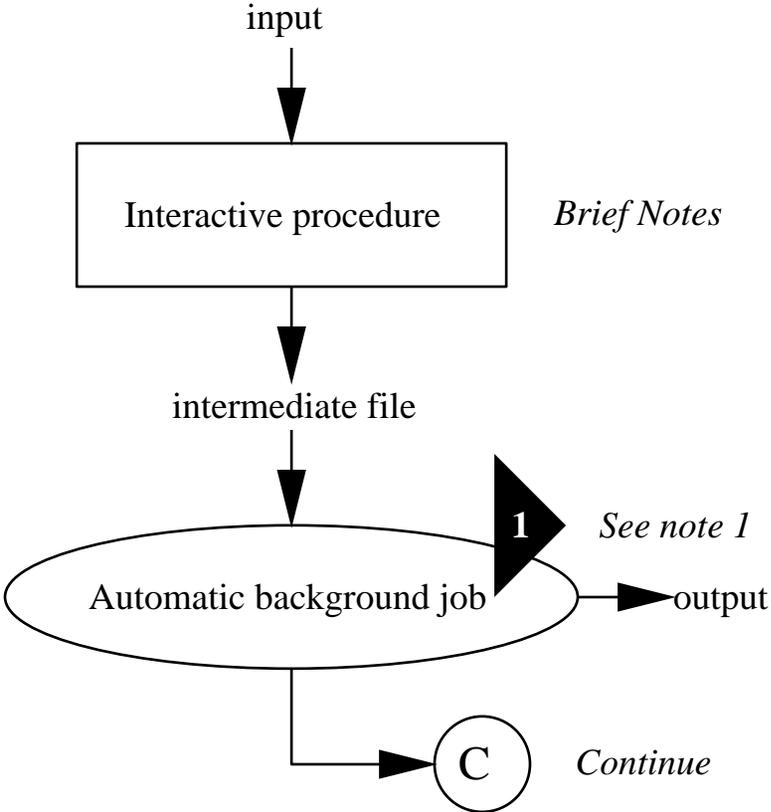# Laue Data Reduction Using `LaueView:` Flow Chart and Notes
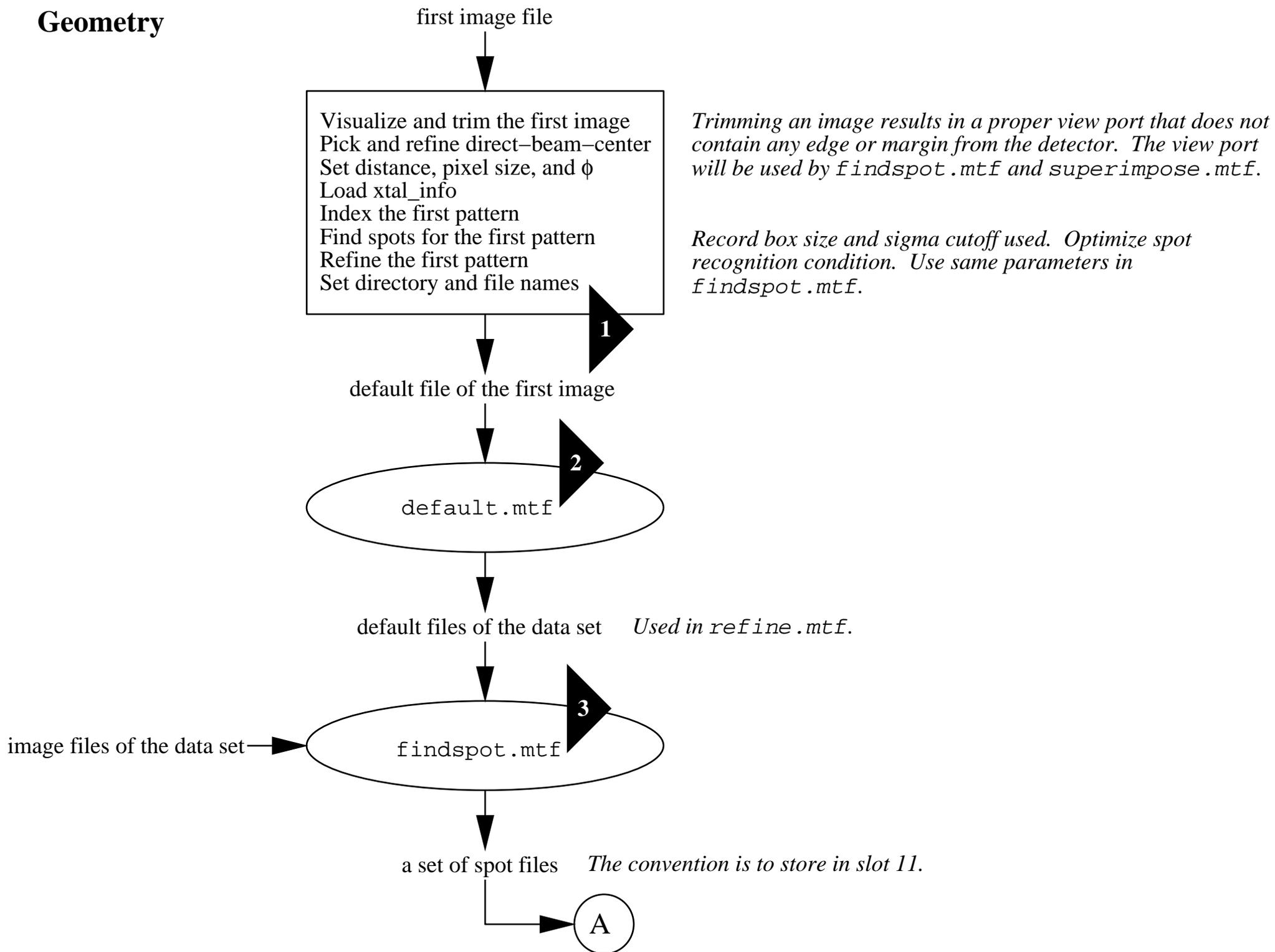
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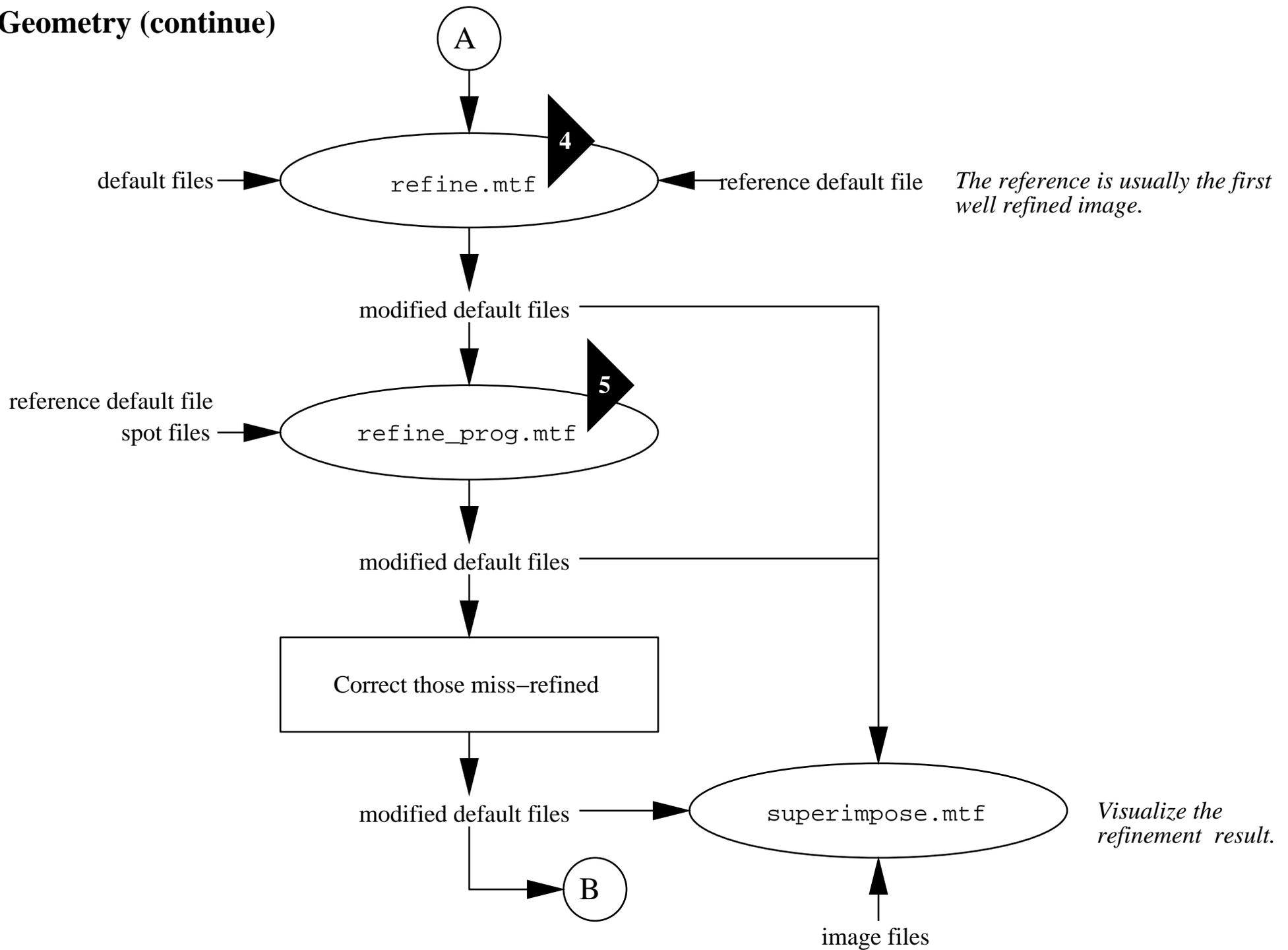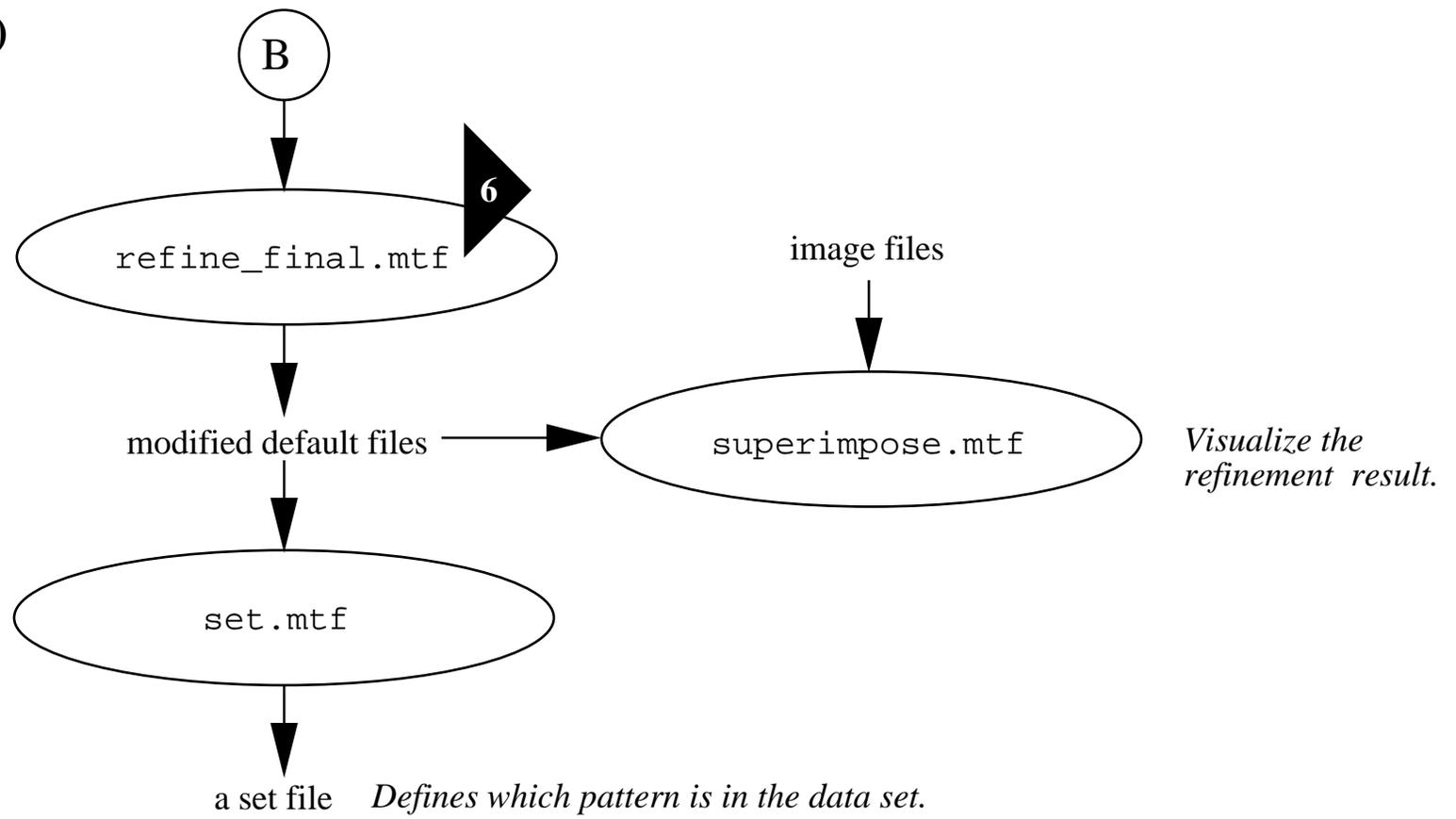*The University of Chicago*

last update April 9, 1997

Notations

input

Interactive procedure   *Brief Notes*

intermediate file

1 *See note 1*

Automatic background job   output

C   *Continue*

Geometry

first image file

Visualize and trim the first image
Pick and refine direct−beam−center
Set distance, pixel size, and φ
Load xtal_info
Index the first pattern
Find spots for the first pattern
Refine the first pattern
Set directory and file names

1

Trimming an image results in a proper view port that does not contain any edge or margin from the detector. The view port will be used by `findspot.mtf` *and* `superimpose.mtf`.

Record box size and sigma cutoff used. Optimize spot recognition condition. Use same parameters in `findspot.mtf`.

default file of the first image

2

`default.mtf`

default files of the data set   *Used in* `refine.mtf`.

3

image files of the data set ⟶ `findspot.mtf`

a set of spot files   *The convention is to store in slot 11.*

A

Geometry (continue)

A

default files → refine.mtf **4** ← reference default file   *The reference is usually the first well refined image.*

↓

modified default files

↓

reference default file
spot files → refine_prog.mtf **5**

↓

modified default files

↓

Correct those miss−refined

↓

modified default files → superimpose.mtf   *Visualize the refinement result.*

B

↑

image files

Geometry (continue)

B

6

refine_final.mtf

image files

modified default files → superimpose.mtf

Visualize the refinement result.

set.mtf

a set file   *Defines which pattern is in the data set.*

Profiles

7

set file
.lam file
a set of default files

.lam file is a two−column file that describes the initial lambda−curve, in which the columns are wavelength in angstrom and relative intensity, respectively.

spoverlap_rdb.mtf
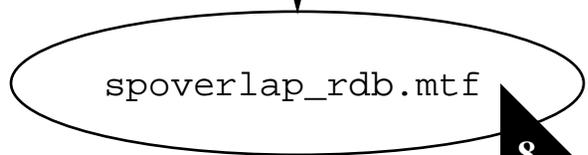
8

Set d_{min} to the best or conservative estimate. The same value should be used in selectsam.mtf and sampling.mtf.

a set of .lnk files

set file
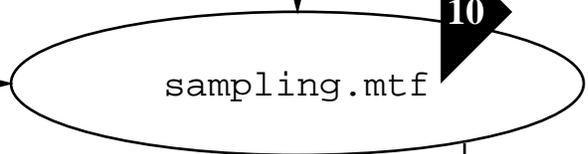a set of image files
a set of default files
a set of spot files

selectsam.mtf

9

more spots added to the spot files

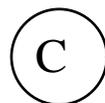*The convention is to store the selected sample reflections in slot 12.*

set file
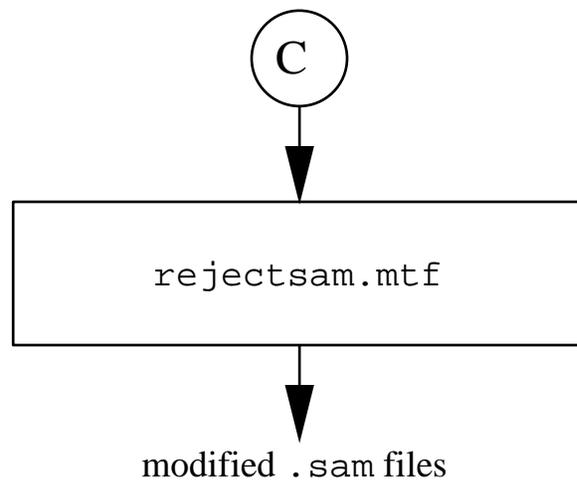a set of image files
a set of default files

sampling.mtf

10

a set of .apf files

a set of .sam files

C

animateProfile.pro

Viewing the fitted profiles by IDL.

Profiles (continue)

```
     ( C )
       │
       ▼
┌─────────────────────────┐
│                         │        Usually rejects a few percent by all parameters of the profiles.
│      rejectsam.mtf       │        This motif uses a utility program LauePlot.
│                         │
└─────────────────────────┘
       │
       ▼
 modified .sam files
```

set file
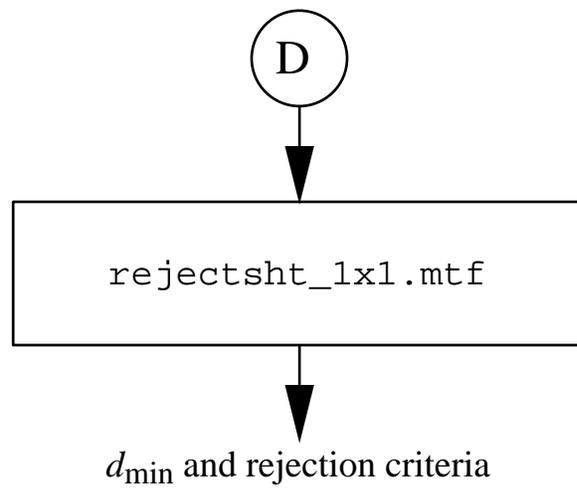`.lam` file
a set of default files

spoverlap_rdb.mtf
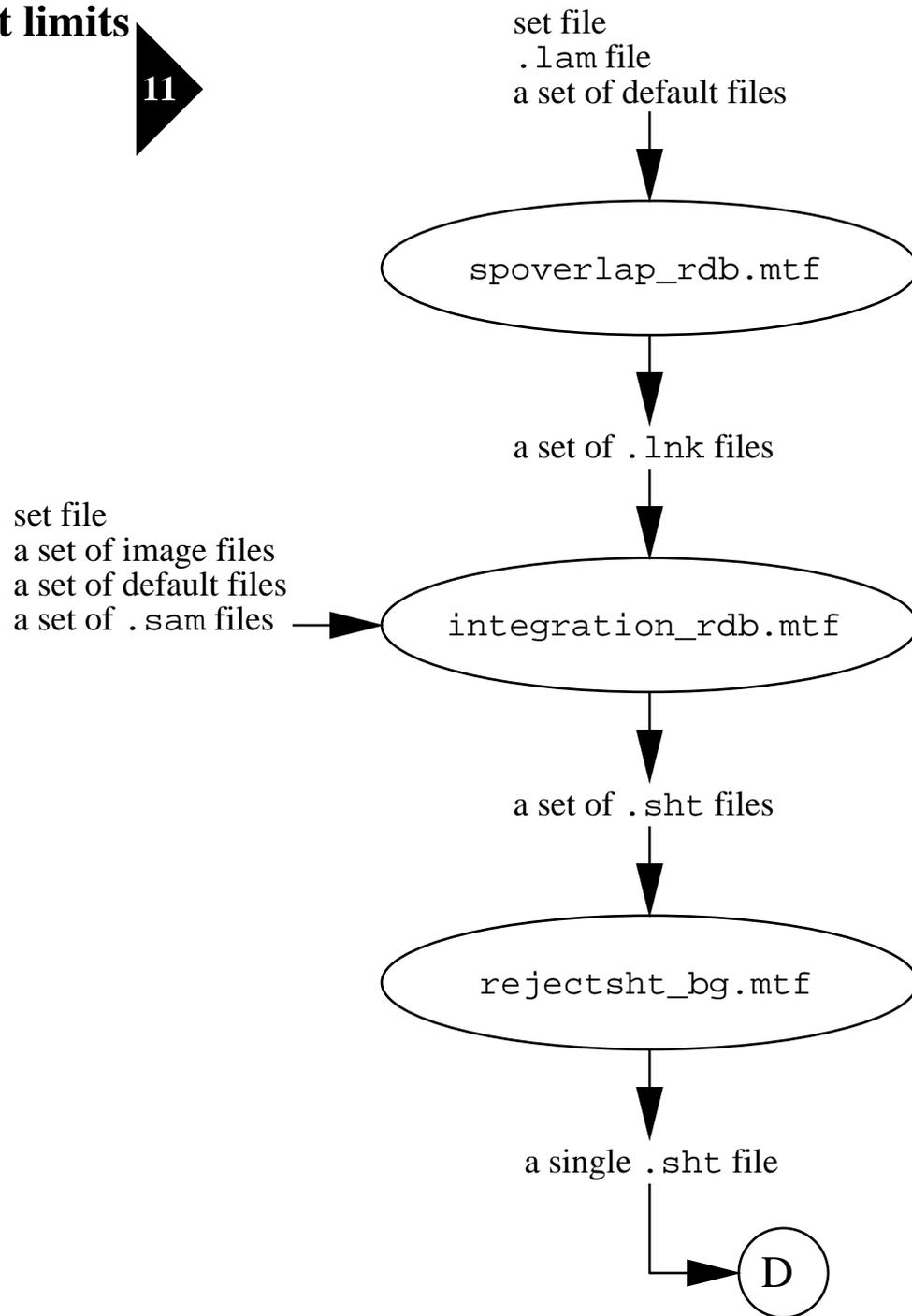
Set d$_{min}$ to a deliberately and liberally overpredicted value, such as 1.5 Å if the best estimated value is 2 Å, and 1.2 Å if the best estimate is 1.5 Å.
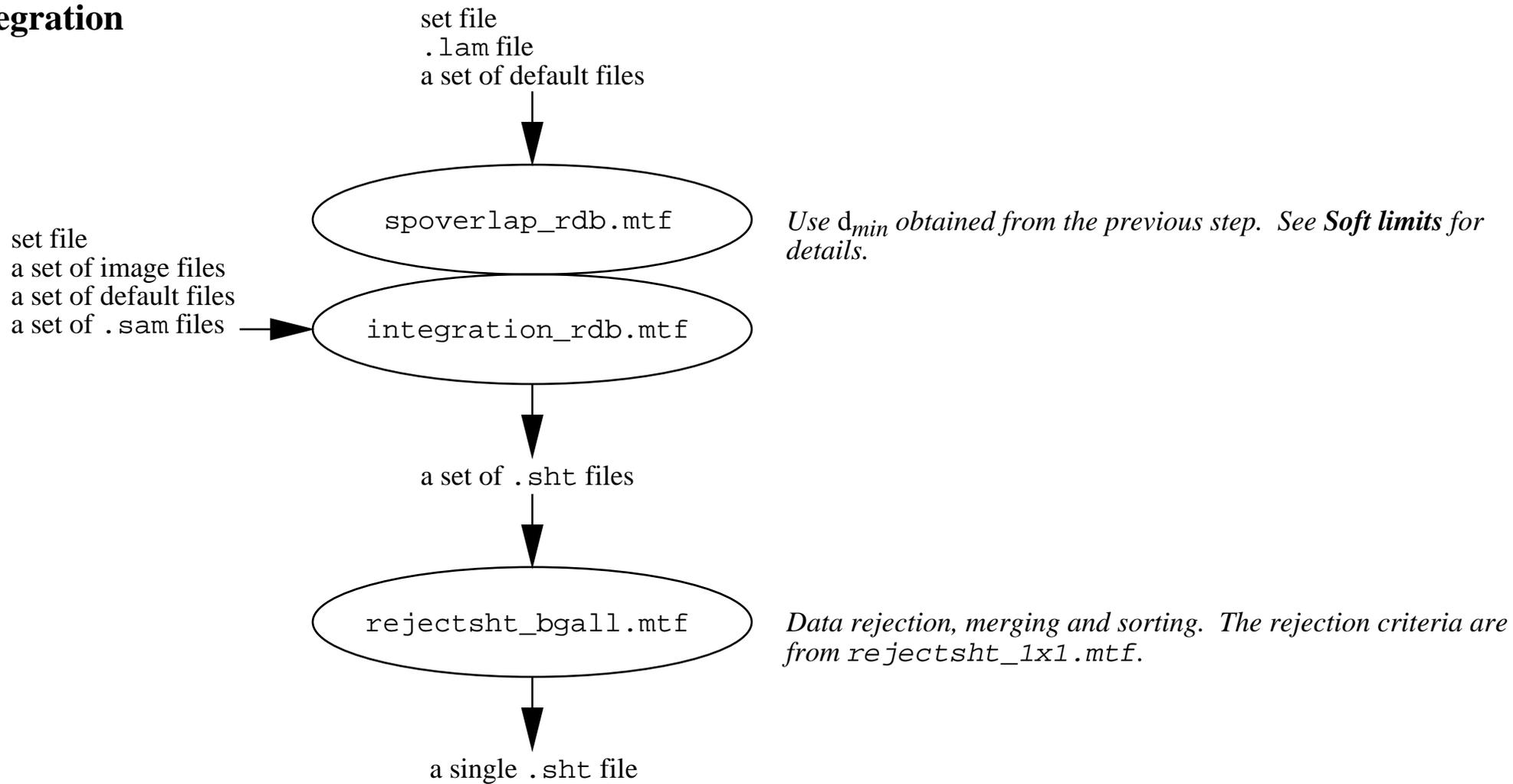
a set of `.lnk` files

set file
a set of image files
a set of default files
a set of `.sam` files

integration_rdb.mtf

a set of `.sht` files

rejectsht_bg.mtf

Data filtering, merging and sorting.

a single `.sht` file

D

Soft limits (continue)
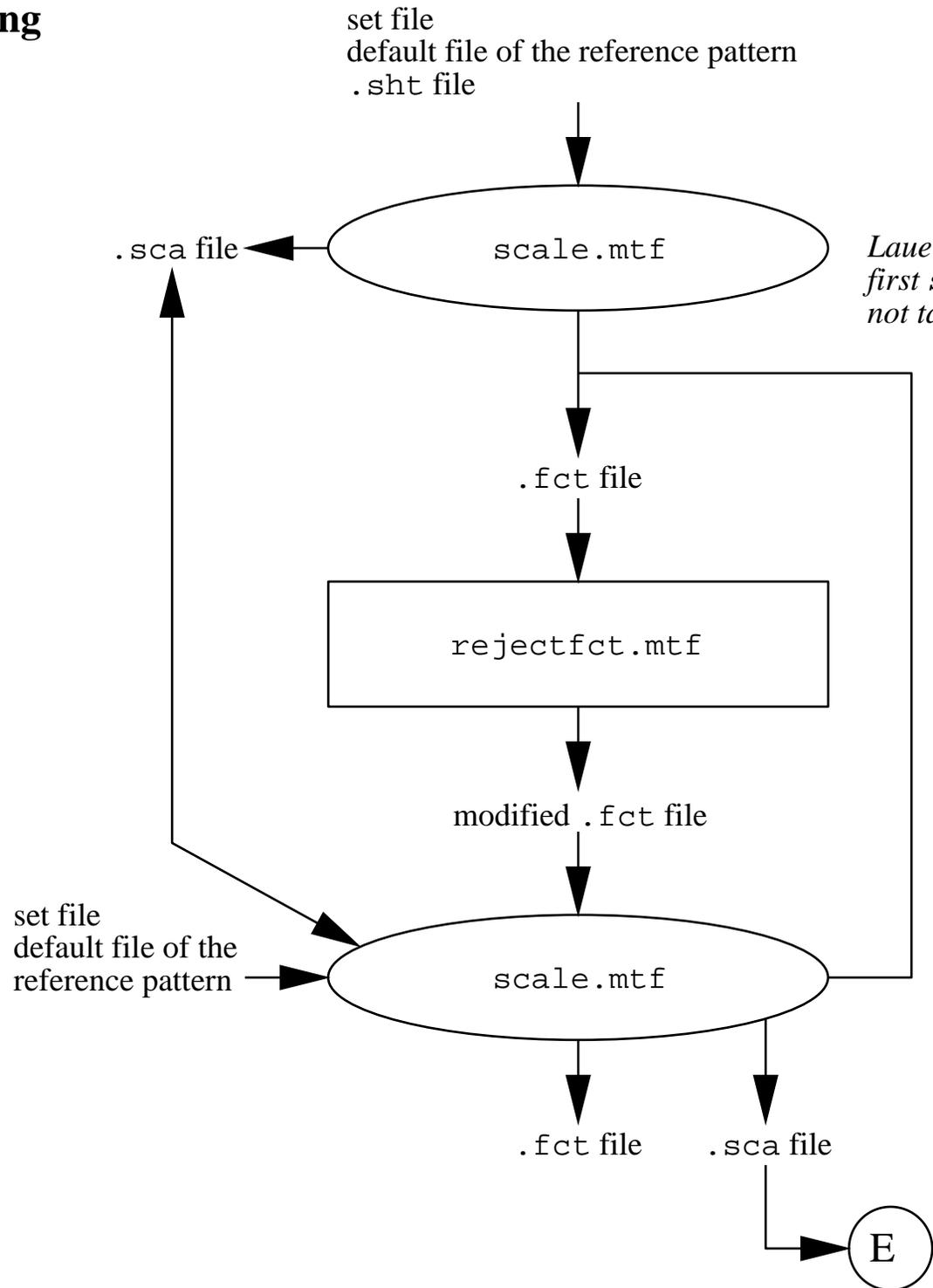
D

rejectsht_1x1.mtf

$d_{\min}$ and rejection criteria

Exam the histogram of resolution vs. I/σ(I), i.e., column 10−15. Select d_{min}. Sometimes reference to histogram of wavelength vs. resolution (11−10) is helpful.
Another purpose of this motif is to exam rejection criteria. Edit `rejectsht_bgall.mtf` *and record these criteria.*

Integration

set file
`.lam` file
a set of default files

spoverlap_rdb.mtf

*Use d$_{min}$ obtained from the previous step. See **Soft limits** for details.*

set file
a set of image files
a set of default files
a set of `.sam` files

integration_rdb.mtf

a set of `.sht` files

rejectsht_bgall.mtf

Data rejection, merging and sorting. The rejection criteria are from `rejectsht_1x1.mtf`.

a single `.sht` file

Scaling

set file
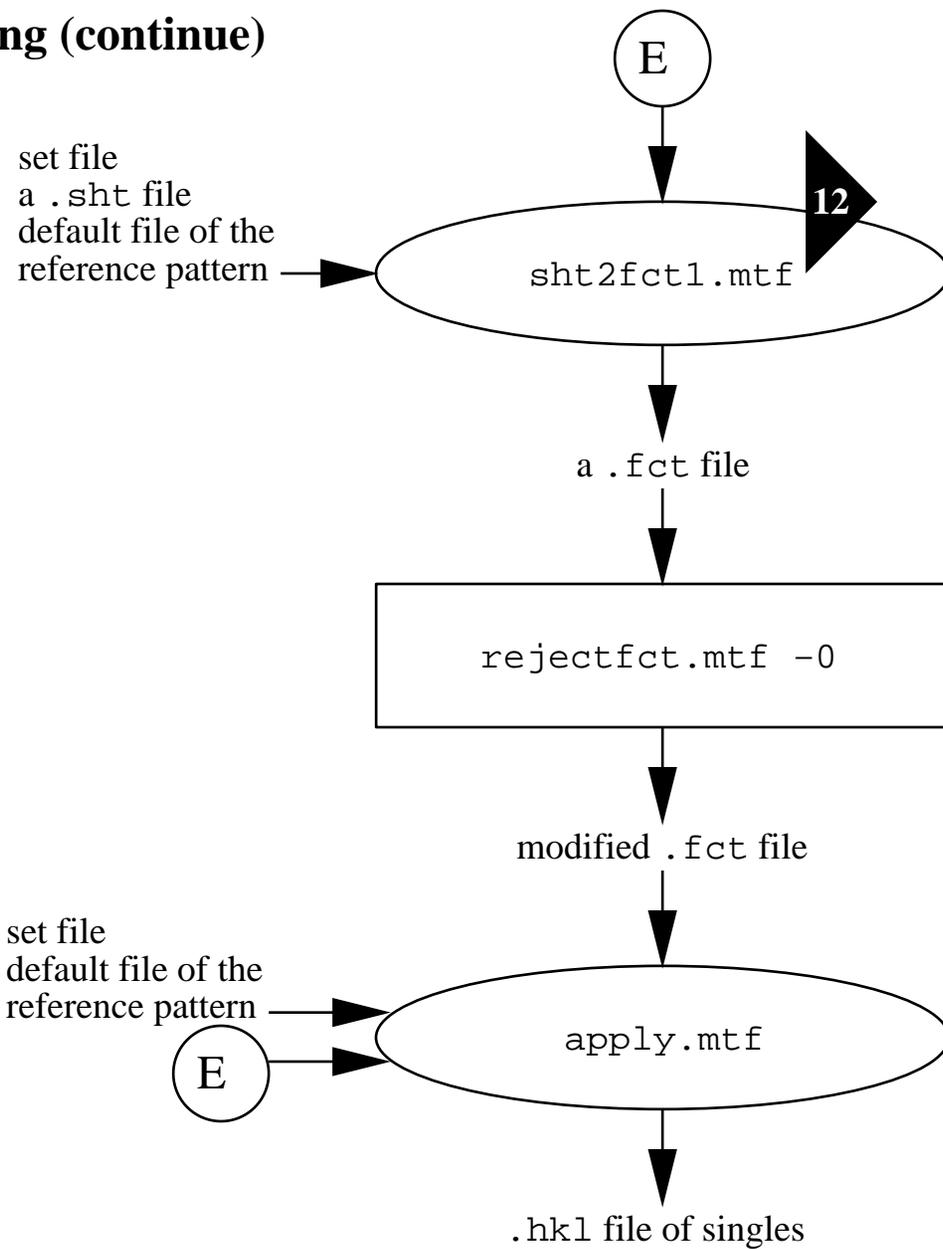default file of the reference pattern
`.sht` file

scale.mtf

.sca file

Laue data scaling including wavelength normalization. The first scale.mtf takes a .sht file as input. It may or may not take a .sca file as the initial values for scaling factors.

.fct file

rejectfct.mtf

modified .fct file

set file
default file of the
reference pattern

scale.mtf

This is a loop of rejectfct.mtf–scale.mtf. But the last step of the loop should be scale.mtf.

.fct file   .sca file

E

Scaling (continue)

E

set file
a `.sht` file
default file of the
reference pattern →

`sht2fct1.mtf` **12**

The input .sht file is usually the output of
`rejectsht_bgall.mtf` *or* `rejectsht_1x1.mtf`*.*

a `.fct` file

`rejectfct.mtf -0`

*Same or more stringent criteria should be used compared to
those in scaleing.*

modified `.fct` file

set file
default file of the
reference pattern →

E →

`apply.mtf`

`.hkl` file of singles

Harmonic reflections
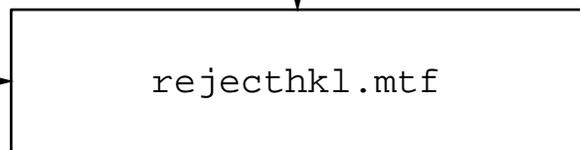
set file
.sca file
a set of .sht files
a default file of the reference pattern

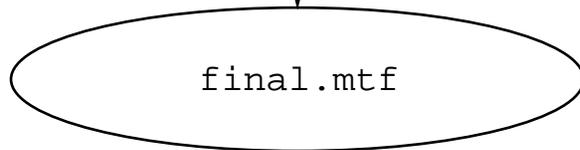*The .sht files are the output of integration_rdb.mtf.*
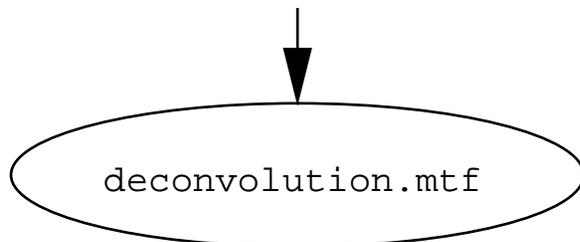
deconvolution.mtf

.hkl file of deconvoluted harmonic reflections

.hkl file of singles ⟶ rejecthkl.mtf

Reject data whose F or σ(F) are non−positive or small F/σ(F).

modified .hkl file of singles
modified .hkl file of multiples

final.mtf ⟶ .hkl file of singles and multiples merged

For the first time of finalizing, this result can be discarded.

modified .hkl file of singles
modified .hkl file of multiples

F

Harmonic reflections (continue)

F

rejecthkl.mtf   *Reject more data according to F/σ(F), if necessary.*

modified `.hkl` file of singles
modified `.hkl` file of multiples

final.mtf   modified `.hkl` file of singles
                              modified `.hkl` file of multiples

`.hkl` file of singles and multiples merged   *The result.*
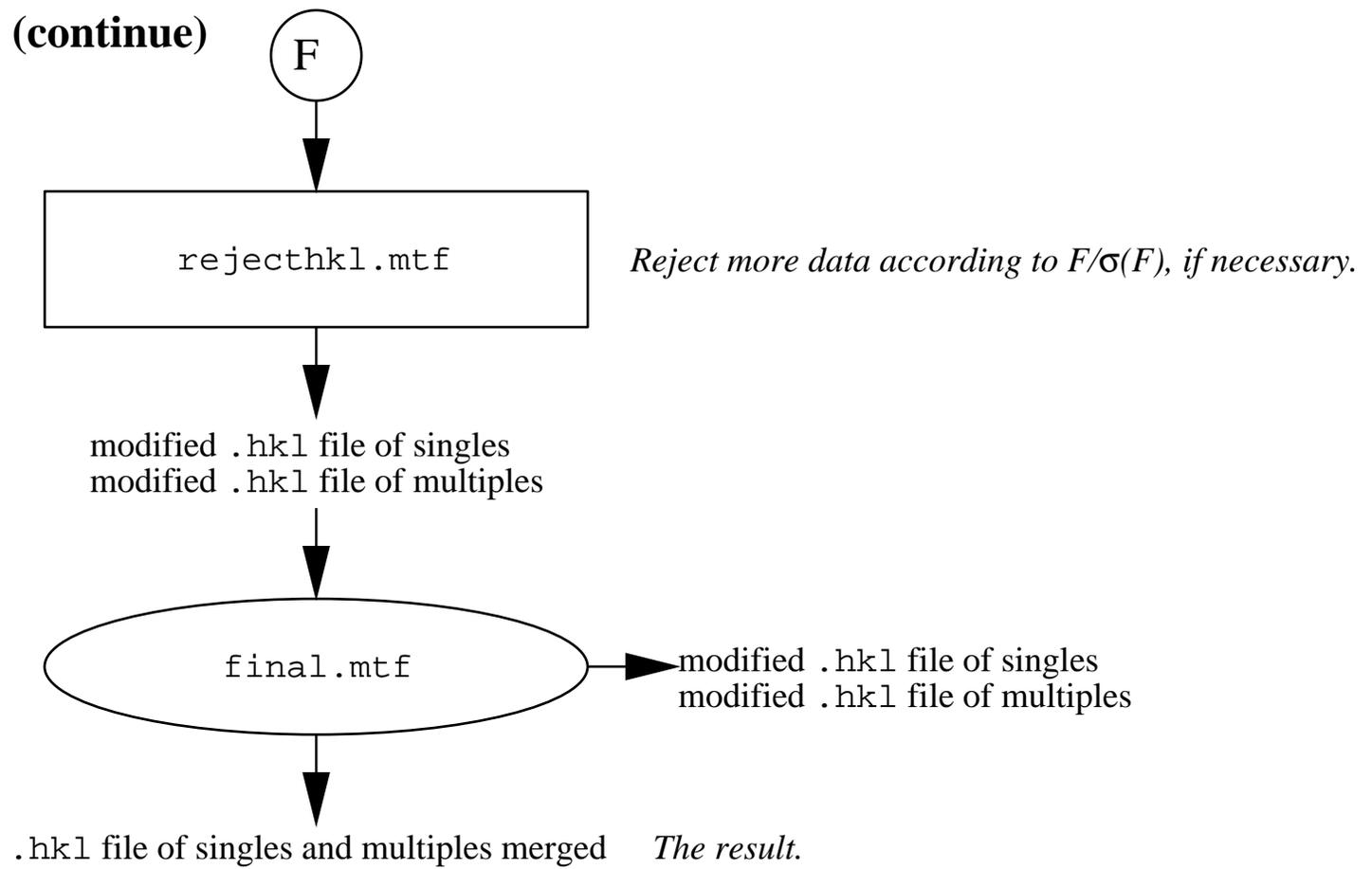
Monochromatic scaling

13

.hkl files whose σ's are to be scaled

.hkl file whose σ's are
the target

scalesigma.mtf **14**

This can be done one file at a time only.

.hkl files with σ's scaled

.hkl file whose σ's are
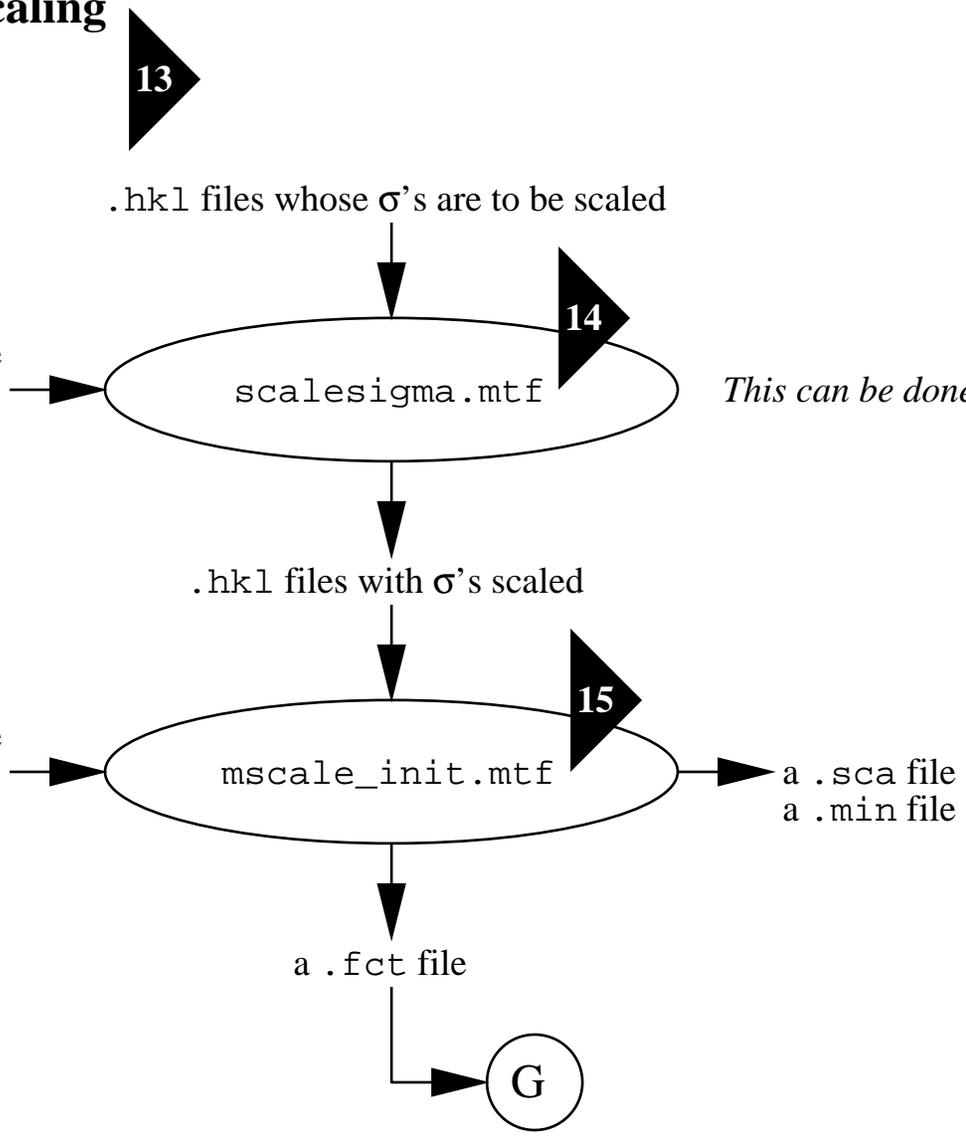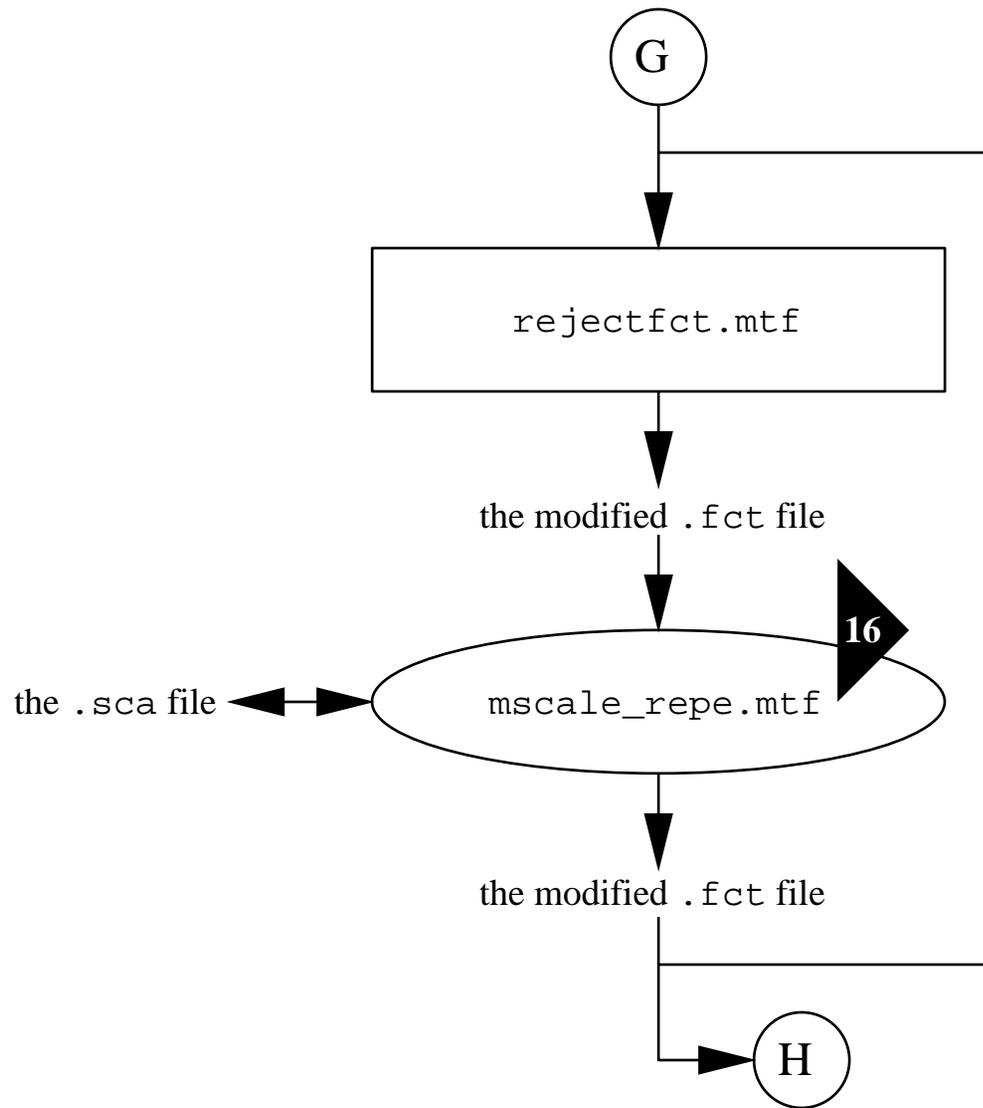the target

mscale_init.mtf **15**

a .sca file
a .min file

The .min file will be used in
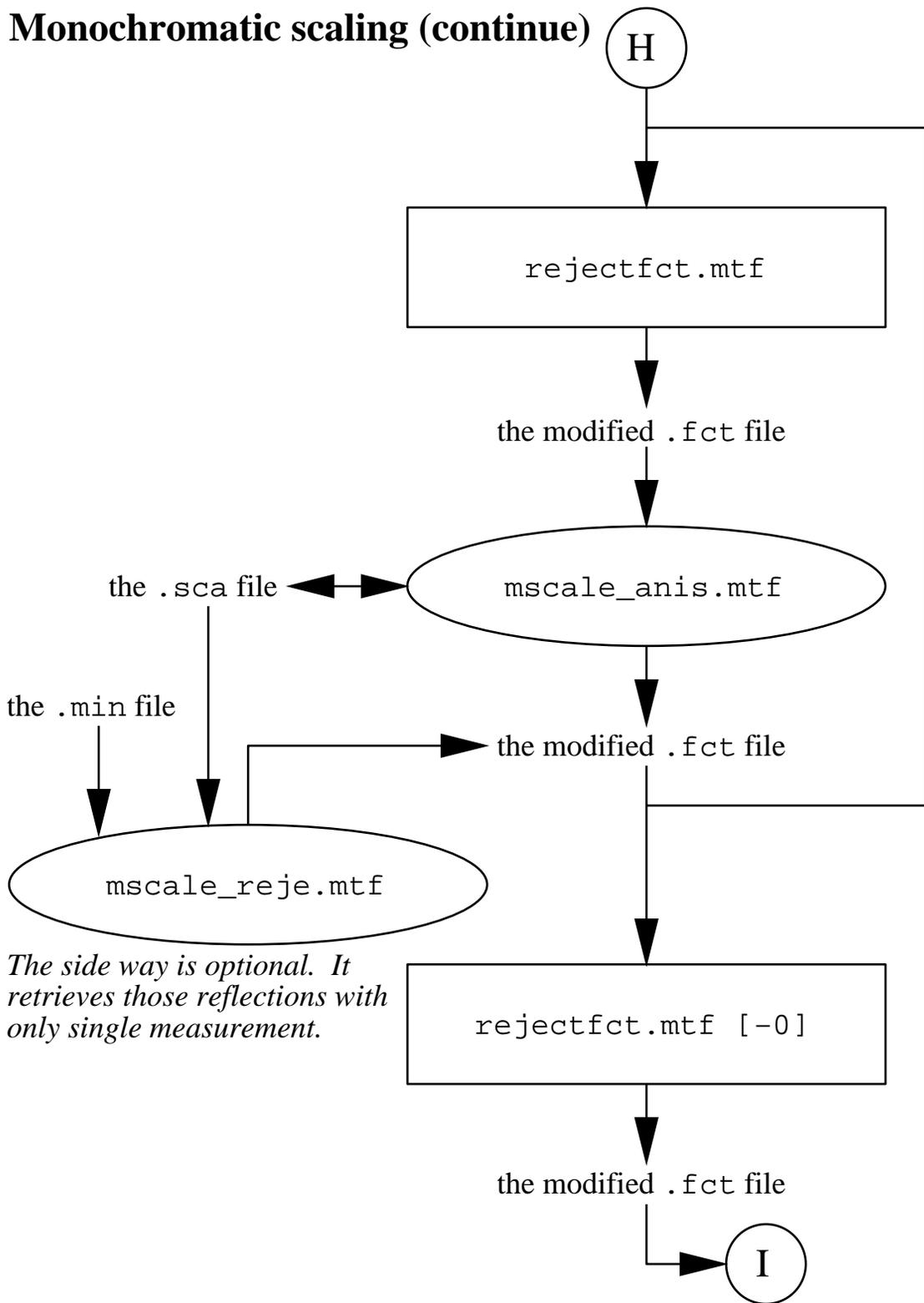*mscale_reje.mtf.*

a .fct file

G

Monochromatic scaling (continue)

G

rejectfct.mtf

the modified .fct file

16

the .sca file ←→ mscale_repe.mtf

the modified .fct file

H

This loop can be run as many as necessary, but normally once or twice.

Monochromatic scaling (continue)

H

rejectfct.mtf

the modified .fct file

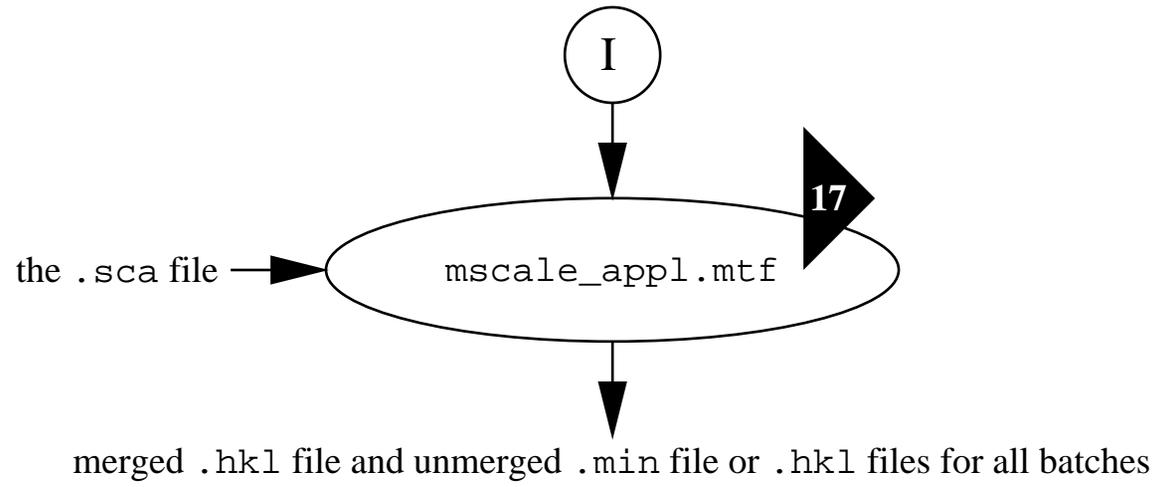the .sca file ⟷ mscale_anis.mtf

Anisotropic scale factors and temperature factors will be scaled. This loop is optional and can be run as many times as necessary, but normally once or twice.

the .min file

the modified .fct file

mscale_reje.mtf

The side way is optional. It retrieves those reflections with only single measurement.

rejectfct.mtf [-0]

Use -0 flag if mscale_reje.mtf *was used.*

the modified .fct file

I

Monochromatic scaling (continue)

I

the `.sca` file → mscale_appl.mtf **17**

merged `.hkl` file and unmerged `.min` file or `.hkl` files for all batches

Notes

1 Before start, make sure that all image file names are not longer than 10 characters.
The directory and file name convention is:

directory 1   where the image files reside
directory 2   the working directory, i.e., "./"
directory 3   the xtal_info directory
directory 4   anything
file name 1   image file name
file name 2   pattern name; for 1−spot pattern this is identical to file name 1
file name 3   data set name
file name 4   anything

2 `default.mtf` generates a set of default files. A default file contains information related to a single Laue pattern, such as crystal orientation, ϕ angle *etc*. Before running this motif, interactively display the first image in a data set, trim the image to remove edges/margins from the detector, save a default file with properly set directory names and file names (see Note 1). The first default file will be an input for this motif. The information contained in the first default file, such as how the image is trimmed, the directories and file names, will be spread out other default files in the data set.

3 `findspot.mtf` finds spots using a pattern recognition program. The coordinates of these spots will be stored in spot files `*.spt` and used in the geometry refinement. Please note that this motif will overwrite the old spot files.

4 `refine.mtf` performs geometry refinement, including crystal orientation, cell constants a, c, α, β, γ, beam center, distance, detector tilt angles, pixel size, bulge effect *etc*. This motif starts with a single well−refined reference image, which may or may not be done interactively. This motif reloads the unit cell constants and resets distance. This motif may also perform a detector edge testing that helps re−determine the beam center better in case that beam center is not stable from image to image. This segment can be commented out if the detector edges are not straight lines. Edge_testing is not applicable to the ESRF CCD detectors. Please note that this motif will overwrite the old default files.

5 `refine_prog.mtf` refines Laue geometry. This motif differs from `refine.mtf` in terms of using the previous refinement as the reference. It does not reload unit cell constants and does not reset distance. This motif refines crystal orientation, cell constants a, c, α, β, γ, beam center, distance, detector tilt angles, pixel size, bulge effect *etc*. A well refined pattern is necessary as the first reference. This motif may also test the detector edges (see Note 4). Please note that this motif will overwrite the old default files.

6 `refine_final.mtf` does the final geometry refinement including crystal orientation, cell parameters, beam center,

distance, detector tilt angles, pixel size, detector bulge effect *etc*. Preliminary refinement should be done before running this motif. Preliminary refinement can be done by `refine.mtf`, `refine_prog.mtf` and/or interactive refinement.

7 This section shows how to obtain the best profiles for the Laue data set. The resolution limit d_{min} should be set to the best or conservative estimate according to the user's knowledge of the crystal. A better estimate can be obtained in the next section.

8 `spoverlap_rdb.mtf` checks spatial overlaps between adjacent spots using resolution–dependent bandpass (RDB). RDB takes into consideration both an initial lambda–curve and the Wilson curve simultaneously. At high resolution, the effective bandpass is far narrower than one at low resolution. Prediction of the Laue diffraction is based on the variable bandpass. This motif does not load the image files; it is fully based on the prediction from the refined cell parameters and detector parameters.

9 `selectsam.mtf` selects sample reflections. A sample reflection is a non–spatially–overlapped and accurately predicted spot with high signal–to–noise ratio.

10 `sampling.mtf` fits the profiles of the selected sample reflections. This motif saves the profiles as `.apf` file which can be played by an `IDL` procedure `animateProfile.pro`.

11 Soft limits are d_{min}, λ_{min}, and λ_{max}. λ_{min} and λ_{max} are usually known, though roughly; d_{min} varies from crystal to crystal. This section shows how to determine d_{min} from overprediction.

12 `sht2fct1.mtf` copies a `.sht` file to a `.fct` format. The observations of redundancy=1 are included in the output. This motif retrievs observations as many as possible. However, the quality of redundancy=1 observations is unknown unless an external reference is available. This motif also calculates the `<F^2>` and the errors for evaluating the data quality of redundante data. LauePlot could be run to reject those reflections which have large errors. The input .sht file must be properly sorted by symmetry, *e.g.*, by `rejectsht_bg.mtf` or `rejectsht_bgall.mtf`. If one doesn't want to include redundancy=1 observations, the other motif `sht2fct2.mtf` should be used, instead.

13 This is not part of Laue data reduction, but it is useful for any scaling that does not involve wavelength–dependent correction factors.

14 This step is not always necessary. But when data from different sources, *e.g.*, different detectors, deferent software, experimental data *vs.* calculated data, the overall $I/\sigma(I)$ or $F/\sigma(F)$ level may be very different from each other. The subsequent steps of scaling may be biased due to the biased weighting scheme derived from the σ's. This step corrects this bias.

15 This motif initializes a monochramatic data scaling or sometimes a data scaling equivalent to monochramatic case, *i.e.*, no

wavelength–dependent correction factors. It takes several files in the free format of h, k, l, I, $\sigma(I)$. Each file contains the integrated intensities from a scan, which is called a batch sometime. The isotropic scale factors and temperature factors will be scaled. Histograms of the `.fct` file should be shown after this motif, and further scaling using `mscale_repe.mtf` is necessary if rejection is applied according to the histograms. The environment variable `CRYSTALINFO` must be set to point to the `xtal_info` directory. The environment variable `CRYSTALNAME` must be set.

16 Repeat monochramatic data scaling. Isotropic scale factors and temperature factors will be scaled again. Before running this motif, check the histograms by `LauePlot` (`rejectfct.mtf`) and reject some outliers. After running this motif, histograms of the `.fct` file could be shown, and further scaling of repeating this motif is necessary if rejection is applied.

17 Apply scale factors in monochramatic data scaling. After several repeats of `mscale_repe.mtf` and rejection using `LauePlot` (`rejectfct.mtf`) this motif applies the scale factors. Merged symmetry related reflections are saved in `$1.apply.hkl` file and unmerged are saved in `$1.apply.min` file. While merging, the square root is taken (I to F). If batch names are supplied after the dataset name, instead of output `$1.apply.min`, data from different batches are separated into `batch*.hkl`. The last step before this motif should be `mscale_repe.mtf` rather than the rejection.