$$\psi = \sum_h \sum_i \sum_m W_{him}(I_{him} - G_m p_{him} I_h)^2 \qquad (11.5.2.5)$$

and, using expression (11.5.1.2), the best least-squares estimate of I_h will then be

$$I_h = \frac{\sum_i \sum_m W_{him} G_m p_{him} I_{him}}{\sum_i \sum_m W_{him} G_m^2 p_{him}^2}. \qquad (11.5.2.6)$$

When all reflections in the data set are fully recorded, expressions (11.5.2.3) and (11.5.2.5) reduce to the 'classical' HRS expression (11.5.1.1), and expressions (11.5.2.4) and (11.5.2.6) reduce to expression (11.5.1.3).

The scale factor G_m can be generalized to incorporate crystal decay (Gewirth, 1996; Otwinowski & Minor, 1997):

$$G_{him} = G_m \exp\left\{-2B_m[\sin(\theta_{hi})/\lambda]^2\right\}, \qquad (11.5.2.7)$$

where B_m is a parameter describing the crystal disorder while frame m was recorded, θ_{hi} is the Bragg angle of reflection h_i and λ is the X-ray wavelength.

Method 1 only allows the refinement of the scale factors while method 2 allows refinement of the scale factors, crystal mosaicity and orientation matrix, as the latter two factors contribute to the calculated partiality. Furthermore, method 2 is essential for scaling of data sets with low redundancy (*e.g.* data collected from low-symmetry crystals or data collected over small rotation ranges). When a reflection h_i spans more than one frame, but there are no other reflections with the same reduced Miller indices h in the data set, the contribution of any partial reflection h_{im} to expression (11.5.2.3) will be zero, as in this case I_h will be the same as I_{hi}. In contrast, in method 2 the reflection h_i can be used for scaling because the estimates of the full intensity I_{hi} are calculated independently from every frame spanned by reflection h_i.

11.5.3. Selection of reflections useful for scaling

Both scaling methods 1 and 2 may take into account any reflection intensity observation, regardless of whether it is a partially or fully recorded reflection. However, there are significant differences between the selection of reflections in the two methods. Method 1 requires that all parts of a reflection are available in order to incorporate the reflection into the generalized HRS target, expression (11.5.2.3). Thus, reflections that occur at the beginning or the end of the crystal orientation, or at gaps within the rotation range, must be rejected. Even when all parts of a reflection are recorded, there might be parts for which there was a problem during integration, thus making the reflection useless for scaling. The decision on whether all parts of a reflection are available for scaling is dependent on knowledge of the crystal mosaicity and of the crystal orientation matrix. Since these might be inaccurate, a reasonable tolerance has to be exercised when deciding if a reflection has been completely measured on consecutive frames. Method 2 allows the use of all reflections for scaling as every observation of a partial reflection is sufficient to estimate the intensity of a full reflection, expression (11.5.2.2). However, a reasonable lower limit of calculated partiality has to be imposed in selecting reflections useful for scaling. The criteria for rejecting reflections prior to scaling and averaging are listed in Table 11.5.3.1.

11.5.4. Restraints and constraints

Scale factors will depend on the variation of the incident X-ray beam intensity, crystal absorption and radiation damage. Hence, in general, scale factors can be constrained to follow an analytical function or restrained to minimize variation between successive frames. The scale factors can be restrained by adding a term $w(G_n - G_{n+1})^2$ to ψ, expression (11.5.1.1), where G_n and G_{n+1} are scale factors for the nth and $(n+1)$th frame and w is a suitably chosen weight. Such procedures will increase $R_{\rm merge}$ but will also increase the accuracy of the scaled intensities as additional reasonable physical conditions have been applied.

The mis-setting angles of a single crystal should remain constant throughout the data set. Thus, in principle, the mis-setting angles should be constrained to be the same for all frames associated with a single crystal in the data set. However, in practice, independent refinement of the mis-setting angles can detect problems in the data set when there are discontinuities in these angles with respect to frame number. Cell dimensions should be the same for all crystals and might therefore be constrained. However, care should be taken, as the exact conditions of freezing may cause some variations in cell dimensions between crystals. As radiation damage proceeds, mosaicity is likely to increase. Hence, constraint between the refined mosaicities of neighbouring frames can be useful.

Table 11.5.3.1. *Hierarchy of criteria for selecting reflections for scaling and averaging procedures*

Methods 1 and 2	
All parts of a reflection are rejected if: (1) There are no successfully integrated parts. (2) There are no parts with significant intensity (for scaling only). (3) There are some parts entering and some parts exiting the Ewald sphere (this implies that the reflection is too close to the rotation axis and is partly in the blind zone). (4) This is a full reflection recorded only once with no other symmetry-equivalent observations.	
Method 1	Method 2
All parts of a reflection are rejected if: (1) There is a part that is not successfully integrated. (2) There is a part that has a significant intensity, but is not predicted by the crystal orientation and mosaicity used in the scaling program. (3) The sum of calculated partialities differs from unity by more than a chosen value.	Any part of a reflection is rejected if: (1) The calculated partiality is less than a chosen value. (2) The intensity is less than a chosen fraction of the error estimate.

references