[combining data]
(Chapter 5.4.1]

Combining Over-Determined Data
Now we illustrate how the over-determined data combine to produce the desired, grand average scattering function. The counting rate in the detector, as a function of the wavelength (time-of-flight) is

$$C_D(Q) = I_o(\lambda)P_s(Q)e^{-\mu d_s}\Delta\Omega_D(\theta_s)\eta_D(\lambda), \tag{5-CD1}$$

where

$$P_s(Q) = d_s N\frac{\partial\sigma}{\partial\Omega}(Q) = d_s\frac{\partial\Sigma}{\partial\Omega}(Q) \tag{5-CD2}$$

is the sample scattering probability per unit solid angle, to be determined, which is a function of $Q(\lambda,\theta_s) = \dfrac{4\pi\sin\left(\theta_s/2\right)}{\lambda} \approx \dfrac{2\pi\sin\theta_s}{\lambda}$. Integrating over the angles and wavelengths that correspond to the same value of scalar Q, gives

$$\Psi_s(Q) = P_s(Q) \times \iiint_{\substack{\lambda_{\min} < \lambda < \lambda_{\max} \\ \theta_{s\min} < \theta_s < \theta_{s\max}}} I_o(\lambda)\eta_D(\lambda)e^{-\mu(\lambda)d_s}\delta\left[Q(\lambda,\theta_s) - Q_k\right]d^2\Omega_D(\theta_s)d\lambda \ , \tag{5-CD3}$$

in which scattering probability $P_s(Q)$ factors out in the integration because each term for which the delta function is satisfied corresponds to the same Q. Then

$$P_s(Q) = \frac{\Psi_s(Q)}{W(Q)}, \tag{5-CD4}$$

where

$$W(Q) = \iiint_{\substack{\lambda_{\min} < \lambda < \lambda_{\max} \\ \theta_{s\min} < \theta_s < \theta_{s\max}}} I_o(\lambda)\eta_D(\lambda)e^{-\mu(\lambda)d_s}\delta\left[Q(\lambda,\theta_s) - Q_k\right]d^2\Omega_D(\theta_s)d\lambda \ , \tag{5-CD6}$$

is a weighting function that applies to the integral of separate values of wavelength and scattering angle. In practice, the integration is determined on a predefined array of discrete Q-values and is a summation over discrete values of wavelength and scattering angle (*pixels*) selected to correspond to the same Q-bin. A separate calibrating measurement using a standard sample whose scattering probability is known determines $W(Q)$, which is called the *instrument weighting function.* In the discretized case, having defined a binning array $\{Q_k, \Delta Q_k\}$,

$$\Psi_s(Q_k) = P_s(Q_k)W(Q_k) =$$

$$P_s(Q_k) \sum_{\substack{\lambda_{\min} < \lambda_i < \lambda_{\max} \\ \theta_{s\,\min} < \theta_{s\,j} < \theta_{s\,\max}}} I_o(\lambda_i)\eta_D(\lambda_i)e^{-\mu(\lambda_i)d_s}U\left[Q(\lambda_i,\theta_j) - Q_k\right]\Delta\Omega_{D\,j}\Delta\lambda_i \qquad (5\text{-CD7})$$

and

$$P_s(Q_k) = \frac{\Psi_s(Q_k)}{W(Q_k)}. \qquad (5\text{-CD8})$$

Here, the function U selects the data corresponding to Q_k,

$$U_k\left[Q(\lambda,\theta) - Q_k\right] = \frac{1}{\Delta Q_k}\begin{cases} 1 \text{ if } |\,Q(\lambda,\theta) - Q_k\,| < \frac{\Delta Q_k}{2}, \text{ and} \\ 0 \text{ otherwise.} \end{cases} \qquad (5\text{-CD9})$$

Resolution or background constraints on which pixels are admitted in the average can also be imposed in the same way in the final binning.

Similarly, to determine the weighting function from measurements on a known calibrating sample,

$$W(Q_k) = \frac{\Psi_{calib}(Q_k)}{P_{calib}(Q_k)}. \qquad (5\text{-CD10})$$

Always, it is necessary to estimate the statistical error in the measured function. In the final analysis, this requires calculating the inverse-variance-weighted average of contributions to $P_s(Q)$, corrected pixel by pixel for background, attenuation, spectral intensity and detector efficiency, and the statistical error of the sum as the weighted sum of statistical errors of each contribution to the sum. This represents a substantial computation because of the large number of pixels in a time-of-flight SANS measurement. Modern computers are capable of calculating these results quite rapidly. But it is not necessary to do it that way for a quick result.

A roughly equivalent result for the statistical error in $P_s(Q_k)$ for each Q_k comes about, without the detailed corrections, because $\Psi_s(Q_k)T_s$, where T_s is the counting time for the sample data, is just a total of counts, subject to Poisson counting statistics. So, accordingly, the error in $\Psi_s(Q_k)T_s$, as measured by the standard deviation, is

$$\varepsilon_{\Psi_s,\,k} = \sqrt{\Psi_s(Q_k)T_s}\;. \qquad (5\text{-CD11})$$

The same can be said about the error in $W(Q_k)$ and the total error computed by the usual error propagation analysis,

$$\frac{\varepsilon^2_{P_s,\,k}}{P_s^2(Q_k)} = \frac{\varepsilon^2_{\Psi_s,\,k}}{\left(\Psi_s(Q_k)T_s\right)^2} + \frac{\varepsilon^2_{\Psi_{calib},\,k}}{\left(\Psi_{calib}(Q_k)T_{calib}\right)^2} \quad , \qquad (5\text{-CD12})$$

However, this is not all that needs to be taken into account in final data reduction—raw data need to be corrected for variations in source intensity during the run as determined by beam monitors, for the various contributions to the net scattering data, and for the backgrounds, measured with the beam blocked with an opaque neutron absorber, detector sensitivity, pixel size, delayed neutrons, etc. Consequently, the simple procedure suggested just previously is inadequate for complete data analysis, only for a simple first cut. Thiyagarajan et al. (1997) discuss the data reduction procedure more thoroughly.

Table 5-CD2. Parameters of the instrument of Fig. 5.22 in *Elements.*

Parameter	Value
$L_c = L_D$	8.0 m
Collimator entrance aperture, $\Delta x = \Delta y$	0.5 cm
Collimator entrance area, X = Y	10 cm
Collimator exit aperture, $\Delta x = \Delta y$	0.25 cm
Collimator exit area, X = Y	5 cm
Detector pixel size, $\Delta x = \Delta y$	0.5 cm
Detector area, X = Y	100 cm
Pulsing frequency	30 Hz
λ_{min}	2 Å
λ_{max}	10 Å
Q_{mim}	6 x 10^{-4} Å^{-1}
Q_{max}	0.3 Å^{-1f}
Flux on sample	2.6 x 10^5 n/cm^2-sec

In an intensity-resolution plot similar to Fig. 5-STO.1 for a monochromatic-beam instrument, the weighting function would appear as in Fig. 5.17 in *Elements*, and the resolution broadening width would be constant because there is no wavelength averaging in that case.

Thiyagarajan et al. (1992) have compared measurements on identical samples carried out at several conventional and time-of-flight SANS instruments. The time-of-flight instruments do not yet quite reach the lowest Q-values accessed in steady-source instruments (Q_{min} ~ 3 x 10^{-3} Å^{-1} vs. Q_{min} ~ 1 x 10^{-3} Å^{-1}); however, the quality of data from all of these is comparable. The measuring times of the time-of-flight instruments in relation to the available neutron fluxes, projects that time-of-flight SANS instruments at the high-power pulsed sources coming into operation as this is written may perform competitively with steady-source instruments, or better. For example, SAD at IPNS with 7.5 kW proton beam was 1/12 as fast as D-11 at ILL. It remains to be seen whether this projection works out in practice when new instruments come into being.

References

Thiyagarajan, P., J. E. Epperson, R. K. Crawford, J. M. Carpenter, T. E. Klippert, and D. G. Wozniak (1997). The time-of-flight small-angle diffractometer (SAD) at IPNS, Argonne National Laboratory. *J. Appl. Crystallogr.* **30**, 280-93.

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Seminar on Structural Investigations at Pulsed Neutron Sources,) Russia, ED3-93-65, pp. 194-211.