SAS program for two-detector system: seamless curve from both detectors

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Abstract. The changes of the SAS program have been made as an attempt to adapt it to a two-detector system for the YuMO spectrometer. It is shown that applying weight algorithm technique for the raw data averaging procedure allows one to avoid a “sewing” problem resulting from using different detectors in rather wide q-range. The operating scheme and the background details of the experiment are discussed as well.

1. Introduction

The methodical specific features of experiment configuration at a small angle neutron scattering spectrometer are essential for the raw data treatment. The YuMO spectrometer located at the 4-th beam-line of the IBR-2 reactor (JINR, Dubna, Russia) has specific features, namely: two-detector system, vanadium standard in front of each detectors, high flux on a sample, a direct view of the reactor core, a central hole of the detectors and special geometry of the beam [1-4].

The methodological specifications of small-angle neutron scattering (SANS) experiments are always beyond the scope of the papers aimed at highlighting the features of measurements [5]. The main feature of YuMO spectrometer is a pulsed reactor. It allows using a wide range of wavelengths (from 0.7 Å to 10 Å) and applying time of flight method [1]. The second feature is two-detector system for small-angle scattered neutrons [3, 4]. Before having been mounted in Dubna in 2000, a similar system did never exist. Now there is at least a couple of known SANS instruments which have two-detector system [6-8]. The other point is centered detectors without using a neutron guide or bender. Such geometry allows obtaining a high flux on the sample comparable to the flux of ILL in terms of SANS spectrometer [9], although the power of ILL reactor is much higher. One more point is the usage of a special geometry of scaling rings of gas ³He detectors, i.e. a hole in the center of the detectors. This allows applying a direct-beam detector and decreasing background scattering. Finally, a specific feature of the installation is vanadium standards in front of each detector. They periodically overlap the direct beam of neutrons that have already come through the sample.

In the paper, we investigate one of the problems connected with the experimental data treatment: sewing SAS curves obtained from different detectors. In this case, accurate background calculation and direct-beam detector usage as well as other spectrometer features mentioned above sound crucial.
Detailed answers to these questions are not the goals of the paper. Here we just illustrate the possibilities of the SAS program [4, 13], adapted to the two-detector system, i.e. the seamless curves obtained by two different detectors.

2. Brief description of specific YuMO setup features
The time-of-flight SANS YuMO spectrometer at the high flux pulse IBR-2 reactor [1, 3, 11] was modernized in 2000. One of the goals of the improvement was to increase the dynamic Q-range of the instrument. It was done by using two-detector system with central holes on the YuMO instrument. For this purpose, "OLD" and "NEW" detectors were used. The main view of the setup of the modernized YuMO instrument as well as examples of the SANS experiments are presented in figure 1.

Figure 1. The setup small-angle scattering of neutrons YuMO (4-th channel IBR-2): 1 - reflectors, 2 - active zone of reactor with moderator, 3 - chopper, 4 - changeable collimator, 5 - vacuum tube with additional background collimators, 6 - justified collimator, 7 - thermostat, 8 - holder with samples on the table with thermos boxes, 9 - table of samples, 10 - the vanadium standard, 11, 12 - detectors ("OLD" and "NEW" accordingly), 13 - direct beam detector.

Figure 1 presents a scheme of the small-angle YuMO spectrometer. The neutrons which have arisen as a result of passage of reflectors 1 near to zone 2, then thermalized in moderator. Chopper cuts the background. Neutrons go through the collimation system and scatter at the sample 8 and than and comes on detectors 11, 12 and 13. More detailed description of the spectrometer operation in two-detector variant can be found in [3-4].

3. Mathematical background and realization
In general, processing with SAS includes three main stages:
1. preliminary corrections of the time spectra;
2. normalization of the time spectra over the scattering from the vanadium standard;
3. conversion time spectra into the space of neutron momentum transfer.
4. Conversion into Q-space and averaging spectra

On this final processing stage, we should convert time-channel and angle of scatter to q-space. To check conversion, we used a procedure, describing in [12]. The values of the module q-vector scattering and its dispersion are calculated by the formulas shown below.

Values of the transferred momentum \( q \) of a neutron and its dispersion can be calculated according to:

\[
q = \frac{4\pi \sin(\Theta / 2)}{\lambda} \approx \frac{2\pi \Theta}{\lambda}, \quad \Delta q = q \sqrt{\frac{\sigma_\Theta^2}{\Theta^2} + \frac{1}{12} \left( \frac{\Delta t}{t} \right)^2},
\]

where \( \Theta \) and \( \sigma_\Theta \) – average scattering angle for the corresponding detector (ring of detector) and its dispersion, \( \lambda \) – neutron wavelength, \( t \) and \( \Delta t \) – the time channel center and its width. Average scattering angle and its dispersion can be calculated according to the:

\[
\Theta = \frac{\int_{\Theta_m}^{\Theta} \theta F(\theta) d\theta}{\int_{\Theta_m}^{\Theta} F(\theta) d\theta}, \quad \sigma_\Theta = \sqrt{\frac{\int_{\Theta_m}^{\Theta} \theta^2 F(\theta) d\theta}{\int_{\Theta_m}^{\Theta} F(\theta) d\theta} - \Theta^2},
\]

where \( F(\theta) \) is the instrument resolution function,

\[
\Theta_m = \Theta_{\text{min}} - d\Theta, \quad \Theta_{\text{min}} = \frac{R_{\text{in}}}{d_{\text{sample-detector}}}, \quad \Theta_m = \Theta_{\text{max}} + d\Theta, \quad \Theta_{\text{max}} = \frac{R_{\text{out}}}{d_{\text{sample-detector}}},
\]

\[
d\Theta = \frac{R_{\text{collimator-1}}}{d_{\text{reactor-sample}}} + \frac{R_{\text{collimator-2}}}{d_{\text{reactor-sample}}} + \frac{R_{\text{collimator-2}}}{d_{\text{sample-detector}}},
\]

An averaging procedure on interval \([Q_{\text{min}}, Q_{\text{max}}]\) with step equal to \( \Delta Q \) is follows:

\[
Q_n = \left( \sum_{i,j}^{N_{\text{out}}} \frac{q^{(i)}_{j} dI^{(i)}_{j}}{dQ_{n}} \right)^{-1}
\]

\[
I_n = \left( \sum_{i,j}^{N_{\text{out}}} \frac{1}{dI^{(i)}_{j}} \right)^{-1}
\]
\[ \Delta I_n = \left( \frac{\sum_{i=1}^{N_{\text{det}}} \frac{1}{dI_j^{(i)}}}{\sum_{i=1}^{N_{\text{det}}} \frac{1}{dI_j^{(i)}}} \right)^{-1}, \]

\[ \Delta Q_n = \left( \frac{\sum_{i=1}^{N_{\text{det}}} \frac{q_j^{(i)}}{dI_j^{(i)}}}{\sum_{i=1}^{N_{\text{det}}} \frac{q_j^{(i)}}{dI_j^{(i)}}} \right) \left( \frac{\sum_{i=1}^{N_{\text{det}}} \frac{1}{dI_j^{(i)}}}{\sum_{i=1}^{N_{\text{det}}} \frac{1}{dI_j^{(i)}}} \right)^{-1}, \]

\[ n = 0 \ldots (Q_{\text{max}} - Q_{\text{min}}) / \Delta Q. \]

Summation is made for nonzero values of \( q_j^{(i)} \), \( I_j^{(i)} \) and \( dI_j^{(i)} \). Upper index \( (i) \) refers to the detector ring number (e.g. \( i = 1 \ldots 8 \) refers to the 1st detector and \( i = 9 \ldots 16 \) - to the 2nd detector). In addition, it is possible to exclude some rings from the averaging procedure for some reason.

The program provides an opportunity for non-averaging. In this case, sorting points of the spectrum over neutron momentum transfer is performed.

5. Realization and example
Since SAS [4, 13] is object-oriented, and elementary object deals with a detector ring, it does not really matter to which of two physical detectors the ring belongs. This allows one to process all the rings of both detectors simultaneously in the procedure described above. SAS does NOT operate with “OLD” and “NEW” detectors separately, and does NOT sew spectra from them. Instead, it operates with a set of their rings and produces the final spectrum in a natural way. In other words for realization in SAS [4, 13] seamless merger of curves, we shift a “vector of data treatment” from physical detector to each ring as self-sufficient unit. It means that we have spectra as a file from each of the rings and do averaging of these files.

Below, figure 2 shows the overlapping of the scattering curves from the “OLD” (green triangles) and “NEW” (blue squares) detectors. Insertion shows zoom of the overlapping region. Points with poor statistics (small angles for “OLD” and wide angel for “NEW”) have no influence on the resulting curve (red circles). Also figure 2 demonstrates possibility on dynamical range of q-space by more than 100. Another scale (delta Sigma/ delta Omega - is a differential cross section) is an absolute scale. The given example is not unique. Good overlapping of the scattering curves from the “OLD” and “NEW” detectors simultaneously shows the real q-range which could be used for a part of ranges for small and wide q.
Figure 2. shows overlapping of the scattering curves from the “OLD” (green triangles) and “NEW” (blue squares) detectors. Insertion shows zoom of the overlapping region. Points with poor statistics (small angles for “OLD” and wide angles for “NEW”) have no influence on the resulting curve (red circles).

To demonstrate good quality of the overlapping procedure with different detectors, in figure 3 we presented a view of monitor screen with above-described SAS program data treatment for series of silver alkanoates [14] curves measured at YuMO spectrometer with two-detector system and by using smoothing procedure [10]. As we can see, the different position of peaks does not have asymmetry in different position of q-scale. It is important to stress that only 2 rings of “New” detector “see” peaks and hence take part in averaging of curves. We specially used wide neutron wavelength range to show influence of tail of “New” detector. The stability of curves behaviour in this case has been also demonstrated.
Figure 3. View of monitor screen with above-described SAS program data treatment for series of silver alkanoates [14] curves measured at YuMO spectrometer with two-detector system and by using smoothing procedure [10].

6. Conclusion

The improvement of the SAS program as an attempt to adapt it to a two-detector system for YuMO spectrometer are described. It is shown that applying a weight algorithm technique for raw data averaging procedure allows one to avoid a “sewing” problem resulting from using different detectors in rather wide q-range. In particular, choosing the time range (the wavelength range) has now a mathematical background. On the other hand, it is an additional “advise” from the curves view for maxima and minima q to use for consideration.

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References

[1] Ostanevich Y M 1988 Makromol.Chem. Macromol.Symp. 15 pp 91-103
[2] Kuklin A I, Islamov A K and Gordeliy V I 2005 Neutron News 16(3) pp 16-18
[3] Kuklin A I, Islamov A K, Kovalev Yu S, Utrobin P K and Gordeliy V I 2006 Poverkhnost'. Rentgenovskie, Sinkhrotronnye i Nejtronnye Issledovaniya 6 pp 74-83
[4] Soloviev A G, Solovieva T M, Stadnik A V Islamov A Kh and Kuklin A I 2003 Communication of JINR P10-2003-86
[5] Kuklin A I, Soloviov D V, Rogachev A V et al 2011 J. Phys.: Conf. Series 291 No. 1 012013
[6] Heenan R K, Rogers S E, Turner D, Terry A E, Treadgold J and King S M 2011 Neutron News 22(2) pp 19-21
[7] Dewhurst C D 2008 Measurement Science and Technology 19(3) 034007
[8] Klose F, Constantine P, Kennedy S J and Robinson R A 2014 J. Phys.: Conf. Series 528 No. 1 012026
[9] Kuklin A I, Rogov A D, Gorshkova Yu E, Utrobin P K, Kovalev Yu S, Rogachev A V, Ivankov O I, Kutuzov S A, Soloviev D V and Gordeliy V I 2011 Physics of Particles and Nuclei Letters 8(2) pp 119-128.
[10] Soloviev A G, Litvinenko E I, Ososkov G A, Islamov A K and Kuklin A I 2003 *Nuclear Inst. and Methods in Physics Research*, A. 502/2-3 pp. 498—500.

[11] Kuklin A I, Islamov A H, Balasoiu M, Murugova T N and Gordeliy V I 2012 *J. Phys.: Conf. Series* **351** No. 1 012001

[12] Nyam-Osor M, Soloviov D V, Koyalev Y S, Zhigunov A, Rogachev A V, Ivankov O I, Erhan R V and Kuklin A I 2012 *J. Phys.: Conf. Series* **351** No. 1 012024

[13] http://yumo.jinr.ru/software/sas

[14] Binnemans K, Van Deun R, Thijs B, Vanwelkenhuysen I and Geuens I 2004 *Chemistry of materials* **16**(10) pp 2021-2027