RKH 04/11/14 v3, now with Q resolution

**Data reduction details (hacked from another document, read the second part first.)**

The number of counts recorded at detector radius R and time of flight corresponding to wavelength λ is given by the incident number of neutrons I0(λ) times the scattering cross section ∂Σ(Q)/∂Ω for scattering at a particular value of Q.

 (2)

Ω(R) is a detector pixel solid angle, T(λ) the transmission of the sample, of thickness t and ηM(λ) is the detector efficiency. Following the early work of Seeger, Hjelm & Pynn [1] the data reduction method used for many years on LOQ at ISIS [2] to extract tof data at a particular Q is derived as follows. The incident flux I0(λ) is recorded by a beam monitor detector M(λ) of efficiency ηM(λ).

 (3)

To obtain the scattering cross section we only need the ratio of the efficiency of the main detector to that of the incident beam monitor. In theory, at least the shape of this wavelength dependent function is obtained by removing the beam stop and putting a small hole of area AH, or some other attenuator, at the sample position of normal area AS. “Direct beam” function D(λ) is then measurable as counts CH(λ) on the detector:

 (4)

Rearranging the equations gives us the scattering cross section:

 (5)

The numerator sums neutron counts C(R,λ) over all radii and wavelengths contributing to a particular value of Q, so has a clear Poisson error. The denominator includes three wavelength dependent corrections: for incident beam monitor spectrum M(λ), measured sample transmission T(λ) and the direct beam function D(λ), whilst Ω(R) is a detector pixel solid angle. The scattering volume of the sample is the beam area AS times sample thickness t. In practice the leading scalar AH is determined by a fit to scattering from a “standard sample”, so results do not depend on knowing a precise attenuation factor.

**Discussion of event mode data**

Consider data reduction at fixed wavelength, over a simple ring of detector pixels at radius R, where Q ≈ (2π/λ)(R/L2)

 (B1a / B1b)

The sum over *i* runs over all N(R) pixels with counts Ci(R), at radius R, including those with no counts. The normalising factor *fi* for monitor spectrum & transmission etc is roughly constant at a given Q and wavelength. The total solid angle ΩRING(R) ~ N(R)Ωi.

If the counts arrive or are processed as an event stream I(Q) can still be calculated providing we anticipate the full solid angle in the denominator in (B1b).

The way Mantid averages data in Q1dWeighted.cpp for EQSANS seems to sum over CT individual neutrons (assuming that is what is in Yin) and then divide by the number of items processed (presumed the number of events at that Q):

 (B2a/B2b/B2c)

In (B2b) we regroup the summation from events into counts in each pixel.

 In (B2c) note that actually CT is identical to Σ Ci(R), so they could be cancelled, which is a little odd, but I think this is because in reality we are trying to average 1/f.

Comparing (B2c) with (B1b) this seems to differ from the ideal case by a number of pixels divided by the total counts. These at least are proportional to each other, so if we go to a different Q at this wavelength or the same Q at a different tof wavelength, perhaps all is OK?

I am still musing over the implications for the “zero count pixels” and whether there is a better way to look at this, e.g. when CT is small.

**Q resolution average**

EQSANS uses routine TOFSANSResolution.cpp to average the Q resolution from individual neutrons in the event stream, as might be expected from (B2a) by:

 (B3)

Since ISIS uses, more correctly, equation (5), we need instead:

 (B4)

Where C(R,λ) are the neutron counts at all radii and wavelengths contributing to a particular value of Q.

[The Mantid calculation for this would most easily be achieved inside Q1d. The EQSANS evaluation of (B5) is carried out by a separate summation in TOFSANSResolution.cpp that repeats the summations of Q1dWeighted.cpp, though likely the resolution calculation is optional?]

Mildner and Carpenter’s approximation for Q resolution σQ should be used, though here with some debate as to what to use for the detector pixel size term ΔR for our gas tubes.

 (B5)

Where 

This may appear in slightly different but equivalent forms, often using the small angle approximation Q = 2πR/(λL2). Note here I have used the standard deviation of wavelength σλ rather than the more usual rectangular bin width Δλ, for which the standard deviation is Δ/(12)1/2. Wavelength uncertainty σλ contains two terms, one from the intrinsic time spread of the moderator [as provided for EQSANS by function getTOFResolution in EQSANSResolution.cpp] and the other for whatever histogram time bin width ΔλTOF was used in the tof data collection or histogram regrouping.

 (B6)

[Note there is a units conversion from time to wavelength required for σMODERATOR, as in TOFSANSResolution.cpp. Is there yet such a function for ISIS moderators?]

Equations (B3) and (B4) sum standard deviation σ not variance σ2 as these are independent measurements. The “average” resolution depends on the shape of I(Q) where sharp features are concerned. For example an isolated Bragg peak will give a tall narrow peak at long wavelengths and a lower, broad, peak at short wavelengths due to the 1/λ dependence of resolution in (B5). At the peak position the long wavelengths dominate the average so the mean resolution improves. For a sharp dip in I(Q) the converse is true, the short wavelengths dominate at the dip position and the average Q resolution is worse. If a user looks up the resolution at the peak position, then a Gaussian with that standard deviation should be a reasonable approximation to the resolution function. To improve resolution at the expense of counting statistics it is helpful to remove short wavelength neutrons at smaller radii R on the detector.