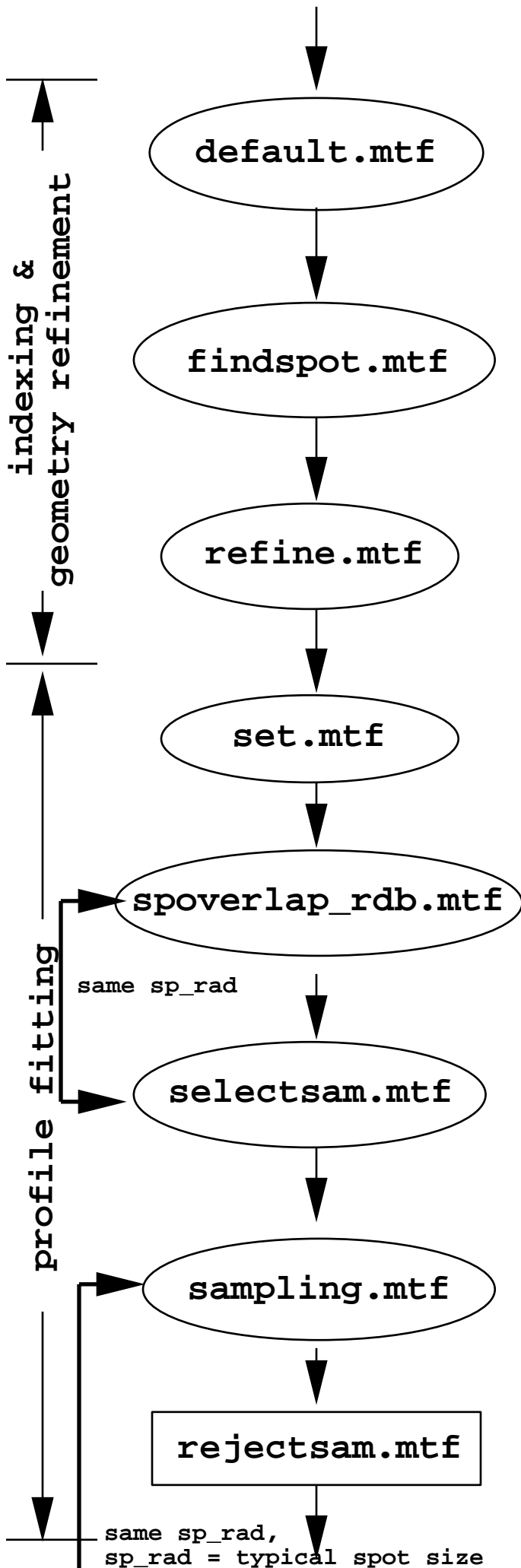


Notes



function: copies ref.def to all other *.def files

input: manually well refined reference default (ref.def)

output: *.def (for those on the image name list)

function: finds spots for geometry refinement

input: *.def

output: *.spt(slot #11)

in **findspot.log** check # of spots actually found (search for "spots")

function: geometry refinement

input: *.def

output: *.def (overwrites the old *.def)

in **refine.log** search for "matched spots"

function: generates a \$.set file

assigning a pattern # to each image

input: *.def files

output: \$.set (\$=data set name)

function: predicts spatially overlapped spots

input: *.def,

\$.set, X-ray-spectrum.lam

output: *.lnk

in **sponverlap_rdb.log** search for "reflections checked"

function: selects non-spatially

overlapped spots (<1000) for profile fitting

input: *.def, *.img, *.spt, \$.set, *.lnk

output: *.spt(slot #12)

in **selectsam.log** search for "spots selected"

function: profile fitting for selected samples

input: *.def, *.img, *.lnk, *.spt, \$.set

output: *.sam

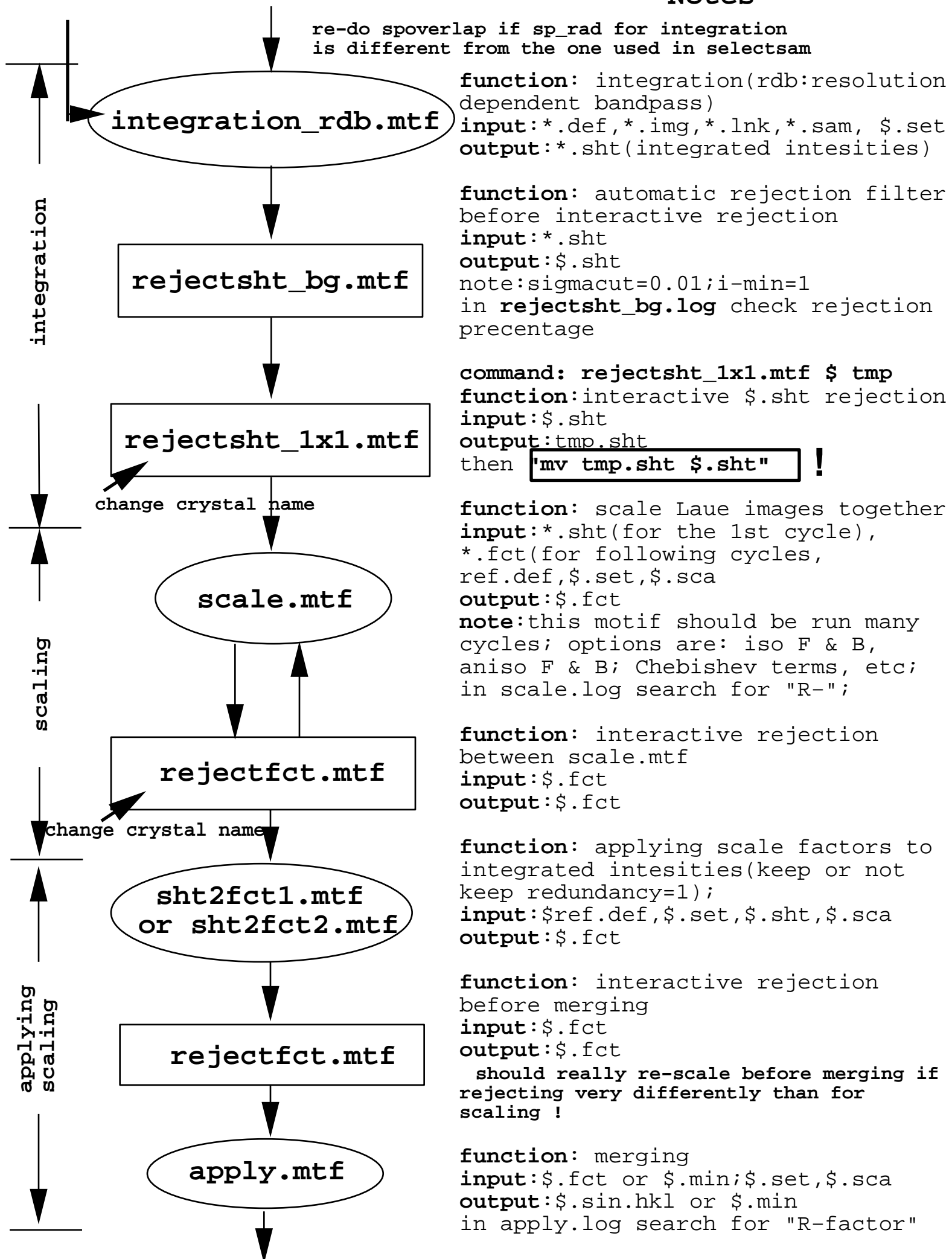
function: interactive rejection of

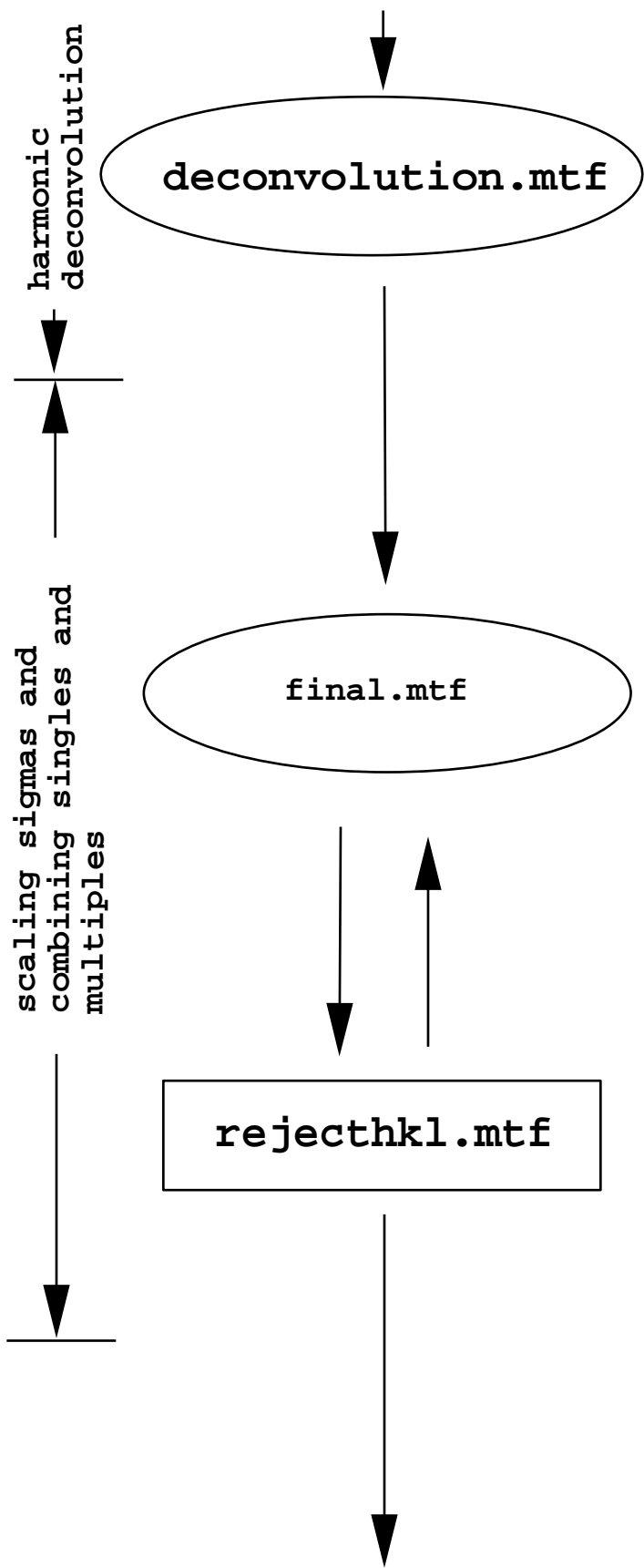
samples by LauePlot

make **note** on half-axis-a and

half-axis-b for typical spots

Notes





function:deconvoluting energy overlaps;
input:*.def,*.sht,\$.set,\$.sca
output:\$dataset.har.hkl
Note: use same sigma cut and i-min criteria as for singles in rejectsht_1x1.mtf or rejectsht_bgall.mtf

command: final.mtf \$
function:calculating true error estimates for singles, scaling multiples' sigmas against singles' and combining singles and multiples
input:\$.sin.hkl,\$.har.hkl
output:modified \$.sin.hkl, \$.har.hkl and \$.hkl (merged singles and multiples)

command: rejecthkl.mtf \$.sin \$.har
function: rejecting data based on $F/\sigma(F)$ if necessary
input: \$.sin.hkl, \$.har.hkl
output:modified \$.sin.hkl, \$.har.hkl

\$dataset.hkl

h k l F σ_F