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Online Data Reduction of SAXS/WAXS Data

Introduction

X-ray detectors with 2048 x 2048 pixels and 16 bit intensity resolution are in routine use for time resolved experiments. Several detectors can be used at the same time to record SAXS and WAXS data.

All detectors require various corrections to convert the measured pixel intensities into absolute differential scattering cross-sections. The online data reduction routines have been developed to make absolute intensities available immediately during the experiment. They include the correction of detector artifacts such as dark current, image distortion and spatial inhomogeneities, as well as normalization of intensities to incident photon flux, sample transmission and spherical angle.

The correction programs can also be used to reprocess offline experimental data. The offline programs are available for a number of different platforms (UNIX, LINUX, WINDOWS).

Description

The online data reduction is automatically applied after exposure. It is called from the SPEC acquisition program. The data transfer between SPEC and the online correction program is mainly done with shared memories.

The acquisition program writes data into shared memories and the correction program gets it from there. The output is written to other shared memories. Each relevant image has an associated header.

The names of the shared image memories are ending with `_data<CCD_U>` and the corresponding header arrays are ending with `_header<CCD_U>`.

`image_data0` `image_header0`

```
dark_data0
corr_data0      corr_header0
azim_data0
ave_data0
```

Header arrays are in principle associated to all image memories. But currently only image_header... and corr_header... can be used.

The command **corimg** <CCD_U> corrects and saves the data of detector <CCD_U> as configured in corimgmenu (see below). It uses as input the data of **image_data**<CCD_U>, **dark_data**<CCD_U> and **image_header**<CCD_U>. The output is written to **corr_data**<CCD_U>, **corr_header**<CCD_U>, **azim_data**<CCD_U> and **ave_data**<CCD_U>.

Header Values

The geometrical setup of the experiment is described by header values.

Dim_1, Dim_2: image dimensions

Offset_1, Offset_2: offset of image coordinates (for ROI)

BSize_1, BSize_2: binning size (pixel size relative to unbinned image)

Center_1, Center_2: point of normal incidence on the detector

PSize_1, PSize_2: pixel sizes in meter

SampleDistance: distance between sample and detector in meter

WaveLength: wavelength in meter

Intensity0: intensity of primary beam before sample (in photons during exposure)

Intensity1: intensity of primary beam after sample (in photons during exposure)

ExposureTime: exposure time in seconds

Dummy: dummy value

Time: start of the exposure (YYYY-MM-DD hh:mm:ss.uuuuuu)

Title: title string

RasterOrientation: orientation of the image (1 to 8)

Graphical Interface

Inside **SPEC** the correction menu is called with the command **corimgmenu**, abbreviated **cm**. It can be followed by the detector number. The detector number starts with 0 and increases to the number of defined detectors minus 1. Inside **SPEC** this number is called **CCD_U**. Without a number the menu of all detectors are sequentially opened.

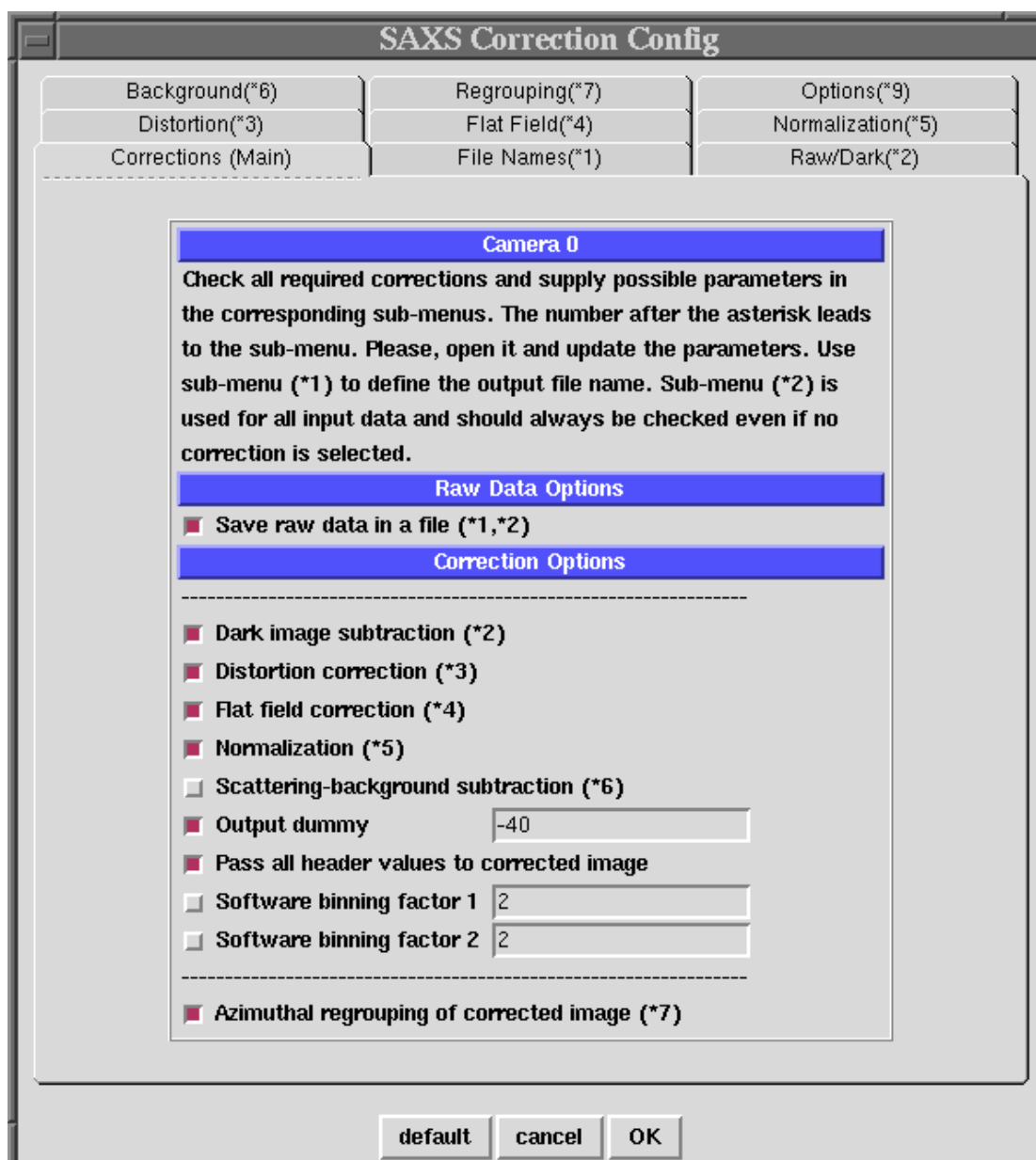


Fig. 1. Main correction menu (**SPEC** command **corimgmenu**, abbreviated **cm**)

The correction menu has a main sheet (see above) to select the data processing options of each detector. An option that requires additional parameters is followed by a number that refers to the additional configuration sheet, e.g. (*4) for the flat field correction.

A horizontal dashed line in the main menu separates the three main parts of the online correction: no correction, correction, regrouping.

With one exception, the corrections are always applied in the order that is shown in the main menu. It is possible to apply the flat field correction before the distortion correction.

To configure the online correction steps for each detector open the main correction menu, select the required options and go through the additional configuration menus.

Description of the Options

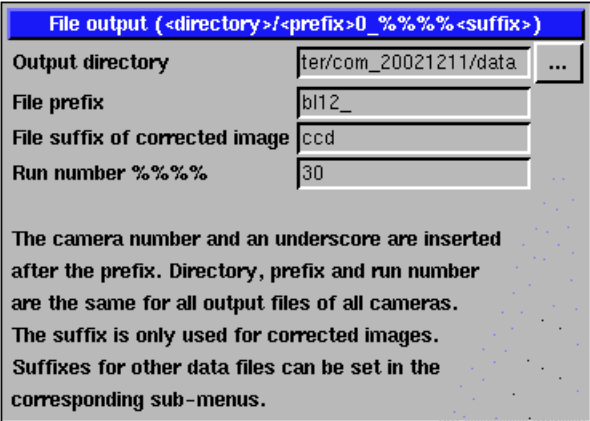
Save raw data in a file

This option must be chosen to save unprocessed detector data. The raw data image and the dark data image is saved to disk before the correction starts. Two additional configuration sheets must be configured (*1, *2).

Configuration sheet *1 is used to define the destination directory and prefix that are common for all output files. Additionally, it is used to define the suffix of the corrected image. The output file names of all detectors have the same form, i.e. directory, prefix, run number and suffix are identical. The detector number <CCD_U> is used to distinguish between data of different detectors:

<directory>/<prefix><CCD_U>_<run number><suffix> ,

where <CCD_U> is the detector number and <run number> a placeholder for a run number with 4 integer digits. It is suggested to use always `ccd` as suffix of the corrected image.



File output (<directory>/<prefix>0_<run number><suffix>)	
Output directory	ter/com_20021211/data ...
File prefix	b112_
File suffix of corrected image	ccd
Run number <run number>	30

The camera number and an underscore are inserted after the prefix. Directory, prefix and run number are the same for all output files of all cameras. The suffix is only used for corrected images. Suffixes for other data files can be set in the corresponding sub-menus.

Fig. 2. File name configuration menu

A dot slash in the output directory field selects the current directory. Instead of configuration sheet *1 the **SPEC** command `ccdnewfile` can be used to define a destination directory and filename.

Configuration sheet *2 is used to define source and output suffix of the raw and dark image. For a correct functioning of the online correction **SPEC** must be selected as image source and the output suffixes should be `ccdraw` for the raw image and `ccddark` for the dark image. The rest of the file name is identical to the file name of the corrected output image.

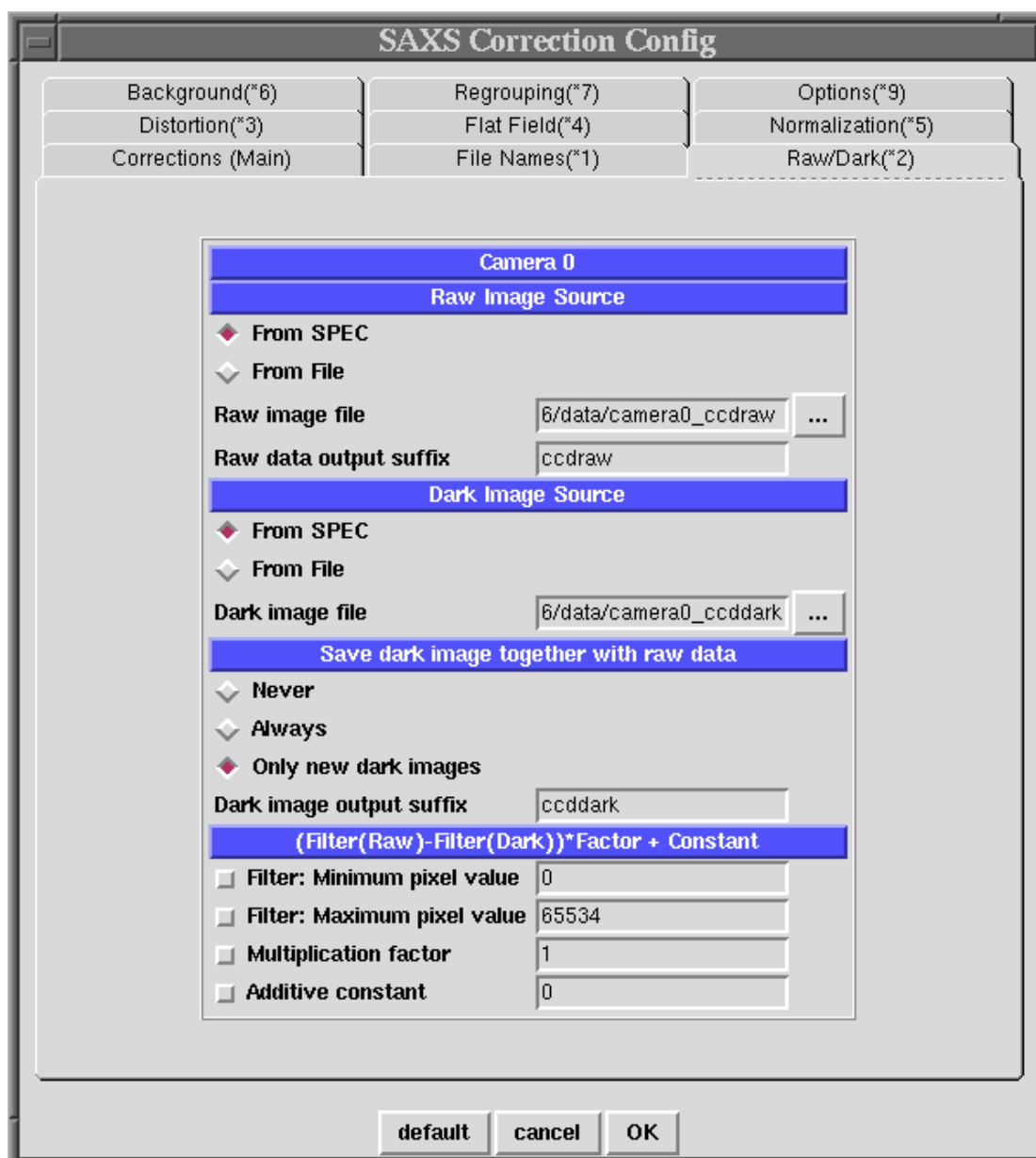


Fig. 3. Raw data configuration menu.

To avoid saving identical dark images it is suggested to save only new dark images. In all cases, a dark image is only saved together with a raw image. A dark image is never saved without a raw image. Raw images and dark images are saved without modification as they are read from the detector.

The filter option at the bottom are only used to calculate a corrected image in the following way:

$$(\text{Filter}(\text{Raw}) - \text{Filter}(\text{Dark})) * \text{Factor} + \text{Constant}$$

The filter function accepts only intensities between a lower and upper limit. Values outside this range are set to the dummy value that can be defined on the main sheet. It is suggested to define a reasonable upper limit for the detector data. After filtering the data can be multiplied by a factor and a constant can be added. For correct functioning of the online normalization the factor should be 1 and the constant 0 or these options should be switched off.

Dark image subtraction

This option must be chosen to subtract a dark image from the raw image. Configuration sheet *2 allows to configure additional options.

Distortion correction

This option must be chosen to do a spatial distortion correction on the image. Configuration sheet *3 allows to configure the required parameters.

Fig. 4. Distortion correction menu

The spatial distortion correction is based on the procedure used in fit2d. Before a spatial distortion correction can be applied the distortion function must be measured. This is usually done with a two-dimensional hole grid that is placed in front of the detector. A diffuse scatterer is placed at the sample position and detector images of the grid are measured at all sample to detector distances that are of interest. For each distance a distortion function is calculated with fit2d and parameterized by a spline function.

The distortion correction is effectively a projection of the detector pattern to the position of the grid. Due to the algorithm, the effective pixel size of the corrected pattern depends on the distance between sample and detector. The files that describe the distortion corrections contain also the fitted pixel size. For correct results it is therefore necessary to use the pixel size of the distortion file.

Internally, the distortion spline file is used to calculate two arrays containing the horizontal and vertical displacements of each pixel. These shift arrays can be saved and can later be used alternatively to the spline file.

Flat field correction

This option must be chosen to divide the detector pattern by a flat-field image. A flat field image contains the relative sensitivities of each pixel. The division can either be

done before or after the distortion correction. Configuration sheet *4 allows to configure the required parameters.

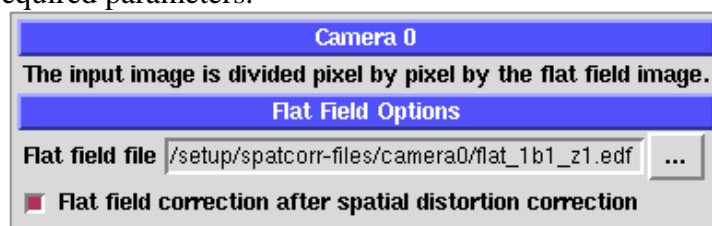


Fig. 5. Flat field correction menu

Normalization

This option must be chosen to normalize the detector pattern to absolute scattering intensities. Configuration sheet *5 allows to configure the normalization.

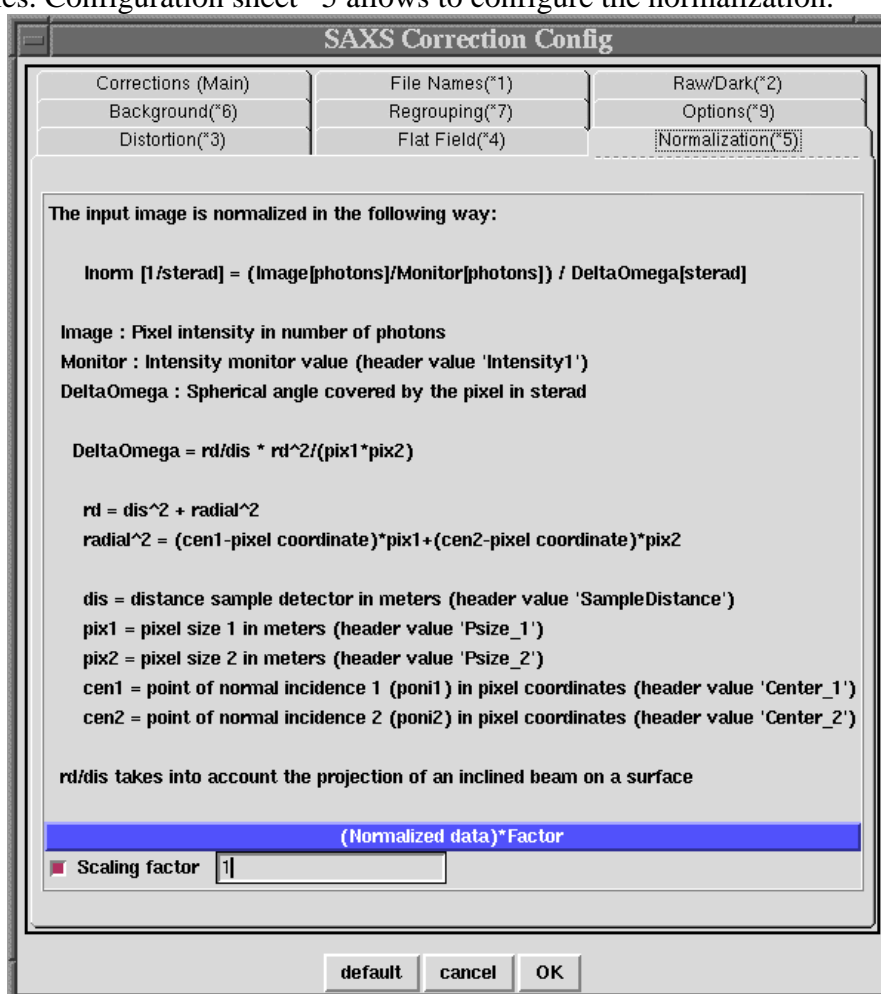


Fig. 6. Normalization menu

Absolute scattering cross sections

The normalization returns the absolute scattering intensity as the ratio between the number of scattered photons per spherical angle to the number of photons in the primary beam after the sample. This is the differential scattering cross section per sample cross section divided by the sample transmission T. The unit is 1/sterad. If the

intensity I_1 of the transmitted beam is measured in the beamstop the normalization does not require an explicit value of the transmission T .

$$I_{\text{norm}} = 1/T \cdot 1/A \cdot ds/dW = ds/dW \cdot 1/(T \cdot I_0) = ds/dW \cdot 1/I_1$$

When this value is divided by the sample thickness d one gets the differential scattering cross section per scattering volume measured in $1/m$ for a non-absorbing sample.

$$I_{\text{norm}}/d = 1/T \cdot 1/V \cdot ds/dW$$

To convert this value into a number of scattering electrons per volume it must be divided by the Thompson scattering cross section.

Calculation

The normalized scattering intensity is given in

$$I_{\text{norm}} [1/\text{sr}] = \text{Image} [\text{ph}] / \text{Monitor} [\text{ph}] / \Delta\Omega [\text{sr}]$$

Usually, the intensities of the input image and of the monitor are not (exactly) calibrated to number of photons. In this case it is necessary to determine a scaling factor with the help of a standard scatterer, e.g. lupolen or water. This factor is energy dependent.

$$\text{Image} [\text{ph}] / \text{Monitor} [\text{ph}] = \text{Image} [\text{arb.}] / \text{Monitor} [\text{arb.}] \cdot \text{factor}$$

The intensities of each pixel of the input image is divided by the value of the intensity monitor (header value 'Intensity1'), multiplied by the scaling factor and is then divided by the covered spherical angle.

Calibration

The absolute SAXS scattering intensity of **water** is **1.6/sr/m**. This value does not depend on the photon energy. The absolute scattering intensity of a 1_mm thick water layer is $1.6e-3/\text{sr}$.

As secondary standard a calibrated **lupolen** sample is available. The absolute scattering intensity in the maximum is **1.8/sr**. This value does not depend on the photon energy.

Scattering-background subtraction

This option must be chosen to subtract a parasitic scattering background. Configuration sheet *6 allows to configure this calculation.

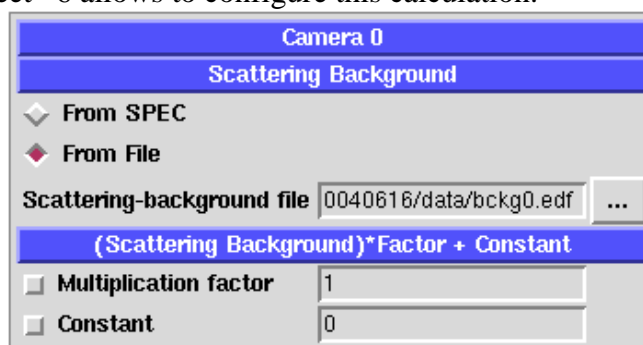


Fig. 7. Scattering background menu

The scattering background should be normalized and must have the same size as the corrected scattering pattern. Additionally, it can also be used to add a permanent mask to a corrected image.

Output dummy

The dummy value should be set to a negative number, e.g. -10 for unbinned images.

A dummy value is a non-zero number that is used to mask invalid pixels, e.g. after a division by zero. A value of zero switches off this feature. If a pixel is set to a dummy value its original value is lost. Pixels with values between $\text{dummy}-0.1 < \text{value} < \text{dummy}+0.1$ are ignored and are not used for calculation. The dummy value should therefore be outside the value range of an image.

To use a beamstop mask it is necessary to define a dummy value different from zero.

Pass all header values to corrected image

This option copies all input header values to the output header. If not set, only the essential header values are copied into the output image.

Software binning factor 1 and Software binning factor 2

These values set the horizontal and vertical binning factors of the corrected image. The raw and dark images are not changed. The output dimensions are reduced by the binning factors, e.g. $\text{Dim}_1' = \text{Dim}_1/\text{bin}_1$ and $\text{Dim}_2' = \text{Dim}_2/\text{bin}_2$.

Azimuthal regrouping of corrected image

This option must be chosen to do an azimuthal regrouping of the corrected image. Configuration sheet *7 must be used to configure it.

Camera 0	
Azimuthal Regrouping Setup	
Lower angle [deg]	0
Width of azimuthal sections [deg]	1
Number of azimuthal sections (0 for default)	0
Number of radial steps (0 for default)	0
Azimuthal Regrouping Options	
<input checked="" type="checkbox"/> Mask data before regrouping.	
Mask file	20040616/data/msk0.edf ...
<input type="checkbox"/> Save regrouped data in a file	
Output file suffix	ccdazim
Azimuthal Average Options	
<input checked="" type="checkbox"/> Save azimuthal average in a text file	
<input checked="" type="checkbox"/> Include header of corrected image	

Fig. 8. Azimuthal regrouping menu