

NAME

MX-calibrate – MX-calibrate

DESCRIPTION

usage: MX-Calibrate **-w** 1.54 **-c** CeO2 file1.cbf file2.cbf ...

Calibrate automatically a set of frames taken at various sample–detector distance. Return the linear regression of the fit in function of the sample-detector distance.

positional arguments:

FILE List of files to calibrate

optional arguments:

-h, --help

show this help message and exit

-V, --version

-v, --verbose

switch to debug/verbose mode

-c FILE, --calibrant FILE

file containing d–spacing of the calibrant reference sample (MANDATORY)

-w WAVELENGTH, --wavelength WAVELENGTH

wavelength of the X–Ray beam in Angstrom

-e ENERGY, --energy ENERGY

energy of the X–Ray beam in keV (hc=12.398419292keV.A)

-P POLARIZATION_FACTOR, --polarization POLARIZATION_FACTOR

polarization factor, from **-1** (vertical) to **+1** (horizontal), default is 0, synchrotrons are around 0.95

-b BACKGROUND, --background BACKGROUND

Automatic background subtraction if no value are provided

-d DARK, --dark DARK

list of dark images to average and subtract

-f FLAT, --flat FLAT

list of flat images to average and divide

-s SPLINE, --spline SPLINE

spline file describing the detector distortion

-p PIXEL, --pixel PIXEL

size of the pixel in micron

-D DETECTOR_NAME, --detector DETECTOR_NAME

Detector name (instead of pixel size+spline)

-m MASK, --mask MASK

file containing the mask (for image reconstruction)

--filter FILTER

select the filter, either mean(default), max or median

--saturation SATURATION

consider all $\text{pixel} > \text{max} * (1 - \text{saturation})$ as saturated and reconstruct them

-r MAX_RINGS, --ring MAX_RINGS

maximum number of rings to extract

--weighted

weight fit by intensity

-l DISTANCE, **--distance** DISTANCE
sample-detector distance in millimeter

--no-tilt
refine the detector tilt

--poni1 PONI1
poni1 coordinate in meter

--poni2 PONI2
poni2 coordinate in meter

--rot1 ROT1
rot1 in radians

--rot2 ROT2
rot2 in radians

--rot3 ROT3
rot3 in radians

--fix-dist
fix the distance parameter

--free-dist
free the distance parameter

--fix-poni1
fix the poni1 parameter

--free-poni1
free the poni1 parameter

--fix-poni2
fix the poni2 parameter

--free-poni2
free the poni2 parameter

--fix-rot1
fix the rot1 parameter

--free-rot1
free the rot1 parameter

--fix-rot2
fix the rot2 parameter

--free-rot2
free the rot2 parameter

--fix-rot3
fix the rot3 parameter

--free-rot3
free the rot3 parameter

--fix-wavelength
fix the wavelength parameter

--free-wavelength
free the wavelength parameter

--no-gui
force the program to run without a Graphical interface

--gui force the program to run with a Graphical interface

--no-interactive

force the program to run and exit without prompting for refinements

--interactive

force the program to prompt for refinements

--peak-picker PEAKPICKER

Uses the 'massif' or the 'blob' peak-picker algorithm (default: blob)

This tool has been developed for ESRF MX-beamlines where an acceptable calibration is usually present in the header of the image. PyFAI reads it and does a "recalib" on each of them before exporting a linear regression of all parameters versus this distance.