beam implies a different wavelength distribution at the sample position (due to inevitable gaps in the continuity of the guides). In general the beam monitor serves primarily to correct for changes in the source intensity; not all the neutrons passing through it reach the sample, and this fraction also depends on the wavelength in use. The incident beam intensity is thus best re-measured using a calibrated strongly scattering sample at the actual sample position. Sets of slabs cut from the same sample of poly-methyl-methacrylate sheet can form the basis for such measurements.

To merge data measured at different wavelengths it is necessary to know the efficiency of the detector as a function of wavelength. Again this can be estimated for the beam transmitted by a calibrated strongly scattering sample.

These same calibrated transmission measurements help to place the data on an absolute scale. We note that the use of water calibrations brings with it questions on the reliability of using a broad range of wavelengths to calibrate the detector. This is usually judged as being an expedient solution, but should be based on previous measurements of known systems, i.e. really using a coherent elastic small angle scattering sample as a primary calibrant. The water normalisation, used in conjunction with this derived cross-section, is then used to correct for both detector efficiency fluctuations, and to set an "absolute" scale on the measurements. Further information on absolute calibration, especially matching neutron and x-ray SAS data is given by Russell et al (1988).

GEOMETRY OF THE SMALL ANGLE SCATTERING MEASUREMENT



$$\text{Offset DETECTOR-O} = \Gamma$$

$$\tan \beta = y/w$$

$$= y / (d \sin \Gamma - x \cos \Gamma)$$

$$\psi = 180 - \beta$$

This diagram shows the general nomenclature of angles

The case is shown for D17 showing x increasing as Γ physically decreases (though the coder value increases). On D16 and D22 the encoding matches geometry that corresponds to x increasing as Γ increases.

4.6 Masking data during analysis

The programs *rmask* and *grund* each produce a file with an identical format, namely a title then a string of characters corresponding to the detector image that are set to “#” if a cell is to be eliminated, or “.” if the contents of the cell are to be used.

```

y      |      CELLS
      |      64 65 66 67 68 69 70 71
      |      0  1  2  3  4  5  6  7
      |-----
                                     x

y      |      Example of bits in mask 1
      |      # # # # # # . .
      |      # # # # # . . .
      |-----
                                     x

y      |      Example of bits in mask 2
      |      . . . . # . . #
      |      . . . . . . # . .
      |-----
                                     x

y      |      Example of
      |      resultant
      |      MASK=MASK 1 OR MASK 2
      |      # # # # # # . #
      |      # # # # # . # .
      |-----
                                     x

```

The program *rmask* allows a definite pattern to be set up to eliminate whole rows or columns, or define a sector or a band. *grund* enables a nominally flat spectrum to be examined and sets up a bit pattern corresponding to cells which are outside an upper and lower limit set by the user. The mask options in treatment programs allow one or a set of these masks to be read in. The normal files output by *rmask* and *grund* have a five character name and add an automatic extension name of .msk The set of masks are used to create a resultant mask and cells are subsequently eliminated when any mask contains a “#”.

Thus quite detailed analyses of anisotropic data may be performed with *rnils* by creating a suitable set of sector or strip masks, the application of each separately leading to new values for the resulting regrouped I(Q).

All cells more than 36 cms from the centre of the D11 or D17 detector ($x = 31.5$, $y = 31.5$ cms) are always eliminated by *rnils* and *areg* (the detectors have no active elements beyond this distance - any counts in data are due to noise and electronic faults).

MASKING SHOULD NOT BE USED TO SQUEEZE SIGNIFICANCE FROM CELLS WHICH MAY SOMETIMES BE PARTIALLY OBSCURED BY THE BEAM STOP.

If data at low Q values from cells close to the beam stop are to be interpreted then all cells which might be partially obscured must be carefully masked, taking into account the irreproducibility in positioning the beam stop.

Inevitably the resolution is poor near the beam stop, and the differences in horizontal and vertical beam divergences may be significant. For these reasons large beam stops are often used, and even larger areas are excluded from subsequent analysis by deliberate masking.

The format of the mask file is in appendix A1, and the subroutine *grundd* which reads the file in most applications is described with other routines in *librlib.a* in appendix A2.

Finding and treating data at the ILL

5

The most convenient organization for files is to store the raw data (copies from the permanent data archive) in one directory. The environment variable associated with this is `SAS_DATA_PATH`. Data treatment is performed with all plotting and listings and treated data stored in a second directory, the current default working directory. This layout works well on all systems.

Although this section principally describes Unix/Linux/Macintosh-OSX systems at the ILL (Unix generic commands) there is a close correspondence between the simple commands proposed here and equivalents on PC systems using a command terminal window. Appendix 4 describes the *prop* GUI for easier use of programs with Windows. All programs use the same environment variable names.

During the start-up and logging-on procedure on network computers a number of commands and variables are defined either by the system manager, or by the user. This has been used at the ILL to pre-define a number of parameters, for example the location of raw data, default printers and type of graphical output.

The user thus works within an environment which may vary between computers. At the ILL this has been used to offer the user identical possibilities transparently on the instrument workstations, and on the LSS Group workstations. The user's command file invoked on the instrument accounts is given in annotated form in the appendix A3. The PC environment is described in appendix A4.

5.1 Logging on and logging off

The user is recommended to login afresh on the instrument workstation e.g. *d22lnx*; this procedure will allocate a personal working directory, and avoid conflicts with previous users

*Logging onto networked
Unix/Linux systems at
the ILL*

In general, commands or data input from terminals are only sent after pressing the RETURN key. Most mouse actions require use of the left-hand button. A default answer is usually shown by a highlighted border. Selection with the mouse, and left click acknowledges a choice. A default proposal may also be accepted using the RETURN key.

1. Type your name if you have a personal account, otherwise give the instrument name.
2. Then give the appropriate password.
3. If you are using the shared instrument account you will be asked for a name to identify your work. Special directories are created and you must give the same identification name at the next login to re-use this disk space.

After logging on you will receive a system prompt, typically %, or on many systems the system name and sometimes the current file directory, terminating in the % symbol. In the following examples these are shown: the user's own typed input then follows, terminated by the RETURN or ENTER key.

4. If you are not using the shared instrument account you should invoke the command file which defines the commands to run the suite of programs by personally giving the sequence of commands below :

```
% setenv SAS_DIR /home/cs/sans
% source $SAS_DIR/sasetup
% setenv SAS_INSTRUMENT d11
% setenv SAS_DATA_PATH /usr/illdata/data/d11/
```

The last two lines signify the instrument and source of raw data from the current reactor cycle for D11. This avoids repetitive typing of this information during treatment. Please note the terminal / in the data path.

5. It is useful to create a sub-directory for each project (mkdir command), and then change to this directory (cd command) to localise all the result files together. It can be especially useful, once a measurement sequence is finished, to retreat systematically all the data when a full overview of the raw results is available. This separates off the files created quickly during the experiment, perhaps when not all component spectra had been fully measured. Most programs have logging output, and the treated data too have information within giving the history of their creation. With all components present in a common location it is easy to detect errors in treatment which give anomalous results.

Setting the display terminal name

When running from a remote system or X-window terminal, the normal logon procedure or ssh -X login should setup the terminal name correctly. To define this manually the environment variable DISPLAY should be set to the host name or IP number and screen number (invariably 0) e.g.

```
% setenv DISPLAY my_Xterminal_IP_address:0
```

Logging off

Type the command exit followed by RETURN . This will logout the current window. On an X-window display there is a logout menu item to click on, which will lead to a confirmation request, logging off and liberating the display.

5.2 Special key functions

If there are typing errors typing RUBOUT (or the key marked $\leftarrow X$) will delete the last character typed, and a sequence of RUBOUTs will progressively eliminate the original line. The keys CTRL+H together have the same effect. To cancel the whole line (Unix) to start again type CTRL + U (hold down the CTRL key while typing U).

To halt the current program type CTRL + C. For Unix CTRL+Z interrupts the current program; type fg to continue (foreground) or bg to allow it to continue as a background process. For Unix the end of data input is signified by a CTRL+D. For the PC the CTRL+Z is used and habitual PC users should note the difference.

5.3 Running programs

Programs are run using the program name

e.g. `% windet`

Most numerical input is checked for illegal characters; numbers can usually be entered omitting the decimal point, or in scientific format. An incomplete input line usually sets the remaining requested input values to zero except where otherwise specified (dividing factors typically default to unity) After each end of program execution the names of the resulting listing file and plot files are given. Empty PostScript graphics files are quietly deleted. You may examine the listing screen page by screen page e.g.:

```
% more rnls052.lis
```

and then perhaps print the file with the command `pri`.

```
% pri rnls052.lis
```

For graphical output a command `plo` is used:

```
% plo mplr057.ps
```

The first time the command `pri` or `plo` is given the user is notified of the name and location of the default printer, and is offered the choice of changing this to a more conveniently located printer. Subsequently, to change the printer, the command

```
% myprinter          or          % myplotter
```

should be given, and an alternative printer may then be selected. These commands allow a fast black/white printer to be used for listings, and a (slower) colour printer for graphical output. The `pri` command tests the file type; PostScript files with an extension `.ps` or `.PS` are sent directly to the printers. Other files are piped through the formatting utility `fpr` which lists and paginates the file as a 132 column listing, interpreting Fortran formatting controls if required. The resultant PostScript file is then piped directly to the default printer set with `myprinter`.

5.4 Other useful commands

Unix commands and filenames are case-sensitive This is not the case for the PC.. A filename has a general form

```
Unix    /path1/path2/path3/filename          PC
D:\path1\path2\path3\filename
```

The shell (or command interpreter), `tcsh` by default for ILL visitors also interprets asterisks as a wild-card instead of part of the filename. A question mark may be used to denote a single character. Some examples are shown below.

To halt a program, type Control-C.

The general command for searching for help on a topic is `% man -k topic`

The manual pages on a specific topic are shown with `% man topic`

The following standard Unix commands perform the following simple functions when typed into a terminal window:

% ls	directory command
e.g.	
% ls g0*	shows all regrouped data files g0nnnnn.mmm
% ls -l g0*	shows all regrouped data files
g0nnnnn.mmm	with details of size, date etc.
% cat filename	types out a file
% rm filename	delete file
% cat g008700.001	types out regrouped data file for 8700, extension 1
% more	types a long file out page by page
e.g.	
% more 022100	types out raw data file
% head -n filename	types first n lines of filename
% tail -n filename	types last n lines of filename
% grep "string" filename	types each line in filename containing string
% pwd	type current directory name
% mkdir samplew	creates a sub-directory samplew
% cd	change to logon directory (\$HOME)
% cd samplew	change to \$HOME/samplew/ directory
% printenv	show environment
% setenv ABCDE wxyz	set environment variable \$ABCDE to wxyz
% echo \$ABCDE	type current string variable ABCDE
% mv file1 file2	rename file1 to file2 (will overwrite an existing file2)
% cp file1 file2	copies file1 to file2 (will overwrite an existing file2)

On the LSS Group's workstations:

% help	starts browser with help on SANS programs
% pri filename	prints a file
% plo filename.ps	prints a graphics file
% nedit myfile &	opens a new window for nedit X window editor

5.5 Environment variables

All the programs described here write treated data, output listing files (*.lis) and graphics files (*.ps) in the current directory (shown by the command `pwd`).

Environment variables are used to designate the instrument in use, the location of the raw data, and for program control, and most notably, for controlling plotting output. The commands to set up the environment are typically included in logon scripts, and this simplifies creating a common layout for visiting scientists. In the PC world the same variables are used in that set of programs.

Designation of instrument and location of data

Raw data are expected to be in the directory designated by `SAS_DATA_PATH` for an instrument defined in `SAS_INSTRUMENT`. Compressed raw data files (names terminating in `.Z`) can be read directly if a suitable decompression utility e.g. `zdarcht` is defined in `SAS_DECOMPRESS`.

As mentioned above, for the instrument visitors' accounts these are automatically set to the appropriate defaults, e.g. for D22 the following commands are already in the logon procedures.

```
% setenv SAS_INSTRUMENT d22
% setenv SAS_DATA_PATH /usr/illdata/data/d22/
note the terminating / for the PC the backslash separators are used.
```

Additional environment variables which are tested by many programs are:

```
% setenv SAS_CHECK limited
% setenv SAS_ERROR none
% setenv SAS_DEBUG true
```

These can be removed e.g.

```
% unsetenv SAS_DEBUG
```

Normally all would be absent. `SAS_CHECK` when set limits the number of error warnings when regrouping information does not match the parameters stored with raw data. When `SAS_ERROR` is defined then the error arrays in 2D data are not written out, saving disk space. When `SAS_DEBUG` is set the data access routines write progress information; this can be useful to find if data files have been damaged.

Extending standard data treatment

Additional environment variables allow external programs to be launched automatically each time a standard regrouped data file `grrrrrr.eee` or 2D data file `tnnnnnn.eee` is produced respectively

Example to create a simple/full xml formatted data files in addition to the standard output

```
% setenv SAS_EXTRA_G g2x
% setenv SAS_EXTRA_G g2xfull

% setenv SAS_EXTRA_T extt
```

In each case the effect is that of giving a command, e.g. after creating `g008700.000` the xml formatted copy is made by `g2x`, with the generated command using the new filename `g2x g008700.000`
Any valid command can be inserted; an initial check should be made with the command line input.

Environment variables on PCs

These are set and cleared with a slightly different syntax e.g.

```
> SET SAS_DEBUG=true
> SET SAS_DEBUG=
```

Control of Plotting

All graphics are performed using the PGPLOT library of Prof. Tim Pearson of the California Institute of Technology. A number of adaptations have been made at the ILL (<http://www.ill.fr/Computing/pgplotSS.html>) to provide systematic filename generation, and easy switching between devices. Output files have a unique sequence number and the name starts with an indication of the originating program. In addition to PostScript output on PCs the/GW option (using GRWIND.EXE from Tsuguhiko Tamaibuchi) allows printing the window directly on a Windows printer. For each type of graphical device a number of environment variables are checked. The principal variables are described here. The default values noted are set up by the standard login setup file (appendix A3) or by *prop* on PCs (appendix A4).

The graphical format uses a typical picture width/height aspect ratio of 4:3. Normally two X-Y graphs are plotted on each A4 page in portrait format with the standard environment settings (PGPLOT_ILL_PPAGE).

Table 5.1. Some environment variables used to control PGPLOT graphics.

Environment variable	value	Default	Function
PGPLOT_ILL_DEV_1	/xserve	D	X-terminal graphics device
	/xdisp		X-terminal+cursor
	/GW		PC Windows display
	/tk4100		Tektronix 4105 (colour)
	"?"		Prompt user for device
PGPLOT_ILL_DEV_2	/VCPS	D	hardcopy graphics Colour PostScript/Portrait
	/CPS		Colour PostScript/Landscape
	/GIF		GIF file
	"?"		Prompt user for device
PGPLOT_XW_WIDTH	0.4	D	Fraction of width for screen graphics
PGPLOT_PS_WIDTH	7500	D	Default (A4)
PGPLOT_PS_HEIGHT	11000	D	Default (A4)
PGPLOT_DIR	/usr/ill/lib	D	Location of font and X files
PGPLOT_ILL_PPAGE	2	D	Number of pictures/page 4:3

*minimum login
configuration*

A minimum amount of information to be included in a .cshrc file would usually include the following (e.g. for D11 data) These would usually be setup in the visitor zones in the starting procedures.

```
setenv SAS_INSTRUMENT d11
setenv SAS_DATA_PATH /usr/illdata/data/d11/
setenv PGPLOT_DIR /usr/ill/lib
setenv PGPLOT_ILL_DEV_1 /xserve
setenv PGPLOT_ILL_DEV_2 /VCPS
setenv PGPLOT_ILL_PPAGE 2
setenv PGPLOT_ILL_XW_WIDTH 0.4
```

5.6 Summary of files created by treatment programs

If each set of experiments is associated with a new subdirectory then the systematic naming of the output files is a guide to the sequence of operations used in treating the data. Data files are identified by the run and extension numbers, and also contain history of their creation, with information used in the last stage of treatment. It is thus possible to trace through treatment back to the raw data.

Many of the programs store variables in files so that these previous parameters can be used as defaults on restarting treatment. Most of the regrouping programs use the same file so the parameters are shared. If a parameter file is deleted, or work is started in a new directory the programs will start with built-in defaults. The contents of some of these files is summarised below:

xpolly.his	log file of all xpolly operations
sans.trm	results of all transmission calculations in a simple table
*.ffn	parameter files for <i>fitfun</i> fitting programs
windet.par	window settings and transmission data
colrow.par	windows and normalisation data for <i>colrow</i>
splots2.par	window and normalisation data for <i>splots</i> and <i>xplots</i>
rndx.par	data selection for listing by <i>rundex</i>
sequ.seq	sequence number for listing and graphical output files
sasval.par	file containing regrouping parameters

Listing output files and PostScript graphics files from different programs can be identified by the initial four letter acronym, and the incrementing sequence number. It is therefore easy to identify that the results of *spolly* in spol012.lis was done after the *rnils* regrouping shown in rnl005.lis. A further aid to troubleshooting apparent problems in the data reduction can be found by inspecting the history stored in treated data files (see A.1.2.1)

5.7 Locating raw data

The web server BARNES <http://barns.ill.fr> incorporates a web utility IDA which will search the data catalogue (post 1995) with a number of options. There it is possible to select and download raw data from the online archive. To treat these data it is necessary to refer to personal experiment notes and the log books conserved by the instrument responsables. Data are identified by year/cycle number and instrument name. The data server is *serdon*. Typical archive directory path names are automounted on use of the standard names e.g cycle 1, 1998.

```
/usr/illdata/981/d22/006888
```

The present archive of data for D11 is complete from cycle 743, and for D17 from cycle 771, all treatable with the present programs, with a few absences due to tape errors.

5.8 Retrieval of raw data

Current data and that from the preceding cycle are stored on-line on disk. The standard directories in which the data may be found are, respectively:

```
/usr/illdata/data/instrument/  
/usr/illdata/data-1/instrument/
```

Each run is stored as a separate file with a simple six digit sequence number as filename. This offers compatibility with all computer systems, including the compressed data when an extension *.Z* suffix is added. A summary of the contents, for example for D11 can be obtained using *dirrun*.

dirrun

This program examines a directory for data files, and lists a summary of the sequences of runs found therein. If just the instrument name is given the default directory */usr/illdata/data/instrument* directory is searched, otherwise the named directory is used.

This will show whether all runs have been transferred to the central data store.

```
% dirrun d11  
Data in directory /usr/illdata/d11  
  
numors 005236 to 008858  
3623 data files are stored here
```

Older data are archived in a compressed format (which may be uncompressed with the standard unix command *uncompress* or *gunzip*). Up to date information on retrieval is best found in the ILL WWW pages, from <http://www.ill.fr/Computing/illdata.html> Typically the compressed data are copied to a local disk and uncompressed before standard use. Wildcards can be used as shown in the example to simplify specification of a range of files for transfer. In this case the environment variable should be set to the current raw data directory (in this case a typical directory of archived data from cycle 981, the first reactor cycle in 1998) as follows:

```
21% dirrun /usr/illdata/981/d22  
Data in directory /usr/illdata/981/d22  
numors 000001 to 007063  
7063 data files are stored here  
Some or all data files have been compressed  
22% mkdir myraw981  
23% cd myraw981  
24% cp /usr/illdata/981/d22/00688* .  
25% cp /usr/illdata/981/d22/00689* .  
26% ls  
006880.Z 006882.Z 006884.Z 006886.Z 006888.Z ...  
006881.Z 006883.Z 006885.Z 006887.Z 006889.Z ...  
27% uncompress *.Z (or 27% gunzip *.Z )
```

```

27% ls
006880 006882 006884 006886 006888 006890 006892 ...
006881 006883 006885 006887 006889 006891 006893 ...
28% cd ..
29% setenv SAS_DATA_PATH myraw981/
30% setenv SAS_INSTRUMENT d22

```

If the environment variable `SAS_DECOMPRESS` is set to a decompression utility like `zcat` or `dzarch` then compressed data may be used directly, though if multiple accesses are to be made it is clearly advantageous to decompress the sequence as above (even just showing titles as in `xplots` would require decompressing each file).

rundex

`rundex` will look at the `SAS_DATA_PATH` directory for current raw data, and in the current working directory for regrouped or 2D treated data. It lists a summary of information on the screen in tabular form. For raw data, the table in the more comprehensive listing file can include values selected from the initial experimental data parameters; up to four additional columns are possible. Together with the count rate information, and the possibility of defining repeat sets this program offers a good method for obtaining an overview of a set of measurements.

Inspection of monitor and detector count rates will show up anomalous scattering from samples or unexpected changes in instrument performance.

```

% rundex
rundex - version 1.3 June '05 (R.E. Ghosh)
Summaries from current SANS data files

12-Nov-2006 16:42:32
  100 RAW DATA are stored for d22 in SAS_DATA_PATH=./raw0/
Runs range from 26800 to 26899
  4 1D data files are stored here
Runs range from 10392 to 10451
Exts range from 2 to 2
  0 2D data files are stored here
Runs range from 0 to 0
Exts range from 0 to 0

rundex will list summary information from SANS data files

Options
R      Raw data summaries
S      Select additional parameters for raw lists
G      Grouped data summaries ( 1D )
U      Ungrouped data summaries ( 2D )
E      Exit
H      Help - this text
Option R,S,G,U,E,H or Help : r

Raw data Summary
Runs range from 26800 to 26899
Give First run..Last run...Set repeat length : 26832 26845 7

```

Run	Title	Monitor*	monitor/s	detector/s	Wave	S-Dm
26832	2 H2O	6987	23290.01	431.91	8.0	14.40
26839	2 H2O	6982	23276.32	431.51	8.0	14.40
26833	2 ec	6986	23288.56	231.40	8.0	14.40
26840	2 ec	6984	23282.24	233.28	8.0	14.40
26834	2 B4C	3493	23288.05	6.64	8.0	14.40
26841	2 B4C	3492	23286.07	9.75	8.0	14.40
26835	2 0% virus	13969	23281.71	3606.45	8.0	14.40
26842	2 0% virus	13972	23286.73	3615.46	8.0	14.40
26837	2 67% virus	13968	23280.85	593.37	8.0	14.40
26844	2 67% virus	13971	23285.45	541.00	8.0	14.40
26838	2 100% virus	13972	23287.46	1051.47	8.0	14.40
26845	2 100% virus	13972	23286.68	1049.54	8.0	14.40

```

Option R,S,G,U,E,H or Help : e
Closing listing file rndx007.lis

% pri rndx007.lis
request id is ljl_ill20_2-5281 (standard input)
PRI - rndx007.lis processed as fortran listing.

```

To ensure measurements are reliable it is often useful to divide them into several cycles, with calibrants. The skip factor groups the sets together for easy comparison.

Raw data programs

6

6.1 Setting location of raw data

Most 2D display and treatment programs can access either raw data or treated data. In these cases an extension number of zero will indicate that the input data is in the form of the original measurements from the instruments. The programs presented in this section are usually used in preparing treatment, and in offering simple inspection of the data files from printer listings. The display programs *xplots* and *colrow* described in chapter 10 are also useful at this preliminary stage. *rundex* offers an alternative presentation of producing a tabular summary listing of raw data parameters stored after the measurement.

The location of raw data is defined in the environment variable `SAS_DATA_PATH`, and the instrument name is set in the variable `SAS_INSTRUMENT` (see page 39). Direct use of compressed raw data is also described there.

6.2 *rundex*

This program scans the raw data and will print out an index summarising count rate and configuration information. Up to four experiment parameters from the data can be selected and added to the column form listing. The same program will extract simple summaries from treated data files - see terminal dialogue in 5.8.

6.3 *windet*

Now that text windows with wide, scrolling displays are commonly available they can be used directly to view the tabulated listings of multi-detector results.

This program reads raw data from either the archive disk, or the individual data files on the instrument and lists the raw data cell by cell within a window defined by the **W** command. The **T** command is used to designate a transmission reference run. The sum of the current window is stored, and the peak centre at half height in x and y is calculated, together with the centre of gravity in x and y directions. The **R** command sets up a sequence of runs which can then be listed with the **L** command. The sequence can be interrupted after each run. If a transmission run has been defined then the subsequent data have the sum ratioed to this reference and listed as the transmission.

The transmission results are systematically appended to a file "sans.trm" which serves thus as a summary. If this file is printed it can aid evaluating correction factors for *spolly* or *xpolly*.

One main reason for listing the windows of raw data as the transmissions are assessed is to detect anomalous cells. In general the centres of gravity and the peak centres should be in close agreement. Evaluation of the transmissions during the sequence of measurements will often show up problems with samples.

lass1 42% windet
windet - shows raw data in preset windows

version 1.8 June 1998 (R.E. Ghosh)

Help for WINDET

Command line

windet [first_run] [last_run]
displays data using current window settings
The sequence may be interrupted, returning to Options:

Type W to set window limits
R to set run number(s)
T to set a transmission run/beam centre
L to list window contents
E to exit
H to show this text

Option W,R,L,T,E or Help : w

Current window is 57 <= x <= 68 57 <= y <= 70
Give cell numbers 0<=x<=63 or 127, 0<=y<=15,63,127
RETURN retains present values
xmin...xmax...ymin...ymax : 57 68 57 70
Window has been modified.
There is no valid transmission data now.
Option W,R,L,T,E or Help : t
Give run number of transmission run : 9333

*Note:
column 64
shows
anomalous
counts!*

Y	av	X	057	058	059	060	061	062	063	064	065	066	067	068
070	4		0	1	0	3	10	5	4	5	3	5	4	3
069	34		2	3	6	32	77	85	82	49	53	13	2	0
068	1867		2	1	46	1415	4620	5339	4960	2274	3273	456	7	7
067	6408		3	8	150	4808	15615	18913	17185	7847	10727	1635	5	5
066	7568		6	6	193	5383	18076	22613	20552	9095	12822	2055	8	4
065	13357		3	10	295	9586	31325	39162	36810	15779	23262	4026	17	8
064	11798		1	9	238	8149	27637	33586	33801	14184	20225	3725	13	6
063	11412		5	15	194	7927	29383	33018	30685	12967	18649	4084	9	3
062	11462		4	9	195	7991	30161	32752	29762	13209	18788	4663	10	1
061	7523		4	5	133	5004	19244	21782	20011	8685	12220	3172	11	4
060	2919		5	7	52	1968	7763	8813	7996	3069	4205	1136	8	6
059	216		5	3	8	171	610	667	536	222	271	88	4	5
058	5		4	4	4	8	7	14	5	6	3	2	6	1
057	4		3	3	1	1	2	4	5	6	10	1	6	0
Average			3	6	108	3746	13181	15482	14457	6243	8894	1790	8	4

Total counts 894901 for 57 <= x <= 68 57 <= y <= 70 Monitor 8914439.
Centroid of window Xbar = 62.6 Ybar = 63.8
Peak average:
Xav(col) Maximum 15482. at 62.0 FWHM 4.7 X0 centre 62.8 COFG 62.6
Yav(row) Maximum 13357. at 65.0 FWHM 6.0 Y0 centre 63.8 COFG 63.8

Transmission Run 9333 Empty Hole T 30-APR-98 22:56:43

Option W,R,L,T,E or Help : r
Give first and last run numbers : 9332 9339
Option W,R,L,T,E or Help : l

Y	av	X	057	058	059	060	061	062	063	064	065	066	067	068
070	0		0	1	0	0	0	0	0	0	0	0	0	0
069	0		1	0	0	0	0	0	1	0	0	0	0	1
068	0		0	0	0	0	2	1	0	0	0	0	0	0
067	0		0	1	0	0	0	0	0	0	0	0	0	0
066	0		0	0	0	0	0	1	0	0	0	0	0	0
065	0		0	0	1	0	0	0	0	0	0	0	0	0
064	0		0	0	0	0	0	1	0	0	0	0	1	0
063	0		0	0	0	0	2	0	0	1	0	0	0	0
062	0		1	0	0	0	0	1	0	0	0	0	1	0
061	0		0	0	1	0	0	0	0	0	0	0	0	0
060	0		0	0	0	0	0	0	0	0	0	0	0	0
059	0		0	1	0	1	0	0	1	0	1	0	0	0
058	0		0	0	1	0	0	0	0	0	0	0	1	1
057	0		0	0	0	2	0	0	0	0	0	0	0	0
Average			0	0	0	0	0	0	0	0	0	0	0	0

Total counts 28 for 57 <= x <= 68 57 <= y <= 70 Monitor 8916555.
Centroid of window Xbar = 61.8 Ybar = 63.1
Transmission: 0.00003 compared to run 9333, saved in summary file "sans.trm"

Run 9332 Cd - Bgd T 30-APR-98 22:49:43 Monitor 8916555.

Type return to continue or q to quit sequence :

Y	av	X	057	058	059	060	061	062	063	064	065	066	067	068
070	4	0	1	0	3	10	5	4	5	3	5	4	3	
069	34	2	3	6	32	77	85	82	49	53	13	2	0	
068	1867	2	1	46	1415	4620	5339	4960	2274	3273	456	7	7	
067	6408	3	8	150	4808	15615	18913	17185	7847	10727	1635	5	5	
066	7568	6	6	193	5383	18076	22613	20552	9095	12822	2055	8	4	
065	13357	3	10	295	9586	31325	39162	36810	15779	23262	4026	17	8	
064	11798	1	9	238	8149	27637	33586	33801	14184	20225	3725	13	6	
063	11412	5	15	194	7927	29383	33018	30685	12967	18649	4084	9	3	
062	11462	4	9	195	7991	30161	32752	29762	13209	18788	4663	10	1	
061	7523	4	5	133	5004	19244	21782	20011	8685	12220	3172	11	4	
060	2919	5	7	52	1968	7763	8813	7996	3069	4205	1136	8	6	
059	216	5	3	8	171	610	667	536	222	271	88	4	5	
058	5	4	4	4	8	7	14	5	6	3	2	6	1	
057	4	3	3	1	1	2	4	5	6	10	1	6	0	
Average			3	6	108	3746	13181	15482	14457	6243	8894	1790	8	4

Total counts 894901 for 57 <= x <= 68 57 <= y <= 70 Monitor 8914439.

Centroid of window Xbar = 62.6 Ybar = 63.8

Transmission: 1.00000 compared to run 9333, saved in summary file "sans.trm"

Run 9333 Empty Hole T 30-APR-98 22:56:43 Monitor 8914439.

Type return to continue or q to quit sequence :

Y	av	X	057	058	059	060	061	062	063	064	065	066	067	068
070	2	0	1	0	2	0	5	0	2	1	3	3	3	
069	15	0	3	2	22	30	35	38	19	23	4	0	1	
068	879	3	2	26	668	2187	2548	2280	1113	1504	212	1	3	
067	2944	1	3	62	2094	7240	8763	8015	3445	4888	813	4	4	
066	3479	1	3	71	2450	8271	10557	9487	4181	5727	983	9	5	
065	6166	2	3	156	4315	14560	18144	16975	7369	10641	1819	5	4	
064	5499	2	3	104	3772	13085	15453	15660	6697	9421	1776	8	3	
063	5238	3	4	100	3708	13577	15069	14038	5854	8598	1894	7	3	
062	5239	2	4	90	3552	13604	14919	13872	6130	8596	2092	8	3	
061	3444	2	2	49	2307	8817	10150	9083	3911	5497	1505	6	2	
060	1363	2	2	27	868	3576	4177	3763	1447	1983	510	3	0	
059	96	2	4	3	74	269	305	235	95	107	50	1	2	
058	2	2	0	2	3	4	3	1	3	4	4	1	0	
057	2	0	2	1	3	1	0	4	1	4	2	0	0	
Average			2	3	50	1703	6087	7152	6675	2876	4071	833	4	2

Total counts 412406 for 57 <= x <= 68 57 <= y <= 70 Monitor 8913635.

Centroid of window Xbar = 62.6 Ybar = 63.8

Transmission: 0.46088 compared to run 9333, saved in summary file "sans.trm"

Run 9334 H2O 1mm T 30-APR-98 23:03:41 Monitor 8913635.

Type return to continue or q to quit sequence :etc.

Option W,R,L,T,E or Help :

Option W,R,L,T,E or Help : e

Closing listing file wndt001.lis

lassl 43% cat sans.trm

Run	Trans.	Pos	Title	Xbar	Ybar	Ref.	x-pixels	y-pixels
9333	1.00000	2	Empty Hole T	62.6	63.8	9333	57 68	57 70
9332	0.00003	1	Cd - Bgd T	61.8	63.1	9333		
9333	1.00000	2	Empty Hole T	62.6	63.8	9333		
9334	0.46088	3	H2O 1mm T	62.6	63.8	9333		
9335	0.94626	4	Empty Qtz Cell T	62.6	63.8	9333		
9336	0.95308	5	PTFE T	62.6	63.8	9333		
9337	0.83511	6	D2O 2mm T	62.6	63.8	9333		
9338	0.77422	7	7D1 2mm T	62.6	63.8	9333		
9339	0.80731	8	7D2 2mm T	62.6	63.8	9333		

lassl 44%

6.4 detec

This program reads raw data from either the archive disk, or the individual data files on the instrument and lists the raw data cell by cell. As with other programs accessing raw data the commentary blocks too are printed out, showing the

contents of the scalers etc., and offering options to select a subset of the more relevant other parameters. It is useful to include at least the principal scaler values.

Options exist for printing out selected areas of a spectrum; this avoids the wasteful printing of unwanted output. If zero is given for either the 4K or 16K option then only the comment blocks and scaler contents are printed: the user is then prompted to define a region of the spectrum XMIN, XMAX, YMIN, YMAX which is summed, averaged, and printed (ISUM). This can be useful for checking transmission measurements (see section 4.3 and *windet*).

input requested

1. Comments, scalers and ISUM only 1 page per run
2. 4K options

rows	0-63	outputs	8 pages per run
rows	6-60	outputs	4 pages
central region	x (24-39), y (6-60),		1 page per run
personal choice			up to 16 pages
3. 16K options similarly.
4. parameter print-out choice
5. Run numbers, first and last of sequence.

terminal dialogue

```
% detec
DETEC VERSION V4.5u August '95 (R. E. GHOSH)
OPTIONS FOR PRINT-OUT OF SPECTRA:
0: COMMENTS, SCALERS, PARAMETERS AND ISUM ONLY
1: 4K..X 24-39...Y 6-60 CENTRAL REGION
2: 4K..X 0-63...Y 6-60
3: 4K..X 0-63...Y 0-63
4: 4K PERSONAL CHOICE
5: 16K..X 48-79...Y 40-90 CENTRAL REGION
6: 16K..X 0-127...Y 0-127
7: 16K PERSONAL CHOICE

TYPE 4K SPECTRUM OPTION :0
TYPE 16K SPECTRUM OPTION :7
A MAXIMUM OF 16 COLUMNS (X) MAY BE REQUESTED PER PAGE
ABOUT 55 ROWS (Y) FILL ONE PRINTED PAGE.
PAGE 1 XMIN,XMAX,YMIN,YMAX
56 70 50 80
ANOTHER REGION ? (Y/N)[N] :n

At present only scaler values will be printed
Select experimental parameters for listing output

Type A,D,S,Help, or RETURN when selection is complete :
 5 parameters selected for printing
# START ? # END ? 6880 6883
RUN 6880 LENGTH 16384
RUN 6881 LENGTH 16384
RUN 6882 LENGTH 16384
RUN 6883 LENGTH 16384
ANOTHER SET OF DATA ? (Y/N)[N] :n
Closing listing file detc002.lis
% pri detc002.lis
```

6.5

The programs *xplots*, *splots*, *colrow*, *cont* etc. described in chapter 10 will display raw (and treated) two dimensional data in various representations. The

**display
programs**

general ILL/IDL program LAMP, started with the command % lamp can also be used to view raw data and perform limited treatment

Recommendation

Experimenters are strongly advised to view all data sets measured. This is easily performed using *xplots* (the graphical interface to *splots*). The intensity scale may be fixed and the set of measurements can be compared rapidly using the uniform scaling using the NEXT button. This will often show up anomalous data sets clearly, and help identifying specific problems with either the instrument or samples. Although most programs will open compressed raw data files, users are strongly advised to decompress all raw data files before use as this will greatly speed up subsequent accesses.

Masking

7

7.1 rmask

This program sets the addresses of cells to be excluded from the analysis by *rnils* and other programs. The user can define individual cell addresses, rows, columns, or various rectangles to be deleted. Additional options allow all cells excluding a sector of defined dimensions or a band (both of which may be rotated about an origin on the detector). Any of these possibilities may be used in conjunction with any other, and the resultant mask will exclude all the cells so chosen. This is written on disk in the same format as the file from *grund* (see 7.2). The file is called *maskx.msk*, where *maskx* is a five character name given by the user.

The normal sequence of operations is as follows:

1. The user selects a suitable geometric pattern for cell elimination or reads in an existing mask file.
2. The user may then print or modify this mask, change the title, or zero the memory to create a fresh mask.
3. A choice of options or type of mask is made by typing an appropriate letter. When no more additions are to be made to the mask a title must be added for identification and the file is then saved.
4. The user then again has a choice as in 1. to further modify, or to print the result, or simply to stop.

These possibilities allow this set of isotropic analysis programs to be used on anisotropic distributions by creating a set of masks, e.g. one containing a vertical strip, and one containing a horizontal strip.

terminal dialogue

```
lass2 36% rmask
RMask - Multidetector masks - version 4.5  September '98 (R.E.GHOSH)

Type 0,1, or 2 for 64X64,128X128, or 64X16 MASKS :
rmsk>
OPTIONS:
C      Cells eliminated
R      Rectangles eliminated
X      Line at fixed X eliminated
Y      Line at fixed Y eliminated
B      all but a band eliminated
S      all but a sector eliminated
Z      Zero current mask
I      Input previous mask
F      File current mask
M      Modify mask title
L      List current mask
T      Type current mask
H      this text
E      EXIT program
```

Type control+C to stop program at any time.

```
Option C,R,X,Y,S,B,Z,I,M,F,L,T,E OR HELP :
rmsk>r
0 <= X <= 63  0 <= Y <= 63
Give XMIN..XMAX..YMIN..YMAX to be eliminated
rmsk>26 35 25 36
Option C,R,X,Y,S,B,Z,I,M,F,L,T,E OR HELP :
rmsk>x
Deleting line at constant X (set X to -1 to end)

Give X :
rmsk>0
Give X :
rmsk>1
Give X :
rmsk>62
Give X :
rmsk>63
Give X :
rmsk>-1
Option C,R,X,Y,S,B,Z,I,M,F,L,T,E OR HELP :
rmsk>y
Deleting line at constant Y (set Y to -1 to end)

Give Y :
rmsk>0
Give Y :
rmsk>1
Give Y :
rmsk>62
Give Y :
rmsk>63
Give Y :
rmsk>-1
Option C,R,X,Y,S,B,Z,I,M,F,L,T,E OR HELP :
```

```

rmsk>t
      0      8      16      24      32      40      48      56
63#####|#####|#####|#####|#####|#####|#####|#####
62#####|#####|#####|#####|#####|#####|#####|#####
61#####|#####|#####|#####|#####|#####|#####|#####
60#####|#####|#####|#####|#####|#####|#####|#####
59#####|#####|#####|#####|#####|#####|#####|#####
58#####|#####|#####|#####|#####|#####|#####|#####
57#####|#####|#####|#####|#####|#####|#####|#####
56#####|#####|#####|#####|#####|#####|#####|#####

55#####|#####|#####|#####|#####|#####|#####|#####
54#####|#####|#####|#####|#####|#####|#####|#####
53#####|#####|#####|#####|#####|#####|#####|#####
52#####|#####|#####|#####|#####|#####|#####|#####
51#####|#####|#####|#####|#####|#####|#####|#####
50#####|#####|#####|#####|#####|#####|#####|#####
49#####|#####|#####|#####|#####|#####|#####|#####
48#####|#####|#####|#####|#####|#####|#####|#####

47#####|#####|#####|#####|#####|#####|#####|#####
46#####|#####|#####|#####|#####|#####|#####|#####
45#####|#####|#####|#####|#####|#####|#####|#####
44#####|#####|#####|#####|#####|#####|#####|#####
43#####|#####|#####|#####|#####|#####|#####|#####
42#####|#####|#####|#####|#####|#####|#####|#####
41#####|#####|#####|#####|#####|#####|#####|#####
40#####|#####|#####|#####|#####|#####|#####|#####

39#####|#####|#####|#####|#####|#####|#####|#####
38#####|#####|#####|#####|#####|#####|#####|#####
37#####|#####|#####|#####|#####|#####|#####|#####
36#####|#####|#####|#####|#####|#####|#####|#####
35#####|#####|#####|#####|#####|#####|#####|#####
34#####|#####|#####|#####|#####|#####|#####|#####
33#####|#####|#####|#####|#####|#####|#####|#####
32#####|#####|#####|#####|#####|#####|#####|#####

31#####|#####|#####|#####|#####|#####|#####|#####
30#####|#####|#####|#####|#####|#####|#####|#####
29#####|#####|#####|#####|#####|#####|#####|#####
28#####|#####|#####|#####|#####|#####|#####|#####
27#####|#####|#####|#####|#####|#####|#####|#####
26#####|#####|#####|#####|#####|#####|#####|#####
25#####|#####|#####|#####|#####|#####|#####|#####
24#####|#####|#####|#####|#####|#####|#####|#####

23#####|#####|#####|#####|#####|#####|#####|#####
22#####|#####|#####|#####|#####|#####|#####|#####
21#####|#####|#####|#####|#####|#####|#####|#####
20#####|#####|#####|#####|#####|#####|#####|#####
19#####|#####|#####|#####|#####|#####|#####|#####
18#####|#####|#####|#####|#####|#####|#####|#####
17#####|#####|#####|#####|#####|#####|#####|#####
16#####|#####|#####|#####|#####|#####|#####|#####

15#####|#####|#####|#####|#####|#####|#####|#####
14#####|#####|#####|#####|#####|#####|#####|#####
13#####|#####|#####|#####|#####|#####|#####|#####
12#####|#####|#####|#####|#####|#####|#####|#####
11#####|#####|#####|#####|#####|#####|#####|#####
10#####|#####|#####|#####|#####|#####|#####|#####
9#####|#####|#####|#####|#####|#####|#####|#####
8#####|#####|#####|#####|#####|#####|#####|#####

7#####|#####|#####|#####|#####|#####|#####|#####
6#####|#####|#####|#####|#####|#####|#####|#####
5#####|#####|#####|#####|#####|#####|#####|#####
4#####|#####|#####|#####|#####|#####|#####|#####
3#####|#####|#####|#####|#####|#####|#####|#####
2#####|#####|#####|#####|#####|#####|#####|#####
1#####|#####|#####|#####|#####|#####|#####|#####
0#####|#####|#####|#####|#####|#####|#####|#####
      0      8      16      24      32      40      48      56

```

0 ---- DETECTOR VIEWED FROM SAMPLE ----> 63

*** NO TITLE SET ***

```

Option C,R,X,Y,S,B,Z,I,M,F,L,T,E OR HELP :
rmsk>f
Give new title for mask (20 chars)
or RETURN to retain current title :
rmsk>Bstop 26-35x 25-36y
Give output mask file name (5 chars. e.g. mask1)
rmsk>bedge
File recorded : bedge.msk
Title : Bstop 26-35x 25-36y 29-Jun-1998 18:21:06
Option C,R,X,Y,S,B,Z,I,M,F,L,T,E OR HELP :
rmsk>e

```

lass2 37 %

7.2 grund

This program writes a standard mask file containing a pattern of the addresses of cells to be excluded from analysis by *rnls* etc., and the anisotropic analysis programs.

The elimination is achieved by examining a nominally flat spectrum (or sum of spectra) and excluding all cells with contents outside certain limits supplied by the user. When the upper and lower limits are proposed by the user the program responds by typing the number of cells which would be deleted. If this number seems reasonable then the user can terminate by writing the file, otherwise he can repeat the examination with another set of limits.

1. The program adds specified runs together cell by cell with weighting (dividing factor) given by the user. The default value is 1. This final spectrum can be printed out.

2. The program calculates the average intensity per cell for the whole spectrum (MEAN), and the difference, DIFF, the average of the absolute differences of cell values from the MEAN.

The results of this calculation are listed on the terminal as the proposed minimum and maximum limits for acceptable cells and the number of cells which would then be eliminated. These limits are $\text{MEAN} \pm \text{DIFF}$

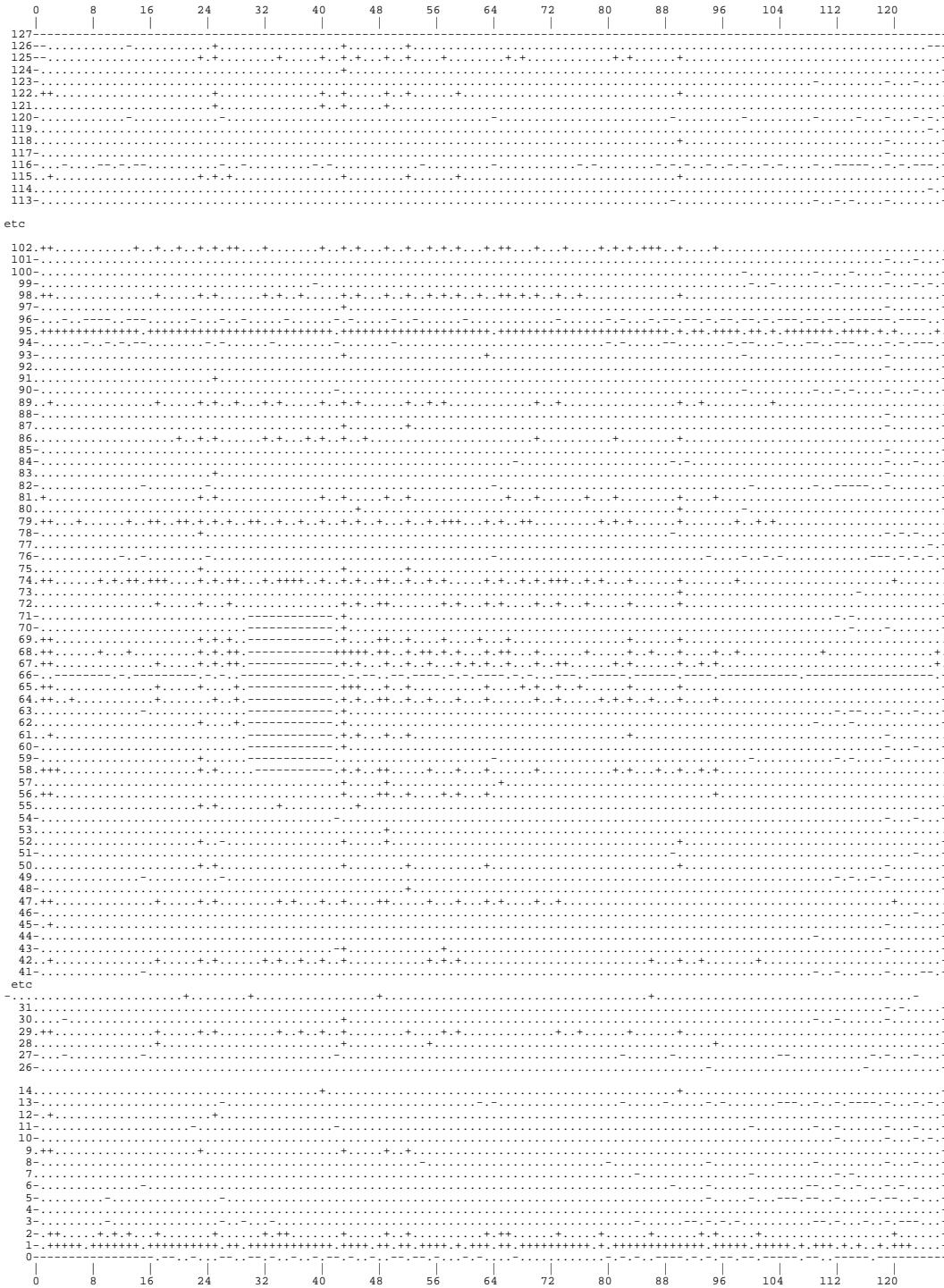
3. The user now sets limits thought reasonable, and sees how many cells are eliminated. When satisfied that only a reasonable number of cells are eliminated the program can be allowed to continue to create the file containing a suitable reference title and a character map of the deleted cells.

4. The user is requested to give a title and a five character name masky to identify the output file (masky.msk). A summary picture of the detector can be written to a listing file. If required a detailed listing may be output containing the values in the eliminated cells.

terminal dialogue

```
lass2 46% grund
GRUND - version 4.2  September 1998 (R. E. Ghosh)
Creates mask by scanning input data with upper and lower limit
RUNS to be added together - sequence ends with a zero run number
RUN NUMBER...EXT...DIVIDER ?
9326
RUN NUMBER...EXT...DIVIDER ?
Average: 679.82495
Proposal
Lower limit: 620.20813 Upper limit: 739.44177
GIVE LOWER AND UPPER LIMITS : 580 800
1902 CELLS KILLED:
Type
L   to set new Limits
D   to display summary of current mask
P   to print all in detail (pages...)
R   to read in a new set of data
F   to write out file of current mask
S   to print display summary
E   to exit
d
```

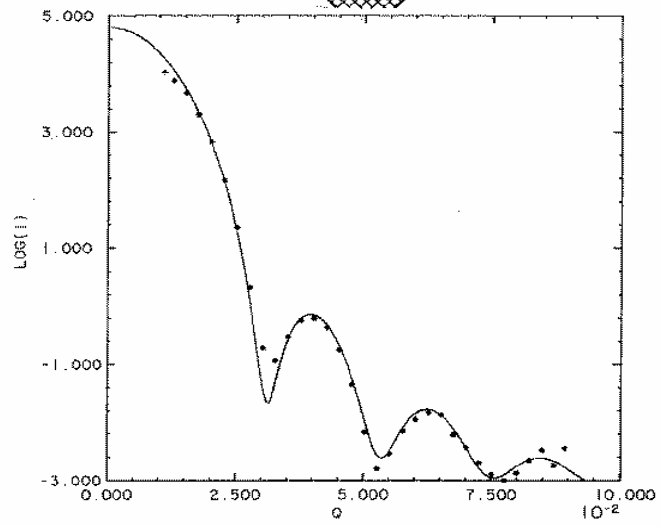
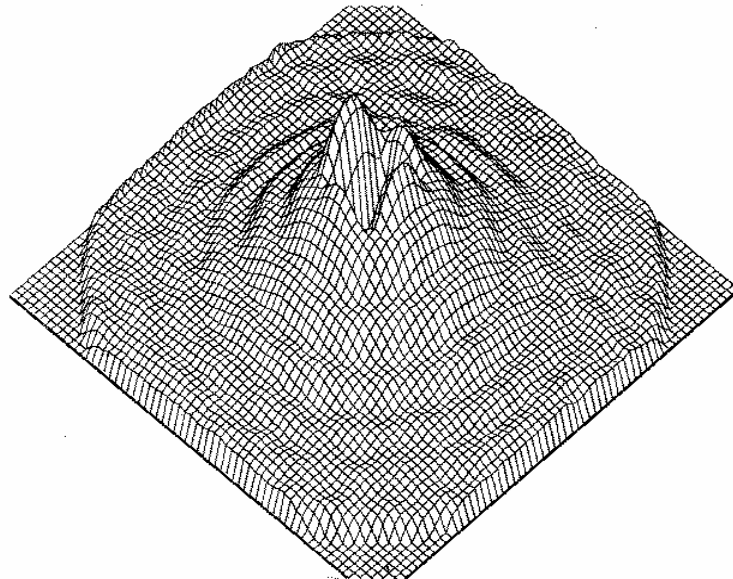
This five minute water run picks out that there are some noisy lines and non-uniformity at the edge of the detector.

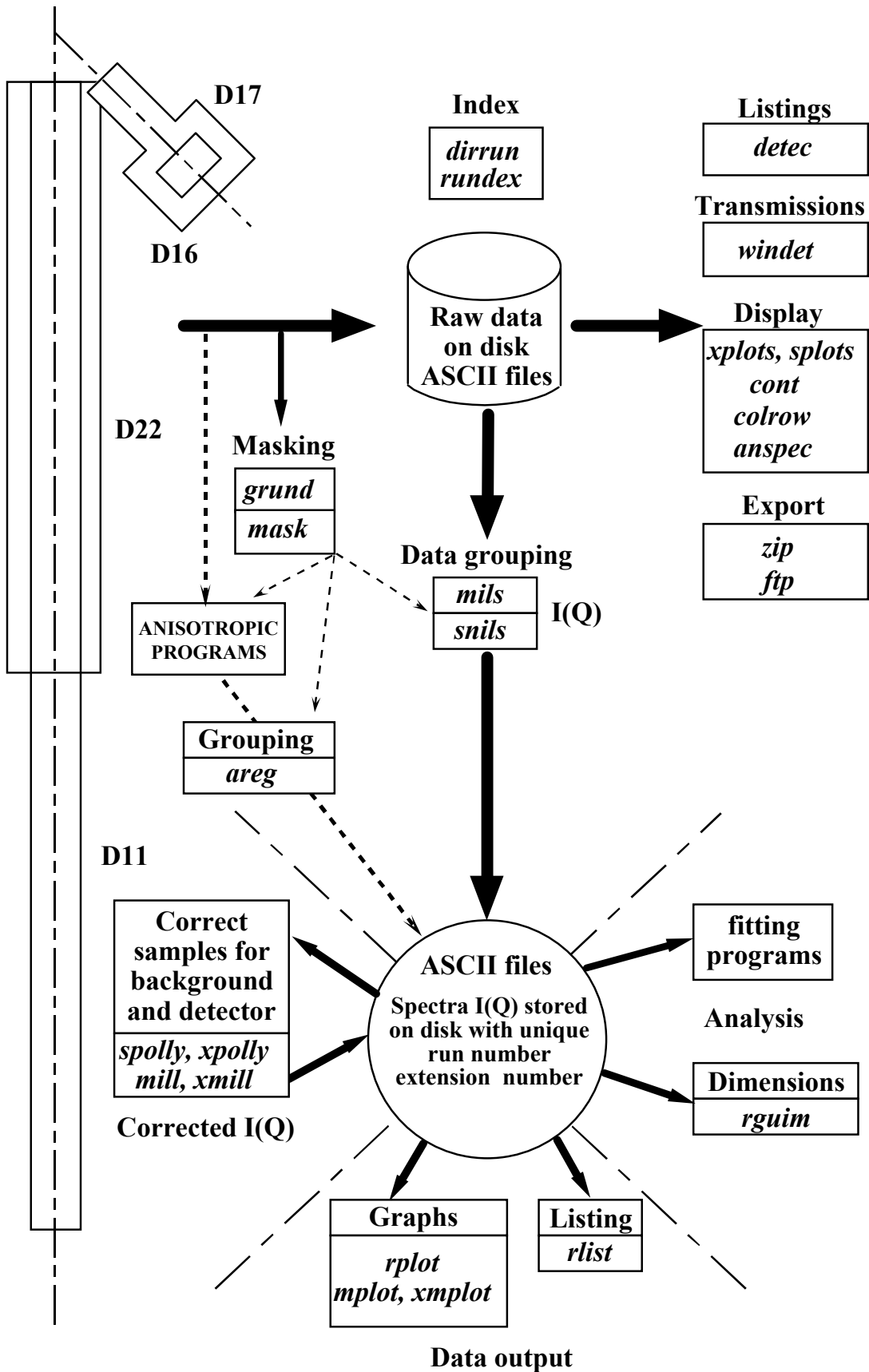


0 ----- DETECTOR VIEWED FROM SAMPLE ----->127
 LIMITS 580. <....< 800.

```
Type
  L   to set new Limits
  D   to display summary of current mask
  P   to print all in detail (pages...)
  R   to read in a new set of data
  F   to write out file of current mask
  S   to print display summary
  E   to exit
f
Give title for mask file (20 chars. max) :
3m 8A May 98
Give output mask file name (5 chars. e.g. mask1)
grund
File recorded : grund.msk
Title : 3m 8A May 98      1-Jul-1998 14:48:37
Type
  L   to set new Limits
  D   to display summary of current mask
  P   to print all in detail (pages...)
  R   to read in a new set of data
  F   to write out file of current mask
  S   to print display summary
  E   to exit
e
lass2 47%
```

TREATMENT OF RADIAL DISTRIBUTION FUNCTIONS





Treatment of radial distribution functions

8

8.1 Regrouped data files

Spectra are stored in individual files with names generated from the principal sample component and an extension version number which is unique. Details of the format are given in appendix 2. There too is given a description of the standard routines for reading and writing data, with instructions on how to invoke them.

For a principal run number nnnnnn filenames have the form

gnnnnnn.eee

where eee will be a unique extension number which starts at 000, and is incremented and checked for uniqueness before a treated data file is written back. The data files contain some history relating to their origins, and subcomponents, and retain the principal experimental parameters in text form. The last part of the file is a three column listing of Q, S, and error in S. The data may also be written out as an XML text file (see the environmental variable SAS_EXTRA_G page 39). A four column output is written including an estimate of the Q resolution. This offers an easier merging with data from other instruments in the future as this standard is adopted. The file names generated are of the form xgnnnnnn_eee.xml

Chapter 13 describes some utility programs to import SAS data measured elsewhere and written in one of a number of formats and convert them for treatment as data from the ILL.

Use by several users simultaneously

The unique version numbers and output listing and graphics files minimise the conflicts due to several simultaneous workers. The normal logon procedure does allow several members to have their own filespace, and it is also useful to use separate sub-directories (`% mkdir ... ; cd ...` see page 38) for separate projects. This keeps all listing and graphics files together with the treated data. Often users are recommended to restart and treat all data systematically after the end of the experiment; when performed in a separate subdirectory this creates a set of files which are more likely to be easier to identify and exploit than work performed under the pressure of the measurements. In general many programs retain parameters from their last use. Some care is required if two users find that they have conflicting needs but are sharing the same directory; in this case a new sub-directory should be created, and any common data files can be copied to this before each continues with their personal set of files.

8.2 radial averaging

rnls

This program produces a radial distribution function $I(Q)$ from a whole or a part of the multidetector spectrum. Using the beam centre definitions described in section 4, cells are allocated to a specific Q value and when this has been performed for all, each set is taken in turn and the actual Q value is calculated, together with the "radius" at which the beam of that Q value would fall on the plane normal to the beam-centre-line.

On reading each spectrum the content of each cell is distributed according to the above pre-allocation of the centre of the cell, and the average intensity is output as $I(Q)$. The average intensity in the region about the beam centre, limited to the region $\pm dx$, and $\pm dy$ cm, is calculated (ISUM), which may be used as a simple check for transmissions.

The radius, average Q , the number of cells within the Q step, and the number of cells actually used after any elimination by masking are written to the output file `rnlsijk.lis`. These are followed by the value of $I(Q)$ and the error $I_{er}(Q) = \sqrt{\text{total counts}/(\text{number of cells})}$. Values of Q , $I(Q)$, and $I_{er}(Q)$ are written into the regrouped data file and are identified by the name containing a run and extension number `gnnnnnn.eee`. If the run and extension number are not unique the extension number is incremented until the combination is so.

1. The current experimental parameters are tabulated. These may be modified by giving the parameter number and a new value. A parameter number of 0 (RETURN) allows the program to progress. The 4 or 16k option requires that the user specifies in advance whether data are expected to be 64x64 or 128x128 pixel images respectively.

The parameters are retained on disk, and will appear in the modified form when the program is next run.

2. The user is asked whether he wants to mask the detector. If the answer is Y (yes), the name of the mask file must be given (up to 5 letters). The mask file is read and the internal title is displayed for a check. If all is well the user can continue and add in a similar fashion other masks, and finally continue to process the data.

3. A selection of parameters stored with the raw data can then be set to be printed with each run treated.

4. The sequence of run numbers is then given, together with a proposed extension number. The latter is normally zero but it is sometimes useful to restart a treatment with all initial extension numbers set to the same integer. During the subsequent retreatment all the extension numbers will then be well ordered.

5. The program runs through the range of raw data and performs the regrouping and saves the regrouped data in standard regrouped files. At the end of the sequence additional runs may be treated, and there is an option to re-use the same regrouping parameters as before.

terminal dialogue

```

% rnils

RNILS - version 6.7 June '06 (R.E. Ghosh)

  1 Detector0 deg.      0.0000      2 x0 address      31.5000
  3 y0 address      31.5000      4 Radial step cms.  1.0000
  5 Sample-detect m.  3.0000      6 Wavelength a     10.0000
  7 Collimation m.   5.0000      8 Concentration     1.0000
  9 isum dx cms.    2.0000     10 isum dy cms.    2.0000
 11 4 or 16k        4.0000

To modify give parameter number and value
to relist type -1 to continue type return

Parameter... value : 2 62.7
Parameter... value : 3 63.7
Parameter... value : 5 10
Parameter... value : 6 8
Parameter... value : 7 11.2
Parameter... value : 11 16
Parameter... value : -1

  1 Detector0 deg.      0.0000      2 x0 address      62.7000
  3 y0 address      63.7000      4 Radial step cms.  1.0000
  5 Sample-detect m.  10.0000     6 Wavelength a     8.0000
  7 Collimation m.   11.2000     8 Concentration     1.0000
  9 isum dx cms.    2.0000     10 isum dy cms.    2.0000
 11 4 or 16k        16.0000

To modify give parameter number and value
to relist type -1 to continue type return

Parameter... value :

Delete cells listed in mask file ? (Y) : y

Give filename (e.g. grund or mask) : cedge

Mask information: April 98 D22          17-Nov-2006  9:32:39
for spectrum size 128 x 128
Type:
    S to stop
    A to read another mask file
    carriage return to continue
Option :

    5 experimental parameters are set for printing
Select experimental parameters for listing output

Type A,D,S,Help, or RETURN when selection is complete :
    5 parameters selected for printing
FIRST RUN...LAST RUN...EXTENSION : 9340 9347

RUN 9340 FOUND
% No warning will now be given if grouping parameters differ from input
data
  recorded g009340.000
RUN 9341 FOUND recorded g009341.000
RUN 9342 FOUND recorded g009342.000
RUN 9343 FOUND recorded g009343.000
RUN 9344 FOUND recorded g009344.000
RUN 9345 FOUND recorded g009345.000
RUN 9346 FOUND recorded g009346.000
RUN 9347 FOUND recorded g009347.000
ANOTHER SET OF DATA (Y) : n
Closing listing file rnls001.lis
%

```


snils

This program is for use on the small angle instruments when there may be spurious counting differing from run to run. The data within each set of successive annuli are compared for approximately consistent values, and outliers are rejected in a simple iterative procedure. The program will list summary maps of eliminated data. The terminal dialogue follows closely that of *rnils*. Because the cells used might differ from one set of data to another the results are less objective than formally masking data, but masking may become impracticable when, occasionally, sporadic miscounting occurs. The program also evaluates the deviation between the contributing pixels in each annulus. This gives notably different results from the deviation of the sum of counts if there is anisotropic scattering.

Regrouping for D16

The output from these programs match the standard SANS data files, and can be viewed and treated as such. Users should be aware of the different formalisms involved in treating data beyond the small angle regime which is assumed throughout this suite of programs.

rnd16, rnd16s

These programs treat data for the D16 multi-detector diffractometer in a similar way to *rnils*. The dialogue is very similar, and the results are stored in files with identical characteristics to the small angle cameras.

rnd16s in addition allows a raw or treated 2D dataset to be used for detector normalisation before the regrouped data are stored.

red16

This program is primarily intended to regroup 2D data from D16 diffraction experiments when the detector is scanned about the sample in small steps. One output option includes writing data in the same format as the SANS suite, and consequently these may be compared directly with SANS measurements, though the regrouping algorithm produces data with a uniform angle increments.

8.3 Normalisation and background subtraction

Several programs are available to perform simple arithmetic on the component spectra to obtain the corrected cross-section. They are stylised to help less experienced users perform their work systematically. In more complex problems the programs may also be used in a more elementary fashion to perform a personally designed treatment scheme.

spolly

This program corrects the sample spectrum $I(Q)$ by combining individual spectra or sets of similar spectra, and outputs the result back into a resultant regrouped data file, from which it may be plotted, and further analysed.

The following spectra or sets of spectra, normalised to the same monitor count are taken :

C cadmium run (neutron + electronic background), or run with beam closed ("electronic" background) $\delta C = \text{ERR}(C)$

V vanadium run, $\delta V = \text{ERR}(V)$

VB vanadium background run, $\delta VB = \text{ERR}(VB)$

S sample run, $\delta S = \text{ERR}(S)$

SB sample background run, $\delta SB = \text{ERR}(SB)$

the following calculations are performed for each Q

$$V_f = V - C - A_1 \times (VB - C) \quad (8.1)$$

$$\delta V_f = \delta V + \delta C \times (1 - A_1) + A_1 \times \delta VB \quad (8.2)$$

$$S_f = S - C - A_2 \times (SB - C) \quad (8.3)$$

$$\delta S_f = \delta S + C \times (1 - A_2) + A_2 \times \delta SB \quad (8.4)$$

A_1 and A_2 are given by the user and in the normal case refer to the absorption (and hence attenuation) of the background scattering by the sample. These attenuation factors are obtained from the essential transmission measurements. The factors could also provide for correcting other variations between the sample and background runs. The program then normalises the corrected sample scattering to corrected vanadium scattering for each Q value giving the cross-section $I(Q)$.

$$I = \frac{S_f}{V_f} \cdot \frac{A_3}{A_4} - A_5 \quad (8.5)$$

$$\delta I = I \sqrt{\left(\frac{\delta V_f}{V_f}\right)^2 + \left(\frac{\delta S_f}{S_f}\right)^2} \quad (8.6)$$

A_3 and A_4 are given by the user and normally refer to the vanadium and sample cross sections. They will include two effects:

(a) The coherent scattering from the sample will be reduced by self-absorption (self-shielding), so A_4 corrects for this and contains $e^{-\Sigma d}$, where Σ is the macroscopic total cross section of the sample, and d the sample thickness. For vanadium, the incoherent scattering is isotropic, and it is only necessary to consider the losses due to the absorption cross-section (which is dominant at long wavelengths), see 2.5. In the case of a water standard the cross-section factor is usually determined experimentally for a given instrument and wavelength, since the measured water level cross-section is a function of detecting the complex scattering processes shown on page 11.

(b) For absolute Scattering Law results $S(Q)$, the cross-section term

$$(d\Sigma_{\text{scattering}} / d\Omega) \cdot d$$

must be removed. Thus for example A_3 and A_4 might be:

$$A_i = \left(d\Sigma_{\text{scattering}}^i / d\Omega \right) d_i e^{-\sum_{\text{total}}^i d_i} \quad (8.7)$$

The term A_5 is subtracted from the corrected intensity and represents a Q independent intensity (e.g. incoherent scattering) which accompanies the coherent small-angle signal. In some measurements where there has been considerable incoherent scattering for the background measurement this must be taken into account in a separate fashion (Horkay et al, 1991), though there remains a problem of assessing what fraction of incoherently scattered neutrons are not counted due to inelastic effects and subsequent losses due to low-efficiency detection.

It is often useful to prepare a table of parameters and run numbers for input to *spolly/xpolly* before treating the data. Mistakes can then be checked against the intended input. The file *sans.term* containing transmission information from *windet* (p 44) can help in preparing this table.

Input: regrouped data files created by *rnils*, *areg*, etc.

Output: standard regrouped data files for subsequent plotting, etc., and also a line-printer listing of "radius", theta (full scattering angle), Q , Q^2 , Q^{-4} , I , dI , IQ^2 , Concent./I , $\text{Log}_e(I)$, $\text{Log}_e(QI)$, S' , B' , where $S' = (S - C)$ and $B' = A_2(SB - C)$.

The program assumes there will only be one set of each of the cadmium, vanadium, and vanadium background runs followed by the series of associated sets of background and sample runs. The intensities used are the sum of the individual runs in the set divided by the sum of the preset values. No interpolation between Q values is attempted; the values stored are the average values from the set of sample runs.

The default values for the extension number and the monitor preset are 0 and 1.0 respectively.

At any stage a negative run number will stop the program

A summary of the runs and factors used is always written to the output listing file, and included in the final output file. If requested a full table of calculated values including Q^2 , Concentration/I(Q), etc can be given on the screen or in the listing file. *rlist* can reconstruct a similar listing from the regrouped data files.

The monitor values are taken from the data files, and it is usual to prescale these large values by 100000 for later use. If prescaling would lead to a very small value then this is not done. Hence treated data, with unit monitors remain unchanged. The actual monitor for use is always shown.

1. The program asks for the cadmium run numbers, extension and preset (each spectrum will be divided by its own preset). A zero run number indicates that the set is complete or absent.
2. The program requests the vanadium run numbers, extension, and preset. A zero run number indicates that the set is complete or absent.
3. If a vanadium run number was given, the information for the vanadium background set is now sought. A zero run number indicates that the set is complete or absent.
4. The user then gives the background correction factor for vanadium absorption (A_1), and the total cross-section of the vanadium (A_3). Defaults are both one.
5. The sequence of samples and backgrounds now begins with a request for the background run numbers, extension, and preset. A zero run number indicates that the set is complete or absent.
6. The sample run numbers are then sought. As before the set of sample runs is terminated by a zero run number. If the initial run number of a set is set to zero the program returns to (5) and asks for a new set of background runs.
7. The user then gives the background factor for the sample absorption (A_2) followed then by the sample "total cross-section" (A_4), the concentration, and a flat background (this value representing an incoherent cross section): default values 1,1, and 0 respectively.
8. The user may then modify a proposed reference title, which is taken from the experiment recording, and the treatment is performed and the output written.
9. A new set of sample run numbers, extension, and preset is sought to be treated with the same background and vanadium data, proceeding as from (6).

Terminal dialogue

This example is from a preliminary look at runs measured quickly (100 seconds) to test samples

```
% spolly
SPOLLY - Version 6.7 June 2003 (R Ghosh)

Table output 0:none 1:Local terminal 2:Printer file
spol>2
Prescale stored monitor by 100000: give new divider
else give <RETURN> :
spol>
CADMIUM/ELECTRONIC BACKGROUND runs:
Run number...Ext
spol>9340
Title : Cd - Bgd                stored monitor  0.22305E+07
Using scaled monitor preset    22.305
Type <RETURN> or give new value:
```

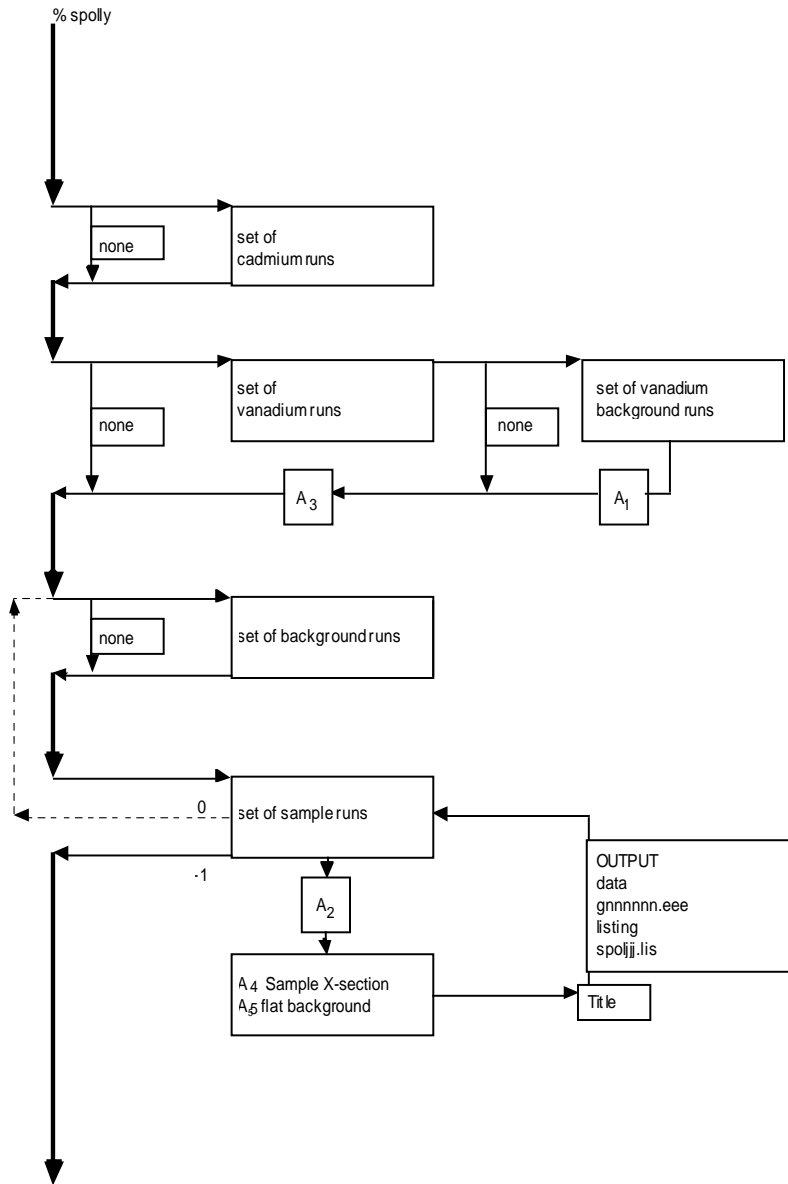
```
spol>
Run number...Ext
spol>
VANADIUM SAMPLE runs:
Run number...Ext
spol>9342
Title : H2O 1mm          stored monitor  0.22296E+07
Using scaled monitor preset  22.296
Type <RETURN> or give new value:
spol>
Run number...Ext
spol>
VANADIUM BACKGROUND runs
Run number...Ext
spol>9343
Title : Empty Qtz Cell   stored monitor  0.22292E+07
Using scaled monitor preset  22.292
Type <RETURN> or give new value:
spol>
Run number...Ext
spol>
Background correction factor for van. absorption (A1)
spol>0.487
Total cross-section of vanadium (A3)
spol>0.0438
SAMPLE-BACKGROUND runs
Run number...Ext
spol>9345
Title : D2O 2mm          stored monitor  0.22299E+07
Using scaled monitor preset  22.299
Type <RETURN> or give new value:
spol>
Run number...Ext
spol>
SAMPLE run numbers
Run number...Ext
spol>9346
Title : 7D1 2mm          stored monitor  0.22296E+07
Using scaled monitor preset  22.296
Type <RETURN> or give new value:
spol>
Run number...Ext
spol>
Background correction factor for sample absorption (A2)
spol>.927
Sample total crosssection (A4)...Concentration...Flat background (A5)
spol>.1636
Default title is : 7D1 2mm
Type return to use this or give new title (20 characters) :
spol>

Saved as file g009346.001  run   9346  ext.  1

SAMPLE run numbers
Run number...Ext
spol>9347
Title : 7D2 2mm          stored monitor  0.22294E+07
Using scaled monitor preset  22.294
Type <RETURN> or give new value:
spol>
Run number...Ext
spol>
Background correction factor for sample absorption (A2)
spol>0.966
Sample total crosssection...Concentration...Flat background
spol>.1706
Default title is : 7D2 2mm
Type return to use this or give new title (20 characters) :
spol>

Saved as file g009347.001  run   9347  ext.  1

SAMPLE run numbers
Run number...Ext
spol>-1
closing listing file spol002.lis
```



% more spoljij.lis

:

% pri spoljij.lis

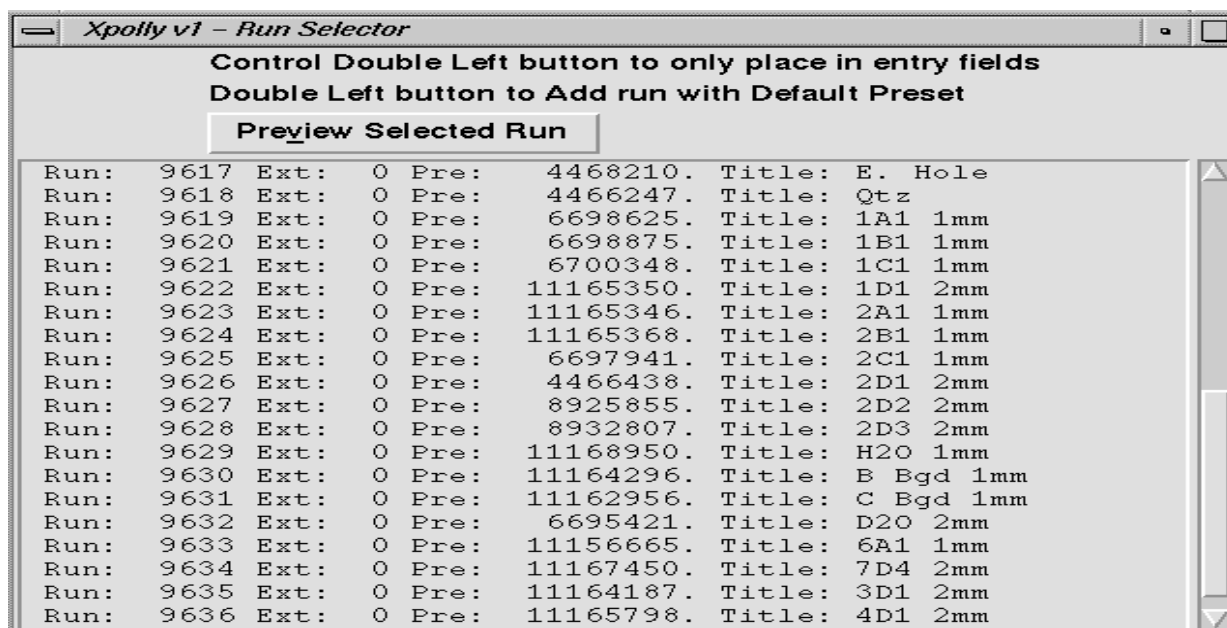
mpolly

When a sequence of measurements is performed, and the transmission of the sample is not changing significantly, mpolly allows such a set to be treated with the same parameters A_1 to A_5 . The first and last run numbers identifying the set are entered for the sample with a single extension number and a stepping factor for the generated sequence. A proposed output extension can be given and an identifying sequence number is added in the short title, the latter is incremented for each spectrum treated. The *Clickfit* GUI (p109) simplifies fitting these sequences of measurements.

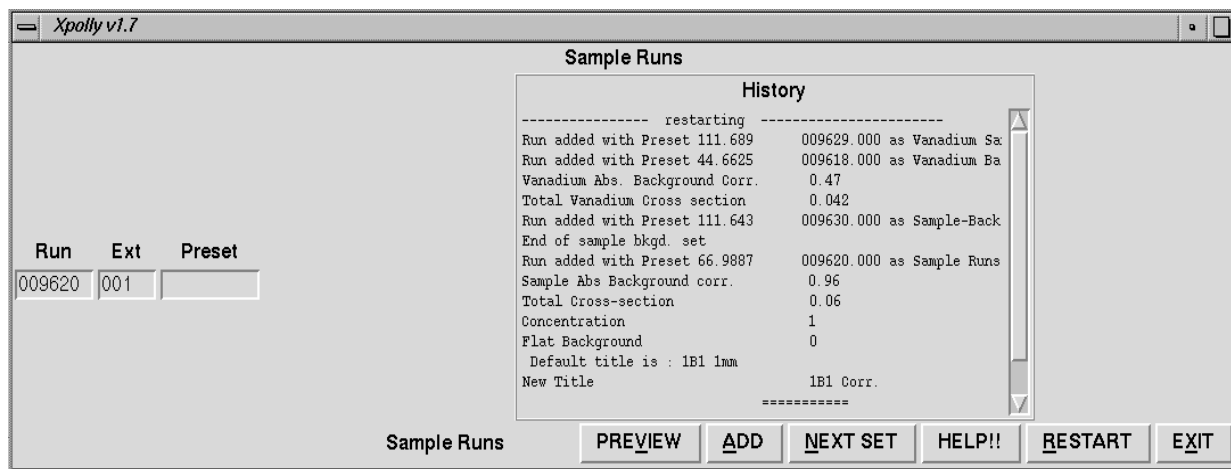
xpolly

This is a tk/tcl program which presents the spolly program with a graphical user interface. Additional facilities include the possibility of previewing the component spectra, and the resultant. In addition to standard listings a summary of the xpolly input is appended to the history file xpolly.his

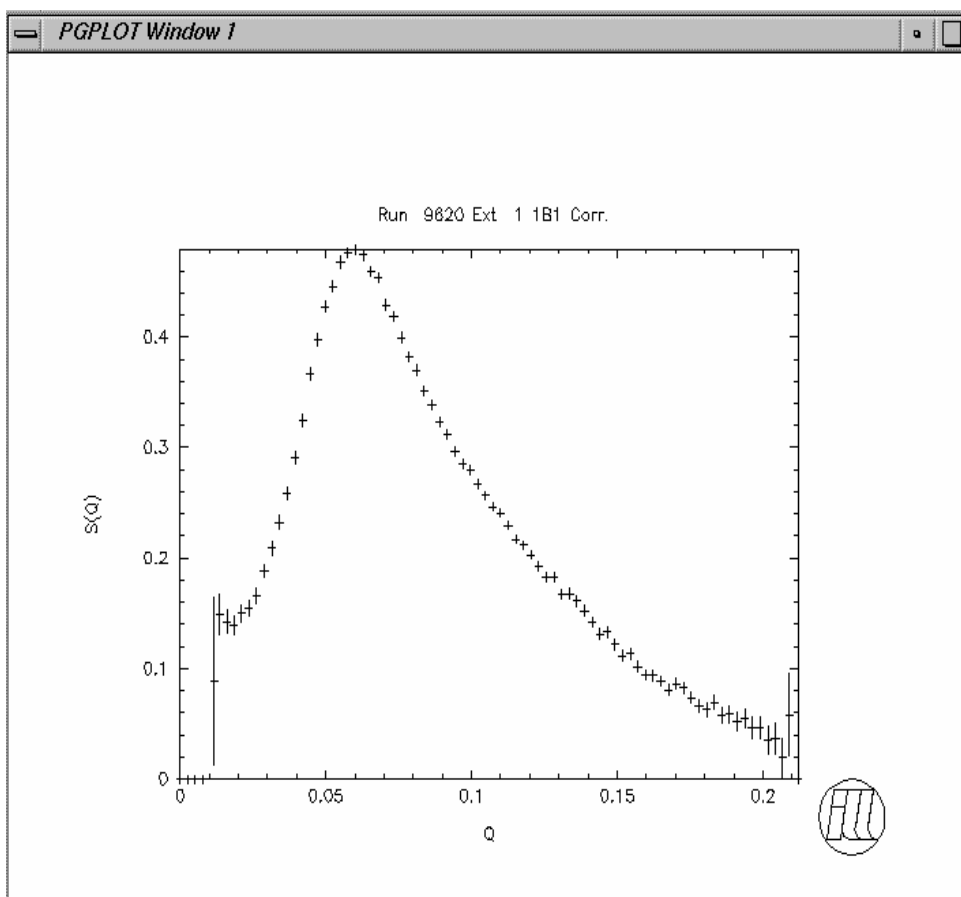
When the program is run, the known regrouped data files are shown in a scrolling box. Double clicking on the selected data enters the run number, extension and preset in the appropriate fields. The NEXT SET button requests the next operation. The corrected data are then displayed.



xpolly - the run selector window



xpolly - main window



xpolly - final results displayed

xmill, mill

These provide simple arithmetic means for treating either regrouped (1D) or two dimensional SANS data especially where a sequence of sample runs has been measured. The significance of the pre-multiplying factors is left to the user. The result is calculated according to the equation shown.

The terminal version is *mill*. It was written in Fortran to perform the calculation for *xmill* a tcl/tk graphical version using the standard library components for accessing either 1D or 2D data.

The sequence of operations for both versions is similar.

Initially the type of treatment must be chosen (1D or 2D). Then the various fields in the equation are filled in. In the case of the graphical version the completion of a set of run/extension and multiplier values for the background or divider is signalled by clicking on the button beside the element name. The program then fetches that component. Finally the sequence of sample runs is set up and the "calculate result" is activated to treat the desired range. The results are displayed in a simple manner by double clicking on the results run and extension numbers. Individual components can also be previewed in *xmill* by entering the run and extension number in the preview box and clicking "preview".

Subsequently the *Clickfit* GUI (p108) simplifies fitting these sequences of measurements.

Terminal dialogue

```
% mill
MILL version 2.2 October 1998 R. Ghosh
Equation for MILL
          Result = m * ( S-(B1*b1+B2*b2+B3*b3+B4*b4))/D*d )
Input data are normalised by a prescaled monitor
B no.(1-4) run ext mul   Background run(s)
D run ext mul           Dividing run details
M mul                   Scaling multiplier
S run [ext] [last] [step] Sample run sequence details
C 1 or 2                Change Dimensions (default 1D)
Z                        Reset
H                        Display this Menu
V                        Verify current settings
E                        Exit

Set to treat regrouped data at present

Option B,D,M,S,C,Z,E,H> b 1 9375 0 .95
Option B,D,M,S,C,Z,E,H> m 2.43
Option B,D,M,S,C,Z,E,H> s 9376 0 9377
Result is in 9376 / 1
Result is in 9377 / 1
Option B,D,M,S,C,Z,E,H> e
% exiting !
Closing listing file mill011.lis
% end !
```

XMILL for 2-D

$$\bar{R} = m * \left\{ \frac{\bar{S} - (\bar{B}_1 * b_1 + \bar{B}_2 * b_2 + \bar{B}_3 * b_3 + \bar{B}_4 * b_4)}{\bar{D} * d} \right\}$$

◆ Regrouped Data '1-D' ◆ Ungrouped data '2-D'

Background Runs

<input checked="" type="checkbox"/> B1 Run No.	<input type="text" value="3112"/>	Ext <input type="text" value="0"/>	Mul b1	<input type="text" value="0.5"/>
<input type="checkbox"/> B2 Run No.	<input type="text" value="unused"/>	Ext <input type="text" value="0"/>	Mul b2	<input type="text" value="1.0"/>
<input type="checkbox"/> B3 Run No.	<input type="text" value="unused"/>	Ext <input type="text" value="0"/>	Mul b3	<input type="text" value="1.0"/>
<input type="checkbox"/> B4 Run No.	<input type="text" value="unused"/>	Ext <input type="text" value="0"/>	Mul b4	<input type="text" value="1.0"/>

Divider Run

<input checked="" type="checkbox"/> D Run No.	<input type="text" value="3114"/>	Ext <input type="text" value="0"/>	Mul d	<input type="text" value="1.4"/>
---	-----------------------------------	------------------------------------	-------	----------------------------------

Sequence of Sample Runs S

First Run No.	<input type="text" value="3118"/>	Ext <input type="text" value="0"/>	Mul m	<input type="text" value="1.0"/>
Last Run No.	<input type="text" value="3120"/>	Step	<input type="text" value="1"/>	

Run No. Ext

Results

Double click to view

3118 /1
3119 /1
3120 /1

xmill - main window

8.4 Simple linear fits

rguim

This program attempts to fit a straight line to any spectrum stored in the standard regrouped data files. Five different functions of intensity versus Q^2 may be fitted within a certain Q range which may be adjusted by the user to optimise the region of Q for which the model may be appropriate. The functions chosen relate to the limiting forms of the scattering function for a number of simple models. From the intercepts and slopes of the fitted line it is possible to derive the radius of gyration of the scattering particles, and these values are also displayed.

Guiner and Fournet (1955, chapter 4) describe models, also giving ranges for the range of QR_G where they are valid, and reasons for deviation from straight lines. Today it is easy to fit the full scattering curve, q.v. *polymer* however *rguim* is frequently used during measurements to follow experiments.

Resolution effects reduce the value of $I(0)$, and the apparent radius of gyration is smaller than the true value (Cotton, 1974). Ullman (1983,1985) describes corrections which take account of measurements at non-optimum values of QR_G , and the second reference deals with corrections which account for several common polydispersity distributions.

A linear plot option of $I(Q)$ versus Q is included to help estimate flat (incoherent) backgrounds.

1. The program prompts for the run number, extension and function option and seeks the data. A zero run number stops the program.
2. On finding the data the concentration, C , is written out, and this value may be altered.
3. The scale limits for the fitting and plotting are now requested, RMIN and RMAX. To simplify the input these values requested are the "radii" described earlier (cm) at the detector normal to the incident direct beam, (section 4.5.2), hence typically two digit values, rather than derived Q values. This helps the experimenter relate to the problems of resolution effects at small radii.

If fewer than two fittable points are found in the desired fitting range a message is written and the request for the new range output. In general zero values for the plotting range lead to the limits either being kept as before or suitably expanded to include any changed fitting range.

Fixed Scale Limits

If RMIN for the fit is set to -3 then the user is prompted to give his own scale limits. Once set these are retained until a model option is changed, allowing a number of spectra to be compared on identical scales. To reset the scales to include all within the plotting range again set RMIN to -3, and when prompted for the new fixed scale limits set all to zero (give a RETURN).

Choosing Another Spectrum

If RMIN for the fit is set to -1 the program returns to (1). The fit type option is remembered, and does not have to be re-entered unless it is to be changed. The values for fitting and plotting too are retained, even on changing this option,

allowing two models to be rapidly compared within the same fitting ranges.

Termination

If RMIN for the fit is set to -2 the program terminates.

4. When the fit has been made and the graphs drawn, the values for the radius of gyration and the error are typed. The user is then asked whether he wants hardcopy output; by default this is a PostScript file (see 5.5).

5. The user can then change the region of the fit, and/or the plotting and so optimise the fit to the region of the spectrum which is actually a straight line. The product QR_G is also shown to indicate when the fit is limited to the region where the model approximations are valid.

Terminal dialogue

```
lass1 55% rguim

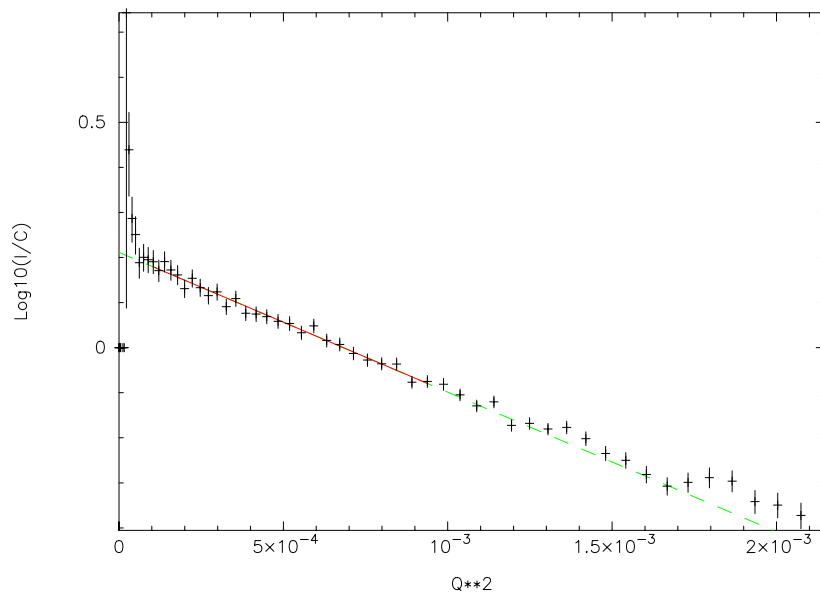
RGUIM - Version 5.9  June 1998 (R.E. Ghosh)

Zero run number stops program
rmin=-1 returns for another spectrum
rmin=-2 stops program
rmin=-3 allows scales to be fixed
Options:
 1 C/I          versus Q**2   Zimm
 2 C/I**0.5     versus Q**2   Debye
 3 Log10(I/C)   versus Q**2   Guinier
 4 Log10(I*Q)   versus Q**2   Thin rods
 5 Log10(IQ**2) versus Q**2   Sheets
 6 I(Q)         versus Q     Incoherent

Run number...Ext.no...Option :
guim>9347 1 3
Concentration = 1.00
New value :
guim>
Fit: rmin..rmax Plot: rmin..rmax :
guim>12 40 0 60
Hardcopy (Y/N) [N] :
guim>y
Fit: rmin..rmax Plot: rmin..rmax :
guim>-2
%PGPLOT, Closing file guim004.ps
```

$y=mx+c$: $m= -310.1$ $dm= 11.$ $c= 0.2115$ $dc= 0.48E-02$
 $0.10E-01 < Q < 0.31E-01$ $0.47 < QR < 1.42$ $0.0 < PLOT < 60.0$
Radius of Gyration = 46.29 error = 0.79 $13.0 < FITR < 39.0$
Intensity/Conc.(Q=0) = 1.628 error = 0.18E-01
Concentration= 1.00 Distance S-D=10.000 M. Wavelength= 8.00 A.

9347/ 1 7D2 2mm RG= 46.29 0.47<QR< 1.42



rguim - Micelles of non-ionic polymeric surfactants can be large. In this example R_g is 46\AA and the range of a Guinier fit has been taken from $0.5 < QR_g < 1.4$ (!)

8.6 Plotting results

rplot

SANS results often result from the subtraction of curves of similar shape; detection of errors in treatment depends on the easy and quantitative comparison of components by quick inspection.

rplot is a general plotting program which will plot functions of intensity and Q , and allow two curves to be compared, showing error bars only for the first curve, to avoid confusion of data which often have identical Q values.

A dialogue is initiated on starting the program which enables a function of the intensity $I(Q)$ to be plotted as a function of Q .

1. The program prompts for the run number, the extension number and the plotting option, and seeks the data. A zero run number stops the program; once given the same plotting option is re-used unless an alternative request is made.
2. On finding the data the concentration value, *CON*, stored may be changed, and the intensity scaled by a dividing factor if non-zero.
3. A second spectrum may also be plotted for comparison; if a second run is requested the user is prompted for the concentration and another scaling factor.
4. The scale limits *XMIN*, *XMAX*, *YMIN*, *YMAX* stored already in the program are printed out, followed by the limits for the recalled spectrum: the user is then prompted for new values. Replying with a carriage return retains all current limits. To modify only the X axis give *XMIN* and *XMAX*. To modify only the Y axis limits give 0 0 *YMIN* *YMAX*.
5. The graph is then plotted and the user is asked if he wants hardcopy output. By default this is set to a PostScript file (see 5.5).
6. There is also the possibility to replot the data with a change of scale, i.e. returning to 4.
7. In addition there is the option of typing and printing values of the points calculated.
8. The program then returns to 1 to plot another spectrum.

terminal dialogue

```

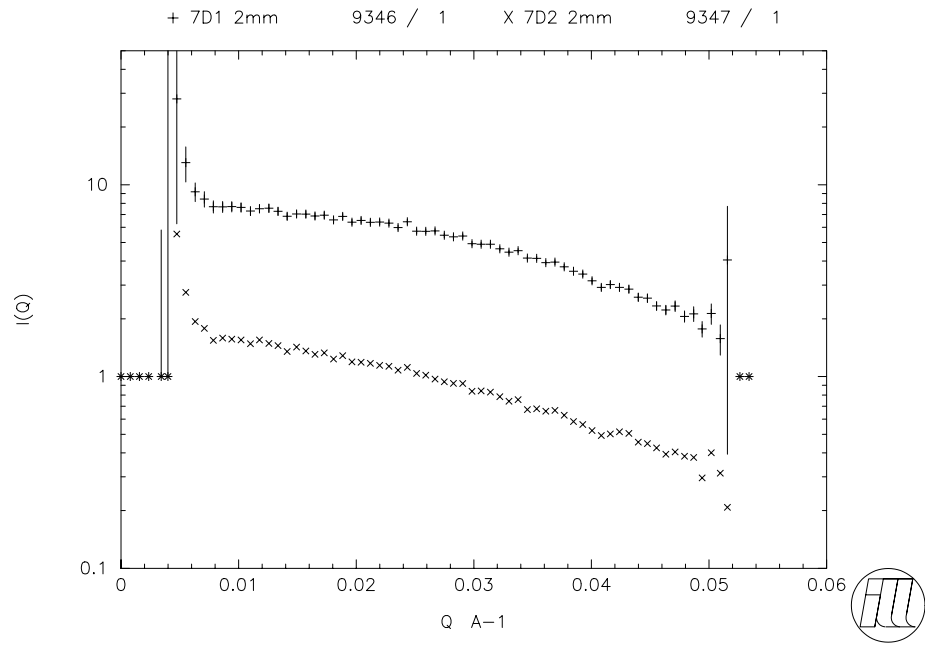
lass2 51% rplot
rplot - version 5.7 May 1997 (R.E. Ghosh)

A zero or negative first run number stops the program

set second run number to zero to treat one spectrum

Plotting options :
 1:I(Q)      versus Q
 2:Log(I)    versus Q
 3:Log(I)    versus Log(Q)
 4:Log(I)    versus Q**2
 5:CON/I     versus Q**2
 6:Log(IQ)   versus Q**2
 7:Log(IQ^2) versus Q**2
 8:IQ**4     versus Q**4
 9:I**A      versus Q**B
10:IQ**A     versus Q**B
11:Log(IQ^A) versus Q**B
12:Log(IQ^A) versus Log(Q**B)
13:IQ**4     versus Q
First run number...ext...option :
rplo>9346 1 2
Concentration = 1.000 divider = 1.000
new values (or 0 to retain old) :
rplo>
Second run number (or 0)...ext :
rplo>9347 1
Concentration = 1.000 divider = 1.000
new values (or 0 to retain old) :
rplo>
Current scale limits x =Q A-1 y =I(Q)
xmin = 0.000000E+00 xmax = 0.534071E-01
ymin = 0.207851 ymax = 28.0385
Spectrum values
xmin = 0.000000E+00 xmax = 0.534071E-01
ymin = 0.207851 ymax = 28.0385
New values: xmin...xmax :
rplo>0 .06
New values: ymin...ymax :
rplo>.1 50
Type r to replot, l to list, p for PostScript
return to continue
rplo>p
Type r to replot, l to list, p for PostScript
return to continue
rplo>
Plotting options :
 1:I(Q)      versus Q
 2:Log(I)    versus Q
 3:Log(I)    versus Log(Q)
 4:Log(I)    versus Q**2
 5:CON/I     versus Q**2
 6:Log(IQ)   versus Q**2
 7:Log(IQ^2) versus Q**2
 8:IQ**4     versus Q**4
 9:I**A      versus Q**B
10:IQ**A     versus Q**B
11:Log(IQ^A) versus Q**B
12:Log(IQ^A) versus Log(Q**B)
13:IQ**4     versus Q
First run number...ext...option :
rplo>-1
%PGPLOT, Closing file rplo005.ps
lass2 52%

```



mplot

This general plotting program superposes up to ten spectra on one graph, displaying this on a screen, and with options including output to files for hardcopy results.

Various functions of the intensity $I(Q)$ as functions of Q , the momentum transfer may be plotted with the same options as in RPLOT.

To simplify the picture error bars are not shown. In general the magnitude of errors is self-evident from the dispersion of the spectral values about an expected smooth scattering function.

The symbols used in the plot are:

Spectrum	#1	#2	#3	#4	#5	#6	#7	#8	#9	#10
	+	x	●	■	▲	*	◆	▼	☆	⊛

1. The program prompts for a sequence of run numbers, extension numbers and dividing scale factors. A zero run number ends the sequence.
2. The functional form for the graph is then requested.
3. The user is then presented with the choice of a number of commands.
 - P to plot the current data in the current mode
 - S to select another choice of functions of $I(Q)$ versus Q
 - W ro write the graphics to an output file (usually PostScript).
 - R to read in a fresh set of data
 - A to add other spectra (up to a grand total of ten) to those already present.
 - X to show current spectrum limits and allow modification of X scale
 - Y to show current spectrum limits and allow modification of Y scale
 - B to choose spectra to be shown with statistical error bars
 - C to turn on the cursor for the next plot
 - D to delete the cursor in the next plot
 - H to give a summary of options and commands
 - E to terminate the program

terminal dialogue

```

lassl 62% mplot
mplot - version 5.5 Jan '99 (R. E. Ghosh)

Superposes plots of SANS spectra

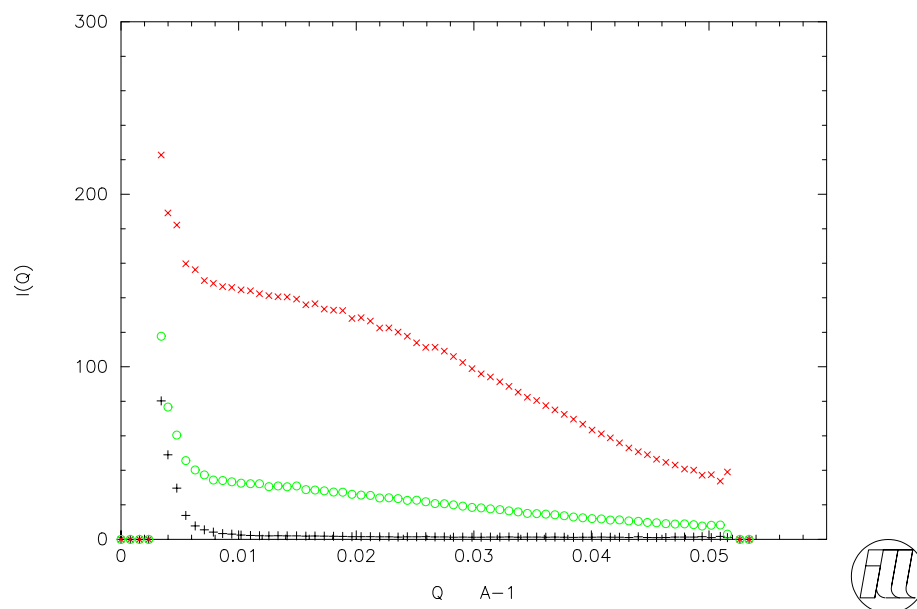
Plotting options:
      Y                X
  1    I(Q)           Q   A-1
  2    Log(I)         Q   A-1
  3    Log(I)         Log(Q)
  4    Log(I)         Q**2   A-2
  5    CON/I         Q**2   A-2
  6    Log(IQ)       Q**2   A-2
  7    Log(IQ^2)     Q**2   A-2
  8    IQ**4         Q**4   A-4
  9    I**A          Q**B
 10    IQ**A         Q**B
 11    Log(IQ^A)     Q**B
 12    Log(IQ^A)     Log(Q**B)
 13    IQ**4         Q   A-1

Command options:
  R    Read in data
  S    Select plotting option
  X    X plot limits
  Y    Y plot limits
  P    PLOT
  W    Write graphics to output file
  B    Bars for statistical errors
  A    Add more runs to set
  C    Cursor on next plot
  D    Delete cursor
  H    HELP (this text)
  E    Exit

Option R,S,X,Y,P,W,A,C,D,HELP or EXIT : r
Read in data, a zero run number ends sequence, -1 to stop
Run number...ext...divider : 9345
Spectrum D20 2mm      read in
Run number...ext...divider : 9346
Spectrum 7D1 2mm     read in
Run number...ext...divider : 9347
Spectrum 7D2 2mm     read in
Run number...ext...divider :
Option R,S,X,Y,P,W,A,C,D,HELP or EXIT : p
Option R,S,X,Y,P,W,A,C,D,HELP or EXIT : y
Y - scale I(Q)
  Spectra min. 0.0000E+00 max 222.7
  Plot min. 0.0000E+00 max 222.7
Type RETURN use values or give new values YMIN YMAX : 0 300
Option R,S,X,Y,P,W,A,C,D,HELP or EXIT : x
X - scale Q   A-1
  Spectra min. 0.0000E+00 max 0.5341E-01
  Plot min. 0.0000E+00 max 0.5341E-01
Type RETURN use values or give new values XMIN XMAX : 0 .06
Option R,S,X,Y,P,W,A,C,D,HELP or EXIT : p
Option R,S,X,Y,P,W,A,C,D,HELP or EXIT : w
Option R,S,X,Y,P,W,A,C,D,HELP or EXIT : e
%PGPLOT, Closing file mplr009.ps
lassl 63%

```

+ 9345/ 0 (1.000) D20 2mm x 9346/ 0 (1.000) 7D1 2mm
o 9347/ 0 (1.000) 7D2 2mm



The graphical results from mplot appear above. The sample here is a hydrogenous surfactant in D_2O at two concentrations. At the higher concentration, the curvature in the raw data at greater intensity shows clear evidence of different extent of aggregation. The raw data also show unusually high background around the beam stop, giving a sharp rise of intensity at small Q .

xmplot

This version of mplot offers the advantage of showing the regrouped data files and the short titles, simplifying selection and plotting sets and subsets. When "Print Plot" is selected the results are sent directly to the default graphical printer (section 5.3), without leaving the program.



xmplot - main window

Options x

Click on "Set x,y" to lock scale

Plotting Option Y vs X	Scale	LowerLimit	UpperLimit
<input checked="" type="radio"/> I(Q) vs Q A-1	X:	<input type="text" value="0.000"/>	<input type="text" value="0.25"/>
<input type="radio"/> Log(I) vs Q A-1	Y:	<input type="text" value="0.000"/>	<input type="text" value="60Q"/>
<input type="radio"/> Log(I) vs Log(Q)	<input type="button" value="Set X Y Limits"/>		<input type="button" value="Auto Scale"/>
<input type="radio"/> Log(I) vs Q**2 A-2	Factor		
<input type="radio"/> CON/I vs Q**2 A-2	A	<input type="text" value="1.00"/>	B <input type="text" value="1.00"/>
<input type="radio"/> Log(IQ) vs Q**2 A-2	<input type="text"/>		
<input type="radio"/> Log(IQ^2) vs Q**2 A-2	Error bars		
<input type="radio"/> IQ**4 vs Q**4 A-4	<input type="radio"/> none		
<input type="radio"/> I**A vs Q**B	<input type="radio"/> on last choice		
<input type="radio"/> IQ**A vs Q**B	<input checked="" type="radio"/> on all choices		
<input type="radio"/> Log(IQ^A) vs Q**B	<input type="button" value="Close"/>		
<input type="radio"/> Log(IQ^A) vs Log(Q**B)	<input type="button" value="Dismiss"/>		
<input type="radio"/> IQ**4 vs Q A-1			

xmplo - option window

8.7 UTILITY PROGRAMS

The regrouped data files are easy to read, but should not be edited as this may affect the expected internal structure. The programs here will list, and also perform some editing functions which may make the data more presentable for publication.

rlist

This program will access any spectrum in a standard regrouped data file and produce a tabulated listing similar to that of SPOLLY. Thus the table includes - "radius", theta (full scattering angle), Q , Q^2 , Q^{-4} , I , dI , IQ^2 , Concentration/ I , $\text{Log}_e(I)$, $\text{Log}_e(QI)$. The history is limited to the last five components.

1. The program asks for the initial spectrum number, extension number and a final spectrum number. Spectra within this range are printed out.
2. Another set may be printed
3. A zero initial run number stops the program.

terminal dialogue

```
lass1 61% rlist
rlist - version 1.3(August 1996 R. E. Ghosh)
Line-printer output of Regrouped SANS Data
Spectrum number = 0 terminates program
Initial spectrum no...ext...Final spectrum no.
9346 1 9347

9346/ 1 found

9347/ 1 found
Initial spectrum no...ext...Final spectrum no.
Closing listing file rlst001.lis
lass1 62%
```

smorger

This program will access any spectrum in a standard regrouped data file and merge it in with others, resequencing in increasing Q values if requested. As data are read in, a subset can be defined to eliminate poor data at the extremes of the measurement. Data may also be rebinned, using simple linear interpolation, and smoothed with a simple 3 point smoothing function.

terminal dialogue

```
lassl 30% smorger
smorger - version 1.0 June '97 (R. E. Ghosh)

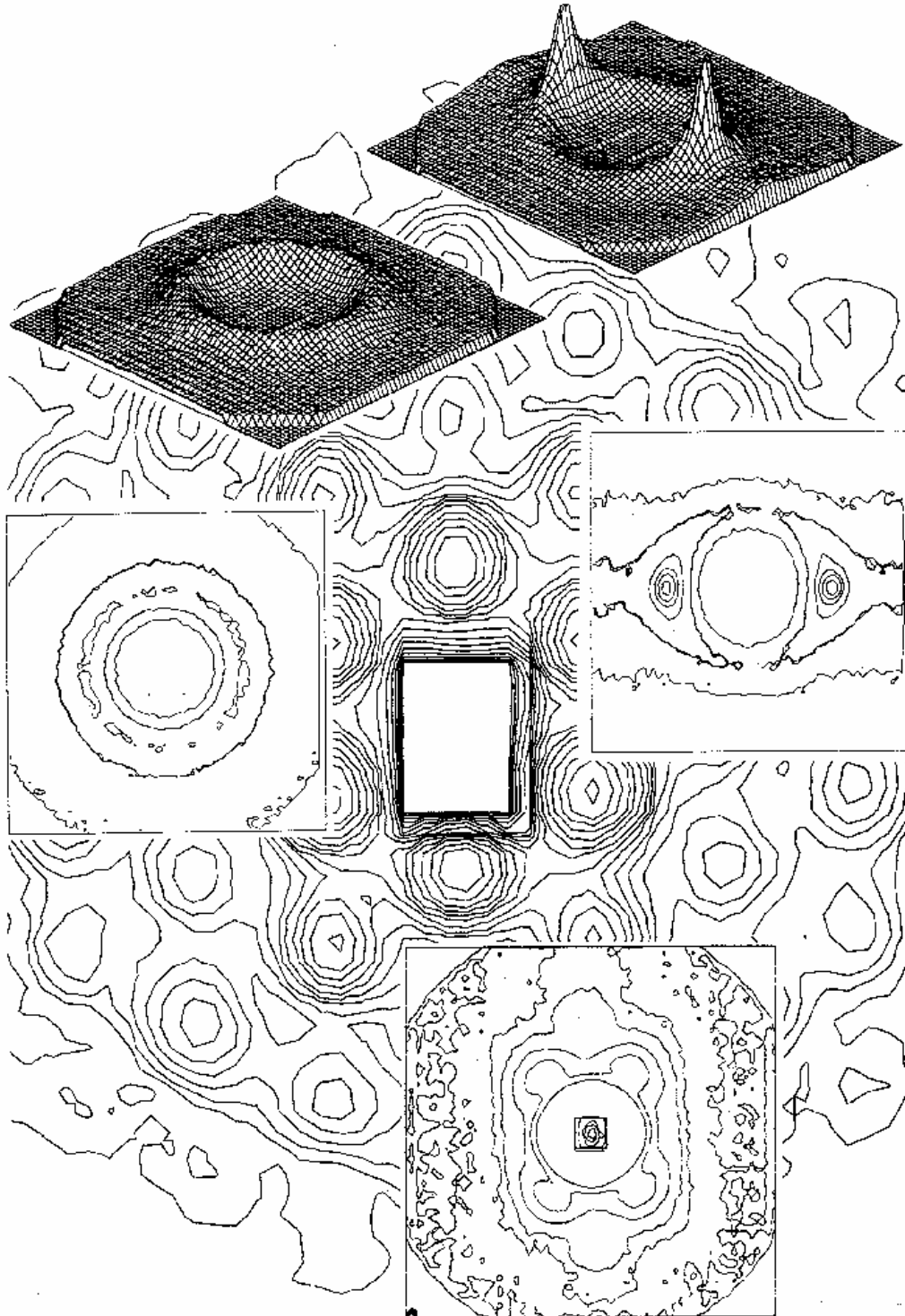
Sorts / merges / smooths /re-bins SANS grouped data

Command options:
  A      Add new data
  O      Order data in increasing Q
  C      Concatenate sets
  S      Smooth data (over 3 points)
  R      Re-bin ordered data
  W      Write out result
  Z      Zero all - reset
  H      HELP (this text)
  E      Exit

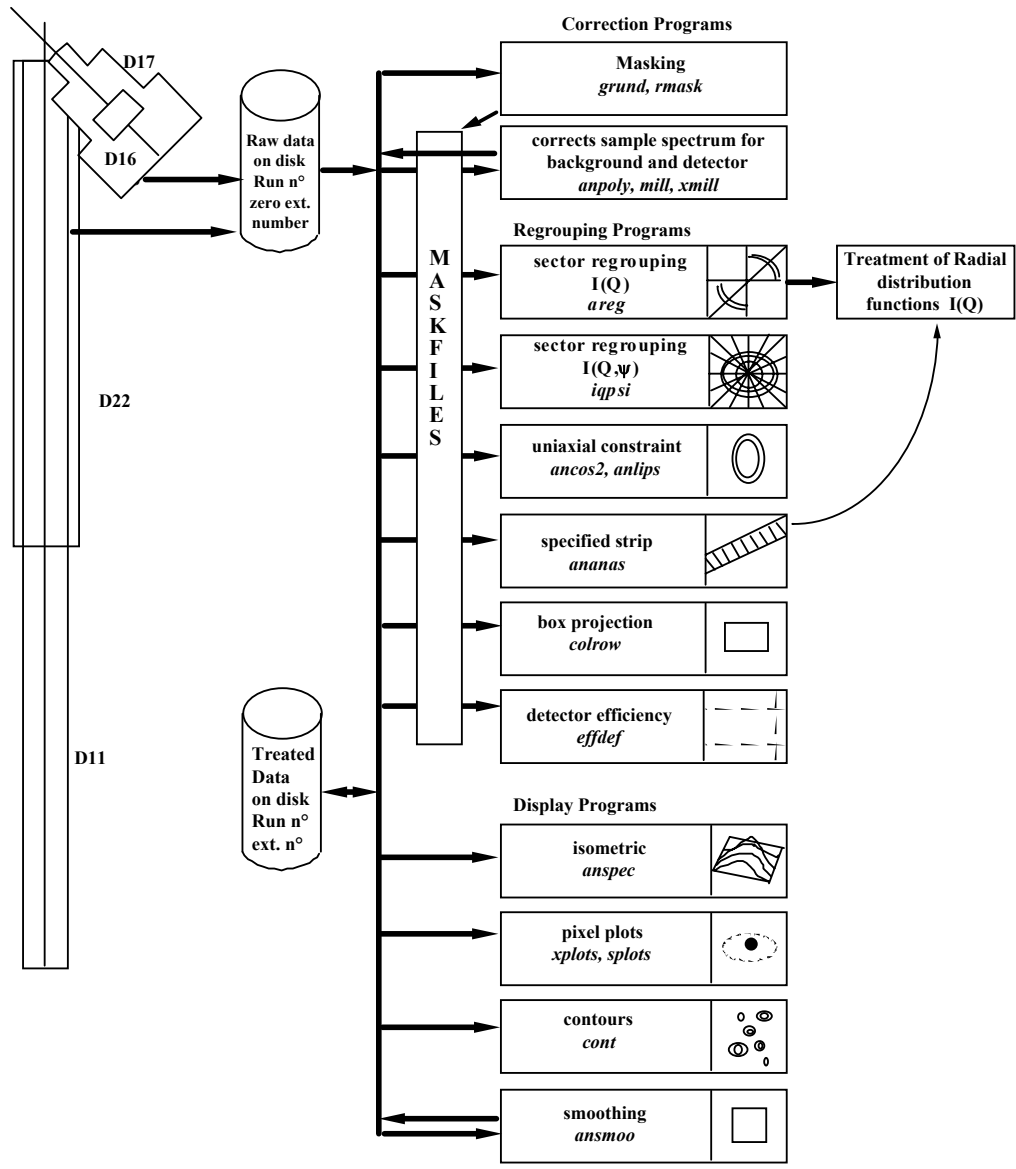
Read in data, a zero run number ends sequence, -1 to stop
Use 1st and last datum (if non-zero, e.g. 4 36) to trim range taken
Run number...ext...divider...1st datum...last : 14177 3 1 5 38
Spectrum SP12 0.5% 5e-3M NaCl read in
Run number...ext...divider...1st datum...last : 14191 3 1 6 36
Spectrum SP12 0.5% 5e-3M NaCl read in
Run number...ext...divider...1st datum...last : 14205 3 1 6 36
Spectrum SP12 0.5% 5e-3M NaCl read in
Run number...ext...divider...1st datum...last : 14234 3 1 6 36
Spectrum SP12 0.5% 5e-3M NaCl read in
Run number...ext...divider...1st datum...last :
Option A,O,C,S,R,W,Z,HELP or EXIT : c
Concatenating sets...
Option A,O,C,S,R,W,Z,HELP or EXIT : o
Ordering in increasing Q values...
Option A,O,C,S,R,W,Z,HELP or EXIT : w
Output will have the following title : SP12 0.5% 5e-3M NaCl

Give new title or <Return> to use this : SP12 ~0.5%/w PS latex
Recorded as 14177 / 4
Option A,O,C,S,R,W,Z,HELP or EXIT : e
lassl 31%
```

ANISOTROPIC DATA TREATMENT



ANISOTROPIC DATA TREATMENT



Treatment of anisotropic data

9

This set of simple programs enables experimental data to be treated on an individual cell basis in a similar fashion to the regrouped data. Consequently it is a fundamental assumption that the data are of good statistical worth cell by cell; this necessitates longer counting times and fewer spectra result than in problems where a simple radial average suffices for analysis. These considerations, and the lack of an acceptable general scheme capable of covering the diverse problems under examination have led to the present choice of method for data treatment. A more comprehensive treatment of these data may be achieved with the Matlab package GRASP (C. Dewhurst, ILL, <http://www.ill.fr/lss/grasp>)

All the programs in this section can access either raw data (when the extension run number requested is zero), or treated data (non-zero extension). Most programs too can use standard masking files before performing their task on the unmasked cells. After corrections etc., it is possible to regroup the data using the program *areg* which will store the regrouped data from defined segments as separate spectra in standard regrouped files, allowing further treatment with the programs which treat radial distributions. When attempting to regroup highly anisotropic data, performing corrections first cell by cell then regrouping is preferable to simple masking and using *rnils* when the detector is not showing a uniform response.

Source of Data

Spectra are referred to by run and extension number. If the extension number is zero then the raw data are assumed to be in an appropriate directory pointed at by SAS_DATA_PATH. Data with non-zero extension numbers are expected to be found in the current directory. Output 2D files are given the systematic names:

tnnnnn.eee

where nnnnn is the run number and eee is the extension number

It is thus simple to find the files

e.g. `% ls t*`

or delete `% rm t*`

The program *rundex* (see page 43) will list a summary of files present, and list titles and internal parameters.

The ASCII File Format is described in appendix 2, together with access routines which are in the library /usr/ill/lib/librllib.a

9.1 Combining spectra

The following programs operate on the full 2D patterns. If the environment variable SAS_ERROR is set to false then the error in intensity is not written out, leading to some economy of disk usage.

anpoly

This program corrects the sample spectrum by combining individual spectra or sets of similar spectra, and rewrites the result back as an anisotropic file, from which it may be plotted, regrouped etc. At the end of the calculation the corrected spectrum may be printed out.

The program uses the same formalism as spolly (see 8.3) with a very similar terminal dialogue; the printout options include output of the whole data array.

mill, xmill

These programs, already described in section 8.3, can be used to treat 2D data. The terminal dialogue and selection operations are identical in the two cases. The two dimensional data are displayed as pixel maps

effdef

This uses the initial formalism of anpoly/spolly to obtain a background corrected spectrum of a uniform scatterer. Masked values are set to a value of -0.1. Results are displayed as a pixel map with a scale 0-200% of the nominal average value. The standard 2D output file can be used later to normalise data in the display programs in chapter 10.

terminal dialogue

```
lassl 27% effdef
effdef - Version 1.1   March '97 (R. Ghosh)

Delete cells listed in mask file ? (Y) : n
VANADIUM/WATER BACKGROUND runs
Run number...Ext
effdf>9325
Title : Empty Hole                stored monitor  0.67007E+07
Using scaled monitor preset      67.007
Type <RETURN> or give new value :
effdf>
Run number...Ext
effdf>9371
Title : E. Hole                    stored monitor  0.66893E+07
Using scaled monitor preset      66.893
Type <RETURN> or give new value :
effdf>
Run number...Ext
effdf>
VANADIUM/WATER SAMPLE runs:
Run number...Ext
effdf>9326
Title : H2O 1mm                   stored monitor  0.13401E+08
Using scaled monitor preset      134.01
Type <RETURN> or give new value :
effdf>
Run number...Ext
effdf>9372
Title : H2O 1mm                   stored monitor  0.66877E+07
Using scaled monitor preset      66.877
Type <RETURN> or give new value :
effdf>
```

```

Run number...Ext
efdf>
Background correction factor for van. absorption (A1)
efdf>0.485
Default title is : H2O 1mm
Type return to use this or give new title (20 characters) :
efdf>H2O efficiency
For 16384 cells the average value is 4.775

Saved as file t009372.001 run 9372 ext. 1

%PGPLOT, Completing PostScript file efdf008.ps
lassl 28%

```

9.2 Regrouping

areg

This program will produce one or more radial distribution functions $I(Q)$ from a whole or masked 4K (64x64) or 16K (128x128) spectrum by selecting segments of cells for each regrouped output spectrum. The regrouped data are written out as standard regrouped data files and may be further treated by the programs in section 8.

The geometry of the SANS measurements is shown adjacent. The segments are selected by defining the centre angle of the first segment (PSI-ZERO) and a segment angular width (PHI). The segment is then stepped NSTEP times producing that number of regrouped spectra.

Setting the segment angle to 180 degrees and selecting a single step reproduces the regrouped results obtained using *rnils*.

By correcting data first with *anpoly* this provides a rapid means of obtaining radial averages for very anisotropic samples, when there are large fluctuations in local detector efficiency and use of *rnils* with simple masking techniques is inadequate.

The cell allocation algorithm is similar to that in *rnils*, see 4.5, and an option permits a full print-out of the values of Q , sector angle, and sector allocation for each cell.

Given the beam centre (where $X0$ and $Y0$ are given in cell coordinates 0 to 63 or 0 to 127, corresponding to displays and listings) and any offset angle the allocations are calculated, then the input data are treated for each sector, after any masking.

In the output are included the nominal sector angle and the average sector angle at each radial value.

1. The current experimental parameters are tabulated. These may be modified by giving the parameter number and new value. A parameter number of 0 (or RETURN) allows the program to progress. The modified parameters are retained on disk for re-use.
2. The user is requested to give masking information.
3. After calculating the cell allocation the user is requested to supply the sequence of run and extension numbers both for input and output. This allows the output set to start with a uniform extension number, distinguishing them from previous program runs.

terminal dialogue

```
$!class1 44% areg

AREG - Version 9.6 June '06 (R.E. Ghosh)

Output options
0: no terminal listing
1: terminal listing
2: Printer output file to include Q/psi/Sector maps
areg>2

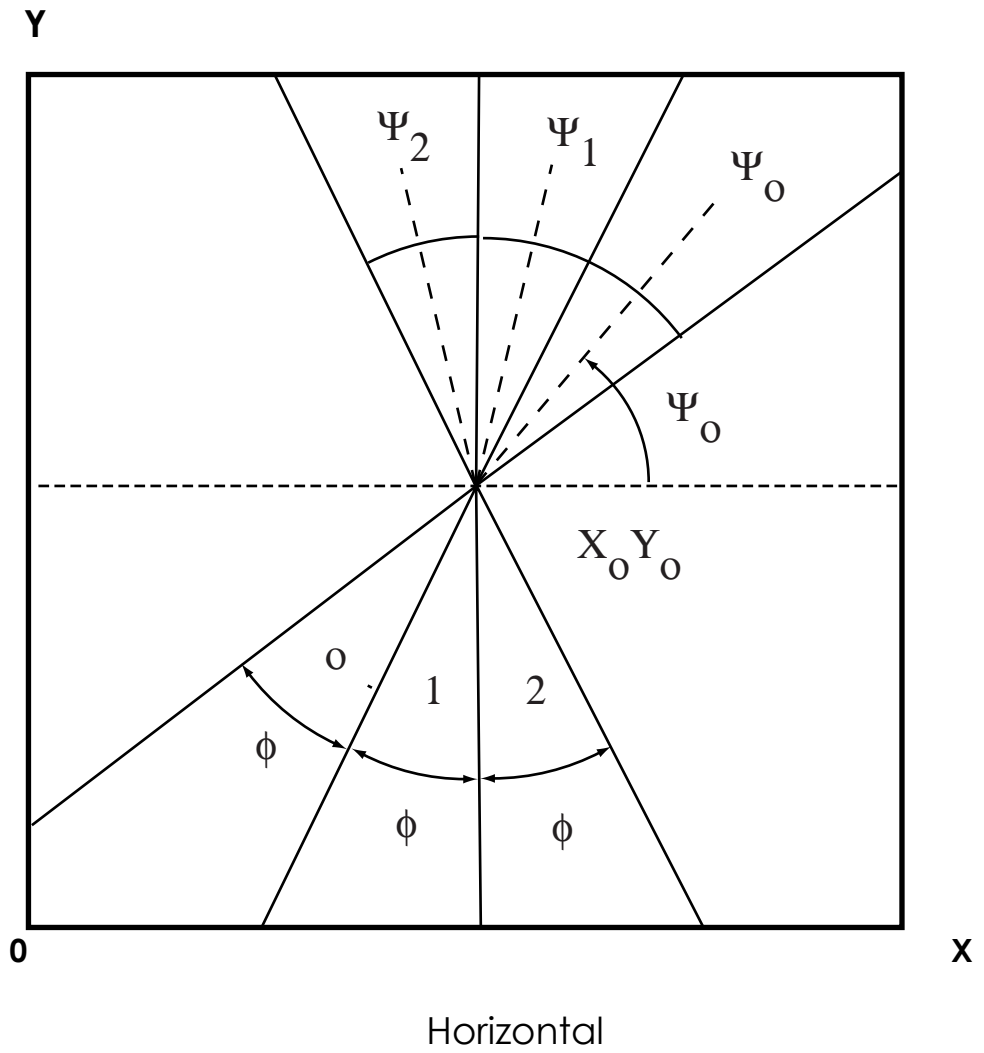
  1  Detector0  deg.    0.0000      2  x0  address      31.6000
  3  y0  address      31.0000      4  Radial step cms.  1.0000
  5  Sample-detect m. 10.0000      6  Wavelength a     6.0000
  7  Collimation  m.  8.0000      8  Concentration     1.0000
  9  isum dx   cms.  2.0000     10  isum dy   cms.  2.0000
 11  4 or 16k           4.0000     12  Sectang phi deg. 180.0000
 13  Sector  psi-0      0.0000     14  No. of  sectors  1.0000

To modify give parameter number and value
to relist type -1 to continue type return

Parameter... value : 12 30
Parameter... value : 14 6
Parameter... value : 7 10
Parameter... value :

Delete cells listed in mask file ? (Y/N) [N] : n
First run...Last...Input extension...Output extension :
areg>14252
SEEKING DATA
RUN 14252 FOUND
SECTOR : 0.0 saved as run 14252 ext. 0
SECTOR : 30.0 saved as run 14252 ext 1
SECTOR : 60.0 saved as run 14252 ext 2
SECTOR : 90.0 saved as run 14252 ext. 3
SECTOR : 120.0 saved as run 14252 ext 4
SECTOR : 150.0 saved as run 14252 ext 5
TREAT ANOTHER SPECTRUM ? (Y/N) [N] :
areg>n
Closing listing file areg016.lis
isl 45%
```

ANGLES USED IN REGROUPING ANISOTROPIC DATA



The detector is viewed from the sample

iqpsi

This program regroups data in annuli and presents the results as a function of the azimuthal angle Ψ . Ψ_0 is set along the X-axis, and the full 180 degrees is then divided by the number of sectors to set the sector width ϕ . The program includes simple graphics, and outputs results in a table for later use,

The user first defines the central cell, wavelength etc. At this stage it is also possible to define a mask file which is to be used.

After selecting the data file, the annuli must be selected by setting the inner and outer radial limits with the Q command. This is limited to 10 sets per grouping action, to avoid the plots becoming too confusing.

The data are regrouped with the G command, and then plotted. The scale limits can be changed at this stage. A hardcopy PostScript file and an output file can be created of all sectors for each radius set, or specific set (number n below).

terminal dialogue

```
% iqpsi
IQPSI version 2.0 May '04 (R.E. GHOSH)

  1 Detector0 deg.      0.0000      2 x0 address          31.5000
  3 y0 address         24.0000      4 4 or 16k            4.0000
  5 Sample-detect m.  10.0000      6 Wavelength a       8.0000

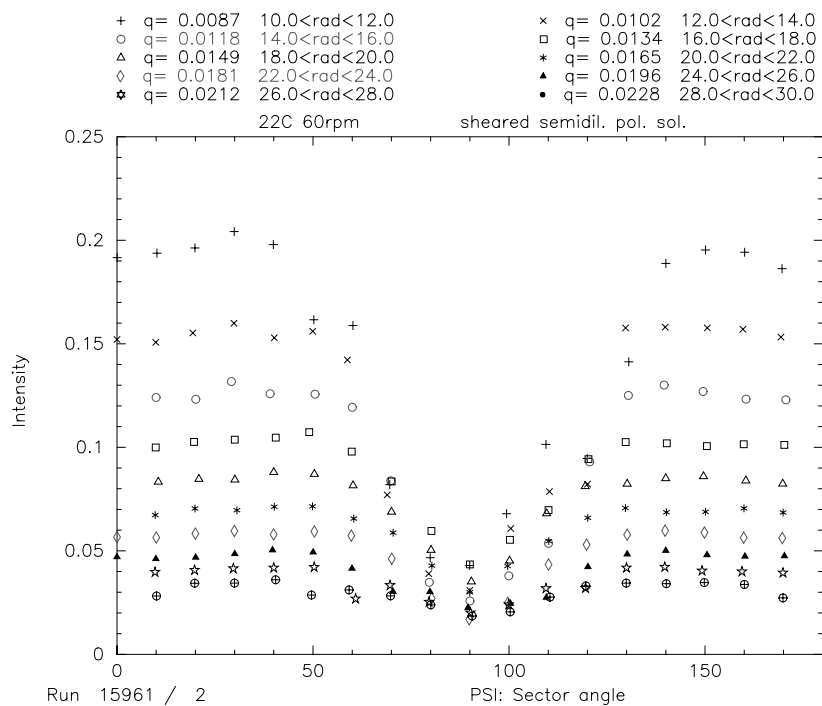
To modify give parameter number and value
to relist type -1 to continue type return

Parameter... value : 2 33.7
Parameter... value : 3 22.8
Parameter... value :

Delete cells listed in mask file ? (Y/N) [N] :
Options:
      R          Read in data
      N          Number of sectors
      Q          Q selection (radii)
      G          Group data
      L [n]      List [nth] results
      P [n]      Plot [nth] results
      W [n]      Write plot file
      Y min max Y scale settings
      F [n]      File output of results
      E          Exit
      Help      this text

IQPSI - Option HELP or R,N,Q,G,L,P,W,Y,F,H,Exit : r
Give RUN...EXT : 15961 2
Data read in
IQPSI - Option HELP or R,N,Q,G,L,P,W,Y,F,H,Exit : q
#  inner radius(cm)  outer radius(cm)  Q(A-1)
  1      10.00         12.00             0.0086
  2      12.00         14.00             0.0102
  3      14.00         16.00             0.0118
  4      16.00         18.00             0.0134
  5      18.00         20.00             0.0149
  6      20.00         22.00             0.0165
  7      22.00         24.00             0.0181
  8      24.00         26.00             0.0196
  9      26.00         28.00             0.0212
 10      28.00         30.00             0.0228

Q : Type -1 to view list, -99 to reset, return to continue
give number...inner radius...step...number of steps :
There are 10 groups set
IQPSI - Option HELP or R,N,Q,G,L,P,W,Y,F,H,Exit : g
IQPSI - Option HELP or R,N,Q,G,L,P,W,Y,F,H,Exit : p
```

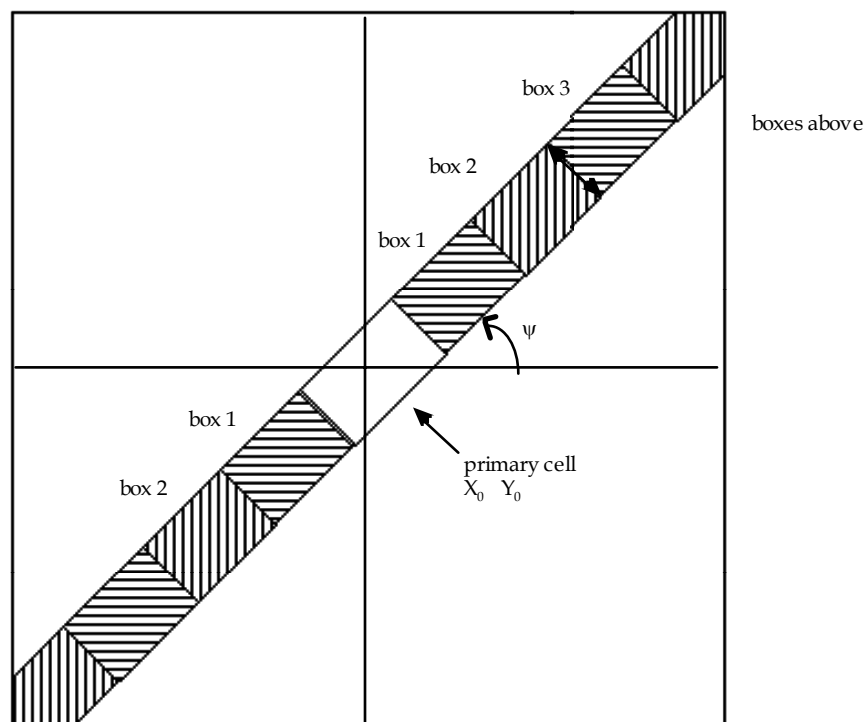


```

IQPSI - Option HELP or R,N,Q,G,L,P,W,Y,F,H,Exit : y
Data maximum 0.20418      ymin 0.00000E+00 ymax 1000.0
IQPSI - Option HELP or R,N,Q,G,L,P,W,Y,F,H,Exit : y 0 0.25
Data maximum 0.20418      ymin 0.00000E+00 ymax 0.25000
IQPSI - Option HELP or R,N,Q,G,L,P,W,Y,F,H,Exit : p
IQPSI - Option HELP or R,N,Q,G,L,P,W,Y,F,H,Exit : w
IQPSI - Option HELP or R,N,Q,G,L,P,W,Y,F,H,Exit : f
Give output filename : b601030.qps
IQPSI - Option HELP or R,N,Q,G,L,P,W,Y,F,H,Exit : e
%PGPLOT, Closing file qpsi025.ps
Closing listing file qpsi024.lis
%
```


ananas

This program calculates the mean intensity per cell for equally spaced boxes in a strip which may be rotated about the primary cell. It is intended for analysis of diffraction from well-ordered uniaxial systems.



The width of the strip is given in cm, and the radial step (cm) is used for the second box dimension. The boxes are symmetric about the primary cell X_0, Y_0 . It is assumed in the calculation that the detector is normal to the axis of the incident beam. The mean intensity per cell for boxes above and below this central box are given separately, ignoring the usual symmetry of the scattering pattern. A mask file from *rmask* or *grund* may be used to eliminate errant cells. The output can be written into standard regrouped data files, with options of averaging the data from each side of the central cell, or storing as two datasets. This allows the resultant to be plotted.

The user must supply the beam origin, the box size and angle with respect to the horizontal plane, ψ , and the runs for treatment.

The data are saved as a standard regrouped data file, which allows the standard plotting programs in section 8.2 to be used to examine these results, and multiple peaks can be analysed by fitting programs described in chapter 11.

terminal dialogue

```

% ananas

ananas - boxes from sans spectral data
version 2.0 - September 2000 (R.E. Ghosh)

  1 x0 address      17.0000      2 y0 address      62.5000
  3 Radial step cms. 1.0000      4 Sample-detect m. 4.5200
  5 Wavelength a     8.0000      6 4 or 16k       16.0000
  7 Sector psi-0     0.0000      8 strip width cms. 0.0000

To modify give parameter number and value
to relist type -1 to continue type return

Parameter... value : 1 62.3
Parameter... value : 2 63
Parameter... value : 4 5
Parameter... value : 5 4.6
Parameter... value : 8 5
Parameter... value : 3 2
Parameter... value :

Delete cells listed in mask file ? (Y/N) [N] : n

Give run number...ext :12131
Data found, title: unicc/5m/4.6 fibre orient. test.

Primary cell box at 62.30 63.00
Intensity 4.3000E+00 error 6.5574E-01

Data are in two sets, one each side of the central box
# Q Intensity-1 error-1 Intensity-2 error-2

  1 0.00546 2.4000E+00 4.8990E-01 3.2000E+00 5.6569E-01
  2 0.01093 2.4000E+00 4.8990E-01 5.3800E+01 2.3195E+00
  3 0.01639 1.0530E+02 3.2450E+00 1.7100E+02 4.1352E+00
  4 0.02185 9.7700E+01 3.1257E+00 8.6600E+01 2.9428E+00
  5 0.02731 6.9800E+01 2.6420E+00 5.7900E+01 2.4062E+00
  6 0.03277 4.5300E+01 2.1284E+00 3.5700E+01 1.8894E+00
  7 0.03823 2.9600E+01 1.7205E+00 3.0200E+01 1.7378E+00
  8 0.04369 2.4900E+01 1.5780E+00 2.4200E+01 1.5556E+00
  9 0.04915 2.0300E+01 1.4248E+00 1.9300E+01 1.3892E+00
 10 0.05460 1.9000E+01 1.3784E+00 2.0700E+01 1.4387E+00
 11 0.06006 1.7600E+01 1.3266E+00 1.8500E+01 1.3601E+00
etc.
 21 0.11443 1.6800E+01 1.2961E+00 1.7400E+01 1.3191E+00
 22 0.11985 2.2600E+01 1.5033E+00 2.2600E+01 1.5033E+00
 23 0.12527 3.0500E+01 1.7464E+00 3.7000E+01 1.9235E+00
 24 0.13068 5.5400E+01 2.3537E+00 6.0600E+01 2.4617E+00
 25 0.13608 6.7900E+01 2.6058E+00 7.3100E+01 2.7037E+00
 26 0.14148 6.5000E+01 2.5495E+00 6.8300E+01 2.6134E+00
 27 0.14688 4.9800E+01 2.2316E+00 4.5100E+01 2.1237E+00
 28 0.15227 2.7300E+01 1.6523E+00 2.5500E+01 1.5969E+00
 29 0.15765 2.0200E+01 1.4213E+00 2.1800E+01 1.4765E+00
 30 0.16303 1.5900E+01 1.2610E+00 1.9100E+01 1.3820E+00
 31 0.16841 1.5900E+01 1.2610E+00
 32 0.17377 1.4800E+01 1.2166E+00

Type A to store average as regrouped data
B to store both separately
M to print allocation map
R to restart (new data/new parameters)
E to exit
Option A,B,M,R,E : b
Saved as run 12131 / 0
Saved as run 12131 / 1

Type A to store average as regrouped data
B to store both separately
M to print allocation map
R to restart (new data/new parameters)
E to exit
Option A,B,M,R,E : e
Closing listing file anas032.lis
%

```

9.3 data smoothing

ansmoo

This program takes raw or treated anisotropic data and performs a simple smoothing operation merging adjacent cell contents in the X and Y directions. The outermost rows and columns remain unsmoothed. To help present the data visually there are two rescaling options, offering conversion to a logarithmic, or a square-root intensity scale. With these options it is possible to use, for example, *anspec* for isometric plots of data with a large range of intensities. In the case of the converted spectra the data error output is suppressed.

The program terminates when a zero run number is given.

terminal dialogue

The data were converted to a square-root scale to visualise a pattern with a large dynamic range.

```
% ansmoo

      ANSMOO : Smoothing program
      Version 1.4 April 1995 (R.E. Ghosh)

Smooths and rescales 4K or 16K spectra

For smoothing only           set TYPE to 0
For conversion to LOG scale  set TYPE to 1
For conversion to SQRT scale set TYPE to 2

Spectrum number = 0 stops program

Give spectrum number...ext...type :10264 0 2
Result copied to disk: Run 12064 Ext. 1
Give spectrum number...ext...type :
%
```

9.4 analysis

ancos2

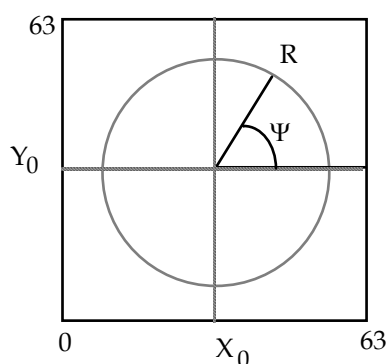
This program was devised with the help of B. Rainford to analyse paramagnetic scattering in an external field (see Marshall and Lovesey, p112, e.q. 5.37).

Here the (R, ψ) variation of the scattered intensity is of the form

$$I(R_i, \psi_j) = A(R_i) + B(R_i) \cos^2 \psi_j$$

where ψ is the angle between the radius vector and the horizontal field direction.

The functions $A(R)$ and $B(R)$ can be readily determined by least-squares methods by analysing data on any annulus, i.e. for a set of cells at fixed R .



$$B_i = \frac{N_i \sum_j \cos^2 \psi_j \sum I_j}{N_i \sum_j \cos^4 \psi_j - (\sum_j \cos^2 \psi_j)^2}$$

$$A_j = \left\{ \sum_j I_j - B_i \sum_j \cos^2 \psi_j \right\} / N_i$$

The error is then:

$$DEL = N^{-1} \sqrt{\sum_j I_j^2 + A^2 N + B^2 \sum_j \cos^2 \psi_j - 2(A \sum_j I_j + B \sum_j I_j \cos^2 \psi_j - A \sum_j \cos^2 \psi_j)}$$

A tabulation of R , $A(R)$, $B(R)$ and $DEL(R)$ is produced for each spectrum.

The input parameters are the primary cell coordinates and the run numbers for treatment. The results are written in an output file name `nnnnnee.ac2` in four columns

terminal dialogue

```
% ancos2
ANCOS2 - Analysis of anisotropic sans spectral data

Version 2.0   November 1999 (REG)
  Spectrum number = 0 returns for new parameters
    < 0 stops program

1  x0  address      31.4000      2  y0  address      30.9000

To modify give parameter number and value
to relist type -1   to continue type return

Parameter... value :
```

Delete cells listed in mask file ? (Y/N) [N] :

Set run number to 0 to change parameters or -1 to finish
Run number ... ext : 11470

Run number 11470 ext. 0
Title: Fe-Alloy A60 field on

Primary cell : X = 31.4 Y = 30.9

R	A	B	DEL	R	A	B	DEL
5	1301.1	7099.7	2044.1	6	1421.0	6590.0	2243.0
7	2293.9	5247.7	2998.2	8	2907.6	3727.7	3221.9
9	2805.6	2928.7	3116.3	10	3388.4	1673.3	3424.2
11	3565.6	513.90	3323.1	12	5512.2	-2655.0	3162.9
13	6001.7	-3969.7	3118.6	14	5242.0	-3525.5	2733.1
15	4463.4	-2987.7	2325.5	16	3675.9	-2348.6	1916.9
17	3019.9	-1860.4	1501.0	18	2505.4	-1464.9	1220.0
19	2084.0	-1169.8	1027.3	20	1789.3	-991.45	880.04
21	1485.0	-746.53	711.65	22	1273.1	-633.52	572.22
23	1106.5	-520.05	506.64	24	941.43	-409.18	414.91
25	930.08	-479.66	324.20	26	907.36	-526.99	244.94
27	842.35	-517.77	206.11	28	786.15	-483.07	159.21
29	712.10	-433.32	137.06	30	639.59	-376.27	115.22
31	572.69	-326.82	129.44	32	499.77	-277.99	139.23
33	486.67	-354.51	136.60	34	461.84	-402.48	135.54
35	433.63	-388.10	112.11	36	404.79	-361.16	96.390
37	359.98	-305.58	87.488	38	334.62	-270.17	70.891
39	314.49	-202.35	49.001	40	294.23	-190.67	41.080
41	301.28	-297.32	50.448	42	345.10	-642.44	55.146
43	158.98	-348.99	45.028	44	-0.85638	10.377	5.0538

Set run number to 0 to change parameters or -1 to finish
Run number ... ext : -1

Closing file acs2799.lis
%

anlips

This program may be used to examine data from materials showing isotropic SANS which are subjected to uniaxial constraints leading to strain distortions and anisotropy in SANS.

Inevitably the program works best when the ellipticity ratio is less than 1:3, and is useful for sets of data with small anisotropy. For greater values it is useful to consider making two measurements to minimise resolution effects.

The spectrum used in this program is searched for sets of cells within certain intensity ranges. The coordinates of any one set are then used to fit an ellipse with principal axes along the detector's x and y axes by a least-squares procedure. The result of these fits is printed as a table of intensity versus Q , the scattering vector, in the X and Y directions. It is assumed that the detector is normal to the beam.

1. The user must give the distance from the sample to the detector (m) and the incident wavelength (\AA) and whether a 4 or 16K spectrum is to be treated. The coordinates of the primary beam coordinates must also be given.
2. The minimum and maximum radius to be treated, and the number of steps in intensity are then entered.
3. A mask file can be included before analysis.
4. The user now gives the run number of the required spectrum. A negative run number returns the user to 2. so he can change the radial parameters. A zero run number will stop the program.
5. The spectrum is scanned, and the number of points within the set minimum and maximum limits are printed out as an aid, showing the typical number of points to be used in any subsequent fitting. At this stage the user can decide to change the chosen intensity range. This range will be divided up into NSTEP sections and each will have an ellipse fitted. The result table includes the mean intensity, dimensions of the major and minor axes in cm, and the corresponding values of Q^2 , with the number of cells, NOP, contributing to the set.

terminal dialogue

```
% anlips
ANLIPS - Ellipse fitting program for SANS data
Version 1.3 July '98 (REG)

  1  x0 address      33.7000      2  y0 address      22.8000
  3  Sample-detect m. 10.0000      4  Wavelength a   5.25000
  5  4 or 16k        4.0000

To modify give parameter number and value
to relist type -1 to continue type return

Parameter... value : 1 31.5
Parameter... value : 2 31.5
Parameter... value :

RMIN...RMAX...NSTEPS : 10 32 20

Delete cells listed in mask file ? (Y/N) [N] : n

RUN NUMBER...EXT. NO. :22100
Radius 10.0 number of points 60 mean intensity 276.65
Radius 32.0 number of points 164 mean intensity 8.2134
Do you wish to change this intensity range ? (Y/N) [N] :
```

Run number 22100 ext. number 0
X0 = 31.5 Y0 = 31.5 Distance S-D = 10.00m Wavelength = 5.2A
RMIN = 10.0 RMAX = 32.0

	INTENSITY	LOG(I)	1/I	RA	RB	QQA	QQB	NOP
1	270.0	5.59842	0.3704E-02	11.7	9.8	0.000195	0.000138	8
2	258.7	5.55554	0.3866E-02	11.7	10.9	0.000197	0.000171	6
3	240.6	5.48302	0.4157E-02	11.9	10.9	0.000203	0.000171	7
4	232.9	5.45061	0.4294E-02	11.9	10.8	0.000203	0.000167	10
5	213.0	5.36129	0.4695E-02	12.5	10.7	0.000224	0.000163	4
6	202.5	5.31096	0.4937E-02	12.2	11.1	0.000212	0.000177	11
7	188.4	5.23868	0.5307E-02	11.6	11.2	0.000193	0.000181	19
8	175.9	5.16989	0.5685E-02	12.4	11.1	0.000220	0.000177	19
9	162.9	5.09343	0.6137E-02	12.7	11.8	0.000232	0.000199	19
10	147.2	4.99206	0.6792E-02	12.8	12.2	0.000235	0.000212	25
11	136.0	4.91300	0.7350E-02	13.2	11.9	0.000248	0.000204	21
12	122.7	4.80986	0.8149E-02	13.1	12.6	0.000244	0.000228	28
13	109.5	4.69563	0.9135E-02	14.0	13.2	0.000281	0.000249	47
14	95.65	4.56073	0.1045E-01	14.1	13.5	0.000286	0.000260	49
15	81.02	4.39468	0.1234E-01	15.2	13.8	0.000329	0.000272	54
16	68.12	4.22126	0.1468E-01	16.2	14.8	0.000376	0.000313	84
17	54.62	4.00033	0.1831E-01	16.9	15.8	0.000410	0.000357	112
18	41.96	3.73669	0.2383E-01	18.0	17.2	0.000464	0.000426	171
19	27.73	3.32260	0.3606E-01	21.7	18.9	0.000672	0.000514	381
20	13.46	2.59974	0.7429E-01	27.8	24.5	0.001107	0.000860	1308

RUN NUMBER...EXT. NO. :
Closing listing file lips810.lis
%

Display of two dimensional data

10

The ILL general plotting routine LAMP based on the commercial IDL package will perform many of the functions described below, may be started with the command `% lamp`. At present it is restricted to raw data, and requires loading the IDL runtime support package. The programs described here are tailored to answer the more pressing needs of the SANS experimenter at ILL and at home.

xplots, xplotc

These offer a good way of rapidly examining a complete set of overnight runs and detecting anomalies

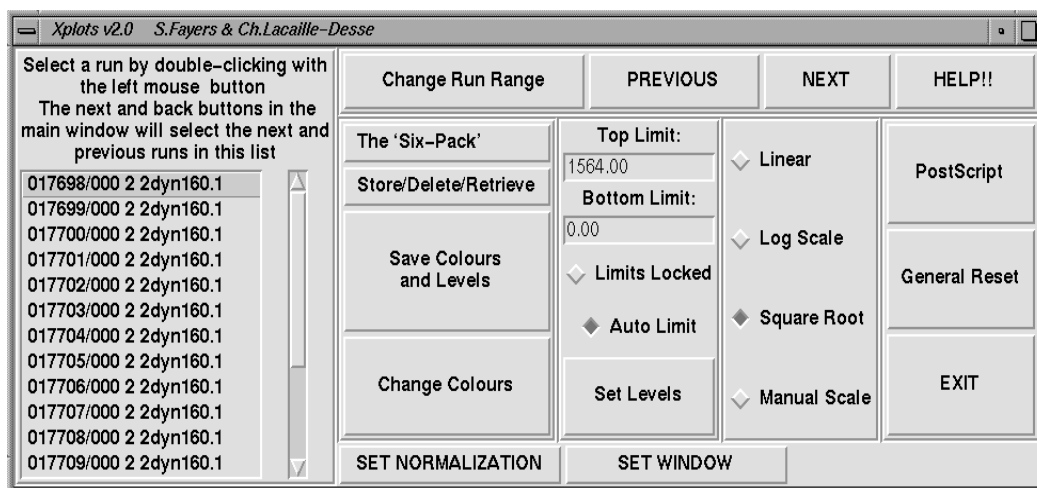
The principal windows of *xplots* are the run selector and the main window. Initially a range of runs is selected from the run selector. These then appear subsequently with their titles in the main window. The images may be selected individually, or by using the PREVIOUS or NEXT buttons. Store/Delete/Retrieve opens access to the six pack for saving images. *xplotc* includes an interactive cursor mode. *xplotc* offers, though this incurs extra cost in cpu time and network activity

xplots run selector



Compressed Data

Although xplots will access compressed data directly users are recommended to decompress all raw data as a set before treatment. There are significant benefits in being able to rapidly view a large sequence of data, and to be able to go back and forth rapidly, without waiting for repeated decompressions at each step.

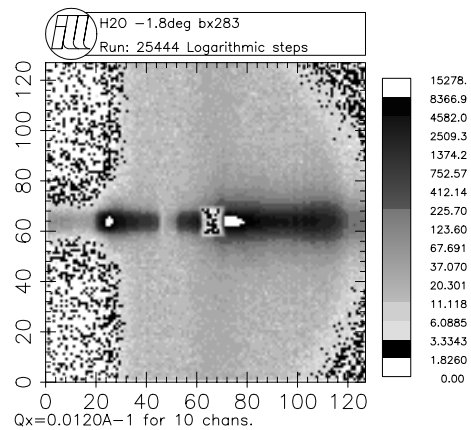
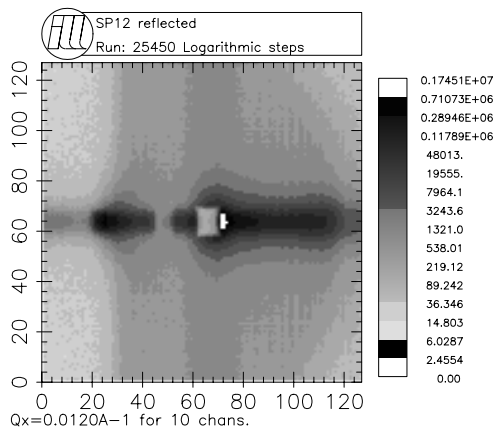
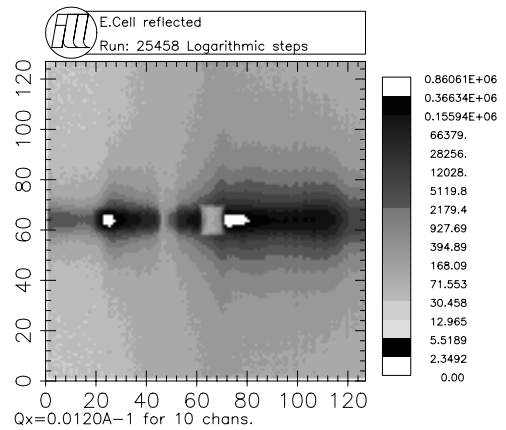
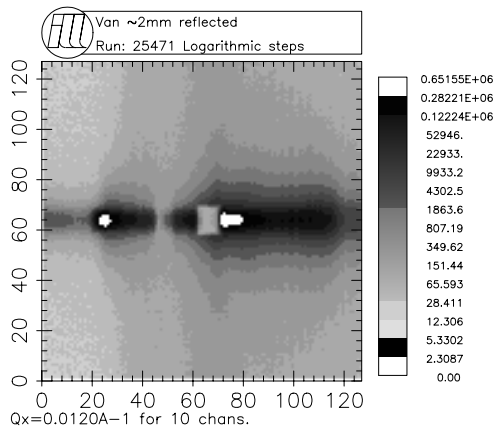
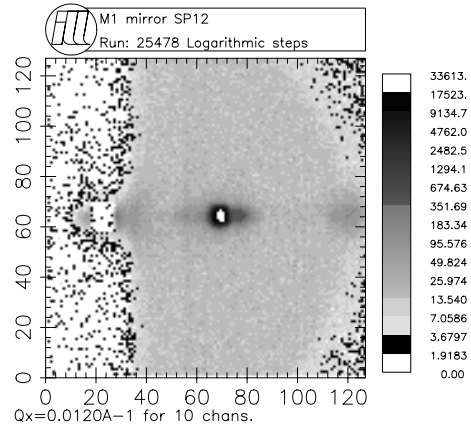
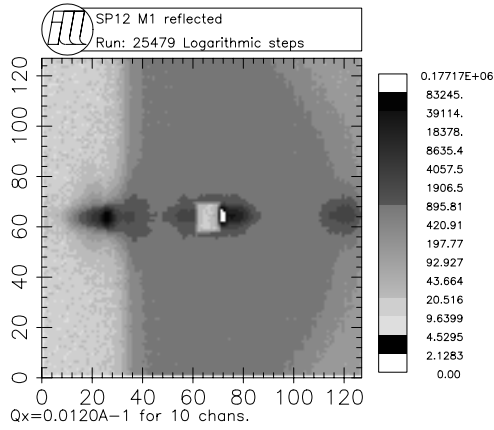
xplots main window**Six-Pack**

Using the Store/Delete/Retrieve button to bring up the SIX-PACK window the current single picture can be saved in a batch of up to six images. If scales limits are preset this offers an excellent means for illustrating subtle differences. Individual pictures can be removed or brought back to the main window, for example to change scales.

**splots**

splots is the underlying graphics program behind *xplots* and *xplotc* and is controlled from a command line interface. It draws the pixel plots of raw or treated data, and includes the possibility of selecting and expanding regions. An important part is the possibility to assemble up to six pictures (the Six-Pack) on a screen or hardcopy page, which helps compare different measurements.

Telling the tale - from the SIX-PACK



10.2 contour plots

cont

Raw or treated data from the instruments can be read and plotted as contour outlines on both screen and PostScript file output devices.

Several line types may be plotted. The lines are shown as continuous (0), dashed (1), dot-dashed (2). The source data may either be raw data or standard corrected anisotropic data files.

The sequence of use is as follows :

1. Define a set of runs to be treated (or just give one run number). A zero number for the first run stops the program.
2. At this stage the user may preselect a number of contour levels to be plotted. Giving a zero level value terminates the set of contours. On returning through this part of the program this set can be overwritten or cancelled.
3. The data are read, and the preset contours plotted. If no contour is found a message is typed out.
4. The user may then propose additional contour levels. These are added one by one to those already preset, and plotted if found.
5. The spectrum is terminated when a level of zero is input.
6. Then, if a set of spectra have been requested, the program proceeds to the next in sequence, otherwise more run numbers are requested.

terminal dialogue

```
lass2 21% cont
  Contour plots of SANS data

version 2.7 April '97 (R.E. Ghosh)
First run...last run...ext
cont>15961 0 2

Run 15961 ext. 2
spectrum minimum : 0.0000E+00 maximum : 0.3707
mean : 0.5036E-01

Two types of contours may be plotted.
for a continuous line type=0
for discontinuous lines type 1,2,3
set level=0 to terminate a set of contours.
Preset level...type
cont>
Level...type
cont>.3
Level...type
cont>.2 1
Level...type
cont>.15
Level...type
cont>.10 2
Level...type
cont>.07 1
Level...type
cont>.04
Level...type
cont>
Hardcopy output (Y/N) [N]
cont>y
First run...last run...ext
cont>
%PGPLOT, Closing file cont045.ps
lass2 22%
```

10.3 isometric plots

anspec draws isometric plots of either raw or treated spectra. The current program uses plotting algorithms originally designed by J.B. Hayter and J. Penfold.

anspec

1. After finding the requested spectrum, the user defines lower and upper clipping limits for the spectrum to be plotted.
2. The left hand and right hand isometric axes are then set up, allowing the view of the spectrum to be changed.
3. The display may be rotated. The sides are named 1, 2, 3, and 4. Side 1 is the normal, horizontal, X axis of the detector.
4. The isometric plot is then made plotting along the left-hand axis. In case the plot is to be abandoned, a prompt arrow is then given. Typing Y, or a return, allows the plotting to continue, and draw the first part of the plots following the right-hand axis. A second prompt occurs after every second line has been drawn. Typing a Y or return allows the picture to be completed, when again the program pauses with a prompt arrow. Should the picture be unsatisfactory typing N at these intermediate stages terminate the isometric plots.
5. The choice of plot can then be modified, or a hardcopy plot selected.

terminal dialogue

```
isl 162% anspec

***** ANSPEC 3-DIMENSIONAL ISOMETRIC PLOT OF SPECTRA.*****
        version 3.1 June '98 (R.E. Ghosh after J.B. Hayter).

Give run number .. ext. : 15961 2
Title: 22C 60rpm          sheared semidil. pol. sol.
Min.intensity is:0.000000E+00 Max.intensity is:0.370700
and mean intensity is:0.503559E-01

Type RETURN to continue or N to select new data

Give lower and upper limits in order to truncate the plot.
CARRIAGE RETURN is default, plotting all the values.

Lower limit...Upper limit ? : 0 .4

Left isometric angle (0<ANG<85) : 15

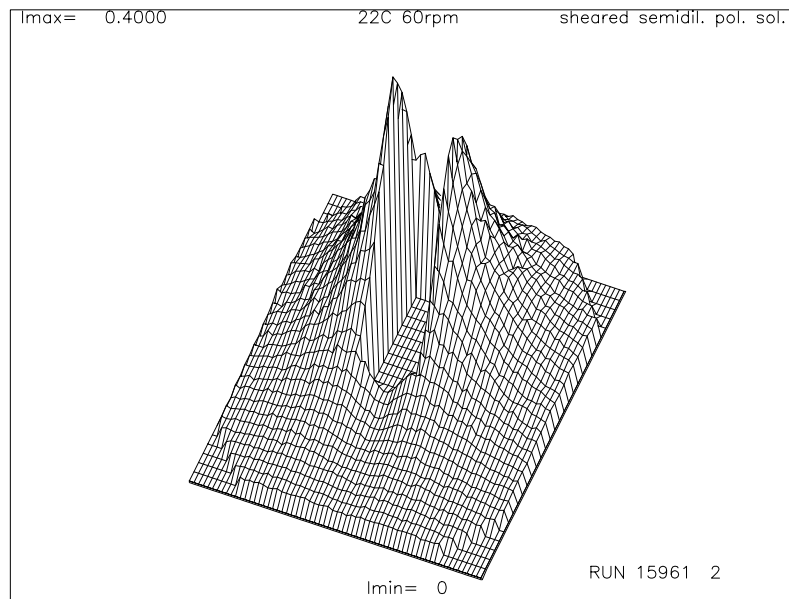
Right isometric angle (10<ANG<65): 65

WILL TAKE LEFT ANGLE AS 18.4 DEGREES
        RIGHT ANGLE AS 63.4 DEGREES

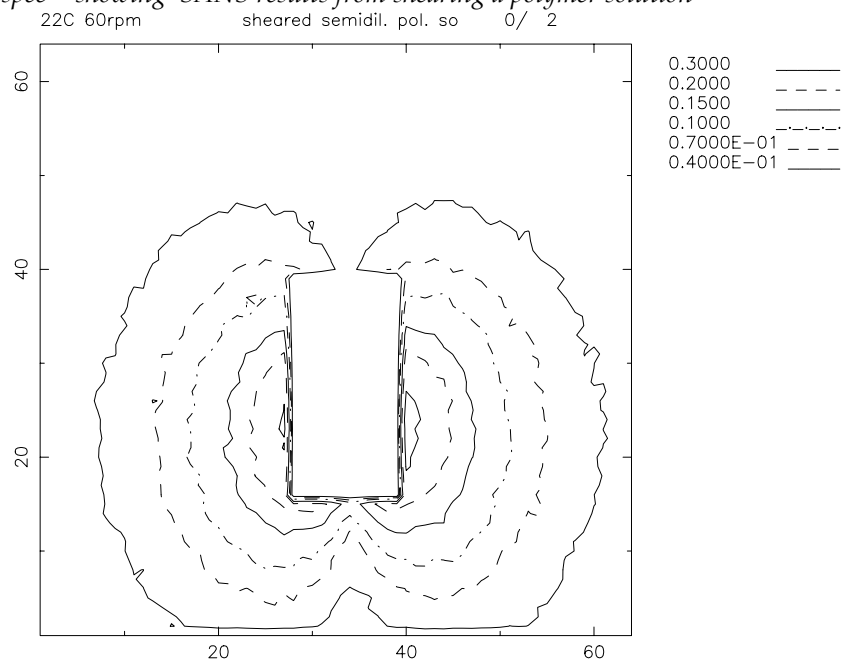
TYPE: 0 TO LEAVE SPECTRUM AS IT IS.
      1 TO ROTATE THE SPECTRUM 90 DEG.
      2 TO ROTATE 180 DEG.
      3 TO ROTATE -90 DEG.           ? : 2
Add second direction (Y/N) [Y] ? : y
Continue with additional lines (Y/N) [Y] ? :

TYPE: RETURN to plot the same data with other isometric angles.
      F For PostScript file of last screen plot.
      R to read and plot new data.
      E To end.                       ? : f

TYPE: RETURN to plot the same data with other isometric angles.
      F For PostScript file of last screen plot.
      R to read and plot new data.
      E To end.                       ? : e
%PGPLOT, Closing file aspc049.ps
%
```



anspec - showing SANS results from shearing a polymer solution



cont - showing the same results as a contour plot

10.4 projection plots

colrow

This program selects a spectrum, and within a defined rectangular window calculates the average intensity per cell for each row or column within that window. The sum may be scaled by a dividing factor, then listed and plotted either on the screen or hardcopy. The highest point in the spectrum is listed, and an indication of peak full width at half maximum is shown on the terminal. Each option is selected by single letter commands.

Commands

R Read in run number and extension number
 I Identify rectangular window: current settings shown, allows modification
 P Plots results and attempts to identify a peak
 W Write graphics to a file.
 O Outputs to the terminal the current averages and errors
 L Logarithmic or Linear scaling (alternates at each L command)
 M Mode of averaging rows or columns is alternated at each M command
 X shows current graph scale limits and allows modification
 Y shows current graph scale limits and allows modification
 C Cursor is toggled on or off for next plot (typing space shows coordinates or RETURN to continue)
 F shows and sets a dividing factor
 N Normalise newly read data with a detector response run
 H types a HELP text
 E EXIT

terminal dialogue

```
% colrow
COLROW - version 2.2 June '98 (R. E. Ghosh)

Sums projections of data and plots averaged results.

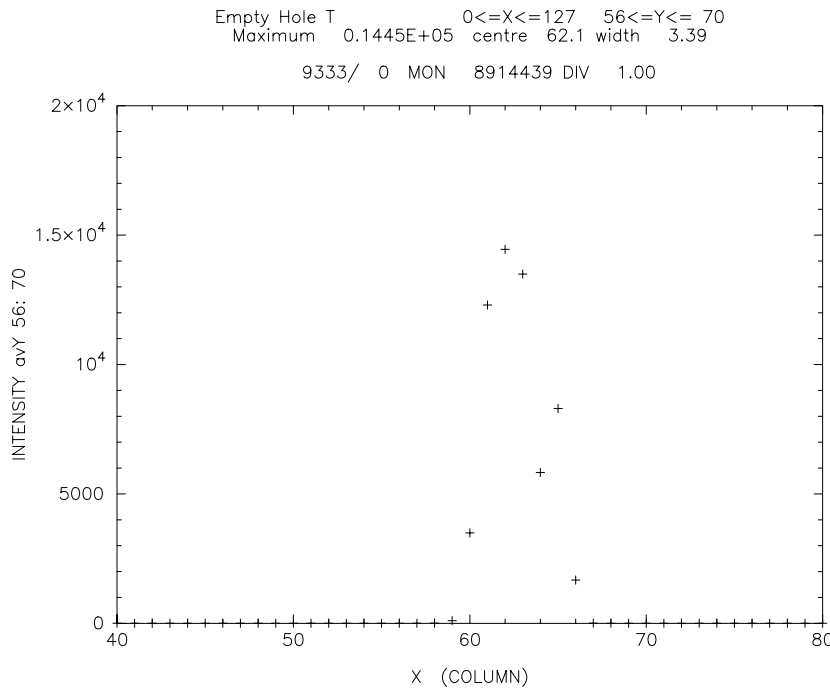
The current rectangular window in use is  0 <= X <= 63    0 <= Y <= 63
Currently the following averages are calculated :X (COLUMNS)
Intensities are scaled linearly

No normalisation data has been selected

Type:
R      Read in data
I      Identify rectangle to be treated
P      PLOT result
W      Write plot file of result
O      Output list of current values
L      Linear or Log plot (toggle)
M      Mode average columns or rows (toggle)
X      X plot limits
Y      Y plot limits
C      Cursor to be toggled for next plot
F      divide Factor for spectrum
N      normalisation of new data for detector response
H      HELP
EXIT

Type EXIT or control+D to terminate
Give RUN NUMBER ... EXT. NUMBER : 9333
Spectrum read in; length 16384
No efficiency normalisation used.
Option I,R,P,W,L,M,N,O,X,Y,C,F,HELP or EXIT : i
Current rectangle X 0 => 63 and Y 0 => 63
Define rectangle of data to be used 0 => X 127 0 => Y 127
Give <RETURN> to re-use these values
Give XMIN XMAX YMIN YMAX : 0 127 56 70
```

Examination of this transmission run shows that $x=64$ has a low efficiency which might affect precise results see windet p44



```

Option I,R,P,W,L,M,N,O,X,Y,C,F,HELP or EXIT : x
Current scale limits
  spectrum 0.0000E+00 127.0
  plot     0.0000E+00 63.00
Type RETURN to use values or give new values XMIN,XMAX : 0 127
Option I,R,P,W,L,M,N,O,X,Y,C,F,HELP or EXIT : y
Current scale limits
  spectrum 0.0000E+00 0.1445E+05
  plot     0.0000E+00 1000.
Type RETURN to use values or give new values YMIN,YMAX : 0 2e5
Option I,R,P,W,L,M,N,O,X,Y,C,F,HELP or EXIT : p
Option I,R,P,W,L,M,N,O,X,Y,C,F,HELP or EXIT : y
Current scale limits
  spectrum 0.0000E+00 0.1445E+05
  plot     0.0000E+00 0.2000E+06
Type RETURN to use values or give new values YMIN,YMAX : 0 .2e5
Option I,R,P,W,L,M,N,O,X,Y,C,F,HELP or EXIT : p
Option I,R,P,W,L,M,N,O,X,Y,C,F,HELP or EXIT : x
Current scale limits
  spectrum 0.0000E+00 127.0
  plot     0.0000E+00 127.0
Type RETURN to use values or give new values XMIN,XMAX : 40 80
Option I,R,P,W,L,M,N,O,X,Y,C,F,HELP or EXIT : p
Option I,R,P,W,L,M,N,O,X,Y,C,F,HELP or EXIT : w
Option I,R,P,W,L,M,N,O,X,Y,C,F,HELP or EXIT : e
%PGPLOT, Closing file clro042.ps
%
```

Analysis Programs for SANS data at the ILL

11

The programs described in earlier chapters have been concerned primarily with correction of raw data, regrouping and inspection. They allow the current experiment to be monitored and ensure that the data are of good quality.

Arising from their own SAS studies a number of scientists have installed programs at ILL for further analysis. In general they are willing to make them available for non-profit applications on individual request, though suitable acknowledgement of use is expected. Some programs have been adapted to read ILL data directly using routines described in appendix 2. Future developments will be posted on the http://www.ill.fr/lss/lss_data_treatment/LSS_treatment.html, and the canSAS (Collective Action for Nomadic Small-Angle Scatterers) initiative also contains useful information on other analysis programs: <http://www.ill.fr/lss/canSAS>

Special thanks are due to Otto Glatter, University of Graz, otto.glatter@kfunigraz.ac.at, Dimitri Svergun, EMBL-Hamburg and the Institute for Crystallography, Moscow, svergun@embl-hamburg.de, and Adrian Rennie, Uppsala University, Adrian.Rennie@fysik.uu.se for their contributions. Roland May, ILL, may@ill.fr has a close involvement in installing and supporting use of the programs from Glatter and Svergun at ILL.

11.1 Model and Peak Fitting

assa

Authors: M. Kozin and D.J. Svergun, EMBL Hamburg

An interactive modelling program for solution scattering performing 3-D rendering and calculations for rigid body sub-unit refinement.

<http://www.embl-hamburg.de/ExternalInfo/Research/Sax/program.html>

cryson and crysol

Author: D.J.Svergun, EMBL Hamburg

Programs to calculate solution scattering for neutrons (cryson) and X-rays (crysol) from atomic coordinates.

<http://www.embl-hamburg.de/ExternalInfo/Research/Sax/program.html>

mshell

Author: Adrian R. Rennie, Department of Physics, Uppsala University

This is a program to fit simultaneously multiple data sets. The model comprises spherical particles with up to 4 concentric shells. The parameters for several different data sets can be linked or varied independently. Interactions between the particles can be included using the rescaled mean spherical approximation of J.B. Hayter and J. Penfold, 'An Analytic Structure Factor for Macroion Solutions', *Molecular Physics* 42, 109-118 (1981). The executable file is `~rennie/mfit/mshell`.

multibody

Author: O. Glatter, University of Graz

A program to calculate scattering curves and distance distribution functions from models made up of little spheres (or other bodies with known scattering function). The ILL version can read ATOM cards of the PDB (protein data base) executable program is `~sans/multib`

polymer

Author: A. R. Rennie, Department of Physics, Uppsala University

This fits simple models appropriate to polymers such as the Debye function, and adaptations for copolymers, polymer blends star polymers and polydisperse systems. Executable code is `/home/cs/sans/polymer`. A short manual is available at http://material.fysik.uu.se/Group_members/adrian/poly.htm which describes the models, with literature references, and how to use the program.

pyshell

Author: A.R. Rennie, Department of Physics, Uppsala University

This fits a core-shell model for interacting, hard spherical colloidal particles. The interactions are calculated with the Ashcroft-Lekner model for hard spheres. The executable code is `~rennie/pyshell` A short manual is available on which describes the models, with literature references, and how to use the program http://material.fysik.uu.se/Group_members/adrian/pyshell.htm.

rfit

Author: A. R. Rennie, Department of Physics, Uppsala University

This fits models to SANS data and includes a parameterised instrument resolution function appropriate to pinhole cameras at fixed wavelength. Models include spheres, polymer coils, Gaussian peaks, Lorentzian broadening and other functions. Executable code is `/home/lss/rennie/rfit`. A description may be found at http://material.fysik.uu.se/Group_members/adrian/rfit.htm

sasfit4

Author: R. Ghosh, ILL

This programs fits up to 4 gaussian, and other peak shapes to regrouped SANS data and permit overlapping peaks to be modelled. *sasfit4* will treat sequences of data. The executable programs is `~sans/sasfit4`

sasha

Authors: D.J. Svergun, EMBL Hamburg

V. Volkov, Institute of Crystallography, Moscow

This program, `~sans/sasha`, offers a generalised analysis of particle shape at low resolution to match scattering curves using spherical harmonic functions; see: <http://www.embl-hamburg.de/ExternalInfo/Research/Sax/program.html>

Clickfit and the fitfun library

Clickfit and *clickfit_m* are GUI extensions to *fitfun* which simplify data fitting. The first is for individual data sets, but will treat a sequence of data either allowing parameters to be reused for the next fit, or reset to starting values. The second is for treating sets of data simultaneously. The library (R. Ghosh, ILL, ron@ill.fr) contains interactive fitting and plotting routines which has allowed rapid prototype development of a number of programs for SANS analysis, a few of which have been presented above. A description of the GUI, library and examples are in

<http://www.ill.fr/Computing/clickfit.html>
<http://www.ill.fr/Computing/fitfun.htm>

The basic package allows fine control over linking and fitting variables. The extensions include fitting multiple data sets simultaneously, (an obvious advantage in contrast variation experiments), and automatically fitting sequences of data after initially setting starting points interactively. The programs typically run either on Unix or PC systems, and use the same plotting environment variables as the standard SANS programs. Some programs using this library are *mshell*, *polymer*, *pyshell*, *rfit*, and *sasfit4*.

11.2 transform methods

dammin

Author: D.J. Svergun, EMBL, Hamburg
This performs ab initio shape determination by simulated annealing analysis of IFT results from gnom using a single phase dummy atom replacement procedure.
<http://www.embl-hamburg.de/ExternalInfo/Research/Sax/program.html>

gnom

Authors: D.J. Svergun, EMBL, Hamburg, and A. Semenyuk, Institute of Crystallography, Moscow
This is an indirect Fourier transform program; the program automatically adjusts the regularisation parameters.
<http://www.embl-hamburg.de/ExternalInfo/Research/Sax/program.html>

itp, ito

Author: O. Glatter, University of Graz
itp is an indirect Fourier transformation program obtaining $g(r)$ as a sum of cubic B-splines. It has been adapted by Roland May for SGI machines at ILL as `~sans/itp`, and `~sans/ito`. The copyright is owned by the University of Graz. Otto Glatter has to give permission prior to copying elsewhere.

11.3 Utilities

decon

Author: O. Glatter, University of Graz
This program deconvolutes distance distribution functions into radial density distribution functions. It has been adapted by Roland May (email: may@ill.fr) to SGI machines at ILL. The copyright conditions are the same as for *itp*.

sdldcalc

Alan Munter, NIST,
<http://www.ncnr.nist.gov/resources/sldcalc.html>
sdldcalc calculates scattering length densities from the chemical formula and information on the density provided by the user.

pdh

Author: O. Glatter, University of Graz
pdh is Otto Glatter's primary data handling program. It has been adapted by Roland May for SGI machines email: may@ill.fr. The copyright conditions are the same as for *itp*.

Exporting data from ILL

12

12.1 data compression using zip

Exporting data from ILL using zip

zip is proposed as a good compression and file packaging utility for transferring data files from ILL both to Unix and non-Unix systems. Documentation on the use of *zip* and *unzip* is available in *man* pages (`% man zip`). The user is recommended to prepare the transfers correctly at ILL, since only certain versions, (e.g. Unix) have all features available. One feature of using *zip* is that the file creation date is conserved and restored correctly. Away from ILL current executable copies of *zip* and *unzip* for most systems can be found at the Sun Archive Site for example (<ftp://sunsite.doc.ic.ac.uk/>). The resulting files are also compatible with PC *pkunzip*, and *winzip*, and the Macintosh *Stuffit/Expander* utilities.

Firewall

The firewall at ILL allows direct ftp transfers to the outside Internet.. To allow for the case where the remote site has a firewall preventing access, it is possible to place data temporarily on the ILL's ftp server, <ftp.ill.fr>, which is located outside the ILL firewall. These data can then be recovered once logged on at the remote site.. Current information on accessing the internet is given in the Computing section of the ILL web pages (<http://www.ill.fr/Computing>).

Means, media and filenames

Introduction

The general introduction of the use of Unix workstations over the past few years has lead inevitably towards complete use of ASCII (text) files both as a raw data storage form, and for treated results. The added overheads of storage are acceptable and the primary advantage is that there is no need for any specialised browser program - the files can be typed or printed directly.

Different computer systems, unfortunately, have different ways of signalling the end of each line. On Unix systems the `\n` or new-line character (LF) is used. On Macintoshes the carriage-return (CR) character is used. On DOS related PCs the terminator is (CR)(LF). Acceptance of any of the three types of character termination of lines is becoming more prevalent in modern software.

In wishing to transfer data to a non-Unix system the simplest method for a small volume of data is to use network services. *ftp*, the file transfer protocol set to ascii mode transfers will deliver a file correctly formatted.

When the data volumes, and also the number of files, are larger then some automation of the transfer process is desirable and because most data are simply regular arrays of numbers the files can be reduced dramatically in size (typically by a factor between 3 and 5) by compression techniques. The *zip* program is recommended as a means to achieve these two effects, yet still be compatible with a wide range of different systems.

A final consideration before transferring many files to remote systems concerns compatibility of file names across heterogeneous systems. From a conservative past many ILL programs produce files which have a simple filename with a single dot separator from a short extension name, and no embedded blanks. Today the DOS 8.3 format can be taken as an acceptable base standard for all systems. The full directory path specification is in general unique to each system type. Unless one is transferring files between similar system types it is easier to transfer contents of individual directories as separate zip files. Because many programs here were developed initially on Unix systems, users are recommended to keep complete filenames short, and to avoid, where possible, using directory path names containing spaces.

The simplest example

```
zip outfile *.dat
zip outfile *.f
```

creates the archive outfile.zip (or adds files to an existing archive file) and puts all xxxxx.dat files into it (the shell ignores files starting with a period) after compression. The second command adds the xxx.f files. If a filename is given which is already in the archive the earlier file is effectively overwritten. No subdirectories are included in this case.

Example for creating a PC compatible zip file

```
zip -jkl outfile *
```

This creates the outfile.zip in MSDOS fashion. The switches have the following actions.

- j Only filenames (not full path) are stored
- k Attempts to convert names(and paths) to MSDOS, marking file as if it were written under MSDOS. Compatible with *pkunzip.*, etc
- l Translates Unix end-of-line character LF into MSDOS convention CR LF.

Remember to transfer zip files to the remote site using ftp in BINARY mode

12.2 raw data files

File names at the ILL were deliberately chosen as six digits to allow data-compression utilities to add an extension as suffix to indicate the compressed status, while still keeping to the DOS and OpenVMS naming standards. Raw data from the current cycle and the preceding cycle are mostly kept on-line in uncompressed format. Older data are systematically compressed using the Unix compress utility, which can be treated by *gnu-compress*, *gunzip*, *gzip*, etc for other systems.

Export of long sequences of data is most simply performed by writing a permanent archive on a CDROM. A standard volume format, ISO9660, allows the disk to be read on most systems equipped with a CDROM drive. The staff of the *Service Informatique* will help visitors write data, and include suitable de-compression utilities on the disk to resurrect data at the destination ('phone 7013, Email:si@ill.fr)

For small quantities of data it is possible to use zip, then transfer the file by a mail attachment or ftp

e.g. for a short sequence of SANS data:

```
% zip -jkl myd11.zip /usr/illdata/data/d11/0145*
% zip -jkl myd11.zip /usr/illdata/data/d11/01460*
```

will compress the raw ascii files for first runs 14500-14599 then add the files 14600-14609 into the file myd11.zip. For D11 a set of one hundred standard 4k datasets occupy about 700Kb when zipped.

Remember to transfer zip files using ftp in BINARY mode

12.3 other data files

These are all standard text files (including the PostScript graphics files), and hence can be exported using ftp in ASCII mode, which will perform any line terminator conversions. Again *zip* can be used very effectively as a compression tool, and this also is a way of conserving the creation date on the files which is usually lost through ftp. Typical compression factors of greater than 10 are easily achieved. The *zip* output can be decompressed with utilities like *winzip*, and *pkunzip* or directly by XP windows..

12.4 IDA and BARNS

Accessing ILL data via Internet using Netscape or Internet Explorer

Website: <http://barns.ill.fr>

The ILL is developing data access methods and simple data treatments which can be initiated using a web-browser such as Netscape or Internet Explorer. These are used interactively to run procedures at ILL. On completion the results can be sent via ftp to the user. The present stage includes accessing the raw data base, and progressively, other programs are being adapted to use this new technique. The first set of SANS programs adapted include *windet*, for assessing transmissions, masking and regrouping programs. These web-procedures help complement the interactive procedures which can be run locally using either the Unix or PC versions of the programs described here.

IDA, Internet Data Access, is already operational, and allows the database of raw data to be examined via <http://barns.ill.fr>, and enables selected runs to be transmitted in compressed or uncompressed form to the remote site.

12.5 XML data

Appendix 6 describes the potential of formatting regrouped data using *g2x* or *g2xfull*. A parallel output of XML data is produced if the environment variable

```
SAS_EXTRA_G
```

is set to either *g2x* or *g2xfull* (which will include all regrouping parameters) This enables the programs to be updated matching newer standards or alternative file converters to be used without changing the program set.

From the command line a file can be converted manually:

```
% g2x g009346.001
producing file: xg009346_001.xml
```

Importing data to the ILL

13

To enable experimenters to merge data obtained elsewhere with that from the ILL a number of conversion programs have been created. Inevitably it is difficult to ensure that these programs remain up to date with other centres. Any information on changes being necessary will be warmly welcomed (email to ron@ill.fr).

colin

This is a general program intended to reconstruct standard ILL regrouped data files from spread sheet input (multi-column) text files.

There is an initial option to skip a certain number of lines, typically header material, which might be complex to decode.

Then up to twenty columns of data can be read in. The user must tell the program in which column it should find the Q, Intensity and error in intensities. The procedure can then be repeated to extract other data from the file.

The parameters for the standard regrouped files are then presented for the user to edit. It is recommended that at least the first eight are given realistic estimates.

ralread

Reads regrouped data files from LOQ at the ISIS Spallation source (colette output), and restores as standard ILL regrouped data files. (Author A.R. Rennie)

nistread

Reads regrouped data files from the SANS spectrometers at NIST, Washington, and restores as standard ILL regrouped data files. (Author A.R. Rennie)

ornlread

Reads data files from the SANS spectrometer at ORNL, Tennessee, and restores as standard ILL treated 2D data files. (Author A.R. Rennie)

nist2dr

Reads ascii-converted raw data files from the SANS spectrometers at NIST, Washington, and restores as standard ILL treated 2D data files.
(Author A.R. Rennie)

tsas

Reads regrouped data files from the SAS spectrometers at the ESRF, Grenoble, and restores as standard ILL regrouped data files. (Author R.E. Ghosh)

bsas

Reads edf raw data files from the ESRF, Grenoble, and restores as standard ILL 2D treated data files (author R.E. Ghosh)

xmlsin

This program is under development to read in regrouped data in xml form using the structure described in A6, saving this as a standard regrouped data file.

cif2ill

This program is under development to read regrouped data from the draft format sasCIF format files and rewrite as standard ILL regrouped data files.

nx2ill

This program is under development to read NeXus SANS data files (e.g. from PSI) and rewrite as a standard ILL data file.

ILL SANS data formats

A1

This appendix describes the raw data formats and the library routines available to read raw data, and read and write the treated data.

A1.1 Raw data

ILL Standard Formatted SANS Raw Data

A.1.1.1. Introduction

A decision was taken in 1994 to change the storage of ILL raw data from binary to text representation (US-ASCII) when it became evident that a wide variety of machine architectures would be in daily use, and that sufficient power was now available to rapidly decode the formatted data for re-use in calculations. In addition the transfer of text files across networks was not only simpler, but the subsequent printing out of the results would rapidly show up any errors.

The sequence of data generation, network transfer and archiving is now as follows. Data are written to disk by the instrument computer, which has sufficient disk capacity for several days operations. The basic inspection programs necessary for monitoring progress of the experiments usually access these data.

The data are transferred to a central data server; further treatment then is performed on distributed workstations which all access this central file-server.

A.1.1.2. Location of data

To allow compatibility with the largest number of systems we decided that the file of data would be simply identified with their sequential run number, six digits (packed with leading zeros) e.g., 000123. The remaining information (reactor cycle, and instrument name) is used in defining the path to the sub-directory containing the run data. This scheme also matches the name changes which are automatically invoked by compaction routines on the different systems. All data-files include further identification information within the file (see below). On a Unix system the final compressed archived file is identified by the pathname of the form:

`/usr/illdata/951/d11/000123.Z`

for the D11 run number 123 from cycle 951, i.e., the first reactor cycle in 1995.

All data are now held on-line in the present format; for D11 the first year/cycle is 743, for D17 this is 771. Some data have been lost due to media failure, and operator error probably lead to some truncation of the earliest files, which were originally recorded with a 20480 byte record lengths, alas too long for unwary transcription on OpenVMS.

At present raw data are stored uncompressed initially, except for instruments like D19 where some reduction in space requirements is necessary. The server data disks are usually mounted on workstations and the data then found:

Current Cycle /usr/illdata/data/instrument/011151 etc

Previous Cycle /usr/illdata/data-1/instrument/000659 etc

Certain instruments, including D16, produce such a large number of files that they have been subdivided into sets of 10000 in subdirectories. Thus:

/usr/illdata/data/d16/d16_0/..... contains runs 1 to 9999

/usr/illdata/data/d16/d16_1/..... contains runs 10000 to 199999 etc.

A.1.1.3. General layout of data files

The text data files can be handled using standard file-utilities available on each system. The internal structure of the data files is delimited by key records indicating the format of the following field. The first part of the file contains information which is common to all runs, and includes the run number, time of recording, experiment name etc. in a specific format, so new ILL utilities (typically Unix shell-scripts) can be developed to emulate functions of the previous database management program SPECTRA. Following the title records, the contents vary from instrument to instrument.

Parameters and data from the counting system are written in blocks of floating - point or integers, each line being padded out to exactly 80 characters of text. Such files can be read in two fashions, either using simple sequential Fortran READs, or using direct access methods (which can have some advantages, allowing data to be skipped, or read in arbitrary order). To allow instruments a further flexibility, variable length data (unspecified text) is also acceptable, providing that the first two fields correspond to the standards described here.

Each instrument, or group of instruments has a specific data format, which evolves in time. To describe the signification of the data elements an optional description may be stored with the raw data within the file.

The second extension is the introduction of a new type of field, the variable length data signified by the key letter V. Standard ILL utilities will not try to interpret data from this key to the end of the file, since the internal structure will be deemed to be specific to the instrument concerned.

Keys, data and text and are written in 80 character fixed length strings (data following the V descriptor have variable length).

A key field signifies a certain type of data field follows, with information on the size of the following field, and how much text (if any) is present describing the field of data.

The text (if present) then follows.

The next records then contain the data.

There then follows another key record for the next data field.

A.1.1.5 Description of stored real parameters

1 contents of preset 1	75 beamstop x /diam mm
2 contents of preset 2	76 beamstop y or 0.
3 time [1/10 s]	77 ISUM X1 cell#
4 total detector counts	78 ISUM X2 cell#
5 total monitor counts	79 ISUM Y1 cell#
6 total selector revs.	80 ISUM Y2 cell#
7 total chopper rev.	81 shear speed (1/min)
15 detector angle (calc)	82 mag. field (Tesla)
16 coder 1 beamstop By mm	83 pressure (bar)
17 coder 2 beamstop Bx mm	84 reactor power (MW)
18 c-3 S-changer trans. mm	85 TOF number of chans
19 c-4 detector distance m	86 TOF delay msec
20 selector speed (1/min)	87 TOF channel width msec
21 chopper1 speed (1/min)	88 TOF channel inc. Factor
22 chopper2 speed (1/min)	89 preset mon/time 0/1
23 voltmeter 1	91 data file version
24 voltmeter 2	92 iris position
25 selector identifier	93 ADC1
26 sample-det distance (calc)	94 ADC2
27 run sequence cycle	95 ADC3
28 run sequence serial	96 ADC4
29 temperature set K	98 DAC2
30 temperature control K	99 DAC3
31 sample temperature K	100 DAC4
32 temp. control off/on 0/1	101 Sample table trans TTR mm
33 IEEE meter -1 at start	102 Sample goniometer angle deg
34 IEEE meter-2 at end	105 TOF/kin current ch start time
35.. further IEEE meters	106 Flipper frequency
:	107 Flipper amplitude
51 beam centre address X0	108 Flipper pickup
52 beam centre address Y0	109 Polarisation
53 wavelength	110 TOF/kin current ch centre time
54 wavelength resolution	111 Current PSU-1 Amp1
55 detector pixel x (mm)	112 Voltage PSU-1 Volt1
56 detector pixel y(mm)	113 Current of PSU-2 Amp2
57 alarms off/on 0/1	114 Voltage of PSU-2 Volt2
58 collimation m	115 Current of PSU-3 Amp3
59 attenuator type	116 Voltage of PSU-3 Volt3
60 attenuator out/in 0/1	
61 det. angle read (deg)	
62 det translation mm	
63 selector angle (deg)	
64 sample distance mm	
65 sample rotation (deg)	
66 changer position	
67 sample height	
68 source ap. left mm	
69 source ap. right mm	
70 source ap. lower mm	
71 source ap. upper mm	
72 source ap. distance mm	
73 sample ap. x /diam mm	
74 sample ap.y or 0. mm	

A1.2 ILL-SANS treated data formats

A.1.2.1 Regrouped data

The generic filenames are derived from nnnnnn, the run number, and eee, the extension, or version number resulting in the name

gnnnnnn.eee

e.g. g006215.000 (from first regrouping)

g006215.001 (from further treatment...)

The first 5 lines of the file are always present and contain information on the internal layout. To simplify use by other packages, the number of Q values and the number of lines to be skipped before the simple table of Q, S(Q) errS(Q) values are found are written in the first line. To allow programs, e.g. *spolly* to annotate the components used in the treated spectra additional text lines may be included. Similarly there is provision for users to develop their own programs, and store additional real parameters in a supplementary region of the file. The overall layout of the file is in sections as follows:

- 1/ - Title line
- 2/ - Key line (identifying the originating instrument)
- 3/ - Indexing for remainder of file
- 4/ - identification of program, date of recording
- 5/ - additional text lines
- 6/ - parameters
- 7/ - user's additional parameters (maximum 20)
- 8/ - PDH parameters
- 9/ - lines of Q, S(Q) and errS(Q)

The following truncated example shows these numbered sections where present.

```
|----- Data File ----->|
1/ Sample - d corrs TEST prot/deutr. ellipt. chs 44 lines+(Q, I(Q), errI(Q))
2/ ILL SANS D11
3/ 8303 1 37 1 42 38
3/ 1 4 32 0 3 1
4/ spol 20-Oct-1995 9:16:09
5/ AvA1 0.0000E+00 AsA2 9.5000E-01 XvA3 1.0000E+00 XsA4 1.0000E+00 XfA5 0.0000E+00
5/ S... 8303 0 1.00E+00 P100 0.5% 221 Sbak 8309 0 2.00E+00 Blank523 193
5/ V... 8301 0 1.00E+00 Hhaps 911
5/
6/ 0.0000 ! Theta-0 Detector offset angle 1
6/ 32.5000 ! X0 cms Beam centre 2
6/ 32.5000 ! Y0 cms Beam centre 3
6/ 1.0000 ! Delta-R cms regrouping step 4
6/ 2.5000 ! SD m Sample-detector distance 5
6/ 10.5400 ! Angstroms incident wavelength 6
6/ 5.6000 ! m collimation distance 7
6/ 1.0000 ! concentration 8
6/ -3. ! ISUM central window sum 9
6/ 1. ! flux monitor counts 10
6/ 180.0000 ! degrees detector sector width 11
6/ 0.0000 ! degrees sector orientation 12
6/ 10.0000 ! % wavelength spread 13
6/ 20.0000 ! mm source slit width x 14
6/ 0.0000 ! mm source slit height y 15
6/ 10.0000 ! mm sample width x 16
6/ 0.0000 ! mm sample height y 17
6/ 10.0000 ! mm detector x pixel size 18
6/ 10.0000 ! mm detector y pixel size 19
6/ 0.0000 ! degrees sample normal/beam 20
6/ 0.0000 ! K sample temperature 21
```

```

6/ 0.0000 ! sample transmission          22
6/ 1.0000 ! mm sample thickness          23
6/ 900.0000 ! counting time secs         24
6/ 0.0000 ! reserved
6/ 0.0000 ! reserved
6/ 0.0000 ! reserved
6/ 0.0000 ! reserved
6/ 0.0000 ! reserved
6/ 0.0000 ! reserved
6/ 0.0000 ! reserved
6/ 0.0000 ! reserved
8/ 37 0 0 0 0 0 6
8/ 0.100000E+01 0.250000E+03 0.000000E+00 0.100000E+01 0.105400E+01
8/ 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
9/ 0.000000E+00 0.000000E+00 0.000000E+00
9/ 2.194656E-03 3.442688E-01 8.329221E-02
9/ 5.466116E-03 3.000000E-01 5.008947E-02
9/ 8.480323E-03 3.877941E-01 4.232426E-02
9/ 1.189216E-02 6.498784E-01 1.519078E-02
9/ 1.497785E-02 7.493181E-01 1.173622E-02
9/ 1.802907E-02 8.019943E-01 1.021966E-02
9/ 2.128347E-02 8.117417E-01 8.385011E-03
9/ 2.433197E-02 8.423974E-01 8.750222E-03
9/ 2.744053E-02 8.300668E-01 7.543748E-03
9/ 3.045397E-02 7.987967E-01 7.683866E-03
9/ 3.403699E-02 7.619627E-01 5.949513E-03
9/ 3.740020E-02 7.112669E-01 6.774296E-03

```

plus additional Q, S(Q), errS(Q) triplets, 37 in all

Details of file format

1/ Title line:

titles short title (20 characters), long title (60 characters)

2/ Key line: 16(A4, 1X) Keys

The first three keys denote ILL SANS data formats are in use, and contain the instrument name.

3/ Indexing for the remainder of the file

IRUN EXT NDATA1 NDATA2 NSKIP NSKIPP

I10, I10, I10, I10, I10, I10

IRUN run number

EXT extension number

NDATA1 number of Q,S(Q),errS(Q) data

NDATA2 dimensionality (see ungrouped data below)

NSKIP the number of lines preceding the Q,S(Q),errS(Q) data from here

NSKIPP the number of lines to skip after this record to find PDF data

IVERS NTXT NPAR NPARX NPDFX IERRS

I10, I10, I10, I10, I10, I10

IVERS version of this data

NTXT number of lines of text in section 5/

NPAR number of parameters in section 6/ (format F10.x)

NPARX number of extra parameters in section 7/ (max=20, format E16.8)

NPDFX number of lines of PDF data

IERRS(for ungrouped data) 0=no errors included, 1=error array follows data

4/ Identification of originating program

PNAM DATE

A4, 1X, A20

Creating program and date and time of file creation

5/ Additional text

Up to 10 lines of additional text may be placed in the data file. In the above case of spolly this contains details of the components used in the corrections: four lines are used hence NTXT=4.

6/ Standard Parameters

One value is given per line (F10), followed by a space, an exclamation mark and a commentary describing the parameter. When circular diaphragms are in use only the widths (x) are non-zero.

7/ Additional parameters

Up to 20 parameters may be placed here in the file. They are stored using the format 5E16.8.

8/ PDH parameters

These three lines contain values which are similar to those used by PDH SAXS data treatment suites.

Integer constants:

8(I9,1x)

I1 number of data points in file

Real Constants

5(E14.6,1X)

R1 concentration

R2 sample-detector distance (cm)

R3 gamma (SAXS)

R4 data scaling multiplier (following=original x R4)

R5 wavelength (nm)

R6 temperature of sample

9/ DATA

NDATA triplets of Q, S(Q) and the statistical error (standard deviation) in S(Q) then follow. Each line has a format 3(E14.6,1X)

A.1.2.2 Data files for Anisotropic Analysis

The generic filenames are derived from nnnnnn, the run number, and eee, the extension, or version number resulting in the name

```

                                tnnnnnn.eee
e.g.                            t006215.001   (from first treatment)
                                t006215.002   (from further treatment...)

```

The layout of the data file follows closely that of the regrouped data. The variables NDATA1 and NDATA2 are used to denote the numbers of x and y cells respectively.

The PDH section is absent, hence NPDFX is set to zero. If IERRS is set to 0 then no array of errors is produced (this occurs when the environment variable SAS_ERROR is set to "none"). The format for the data arrays is 8(E10.3,1X). Thus, even when negative values arise, there is always "white space" between data. As a consequence these lines exceed 80 characters, which has been used as a guide elsewhere to enable files to be printed and, if necessary, edited; this need is not a likely to arise with the full data arrays.

The array ordering is that of successive rows of values,

D(x=1,y=1),D(x=2,y=1),D(x=3,y=1).....D(x=NDAT1,y=1),D(x=1,y=2)...

..... D(x=NDAT1,y=NDAT2)

an example follows:

```

|----- Data File ----->|
1/ Sample - d corrs      TEST prot/deutr. ellipt. chs  40 lines+ I(x,y)//errI(x,y)
2/ ILL SANS D11
3/      8303           1           64           64           38           0
3/      2             4           32           0           0           1
4/ apol 20-Oct-2006 12:44:23
5/ AvA1 0.0000E+00 AsA2 9.5000E-01 XvA3 1.0000E+00 XsA4 1.0000E+00 XfA5 0.0000E+00
5/ S... 8303 0 1.00E+00 P100 0.5% 221 Sbak 8309 0 2.00E+00 Blank523 193
5/ V... 8301 0 1.00E+00 Hhaps 911
5/
6/ 0.0000 ! Theta-0 Detector offset angle 1
6/ 32.5000 ! X0 cms Beam centre 2
6/ 32.5000 ! Y0 cms Beam centre 3
6/ 1.0000 ! Delta-R cms regrouping step 4
6/ 2.5000 ! SD m Sample-detector distance 5
6/ 10.5400 ! Angstroms incident wavelength 6
6/ 5.6000 ! m collimation distance 7
6/ 1.0000 ! concentration 8
6/ -3.0000 ! ISUM central window sum 9
6/ 1.0000 ! flux monitor counts 10
6/ 80.0000 ! degrees detector sector width 11
6/ 0.0000 ! degrees sector orientation 12
6/ 10.0000 ! % wavelength spread 13
6/ 20.0000 ! mm source slit width x 14
6/ 0.0000 ! mm source slit height y 15
6/ 10.0000 ! mm sample width x 16
6/ 0.0000 ! mm sample height y 17
6/ 10.0000 ! mm detector x pixel size 18
6/ 10.0000 ! mm detector y pixel size 19
6/ 0.0000 ! degrees sample normal/beam 20
6/ 0.0000 ! K sample temperature 21
6/ 0.0000 ! sample transmission 22
6/ 1.0000 ! mm sample thickness 23

```

```

6/ 935.0000 ! counting time secs          24
6/ 0.0000 ! reserved
6/ 0.0000 ! reserved
6/ 0.0000 ! reserved
6/ 0.0000 ! reserved
6/ 0.0000 ! reserved
6/ 0.0000 ! reserved
6/ 0.0000 ! reserved
6/ 0.0000 ! reserved
6/ 0.0000 ! reserved
9/ 0.000E+00 6.833E-01 -2.375E-01 2.625E-01 2.000E-01 0.000E+00 1.000E+00 1.750E-01
9/ 0.000E+00 1.000E+00 1.667E-02 1.000E+00 1.150E-01 8.434E-02 6.612E-02 1.373E-01
9/ 1.475E-01 9.699E-02 1.472E-01 9.640E-02 1.129E-01 1.792E-01 1.801E-01 1.757E-01
9/ 1.384E-01 1.271E-01 2.322E-01 1.743E-01 1.313E-01 1.671E-01 1.757E-01 1.733E-01
9/ 1.583E-01 1.632E-01 1.868E-01 1.901E-01 1.880E-01 1.982E-01 1.326E-01 1.559E-01
9/ 1.374E-01 1.922E-01 1.093E-01 1.762E-01 1.415E-01 1.772E-01 1.526E-01 1.466E-01
9/ 1.016E-01 1.033E-01 8.145E-02 -2.375E-01 2.929E-01 0.000E+00 1.000E+00 5.250E-01

```

a total of 64 x 64 values of intensity, followed by the same number of error values

A.1.2.3. Mask files

These are printable ascii files which contain the detector image viewed from the reactor where cells to be eliminated are marked with a # symbol, and cells to be used are shown with a period.

First line Title(a20),Date(a20)

Second line NDATA(I8)

size of following mask NDATA=1024 (64x16), 4096 (64x64), or 16384 (128x128)

There then follow 16, 64 or 128 lines containing the detector image, starting at the top of the detector, with either 64 or 128 characters showing the current mask.

Note: in all other types of 2-D data files the storage commences with the bottom row of data. The mask file has this alternative row order to have a correctly printed image of the detector mask, viewed from the sample.

Routines for accessing data

A2

The following routines are incorporated in the library /usr/ill/lib/librllib.a, and in the PC library librllib.a

If the environment variable "SAS_DEBUG" is set to true then messages are written out as the data are read in which can help find errors in input files.

A.2.1 RGIO, reads and writes regrouped data

```

SUBROUTINE RGIO(IER, MM, IRUN, IRUNX, TEXT, PAR, NDATA, Q, S, ES, PNAME)

IER      integer      out    0 no error, -1 error
MM       character*1  in     set to 'R' read or 'W' write
IRUN     integer      in     run number
IRUNX    integer      in     extension number
TEXT     character*50 i/o    TEXT(1:20) short title, TEXT(21:50) long title
PAR      real array   i/o    standard ILL-SANS parameters
                               (1-8) THETA0,X0,Y0,DR,SD,WAV,COLL,CONC
                               (9-16)
ISUM,MONITOR,SECT,PHI0,WAV%,SOURCEx,SOURCEy,SAMx
                               (17-24) SAMPLE-
y,PIXx,PIXy,ANGSAMNOR,TEMP,TRANS,THICK,duration
                               (25-32) reserved
                               (33-40) unused
                               dimension (40)
NDATA    integer      i/o    number of Q values in file
Q        real array   i/o    Q ( )
S        real array   i/o    S(Q) ( ) typically a maximum of 180 values
ES       real array   i/o    error in S(Q) ) see "LIMDAT" below
PNAME    character*4  in     calling program's name

```

For additional control of the functions of this routine the following COMMON blocks contain useful variables, while keeping the basic call as simple as possible. The COMMON blocks are pre-initialised within the standard library.

```

COMMON/RGIOX/NTXT,NPARX
NTXT     integer      in/out Number of extra lines of text set in XTXT
NPARX    integer      in/out Number of extra parameters in PARX (max=20)

COMMON/RGIOC/XTXT(10)
XTXT     character*80 in/out extra text data for storage from retrieval

COMMON/RGIOP/PARX(20)
PARX     real          in/out array of extra parameters

COMMON/RGIOY/NUNIT,NTTY
NUNIT    integer      in     unit number for i/o operations - default is 32
NTTY     integer      in     output for error messages - default is 6

COMMON/RGIOL/NDIM,LIMDAT,LIMTXT,LIMPX,IONCE
          default
NDIM     integer      1      dimensionality of data
LIMDAT   integer      180    maximum number of data points
LIMTXT   integer      10     maximum number of lines of added text
LIMPX    integer      20     maximum number of extra parameters
IONCE    integer      0      flag showing initialisations complete

```

RSIO, reads and writes ungrouped data

```

SUBROUTINE RSIO(IER, MM, IRUN, IRUNX, NSET, TEXT, PAR, DAT, ERD, PNAME)

IER      integer      out    0 no error, -1 error
MM       character*1  in     set to 'R' read or 'W' write
IRUN     integer      in     run number
IRUNX    integer      in     extension number
NSET     integer array i/o
          NSET(1) number of characters in extra text
          NSET(2) number of parameters in PAR (40)
          NSET(3) number of parameters in PARX
          NSET(4) NX number of column data (x)
          NSET(5) NY number of row data (y)
          NSET(6) set to 1 if standard errors follow data

TEXT     character*50 i/o    TEXT(1:20) short title, TEXT(21:50) long title
PAR      real array   i/o    standard ILL-SANS parameters
          (1-8) THETA0,X0,Y0,DR,SD,WAV,COLL,CONC
          (9-16)
ISUM,MONITOR,SECT,PHI0,WAV%,SOURCEx,SOURCEy,SAMx
          (17-24) SAMPLE-
y,PIXx,PIXy,ANGSAMNOR,TEMP,TRANS,THICK,spare
          (25-32) reserved
          (33-40) unused
          dimension (40)
DAT      real array   i/o    intensity/cell for nset(4) x nset(5) cells
ERD      real array   i/o    error/cell for nset(4) x nset(5) cells
PNAME    character*4  in     calling program's name

```

Again a number of COMMON blocks contain useful additional control parameters.

```

COMMON/RGIOC/XTXT(10)
XTXT     character*80 in/out extra text data for storage from retrieval

COMMON/RGIOP/PARX(20)
PARX     real          in/out array of extra parameters

COMMON/RSUNIT/NUNIT
NUNIT    integer      in     unit number for i/o operations (default 33)

COMMON/MAXARR/LTITL,LPARR,LPARX,LDATX
LTITL    integer      in     maximum number of characters from raw
          data (default=512)
LPARR    integer      in     maximum number of raw data parameters (128)
LPARX    integer      in     maximum number of extra parameters PARX (20)
LDATX    integer      in     maximum number of data (16384)

```

When IRUNX is zero this subroutine calls SASAS, and reads the raw data. Otherwise the data are written back and read from files with names:

```

          tnnnnnn.eee
e.g.     t002359.001

```

where nnnnnn is the run number
and eee is the extension number

For use with raw data the following environment variables must be defined

```

SAS_INSTRUMENT  name of instrument
SAS_DATA_PATH   directory in which the raw data is stored

```

```

e.g. % setenv SAS_INSTRUMENT d22
      % setenv SAS_DATA_PATH /data/d22/      (for the current cycle)

```

If the environment variable SAS_ERROR is set to NONE then no errors for 2D data will be stored. The resultant datasets are then approximately half-size; statistical errors are still reflected to some degree in the dispersion of local data values about the mean.

A.2.2 SASAS, reads raw data

```
SUBROUTINE SASAS( IER, IRUN, INST, NOMEKP, DDATE, NT, TITL, NP, PARR, ND, IDON)
```

```

      reading standard ILL-SANS ascii files
IER      integer                out  0 ok, else -1
IRUN     integer                in   1<=IRUN<=999999 run number
INST     character*4            out  inst field in file
NOMEKP   character*10          out  nomexp in file
DDATE    character*20          out  data and time of recording
NT       integer                out  number of titl characters (a1)
TITL     character*1 array     out  titl array
NP       integer                out  number of real parameters PARR
PARR     real array             out  real parameters
ND       integer                out  number of integers in spectrum
IDON     integer array         out  spectrum

```

Data are read on unit 31, set as default in a common block,

```
COMMON/SASASC/NUNIT
```

Another common block /LIMINP/ allows reading to be terminated after having read LIMIT data fields. It can be used to read the titles, for example, without the 4k or 16 k data, when limit=2

```
COMMON/LIMINP/LIMIT
```

The routine SASAS limits input from data files to protect the calling program from being overwritten. These limits are set in a common block.

```

COMMON/MAXARR/NTITL,NPAR,NPARX,ND
NTITL   integer                max number of characters in title record (512)
NPAR    integer                max number of parameters (128)
NPARX   integer                maximum number of additional parameters (20)
ND      integer                maximum number of data (16384)

```

SASAS uses the environment variables SAS_INSTRUMENT, SAS_DATA_PATH and SAS_DEBUG.

A.2.3 GRUNDD, reads in a mask file

```

SUBROUTINE GRUNDD(IGRU)
IGRU     character*1            out  2D array containing # or . symbols

```

Data are read on unit 1 set as default in a common block

```
COMMON/MSKUNIT/NU
```

The expected spectrum length is set with ND (1024, 4096, 16384) corresponding to spectra which are 64x16, 64x64, and 128x128 respectively.

```
COMMON/MAXARR/NTITLE,NPAR,NPARX,ND
```

The terminal input unit is INP, output is KOUT

```
COMMON/TTYIO/INP,KOUT,IERT
```

The unit LOUT logs the successful reading of the mask

```
COMMON/LPOUTC/LOUT
```

A.2.4 Data ordering in 2D data

2D data are returned as 1D vectors, length 1024, 4096 or 16384, read explicitly by Fortran as ((V(IX,IY),IX=1,NX),IY=1,NY), but usually as equivalenced 1D arrays (see addresses pp33,123)

Unix environment for SANS treatment at ILL

A3

.cshrc setup files

To define the SANS computing environment the setup procedure is usually invoked by the source command. For Macintosh OSX the programs are run in an Xterm window; the distribution includes a standard copy of tk/tcl software for the GUIs.

```
% source /home/cs/sans/sassetup
```

This follows the system login files which, on the instrument visitor zones, define the instrument name and the default data path, and, usually, default printers/plotters. These include the following variables which are not in the sassetup procedure.

```
SAS_DATA_PATH
SAS_INSTRUMENT
SAS_DEF_PRINTER
SAS_DEF_PLOTTER
```

sassetup

```
# SANS setup file at ILL for SGI-IRIX, Linux, Macintosh OS-X
# invoked as % source /home/cs/sans/sassetup
#
# requires modifications to /etc/cshrc reflect location of host
# instrument specific parts are placed in
# .login for standard users, or
# e.g. /home/vis/d22/.login.group for visitor_d22 zones etc.
# (this is invoked by getname procedure in F. Pinet's login routine)
#
# started 29-Oct-1995 R.E. Ghosh
#-----
#                               /etc/cshrc
# 1. /etc/cshrc could define SAS_ROOT (the present directory)
# 2. /etc/cshrc should define SAS_DEF_PRINTER a local printer (host
# dependent)
# =====
# .login or .login.group e.g. for D11
# setenv SAS_INSTRUMENT d11
# setenv SAS_DATA_PATH /usr/illdata/data/d11
# source $SAS_ROOT/sassetup
#-----
# The .login files in /home/group/xxxx set an absolute path, requiring
# the re-invocation of /etc/cshrc
#=====
#                               Mounted filesystems
# This setup file assumes that the SAS program root directory SAS_ROOT
# has been mounted (SAS_ROOT ==> /home/cs/sans) and that, for Linux, the
# filesystem /usr/public/ has been mounted too.
# The standard mountpoint for data is /usr/illdata
# these are set in standard automount maps.
# manually:
# mount serhom:/home/cs /home/cs
# mount serdon:/illdata /usr/illdata
# for linux
# mount serhom:/usr/idefix/public/linux /usr/public
#                               expectk
# This is the primary gui and is system dependent and may not
# be moved from its place of installation - only linked.
# For SGI it was installed in SAS_ROOT
# For OSX it was installed in /sw (copy in $SASROOT/Osx/expect5.39.zip)
# For Linux it was installed in /usr/public/bin/expectk
# in each case the expectk in the $SAS_ROOT/system/expectk is linked
# to the appropriate expectk
#=====
# This present file contains environment variables primarily, rather than
```

```
# executables which are all in SAS_DIR
if ( $?NEW_SAS_SETUP == 0 ) then
# remaining steps 1,2,3,4,5 will be skipped
set OSNAME=`uname -s`
setenv SAS_ROOT /home/cs/sans
echo "OSNAME is " $OSNAME
switch ($OSNAME)
  case 'IRIX*' :
    setenv SAS_DIR $SAS_ROOT
    setenv COMPILER_DEFAULTS_PATH /home/cs/sans
    alias help "$SAS_ROOT/help"
    alias oldsetup "setenv NEW_SAS_SETUP undefined;source
/home/cs/sans/sassetup-1"
    echo New sassetup procedure for SGI-IRIX
    echo For previous setup give command oldsetup
    breaksw
  case 'Linux' :
    setenv SAS_DIR $SAS_ROOT/Linux
    alias help "/usr/local/bin/mozilla
http://www.ill.fr/data_treat/sanstreat.html"
    breaksw
  case 'Darwin' :
    setenv SAS_DIR $SAS_ROOT/Osx
    alias help "/Applications/Safari.app/Contents/MacOS/Safari
http://www.ill.fr/data_treat/sanstreat.html"
    breaksw
endsw
setenv MY_INST NONE
switch ($USER)
  case 'd11'
    setenv MY_INST d11
  breaksw
  case 'd16'
    setenv MY_INST d16
  breaksw
  case 'd22'
    setenv MY_INST d22
  breaksw
endsw
# note if the DATA_PATH is predefined this is used (e.g. at instrument)
if ($MY_INST !~ "NONE") then
  if($?SAS_INSTRUMENT == 0) then
    setenv SAS_INSTRUMENT $MY_INST
  endif
  if ($?SAS_DATA_PATH == 0) then
    setenv SAS_DATA_PATH "/usr/illdata/data/"$MY_INST/"
  endif
  else
    setenv SAS_INSTRUMENT $MY_INST
    setenv SAS_DATA_PATH $MY_INST
  endif
endif
# to get non-US date formats on some systems
unsetenv LANG
#echo "#1"
if (! $?SAS_DEF_PRINTER ) then
  setenv SAS_DEF_PRINTER lp
  echo "Not standard SAS_DEF_PRINTER"
endif
if (! $?SAS_DEF_PLOTTER ) then
  setenv SAS_DEF_PLOTTER lp
  echo "Not standard SAS_DEF_PLOTTER"
endif
#echo "#1b"
echo "$SAS_DIR" is being added to path"
set path = ( . $SAS_DIR $SAS_ROOT $path )
rehash
#echo "#2"
setenv SAS_CHECK limited
setenv SAS_DECOMPRESS zcat
# places executables in current path
setenv ILLUSER_DIR "$SAS_ROOT/"
# for graphics:
setenv PGPLOT_XW_WIDTH 0.45
setenv PGPLOT_ILL_DEV_1 /xserv
setenv PGPLOT_ILL_DEV_2 /vcps
setenv PGPLOT_ILL_DEV_3 /null
setenv PGPLOT_ILL_PPAGE 2
setenv PGPLOT_ILL_PGRUNFIGDISP figdisp
setenv PGPLOT_DIR $SAS_DIR
# for mosaic 2.75
setenv http_proxy "http://proxy.ill.fr:8888/"
setenv ftp_proxy "http://proxy.ill.fr:8888/"
setenv gopher_proxy "http://proxy.ill.fr:8888/"
```


PC environment for ILL SANS data treatment

A4

SANS programs for PCs

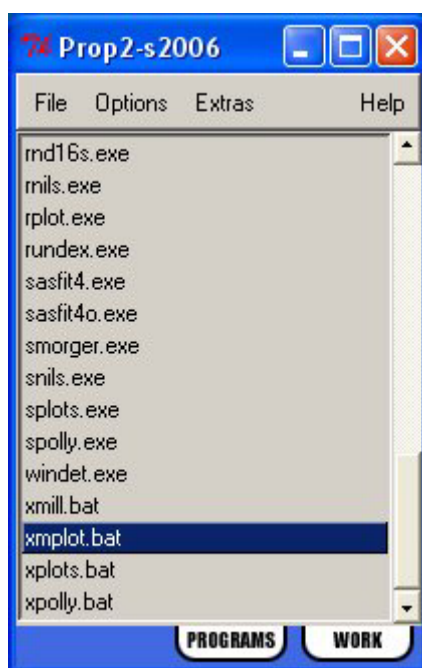
The full set of programs to analyse the ILL SANS data on PCs is available on the ILL anonymous ftp-server, ftp.ill.fr They may be copied from here, together with useful library routines librlib.a, and fitting and plotting libraries. All have been created with free Open source GNU compilers from the MinGW distribution. .

ILL does not guarantee the correctness of the programs, though all have been subjected to tests; any comments concerning errors or improvements will be welcomed as will requests for programs not yet included in this PC set. Emails to R. Ghosh (ron@ill.fr)

Prop

running programs

PC users expect easy operations of clicking to run programs, print etc, using Windows printers. To provide an environment for opening programs originating in linux (and before!) the *prop* program was written to launch programs and bring back results in an editor for viewing and printing. It also manages the many environment variables described in chapter 5, avoiding modifying system files.



The program includes on-line help, and a description is also available at

<http://www.ill.fr/Computing/prop>

When the program is started for the first time the raw data, program, and work directories must be defined. Using the browse button will simplify finding a target directory. To change disk drive type a drive name, e.g. D: in the directory name space and click on Go To in order to browse for the directory. In general you are recommended to use short directory names with no embedded spaces!

Prop uses the notion of projects to group together these sets of programs, raw data, and current work directories. It remembers a number of previous projects which can be recalled, resetting these directories to their prior values. Once defined the main window of *prop*, shown above, has two main tabs, one to view the program list, where clicking on the name starts the program. The WORK tab shows the files in the current work directory. Clicking on these file names brings these result files into an editor, from where they can be examined and printed.

The Extras menu includes the possibility of creating a DOS shell window with the predefined working directory and environment using the `cmd` command. This offers a simple way to use `zip` and other command line programs.

plotting output

The Windows output uses the GRWIND.EXE program of Tsuguhiro Tamaribuchi. This produces display output which can then be printed on standard Windows printers. The optional PostScript file and GIF output are also available (see p. 40)..

Obtaining the program set

We assume the PC users will be using *prop* hence part of the necessary components to run the programs are already packaged in the *prop* distribution to be found with descriptions at

`ftp://ftp.ill.fr/pub/cs/prop`

The programs may be obtained from:

`ftp://ftp.ill.fr/pub/cs/sans`

This contains the program directory with the necessary configuration files for *prop* and includes a small amount of test data and examples.

These programs are the property of the ILL. The programs are made available for use on academic sites with no charge on the condition that no commercial use is made of the results.

SANS Experiment Check List

A5

Actions and Programs

This short section summarises performing an experiment, naming programs which can be used in a systematic fashion which will help prepare for objective data treatment.

Set-up and measurements

1. Decide on the instrument configuration or configurations for the Q range and Q resolution. Often several experiment set-ups will be needed, and the items in this check list will have to be repeated for each setting.
2. Set wavelength, collimation, apertures and sample-to-detector distance.
3. Align sample holder and/or sample changer. Check positions near both ends of the sample changer racks. For precise work it may be necessary to evaluate the transmission of each cell or position in a sample rack separately.
4. Determine the beam centre from a scattering sample (e.g. PTFE) or the attenuated direct beam. Use *windet* (p 44) to evaluate results. Enter X0 and Y0 in the instrument control parameters.
5. Align beam stop. Note position and decide on an offset position for transmission measurements.
6. Check scattering from an empty sample holder to see there are no reflections or other parasitic scattering. Use *xplots* (p 101) to look at the whole detector image.
7. Measure “beam-blocked” background to make sure there is not an excessive electronic or other spurious background when B₄C is in the beam. This signal may be so low that it may be ignored as statistically insignificant in the subsequent analysis.
8. Run short measurements on detector calibration materials (V, H₂O, or plastic sample with appropriate background) to see that the detector response is reasonable. Measure transmissions and check that the background subtraction is reasonable. Use *xplots*, *rnils* (p 58), and *mplot* (p 76) to look at data.
9. Set up a mask file from the test calibrant runs. Use *rmask* (p 49) to create the file. Look for poor lines or areas obscured by the beam stop with *colrow* (p 105) or *xplotc* (p 99).
10. Run a wavelength calibrant such as silver behenate (p 24) to check Q calibration. Average data with *rnils* and use *sasgau* (p 108) to fit the peak.
11. Measure samples. Use repetitive cycles if individual data acquisition periods exceed 10 to 15 minutes, and use *rundex* (p 47) to check that count rates in these sets are stable. Inspect each data set with *xplots*, or use *rnils* and *mplot*. Each cycle should contain calibrant and empty cell. Once checked the individual runs can be added together.

Data Analysis
Check List

12. Measure the transmission of each sample. Use *windet* to evaluate the transmissions.
13. Check that all necessary contrasts and the corresponding backgrounds have been measured. This avoids possible inaccuracies arising through interpolation or scaling results. Compare the regrouped intensities of different samples (*rnils*) to see that they follow expected variations with contrast, concentration and incoherent scattering background. Use the divider in *mplot* to scale data for quick preliminary checks.
14. Produce summary lists of data acquisition with *rundex* (p 47). Check there are no unexpected changes in detector or monitor count rates.
15. Make copy of experiment entries from the instrument log book
16. For the full analysis it is often convenient to make a new sub-directory, *mkdir* (p 38), to separate these results from earlier trials, and change to this as the current work directory *cd* (p 38).
17. Use a *rundex* listing to provide summaries of measurements on each sample and background in different configurations.
18. Check all sample transmissions. These are calculated with *windet*. The values are recorded in file *sans.trm*
19. Check masks. Use *grund* (p 52) if necessary on flat calibrant runs.
20. Prepare information for data reduction with *spolly*, *xpolly* (pp 61,66) or *anpoly* (p 86). This will involve sample thickness, transmission and data for the calibrant sample.
21. Average data if required with *rnils* (p 58) or *areg* (p 87) using masks. If a fresh directory has been used (step 16) the extension numbers will be sequenced systematically.
22. Correct data with *spolly*, *xpolly*, etc.
23. Check results and repeat calculations if the data appear anomalous. Look at the stored history in the reduced data files if there are unresolved problems. Typical problems arise from use of data measured in different configurations, mistyping a run number or transmission or including a transmission measurement in place of cross-section data. Use *xmplot* or *xplots* to look at the results. Data from different configurations with suitable corrections can be merged using *smorger*, (p 82).
24. Make a copy of reduced data to take home for further analysis. Use *zip* (p 111) to create a convenient data file to send by ftp (in binary mode).

XML Data Output

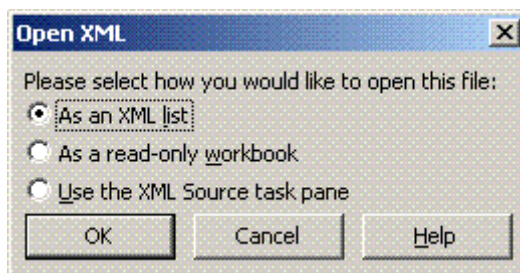
A6

Introduction

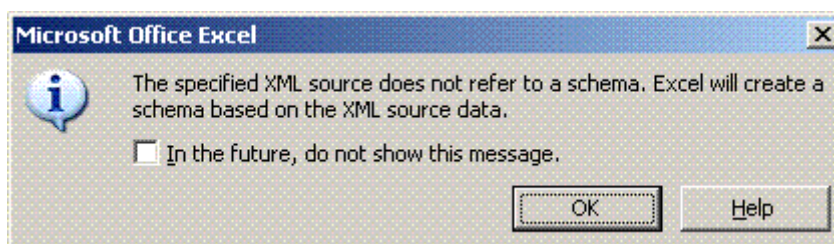
Once data are represented in an XML text file an increasing number of standard tools can be used to transpose the contents to a second standard form, and such transformations can be automated. Of more practical importance to occasional users of SAS facilities is that Excel 2003 will read datafiles produced from *g2x* and *g2xfull* placing the data for Q, I, Idev and Qdev in the first four columns, automatically linking each row. By including white-space around the column values other spreadsheet programs too can read these data with some ease. The future therefore will offer more opportunities for exploiting these files. This appendix has been added to stimulate the discussion and potential standardisation of such data files for small angle scattering

Excel 2003

The XML files can be opened easily using Microsoft Excel 2003. A simple approach is to start Excel and either use the File Open menu or to drag the file on to a blank Worksheet. In either case the following dialogue box will appear:



You can then select "As an XMLlist" and a further query will appear:



Simply choosing OK allows Excel to create a schema itself.

The data will then appear in columns in the Excel spreadsheet, and the first four columns of Q, I, Idev and Qdev will remain coupled if, for example, resorted.

	A	B	C	D	E	F	G	H	I
	Q_A-1	I_cm-1	Idev_cm-1	Qdev_A-1	Title	Source_file	Flux_monitor	Count_time_secs	Q_resolution
1	0	0	0	0	7D1 2mm	"g009346.001"	1	100	"estimated"
2	0.000785398	0	0	0.000529052	7D1 2mm	"g009346.001"	1	100	"estimated"
3	0.001570796	0	0	0.000546264	7D1 2mm	"g009346.001"	1	100	"estimated"
4	0.002356194	0	0	0.000573805	7D1 2mm	"g009346.001"	1	100	"estimated"
5	0.003423113	-10.13887	-15.95304	0.000625238	7D1 2mm	"g009346.001"	1	100	"estimated"
6	0.003986425	-104.0687	-604.0934	0.000657775	7D1 2mm	"g009346.001"	1	100	"estimated"
7	0.004747937	28.03847	21.78166	0.000706535	7D1 2mm	"g009346.001"	1	100	"estimated"
8	0.005511106	13.05283	2.717132	0.000759933	7D1 2mm	"g009346.001"	1	100	"estimated"
9	0.006312272	9.199719	1.025447	0.000819901	7D1 2mm	"g009346.001"	1	100	"estimated"
10	0.007086647	8.427243	0.7807953	0.000880835	7D1 2mm	"g009346.001"	1	100	"estimated"
11	0.007858813	7.684547	0.5645913	0.000944158	7D1 2mm	"g009346.001"	1	100	"estimated"
12	0.008645013	7.676375	0.5031449	0.001010548	7D1 2mm	"g009346.001"	1	100	"estimated"
13	0.009420658	7.693844	0.4735682	0.001077662	7D1 2mm	"g009346.001"	1	100	"estimated"
14	0.01021134	7.626715	0.4288891	0.001147435	7D1 2mm	"g009346.001"	1	100	"estimated"
15	0.0110032	7.296264	0.3833572	0.001218451	7D1 2mm	"g009346.001"	1	100	"estimated"
16	0.01178024	7.506202	0.3720536	0.001289065	7D1 2mm	"g009346.001"	1	100	"estimated"
17	0.01257099	7.551725	0.3677744	0.001361718	7D1 2mm	"g009346.001"	1	100	"estimated"
18	0.01335339	7.271583	0.3373113	0.001434273	7D1 2mm	"g009346.001"	1	100	"estimated"
19	0.01412778	6.848637	0.2879251	0.001506647	7D1 2mm	"g009346.001"	1	100	"estimated"
20	0.01492401	7.045397	0.2919511	0.001581563	7D1 2mm	"g009346.001"	1	100	"estimated"
21	0.01571944	7.026912	0.2918268	0.001656843	7D1 2mm	"g009346.001"	1	100	"estimated"
22									

g2x, g2xfull

These programs operate on a standard regrouped data file `gnnnnn.eee` and convert it to an XML file `xgnnnnnn_eee.xml`. The principal results are the same from both programs, notably including a fourth table column estimating the Q resolution. `g2xfull` adds the parameters suitably annotated in XML. The XML files will be produced as each standard file is produced if the environment variable `SAS EXTRA G` is set to `g2x` or `g2xfull` with typical output following:

```
<?xml version="1.0" encoding="utf-8" ?>
<SASroot>
  <SASentry>
    <SASdata>
      <Idatum><Q_A-1> 0.000000E+00 </Q_A-1><I_cm-1> 0.000000E+00 </I_cm-1><Idev_cm-1> 0.000000E+00 </Idev_cm-1><Qdev_A-1>
0.000000E+00 </Qdev_A-1></Idatum>
      <Idatum><Q_A-1> 7.853982E-04 </Q_A-1><I_cm-1> 0.000000E+00 </I_cm-1><Idev_cm-1> 0.000000E+00 </Idev_cm-1><Qdev_A-1>
5.290519E-04 </Qdev_A-1></Idatum>
      <Idatum><Q_A-1> 1.570796E-03 </Q_A-1><I_cm-1> 0.000000E+00 </I_cm-1><Idev_cm-1> 0.000000E+00 </Idev_cm-1><Qdev_A-1>
5.462641E-04 </Qdev_A-1></Idatum>
      <Idatum><Q_A-1> 2.356194E-03 </Q_A-1><I_cm-1> 0.000000E+00 </I_cm-1><Idev_cm-1> 0.000000E+00 </Idev_cm-1><Qdev_A-1>
5.738046E-04 </Qdev_A-1></Idatum>
      <Idatum><Q_A-1> 3.423113E-03 </Q_A-1><I_cm-1> -1.013887E+01 </I_cm-1><Idev_cm-1> -1.595304E+01 </Idev_cm-1><Qdev_A-1>
6.252376E-04 </Qdev_A-1></Idatum>
      <Idatum><Q_A-1> 3.986425E-03 </Q_A-1><I_cm-1> -1.040687E+02 </I_cm-1><Idev_cm-1> -6.040934E+02 </Idev_cm-1><Qdev_A-1>
6.577747E-04 </Qdev_A-1></Idatum>
      <Idatum><Q_A-1> 4.747937E-03 </Q_A-1><I_cm-1> 2.803847E+01 </I_cm-1><Idev_cm-1> 2.178166E+01 </Idev_cm-1><Qdev_A-1>
7.065347E-04 </Qdev_A-1></Idatum>
      Omitting the middle section of the data table
      <Idatum><Q_A-1> 5.018928E-02 </Q_A-1><I_cm-1> 2.132738E+00 </I_cm-1><Idev_cm-1> 2.599679E-01 </Idev_cm-1><Qdev_A-1>
5.046520E-03 </Qdev_A-1></Idatum>
      <Idatum><Q_A-1> 5.095456E-02 </Q_A-1><I_cm-1> 1.576560E+00 </I_cm-1><Idev_cm-1> 2.831447E-01 </Idev_cm-1><Qdev_A-1>
5.122649E-03 </Qdev_A-1></Idatum>
      <Idatum><Q_A-1> 5.156558E-02 </Q_A-1><I_cm-1> 4.056215E+00 </I_cm-1><Idev_cm-1> 3.662568E+00 </Idev_cm-1><Qdev_A-1>
5.183439E-03 </Qdev_A-1></Idatum>
      <Idatum><Q_A-1> 5.262168E-02 </Q_A-1><I_cm-1> 0.000000E+00 </I_cm-1><Idev_cm-1> 0.000000E+00 </Idev_cm-1><Qdev_A-1>
5.288529E-03 </Qdev_A-1></Idatum>
      <Idatum><Q_A-1> 5.340708E-02 </Q_A-1><I_cm-1> 0.000000E+00 </I_cm-1><Idev_cm-1> 0.000000E+00 </Idev_cm-1><Qdev_A-1>
5.366696E-03 </Qdev_A-1></Idatum>
    </SASdata>
    <Title>7D1 2mm </Title>
    <Source_file>"g009346.001"</Source_file>
    <Flux_monitor> 1.00</Flux_monitor>
    <Count_time_secs> 100.000</Count_time_secs>
    <Q_resolution>"estimated"</Q_resolution>
  </SASsample>

```

```

<sample_temperature>    0.0000 </sample_temperature>
<sample_offset_angle_deg>    0.000 </sample_offset_angle_deg>
<sample_x_mm>    8.00 </sample_x_mm>
<sample_y_mm>    0.00 </sample_y_mm>
<sample_transmission>    0.0000 </sample_transmission>
<sample_thickness_mm>    0.00 </sample_thickness_mm>
</SASsample>
<SASinstrument name="D22 " >
<SASsource>
<radiation> neutron </radiation>
<beam_x_mm>    30.00 </beam_x_mm>
<beam_y_mm>    0.00 </beam_y_mm>
<wavelength_A>    8.00 </wavelength_A>
<wavelength_spread>    0.10 </wavelength_spread>
</SASsource>
<SAScollimator>
<distance_coll_m>    11.200 </distance_coll_m>
</SAScollimator>
<SASdetector>
<offset_angle_deg>    0.00 </offset_angle_deg>
<x0_cm>    47.03 </x0_cm>
<y0_cm>    47.78 </y0_cm>
<distance_SD_m>    10.000 </distance_SD_m>
<pixel_x_mm>    7.50 </pixel_x_mm>
<pixel_y_mm>    7.50 </pixel_y_mm>
</SASdetector>
</SASinstrument>
<SASprocess name="spol" >
<date> 1-Jul-1998 14:57:37 </date>
<radialstep_cm>    1.000 </radialstep_cm>
<sector_width_deg>    180.0 </sector_width_deg>
<sector_orient_deg>    0.0 </sector_orient_deg>
<SASnote_01> AvA1 4.8700E-01 AsA2 9.2700E-01 XvA3 4.3800E-02 XsA4 1.6360E-01 XfA5 0.0000E+00 </SASnote_01>
<SASnote_02> S... 9346 0 2.23E+01 7D1 2mm          Sbak 9345 0 2.23E+01 D20 2mm          </SASnote_02>
<SASnote_03> Vbak 9343 0 2.23E+01 Empty Qtz Cell V... 9342 0 2.23E+01 H2O 1mm          </SASnote_03>
<SASnote_04> Cd/E 9340 0 2.23E+01 Cd - Bgd          </SASnote_04>
</SASprocess>
</SASentry>
</SASroot>

```

The minimal output of `g2x` omits the sections `SASsample`, `SASinstrument`, and `SASprocess`.

Recommended formatting and units Column data items are surrounded by white space; this allows the data to be read by a number of spreadsheet programs in addition to Excel. XML tag names include units explicitly

The XML data format implicitly expects the file to be analysed by parsing software. This allows some flexibility in choice of, say units. Here `g2x*` will set the units for intensity as either `counts` or `cm-1` depending on whether raw data or treated data are present. The Q units may be either `Å-1`, or `nm-1`. The output of `g2x*` is in `Å-1`.

Updates 2012

Introduction

There have been numerous internal changes to programs described in this manual since the last full edition in 2006. For the user most features are transparent and the main text here consequently has not been edited. The 2006 edition was created by Macintosh-Word5 to PC-Word10, with a mixture of picture-file formats. The pagination is consequently fragile and making many fine detail corrections to this manual would probably lead to more errors than being mildly inconvenienced by the small changes introduced to control the present programs. This appendix summarises new program variants, and is followed by a more technical section on changes to improve shareability and general performance.

The main change in usage of the original programs has been the extension to majority usage on PC-Windows and Macintosh laptops. The *prop* program has proved very useful for the PC. For the Macintosh the retention of use of the terminal utility approach offers the advantages of the Unix features though initially requiring some understanding by the user; however the usage closely resembles the scripts illustrated here in the main text for Linux systems. The choice of operating system and whether to use a graphical user interface (GUI) or command line input for the most common programs allows users with different levels of experience and expertise to use the same software.

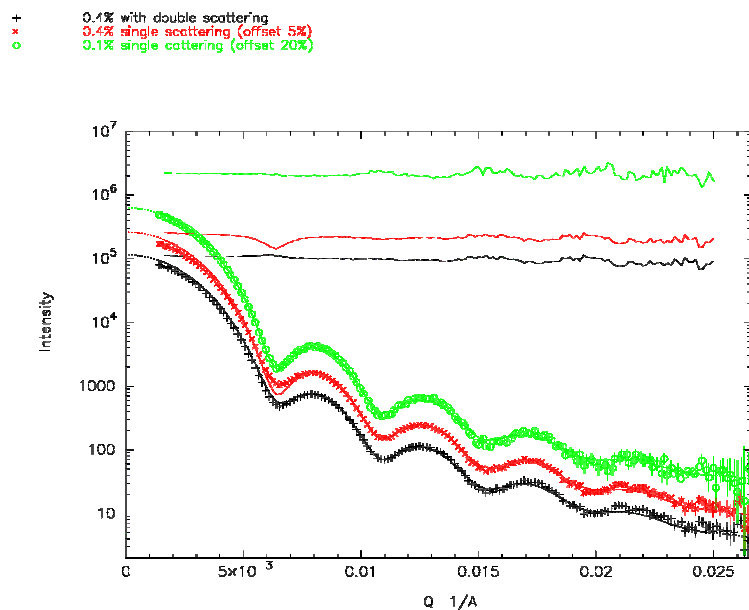
New programs and modifications

spod16, sumraw

rreg, xreg

The instruments have been re-equipped with new detectors; in the case of D16 the Miland detector (320x320 pixels) has deliberately lead to a wider programme of use with single crystals as well as requiring the expansion of arrays in existing programs. Regrouping programs *rnd16*, *rnd16s* and *red16*, masking etc have been updated to cope, and *spod16* can scan through large sequences of data looking for spots of intensity as a preliminary for further analysis, and *sumraw* will sum together a set of raw data files output as a treated 2D data file. For the standard SANS instruments the regrouping programs *rnils*, *snils* now can save the parameters in named files *mynewname.rrg*. This simplifies treatment of sequences of data measured in repeating alternate configurations. The program *rreg* (and GUI version *xreg*) can reread these *_rrg* files and treat raw data; if no file name is given the standard file *sasval.par* is used.

Improved controllability of diaphragms now allows resolution to be modelled and tested well. The canSAS XML 1D data format includes resolution estimates; instruments with velocity selectors and pinhole geometry are simplest in treatment. Earlier work on spherical viruses (*ssqfun*, Zulauf) and micelles and coated spheres (Harris & Ottewill) refined the radial structures using differing scattering densities and contrast variation taking into account basic pinhole resolution. Today the effects of multiple scattering in favourable cases can also be quantified (*hs2*).



The above illustration shows fitting of scattering from mono-disperse hard spheres in dilute solution. At 0.4% concentration (95% transmission) the model including first and second SANS fits better than simple single scattering. At lower concentrations (0.1%) the second scattering is negligible, and the effects of interaction, which reduce $S(0)$, are smaller.

The fitting routines in *clickfit* which are used in a number of model fitting programs *sasfit4*, *polymer*, *rfit*, *hs2*, ... now display statistical data error bars and resolution estimates reflecting the better reliability of the instrument configurations currently stored. Automatic fitting to sequences of data with output of parameters to files for subsequent display is available for all these programs. Options too have been added to *mplot* and *xmplot* to illustrate the q uncertainty.

Plug-ins

inxmpl1, *inxmpl2gin*

Standardised data formats enable data from different facilities to be compared and even fitted simultaneously. Basic display programs *sasmpl* and the current *fitfun* library can utilize external helper programs to read novel data formats. This allows the program functionality to be extended without need for modifying the core distributed programs (see technical notes below)

Distributions

Copies of the programs together with some test data are to be found on the ILL anonymous ftp web server <ftp://ftp.ill.fr/pub/cs/sans>. The source code is essentially identical for the three system versions, Linux, Macintosh OSX and PC-Windows and these distributions have been tested on 32 and 64 bit systems (see technical notes below). The distributions also include libraries for those wishing to extend the functions of the programs.

Websites

Current locations of useful websites follow:

<http://www.ill.eu/html/instruments-support/computing-for-science/data-analysis/raw-data/>

This contains a description of the raw data structures in use at the ILL and tools to check validity e.g. *anadat*.

<http://www.ill.eu/html/instruments-support/computing-for-science/data-analysis/data-treatment/newsans/>

A summary site showing distribution links.

<http://www.ill.eu/html/instruments-support/computing-for-science/cs-software/all-software/sans/>

Summarises software described here, with news on updates.

<http://www.ill.eu/html/instruments-support/computing-for-science/cs-software/all-software/clickfit/>

This describes use of the GUI interface for programs using the *fitfun* package, together with more detailed information on the fitting procedures.

<http://www.ill.eu/instruments-support/computing-for-science/cs-software/all-software/sans/analysis-programs/>

Analysis programs are summarised here together with their associated websites.

http://www.ncnr.nist.gov/staff/hammouda/the_SANS_toolbox.pdf

Boualem Hammouda's broad-ranging compendium of probing nanometer structures with neutrons.

<ftp://ftp.ill.fr/pub/cs/sans>

This site contains the distributions for PC-Windows, Macintosh and Linux together with more documentation on the features introduced in this section.

Current
Programs

Program	Page	Function
<i>ampl</i>		Multi-plot ascii regrouped data in columns
<i>anadat</i>		Analyses ILL raw data file structure
<i>ananas</i>	92	Sums strip of boxes
<i>ancos2</i>	95	Analyses uniaxial data
<i>anlips</i>	97	Analyses uniaxial data
<i>anpoly</i>	86	Background and efficiency correction for 2D data
<i>ansmoo</i>	94	Smooths/places 2D data on log scale
<i>anspec</i>	104	Isometric plot of 2D data
<i>areg</i>	87	Radial regrouping of 2D data in sectors
<i>colin</i>	113	Output columns of ascii regrouped data as ILL or XML
<i>colrow</i>	105	Vertical/Horizontal data sums
<i>cont</i>	102	Contour plots of 2D data
<i>detec</i>	47	Listing raw detector data
<i>dirrun</i>	42	Summary of store raw and treated data
<i>effdef</i>		Detector efficiency file writer
<i>g2x</i>		Converts ILL 1D data to canSAS-XML
<i>g2xfull</i>		Converts ILL 1D data to canSAS-XML
<i>grund</i>	52	Scans raw data file and writes mask of threshold data
<i>hs2</i>		Fits hard spheres and secondscattering
<i>hs2m</i>		Fits hard spheres and second scattering
<i>inillp1</i>		Plug-in reads ILL regrouped data
<i>inxml2gin</i>		Plug-in reads canSAS-XML data using dictionary
<i>inxmlp1</i>		Plug-in read canSAS-XML data command-line
<i>iqpsi</i>	90	Intensity as function of sector angle for 2D data
<i>mill</i>	68,86	Subtracts background/Eff. correction for 1D or 2D data
<i>mplot</i>	76	Multi-plot 1D data
<i>mpolly</i>		Background/efficiency corrections - 1D data sequences
<i>mshell</i>		Fits interacting hard spheres
<i>plfi</i>		Plots/superposes multiple fits from fitfun plot files
<i>polymer</i>		Fitting polymer models to 1D data
<i>ralread</i>		Converts ISIS 1D data to ILL
<i>rcard</i>		Writes out 1D data as multi-column
<i>red16</i>	60	Regroups/normalizes D16 scan data
<i>rfit</i>		Fits models to 1D data: includes resolution
<i>rguim</i>	70	Straight line analysis of 1D data
<i>rlist</i>	81	Outputs multicolumn listing of 1D data
<i>rmask</i>	49	Sets up detector masks for other programs
<i>rnls</i>	29	Regroups raw data
<i>rreg</i>		Regroups raw data using previously set parameters
<i>rnd16</i>	60	Regroups D16 data
<i>rnd16s</i>		Regroups D16 data pre-normalised
<i>rundex</i>	43	Lists sets of raw/treated data and selected parameters
<i>sasfit4</i>		Fits up to 4 peaks to 1D data
<i>sasmpl</i>		Plots 1D data from various inputs (using plug-ins)
<i>smorger</i>	82	Smooths/merges 1D data
<i>snls</i>	60	Regroups raw data with statistical tests for outliers

<i>xplots</i>	99	Pixel plots of 2d data
<i>spolly</i>	61	Background and efficiency corrections for 1D data
<i>ssqfun</i>		Fits concentric shells
<i>sumraw</i>		Sums raw data files writing a standard 2D data file
<i>windet</i>	44	Shows window of raw data; transmission calculations
<i>xmill</i>	68	GUI for mill
<i>xmplot</i>	79	GUI for mplot
<i>xpolly</i>	66	GUI for spolly
<i>xreg</i>		GUI for rreg
<i>utilities</i>		<i>pchead, pdqheads, pdqpg, pdqpt, pdqtitle</i>
<i>clickfit</i>		GUI for <i>polymer, rfit, sasfit4, ssqfun, hs2</i> fits
<i>clickfit_m</i>		GUI for multiple data set fits <i>hs2m, mshell</i>

Technical Changes

running programs

Use of a cache for raw data

Initial compressed data inspection for each run is often performed using *xplots*. Improving the response time to read swathes of data has been achieved by conserving the uncompressed data in a sub-directory in the work directory; by default this is named *cashas* and the uncompressed data are deleted when *xplots* terminates. If the SAS_CACHE environment variable is set to a name, say *mycache* then this is used and the data are not deleted when *xplots* terminates (this is an incentive to visualise all useful raw data before analysis). Implicitly this requires some monitoring of disk space usage. Most other programs also test for raw data being cached and will use the uncompressed data if available. This is further described in the document *auto_decompress.pdf*.

Resolution

A number of programs use the wavelength and diaphragm information in the regrouped data files. The stored (or absent) values are replaced if the environment variable SAS_RESOLUTION is defined. This can contain the following six values: *Sou_x_mm, Sou_y_mm, Sam_x_mm, Sam_y_mm, Dlambd/lambd, Coll_m* for the source and sample apertures (setting the y value to zero for circular diaphragms), wavelength spread and collimation distance.

Plug-in programs to read alternative data formats

A number of programs, *sasfit4, polymer, sasmpl, rfit* etc (but principally fitting programs) identify data using the file name. For data of ILL origin *gnnnnnn.ddd* files are recognized by the three digit extension and are read directly. For other formats a "plug-in" program is invoked to read the alien data and transcribe this for use. For example, an XML file, with extension *.xml* will look for a helper program defined in the environment variable SAS_XML (*inxmlp1* will read canSAS files. More generally *inxml2gin* uses a dictionary *inxml2gin.dcy* to convert data from unexpected units and add titles where absent. An intermediate file is created with the transcribed data e.g. *polymer.gin*. This remains after the end of the program and may help to trace errors. For a specific executable program say *xxx* rather than share the default SAS_XML variable, the variable *XXX_XML* may be specifically selected. Further description of these helper programs and intermediate file formats are included in the distributions (*dataplugins.pdf*)

Summary of Environment Variables

These are set initially in the setup files *sassetup* for Linux and Macintosh, and in the environment file *env.pro* in the program directory for PC-Windows.

Env_Variable	Default Blank=unset	Function
COM_DEBUG		Shows GUI dialogue
SAS_CACHE		Sets permanent cache directory
SAS_CHECK	limited	Suppresses mismatching parameter notification
SAS_DATA_PATH	(mandatory)	Directory for raw data
SAS_DEBUG		Show data reading progress
SAS_DECOMPRESS	zcat	decompress routine linux...
	gunzip -c	decompress (Macintosh)
SAS_DIR		Program directory
SAS_ERROR		Set to false to suppress 2D error data
SAS_EXTRA_G	g2x	Use reformater after storing 1D data
SAS_INSTRUMENT	(mandatory)	ILL instrument name (page 41)
SAS_RESOLUTION		See above for description.
SAS_XML	inxmlp1	Plug-in to read 1D canSAS data
<i>Plotting (also see page 40)</i>		
PGPLOT_DIR	(mandatory)	Usually the program directory
PGPLOT_ILL_DEV_1	/XSERVE	Linux, Macintosh <i>pgxwin_server</i>
	/GW	Windows <i>GRWND.EXE</i>
PGPLOT_ILL_DEV_2	/VCPS	

Distributions

The hardware and software of personal computers have changed much since the initial distributions were constructed and tested. To insulate and maximise independence of these programs from the systems the present distributions have been compiled and linked with certain characteristics described below. All systems use the same code for the GUI interfaces (for uniformity they are named as *.bat* files). Although a considerable effort has been made to test the programs, users are requested to return their comments when problems arise. (mail to reghosh@gmail.com)

Linux

The programs have been compiled using the gnu g77 fortran compiler version 3.4.2 and linked statically. The programs have operated normally on systems ranging from RedHat9 (32bit) to Ubuntu (64bit) version 10. All the unix commands in this manual pertain to use in a terminal window with the *tcsh* shell. A setup file *sassetup* is included in the zip-file distribution to set the basic environment variables; this is a simplified version of that shown on page 128. If an alternate shell is the default, it will be necessary to start the *tcsh* using this command before `%source sassetup`. The wish program used to run the GUI is usually available on linux systems.

Macintosh

All the Unix commands in this manual pertain to use in the terminal utility window with the *tcsh* shell. A setup file *sassetup* is included in the zip-file distribution to set up the basic environment variables; this is a simplified version of that shown on page 128. The OSX systems explicitly require use of shared libraries. For the Macintosh the programs have been compiled with the 32-bit gfortran version 4.2.3 compiler on a Leopard system (10.5). To enable the programs to run on Tiger(10.4), Leopard(10.5), Snow-Leopard (10.6) and Lion (10.7) the additional libraries required by the programs at run time are included with the program files; the *sassetup* procedure also there sets up the environment variable `DYLD_LIBRARY_PATH` directing the programs to find them. No privileges are thus required to install the programs which run on both 32 and 64 bit systems. This procedure works simply; it would help the community if problems were reported. If an alternate shell is the default, it will be necessary to start the *tcsh* using this command before `%source sassetup`. The *wish* program used to run the GUIs is usually available on all OSX systems.

PC-Windows

The earlier distributions worked well on Windows2000 and Windows-XP. Conflicts between the graphics and the file systems arose with Vista. These have been resolved and the programs, compiled with g77 version 3.4.2 now run without problems on all systems Windows2000 to Windows-8 using the *prop* interface included in the distribution, which also installs the *wish* program used for the GUI routines.

Epilogue

The programs here allow any data from the ILL instruments dating back to about 1974 to be displayed and treated. Displaying data from the earliest times in colour today show the results of many careful man-hours of detector adjustments by Jacobe and his team to obtain uniform response; the tradition of measuring calibration information with each configuration means that these data remain totally exploitable from the archives.

The current instruments are better automated, and hence more comfortable to use. The fluxes at the sample have little changed though detector areas have increased. The range of measurements performed is now much wider, with temperature and environment scans easily achieved, though measuring times for good quality data remain similar. The chemist and biologist still measure sequences of samples, concentrations and other variables. The approach in this suite of programs to store the subcomponents of the final treated data still has great value in chasing up anomalous results. For the physicist the controllable environment leads to sequences of measurements varying external constraints. The advantages of using the programs like *xplots* to examine raw data rapidly and store for comparison in its six-pack helps comparisons greatly. For treated data, *xmplot* allows the superposition of results to aid interpretation. Maintaining a one step history within the data files enables an audited trail of treatment steps, helping identify anomalies easily. The extensions to include other data formats (q.v. *plug-ins*) described above allow the data to be mixed and merged with other instruments around the world. The *canSAS XML 1D* format being adopted has made this much more practicable. In addition, this has led to discussion and better presentation of resolution effects in general. Facile input of treated data to a broad range of analysis programs allows more extensive sharing and comparison of model fitting.

The main basis of successful experiments, however, lies with well-prepared and characterised samples.

All comments on these programs from current and future experimenters will be welcomed by the authors, who in turn offer their encouragements to newer generations of researchers.

Ron Ghosh, Adrian Rennie
Epsom, Uppsala
April 2012

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