
pyFAI Documentation

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CONTENTS

This document starts with a general descriptions of the pyFAI library in the first chapter. This first chapter contains an introduction to pyFAI, what it is, what it aims at and how it works (for scientists). Especially, geometry, calibration, azimuthal integration algorithms are described and pixel splitting schemes are explained.

The second chapter is the concatenation of the manual pages of all (relevant) scripts. Those are programs to be launched at the command line allowing the treatment of a diffraction experiment without knowing anything about Python.

The third chapter contains a comprehensive description of most Python modules contained in pyFAI. Some minor submodules as well as the documentation of the Cython sub-modules are not included for concision purposes. The last chapter is an appendix giving some figures about the project and its management.

GENERAL INTRODUCTION TO PYFAI

1.1 Python Fast Azimuthal Integration

PyFAI is implemented in [Python](#) programming language, which is open source and already very popular for scientific data analysis ([PyMca], [PyNX], ...). It relies on the scientific stack of python composed of [NumPy], [SciPy] and [Matplotlib] plus the [OpenCL] binding [PyOpenCL] for performances.

2D area detectors like CCD or pixel detectors have become popular in the last 15 years for diffraction experiments (e.g. for WAXS, SAXS, single crystal and powder diffraction). These detectors have a large sensitive area of millions of pixels with high spatial resolution. The software package pyFAI ([SRI2012], [EPDIC13]) has been designed to reduce SAXS, WAXS and XRPD images taken with those detectors into 1D curves (azimuthal integration) usable by other software for in-depth analysis such as Rietveld refinement, or 2D images (a radial transformation named *caking* in [FIT2D]). As a library, the aim of pyFAI is to be integrated into other tools like [PyMca] or [EDNA] or [LImA] with a clean pythonic interface. However pyFAI features also command line and graphical tools for batch processing, converting data into *q-space* (q being the momentum transfer) or 2θ -space (θ being the Bragg angle) and a calibration graphical interface for optimizing the geometry of the experiment using the Debye-Scherrer rings of a reference sample. PyFAI shares the geometry definition of SPD but can directly import geometries determined by the software FIT2D. PyFAI has been designed to work with any kind of detector and geometry (transmission or reflection) and relies on FabIO, a library able to read more than 20 image formats produced by detectors from 12 different manufacturers. During the transformation from cartesian space (x, y) to polar space $(2\theta, \chi)$, both local and total intensities are conserved in order to obtain accurate quantitative results. Technical details on how this integration is implemented and how it has been ported to native code and parallelized on graphic cards are discussed in this paper.

1.2 Introduction

With the advent of hyperspectral experiments like diffraction tomography in the world of synchrotron radiation, existing software tools for azimuthal integration like [FIT2D] and [SPD] reached their performance limits owing to the fast data rate needed by such experiments. Even when integrated into massively parallel frameworks like [EDNA], such stand-alone programs, due to their monolithic nature, cannot keep the pace with the data flow of new detectors. Therefore we decided to implement from scratch a novel azimuthal integration tool which is designed to take advantage of modern parallel hardware features. PyFAI assumes the setup does not change during the experiment and tries to reuse a maximum number of data (using [memoization](#)), moreover those calculation are performed only when needed ([lazy_evaluation](#)).

1.3 Geometry and calibration

PyFAI and spd share the same 6-parameter geometry definition: distance, point of normal incidence (2 coordinates) and 3 rotations around the main axis; these parameters are saved in text files usually with the *.poni* extension. The program *pyFAI-calib* helps calibrating the experimental setup using a constrained least squares optimization on the Debye-Scherrer rings of a reference sample (*LaB₆*, silver behenate, ...). Alternatively, geometries calibrated using *fit2d* can be imported into pyFAI, including geometric distortions (i.e. optical-fiber tapers distortion) described as *spline-files*.

1.3.1 Geometry

PyFAI takes diffraction images as 2D numpy arrays. The origin of the image is considered to be at the lower-left corner of the image. Axis 1 and 2 on the image (like in *poni1* & *poni2*) refer to the slow and fast dimension of the image, so usually to the y and x axis (and not the opposite)

$(p1,2) = (y, x)$

In the same idea *rot1*, *rot2* and *rot3* are rotation along axis 1, 2 and 3, always expressed in radians. Axis 3 is built in such a way to be orthogonal and (1,2,3) is a direct orientation Rotations applied in the same order: *rot1* then *rot2* then *rot3*.

Poni1 and *poni2* are distances in meter, like the distance, letting the calibration be independent to pixel size hence to binning.

1.3.2 Calibration

The determination of the geometry of the experimental setup for the diffraction pattern of a reference sample is called calibration in pyFAI. A geometry setup is composed of a detector, the six refined parameters like the distance and fixed parameters like the wavelength (or the energy of the beam), they are all saved together into a text files named ".poni" (as a reference to the point of normal incidence) which is subsequently used for processing the experiment.

By storing all parameters together in a single small file, the risk of mixing two parameters is highly reduced and we believe this helps performing better science with fewer mistakes.

While entering the geometry of the experiment in a *poni-file* is possible it is easier to perform a calibration, using the Debye-Sherrer rings of a reference sample called calibrant. About 10 calibrant description files are shipped with the default installation of pyFAI, like *LaB₆*, silicon, ceria, corundum or silver behenate. The user can choose to provide their own calibrant description files which are simple text-file containing the largest d-spacing (in Angstrom) for a set of Miller plans. A useful reference is the American Mineralogist database [AMD] or the Crystallographic Open database [COD].

The calibration is divided into 4 major steps:

Pre-processing of images:

The typical pre-processing consists of the averaging (or median filter) of darks images. Dark current images are then subtracted from data and corrected for flat.

If saturated pixels exists, they are likely to be treated like peaks but their positions will be wrong. It is advised to either mask them out or to desaturate them (pyFAI provides an option, but it is expensive in calculation time)

Peak-picking

The Peak-picking consists in the identification of peaks and groups of peaks belonging to same ring. It can be performed by two methods : blob detection or massif detection.

Massif detection

This method consists in making the difference of the original image and a blurred image. Then we look for a chain of positives values, corresponding to a single group of peak. The blurring parameter can be adjusted using the “-g” option in pyFAI-calib.

Blob detection

The approach is based on difference of gaussians (DoGs) as described in the [blob_detection](#) article of wikipedia.

It consists in blurring the image by convolution with a 2D gaussian kernel and making differences between two successive blurs (called Difference Of Gaussian). In these DoGs, keypoints are defined as the maxima in the 3D space (y,x,size of the gaussian). After their localization, keypoints are refined by Savitzky Golay algorithm or by an interpolation at the second order which is equivalent but uses less points. At this step, if the estimation of the maximum is too far from the maximum, the keypoint will be considered as a fake maximum and removed.

Steepest ascent

This is very naive implementation which looks for the nearest local maximum. Subsequently a sub-pixel optimization is performed based on the local gradient and hessian.

Monte-Carlo sampling

Series of peaks can be extracted using the Steepest Ascent on randomly selected seeds.

Refinement of the parameters

After grouping of peaks, groups of peak are assigned to a Debye-Scherrer ring and to a d-spacing. PyFAI uses a least-squares refinement of the geometry parameters on peak position.

The optimization procedure is the Sequential Least Squares Programming implemented in `scipy.optimize.slsqp`. The cost function is the sum of the square of the difference between the expected and calculated 2θ values for the various peaks. This sum is dependent on the number of control-points.

Validation of the calibration

Validation by an human being of the geometry is an essential step: pyFAI will overlay to the diffraction image, the lines corresponding to the various diffraction rings expected from the calibrant. Those lines should be in pretty good agreement with the rings of the scattering image.

Once the calibration is finished, one can use the `validate` option to check the offset between the input image and the generated one from the diffraction pattern.

1.3.3 PyFAI executables

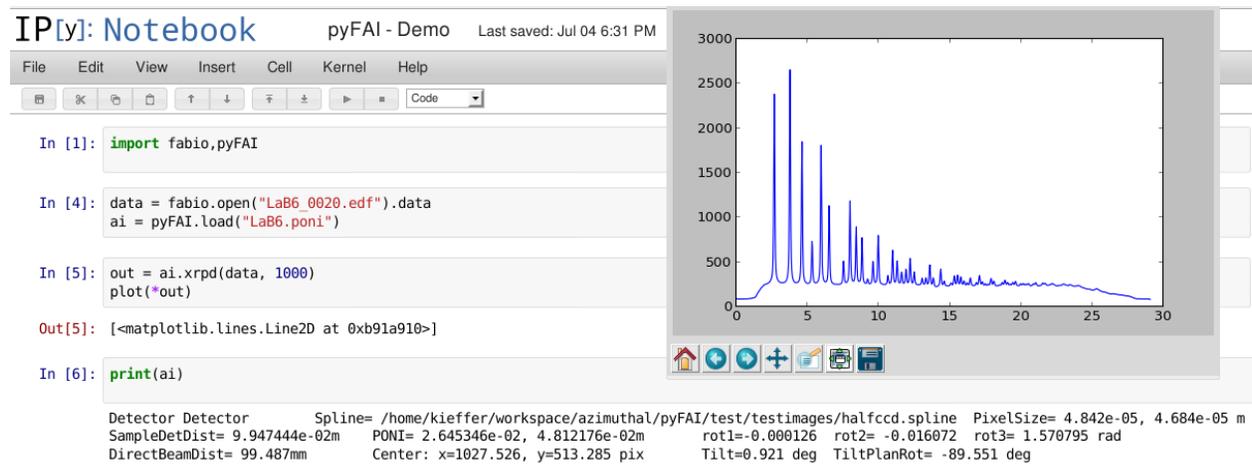
PyFAI was designed to be used by scientists needing a simple and effective tool for azimuthal integration. Two command line programs *pyFAI-waxs* and *pyFAI-saxs* are provided with pyFAI for performing the integration of one or more images on the command line. The waxs version outputs result in $2\theta/I$, whereas the saxs version outputs result in $q/I(\sigma)$. Options for these programs are parameter file (*poni-file*) describing the geometry and the mask file. They can also do some pre-processing like dark-noise subtraction and flat-field correction (solid-angle correction is done by default).

A new Graphical interface based on Qt called *pyFAI-integrate* is now available, offers all options possible for azimuthal integration (dark/flat/polarization, ...) in addition to a finer tuning for the computing device selection (CPU/GPU).

Finally a specialized tool called *diff_tomo* is available to reduce a mapping of 2D images into a 3D volume (math:*x, y, 2theta* for mapping or math:*rot, trans, 2theta* for tomography)

1.3.4 Python library

PyFAI is first and foremost a library: a tool of the scientific toolbox built around [IPython] and [NumPy] to perform data analysis either interactively or via scripts. Figure [notebook] shows an interactive session where an integrator is created, and an image loaded and integrated before being plotted.



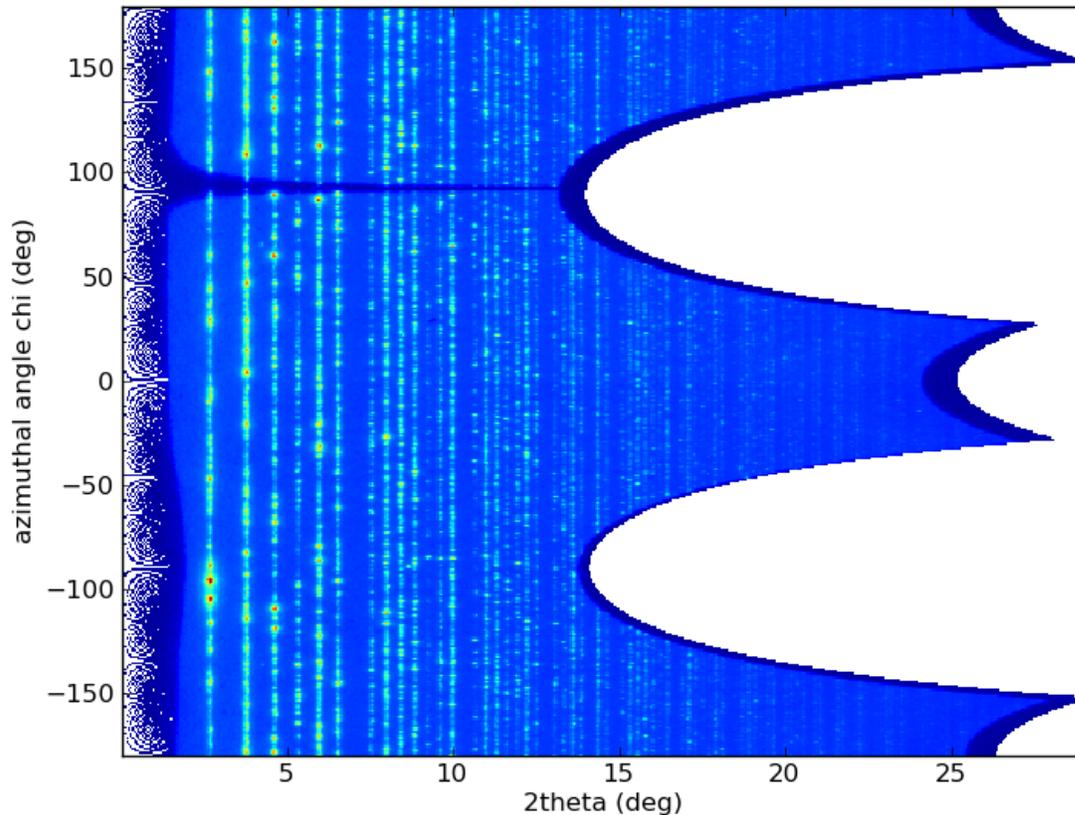
1.4 Regrouping mechanism

In pyFAI, regrouping is performed using a histogram-like algorithm. Each pixel of the image is associated to its polar coordinates ($2\theta, \chi$) or (q, χ), then a pair of histograms versus 2θ (or q) are built, one non weighted for measuring the number of pixels falling in each bin and another weighted by pixel intensities (after dark-current subtraction, and corrections for flat-field, solid-angle and polarization). The division of the weighted histogram by the number of pixels per bin gives the diffraction pattern. $2D$ regrouping (called *caking* in FIT2D) is obtained in the same way using two-dimensional histograms over radial (2θ or q) and azimuthal angles (χ).

1.4.1 Pixel splitting algorithm

Powder diffraction patterns obtained by histogramming have a major weakness where pixel statistics are low. A manifestation of this weakness becomes apparent in the $2D$ -regrouping where most of the bins close to the beam-stop are not populated by any pixel. In this figure, many pixels are missing in the low 2θ region, due to the arbitrary

discretization of the space in pixels as intensities were assigned to each pixel center which does not reflect the physical reality of the scattering experiment.



PyFAI solves this problem by pixel splitting : in addition to the pixel position, its spatial extension is calculated and each pixel is then split and distributed over the corresponding bins, the intensity being considered as homogeneous within a pixel and spread accordingly. The drawback of this is the correlation introduced between two adjacent bins. To simplify calculations, this was initially done by abstracting the pixel shape with a bounding box that circumscribes the pixel. In an effort to better the quality of the results this method was dropped in favour of a full

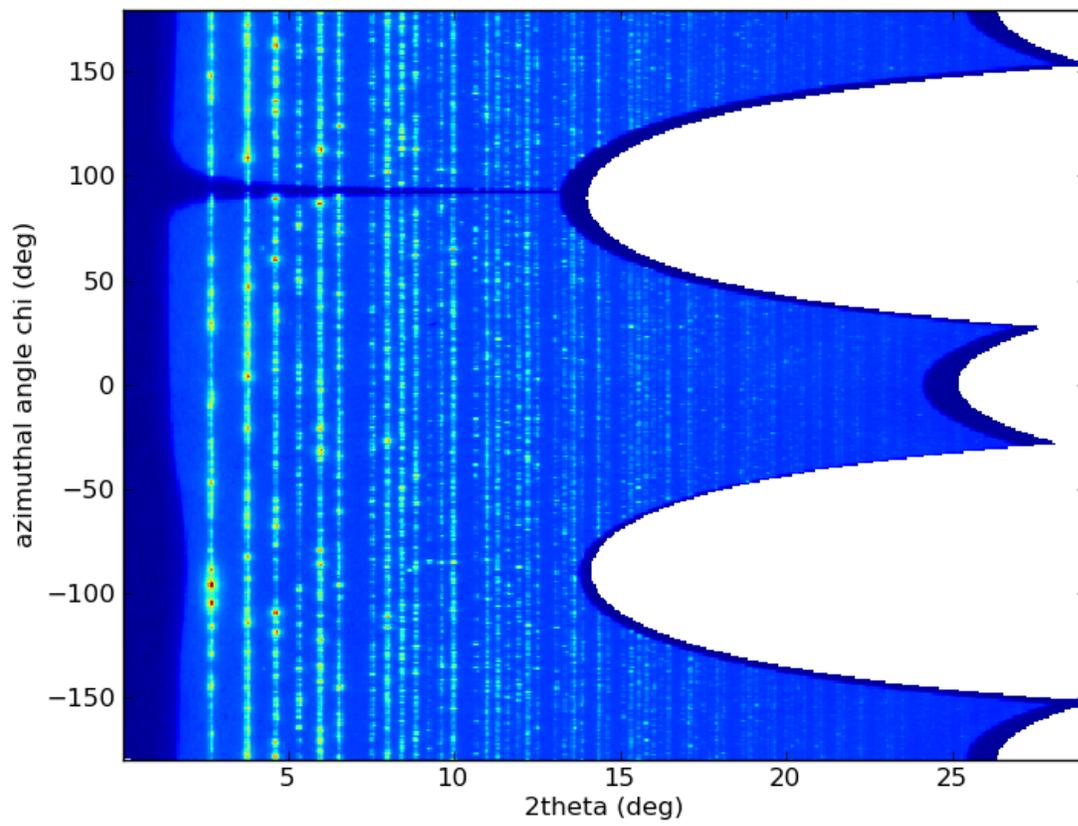
pixel splitting scheme that actually uses the actual pixel geometry for its calculations.

1.4.2 Performances and migration to native code

Originally, regrouping was implemented using the histogram provided by [NumPy], then re-implemented in [Cython] with pixel splitting to achieve a four-fold speed-up. The computation time scales like $O(N)$ with the size of the input image. The number of output bins shows only little influence; overall the single threaded [Cython] implementation has been stated at 30 Mpix/s (on a 3.4 GHz Intel core i7-2600).

1.4.3 Parallel implementation

The method based on histograms works well on a single processor but runs into problems requiring so called “atomic operations” when run in parallel. Processing pixels in the input data order causes write access conflicts which become



less efficient with the increase of number of computing units (need of `atomic_operation`). This is the main limit of the method exposed previously; especially on GPU where hundreds of threads are executed simultaneously.

To overcome this limitation; instead of looking at where input pixels GO TO in the output image, we instead look at where the output pixels COME FROM in the input image. This transformation is called a “scatter to gather” transformation in parallel programming.

The correspondence between pixels and output bins can be stored in a look-up table (LUT) together with the pixel weight which make the integration look like a simple (if large and sparse) matrix vector product. This look-up table size depends on whether pixels are split over multiple bins and to exploit the sparse structure, both index and weight of the pixel have to be stored. We measured that 500 Mbytes are needed to store the LUT to integrate a 16 megapixels image, which fits onto a reasonable quality graphics card nowadays but can still be too large to fit on an entry-level graphics card.

By making this change we switched from a “linear read / random write” forward algorithm to a “random read / linear write” backward algorithm which is more suitable for parallelization. As a further improvement on the algorithm, the use of compressed sparse row (CSR) format was introduced, to store the LUT data. This algorithm was implemented both in [Cython]-OpenMP and OpenCL. The CSR approach has a double benefit: first, it reduces the size of the storage needed compared to the LUT by a factor two to three, offering the opportunity of working with larger images on the same hardware. Secondly, the CSR implementation in OpenCL is using an algorithm based on multiple parallel reductions where many execution threads are collaborating to calculate the content of a single bin. This makes it very well suited to run on GPUs and accelerators where hundreds to thousands of simultaneous threads are available.

When using OpenCL for the GPU we used a compensated (or [Kahan_summation](#)), to reduce the error accumulation in the histogram summation (at the cost of more operations to be done). This allows accurate results to be obtained on cheap hardware that performs calculations in single precision floating-point arithmetic (32 bits) which are available on consumer grade graphic cards. Double precision operations are currently limited to high price and performance computing dedicated GPUs. The additional cost of Kahan summation, 4x more arithmetic operations, is hidden by smaller data types, the higher number of single precision units and that the GPU is usually limited by the memory bandwidth anyway.

The performances of the parallel implementation based on a LUT, stored in CSR format, can reach 750 MPix/s on recent multi-core computer with a mid-range graphics card. On multi-socket server featuring high-end GPUs like Tesla cards, the performances are similar with the additional capability to work on multiple detector simultaneously.

1.5 Conclusion

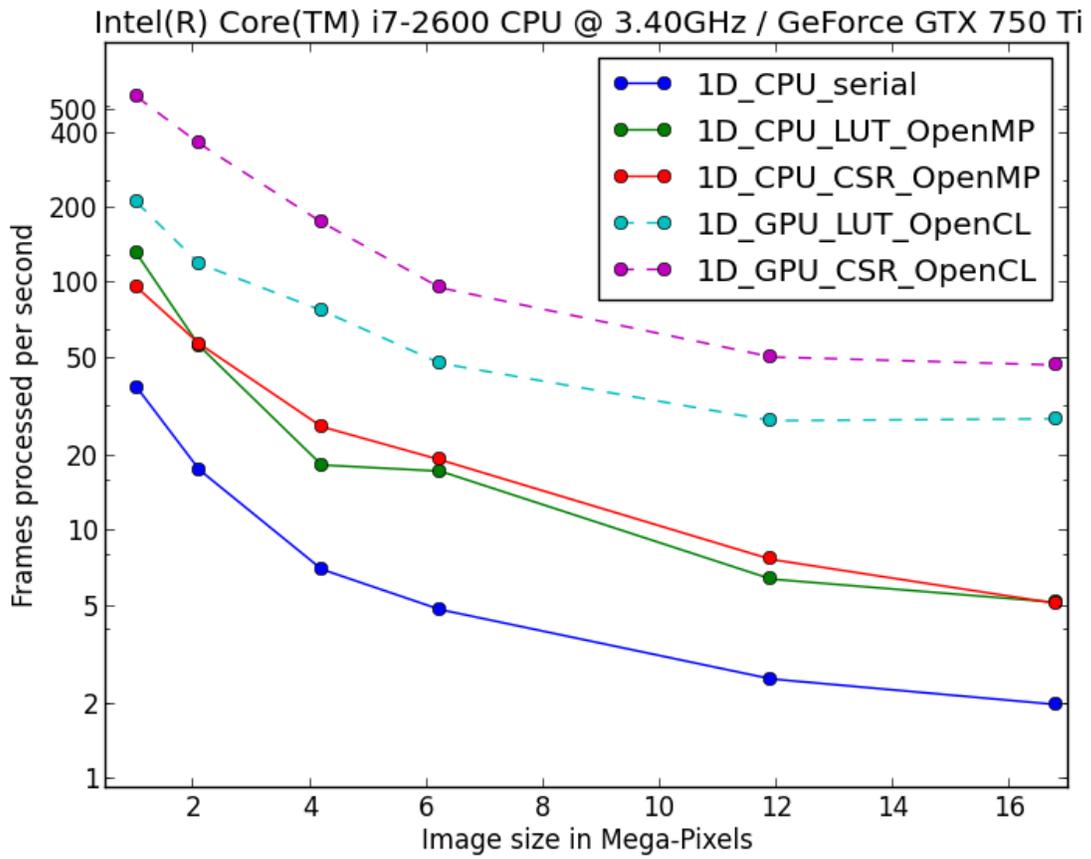
The library pyFAI was developed with two main goals:

- Performing azimuthal integration with a clean programming interface.
- No compromise on the quality of the results is accepted: a careful management of the geometry and precise pixel splitting ensures total and local intensity preservation.

PyFAI is the first implementation of an azimuthal integration algorithm on a GPUs as far as we are aware of, and the stated twenty-fold speed up opens the door to a new kind of analysis, not even considered before. With a good interface close to the camera, we believe PyFAI is able to sustain the data streams from the next generation high-speed detectors.

1.5.1 Acknowledgments

Porting pyFAI to GPU would have not been possible without the financial support of LinkSCEEM-2 (RI-261600).



PYFAI SCRIPTS MANUAL

While pyFAI is first and foremost a Python library to be used by developers, a set of scripts is provided to process a full diffraction experiment on the command line without knowing anything about Python. Those scripts can be divided into 3 categories: pre-processing tools which prepare the dataset for the calibration tool. The calibration is the determination of the geometry of the experimental setup using Debye-Scherrer rings of a reference compound (or calibrant). Finally a full dataset can be integrated using different tools targeted at different experiments.

Pre-processing tools:

- drawMask_pymca: tool for drawing a mask on top of an image
- pyFAI-average: tool for averaging/median/... filtering images (i.e. for dark current)

Calibration tools:

- pyFAI-calib: manually select the rings and refine the geometry
- pyFAI-recalib: automatic ring extraction to refine the geometry (deprecated: see “recalib” option in pyFAI-calib)
- MX-calibrate: Calibrate automatically a set of images taken at various detector distances
- check_calib: checks the calibration of an image at the sub-pixel level (deprecated: see “validate” option in pyFAI-calib)

Azimuthal integration tools:

- pyFAI-integrate: the only graphical interface for integration
- pyFAI-saxs: command line interface for small-angle scattering
- pyFAI-waxs: command line interface for powder diffraction
- diff_tomo: diffraction mapping&tomography tool

2.1 Preprocessing tool: pyFAI-average

2.1.1 Purpose

This tool can be used to average out a set of dark current images using mean or median filter (along the image stack). One can also reject outliers by specifying a cutoff (remove cosmic rays / zingers from dark)

It can also be used to merge many images from the same sample when using a small beam and reduce the spotty-ness of Debye-Scherrer rings. In this case the “max-filter” is usually recommended.

2.1.2 Options:

Usage: pyFAI-average [options] -o output.edf file1.edf file2.edf ...

Options:

- version** show program's version number and exit
- h, --help** show help message and exit
- o OUTPUT, --output=OUTPUT** Output/ destination of average image
- m METHOD, --method=METHOD** Method used for averaging, can be 'mean'(default) or 'median', 'min' or 'max'
- c CUTOFF, --cutoff=CUTOFF** Take the mean of the average +/- cutoff * std_dev.
- f FORMAT, --format=FORMAT** Output file/image format (by default EDF)
- v, --verbose** switch to verbose/debug mode

2.2 Mask generation tool: drawMask_pymca

2.2.1 Purpose

Draw a mask, i.e. an image containing the list of pixels which are considered invalid (no scintillator, module gap, beam stop shadow, ...).

This will open a PyMca window and let you draw on the first image (provided) with different tools (brush, rectangle selection, ...). When you are finished, come back to the console and press enter. The mask image is saved into file1-masked.edf. Optionally the script will print the number of pixel masked and the intensity masked (as well on other files provided in input)

Usage: drawMask_pymca [options] file1.edf file2.edf ...

2.2.2 Options:

- version** show program's version number and exit
- h, --help** show help message and exit

Optionally the script will print the number of pixel masked and the intensity masked (as well on other files provided in input)

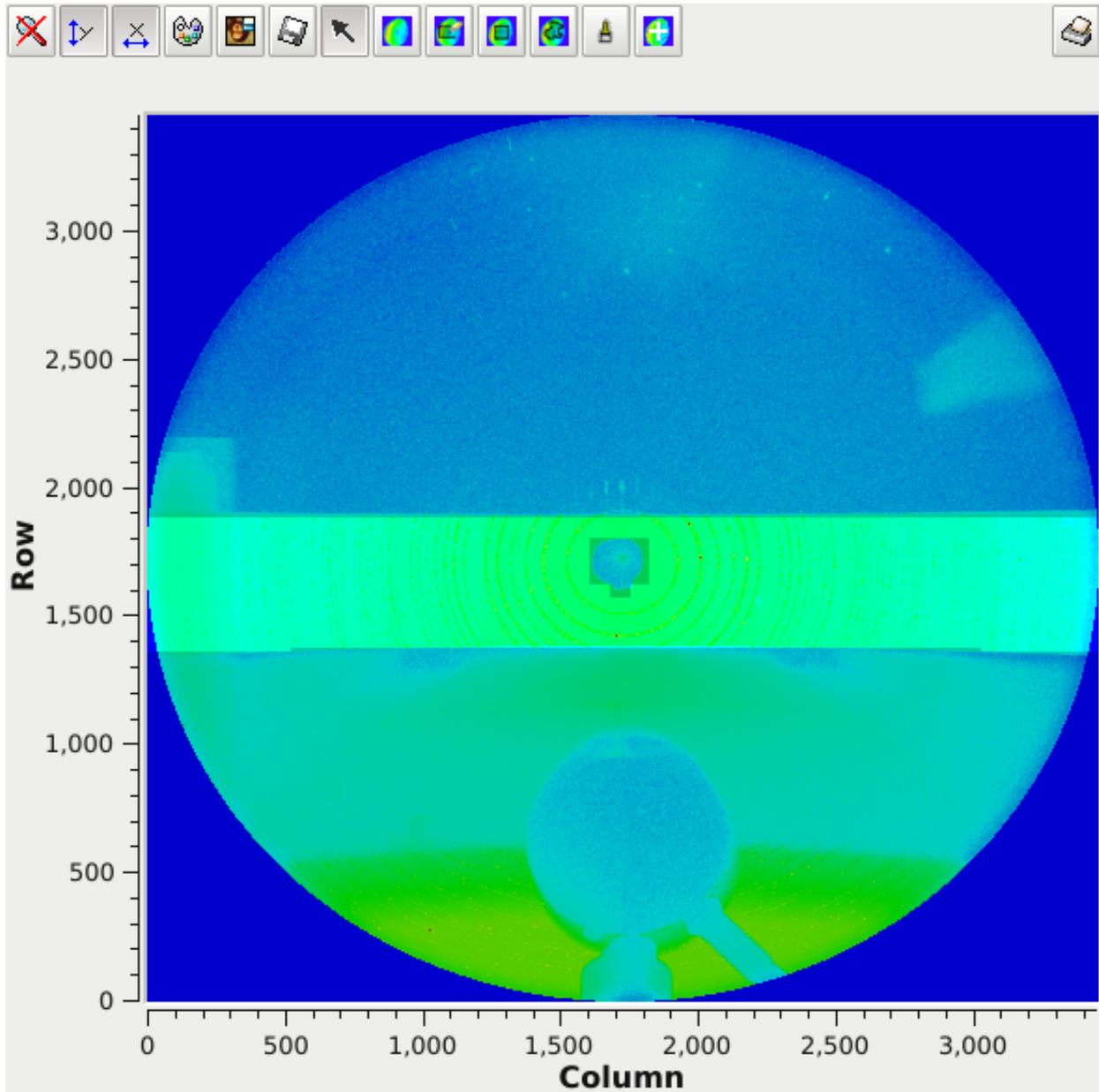
2.3 Calibration tool: pyFAI-calib

2.3.1 Purpose

Calibrate the diffraction setup geometry based on Debye-Sherrer rings images without a priori knowledge of your setup. You will need to provide a calibrant or a "d-spacing" file containing the spacing of Miller plans in Angstrom (in decreasing order). If you are using a standard calibrant, look at <https://github.com/kif/pyFAI/tree/master/calibration> or search in the American Mineralogist database: [AMD] or in the [COD]. The `-calibrant` option is mandatory !

You will need in addition:

- The radiation energy (in keV) or its wavelength (in Å)



- The description of the detector: its name or its pixel size or the spline file describing its distortion

Many options are available among those:

- dark-current / flat field corrections
- Masking of bad regions
- reconstruction of missing region (module based detectors)
- Polarization correction
- Automatic desaturation (time consuming!)
- Intensity weighted least-squares refinements

The output of this program is a “PONI” file containing the detector description and the 6 refined parameters (distance, center, rotation) and wavelength. An 1D and 2D diffraction patterns are also produced. (.dat and .azim files)

2.3.2 Usage:

```
pyFAI-calib [options] -w 1 -D detector -c calibrant.D imagefile.edf
```

2.3.3 Options:

- version** show program’s version number and exit
- h, --help** show this help message and exit
- o FILE, --out=FILE** Filename where processed image is saved
- v, --verbose** switch to debug/verbose mode
- c FILE, --calibrant=FILE** Calibrant name or file containing d-spacing of the 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 None (no correction), 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
- D DETECTOR_NAME, --detector=DETECTOR_NAME** Detector name (instead of pixel size+spline)
- m MASK, --mask=MASK** file containing the mask (for image reconstruction)
- n NPT, --pt=NPT** file with datapoints saved. Default: basename.npt

--filter=FILTER select the filter, either mean(default), max or median
-l DISTANCE, --distance=DISTANCE sample-detector distance in millimeter
--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
--saturation=SATURATION consider all pixel>max*(1-saturation) as saturated and reconstruct them
--weighted weight fit by intensity, by default not.
--npt=NPT_1D Number of point in 1D integrated pattern, Default: 1024
--npt-azim=NPT_2D_AZIM Number of azimuthal sectors in 2D integrated images. Default: 360
--npt-rad=NPT_2D_RAD Number of radial bins in 2D integrated images. Default: 400
--unit=UNIT Valid units for radial range: 2th_deg, 2th_rad, q_nm^-1, q_A^-1, r_mm. Default: 2th_deg
--no-gui force the program to run without a Graphical interface
--no-interactive force the program to run and exit without prompting for refinements
-r, --reconstruct Reconstruct image where data are masked or <0 (for Pilatus detectors or detectors with modules)
-g GAUSSIAN, --gaussian=GAUSSIAN Size of the gaussian kernel. Size of the gap (in pixels) between two consecutive rings, by default 100 Increase the value if the arc is not complete; decrease the value if arcs are mixed together.

--square Use square kernel shape for neighbor search instead of diamond shape
-p PIXEL, --pixel=PIXEL size of the pixel in micron

2.3.4 Example of usage:

Pilatus 1M image of Silver Behenate taken at ESRF-BM26:

```
pyFAI-calib -D Pilatus1M -c AgBh -r -w 1.0 test/testimages/Pilatus1M.edf
```

We use the parameter `-r` to reconstruct the missing part between the modules of the Pilatus detector.

Half a FReLoN CCD image of Lanthanide hexaboride taken at ESRF-ID11:

```
pyFAI-calib -s test/testimages/halfccd.spline -c LaB6 -w 0.3 test/testimages/halfccd.edf -g 250
```

This image is rather spotty. We need to blur a lot to get the continuity of the rings. This is achieved by the `-g` parameter. While the sample is well diffracting and well known, the wavelength has been guessed. One should refine the wavelength when the peaks extracted are correct

All those images are part of the test-suite of pyFAI. To download them from internet, run

```
python setup.py build test
```

Downloaded test images are located in `tests/testimages`

2.4 Calibration tool: pyFAI-recalib

2.4.1 Purpose

Calibrate the diffraction setup geometry based on Debye-Sherrer rings images with a priori knowledge of your setup (an input PONI-file). You will need to provide a calibrant or a “d-spacing” file containing the spacing of Miller plans in Angstrom (in decreasing order). If you are using a standard calibrant, look at <https://github.com/kif/pyFAI/tree/master/calibration> Else, you will need a “d-spacing” file containing the spacing of Miller plans in Angstrom (in decreasing order), they can be found on the American Mineralogist database [AMD] or in the [COD]. The `-calibrant` option is mandatory !

You will need in addition:

- The radiation energy (in keV) or its wavelength (in Å)

Many option are available among those:

- dark-current / flat field corrections
- Masking of bad regions
- Polarization correction
- Automatic desaturation (time consuming!)
- Intensity weighted least-squares refinements

The output of this program is a “PONI” file containing the detector description and the 6 refined parameters (distance, center, rotation) and wavelength. An 1D and 2D diffraction patterns are also produced. (.dat and .azim files)

The main difference with pyFAI-calib is the way control-point hence Debye-Sherrer rings are extracted. While pyFAI-calib relies on the contiguity of a region of peaks called massif; pyFAI-recalib knows approximately the geometry and is able to select the region where the ring should be. From this region it selects automatically the various peaks; making pyFAI-recalib able to run without graphical interface and without human intervention (–no-gui –no-interactive options).

2.4.2 Usage:

```
pyFAI-recalib [options] -w 1 -p imagefile.poni -S calibrant.D imagefile.edf
```

2.4.3 Options:

- h, --help** show help message and exit
- V, --version** print version of the program and quit
- o FILE, --out=FILE** Filename where processed image is saved
- v, --verbose** switch to debug/verbose mode
- S FILE, --spacing=FILE** file containing d-spacing of the 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 None (no correction), 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
- D DETECTOR_NAME, --detector=DETECTOR_NAME** Detector name (instead of pixel size+spline)
- m MASK, --mask=MASK** file containing the mask (for image reconstruction)
- n NPT, --pt=NPT** file with datapoints saved. Default: basename.npt
- filter=FILTER** select the filter, either mean(default), max or median
- l DISTANCE, --distance=DISTANCE** sample-detector distance in millimeter
- 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
--saturation=SATURATION consider all pixel>max*(1-saturation) as saturated and reconstruct them
--weighted weight fit by intensity, by default not.
--npt=NPT_1D Number of point in 1D integrated pattern, Default: 1024
--npt-azim=NPT_2D_AZIM Number of azimuthal sectors in 2D integrated images. Default: 360
--npt-rad=NPT_2D_RAD Number of radial bins in 2D integrated images. Default: 400
--unit=UNIT Valid units for radial range: 2th_deg, 2th_rad, q_nm^-1, q_A^-1, r_mm. Default: 2th_deg
--no-gui force the program to run without a Graphical interface
--no-interactive force the program to run and exit without prompting for refinements
-r MAX_RINGS, --ring=MAX_RINGS maximum number of rings to extract. Default: all accessible
-p FILE, --poni=FILE file containing the diffraction parameter (poni-file). MANDATORY
-k, --keep Keep existing control point and append new

2.4.4 Tips & Tricks

PONI files are ASCII files and each new refinement adds an entry into the file. So if you are unhappy with the last step, just edit this file and remove the last entry (timestamps will help you).

2.5 Calibration tool: check_calib

2.5.1 Purpose

Check_calib is a research tool aiming at validating both the geometric calibration and everything else like flat-field correction, distortion correction, at a sub-pixel level.

Note that *check_calib* program is obsolete as the same functionality is available from within pyFAI-calib, using the *validate* command in the refinement process.

2.5.2 Usage:

```
check_calib [options] -p param.poni image.edf
```

2.5.3 Options:

-h, --help show this help message and exit

-V, --version -v, --verbose switch to debug mode **-d FILE, --dark FILE** file containing the dark images to subtract **-f FILE, --flat FILE** file containing the flat images to divide **-m FILE, --mask FILE** file containing the mask **-p FILE, --poni FILE** file containing the diffraction parameter (poni-file) **-e ENERGY, --energy ENERGY** energy of the X-Ray beam in keV (hc=12.398419292keV.A)

-w WAVELENGTH, --wavelength WAVELENGTH wavelength of the X-Ray beam in Angstrom

2.5.4 Arguments:

FILE Image file to check calibration for

2.6 Calibration tool: MX-calibrate

2.6.1 Purpose

Calibrate automatically a set of frames taken at various sample-detector distance.

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.

Most standard calibrants are directly installed together with pyFAI. If you prefer using your own, you can provide a “d-spacing” file containing the spacing of Miller plans in Angstrom (in decreasing order). Most crystal powders used for calibration are available in the American Mineralogist database [AMD] or in the [COD].

2.6.2 Usage:

```
MX-Calibrate -w 1.54 -c CeO2 file1.cbf file2.cbf ...
```

2.6.3 Options:

- h, --help** show this help message and exit
- V, --version** print version of the program and quit
- v, --verbose** switch to debug/verbose mode
- c FILE, --calibrant FILE** calibrant name or 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 pixel>max*(1-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)

2.7 Integration tool: pyFAI-integrate

2.7.1 Purpose

PyFAI-integrate is a graphical interface (based on Python/Qt4) to perform azimuthal integration on a set of files. It exposes most of the important options available within pyFAI and allows you to select a GPU (or an openCL platform) to perform the calculation on.

2.7.2 Usage

```
pyFAI-integrate [options] file1.edf file2.edf ...
```

2.7.3 Options:

--version	show program's version number and exit
-h, --help	show help message and exit
-v, --verbose	switch to verbose/debug mode
-o OUTPUT, --output=OUTPUT	Directory or file where to store the output data

Poni File ...

Detector Wavelength (m)

Pixel1 (m) Pixel2 (m)

Spline file ...

Distance (m) Rotation 1 (rad)

Poni 1 (m) Rotation 2 (rad)

Poni 2 (m) Rotation 3 (rad)

Mask File ...

Dark Current ...

Flat Field ...

Dummy value delta dummy

Polarization factor Solid Angle corrections

Radial units: 2θ (°) 2θ (rad) q (1/nm) q (1/Å) r (mm)

Number of radial points Std-err (Poisson law)

Number of azimuthal points (2D) χ discontinuity at 0

Radial range

Azimuthal range

Use OpenCL Platform Device

2.7.4 Tips & Tricks:

PyFAI-integrate saves all parameters in a .azimint.json (hidden) file. This JSON file is an ascii file which can be edited and used to configure online data analysis using the LImA plugin of pyFAI.

Nota: there is bug in debian6 making the GUI crash (to be fixed inside pyqt) <http://bugs.debian.org/cgi-bin/bugreport.cgi?bug=697348>

2.8 Integration tool: diff_tomo

2.8.1 Purpose

Azimuthal integration for diffraction tomography.

Diffraction tomography is an experiment where 2D diffraction patterns are recorded while performing a 2D scan, one (the slowest) in rotation around the sample center and the other (the fastest) along a translation through the sample. Diff_tomo is a script (based on pyFAI and h5py) which allows the reduction of this 4D dataset into a 3D dataset containing the rotations angle (hundreds), the translation step (hundreds) and the many diffraction angles (thousands). The resulting dataset can be opened using PyMca roitool where the 1d dataset has to be selected as last dimension. This file is not (yet) NeXus compliant.

This tool can be used for mapping experiments if one considers the slow scan direction as the rotation.

tips: If the number of files is too large, use double quotes around “*.edf”

2.8.2 Usage:

```
diff_tomo [options] -p ponifile imagefiles*
```

2.8.3 Options:

- version** show program's version number and exit
- h, --help** show help message and exit
- o FILE, --output=FILE** HDF5 File where processed sinogram was saved
- v, --verbose** switch to verbose/debug mode
- P FILE, --prefix=FILE** Prefix or common base for all files
- e EXTENSION, --extension=EXTENSION** Process all files with this extension
- t NTRANS, --nTrans=NTRANS** number of points in translation
- r NROT, --nRot=NROT** number of points in rotation
- c NDIFF, --nDiff=NDIFF** number of points in diffraction powder pattern
- d FILE, --dark=FILE** list of dark images to average and subtract
- f FILE, --flat=FILE** list of flat images to average and divide
- m FILE, --mask=FILE** file containing the mask
- p FILE, --poni=FILE** file containing the diffraction parameter (poni-file)
- O OFFSET, --offset=OFFSET** do not process the first files

-g, --gpu process using OpenCL on GPU

Most of those options are mandatory to define the structure of the dataset.

2.9 Integration tool: pyFAI-saxs

2.9.1 Purpose

Azimuthal integration for SAXS users.

pyFAI-saxs is the SAXS script of pyFAI that allows data reduction (azimuthal integration) for Small Angle Scattering with output axis in q space.

2.9.2 Usage:

```
pyFAI-saxs -p=param.poni -w1.54e-9 file.edf file2.edf file3.edf
```

Options:

--version show program's version number and exit

-h, --help show this help message and exit

-p PONIFILE PyFAI parameter file (.poni)

-n NPT Number of points in radial dimension

-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)

-u DUMMY, --dummy=DUMMY dummy value for dead pixels

-U DELTA_DUMMY, --delta_dummy=DELTA_DUMMY delta dummy value

-m MASK, --mask=MASK name of the file containing the mask image

-d DARK, --dark=DARK name of the file containing the dark current

-f FLAT, --flat=FLAT name of the file containing the flat field

-P POLARIZATION_FACTOR, --polarization=POLARIZATION_FACTOR Polarization factor, from -1 (vertical) to +1 (horizontal), default is None for no correction, synchrotrons are around 0.95

--error-model=ERROR_MODEL Error model to use. Currently on 'poisson' is implemented

--unit=UNIT unit for the radial dimension: can be q_nm^-1, q_A^-1, 2th_deg, 2th_rad or r_mm

--ext=EXT extension of the regrouped filename (.dat)

2.10 Integration tool: pyFAI-saxs

2.10.1 Purpose

Azimuthal integration for WAXS users.

pyFAI-wax is the script of pyFAI that allows data reduction (azimuthal integration) for Wide Angle Scattering to produce X-Ray Powder Diffraction Pattern with output axis in 2-theta space.

2.10.2 Usage:

```
pyFAI-wax -p param.poni [options] file1.edf file2.edf ...
```

2.10.3 Options:

- version** show program's version number and exit
- h, --help** show this help message and exit
- p PONIFILE** PyFAI parameter file (.poni) MANDATORY
- n NPT** Number of points in radial dimension
- 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)
- u DUMMY, --dummy=DUMMY** dummy value for dead pixels
- U DELTA_DUMMY, --delta_dummy=DELTA_DUMMY** delta dummy value
- m MASK, --mask=MASK** name of the file containing the mask image
- d DARK, --dark=DARK** name of the file containing the dark current
- f FLAT, --flat=FLAT** name of the file containing the flat field
- P POLARIZATION_FACTOR, --polarization=POLARIZATION_FACTOR**
Polarization factor, from -1 (vertical) to +1 (horizontal), default is None for no correction, synchrotrons are around 0.95
- error-model=ERROR_MODEL** Error model to use. Currently on 'poisson' is implemented
- unit=UNIT** unit for the radial dimension: can be q_nm^-1, q_A^-1, 2th_deg, 2th_rad or r_mm
- ext=EXT** extension of the regrouped filename (.xy)
- multi** Average out all frame in a file before integrating
- average AVERAGE** Method for averaging out: can be 'mean' (default), 'min', 'max' or 'median'
- do-2D** Perform 2D integration in addition to 1D

pyFAI-wax is the script of pyFAI that allows data reduction (azimuthal integration) for Wide Angle Scattering to produce X-Ray Powder Diffraction Pattern with output axis in 2-theta space.

PYFAI API

This chapter describes the programming interface of pyFAI, so what you can expect after having launched ipython and typed: ..

```
import pyFAI
```

The most important class is `AzimuthalIntegrator` which is an object containing both the geometry (it inherits from `Geometry`, another class) and exposes important methods (functions) like `integrate1d` and `integrate2d`.

3.1 pyFAI Package

3.2 azimuthalIntegrator Module

```
class pyFAI.azimuthalIntegrator.AzimuthalIntegrator (dist=1, poni1=0, poni2=0, rot1=0, rot2=0, rot3=0, pixel1=None, pixel2=None, splineFile=None, detector=None, wavelength=None)
```

Bases: `pyFAI.geometry.Geometry`

This class is an azimuthal integrator based on P. Boesecke's geometry and histogram algorithm by Manolo S. del Rio and V.A Sole

All geometry calculation are done in the `Geometry` class

main methods are:

```
>>> tth, I = ai.integrate1d(data, npt, unit="2th_deg")
>>> q, I, sigma = ai.integrate1d(data, npt, unit="q_nm^-1", error_model="poisson")
>>> regrouped = ai.integrate2d(data, npt_rad, npt_azim, unit="q_nm^-1")[0]
```

```
array_from_unit (shape, typ='center', unit=2th_deg)
```

Generate an array of position in different dimentions (R, Q, 2Theta)

Parameters

- **shape** (`ndarray.shape`) – shape of the expected array
- **typ** (`str`) – “center”, “corner” or “delta”
- **unit** (`pyFAI.units.Enum`) – can be Q, TTH, R for now

Returns R, Q or 2Theta array depending on unit

Return type `ndarray`

dark_correction (*data*, *dark=None*)

Correct for Dark-current effects. If dark is not defined, correct for a dark set by “set_darkfiles”

Parameters

- **data** – input ndarray with the image
- **dark** – ndarray with dark noise or None

Returns 2tuple: corrected_data, dark_actually used (or None)

darkcurrent

flat_correction (*data*, *flat=None*)

Correct for flat field. If flat is not defined, correct for a flat set by “set_flatfiles”

Parameters

- **data** – input ndarray with the image
- **dark** – ndarray with dark noise or None

Returns 2tuple: corrected_data, flat_actually used (or None)

flatfield

get_darkcurrent ()

get_flatfield ()

get_mask ()

get_maskfile ()

integrate1d (*data*, *npt*, *filename=None*, *correctSolidAngle=True*, *variance=None*, *error_model=None*, *radial_range=None*, *azimuth_range=None*, *mask=None*, *dummy=None*, *delta_dummy=None*, *polarization_factor=None*, *dark=None*, *flat=None*, *method='lut'*, *unit=q_nm^-1*, *safe=True*, *normalization_factor=None*, *block_size=32*, *profile=False*)

Calculate the azimuthal integrated Saxes curve in $q(\text{nm}^{-1})$ by default

Multi algorithm implementation (tries to be bullet proof), suitable for SAXS, WAXS, ... and much more

Parameters

- **data** (*ndarray*) – 2D array from the Detector/CCD camera
- **npt** (*int*) – number of points in the output pattern
- **filename** (*str*) – output filename in 2/3 column ascii format
- **correctSolidAngle** (*bool*) – correct for solid angle of each pixel if True
- **variance** (*ndarray*) – array containing the variance of the data. If not available, no error propagation is done
- **error_model** (*str*) – When the variance is unknown, an error model can be given: “poisson” (variance = I), “azimuthal” (variance = $(I - \langle I \rangle)^2$)
- **radial_range** (*(float, float)*, *optional*) – The lower and upper range of the radial unit. If not provided, range is simply (data.min(), data.max()). Values outside the range are ignored.
- **azimuth_range** (*(float, float)*, *optional*) – The lower and upper range of the azimuthal angle in degree. If not provided, range is simply (data.min(), data.max()). Values outside the range are ignored.
- **mask** (*ndarray*) – array (same size as image) with 1 for masked pixels, and 0 for valid pixels

- **dummy** (*float*) – value for dead/masked pixels
- **delta_dummy** (*float*) – precision for dummy value
- **polarization_factor** (*float*) – polarization factor between -1 (vertical) and +1 (horizontal). 0 for circular polarization or random, None for no correction
- **dark** (*ndarray*) – dark noise image
- **flat** (*ndarray*) – flat field image
- **method** (*str*) – can be “numpy”, “cython”, “BBox” or “splitpixel”, “lut”, “csr”, “nosplit_csr”, “lut_ocl” and “csr_ocl” if you want to go on GPU. To Specify the device: “csr_ocl_1,2”
- **unit** (*pyFAI.units.Enum*) – Output units, can be “q_nm⁻¹”, “q_A⁻¹”, “2th_deg”, “2th_rad”, “r_mm” for now
- **safe** (*bool*) – Do some extra checks to ensure LUT/CSR is still valid. False is faster.
- **normalization_factor** (*float*) – Value of a normalization monitor

Returns q/2th/r bins center positions and regrouped intensity (and error array if variance or variance model provided).

Return type 2 or 3-tuple of ndarrays

```
integrate2d(data, npt_rad, npt_azim=360, filename=None, correctSolidAngle=True, variance=None, error_model=None, radial_range=None, azimuth_range=None, mask=None, dummy=None, delta_dummy=None, polarization_factor=None, dark=None, flat=None, method='bbox', unit=q_nm-1, safe=True, normalization_factor=None)
```

Calculate the azimuthal regrouped 2d image in q(nm⁻¹)/chi(deg) by default

Multi algorithm implementation (tries to be bullet proof)

Parameters

- **data** (*ndarray*) – 2D array from the Detector/CCD camera
- **npt_rad** (*int*) – number of points in the radial direction
- **npt_azim** (*int*) – number of points in the azimuthal direction
- **filename** (*str*) – output image (as edf format)
- **correctSolidAngle** (*bool*) – correct for solid angle of each pixel if True
- **variance** (*ndarray*) – array containing the variance of the data. If not available, no error propagation is done
- **error_model** (*str*) – When the variance is unknown, an error model can be given: “poisson” (variance = I), “azimuthal” (variance = (I-<I>)²)
- **radial_range** (*(float, float), optional*) – The lower and upper range of the radial unit. If not provided, range is simply (data.min(), data.max()). Values outside the range are ignored.
- **azimuth_range** (*(float, float), optional*) – The lower and upper range of the azimuthal angle in degree. If not provided, range is simply (data.min(), data.max()). Values outside the range are ignored.
- **mask** (*ndarray*) – array (same size as image) with 1 for masked pixels, and 0 for valid pixels
- **dummy** (*float*) – value for dead/masked pixels
- **delta_dummy** (*float*) – precision for dummy value

- **polarization_factor** (*float*) – polarization factor between -1 (vertical) and +1 (horizontal). 0 for circular polarization or random, None for no correction
- **dark** (*ndarray*) – dark noise image
- **flat** (*ndarray*) – flat field image
- **method** (*str*) – can be “numpy”, “cython”, “BBox” or “splitpixel”, “lut”, “csr”, “lut_ocl” and “csr_ocl” if you want to go on GPU. To Specify the device: “csr_ocl_1,2”
- **unit** (*pyFAI.units.Enum*) – Output units, can be “q_nm⁻¹”, “q_A⁻¹”, “2th_deg”, “2th_rad”, “r_mm” for now
- **safe** (*bool*) – Do some extra checks to ensure LUT is still valid. False is faster.
- **normalization_factor** (*float*) – Value of a normalization monitor

Returns azimuthally regrouped intensity, q/2theta/r pos. and chi pos.

Return type 3-tuple of ndarrays (2d, 1d, 1d)

makeHeaders (*hdr='#', dark=None, flat=None, polarization_factor=None, normalization_factor=None*)

Parameters

- **hdr** (*str*) – string used as comment in the header
- **dark** – save the darks filenames (default: no)
- **flat** – save the flat filenames (default: no)
- **polarization_factor** (*float*) – the polarization factor

Returns the header

Return type str

makeMask (*data, mask=None, dummy=None, delta_dummy=None, mode='normal'*)

Combines various masks into another one.

Parameters

- **data** (*ndarray*) – input array of data
- **mask** (*ndarray*) – input mask (if none, self.mask is used)
- **dummy** (*float*) – value of dead pixels
- **delta_dummy** – precision of dummy pixels
- **mode** (*str*) – can be “normal” or “numpy” (inverted) or “where” applied to the mask

Returns the new mask

Return type ndarray of bool

This method combine two masks (dynamic mask from *data* & *dummy* and *mask*) to generate a new one with the ‘or’ binary operation. One can adjust the level, with the *dummy* and the *delta_dummy* parameter, when you consider the *data* values needs to be masked out.

This method can work in two different *mode*:

- “normal”: False for valid pixels, True for bad pixels
- “numpy”: True for valid pixels, false for others

This method tries to accomodate various types of masks (like valid=0 & masked=-1, ...) and guesses if an input mask needs to be inverted.

mask

maskfile

reset ()

Reset azimuthal integrator in addition to other arrays.

save1D (*filename, dim1, I, error=None, dim1_unit=2th_deg, dark=None, flat=None, polarization_factor=None, normalization_factor=None*)

Parameters

- **filename** (*str*) – the filename used to save the 1D integration
- **dim1** (*numpy.ndarray*) – the x coordinates of the integrated curve
- **I** (*numpy.ndarray*) – The integrated intensity
- **error** (*numpy.ndarray or None*) – the error bar for each intensity
- **dim1_unit** (*pyFAI.units.Unit*) – the unit of the dim1 array
- **dark** – save the darks filenames (default: no)
- **flat** – save the flat filenames (default: no)
- **polarization_factor** (*float*) – the polarization factor
- **normalization_factor** (*float*) – the monitor value

This method save the result of a 1D integration.

save2D (*filename, I, dim1, dim2, error=None, dim1_unit=2th_deg, dark=None, flat=None, polarization_factor=None, normalization_factor=None*)

Parameters

- **filename** (*str*) – the filename used to save the 2D histogram
- **dim1** (*numpy.ndarray*) – the 1st coordinates of the histogram
- **dim2** – the 2nd coordinates of the histogram
- **I** (*numpy.ndarray*) – The integrated intensity
- **error** (*numpy.ndarray or None*) – the error bar for each intensity
- **dim1_unit** (*pyFAI.units.Unit*) – the unit of the dim1 array
- **dark** – save the darks filenames (default: no)
- **flat** – save the flat filenames (default: no)
- **polarization_factor** (*float*) – the polarization factor
- **normalization_factor** (*float*) – the monitor value

This method save the result of a 2D integration.

saxs (*data, npt, filename=None, correctSolidAngle=True, variance=None, error_model=None, qRange=None, chiRange=None, mask=None, dummy=None, delta_dummy=None, polarization_factor=None, dark=None, flat=None, method='bbox', unit=q_nm^-1*)
Calculate the azimuthal integrated Saxs curve in q in nm⁻¹.

Wrapper for integrate1d emulating behaviour of old saxs method

Parameters

- **data** (*ndarray*) – 2D array from the CCD camera

- **npt** (*int*) – number of points in the output pattern
- **filename** (*str*) – file to save data to
- **correctSolidAngle** (*bool*) – if True, the data are divided by the solid angle of each pixel
- **variance** (*ndarray*) – array containing the variance of the data, if you know it
- **error_model** (*str*) – When the variance is unknown, an error model can be given: “poisson” (variance = I), “azimuthal” (variance = $(I-\langle I \rangle)^2$)
- **qRange** (*(float, float), optional*) – The lower and upper range of the scatter vector q. If not provided, range is simply (data.min(), data.max()). Values outside the range are ignored.
- **chiRange** (*(float, float), optional*) – The lower and upper range of the chi angle. If not provided, range is simply (data.min(), data.max()). Values outside the range are ignored.
- **mask** (*ndarray*) – array (same size as image) with 1 for masked pixels, and 0 for valid pixels
- **dummy** (*float*) – value for dead/masked pixels
- **delta_dummy** (*float*) – precision for dummy value
- **polarization_factor** (*float*) – polarization factor between -1 and +1. 0 for no correction
- **dark** (*ndarray*) – dark noise image
- **flat** (*ndarray*) – flat field image
- **method** (*str*) – can be “numpy”, “cython”, “BBox” or “splitpixel”

Returns azimuthally regrouped data, 2theta pos. and chi pos.

Return type 3-tuple of ndarrays

separate (*data, npt_rad=1024, npt_azim=512, unit='2th_deg', percentile=50, mask=None, restore_mask=True*)

Separate bragg signal from powder/amorphous signal using azimuthal integration, median filtering and projected back before subtraction.

Parameters

- **data** – input image as numpy array
- **npt_rad** – number of radial points
- **npt_azim** – number of azimuthal points
- **unit** – unit to be used for integration
- **percentile** – which percentile use for cutting out
- **mask** – masked out pixels array
- **restore_mask** – masked pixels have the same value as input data provided

Returns bragg, amorphous

set_darkcurrent (*dark*)

set_darkfiles (*files=None, method='mean'*)

Parameters

- **files** (*str or list(str) or None*) – file(s) used to compute the dark.
- **method** (*str*) – method used to compute the dark, “mean” or “median”

Set the dark current from one or multiple files, averaged according to the method provided

set_flatfield (*flat*)

set_flatfiles (*files, method='mean'*)

Parameters

- **files** (*str or list(str) or None*) – file(s) used to compute the dark.
- **method** (*str*) – method used to compute the dark, “mean” or “median”

Set the flat field from one or mutliple files, averaged according to the method provided

set_mask (*mask*)

set_maskfile (*maskfile*)

setup_CSR (*shape, npt, mask=None, pos0_range=None, pos1_range=None, mask_checksum=None, unit=2th_deg, split='bbox'*)

Prepare a look-up-table

Parameters

- **shape** (*(int, int)*) – shape of the dataset
- **npt** (*int or (int, int)*) – number of points in the the output pattern
- **mask** (*ndarray*) – array with masked pixel (1=masked)
- **pos0_range** (*(float, float)*) – range in radial dimension
- **pos1_range** (*(float, float)*) – range in azimuthal dimension
- **mask_checksum** (*int (or anything else ...)*) – checksum of the mask buffer
- **unit** (*pyFAI.units.Enum*) – use to propagate the LUT object for further checkings
- **split** – Splitting scheme: valid options are “no”, “bbox”, “full”

This method is called when a look-up table needs to be set-up. The *shape* parameter, correspond to the shape of the original dataset. It is possible to customize the number of point of the output histogram with the *npt* parameter which can be either an integer for an 1D integration or a 2-tuple of integer in case of a 2D integration. The LUT will have a different shape: (npt, lut_max_size), the later parameter being calculated during the instantiation of the splitBBoxLUT class.

It is possible to prepare the LUT with a predefine *mask*. This operation can speedup the computation of the later integrations. Instead of applying the patch on the dataset, it is taken into account during the histogram computation. If provided the *mask_checksum* prevent the re-calculation of the mask. When the mask changes, its checksum is used to reset (or not) the LUT (which is a very time consuming operation !)

It is also possible to restrain the range of the 1D or 2D pattern with the *pos1_range* and *pos2_range*.

The *unit* parameter is just propagated to the LUT integrator for further checkings: The aim is to prevent an integration to be performed in 2th-space when the LUT was setup in q space.

setup_LUT (*shape, npt, mask=None, pos0_range=None, pos1_range=None, mask_checksum=None, unit=2th_deg*)

Prepare a look-up-table

Parameters

- **shape** (*(int, int)*) – shape of the dataset
- **npt** (*int or (int, int)*) – number of points in the the output pattern
- **mask** (*ndarray*) – array with masked pixel (1=masked)
- **pos0_range** (*(float, float)*) – range in radial dimension

- **pos1_range** (*float, float*) – range in azimuthal dimension
- **mask_checksum** (*int (or anything else ...)*) – checksum of the mask buffer
- **unit** (*pyFAI.units.Enum*) – use to propagate the LUT object for further checkings

This method is called when a look-up table needs to be set-up. The *shape* parameter, correspond to the shape of the original dataset. It is possible to customize the number of point of the output histogram with the *npt* parameter which can be either an integer for an 1D integration or a 2-tuple of integer in case of a 2D integration. The LUT will have a different shape: (*npt, lut_max_size*), the later parameter being calculated during the instantiation of the `splitBBoxLUT` class.

It is possible to prepare the LUT with a predefined *mask*. This operation can speedup the computation of the later integrations. Instead of applying the patch on the dataset, it is taken into account during the histogram computation. If provided the *mask_checksum* prevent the re-calculation of the mask. When the mask changes, its checksum is used to reset (or not) the LUT (which is a very time consuming operation !)

It is also possible to restrain the range of the 1D or 2D pattern with the *pos1_range* and *pos2_range*.

The *unit* parameter is just propagated to the LUT integrator for further checkings: The aim is to prevent an integration to be performed in 2th-space when the LUT was setup in q space.

xrpd (*data, npt, filename=None, correctSolidAngle=True, tthRange=None, chiRange=None, mask=None, dummy=None, delta_dummy=None, polarization_factor=None, dark=None, flat=None*)

Calculate the powder diffraction pattern from a set of data, an image.

Cython implementation

Parameters

- **data** (*ndarray*) – 2D array from the CCD camera
- **npt** (*integer*) – number of points in the output pattern
- **filename** (*str*) – file to save data in ascii format 2 column
- **correctSolidAngle** (*bool or int*) – solid angle correction, order 1 or 3 (like fit2d)
- **tthRange** (*(float, float), optional*) – The lower and upper range of the 2theta
- **chiRange** (*(float, float), optional, disabled for now*) – The lower and upper range of the chi angle.
- **mask** (*ndarray*) – array with 1 for masked pixels, and 0 for valid pixels
- **dummy** (*float*) – value for dead/masked pixels (dynamic mask)
- **delta_dummy** (*float*) – precision for dummy value
- **polarization_factor** (*float*) – polarization factor correction
- **dark** (*ndarray*) – dark noise image
- **flat** (*ndarray*) – flat field image

Returns (2theta, I) in degrees

Return type 2-tuple of 1D arrays

This method compute the powder diffraction pattern, from a given *data* image. The number of point of the pattern is given by the *npt* parameter. If you give a *filename*, the powder diffraction is also saved as a two column text file.

It is possible to correct or not the powder diffraction pattern using the *correctSolidAngle* parameter. The weight of a pixel is ponderate by its solid angle.

The 2theta range of the powder diffraction pattern can be set using the *tthRange* parameter. If not given the maximum available range is used. Indeed pixel outside this range are ignored.

Each pixel of the *data* image as also a chi coordinate. So it is possible to restrain the chi range of the pixels to consider in the powder diffraction pattern. you just need to set the range with the *chiRange* parameter. like the *tthRange* parameter, value outside this range are ignored.

Sometimes one needs to mask a few pixels (beamstop, hot pixels, ...), to ignore a few of them you just need to provide a *mask* array with a value of 1 for those pixels. To take a pixel into account you just need to set a value of 0 in the mask array. Indeed the shape of the mask array should be identical to the data shape (size of the array *_must_* be the same). Pixels can also be maseked by seting them to an

Bad pixels can be masked out by setting them to an impossible value (-1) and calling this value the “dummy value”. Some Pilatus detectors are setting non existing pixel to -1 and dead pixels to -2. Then use *dummy=-2 & delta_dummy=1.5* so that any value between -3.5 and -0.5 are considered as bad.

Some Pilatus detectors are setting non existing pixel to -1 and dead pixels to -2. Then use *dummy=-2 & delta_dummy=1.5* so that any value between -3.5 and -0.5 are considered as bad.

The polarisation correction can be taken into account with the *polarization_factor* parameter. Set it between [-1, 1], to correct your data. If set to 0 there is no correction at all.

The *dark* and the *flat* can be provided to correct the data before computing the radial integration.

```
xrpd2 (data, npt_rad, npt_azim=360, filename=None, correctSolidAngle=True, tthRange=None, chiRange=None, mask=None, dummy=None, delta_dummy=None, polarization_factor=None, dark=None, flat=None)
```

Calculate the 2D powder diffraction pattern (2Theta,Chi) from a set of data, an image

Split pixels according to their coordinate and a bounding box

Parameters

- **data** (*ndarray*) – 2D array from the CCD camera
- **npt_rad** – number of bin of the Radial (horizontal) axis (2Theta)
- **npt_azim** (*int*) – number of bin of the Azimuthal (vertical) axis (chi)
- **filename** (*str*) – file to save data in
- **correctSolidAngle** (*bool or int*) – solid angle correction, order 1 or 3 (like fit2d)
- **tthRange** (*(float, float)*) – The lower and upper range of 2theta
- **chiRange** (*(float, float), disabled for now*) – The lower and upper range of the chi angle.
- **mask** (*ndarray*) – array with 1 for masked pixels, and 0 for valid pixels
- **dummy** (*float*) – value for dead/masked pixels (dynamic mask)
- **delta_dummy** (*float*) – precision for dummy value
- **polarization_factor** (*float*) – polarization factor correction
- **dark** (*ndarray*) – dark noise image
- **flat** (*ndarray*) – flat field image

Returns azimuthally regrouped data, 2theta pos. and chi pos.

Return type 3-tuple of ndarrays

This method convert the *data* image from the pixel coordinates to the 2theta, chi coordinates. This is similar to a rectangular to polar conversion. The number of point of the new image is given by *npt_rad* and *npt_azim*. If you give a *filename*, the new image is also saved as an edf file.

It is possible to correct the 2theta/chi pattern using the *correctSolidAngle* parameter. The weight of a pixel is ponderate by its solid angle.

The 2theta and range of the new image can be set using the *tthRange* parameter. If not given the maximum available range is used. Indeed pixel outside this range are ignored.

Each pixel of the *data* image has a 2theta and a chi coordinate. So it is possible to restrain on any of those ranges ; you just need to set the range with the *tthRange* or thee *chiRange* parameter. like the *tthRange* parameter, value outside this range are ignored.

Sometimes one needs to mask a few pixels (beamstop, hot pixels, ...), to ignore a few of them you just need to provide a *mask* array with a value of 1 for those pixels. To take a pixel into account you just need to set a value of 0 in the mask array. Indeed the shape of the mask array should be identical to the data shape (size of the array *_must_* be the same).

Masking can also be achieved by setting masked pixels to an impossible value (-1) and calling this value the “dummy value”. Some Pilatus detectors are setting non existing pixel to -1 and dead pixels to -2. Then use *dummy=-2* & *delta_dummy=1.5* so that any value between -3.5 and -0.5 are considered as bad.

the polarisation correction can be taken into account with the *polarization_factor* parameter. Set it between [-1, 1], to correct your data. If set to 0 there is no correction at all.

The *dark* and the *flat* can be provided to correct the data before computing the radial integration.

```
xrpd2_histogram(data, npt_rad, npt_azim=360, filename=None, correctSolidAngle=True,
                 dark=None, flat=None, tthRange=None, chiRange=None, mask=None,
                 dummy=None, delta_dummy=None)
```

Calculate the 2D powder diffraction pattern (2Theta,Chi) from a set of data, an image

Cython implementation: fast but inaccurate

Parameters

- **data** (*ndarray*) – 2D array from the CCD camera
- **npt_rad** – number of bin of the Radial (horizontal) axis (2Theta)
- **npt_azim** (*int*) – number of bin of the Azimuthal (vertical) axis (chi)
- **filename** (*str*) – file to save data in
- **correctSolidAngle** (*bool or int*) – solid angle correction, order 1 or 3 (like fit2d)
- **tthRange** (*(float, float)*) – The lower and upper range of 2theta
- **chiRange** (*(float, float), disabled for now*) – The lower and upper range of the chi angle.
- **mask** (*ndarray*) – array with 1 for masked pixels, and 0 for valid pixels
- **dummy** (*float*) – value for dead/masked pixels (dynamic mask)
- **delta_dummy** (*float*) – precision for dummy value

Returns azimuthally regrouped data, 2theta pos and chipos

Return type 3-tuple of ndarrays

This method convert the *data* image from the pixel coordinates to the 2theta, chi coordinates. This is similar to a rectangular to polar conversion. The number of point of the new image is given by *npt_rad* and *npt_azim*. If you give a *filename*, the new image is also saved as an edf file.

It is possible to correct the 2theta/chi pattern using the *correctSolidAngle* parameter. The weight of a pixel is ponderate by its solid angle.

The 2theta and range of the new image can be set using the *tthRange* parameter. If not given the maximum available range is used. Indeed pixel outside this range are ignored.

Each pixel of the *data* image has a 2theta and a chi coordinate. So it is possible to restrain on any of those ranges ; you just need to set the range with the *tthRange* or thee *chiRange* parameter. like the *tthRange* parameter, value outside this range are ignored.

Sometimes one needs to mask a few pixels (beamstop, hot pixels, ...), to ignore a few of them you just need to provide a *mask* array with a value of 1 for those pixels. To take a pixel into account you just need to set a value of 0 in the mask array. Indeed the shape of the mask array should be identical to the data shape (size of the array *_must_* be the same).

Masking can also be achieved by setting masked pixels to an impossible value (-1) and calling this value the “dummy value”. Some Pilatus detectors are setting non existing pixel to -1 and dead pixels to -2. Then use *dummy=-2* & *delta_dummy=1.5* so that any value between -3.5 and -0.5 are considered as bad.

```
xrpd2_numpy (data, npt_rad, npt_azim=360, filename=None, correctSolidAngle=True, dark=None,
             flat=None, tthRange=None, chiRange=None, mask=None, dummy=None,
             delta_dummy=None)
```

Calculate the 2D powder diffraction pattern (2Theta, Chi) from a set of data, an image

Pure numpy implementation (VERY SLOW !!!)

Parameters

- **data** (*ndarray*) – 2D array from the CCD camera
- **npt_rad** – number of bin of the Radial (horizontal) axis (2Theta)
- **npt_azim** (*int*) – number of bin of the Azimuthal (vertical) axis (chi)
- **filename** (*str*) – file to save data in
- **correctSolidAngle** (*bool or int*) – solid angle correction, order 1 or 3 (like fit2d)
- **tthRange** (*(float, float)*) – The lower and upper range of 2theta
- **chiRange** (*(float, float), disabled for now*) – The lower and upper range of the chi angle.
- **mask** (*ndarray*) – array with 1 for masked pixels, and 0 for valid pixels
- **dummy** (*float*) – value for dead/masked pixels (dynamic mask)
- **delta_dummy** (*float*) – precision for dummy value

Returns azimuthally regrouped data, 2theta pos and chipos

Return type 3-tuple of ndarrays

This method convert the *data* image from the pixel coordinates to the 2theta, chi coordinates. This is similar to a rectangular to polar conversion. The number of point of the new image is given by *npt_rad* and *npt_azim*. If you give a *filename*, the new image is also saved as an edf file.

It is possible to correct the 2theta/chi pattern using the *correctSolidAngle* parameter. The weight of a pixel is ponderate by its solid angle.

The 2theta and range of the new image can be set using the *tthRange* parameter. If not given the maximum available range is used. Indeed pixel outside this range are ignored.

Each pixel of the *data* image has a 2theta and a chi coordinate. So it is possible to restrain on any of those ranges ; you just need to set the range with the *tthRange* or thee *chiRange* parameter. like the *tthRange* parameter, value outside this range are ignored.

Sometimes one needs to mask a few pixels (beamstop, hot pixels, ...), to ignore a few of them you just need to provide a *mask* array with a value of 1 for those pixels. To take a pixel into account you just need to set a value of 0 in the mask array. Indeed the shape of the mask array should be identical to the data shape (size of the array *_must_* be the same).

Masking can also be achieved by setting masked pixels to an impossible value (-1) and calling this value the “dummy value”. Some Pilatus detectors are setting non existing pixel to -1 and dead pixels to -2. Then use `dummy=-2 & delta_dummy=1.5` so that any value between -3.5 and -0.5 are considered as bad.

```
xrpd2_splitBBox (data, npt_rad, npt_azim=360, filename=None, correctSolidAngle=True, tthRange=None, chiRange=None, mask=None, dummy=None, delta_dummy=None, polarization_factor=None, dark=None, flat=None)
```

Calculate the 2D powder diffraction pattern (2Theta,Chi) from a set of data, an image

Split pixels according to their coordinate and a bounding box

Parameters

- **data** (*ndarray*) – 2D array from the CCD camera
- **npt_rad** – number of bin of the Radial (horizontal) axis (2Theta)
- **npt_azim** (*int*) – number of bin of the Azimuthal (vertical) axis (chi)
- **filename** (*str*) – file to save data in
- **correctSolidAngle** (*bool or int*) – solid angle correction, order 1 or 3 (like fit2d)
- **tthRange** (*(float, float)*) – The lower and upper range of 2theta
- **chiRange** (*(float, float), disabled for now*) – The lower and upper range of the chi angle.
- **mask** (*ndarray*) – array with 1 for masked pixels, and 0 for valid pixels
- **dummy** (*float*) – value for dead/masked pixels (dynamic mask)
- **delta_dummy** (*float*) – precision for dummy value
- **polarization_factor** (*float*) – polarization factor correction
- **dark** (*ndarray*) – dark noise image
- **flat** (*ndarray*) – flat field image

Returns azimuthally regrouped data, 2theta pos. and chi pos.

Return type 3-tuple of ndarrays

This method convert the *data* image from the pixel coordinates to the 2theta, chi coordinates. This is similar to a rectangular to polar conversion. The number of point of the new image is given by *npt_rad* and *npt_azim*. If you give a *filename*, the new image is also saved as an edf file.

It is possible to correct the 2theta/chi pattern using the *correctSolidAngle* parameter. The weight of a pixel is ponderate by its solid angle.

The 2theta and range of the new image can be set using the *tthRange* parameter. If not given the maximum available range is used. Indeed pixel outside this range are ignored.

Each pixel of the *data* image has a 2theta and a chi coordinate. So it is possible to restrain on any of those ranges ; you just need to set the range with the *tthRange* or thee *chiRange* parameter. like the *tthRange* parameter, value outside this range are ignored.

Sometimes one needs to mask a few pixels (beamstop, hot pixels, ...), to ignore a few of them you just need to provide a *mask* array with a value of 1 for those pixels. To take a pixel into account you just need to set a value of 0 in the mask array. Indeed the shape of the mask array should be identical to the data shape (size of the array `_must_` be the same).

Masking can also be achieved by setting masked pixels to an impossible value (-1) and calling this value the “dummy value”. Some Pilatus detectors are setting non existing pixel to -1 and dead pixels to -2. Then use `dummy=-2 & delta_dummy=1.5` so that any value between -3.5 and -0.5 are considered as bad.

the polarisation correction can be taken into account with the *polarization_factor* parameter. Set it between [-1, 1], to correct your data. If set to 0 there is no correction at all.

The *dark* and the *flat* can be provided to correct the data before computing the radial integration.

```
xrpd2_splitPixel (data, npt_rad, npt_azim=360, filename=None, correctSolidAngle=True, tthRange=None, chiRange=None, mask=None, dummy=None, delta_dummy=None, polarization_factor=None, dark=None, flat=None)
```

Calculate the 2D powder diffraction pattern (2Theta,Chi) from a set of data, an image

Split pixels according to their corner positions

Parameters

- **data** (*ndarray*) – 2D array from the CCD camera
- **npt_rad** – number of bin of the Radial (horizontal) axis (2Theta)
- **npt_azim** (*int*) – number of bin of the Azimuthal (vertical) axis (chi)
- **filename** (*str*) – file to save data in
- **correctSolidAngle** (*bool or int*) – solid angle correction, order 1 or 3 (like fit2d)
- **tthRange** (*(float, float)*) – The lower and upper range of 2theta
- **chiRange** (*(float, float)*, *disabled for now*) – The lower and upper range of the chi angle.
- **mask** (*ndarray*) – array with 1 for masked pixels, and 0 for valid pixels
- **dummy** (*float*) – value for dead/masked pixels (dynamic mask)
- **delta_dummy** (*float*) – precision for dummy value
- **polarization_factor** (*float*) – polarization factor correction
- **dark** (*ndarray*) – dark noise image
- **flat** (*ndarray*) – flat field image

Returns azimuthally regrouped data, 2theta pos. and chi pos.

Return type 3-tuple of ndarrays

This method convert the *data* image from the pixel coordinates to the 2theta, chi coordinates. This is similar to a rectangular to polar conversion. The number of point of the new image is given by *npt_rad* and *npt_azim*. If you give a *filename*, the new image is also saved as an edf file.

It is possible to correct the 2theta/chi pattern using the *correctSolidAngle* parameter. The weight of a pixel is ponderate by its solid angle.

The 2theta and range of the new image can be set using the *tthRange* parameter. If not given the maximum available range is used. Indeed pixel outside this range are ignored.

Each pixel of the *data* image has a 2theta and a chi coordinate. So it is possible to restrain on any of those ranges ; you just need to set the range with the *tthRange* or thee *chiRange* parameter. like the *tthRange* parameter, value outside this range are ignored.

Sometimes one needs to mask a few pixels (beamstop, hot pixels, ...), to ignore a few of them you just need to provide a *mask* array with a value of 1 for those pixels. To take a pixel into account you just need to set a value of 0 in the mask array. Indeed the shape of the mask array should be identical to the data shape (size of the array *_must_* be the same).

Masking can also be achieved by setting masked pixels to an impossible value (-1) and calling this value the “dummy value”. Some Pilatus detectors are setting non existing pixel to -1 and dead pixels to -2. Then use *dummy*=-2 & *delta_dummy*=1.5 so that any value between -3.5 and -0.5 are considered as bad.

the polarisation correction can be taken into account with the *polarization_factor* parameter. Set it between [-1, 1], to correct your data. If set to 0 there is no correction at all.

The *dark* and the *flat* can be provided to correct the data before computing the radial integration.

xrpd_CSR_OCL (*data*, *npt*, *filename=None*, *correctSolidAngle=True*, *tthRange=None*, *mask=None*, *dummy=None*, *delta_dummy=None*, *dark=None*, *flat=None*, *chiRange=None*, *safe=True*, *devicetype='all'*, *platformid=None*, *deviceid=None*, *block_size=32*, *padded=False*)

Calculate the powder diffraction pattern from a set of data, an image.

PyOpenCL implementation using a CSR version of the Look-Up Table (OpenCL). The look-up table is a Cython module.

Parameters

- **data** (*ndarray*) – 2D array from the CCD camera
- **npt** (*integer*) – number of points in the output pattern
- **filename** (*str*) – file to save data in ascii format 2 column
- **correctSolidAngle** (*bool or int*) – solid angle correction, order 1 or 3 (like fit2d)
- **tthRange** (*(float, float)*) – The lower and upper range of 2theta
- **chiRange** (*(float, float)*) – The lower and upper range of the chi angle in degrees.
- **mask** (*ndarray*) – array with 1 for masked pixels, and 0 for valid pixels
- **dummy** (*float*) – value for dead/masked pixels (dynamic mask)
- **delta_dummy** (*float*) – precision for dummy value

LUT specific parameters:

Parameters **safe** (*bool*) – set to False if your LUT & GPU is already set-up correctly

OpenCL specific parameters:

Parameters

- **devicetype** (*str*) – can be “all”, “cpu”, “gpu”, “acc” or “def”
- **platformid** (*int*) – platform number
- **deviceid** (*int*) – device number

Returns (2theta, I) in degrees

Return type 2-tuple of 1D arrays

This method compute the powder diffraction pattern, from a given *data* image. The number of point of the pattern is given by the *npt* parameter. If you give a *filename*, the powder diffraction is also saved as a two column text file.

It is possible to correct or not the powder diffraction pattern using the *correctSolidAngle* parameter. The weight of a pixel is ponderate by its solid angle.

The 2theta range of the powder diffraction pattern can be set using the *tthRange* parameter. If not given the maximum available range is used. Indeed pixel outside this range are ignored.

Each pixel of the *data* image has also a chi coordinate. So it is possible to restrain the chi range of the pixels to consider in the powder diffraction pattern by setting the *chiRange* parameter. Like the *tthRange* parameter, value outside this range are ignored.

Sometimes one needs to mask a few pixels (beamstop, hot pixels, ...), to ignore a few of them you just need to provide a *mask* array with a value of 1 for those pixels. To take a pixel into account you just need to set

a value of 0 in the mask array. Indeed the shape of the mask array should be identical to the data shape (size of the array `_must_` be the same).

Dynamic masking (i.e recalculated for each image) can be achieved by setting masked pixels to an impossible value (-1) and calling this value the “dummy value”. Dynamic masking is computed at integration whereas static masking is done at LUT-generation, hence faster.

Some Pilatus detectors are setting non existing pixel to -1 and dead pixels to -2. Then use `dummy=-2` & `delta_dummy=1.5` so that any value between -3.5 and -0.5 are considered as bad.

The `safe` parameter is specific to the OpenCL/LUT implementation, you can set it to false if you think the LUT calculated is already the correct one (setup, mask, 2theta/chi range) and the device set-up is the expected one.

`devicetype`, `platformid` and `deviceid`, parameters are specific to the OpenCL implementation. If you set `devicetype` to ‘all’, ‘cpu’, or ‘gpu’ you can force the device used to perform the computation. By providing the `platformid` and `deviceid` you can chose a specific device (computer specific).

xrpd_LUT (*data*, *npt*, *filename=None*, *correctSolidAngle=True*, *tthRange=None*, *chiRange=None*, *mask=None*, *dummy=None*, *delta_dummy=None*, *safe=True*, *dark=None*, *flat=None*)
Calculate the powder diffraction pattern from an image.

Parallel Cython implementation using a Look-Up Table (OpenMP).

Parameters

- **data** (*ndarray*) – 2D array from the CCD camera
- **npt** (*integer*) – number of points in the output pattern
- **filename** (*str*) – file to save data in ascii format 2 column
- **correctSolidAngle** (*bool or int*) – solid angle correction, order 1 or 3 (like fit2d)
- **tthRange** (*(float, float), optional*) – The lower and upper range of the 2theta angle
- **chiRange** (*(float, float), optional*) – The lower and upper range of the chi angle.
- **mask** (*ndarray*) – array with 1 for masked pixels, and 0 for valid pixels
- **dummy** (*float*) – value for dead/masked pixels (dynamic mask)
- **delta_dummy** (*float*) – precision for dummy value

LUT specific parameters:

Parameters safe (*bool*) – set to False if your LUT is already set-up correctly (mask, ranges, ...).

Returns (2theta, I) with 2theta angle in degrees

Return type 2-tuple of 1D arrays

This method compute the powder diffraction pattern, from a given *data* image. The number of point of the pattern is given by the *npt* parameter. If you give a *filename*, the powder diffraction is also saved as a two column text file.

It is possible to correct or not the powder diffraction pattern using the *correctSolidAngle* parameter. The weight of a pixel is ponderate by its solid angle.

The 2theta range of the powder diffraction pattern can be set using the *tthRange* parameter. If not given the maximum available range is used. Indeed pixel outside this range are ignored.

Each pixel of the *data* image as also a chi coordinate. So it is possible to restrain the chi range of the pixels to consider in the powder diffraction pattern by setting the range with the *chiRange* parameter. Like the *tthRange* parameter, value outside this range are ignored.

Sometimes one needs to mask a few pixels (beamstop, hot pixels, ...), to ignore a few of them you just need to provide a *mask* array with a value of 1 for those pixels. To take a pixel into account you just need to set a value of 0 in the mask array. Indeed the shape of the mask array should be identical to the data shape (size of the array *_must_* be the same).

Dynamic masking (i.e recalculated for each image) can be achieved by setting masked pixels to an impossible value (-1) and calling this value the “dummy value”. Dynamic masking is computed at integration whereas static masking is done at LUT-generation, hence faster.

Some Pilatus detectors are setting non existing pixel to -1 and dead pixels to -2. Then use *dummy=-2* & *delta_dummy=1.5* so that any value between -3.5 and -0.5 are considered as bad.

The *safe* parameter is specific to the LUT implementation, you can set it to false if you think the LUT calculated is already the correct one (setup, mask, 2theta/chi range).

TODO: replace with *inegrate1D*

xrpd_LUT_OCL (*data*, *npt*, *filename=None*, *correctSolidAngle=True*, *tthRange=None*, *chiRange=None*, *mask=None*, *dummy=None*, *delta_dummy=None*, *safe=True*, *devicetype='all'*, *platformid=None*, *deviceid=None*, *dark=None*, *flat=None*)

Calculate the powder diffraction pattern from a set of data, an image.

PyOpenCL implementation using a Look-Up Table (OpenCL). The look-up table is a Cython module.

Parameters

- **data** (*ndarray*) – 2D array from the CCD camera
- **npt** (*integer*) – number of points in the output pattern
- **filename** (*str*) – file to save data in ascii format 2 column
- **correctSolidAngle** (*bool or int*) – solid angle correction, order 1 or 3 (like *fit2d*)
- **tthRange** (*(float, float)*) – The lower and upper range of 2theta
- **chiRange** (*(float, float)*) – The lower and upper range of the chi angle in degrees.
- **mask** (*ndarray*) – array with 1 for masked pixels, and 0 for valid pixels
- **dummy** (*float*) – value for dead/masked pixels (dynamic mask)
- **delta_dummy** (*float*) – precision for dummy value

LUT specific parameters:

Parameters safe (*bool*) – set to False if your LUT & GPU is already set-up correctly

OpenCL specific parameters:

Parameters

- **devicetype** (*str*) – can be “all”, “cpu”, “gpu”, “acc” or “def”
- **platformid** (*int*) – platform number
- **deviceid** (*int*) – device number

Returns (2theta, I) in degrees

Return type 2-tuple of 1D arrays

This method compute the powder diffraction pattern, from a given *data* image. The number of point of the pattern is given by the *npt* parameter. If you give a *filename*, the powder diffraction is also saved as a two column text file.

It is possible to correct or not the powder diffraction pattern using the *correctSolidAngle* parameter. The weight of a pixel is ponderate by its solid angle.

The 2theta range of the powder diffraction pattern can be set using the *tthRange* parameter. If not given the maximum available range is used. Indeed pixel outside this range are ignored.

Each pixel of the *data* image has also a chi coordinate. So it is possible to restrain the chi range of the pixels to consider in the powder diffraction pattern by setting the *chiRange* parameter. Like the *tthRange* parameter, value outside this range are ignored.

Sometimes one needs to mask a few pixels (beamstop, hot pixels, ...), to ignore a few of them you just need to provide a *mask* array with a value of 1 for those pixels. To take a pixel into account you just need to set a value of 0 in the mask array. Indeed the shape of the mask array should be identical to the data shape (size of the array *_must_* be the same).

Dynamic masking (i.e recalculated for each image) can be achieved by setting masked pixels to an impossible value (-1) and calling this value the “dummy value”. Dynamic masking is computed at integration whereas static masking is done at LUT-generation, hence faster.

Some Pilatus detectors are setting non existing pixel to -1 and dead pixels to -2. Then use *dummy=-2* & *delta_dummy=1.5* so that any value between -3.5 and -0.5 are considered as bad.

The *safe* parameter is specific to the OpenCL/LUT implementation, you can set it to false if you think the LUT calculated is already the correct one (setup, mask, 2theta/chi range) and the device set-up is the expected one.

devicetype, *platformid* and *deviceid*, parameters are specific to the OpenCL implementation. If you set *devicetype* to ‘all’, ‘cpu’, or ‘gpu’ you can force the device used to perform the computation. By providing the *platformid* and *deviceid* you can chose a specific device (computer specific).

```
xrpd_OpenCL(data, npt, filename=None, correctSolidAngle=True, dark=None, flat=None,
             tthRange=None, mask=None, dummy=None, delta_dummy=None, devicetype='gpu',
             useFp64=True, platformid=None, deviceid=None, safe=True)
```

Calculate the powder diffraction pattern from a set of data, an image.

This is (now) a pure pyopencl implementation so it just needs pyopencl which requires a clean OpenCL installation. This implementation is not slower than the previous Cython and is less problematic for compilation/installation.

Parameters

- **data** (*ndarray*) – 2D array from the CCD camera
- **npt** (*integer*) – number of points in the output pattern
- **filename** (*str*) – file to save data in ascii format 2 column
- **correctSolidAngle** (*bool or int*) – solid angle correction, order 1 or 3 (like fit2d)
- **tthRange** (*(float, float), optional*) – The lower and upper range of the 2theta
- **mask** (*ndarray*) – array with 1 for masked pixels, and 0 for valid pixels
- **dummy** (*float*) – value for dead/masked pixels (dynamic mask)
- **delta_dummy** (*float*) – precision for dummy value

OpenCL specific parameters:

Parameters

- **devicetype** (*str*) – possible values “cpu”, “gpu”, “all” or “def”
- **useFp64** (*bool*) – shall histogram be done in double precision (strongly advised)
- **platformid** (*int*) – platform number
- **deviceid** (*int*) – device number

- **safe** (*bool*) – set to False if your GPU is already set-up correctly

Returns (2theta, I) angle being in degrees

Return type 2-tuple of 1D arrays

This method compute the powder diffraction pattern, from a given *data* image. The number of point of the pattern is given by the *npt* parameter. If you give a *filename*, the powder diffraction is also saved as a two column text file. The powder diffraction is computed internally using an histogram which by default use should be done in 64bits. One can switch to 32 bits with the *useFp64* parameter set to False. In 32bit mode; do not expect better than 1% error and one can even observe overflows ! 32 bits is only left for testing hardware capabilities and should NEVER be used in any real experiment analysis.

It is possible to correct or not the powder diffraction pattern using the *correctSolidAngle* parameter. The weight of a pixel is ponderate by its solid angle.

The 2theta range of the powder diffraction pattern can be set using the *tthRange* parameter. If not given the maximum available range is used. Indeed pixel outside this range are ignored.

Each pixel of the *data* image has also a chi coordinate. So it is possible to restrain the chi range of the pixels to consider in the powder diffraction pattern. You just need to set the range with the *chiRange* parameter; like the *tthRange* parameter, value outside this range are ignored.

Sometimes one needs to mask a few pixels (beamstop, hot pixels, ...), to ignore a few of them you just need to provide a *mask* array with a value of 1 for those pixels. To take a pixel into account you just need to set a value of 0 in the mask array. Indeed the shape of the mask array should be identical to the data shape (size of the array *_must_* be the same).

Bad pixels can also be masked by setting them to an impossible value (-1) and calling this value the “dummy value”. Some Pilatus detectors are setting non existing pixel to -1 and dead pixels to -2. Then use *dummy=-2 & delta_dummy=1.5* so that any value between -3.5 and -0.5 are considered as bad.

devicetype, *platformid* and *deviceid*, parameters are specific to the OpenCL implementation. If you set *devicetype* to ‘all’, ‘cpu’, ‘gpu’, ‘def’ you can force the device used to perform the computation; the program will select the device accordinly. By setting *platformid* and *deviceid*, you can directly address a specific device (which is computer specific).

The *safe* parameter is specific to the integrator object, located on the OpenCL device. You can set it to False if you think the integrator is already setup correcty (device, geometric arrays, mask, 2theta/chi range). Unless many tests will be done at each integration.

xrpd_cython (*data*, *npt*, *filename=None*, *correctSolidAngle=True*, *tthRange=None*, *mask=None*, *dummy=None*, *delta_dummy=None*, *polarization_factor=None*, *dark=None*, *flat=None*, *pixelSize=None*)

Calculate the powder diffraction pattern from a set of data, an image.

Cython multithreaded implementation: fast but still lacks pixels splitting as numpy implementation. This method should not be used in production, it remains to explain why histograms are hard to implement in parallel. Use *xrpd_splitBBox* instead

xrpd_numpy (*data*, *npt*, *filename=None*, *correctSolidAngle=True*, *tthRange=None*, *mask=None*, *dummy=None*, *delta_dummy=None*, *polarization_factor=None*, *dark=None*, *flat=None*)

Calculate the powder diffraction pattern from a set of data, an image.

Numpy implementation: slow and without pixels splitting. This method should not be used in production, it remains to explain how other more sophisticated algorithms works. Use *xrpd_splitBBox* instead

Parameters

- **data** (*ndarray*) – 2D array from the CCD camera
- **npt** (*integer*) – number of points in the output pattern

- **filename** (*str*) – file to save data in ascii format 2 column
- **correctSolidAngle** (*bool or int*) – solid angle correction, order 1 or 3 (like fit2d)
- **tthRange** (*(float, float), optional*) – The lower and upper range of the 2theta
- **mask** (*ndarray*) – array with 1 for masked pixels, and 0 for valid pixels
- **dummy** (*float*) – value for dead/masked pixels (dynamic mask)
- **delta_dummy** (*float*) – precision for dummy value
- **polarization_factor** (*float*) – polarization factor correction
- **dark** (*ndarray*) – dark noise image
- **flat** (*ndarray*) – flat field image

Returns (2theta, I) in degrees

Return type 2-tuple of 1D arrays

This method compute the powder diffraction pattern, from a given *data* image. The number of point of the pattern is given by the *npt* parameter. If you give a *filename*, the powder diffraction is also saved as a two column text file.

It is possible to correct or not the powder diffraction pattern using the *correctSolidAngle* parameter. The weight of a pixel is ponderate by its solid angle.

The 2theta range of the powder diffraction pattern can be set using the *tthRange* parameter. If not given the maximum available range is used. Indeed pixel outside this range are ignored.

Sometimes one needs to mask a few pixels (beamstop, hot pixels, ...), to ignore a few of them you just need to provide a *mask* array with a value of 1 for those pixels. To take a pixel into account you just need to set a value of 0 in the mask array. Indeed the shape of the mask array should be identical to the data shape (size of the array *_must_* be the same).

Bad pixels can be masked out by setting them to an impossible value (-1) and calling this value the “dummy value”. Some Pilatus detectors are setting non existing pixel to -1 and dead pixels to -2. Then use *dummy=-2 & delta_dummy=1.5* so that any value between -3.5 and -0.5 are considered as bad.

The polarisation correction can be taken into account with the *polarization_factor* parameter. Set it between [-1, 1], to correct your data. If set to 0 there is no correction at all.

The *dark* and the *flat* can be provided to correct the data before computing the radial integration.

xrpd_splitBBox (*data, npt, filename=None, correctSolidAngle=True, tthRange=None, chiRange=None, mask=None, dummy=None, delta_dummy=None, polarization_factor=None, dark=None, flat=None*)

Calculate the powder diffraction pattern from a set of data, an image.

Cython implementation

Parameters

- **data** (*ndarray*) – 2D array from the CCD camera
- **npt** (*integer*) – number of points in the output pattern
- **filename** (*str*) – file to save data in ascii format 2 column
- **correctSolidAngle** (*bool or int*) – solid angle correction, order 1 or 3 (like fit2d)
- **tthRange** (*(float, float), optional*) – The lower and upper range of the 2theta
- **chiRange** (*(float, float), optional, disabled for now*) – The lower and upper range of the chi angle.

- **mask** (*ndarray*) – array with 1 for masked pixels, and 0 for valid pixels
- **dummy** (*float*) – value for dead/masked pixels (dynamic mask)
- **delta_dummy** (*float*) – precision for dummy value
- **polarization_factor** (*float*) – polarization factor correction
- **dark** (*ndarray*) – dark noise image
- **flat** (*ndarray*) – flat field image

Returns (2theta, I) in degrees

Return type 2-tuple of 1D arrays

This method compute the powder diffraction pattern, from a given *data* image. The number of point of the pattern is given by the *npt* parameter. If you give a *filename*, the powder diffraction is also saved as a two column text file.

It is possible to correct or not the powder diffraction pattern using the *correctSolidAngle* parameter. The weight of a pixel is ponderate by its solid angle.

The 2theta range of the powder diffraction pattern can be set using the *tthRange* parameter. If not given the maximum available range is used. Indeed pixel outside this range are ignored.

Each pixel of the *data* image as also a chi coordinate. So it is possible to restrain the chi range of the pixels to consider in the powder diffraction pattern. you just need to set the range with the *chiRange* parameter. like the *tthRange* parameter, value outside this range are ignored.

Sometimes one needs to mask a few pixels (beamstop, hot pixels, ...), to ignore a few of them you just need to provide a *mask* array with a value of 1 for those pixels. To take a pixel into account you just need to set a value of 0 in the mask array. Indeed the shape of the mask array should be identical to the data shape (size of the array *_must_* be the same). Pixels can also be maseked by seting them to an

Bad pixels can be masked out by setting them to an impossible value (-1) and calling this value the “dummy value”. Some Pilatus detectors are setting non existing pixel to -1 and dead pixels to -2. Then use *dummy=-2 & delta_dummy=1.5* so that any value between -3.5 and -0.5 are considered as bad.

Some Pilatus detectors are setting non existing pixel to -1 and dead pixels to -2. Then use *dummy=-2 & delta_dummy=1.5* so that any value between -3.5 and -0.5 are considered as bad.

The polarisation correction can be taken into account with the *polarization_factor* parameter. Set it between [-1, 1], to correct your data. If set to 0 there is no correction at all.

The *dark* and the *flat* can be provided to correct the data before computing the radial integration.

xrpd_splitPixel (*data*, *npt*, *filename=None*, *correctSolidAngle=True*, *tthRange=None*, *chiRange=None*, *mask=None*, *dummy=None*, *delta_dummy=None*, *polarization_factor=None*, *dark=None*, *flat=None*)

Calculate the powder diffraction pattern from a set of data, an image.

Cython implementation (single threaded)

Parameters

- **data** (*ndarray*) – 2D array from the CCD camera
- **npt** (*integer*) – number of points in the output pattern
- **filename** (*str*) – file to save data in ascii format 2 column
- **correctSolidAngle** (*bool or int*) – solid angle correction, order 1 or 3 (like fit2d)
- **tthRange** (*(float, float), optional*) – The lower and upper range of the 2theta

- **chiRange** ((float, float), optional, disabled for now) – The lower and upper range of the chi angle.
- **mask** (ndarray) – array with 1 for masked pixels, and 0 for valid pixels
- **dummy** (float) – value for dead/masked pixels (dynamic mask)
- **delta_dummy** (float) – precision for dummy value
- **polarization_factor** (float) – polarization factor correction
- **dark** (ndarray) – dark noise image
- **flat** (ndarray) – flat field image

Returns (2theta, I) in degrees

Return type 2-tuple of 1D arrays

This method compute the powder diffraction pattern, from a given *data* image. The number of point of the pattern is given by the *npt* parameter. If you give a *filename*, the powder diffraction is also saved as a two column text file.

It is possible to correct or not the powder diffraction pattern using the *correctSolidAngle* parameter. The weight of a pixel is ponderate by its solid angle.

The 2theta range of the powder diffraction pattern can be set using the *tthRange* parameter. If not given the maximum available range is used. Indeed pixel outside this range are ignored.

Each pixel of the *data* image as also a chi coordinate. So it is possible to restrain the chi range of the pixels to consider in the powder diffraction pattern. you just need to set the range with the *chiRange* parameter. like the *tthRange* parameter, value outside this range are ignored.

Sometimes one needs to mask a few pixels (beamstop, hot pixels, ...), to ignore a few of them you just need to provide a *mask* array with a value of 1 for those pixels. To take a pixel into account you just need to set a value of 0 in the mask array. Indeed the shape of the mask array should be identical to the data shape (size of the array *_must_* be the same).

Bad pixels can be masked out by setting them to an impossible value (-1) and calling this value the “dummy value”. Some Pilatus detectors are setting non existing pixel to -1 and dead pixels to -2. Then use *dummy=-2 & delta_dummy=1.5* so that any value between -3.5 and -0.5 are considered as bad.

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The polarisation correction can be taken into account with the *polarization_factor* parameter. Set it between [-1, 1], to correct your data. If set to 0 there is no correction at all.

The *dark* and the *flat* can be provided to correct the data before computing the radial integration.

3.3 integrate_widget Module

pyFAI-integrate

A graphical tool (based on PyQt4) for performing azimuthal integration on series of files.

```
class pyFAI.integrate_widget.AIWidget (input_data=None)
    Bases: PyQt4.QtGui.QWidget

    detector_changed()

    die()
```

dump (*filename*='.azimint.json')

Dump the status of the current widget to a file in JSON

Parameters **filename** (*str*) – path where to save the config

help ()

openCL_changed ()

platform_changed ()

proceed ()

restore (*filename*='.azimint.json')

restore from JSON file the status of the current widget

Parameters **filename** (*str*) – path where the config was saved

select_darkcurrent ()

select_flatfield ()

select_maskfile ()

select_ponifile ()

select_splinefile ()

setBackgroundImage (*dark*=None)

PyMca Plugin specific

Parameters **dark** – 2D array with the dark-current

setSelectionMask (*mask*=None)

PyMca Plugin specific

Parameters **mask** – 2D array with the masked region

setStackDataObject (*stack*, *stack_name*=None)

set_ai ()

set_input_data (*stack*, *stack_name*=None)

set_ponifile (*ponifile*=None)

set_validators ()

Set all validators for text entries

class pyFAI.integrate_widget.**Browser** (*default_url*='http://google.com')

Bases: PyQt4.QtGui.QMainWindow

browse ()

Make a web browse on a specific url and show the page on the Webview widget.

3.4 geometry Module

class pyFAI.geometry.**Geometry** (*dist*=1, *poni1*=0, *poni2*=0, *rot1*=0, *rot2*=0, *rot3*=0, *pixel1*=None, *pixel2*=None, *splineFile*=None, *detector*=None, *wavelength*=None)

Bases: object

This class is an azimuthal integrator based on P. Boesecke's geometry and histogram algorithm by Manolo S. del Rio and V.A Sole

Detector is assumed to be corrected from “raster orientation” effect. It is not addressed here but rather in the Detector object or at read time. Considering there is no tilt:

- Detector fast dimension (dim2) is supposed to be horizontal (dimension X of the image)
- Detector slow dimension (dim1) is supposed to be vertical, upwards (dimension Y of the image)
- The third dimension is chose such as the referential is orthonormal, so dim3 is along incoming X-ray beam

Axis 1 is along first dimension of detector (when not tilted), this is the slow dimension of the image array in C or Y $x1=\{1,0,0\}$

Axis 2 is along second dimension of detector (when not tilted), this is the fast dimension of the image in C or X $x2=\{0,1,0\}$

Axis 3 is along the incident X-Ray beam $x3=\{0,0,1\}$

We define the 3 rotation around axis 1, 2 and 3:

$rotM1 = \text{RotationMatrix}[rot1,x1] = \{\{1,0,0\},\{0,\cos[rot1],-\sin[rot1]\},\{0,\sin[rot1],\cos[rot1]\}\}$ $rotM2 = \text{RotationMatrix}[rot2,x2] = \{\{\cos[rot2],0,\sin[rot2]\},\{0,1,0\},\{-\sin[rot2],0,\cos[rot2]\}\}$ $rotM3 = \text{RotationMatrix}[rot3,x3] = \{\{\cos[rot3],-\sin[rot3],0\},\{\sin[rot3],\cos[rot3],0\},\{0,0,1\}\}$

Rotations of the detector are applied first Rot around axis 1, then axis 2 and finally around axis 3:

$R = rotM3.rotM2.rotM1$

$R = \{\{\cos[rot2] \cos[rot3], \cos[rot3] \sin[rot1] \sin[rot2] - \cos[rot1] \sin[rot3], \cos[rot1] \cos[rot3] \sin[rot2] + \sin[rot1] \sin[rot3]\}, \{\cos[rot2] \sin[rot3], \cos[rot1] \cos[rot3] + \sin[rot1] \sin[rot2] \sin[rot3], -\cos[rot3] \sin[rot1] + \cos[rot1] \sin[rot2] \sin[rot3]\}, \{-\sin[rot2], \cos[rot2] \sin[rot1], \cos[rot1] \cos[rot2]\}\}$

In Python notation:

$R.x1 = [\cos(rot2)*\cos(rot3), \cos(rot2)*\sin(rot3), -\sin(rot2)]$

$R.x2 = [\cos(rot3)*\sin(rot1)*\sin(rot2) - \cos(rot1)*\sin(rot3), \cos(rot1)*\cos(rot3) + \sin(rot1)*\sin(rot2)*\sin(rot3), \cos(rot2)*\sin(rot1)]$

$R.x3 = [\cos(rot1)*\cos(rot3)*\sin(rot2) + \sin(rot1)*\sin(rot3), -\cos(rot3)*\sin(rot1) + \cos(rot1)*\sin(rot2)*\sin(rot3), \cos(rot1)*\cos(rot2)]$

- Coordinates of the Point of Normal Incidence:

$PONI = R.\{0,0,L\}$

$PONI = [L*(\cos(rot1)*\cos(rot3)*\sin(rot2) + \sin(rot1)*\sin(rot3)), L*(-\cos(rot3)*\sin(rot1) + \cos(rot1)*\sin(rot2)*\sin(rot3)), L*\cos(rot1)*\cos(rot2)]$

- Any pixel on detector plan at coordinate (d1, d2) in meters. Detector is at z=L

$P=\{d1,d2,L\}$

$R.P = [t1, t2, t3]$ $t1 = R.P.x1 = d1*\cos(rot2)*\cos(rot3) + d2*(\cos(rot3)*\sin(rot1)*\sin(rot2) - \cos(rot1)*\sin(rot3)) + L*(\cos(rot1)*\cos(rot3)*\sin(rot2) + \sin(rot1)*\sin(rot3))$ $t2 = R.P.x2 = d1*\cos(rot2)*\sin(rot3) + d2*(\cos(rot1)*\cos(rot3) + \sin(rot1)*\sin(rot2)*\sin(rot3)) + L*(-\cos(rot3)*\sin(rot1) + \cos(rot1)*\sin(rot2)*\sin(rot3))$ $t3 = R.P.x3 = d2*\cos(rot2)*\sin(rot1) - d1*\sin(rot2) + L*\cos(rot1)*\cos(rot2)$

- Distance sample (origin) to detector point (d1,d2)

$R.P.I = \sqrt{(\text{pow}(\text{Abs}(L*\cos(rot1)*\cos(rot2) + d2*\cos(rot2)*\sin(rot1) - d1*\sin(rot2)),2) + \text{pow}(\text{Abs}(d1*\cos(rot2)*\cos(rot3) + d2*(\cos(rot3)*\sin(rot1)*\sin(rot2) - \cos(rot1)*\sin(rot3)) + L*(\cos(rot1)*\cos(rot3)*\sin(rot2) + \sin(rot1)*\sin(rot3))),2) + \text{pow}(\text{Abs}(d1*\cos(rot2)*\sin(rot3) + L*(-\cos(rot3)*\sin(rot1) + \cos(rot1)*\sin(rot2)*\sin(rot3)) + d2*(\cos(rot1)*\cos(rot3) + \sin(rot1)*\sin(rot2)*\sin(rot3))),2)}$

•cos(2theta) is defined as (R.P component along x3) over the distance from origin to data point **|R.P|**

$$tth = \text{ArcCos} [-(R.P).x3/|R.P|]$$

$$tth = \text{Arccos}((-L*\cos(rot1)*\cos(rot2)) - d2*\cos(rot2)*\sin(rot1) + d1*\sin(rot2))/$$

$$\text{sqrt}(\text{pow}(\text{Abs}(L*\cos(rot1)*\cos(rot2) + d2*\cos(rot2)*\sin(rot1) - d1*\sin(rot2)),2) +$$

$$\text{pow}(\text{Abs}(d1*\cos(rot2)*\cos(rot3) + d2*(\cos(rot3)*\sin(rot1)*\sin(rot2) - \cos(rot1)*\sin(rot3)) +$$

$$L*(\cos(rot1)*\cos(rot3)*\sin(rot2) + \sin(rot1)*\sin(rot3))),2) + \text{pow}(\text{Abs}(d1*\cos(rot2)*\sin(rot3) +$$

$$L*(-(\cos(rot3)*\sin(rot1)) + \cos(rot1)*\sin(rot2)*\sin(rot3)) +$$

$$d2*(\cos(rot1)*\cos(rot3) + \sin(rot1)*\sin(rot2)*\sin(rot3))),2)))$$

•tan(2theta) is defined as $\text{sqrt}(t1^{**2} + t2^{**2}) / t3$

$$tth = \text{ArcTan2} [\text{sqrt}(t1^{**2} + t2^{**2}) , t3]$$

Getting 2theta from it's tangeant seems both more precise (around beam stop very far from sample) and faster by about 25% Currently there is a swich in the method to follow one path or the other.

•Tangeant of angle chi is defined as (R.P component along x1) over (R.P component along x2). Arctan2 should be used in actual calculation

$$\text{chi} = \text{ArcTan} [((R.P).x1) / ((R.P).x2)]$$

$$\text{chi} = \text{ArcTan2}(d1*\cos(rot2)*\cos(rot3) + d2*(\cos(rot3)*\sin(rot1)*\sin(rot2) - \cos(rot1)*\sin(rot3)) +$$

$$L*(\cos(rot1)*\cos(rot3)*\sin(rot2) + \sin(rot1)*\sin(rot3)),$$

$$d1*\cos(rot2)*\sin(rot3) + L*(-(\cos(rot3)*\sin(rot1)) + \cos(rot1)*\sin(rot2)*\sin(rot3)) +$$

$$d2*(\cos(rot1)*\cos(rot3) + \sin(rot1)*\sin(rot2)*\sin(rot3)))$$

calc_pos_zyx (*d0=None, d1=None, d2=None, param=None*)

Allows you to calculate the position of a set of points in space in the sample re

Parameters

- **d0** – altitude on the point compared to the detector (i.e. z)
- **d1** – position on the detector along the slow dimention (i.e. y)
- **d2** – position on the detector along the fastest dimention (i.e. x)

:return zyx array, so 3D array with dim0=along the beam, dim1=along slowest dimension
 dim2=along fastest dimension unless rotations are too large

calc_transmission (*t0, shape=None*)

Defines the absorption correction for a phosphor screen or a scintillator from t0, the normal transmission of the screen.

$$\text{Icor} = \text{Iobs}(1-t0)/(1-\exp(\ln(t0)/\cos(\text{incidence}))) \quad 1-\exp(\ln(t0)/\cos(\text{incidence}))$$

$$\text{let } t = \frac{\text{Icor}}{1 - t0}$$

See reference on: J. Appl. Cryst. (2002). 35, 356–359 G. Wu et al. CCD phosphor

Parameters

- **t0** – value of the normal transmission (from 0 to 1)

- **shape** – shape of the array

Returns actual

calcfrom1d (*tth, I, shape=None, mask=None, dim1_unit=2th_deg, correctSolidAngle=True*)

Computes a 2D image from a 1D integrated profile

Parameters

- **tth** – 1D array with 2theta in degrees
- **I** – scattering intensity

Returns 2D image reconstructed

chi (*d1, d2, path='cython'*)

Calculate the chi (azimuthal angle) for the centre of a pixel at coordinate d1,d2 which in the lab ref has coordinate:

$$\begin{aligned} X1 &= p1*\cos(\text{rot}2)*\cos(\text{rot}3) + p2*(\cos(\text{rot}3)*\sin(\text{rot}1)*\sin(\text{rot}2) - \cos(\text{rot}1)*\sin(\text{rot}3)) \\ &- L*(\cos(\text{rot}1)*\cos(\text{rot}3)*\sin(\text{rot}2) + \sin(\text{rot}1)*\sin(\text{rot}3)) \quad X2 = p1*\cos(\text{rot}2)*\sin(\text{rot}3) \\ &- L*(-\cos(\text{rot}3)*\sin(\text{rot}1)) + \cos(\text{rot}1)*\sin(\text{rot}2)*\sin(\text{rot}3) + p2*(\cos(\text{rot}1)*\cos(\text{rot}3) + \\ &\sin(\text{rot}1)*\sin(\text{rot}2)*\sin(\text{rot}3)) \quad X3 = -(L*\cos(\text{rot}1)*\cos(\text{rot}2)) + p2*\cos(\text{rot}2)*\sin(\text{rot}1) - p1*\sin(\text{rot}2) \end{aligned}$$

hence $\tan(\text{Chi}) = X2 / X1$

Parameters

- **d1** (*float or array of them*) – pixel coordinate along the 1st dimation (C convention)
- **d2** (*float or array of them*) – pixel coordinate along the 2nd dimation (C convention)
- **path** – can be “tan” (i.e via numpy) or “cython”

Returns chi, the azimuthal angle in rad

chiArray (*shape*)

Generate an array of the given shape with chi(i,j) (azimuthal angle) for all elements.

Parameters **shape** (*ndarray.shape*) – the shape of the chi array

Returns the chi array

Return type ndarray

chi_corner (*d1, d2*)

Calculate the chi (azimuthal angle) for the corner of a pixel at coordinate d1,d2 which in the lab ref has coordinate:

$$\begin{aligned} X1 &= p1*\cos(\text{rot}2)*\cos(\text{rot}3) + p2*(\cos(\text{rot}3)*\sin(\text{rot}1)*\sin(\text{rot}2) - \cos(\text{rot}1)*\sin(\text{rot}3)) \\ &- L*(\cos(\text{rot}1)*\cos(\text{rot}3)*\sin(\text{rot}2) + \sin(\text{rot}1)*\sin(\text{rot}3)) \quad X2 = p1*\cos(\text{rot}2)*\sin(\text{rot}3) \\ &- L*(-\cos(\text{rot}3)*\sin(\text{rot}1)) + \cos(\text{rot}1)*\sin(\text{rot}2)*\sin(\text{rot}3) + p2*(\cos(\text{rot}1)*\cos(\text{rot}3) + \\ &\sin(\text{rot}1)*\sin(\text{rot}2)*\sin(\text{rot}3)) \quad X3 = -(L*\cos(\text{rot}1)*\cos(\text{rot}2)) + p2*\cos(\text{rot}2)*\sin(\text{rot}1) - p1*\sin(\text{rot}2) \end{aligned}$$

hence $\tan(\text{Chi}) = X2 / X1$

Parameters

- **d1** (*float or array of them*) – pixel coordinate along the 1st dimation (C convention)
- **d2** (*float or array of them*) – pixel coordinate along the 2nd dimation (C convention)

Returns chi, the azimuthal angle in rad

chia

chi array in cache

cornerArray (*shape*)

Generate a 3D array of the given shape with (i,j) (radial angle 2th, azimuthal angle chi) for all elements.

Parameters **shape** (*ndarray.shape*) – expected shape

Returns 3d array with shape=(**shape*,2) the two elements are (radial angle 2th, azimuthal angle chi)

cornerQArray (*shape*)

Generate a 3D array of the given shape with (i,j) (azimuthal angle) for all elements.

cornerRArray (*shape*)

Generate a 3D array of the given shape with (i,j) (azimuthal angle) for all elements.

correct_SA_spline**cosIncidence** (*d1*, *d2*)

Calculate the incidence angle (alpha) for current pixels (P). The poni is at incidence angle=1 so $\cos(\alpha) = 1$

del_chia ()**del_dssa** ()**del_qa** ()**del_ttha** ()**delta2Theta** (*shape*)

Generate a 3D array of the given shape with (i,j) with the max distance between the center and any corner in 2 theta

Parameters **shape** – The shape of the detector array: 2-tuple of integer

Returns 2D-array containing the max delta angle between a pixel center and any corner in 2theta-angle (rad)

deltaChi (*shape*)

Generate a 3D array of the given shape with (i,j) with the max distance between the center and any corner in chi-angle (rad)

Parameters **shape** – The shape of the detector array: 2-tuple of integer

Returns 2D-array containing the max delta angle between a pixel center and any corner in chi-angle (rad)

deltaQ (*shape*)

Generate a 2D array of the given shape with (i,j) with the max distance between the center and any corner in q_vector unit (nm^{-1})

Parameters **shape** – The shape of the detector array: 2-tuple of integer

Returns array 2D containing the max delta Q between a pixel center and any corner in q_vector unit (nm^{-1})

deltaR (*shape*)

Generate a 2D array of the given shape with (i,j) with the max distance between the center and any corner in radius unit (mm)

Parameters **shape** – The shape of the detector array: 2-tuple of integer

Returns array 2D containing the max delta Q between a pixel center and any corner in q_vector unit (nm^{-1})

diffSolidAngle (*d1*, *d2*)

Calculate the solid angle of the current pixels (P) versus the PONI (C)

$$\Omega(P) = A \cos(a) \frac{SC^2}{3 SC^3}$$

$$d\Omega = \frac{d\Omega(P)}{d\Omega(C)} = \frac{d\Omega(P)}{d\Omega(C)} \times \frac{d\Omega(C)}{d\Omega(C)} = \cos(a) = \frac{SC}{SP} \frac{\Omega(C)}{SP^2} \frac{A \cos(0)}{SP^3}$$

$$\cos(a) = SC/SP$$

Parameters

- **d1** – 1d or 2d set of points
- **d2** – 1d or 2d set of points (same size&shape as d1)

Returns solid angle correction array

dist

dssa

solid angle array in cache

getFit2D ()

Export geometry setup with the geometry of Fit2D

Returns dict with parameters compatible with fit2D geometry

getPyFAI ()

Export geometry setup with the geometry of PyFAI

Returns dict with the parameter-set of the PyFAI geometry

getSPD ()

get the SPD like parameter set: For geometry description see Peter Boesecke J.Appl.Cryst.(2007).40, s423–s427

Basically the main difference with pyFAI is the order of the axis which are flipped

Returns dictionary with those parameters: SampleDistance: distance from sample to detector at the PONI (orthogonal projection) Center_1, pixel position of the PONI along fastest axis Center_2: pixel position of the PONI along slowest axis Rot_1: rotation around the fastest axis (x) Rot_2: rotation around the slowest axis (y) Rot_3: rotation around the axis ORTHOGONAL to the detector plan PSize_1: pixel size in meter along the fastest dimation PSize_2: pixel size in meter along the slowst dimation splineFile: name of the file containing the spline BSize_1: pixel binning factor along the fastest dimation BSize_2: pixel binning factor along the slowst dimation WaveLength: wavelength used in meter

get_chia ()

get_correct_solid_angle_for_spline ()

get_dist ()

get_dssa ()

get_pixel1 ()

get_pixel2 ()

get_poni1 ()

get_poni2 ()

get_qa ()

get_rot1 ()

`get_rot2()`

`get_rot3()`

`get_spline()`

`get_splineFile()`

`get_ttha()`

`get_wavelength()`

`load(filename)`

Load the refined parameters from a file.

Parameters `filename` (*string*) – name of the file to load

`oversampleArray(myarray)`

`pixel1`

`pixel2`

`polarization(shape=None, factor=None, axis_offset=0)`

Calculate the polarization correction according to the polarization factor:

- If the polarization factor is None, the correction is not applied (returns 1)
- If the polarization factor is 0 (circular polarization), the correction correspond to $(1+(\cos 2\theta)^2)/2$
- If the polarization factor is 1 (linear horizontal polarization), there is no correction in the vertical plane and a node at $2\theta=90$, $\chi=0$
- If the polarization factor is -1 (linear vertical polarization), there is no correction in the horizontal plane and a node at $2\theta=90$, $\chi=90$
- If the polarization is elliptical, the polarization factor varies between -1 and +1.

The `axis_offset` parameter allows correction for the misalignment of the polarization plane (or ellipse main axis) and the the detector's X axis.

Parameters

- **factor** – $(I_h - I_v)/(I_h + I_v)$: varies between 0 (no polarization) and 1 (where division by 0 could occur at $2\theta=90$, $\chi=0$)
- **axis_offset** – Angle between the polarization main axis and detector X direction (in radians !!!)

Returns 2D array with polarization correction array (intensity/polarisation)

`poni1`

`poni2`

`qArray(shape)`

Generate an array of the given shape with $q(i,j)$ for all elements.

`qCornerFunct(d1, d2)`

Calculate the q_vector for any pixel corner (in nm^{-1})

`qFunction(d1, d2, param=None, path='cython')`

Calculates the q value for the center of a given pixel (or set of pixels) in nm^{-1}

$q = 4\pi/\lambda \sin(2\theta / 2)$

Parameters

- **d1** (*scalar or array of scalar*) – position(s) in pixel in first dimension (c order)
- **d2** (*scalar or array of scalar*) – position(s) in pixel in second dimension (c order)

Returns q in nm^{-1}

Return type float or array of floats.

qa

Q array in cache

rArray (*shape*)

Generate an array of the given shape with $r(i,j)$ for all elements; r in mm.

Parameters **shape** – expected shape

Returns 2d array of the given shape with radius in mm from beam stop.

rCornerFunct (*d1, d2*)

Calculate the radius array for any pixel corner (in mm)

rFunction (*d1, d2, param=None, path='numpy'*)

Calculates the radius value for the center of a given pixel (or set of pixels) in mm

$r = \text{direct_distance} * \tan(2\theta)$

Parameters

- **d1** (*scalar or array of scalar*) – position(s) in pixel in first dimension (c order)
- **d2** (*scalar or array of scalar*) – position(s) in pixel in second dimension (c order)

Returns r in mm

Return type float or array of floats.

read (*filename*)

Load the refined parameters from a file.

Parameters **filename** (*string*) – name of the file to load

reset ()

reset most arrays that are cached: used when a parameter changes.

rot1

rot2

rot3

save (*filename*)

Save the refined parameters.

Parameters **filename** (*string*) – name of the file where to save the parameters

setChiDiscAtPi ()

Set the position of the discontinuity of the chi axis between $-\pi$ and $+\pi$. This is the default behaviour

setChiDiscAtZero ()

Set the position of the discontinuity of the chi axis between 0 and 2π . By default it is between π and $-\pi$

setFit2D (*directDist, centerX, centerY, tilt=0.0, tiltPlanRotation=0.0, pixelX=None, pixelY=None, splineFile=None*)

Set the Fit2D-like parameter set: For geometry description see HPR 1996 (14) pp-240

Warning: Fit2D flips automatically images depending on their file-format. By reverse engineering we noticed this behaviour for Tiff and Mar345 images (at least). To obtain correct result you will have to flip images using `numpy.flipud`.

Parameters

- **direct** – direct distance from sample to detector along the incident beam (in millimeter as in fit2d)
- **tilt** – tilt in degrees
- **tiltPlanRotation** – Rotation (in degrees) of the tilt plan around the Z-detector axis * 0deg -> Y does not move, +X goes to Z<0 * 90deg -> X does not move, +Y goes to Z<0 * 180deg -> Y does not move, +X goes to Z>0 * 270deg -> X does not move, +Y goes to Z>0
- **pixelX,pixelY** – as in fit2d they are given in micron, not in meter
- **centerY** (*centerX*,) – pixel position of the beam center
- **splineFile** – name of the file containing the spline

setOversampling (*iOversampling*)
set the oversampling factor

setPyFAI (***kwargs*)
set the geometry from a pyFAI-like dict

setSPD (*SampleDistance, Center_1, Center_2, Rot_1=0, Rot_2=0, Rot_3=0, PSize_1=None, PSize_2=None, splineFile=None, BSize_1=1, BSize_2=1, WaveLength=None*)
Set the SPD like parameter set: For geometry description see Peter Boesecke J.Appl.Cryst.(2007).40, s423–s427

Basically the main difference with pyFAI is the order of the axis which are flipped

Parameters SampleDistance – distance from sample to detector at the PONI (orthogonal projection)

:param Center_1, pixel position of the PONI along fastest axis :param Center_2: pixel position of the PONI along slowest axis :param Rot_1: rotation around the fastest axis (x) :param Rot_2: rotation around the slowest axis (y) :param Rot_3: rotation around the axis ORTHOGONAL to the detector plan :param PSize_1: pixel size in meter along the fastest dimension :param PSize_2: pixel size in meter along the slowest dimension :param splineFile: name of the file containing the spline :param BSize_1: pixel binning factor along the fastest dimension :param BSize_2: pixel binning factor along the slowest dimension :param WaveLength: wavelength used

set_chia (_)

set_correct_solid_angle_for_spline (*value*)

set_dist (*value*)

set_dssa (_)

set_pixel1 (*pixel1*)

set_pixel2 (*pixel2*)

set_poni1 (*value*)

set_poni2 (*value*)

set_qa (_)

set_rot1 (*value*)

set_rot2 (*value*)

set_rot3 (*value*)

set_spline (*spline*)

set_splineFile (*splineFile*)

set_ttha (*_*)

set_wavelength (*value*)

classmethod sload (*filename*)

A static method combining the constructor and the loader from a file

Parameters **filename** (*string*) – name of the file to load

Returns instance of Geometry of AzimuthalIntegrator set-up with the parameter from the file.

solidAngleArray (*shape, order=3*)

Generate an array of the given shape with the solid angle of the current element two-theta(i,j) for all elements.

Parameters

- **shape** – shape of the array expected
- **order** –

spline

splineFile

tth (*d1, d2, param=None, path='cython'*)

Calculates the 2theta value for the center of a given pixel (or set of pixels)

Parameters

- **d1** (*scalar or array of scalar*) – position(s) in pixel in first dimension (c order)
- **d2** (*scalar or array of scalar*) – position(s) in pixel in second dimension (c order)
- **path** – can be “cos”, “tan” or “cython”

Returns 2theta in radians

Return type float or array of floats.

tth_corner (*d1, d2*)

Calculates the 2theta value for the corner of a given pixel (or set of pixels)

Parameters

- **d1** (*scalar or array of scalar*) – position(s) in pixel in first dimension (c order)
- **d2** (*scalar or array of scalar*) – position(s) in pixel in second dimension (c order)

Returns 2theta in radians

Return type float or array of floats.

ttha

2theta array in cache

twoThetaArray (*shape*)

Generate an array of the given shape with two-theta(i,j) for all elements.

wavelength

write (*filename*)

Save the refined parameters.

Parameters **filename** (*string*) – name of the file where to save the parameters

3.5 geometryRefinement Module

```
class pyFAI.geometryRefinement.GeometryRefinement (data, dist=1, poni1=None,
                                                    poni2=None, rot1=0, rot2=0, rot3=0,
                                                    pixell=None, pixel2=None, spline-
                                                    File=None, detector=None, wave-
                                                    length=None, calibrant=None)
```

Bases: pyFAI.azimuthalIntegrator.AzimuthalIntegrator

anneal (*maxiter=1000000*)

calc_2th (*rings, wavelength=None*)

Parameters

- **rings** – indices of the rings. starts at 0 and self.dSpacing should be long enough !!!
- **wavelength** – wavelength in meter

chi2 (*param=None*)

chi2_wavelength (*param=None*)

dist_max

dist_min

get_dist_max ()

get_dist_min ()

get_poni1_max ()

get_poni1_min ()

get_poni2_max ()

get_poni2_min ()

get_rot1_max ()

get_rot1_min ()

get_rot2_max ()

get_rot2_min ()

get_rot3_max ()

get_rot3_min ()

get_wavelength_max ()

get_wavelength_min ()

guess_poni ()

Poni can be guessed by the centroid of the ring with lowest 2Theta

poni1_max

poni1_min

poni2_max

poni2_min

refine1 ()

```

refine2 (maxiter=1000000, fix=['wavelength'])
refine2_wavelength (maxiter=1000000, fix=['wavelength'])
residu1 (param, d1, d2, rings)
residu1_wavelength (param, d1, d2, rings)
residu2 (param, d1, d2, rings)
residu2_wavelength (param, d1, d2, rings)
residu2_wavelength_weighted (param, d1, d2, rings, weight)
residu2_weighted (param, d1, d2, rings, weight)
roca ()
    run roca to optimise the parameter set
rot1_max
rot1_min
rot2_max
rot2_min
rot3_max
rot3_min
set_dist_max (value)
set_dist_min (value)
set_poni1_max (value)
set_poni1_min (value)
set_poni2_max (value)
set_poni2_min (value)
set_rot1_max (value)
set_rot1_min (value)
set_rot2_max (value)
set_rot2_min (value)
set_rot3_max (value)
set_rot3_min (value)
set_tolerance (value=10)
    Set the tolerance for a refinement of the geometry; in percent of the original value
    Parameters value – Tolerance as a percentage
set_wavelength_max (value)
set_wavelength_min (value)
simplex (maxiter=1000000)
wavelength_max
wavelength_min

```

3.6 detectors Module

Module containing the description of all detectors with a factory to instantiate them

class `pyFAI.detectors.Basler` (*pixel=3.75e-06*)

Bases: `pyFAI.detectors.Detector`

Basler camera are simple CCD camera over GigaE

MAX_SHAPE = (966, 1296)

aliases = ['aca1300']

force_pixel = True

class `pyFAI.detectors.Detector` (*pixel1=None, pixel2=None, splineFile=None*)

Bases: `object`

Generic class representing a 2D detector

aliases = []

binning

calc_cartesian_positions (*d1=None, d2=None*)

Calculate the position of each pixel center in cartesian coordinate and in meter of a couple of coordinates. The half pixel offset is taken into account here !!!

Parameters

- **d1** (*ndarray (1D or 2D)*) – the Y pixel positions (slow dimension)
- **d2** (*ndarray (1D or 2D)*) – the X pixel positions (fast dimension)

Returns position in meter of the center of each pixels.

Return type `ndarray`

d1 and d2 must have the same shape, returned array will have the same shape.

calc_mask ()

Detectors with gaps should overwrite this method with something actually calculating the mask!

classmethod **factory** (*name, config=None*)

A kind of factory...

Parameters

- **name** (*str*) – name of a detector
- **config** (*dict or JSON representation of it.*) – configuration of the detector

Returns an instance of the right detector, set-up if possible

Return type `pyFAI.detectors.Detector`

force_pixel = False

getFit2D ()

Helper method to serialize the description of a detector using the Fit2d units

Returns representation of the detector easy to serialize

Return type `dict`

getPyFAI ()

Helper method to serialize the description of a detector using the pyFAI way with everything in S.I units.

Returns representation of the detector easy to serialize

Return type dict

get_binning ()

get_mask ()

get_maskfile ()

get_name ()

Get a meaningful name for detector

get_pixel1 ()

get_pixel2 ()

get_pixel_corners ()

Calculate the position of the corner of the pixels

This should be overwritten by class representing non-contiguous detector (Xpad, ...)

Returns 4D array containing: pixel index (slow dimension) pixel index (fast dimension) corner index (A, B, C or D), triangles or hexagons can be handled the same way vertex position (z,y,x)

get_splineFile ()

guess_binning (*data*)

Guess the binning/mode depending on the image shape :param data: 2-tuple with the shape of the image or the image with a .shape attribute.

mask

maskfile

name

Get a meaningful name for detector

pixel1

pixel2

registry = {'imxpads70': <class 'pyFAI.detectors.ImXPadS70'>, 'rayonix_mx225': <class 'pyFAI.detectors.RayonixM

save (*filename*)

Saves the detector description into a NeXus file, adapted from: http://download.nexusformat.org/sphinx/classes/base_classes/NXdetector.html Main differences:

- differentiate pixel center from pixel corner offsets
- store all offsets are ndarray according to slow/fast dimension (not x, y)

Parameters filename – name of the file on the disc

setFit2D (***kwarg*)

Twin method of getFit2D: setup a detector instance according to a description

Parameters kwarg – dictionary containing pixel1, pixel2 and splineFile

setPyFAI (***kwarg*)

Twin method of getPyFAI: setup a detector instance according to a description

Parameters kwarg – dictionary containing detector, pixel1, pixel2 and splineFile

set_binning (*bin_size=(1, 1)*)

Set the “binning” of the detector,

Parameters **bin_size** (*(int, int)*) – binning as integer or tuple of integers.

set_config (*config*)

Sets the configuration of the detector. This implies: - Orientation: integers - Binning - ROI

The configuration is either a python dictionary or a JSON string or a file containing this JSON configuration

keys in that dictionary are : “orientation”: integers from 0 to 7 “binning”: integer or 2-tuple of integers.

If only one integer is provided, “offset”: coordinate (in pixels) of the start of the detector

set_dx (*dx=None*)

set the pixel-wise displacement along X (dim2):

set_dy (*dy=None*)

set the pixel-wise displacement along Y (dim1):

set_mask (*mask*)

set_maskfile (*maskfile*)

set_pixel1 (*value*)

set_pixel2 (*value*)

set_splineFile (*splineFile*)

splineFile

uniform_pixel = True

class pyFAI.detectors.**DetectorMeta** (*name, bases, dct*)

Bases: type

Metaclass used to register all detector classes inheriting from Detector

class pyFAI.detectors.**Dexela2923** (*pixel1=7.5e-05, pixel2=7.5e-05*)

Bases: pyFAI.detectors.Detector

Dexela CMOS family detector

MAX_SHAPE = (3888, 3072)

aliases = ['Dexela 2923']

force_pixel = True

class pyFAI.detectors.**Eiger** (*pixel1=7.5e-05, pixel2=7.5e-05*)

Bases: pyFAI.detectors.Detector

Eiger detector: generic description containing mask algorithm

MODULE_GAP = (37, 10)

MODULE_SIZE = (1065, 1030)

calc_cartesian_positions (*d1=None, d2=None*)

Calculate the position of each pixel center in cartesian coordinate and in meter of a couple of coordinates.

The half pixel offset is taken into account here !!!

Parameters

- **d1** (*ndarray (1D or 2D)*) – the Y pixel positions (slow dimension)
- **d2** (*ndarray (1D or 2D)*) – the X pixel positions (fast dimension)

Returns position in meter of the center of each pixels.

Return type ndarray

d1 and d2 must have the same shape, returned array will have the same shape.

calc_mask ()

Returns a generic mask for Pilatus detectors...

force_pixel = True

class pyFAI.detectors.**Eiger16M** (*pixel1=7.5e-05, pixel2=7.5e-05*)

Bases: pyFAI.detectors.Eiger

Eiger 16M detector

MAX_SHAPE = (4371, 4150)

class pyFAI.detectors.**Eiger1M** (*pixel1=7.5e-05, pixel2=7.5e-05*)

Bases: pyFAI.detectors.Eiger

Eiger 1M detector

MAX_SHAPE = (1065, 1030)

class pyFAI.detectors.**Eiger4M** (*pixel1=7.5e-05, pixel2=7.5e-05*)

Bases: pyFAI.detectors.Eiger

Eiger 4M detector

MAX_SHAPE = (2167, 2070)

class pyFAI.detectors.**Eiger9M** (*pixel1=7.5e-05, pixel2=7.5e-05*)

Bases: pyFAI.detectors.Eiger

Eiger 9M detector

MAX_SHAPE = (3269, 3110)

class pyFAI.detectors.**FReLoN** (*splineFile=None*)

Bases: pyFAI.detectors.Detector

FReLoN detector: The spline is mandatory to correct for geometric distortion of the taper

TODO: create automatically a mask that removes pixels out of the “valid region”

calc_mask ()

Returns a generic mask for Frelon detectors... All pixels which (center) turns to be out of the valid region are by default discarded

class pyFAI.detectors.**Fairchild** (*pixel1=1.5e-05, pixel2=1.5e-05*)

Bases: pyFAI.detectors.Detector

Fairchild Condor 486:90 detector

MAX_SHAPE = (4096, 4096)

aliases = ['Fairchild', 'Condor', 'Fairchild Condor 486:90']

force_pixel = True

uniform_pixel = True

class pyFAI.detectors.**ImXPadS10** (*pixel1=0.00013, pixel2=0.00013*)

Bases: pyFAI.detectors.Detector

ImXPad detector: ImXPad s10 detector with 1x1modules

```
BORDER_SIZE_RELATIVE = 2.5
```

```
MAX_SHAPE = (120, 80)
```

```
MODULE_SIZE = (120, 80)
```

```
PIXEL_SIZE = (0.00013, 0.00013)
```

```
aliases = ['Imxpad S10']
```

```
calc_cartesian_positions (d1=None, d2=None)
```

Calculate the position of each pixel center in cartesian coordinate and in meter of a couple of coordinates. The half pixel offset is taken into account here !!!

Parameters

- **d1** (*ndarray (1D or 2D)*) – the Y pixel positions (slow dimension)
- **d2** (*ndarray (1D or 2D)*) – the X pixel positions (fast dimension)

Returns position in meter of the center of each pixels.

Return type ndarray

d1 and d2 must have the same shape, returned array will have the same shape.

```
calc_mask ()
```

Calculate the mask

```
calc_pixels_edges ()
```

Calculate the position of the pixel edges

```
force_pixel = True
```

```
uniform_pixel = False
```

```
class pyFAI.detectors.ImXPadS140 (pixel1=0.00013, pixel2=0.00013)
```

Bases: pyFAI.detectors.ImXPadS10

ImXPad detector: ImXPad s140 detector with 2x7modules

```
BORDER_PIXEL_SIZE_RELATIVE = 2.5
```

```
MAX_SHAPE = (240, 560)
```

```
MODULE_SIZE = (120, 80)
```

```
PIXEL_SIZE = (0.00013, 0.00013)
```

```
aliases = ['Imxpad S140']
```

```
force_pixel = True
```

```
class pyFAI.detectors.ImXPadS70 (pixel1=0.00013, pixel2=0.00013)
```

Bases: pyFAI.detectors.ImXPadS10

ImXPad detector: ImXPad s70 detector with 1x7modules

```
BORDER_SIZE_RELATIVE = 2.5
```

```
MAX_SHAPE = (120, 560)
```

```
MODULE_SIZE = (120, 80)
```

```
PIXEL_EDGES = None
```

```
PIXEL_SIZE = (0.00013, 0.00013)
```

```
aliases = ['Imxpad S70']
```

force_pixel = True

class pyFAI.detectors.**Mar345** (*pixel1=0.0001, pixel2=0.0001*)

Bases: pyFAI.detectors.Detector

Mar345 Imaging plate detector

In this detector, pixels are always square The valid image size are 2300, 2000, 1600, 1200, 3450, 3000, 2400, 1800

MAX_SHAPE = (3450, 3450)

VALID_SIZE = {2000: 0.00015, 1600: 0.00015, 3000: 0.0001, 2400: 0.0001, 3450: 0.0001, 1200: 0.00015, 2300: 0.00015, 1800: 0.00015}

aliases = ['MAR 345', 'Mar3450']

calc_mask ()

force_pixel = True

guess_binning (data)

Guess the binning/mode depending on the image shape :param data: 2-tuple with the shape of the image or the image with a .shape attribute.

class pyFAI.detectors.**NexusDetector** (*filename=None*)

Bases: pyFAI.detectors.Detector

Class representing a 2D detector loaded from a NeXus file

calc_cartesian_positions (d1=None, d2=None, center=True)

Calculate the position of each pixel center in cartesian coordinate and in meter of a couple of coordinates. The half pixel offset is taken into account here !!! Adapted to Nexus detector definition

Parameters

- **d1** (*ndarray (1D or 2D)*) – the Y pixel positions (slow dimension)
- **d2** (*ndarray (1D or 2D)*) – the X pixel positions (fast dimension)
- **center** – retrieve the coordinate of the center of the pixel

Returns position in meter of the center of each pixels.

Return type ndarray

d1 and d2 must have the same shape, returned array will have the same shape.

get_pixel_corners (use_cython=True)

Calculate the position of the corner of the pixels

This should be overwritten by class representing non-contiguous detector (Xpad, ...)

Returns 4D array containing: pixel index (slow dimension) pixel index (fast dimension) corner index (A, B, C or D), triangles or hexagons can be handled the same way vertex position (z,y,x)

load (filename)

Loads the detector description from a NeXus file, adapted from: http://download.nexusformat.org/sphinx/classes/base_classes/NXdetector.html

Parameters filename – name of the file on the disc

class pyFAI.detectors.**Perkin** (*pixel=0.0002*)

Bases: pyFAI.detectors.Detector

Perkin detector

MAX_SHAPE = (2048, 2048)

aliases = ['Perkin detector']

force_pixel = True

class pyFAI.detectors.**Pilatus** (*pixel1=0.000172, pixel2=0.000172, x_offset_file=None, y_offset_file=None*)

Bases: pyFAI.detectors.Detector

Pilatus detector: generic description containing mask algorithm

Sub-classed by Pilatus1M, Pilatus2M and Pilatus6M

MODULE_GAP = (17, 7)

MODULE_SIZE = (195, 487)

calc_cartesian_positions (*d1=None, d2=None*)

Calculate the position of each pixel center in cartesian coordinate and in meter of a couple of coordinates. The half pixel offset is taken into account here !!!

Parameters

- **d1** (*ndarray (1D or 2D)*) – the Y pixel positions (slow dimension)
- **d2** (*ndarray (1D or 2D)*) – the X pixel positions (fast dimension)

Returns position in meter of the center of each pixels.

Return type ndarray

d1 and d2 must have the same shape, returned array will have the same shape.

calc_mask ()

Returns a generic mask for Pilatus detectors...

force_pixel = True

get_splineFile ()

set_splineFile (*splineFile=None*)

In this case splinefile is a couple filenames

splineFile

class pyFAI.detectors.**Pilatus100k** (*pixel1=0.000172, pixel2=0.000172*)

Bases: pyFAI.detectors.Pilatus

Pilatus 100k detector

MAX_SHAPE = (195, 487)

class pyFAI.detectors.**Pilatus1M** (*pixel1=0.000172, pixel2=0.000172*)

Bases: pyFAI.detectors.Pilatus

Pilatus 1M detector

MAX_SHAPE = (1043, 981)

class pyFAI.detectors.**Pilatus200k** (*pixel1=0.000172, pixel2=0.000172*)

Bases: pyFAI.detectors.Pilatus

Pilatus 200k detector

MAX_SHAPE = (407, 487)

```

class pyFAI.detectors.Pilatus2M(pixel1=0.000172, pixel2=0.000172)
    Bases: pyFAI.detectors.Pilatus
    Pilatus 2M detector
    MAX_SHAPE = (1679, 1475)
class pyFAI.detectors.Pilatus300k(pixel1=0.000172, pixel2=0.000172)
    Bases: pyFAI.detectors.Pilatus
    Pilatus 300k detector
    MAX_SHAPE = (619, 487)
class pyFAI.detectors.Pilatus300kw(pixel1=0.000172, pixel2=0.000172)
    Bases: pyFAI.detectors.Pilatus
    Pilatus 300k-wide detector
    MAX_SHAPE = (195, 1475)
class pyFAI.detectors.Pilatus6M(pixel1=0.000172, pixel2=0.000172)
    Bases: pyFAI.detectors.Pilatus
    Pilatus 6M detector
    MAX_SHAPE = (2527, 2463)
class pyFAI.detectors.Rayonix(pixel1=None, pixel2=None)
    Bases: pyFAI.detectors.Detector
    BINNED_PIXEL_SIZE = {}
    MAX_SHAPE = (4096, 4096)
    binning
    force_pixel = True
    get_binning()
    guess_binning(data)
        Guess the binning/mode depending on the image shape :param data: 2-tuple with the shape of the image
        or the image with a .shape attribute.
    set_binning(bin_size=(1, 1))
        Set the "binning" of the detector,
        Parameters bin_size (int or (int, int)) – set the binning of the detector
class pyFAI.detectors.Rayonix133
    Bases: pyFAI.detectors.Rayonix
    Rayonix 133 2D CCD detector detector also known as mar133
    Personnal communication from M. Blum
    What should be the default binning factor for those cameras ?
    Circular detector
    BINNED_PIXEL_SIZE = {8: 0.000256, 1: 3.2e-05, 2: 6.4e-05, 4: 0.000128}
    MAX_SHAPE = (4096, 4096)
    aliases = ['MAR133']

```

```
calc_mask ()  
    Circular mask
```

```
force_pixel = True
```

```
class pyFAI.detectors.RayonixLx170
```

```
    Bases: pyFAI.detectors.Rayonix
```

```
    Rayonix lx170 2d CCD Detector (2x1 CCDs).
```

```
    Nota: this is the same for lx170hs
```

```
BINNED_PIXEL_SIZE = {1: 4.42708e-05, 2: 8.85417e-05, 3: 0.0001328125, 4: 0.0001770833, 5: 0.0002213542, 6: 0.0002657083}
```

```
MAX_SHAPE = (1920, 3840)
```

```
aliases = ['Rayonix lx170']
```

```
force_pixel = True
```

```
class pyFAI.detectors.RayonixLx255
```

```
    Bases: pyFAI.detectors.Rayonix
```

```
    Rayonix lx255 2d Detector (3x1 CCDs)
```

```
    Nota: this detector is also called lx255hs
```

```
BINNED_PIXEL_SIZE = {1: 4.42708e-05, 2: 8.85417e-05, 3: 0.0001328125, 4: 0.0001770833, 5: 0.0002213542, 6: 0.0002657083}
```

```
MAX_SHAPE = (1920, 5760)
```

```
aliases = ['Rayonix lx225']
```

```
class pyFAI.detectors.RayonixMx170
```

```
    Bases: pyFAI.detectors.Rayonix
```

```
    Rayonix mx170 2d CCD Detector (2x2 CCDs).
```

```
    Nota: this is the same for mx170hs
```

```
BINNED_PIXEL_SIZE = {1: 4.42708e-05, 2: 8.85417e-05, 3: 0.0001328125, 4: 0.0001770833, 5: 0.0002213542, 6: 0.0002657083}
```

```
MAX_SHAPE = (3840, 3840)
```

```
aliases = ['Rayonix mx170']
```

```
class pyFAI.detectors.RayonixMx225
```

```
    Bases: pyFAI.detectors.Rayonix
```

```
    Rayonix mx225 2D CCD detector detector
```

```
    Nota: this is the same definition for mx225he Personal communication from M. Blum
```

```
BINNED_PIXEL_SIZE = {8: 0.000292969, 1: 3.6621e-05, 2: 7.3242e-05, 3: 0.000109971, 4: 0.000146484}
```

```
MAX_SHAPE = (6144, 6144)
```

```
aliases = ['Rayonix mx225']
```

```
force_pixel = True
```

```
class pyFAI.detectors.RayonixMx225hs
```

```
    Bases: pyFAI.detectors.Rayonix
```

```
    Rayonix mx225hs 2D CCD detector detector
```

```
    Pixel size from a personal communication from M. Blum
```

```
BINNED_PIXEL_SIZE = {1: 3.90625e-05, 2: 7.8125e-05, 3: 0.0001171875, 4: 0.00015625, 5: 0.0001953125, 6: 0.000234375}
```

```

MAX_SHAPE = (5760, 5760)
aliases = ['Rayonix mx225hs']
force_pixel = True
class pyFAI.detectors.RayonixMx300
  Bases: pyFAI.detectors.Rayonix
  Rayonix mx300 2D detector (4x4 CCDs)
  Pixel size from a personal communication from M. Blum
BINNED_PIXEL_SIZE = {8: 0.000292969, 1: 3.6621e-05, 2: 7.3242e-05, 3: 0.000109971, 4: 0.000146484}
MAX_SHAPE = (8192, 8192)
aliases = ['Rayonix mx300']
force_pixel = True
class pyFAI.detectors.RayonixMx300hs
  Bases: pyFAI.detectors.Rayonix
  Rayonix mx300hs 2D detector (4x4 CCDs)
  Pixel size from a personal communication from M. Blum
BINNED_PIXEL_SIZE = {1: 3.90625e-05, 2: 7.8125e-05, 3: 0.0001171875, 4: 0.00015625, 5: 0.0001953125, 6: 0.000234375}
MAX_SHAPE = (7680, 7680)
aliases = ['Rayonix mx300hs']
force_pixel = True
class pyFAI.detectors.RayonixMx325
  Bases: pyFAI.detectors.Rayonix
  Rayonix mx325 and mx325he 2D detector (4x4 CCD chips)
  Pixel size from a personal communication from M. Blum
BINNED_PIXEL_SIZE = {8: 0.000317383, 1: 3.9673e-05, 2: 7.9346e-05, 3: 0.000119135, 4: 0.000158691}
MAX_SHAPE = (8192, 8192)
aliases = ['Rayonix mx325']
class pyFAI.detectors.RayonixMx340hs
  Bases: pyFAI.detectors.Rayonix
  Rayonix mx340hs 2D detector (4x4 CCDs)
  Pixel size from a personal communication from M. Blum
BINNED_PIXEL_SIZE = {1: 4.42708e-05, 2: 8.85417e-05, 3: 0.0001328125, 4: 0.0001770833, 5: 0.0002213542, 6: 0.000265729}
MAX_SHAPE = (7680, 7680)
aliases = ['Rayonix mx340hs']
force_pixel = True
class pyFAI.detectors.RayonixMx425hs
  Bases: pyFAI.detectors.Rayonix
  Rayonix mx425hs 2D CCD camera (5x5 CCD chip)
  Pixel size from a personal communication from M. Blum

```

```
BINNED_PIXEL_SIZE = {1: 4.42708e-05, 2: 8.85417e-05, 3: 0.0001328125, 4: 0.0001770833, 5: 0.0002213542, 6: 0.000265625}
```

```
MAX_SHAPE = (9600, 9600)
```

```
aliases = ['Rayonix mx425hs']
```

```
class pyFAI.detectors.RayonixSx165
```

```
    Bases: pyFAI.detectors.Rayonix
```

```
    Rayonix sx165 2d Detector also known as MAR165.
```

```
    Circular detector
```

```
BINNED_PIXEL_SIZE = {8: 0.000316, 1: 3.95e-05, 2: 7.9e-05, 3: 0.000118616, 4: 0.000158}
```

```
MAX_SHAPE = (4096, 4096)
```

```
aliases = ['MAR165', 'Rayonix Sx165']
```

```
calc_mask ()
```

```
    Circular mask
```

```
force_pixel = True
```

```
class pyFAI.detectors.RayonixSx200
```

```
    Bases: pyFAI.detectors.Rayonix
```

```
    Rayonix sx200 2d CCD Detector.
```

```
    Pixel size are personal communication from M. Blum.
```

```
BINNED_PIXEL_SIZE = {8: 0.000384, 1: 4.8e-05, 2: 9.6e-05, 3: 0.000144, 4: 0.000192}
```

```
MAX_SHAPE = (4096, 4096)
```

```
aliases = ['Rayonix sx200']
```

```
class pyFAI.detectors.RayonixSx30hs
```

```
    Bases: pyFAI.detectors.Rayonix
```

```
    Rayonix sx30hs 2D CCD camera (1 CCD chip)
```

```
    Pixel size from a personal communication from M. Blum
```

```
BINNED_PIXEL_SIZE = {1: 1.5625e-05, 2: 3.125e-05, 3: 4.6875e-05, 4: 6.25e-05, 5: 7.8125e-05, 6: 9.375e-05, 8: 0.000125}
```

```
MAX_SHAPE = (1920, 1920)
```

```
aliases = ['Rayonix Sx30hs']
```

```
class pyFAI.detectors.RayonixSx85hs
```

```
    Bases: pyFAI.detectors.Rayonix
```

```
    Rayonix sx85hs 2D CCD camera (1 CCD chip)
```

```
    Pixel size from a personal communication from M. Blum
```

```
BINNED_PIXEL_SIZE = {1: 4.42708e-05, 2: 8.85417e-05, 3: 0.0001328125, 4: 0.0001770833, 5: 0.0002213542, 6: 0.000265625}
```

```
MAX_SHAPE = (1920, 1920)
```

```
aliases = ['Rayonix Sx85hs']
```

```
class pyFAI.detectors.Titan (pixel1=6e-05, pixel2=6e-05)
```

```
    Bases: pyFAI.detectors.Detector
```

```
    Titan CCD detector from Agilent. Mask not handled
```

```
MAX_SHAPE = (2048, 2048)
```

```
aliases = ['Titan 2k x 2k', 'OXD Titan', 'Agilent Titan']
```

```
force_pixel = True
```

```
uniform_pixel = True
```

```
class pyFAI.detectors.Xpad_flat (pixel1=0.00013, pixel2=0.00013)
```

```
Bases: pyFAI.detectors.ImXPadS10
```

Xpad detector: generic description for ImXPad detector with 8x7modules

```
BORDER_PIXEL_SIZE_RELATIVE = 2.5
```

```
MAX_SHAPE = (960, 560)
```

```
MODULE_GAP = (0.00357, 0)
```

```
MODULE_SIZE = (120, 80)
```

```
PIXEL_SIZE = (0.00013, 0.00013)
```

```
aliases = ['Xpad S540 flat']
```

```
calc_cartesian_positions (d1=None, d2=None, center=True)
```

Calculate the position of each pixel center in cartesian coordinate and in meter of a couple of coordinates. The half pixel offset is taken into account here !!! Adapted to Nexus detector definition

Parameters

- **d1** (*ndarray (1D or 2D)*) – the Y pixel positions (slow dimension)
- **d2** (*ndarray (1D or 2D)*) – the X pixel positions (fast dimension)
- **center** – retrieve the coordinate of the center of the pixel

Returns position in meter of the center of each pixels.

Return type ndarray

d1 and d2 must have the same shape, returned array will have the same shape.

```
calc_mask ()
```

Returns a generic mask for Xpad detectors... discards the first line and raw form all modules: those are 2.5x bigger and often mis - behaving

```
force_pixel = True
```

```
get_pixel_corners ()
```

Calculate the position of the corner of the pixels

Returns 4D array containing: pixel index (slow dimension) pixel index (fast dimension) corner index (A, B, C or D), triangles or hexagons can be handled the same way vertex position (z,y,x)

```
uniform_pixel = False
```

3.7 spline Module

This is piece of software aims at manipulating spline files describing for geometric corrections of the 2D detectors using cubic-spline.

Mainly used at ESRF with FReLoN CCD camera.

class `pyFAI.spline.Spline` (*filename=None*)

Bases: `object`

This class is a python representation of the spline file

Those file represent cubic splines for 2D detector distortions and makes heavy use of fitpack (dierckx in netlib) — A Python-C wrapper to FITPACK (by P. Dierckx). FITPACK is a collection of FORTRAN programs for curve and surface fitting with splines and tensor product splines. See [_http://www.cs.kuleuven.ac.be/cwis/research/nalag/research/topics/fitpack.html](http://www.cs.kuleuven.ac.be/cwis/research/nalag/research/topics/fitpack.html) or [_http://www.netlib.org/dierckx/index.html](http://www.netlib.org/dierckx/index.html)

array2spline (*smoothing=1000, timing=False*)

Calculates the spline coefficients from the displacements matrix using fitpack.

Parameters

- **smoothing** (*float*) – the greater the smoothing, the fewer the number of knots remaining
- **timing** (*bool*) – print the profiling of the calculation

bin (*binning=None*)

Performs the binning of a spline (same camera with different binning)

Parameters **binning** – binning factor as integer or 2-tuple of integers

Type `int` or `(int, int)`

comparison (*ref, verbose=False*)

Compares the current spline distortion with a reference

Parameters

- **ref** (*Spline instance*) – another spline file
- **verbose** (*bool*) – print or not pylab plots

Returns `True` or `False` depending if the splines are the same or not

Return type `bool`

correct (*pos*)

getPixelSize ()

Return the size of the pixel from as a 2-tuple of floats expressed in meters.

Returns the size of the pixel from a 2D detector

Return type 2-tuple of floats expressed in meter.

read (*filename*)

read an ascii spline file from file

Parameters **filename** (*str*) – file containing the cubic spline distortion file

setPixelSize (*pixelSize*)

Sets the size of the pixel from a 2-tuple of floats expressed in meters.

Param pixel size in meter

spline2array (*timing=False*)

Calculates the displacement matrix using fitpack `bisplev(x, y, tck, dx = 0, dy = 0)`

Parameters **timing** (*bool*) – profile the calculation or not

Returns Nothing !

Return type `float` or `ndarray`

Evaluate a bivariate B-spline and its derivatives. Return a rank-2 array of spline function values (or spline derivative values) at points given by the cross-product of the rank-1 arrays x and y. In special cases, return an array or just a float if either x or y or both are floats.

splineFuncX (*x*, *y*)

Calculates the displacement matrix using fitpack for the X direction on the given grid.

Parameters

- **x** (*ndarray*) – points of the grid in the x direction
- **y** (*ndarray*) – points of the grid in the y direction

Returns displacement matrix for the X direction

Return type ndarray

splineFuncY (*x*, *y*)

calculates the displacement matrix using fitpack for the Y direction

Parameters

- **x** (*ndarray*) – points in the x direction
- **y** (*ndarray*) – points in the y direction

Returns displacement matrix for the Y direction

Return type ndarray

tilt (*center=(0.0, 0.0)*, *tiltAngle=0.0*, *tiltPlanRot=0.0*, *distanceSampleDetector=1.0*, *timing=False*)

The tilt method apply a virtual tilt on the detector, the point of tilt is given by the center

Parameters

- **center** (*2-tuple of floats*) – position of the point of tilt, this point will not be moved.
- **tiltAngle** (*float in the range [-90:+90] degrees*) – the value of the tilt in degrees
- **tiltPlanRot** (*Float in the range [-180:180]*) – the rotation of the tilt plan with the Ox axis (0 deg for y axis invariant, 90 deg for x axis invariant)
- **distanceSampleDetector** (*float*) – the distance from sample to detector in meter (along the beam, so distance from sample to center)

Returns tilted Spline instance

Return type Spline

write (*filename*)

save the cubic spline in an ascii file usable with Fit2D or SPD

Parameters **filename** (*str*) – name of the file containing the cubic spline distortion file

writeEDF (*basename*)

save the distortion matrices into a couple of files called *basename-x.edf* and *basename-y.edf*

Parameters **basename** (*str*) – base of the name used to save the data

zeros (*xmin=0.0*, *ymin=0.0*, *xmax=2048.0*, *ymax=2048.0*, *pixSize=None*)

Defines a spline file with no (zero) displacement.

Parameters

- **xmin** (*float*) – minimum coordinate in x, usually zero
- **xmax** (*float*) – maximum coordinate in x (+1) usually 2048

- **ymin** (*float*) – minimum coordinate in y, usually zero
- **ymax** (*float*) – maximum coordinate y (+1) usually 2048
- **pixSize** (*float*) – size of the pixel

zeros_like (*other*)

Defines a spline file with no (zero) displacement with the same shape as the other one given.

Parameters *other* (*Spline instance*) – another Spline instance

`pyFAI.spline.main()`

Some tests

3.8 openc1 Module

class `pyFAI.openc1.Device` (*name='None', dtype=None, version=None, driver_version=None, extensions='', memory=None, available=None, cores=None, frequency=None, flop_core=None, idx=0*)

Bases: `object`

Simple class that contains the structure of an OpenCL device

pretty_print ()

Complete device description

Returns string

class `pyFAI.openc1.OpenCL`

Bases: `object`

Simple class that wraps the structure `ocl_tools_extended.h`

comput_cap = (2, 1)

create_context (*devicetype='ALL', useFp64=False, platformid=None, deviceid=None*)

Choose a device and initiate a context.

Devicetypes can be GPU,gpu,CPU,cpu,DEF,ACC,ALL. Suggested are GPU,CPU. For each setting to work there must be such an OpenCL device and properly installed. E.g.: If Nvidia driver is installed, GPU will succeed but CPU will fail. The AMD SDK kit is required for CPU via OpenCL. :param devicetype: string in ["cpu","gpu", "all", "acc"] :param useFp64: boolean specifying if double precision will be used :param platformid: integer :param devid: integer :return: OpenCL context on the selected device

flop_core = 4

get_platform (*key*)

Return a platform according

Parameters *key* (*int or str*) – identifier for a platform, either an Id (int) or it's name

idd = 0

idx = 2

platforms = [Intel(R) OpenCL, NVIDIA CUDA, AMD Accelerated Parallel Processing]

select_device (*dtype='ALL', memory=None, extensions=[], best=True, **kwargs*)

Select a device based on few parameters (at the end, keep the one with most memory)

Parameters

- **type** – “gpu” or “cpu” or “all”

- **memory** – minimum amount of memory (int)
- **extensions** – list of extensions to be present
- **best** – shall we look for the

```
class pyFAI.opencl.Platform (name='None', vendor='None', version=None, extensions=None,  
                             idx=0)
```

Bases: object

Simple class that contains the structure of an OpenCL platform

add_device (*device*)

get_device (*key*)

Return a device according to key

Parameters *key* (*int or str*) – identifier for a device, either it's id (int) or it's name

3.9 ocl_azim Module

C++ less implementation of Dimitris' code based on PyOpenCL

TODO and trick from dimitris still missing:

- dark-current subtraction is still missing
- In fact you might want to consider doing the conversion on the GPU when possible. Think about it, you have a uint16 to float which for large arrays was slow.. You load on the graphic card a uint16 (2x transfer speed) and you convert to float inside so it should be blazing fast.

```
class pyFAI.ocl_azim.Integrator1d (filename=None)
```

Bases: object

Attempt to implements ocl_azim using pyopencl

clean (*preserve_context=False*)

Free OpenCL related resources allocated by the library.

clean() is used to reinitiate the library back in a vanilla state. It may be asked to preserve the context created by init or completely clean up OpenCL. Guard/Status flags that are set will be reset.

Parameters *preserve_context* (*bool*) – preserves or destroys all OpenCL resources

configure (*kernel=None*)

The method configure() allocates the OpenCL resources required and compiled the OpenCL kernels. An active context must exist before a call to configure() and getConfiguration() must have been called at least once. Since the compiled OpenCL kernels carry some information on the integration parameters, a change to any of the parameters of getConfiguration() requires a subsequent call to configure() for them to take effect.

If a configuration exists and configure() is called, the configuration is cleaned up first to avoid OpenCL memory leaks

Parameters *kernel_path* – is the path to the actual kernel

execute (*image*)

Perform a 1D azimuthal integration

execute() may be called only after an OpenCL device is configured and a Tth array has been loaded (at least once) It takes the input image and based on the configuration provided earlier it performs the 1D integration. Notice that if the provided image is bigger than N then only N points will be taken into account,

while if the image is smaller than N the result may be catastrophic. `set/unset` and `loadTth` methods have a direct impact on the `execute()` method. All the rest of the methods will require at least a new configuration via `configure()`.

Takes an image, integrate and return the histogram and weights

Parameters `image` – image to be processed as a numpy array

Returns `tth_out`, histogram, bins

TODO: to improve performances, the image should be casted to float32 in an optimal way: currently using numpy machinery but would be better if done in OpenCL

getConfiguration (*Nimage, Nbins, useFp64=None*)

`getConfiguration` gets the description of the integrations to be performed and keeps an internal copy

Parameters

- **Nimage** – number of pixel in image
- **Nbins** – number of bins in regrouped histogram
- **useFp64** – use double precision. By default the same as `init!`

get_status ()

return a dictionary with the status of the integrator: for compatibilty with former implementation

init (*devicetype='GPU', useFp64=True, platformid=None, deviceid=None*)

Initial configuration: Choose a device and initiate a context. Devicetypes can be GPU, gpu, CPU, cpu, DEF, ACC, ALL. Suggested are GPU,CPU. For each setting to work there must be such an OpenCL device and properly installed. E.g.: If Nvidia driver is installed, GPU will succeed but CPU will fail. The AMD SDK kit (AMD APP) is required for CPU via OpenCL.

Parameters

- **devicetype** – string in [”cpu”,”gpu”, “all”, “acc”]
- **useFp64** – boolean specifying if double precision will be used
- **platformid** – integer
- **devid** – integer

loadTth (*tth, dtth, tth_min=None, tth_max=None*)

Load the 2th arrays along with the min and max value.

`loadTth` maybe be recalled at any time of the execution in order to update the 2th arrays.

`loadTth` is required and must be called at least once after a `configure()`

log (***kwarg*)

log in a file all opencl events

setDummyValue (*dummy, delta_dummy*)

Enables dummy value functionality and uploads the value to the OpenCL device.

Image values that are similar to the dummy value are set to 0.

Parameters

- **dummy** – value in image of missing values (masked pixels?)
- **delta_dummy** – precision for dummy values

setMask (*mask*)

Enables the use of a Mask during integration. The Mask can be updated by recalling `setMask` at any point.

The Mask must be a PyFAI Mask. Pixels with 0 are masked out. TODO: check and invert!

Parameters **mask** – numpy.ndarray of integer.

setRange (*lowerBound*, *upperBound*)

Instructs the program to use a user - defined range for 2th values

setRange is optional. By default the integration will use the `tth_min` and `tth_max` given by `loadTth()` as integration range. When `setRange` is called it sets a new integration range without affecting the 2th array. All values outside that range will then be discarded when interpolating. Currently, if the interval of 2th (`2th + -d2th`) is not all inside the range specified, it is discarded. The bins of the histogram are RESCALED to the defined range and not the original `tth_max - tth_min` range.

`setRange` can be called at any point and as many times required after a valid configuration is created.

Parameters

- **lowerBound** (*float*) – lower bound of the integration range
- **upperBound** (*float*) – upper bound of the integration range

setSolidAngle (*solidAngle*)

Enables SolidAngle correction and uploads the suitable array to the OpenCL device.

By default the program will assume no solidangle correction unless `setSolidAngle()` is called. From then on, all integrations will be corrected via the SolidAngle array.

If the SolidAngle array needs to be changes, one may just call `setSolidAngle()` again with that array

Parameters **solidAngle** (*ndarray*) – the solid angle of the given pixel

unsetDummyValue ()

Disable a dummy value. May be re-enabled at any time by `setDummyValue`

unsetMask ()

Disables the use of a Mask from that point. It may be re-enabled at any point via `setMask`

unsetRange ()

Disable the use of a user-defined 2th range and revert to `tth_min,tth_max` range

`unsetRange` instructs the program to revert to its default integration range. If the method is called when no user-defined range had been previously specified, no action will be performed

unsetSolidAngle ()

Instructs the program to not perform solidangle correction from now on.

SolidAngle correction may be turned back on at any point

3.10 ocl_azim_lut Module

```
class pyFAI.ocl_azim_lut.OCL_LUT_Integrator(lut, image_size, devicetype='all', platformid=None, deviceid=None, checksum=None, profile=False)
```

Bases: object

```
integrate(data, dummy=None, delta_dummy=None, dark=None, flat=None, solidAngle=None, polarization=None, dark_checksum=None, flat_checksum=None, solidAngle_checksum=None, polarization_checksum=None, preprocess_only=False)
```

```
log_profile()
```

If we are in profiling mode, prints out all timing for every single OpenCL call

3.11 ocl_azim_csr Module

```
class pyFAI.ocl_azim_csr.OCL_CSR_Integrator(lut, image_size, devicetype='all',
                                             block_size=32, platformid=None, deviceid=None, checksum=None, profile=False)
```

Bases: object

```
integrate(data, dummy=None, delta_dummy=None, dark=None, flat=None, solidAngle=None, polarization=None, dark_checksum=None, flat_checksum=None, solidAngle_checksum=None, polarization_checksum=None)
```

```
log_profile()
```

If we are in profiling mode, prints out all timing for every single OpenCL call

3.12 ocl_azim_csr_dis Module

```
class pyFAI.ocl_azim_csr_dis.OCL_CSR_Integrator(lut, image_size, devicetype='all',
                                                block_size=32, platformid=None, deviceid=None, checksum=None, profile=False)
```

Bases: object

```
integrate(data, dummy=None, delta_dummy=None, dark=None, flat=None, solidAngle=None, polarization=None, dark_checksum=None, flat_checksum=None, solidAngle_checksum=None, polarization_checksum=None)
```

```
log_profile()
```

If we are in profiling mode, prints out all timing for every single OpenCL call

3.13 worker Module

This module contains the Worker class:

A tool able to perform azimuthal integration with: additional saving capabilities like - save as 2/3D structure in a HDF5 File - read from HDF5 files

Aims at being integrated into a plugin like LImA or as model for the GUI

The configuration of this class is mainly done via a dictionary transmitted as a JSON string: Here are the valid keys:

“dist”, “poni1”, “poni2”, “rot1” “rot3” “rot2” “pixel1” “pixel2”

“splineFile” “wavelength”

“poni” #path of the file

“chi_discontinuity_at_0” “do_mask” “do_dark” “do_azimuthal_range” “do_flat” “do_2D” “azimuth_range_min” “azimuth_range_max”

“polarization_factor” “nbpt_rad” “do_solid_angle” “do_radial_range” “do_poisson” “delta_dummy” “nbpt_azim” “flat_field” “radial_range_min” “dark_current” “do_polarization” “mask_file” “detector” “unit” “radial_range_max” “val_dummy” “do_dummy” “method”

```
}
```

```

class pyFAI.worker.PixelwiseWorker (dark=None, flat=None, solidangle=None, polariza-
                                     tion=None, mask=None, dummy=None, delta_dummy=None,
                                     device=None)

    Bases: object

    Simple worker doing dark, flat, solid angle and polarization correction

    process (data, normalization=None)
        Process the data and apply a normalization factor :param data: input data :param normalization: normal-
        ization factor :return processed data

class pyFAI.worker.Worker (azimuthalIntegrator=None, shapeIn=(2048, 2048), shapeOut=(360, 500),
                            unit='r_mm')

    Bases: object

    do_2D ()

    get_config ()
        return configuration as a dictionary

    get_json_config ()
        return configuration as a JSON string

    get_unit ()

    process (data)
        Process a frame #TODO: dark, flat, sa are missing

        Param data: numpy array containing the input image

    reconfig (shape=(2048, 2048), sync=False)
        This is just to force the integrator to initialize with a given input image shape

        Parameters
            • shape – shape of the input image
            • sync – return only when synchronized

    reset ()
        this is just to force the integrator to initialize

    save_config (filename=None)

    setDarkcurrentFile (imagefile)

    setExtension (ext)
        enforce the extension of the processed data file written

    setFlatfieldFile (imagefile)

    setJsonConfig (jsonconfig)

    setSubdir (path)
        Set the relative or absolute path for processed data

    set_normalization_factor (value)

    set_unit (value)

    unit

    warmup (sync=False)
        Process a dummy image to ensure everything is initialized

        Parameters sync – wait for processing to be finished

```

3.14 io Module

Module for “high-performance” writing in either 1D with Ascii , or 2D with FabIO or even nD with n varying from 2 to 4 using HDF5

Stand-alone module which tries to offer interface to HDF5 via H5Py and capabilities to write EDF or other formats using fabio.

Can be imported without h5py but then limited to fabio & ascii formats.

TODO: * add monitor to HDF5

```
class pyFAI.io.AsciiWriter (filename=None, prefix='fai_', extension='.dat')
```

Bases: pyFAI.io.Writer

Ascii file writer (.xy or .dat)

```
init (fai_cfg=None, lima_cfg=None)
```

Creates the directory that will host the output file(s)

```
write (data, index=0)
```

```
class pyFAI.io.FabioWriter (filename=None)
```

Bases: pyFAI.io.Writer

Image file writer based on FabIO

TODO !!!

```
init (fai_cfg=None, lima_cfg=None)
```

Creates the directory that will host the output file(s)

```
write (data, index=0)
```

```
class pyFAI.io.HDF5Writer (filename, hpath='data', fast_scan_width=None)
```

Bases: pyFAI.io.Writer

Class allowing to write HDF5 Files.

```
CONFIG = 'pyFAI'
```

```
DATASET_NAME = 'data'
```

```
close ()
```

```
flush (radial=None, azimuthal=None)
```

Update some data like axis units and so on.

Parameters

- **radial** – position in radial direction
- **azimuthal** – position in azimuthal direction

```
init (fai_cfg=None, lima_cfg=None)
```

Initializes the HDF5 file for writing :param fai_cfg: the configuration of the worker as a dictionary

```
write (data, index=0)
```

Minimalistic method to limit the overhead. :param data: array with intensities or tuple (2th,I) or (I,2th,chi)

```
class pyFAI.io.Nexus (filename, mode='r')
```

Bases: object

Writer class to handle Nexus/HDF5 data Manages: entry

pyFAI-subentry detector

#TODO: make it thread-safe !!!

close ()

close the filename and update all entries

find_detector (*all=False*)

Tries to find a detector within a NeXus file, takes the first compatible detector

Parameters **all** – return all detectors found as a list

get_class (*grp, class_type='NXcollection'*)

return all sub-groups of the given type within a group

Parameters

- **grp** – HDF5 group
- **class_type** – name of the NeXus class

get_data (*grp, class_type='NXdata'*)

return all dataset of the the NeXus class NXdata

Parameters

- **grp** – HDF5 group
- **class_type** – name of the NeXus class

get_entries ()

retrieves all entry sorted the latest first.

Returns list of HDF5 groups

get_entry (*name*)

Retrieves an entry from its name

Parameters **name** – name of the entry to retrieve

Returns HDF5 group of NXclass == NXentry

new_class (*grp, name, class_type='NXcollection'*)

create a new sub-group with type class_type :param grp: parent group :param name: name of the sub-group
:param class_type: NeXus class name :return: subgroup created

new_detector (*name='detector', entry='entry', subentry='pyFAI'*)

Create a new entry/pyFAI/Detector

Parameters

- **detector** – name of the detector
- **entry** – name of the entry
- **subentry** – all pyFAI description of detectors should be in a pyFAI sub-entry

new_entry (*entry='entry'*)

Create a new entry

Parameters **entry** – name of the entry

Returns the corresponding HDF5 group

new_instrument (*entry='entry', instrument_name='id00'*)

Create an instrument in an entry or create both the entry and the instrument if

class `pyFAI.io.Writer` (*filename=None, extension=None*)

Bases: `object`

Abstract class for writers.

CONFIG_ITEMS = ['filename', 'dirname', 'extension', 'subdir', 'hpath']

flush (**arg, **kwarg*)

To be implemented

init (*fai_cfg=None, lima_cfg=None*)

Creates the directory that will host the output file(s) :param `fai_cfg`: configuration for worker :param `lima_cfg`: configuration for acquisition

setJsonConfig (*json_config=None*)

Sets the JSON configuration

write (*data*)

To be implemented

`pyFAI.io.from_isotime` (*text, use_tz=False*)

Parameters `text` – string representing the time in iso format

`pyFAI.io.get_isotime` (*forceTime=None*)

Parameters `forceTime` (*float*) – enforce a given time (current by default)

Returns the current time as an ISO8601 string

Return type string

`pyFAI.io.is_hdf5` (*filename*)

Check if a file is actually a HDF5 file

Parameters `filename` – this file has better to exist

3.15 calibration Module

`pyFAI-calib`

A tool for determining the geometry of a detector using a reference sample.

class `pyFAI.calibration.AbstractCalibration` (*dataFiles=None, darkFiles=None, flatFiles=None, pixelSize=None, splineFile=None, detector=None, wavelength=None, calibrant=None*)

Bases: `object`

Everything that is common to Calibration and Recalibration

HELP = {'set': "set the value of a parameter to the given value, i.e 'set wavelength 1e-10'", 'help': "Try to get the help of a"}

PARAMETERS = ['dist', 'poni1', 'poni2', 'rot1', 'rot2', 'rot3', 'wavelength']

UNITS = {'poni1': 'meter', 'poni2': 'meter', 'rot1': 'radian', 'rot3': 'radian', 'rot2': 'radian', 'wavelength': 'meter', 'dist': 'meter'}

analyse_options (*options=None, args=None*)

Analyse options and arguments

Returns option,arguments

configure_parser (*version='calibration from pyFAI version 0.10.0: 2014-10', usage='pyFAI-calib [options] input_image.edf', description=None, epilog=None*)
Common configuration for parsers

extract_cpt (*method='massif'*)
Performs an automatic keypoint extraction: Can be used in recalib or in calib after a first calibration has been performed

get_pixelSize (*ans*)
convert a comma separated sting into pixel size

postProcess ()
Common part: shows the result of the azimuthal integration in 1D and 2D

preprocess ()
Common part: do dark, flat correction thresholding, ... and read missing data from keyboard if needed

prompt ()
prompt for commands to guide the calibration process

Returns True when the user is happy with what he has, False to request another refinement

read_dSpacingFile (*verbose=True*)
Read the name of the calibrant / file with d-spacing

read_pixelsSize ()
Read the pixel size from prompt if not available

read_wavelength ()
Read the wavelength

refine ()
Contains the common geometry refinement part

set_data (*data*)
call-back function for the peak-picker

validate_calibration ()
Validate the calivration and calculate the offset in the diffraction image

win_error = 'We are under windows, matplotlib is not able to display too many images without crashing, this is why the'

class pyFAI.calibration.**Calibration** (*dataFiles=None, darkFiles=None, flatFiles=None, pixelSize=None, splineFile=None, detector=None, gaussianWidth=None, wavelength=None, calibrant=None*)
Bases: pyFAI.calibration.AbstractCalibration
class doing the calibration of frames

gui_peakPicker ()

parse ()
parse options from command line

preprocess ()
do dark, flat correction thresholding, ...

refine ()
Contains the geometry refinement part specific to Calibration

class pyFAI.calibration.**CheckCalib** (*poni=None, img=None, unit='2th_deg'*)
Bases: object

get_1dsize ()

integrate ()

parse ()

rebuild ()

Rebuild the diffraction image and measures the offset with the reference :return: offset

show ()

Show the image with the the errors

sizeId

smooth_mask (hwhm=5)

smooth out around the mask to avoid aligning on the mask

class pyFAI.calibration.**MultiCalib** (*dataFiles=None, darkFiles=None, flatFiles=None, pixelSize=None, splineFile=None, detector=None*)

Bases: object

get_pixelSize (ans)

convert a comma separated sting into pixel size

parse ()

parse options from command line

process ()

read_dSpacingFile ()

Read the name of the calibrant or the file with d-spacing

read_pixelsSize ()

Read the pixel size from prompt if not available

read_wavelength ()

Read the wavelength

regression ()

class pyFAI.calibration.**Recalibration** (*dataFiles=None, darkFiles=None, flatFiles=None, pixelSize=None, splineFile=None, detector=None, wavelength=None, calibrant=None*)

Bases: pyFAI.calibration.AbstractCalibration

class doing the re-calibration of frames

parse ()

parse options from command line

preprocess ()

do dark, flat correction thresholding, ...

read_dSpacingFile ()

Read the name of the file with d-spacing

refine ()

Contains the geometry refinement part specific to Recalibration

pyFAI.calibration.**get_detector** (*detector, datafiles=None*)

Detector factory taking into account the binning knowing the datafiles :param detector: string or detector or other junk :param datafiles: can be a list of images to be opened and their shape used. :return pyFAI.detector.Detector instance

3.16 peak_picker Module

class `pyFAI.peak_picker.ControlPoints` (*filename=None, calibrant=None, wavelength=None*)

Bases: `object`

This class contains a set of control points with (optionally) their ring number hence d-spacing and diffraction 2Theta angle ...

append (*points, angle=None, ring=None*)

Parameters

- **point** – list of points
- **angle** – 2-theta angle in radians

append_2theta_deg (*points, angle=None, ring=None*)

Parameters

- **point** – list of points
- **angle** – 2-theta angle in degrees

check ()

check internal consistency of the class

dSpacing

getList ()

Retrieve the list of control points suitable for geometry refinement with ring number

getList2theta ()

Retrieve the list of control points suitable for geometry refinement

getListRing ()

Retrieve the list of control points suitable for geometry refinement with ring number

getWeightedList (*image*)

Retrieve the list of control points suitable for geometry refinement with ring number and intensities :param image: :return: a (x,4) array with pos0, pos1, ring nr and intensity

get_dSpacing ()

get_wavelength ()

load (*filename*)

load all control points from a file

load_dSpacing (**arg, **kw*)

decorator that deprecates the use of a function

pop (*idx=None*)

Remove the set of points at given index (by default the last)

Parameters **idx** – number of the ring to remove

readAngleFromKeyboard ()

Ask the 2theta values for the given points

readRingNrFromKeyboard ()

Ask the ring number values for the given points

reset ()

remove all stored values and resets them to default

save (*filename*)
 Save a set of control points to a file :param filename: name of the file :return: None

save_dSpacing (**arg, **kw*)
 decorator that deprecates the use of a function

setWavelength_change2th (*value=None*)

setWavelength_changeDs (*value=None*)
 This is probably not a good idea, but who knows !

set_dSpacing (*lst*)

set_wavelength (*value=None*)

wavelength

class pyFAI.peak_picker.**PeakPicker** (*strFilename, reconst=False, mask=None, pointfile=None, calibrant=None, wavelength=None, method='massif'*)

Bases: object

This class is in charge of peak picking, i.e. find bragg spots in the image Two methods can be used : massif or blob

VALID_METHODS = ['massif', 'blob']

closeGUI ()

contour (*data*)
 Overlay a contour-plot

Parameters data – 2darray with the 2theta values in radians...

display_points (*minIndex=0*)
 display all points and their ring annotations :param minIndex: ring index to start with

finish (*filename=None, callback=None*)
 Ask the ring number for the given points

Parameters filename – file with the point coordinates saved

gui (*log=False, maximize=False, pick=True*)

Parameters log – show z in log scale

init (*method, sync=True*)
 Unified initializer

init_blob (*sync=True*)
 Initialize PeakPicker for blob based detection

init_massif (*sync=True*)
 Initialize PeakPicker for massif based detection

load (*filename*)
 load a filename and plot data on the screen (if GUI)

massif_contour (*data*)
 Overlays a mask over a diffraction image

Parameters data – mask to be overlaid

on_minus_pts_clicked (**args*)
 callback function

on_option_clicked (**args*)
 callback function

on_plus_pts_clicked (*args)
callback function

on_refine_clicked (*args)
callback function

onclick (event)

peaks_from_area (mask, Imin, keep=1000, refine=True, method=None)
Return the list of peaks within an area

Parameters

- **mask** – 2d array with mask.
- **Imin** – minimum of intensity above the background to keep the point
- **keep** – maximum number of points to keep
- **method** – enforce the use of detection using “massif” or “blob”

Returns list of peaks [y,x], [y,x], ...]

reset ()
Reset control point and graph (if needed)

sync_init ()

3.17 massif Module

class pyFAI.massif.Massif (data=None)

Bases: object

A massif is defined as an area around a peak, it is used to find neighbouring peaks

calculate_massif (x)
defines a map of the massif around x and returns the mask

delValleySize ()

find_peaks (x, nmax=200, annotate=None, massif_contour=None, stdout=<open file '<stdout>', mode 'w' at 0x7fb2185381e0>)

All in one function that finds a maximum from the given seed (x) then calculates the region extension and extract position of the neighboring peaks. :param x: seed for the calculation, input coordinates :param nmax: maximum number of peak per region :param annotate: call back method taking number of points + coordinate as input. :param massif_contour: callback to show the contour of a massif with the given index. :param stdout: this is the file where output is written by default. :return: list of peaks

getBinnedData ()
:return binned data

getBlurredData ()

Returns a blurred image

getLabeledMassif (pattern=None)

Returns an image composed of int with a different value for each massif

getMedianData ()

Returns a spacial median filtered image

getValleySize ()

initValleySize ()

nearest_peak (*x*)

Parameters *x* – coordinates of the peak

:returns the coordinates of the nearest peak

peaks_from_area (*mask*, *Imin=None*, *keep=1000*, ***kwarg*)

Return the list of peaks within an area

Parameters

- **mask** – 2d array with mask.
- **Imin** – minimum of intensity above the background to keep the point
- **keep** – maximum number of points to keep
- **kwarg** – ignored parameters

Returns list of peaks [*y,x*], [*y,x*], ...]

setValleySize (*size*)

valley_size

Defines the minimum distance between two massifs

3.18 blob_detection Module

class pyFAI.blob_detection.**BlobDetection** (*img*, *cur_sigma=0.25*, *init_sigma=0.5*, *dest_sigma=1*, *scale_per_octave=2*, *mask=None*)

Bases: object

Performs a blob detection: http://en.wikipedia.org/wiki/Blob_detection using a Difference of Gaussian + Pyramid of Gaussians

direction ()

Perform and plot the two main directions of the peaks, considering their previously calculated scale ,by calculating the Hessian at different sizes as the combination of gaussians and their first and second derivatives

nearest_peak (*p*, *refine=True*, *Imin=None*)

Return the nearest peak from a position

Parameters

- **p** – input position (*y,x*) 2-tuple of float
- **refine** – shall the position be refined on the raw data
- **Imin** – minimum of intensity above the background

peaks_from_area (*mask*, *keep=None*, *refine=True*, *Imin=None*, ***kwargs*)

Return the list of peaks within an area

Parameters

- **mask** – 2d array with mask.
- **refine** – shall the position be refined on the raw data
- **Imin** – minimum of intensity above the background
- **kwarg** – ignored parameters

Returns list of peaks [y,x], [y,x], ...]

process (*max_octave=None*)

Perform the keypoint extraction for max_octave cycles or until all octaves have been processed. :param max_octave: number of octave to process

refine_Hessian (*kpx, kpy, kps*)

Refine the keypoint location based on a 3 point derivative, and delete uncoherent keypoints

Parameters

- **kpx** – x_pos of keypoint
- **kpy** – y_pos of keypoint
- **kps** – s_pos of keypoint

:return arrays of corrected coordinates of keypoints, values and locations of keypoints

refine_Hessian_SG (*kpx, kpy, kps*)

Savitzky Golay algorithm to check if a point is really the maximum :param kpx: x_pos of keypoint :param kpy: y_pos of keypoint :param kps: s_pos of keypoint :return array of corrected keypoints

refinement ()

show_neighbor ()

show_stats ()

Shows a window with the repartition of keypoint in function of scale/intensity

tresh = 0.6

pyFAI.blob_detection.**image_test** ()

pyFAI.blob_detection.**local_max** (*dogs, mask=None, n_5=True*)

Parameters **dogs** – 3d array with (sigma,y,x) containing difference of gaussians

@parm **mask**: mask out keypoint next to the mask (or inside the mask) :param **n_5**: look for a larger neighborhood

pyFAI.blob_detection.**make_gaussian** (*im, sigma, xc, yc*)

3.19 calibrant Module

Calibrant

A module containing classical calibrant and also tools to generate d-spacing.

class pyFAI.calibrant.**Calibrant** (*filename=None, dSpacing=None, wavelength=None*)

Bases: object

A calibrant is a reference compound where the d-spacing (interplanar distances) are known. They are expressed in Angstrom (in the file)

append_2th (*value*)

append_dSpacing (*value*)

dSpacing

fake_calibration_image (*ai, shape=None, Imax=1.0, U=0, V=0, W=0.0001*)

Generates a fake calibration image from an azimuthal integrator

Parameters

- **ai** – azimuthal integrator
- **Imax** – maximum intensity of rings
- **V, W (U,)** – width of the peak ($FWHM = U \tan(\theta)^2 + V \tan(\theta) + W$)

get_2th ()

get_2th_index (*angle*)

return the index in the 2theta angle index

get_dSpacing ()

get_wavelength ()

load_file (*filename=None*)

save_dSpacing (*filename=None*)

save the d-spacing to a file

setWavelength_change2th (*value=None*)

setWavelength_changeDs (*value=None*)

This is probably not a good idea, but who knows !

set_dSpacing (*lst*)

set_wavelength (*value=None*)

wavelength

class pyFAI.calibrant.**calibrant_factory** (*basedir=None*)

Bases: object

Behaves like a dict but is actually a factory: Each time one retrieves an object it is a new genuine new calibrant (unmodified)

get (*what, notfound=None*)

has_key (*k*)

items ()

keys ()

values ()

3.20 distortion Module

class pyFAI.distortion.**Distortion** (*detector='detector', shape=None, method='LUT', device=None, workgroup=8*)

Bases: object

This class applies a distortion correction on an image.

New version compatible both with CSR and LUT...

calc_LUT (**arg, **kw*)

calc_init ()

initialize all arrays

calc_pos (**arg, **kw*)

calc_size (*arg, **kw)

Considering the “half-CCD” spline from ID11 which describes a (1025,2048) detector, the physical location of pixels should go from: [-17.48634 : 1027.0543, -22.768829 : 2028.3689] We chose to discard pixels falling outside the [0:1025,0:2048] range with a lose of intensity

correct (image)

Correct an image based on the look-up table calculated ...

Parameters **image** – 2D-array with the image

Returns corrected 2D image

reset (method=None, device=None, workgroup=None)

reset the distortion correction and re-calculate the look-up table

Parameters

- **method** – can be “lut” or “csr”, “lut” looks faster
- **device** – can be None, “cpu” or “gpu” or the id as a 2-tuple of integer
- **workgroup** – enforce the workgroup size for CSR.

uncorrect (image)

Take an image which has been corrected and transform it into it’s raw (with loss of information)

Parameters **image** – 2D-array with the image

Returns uncorrected 2D image and a mask (pixels in raw image)

class pyFAI.distortion.**Quad** (buffer)

Bases: object

```

                xxxxA
            xxxxxxI'xxxxxxx x
        xxxxxxxxIxxxxx | x
    Bxxxxxxxxxxxx || x x || x x || x
        x || x x || x x || x x || x x || x
            x || x x || x x || x x O | P A' x

-----J-----+-----L----- x | x x | x x | x
x | xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxD CxxxxxxxxxxxxxxxxxxxxKxxxxx

```

calc_area ()

calc_area_AB (I1, I2)

calc_area_BC (J1, J2)

calc_area_CD (K1, K2)

calc_area_DA (L1, L2)

```
calc_area_old()
calc_area_vectorial()
get_box(i,j)
get_box_size0()
get_box_size1()
get_idx(i,j)
get_offset0()
get_offset1()
init_slope()
integrateAB(start, stop, calc_area)
populate_box()
reinit(A0, A1, B0, B1, C0, C1, D0, D1)
pyFAI.distortion.test()
```

3.21 units Module

```
class pyFAI.units.Enum
```

```
    Bases: dict
```

Simple class half way between a dict and a class, behaving as an enum

```
pyFAI.units.to_unit(obj)
```

3.22 utils Module

Utilities, mainly for image treatment

```
pyFAI.utils.averageDark(lstimg, center_method='mean', cutoff=None)
```

Averages a serie of dark (or flat) images. Centers the result on the mean or the median ... but averages all frames within cutoff*std

Parameters

- **lstimg** – list of 2D images or a 3D stack
- **center_method** – is the center calculated by a “mean” or a “median”
- **cutoff** – keep all data where $(I-center)/std < cutoff$

Returns 2D image averaged

```
pyFAI.utils.averageImages(listImages, output=None, threshold=0.1, minimum=None, maximum=None, darks=None, flats=None, filter_='mean', correct_flat_from_dark=False, cutoff=None, format='edf')
```

Takes a list of filenames and create an average frame discarding all saturated pixels.

Parameters

- **listImages** – list of string representing the filenames
- **output** – name of the optional output file

- **threshold** – what is the upper limit? all pixel $> \max*(1-\text{threshold})$ are discarded.
- **minimum** – minimum valid value or True
- **maximum** – maximum valid value
- **darks** – list of dark current images for subtraction
- **flats** – list of flat field images for division
- **filter** – can be maximum, mean or median (default=mean)
- **correct_flat_from_dark** – shall the flat be re-corrected ?
- **cutoff** – keep all data where $(I-\text{center})/\text{std} < \text{cutoff}$

Returns filename with the data or the data ndarray in case format=None

`pyFAI.utils.binning` (*input_img*, *binsize*)

Parameters

- **input_img** – input ndarray
- **binsize** – int or 2-tuple representing the size of the binning

Returns binned input ndarray

`pyFAI.utils.boundingBox` (*img*)

Tries to guess the bounding box around a valid massif

Parameters *img* – 2D array like

Returns 4-tuple (d0_min, d1_min, d0_max, d1_max)

`pyFAI.utils.center_of_mass` (*img*)

Calculate the center of mass of of the array. Like `scipy.ndimage.measurements.center_of_mass` :param *img*: 2-D array :return: 2-tuple of float with the center of mass

`pyFAI.utils.convert_CamelCase` (*name*)

convert a function name in CamelCase into camel_case

`pyFAI.utils.deg2rad` (*dd*)

Convert degrees to radian in the range $-\pi \rightarrow \pi$

Parameters *dd* – angle in degrees

Nota: depending on the platform it could be $0 < 2\pi$ A branch is cheaper than a trigo operation

`pyFAI.utils.deprecated` (*func*)

`pyFAI.utils.dog` (*s1*, *s2*, *shape=None*)

2D difference of gaussian typically 1 to 10 parameters

`pyFAI.utils.dog_filter` (*input_img*, *sigma1*, *sigma2*, *mode='reflect'*, *cval=0.0*)

2-dimensional Difference of Gaussian filter implemented with FFTw

Parameters

- **input_img** (*array-like*) – input_img array to filter
- **sigma** (*scalar or sequence of scalars*) – standard deviation for Gaussian kernel. The standard deviations of the Gaussian filter are given for each axis as a sequence, or as a single number, in which case it is equal for all axes.
- **mode** – {‘reflect’, ‘constant’, ‘nearest’, ‘mirror’, ‘wrap’}, optional The *mode* parameter determines how the array borders are handled, where *cval* is the value when *mode* is equal to ‘constant’. Default is ‘reflect’

- **cval** – scalar, optional Value to fill past edges of input if mode is ‘constant’. Default is 0.0

`pyFAI.utils.expand(input_img, sigma, mode='constant', cval=0.0)`

Expand array a with its reflection on boundaries

Parameters

- **a** – 2D array
- **sigma** – float or 2-tuple of floats.

:param mode: “constant”, “nearest”, “reflect” or mirror :param cval: filling value used for constant, 0.0 by default

Nota: sigma is the half-width of the kernel. For gaussian convolution it is advised that it is 4*sigma_of_gaussian

`pyFAI.utils.expand_args(args)`

Takes an argv and expand it (under Windows, cmd does not convert *.tif into a list of files. Keeps only valid files (thanks to glob)

Parameters **args** – list of files or wilcards

Returns list of actual args

`pyFAI.utils.float_(val)`

Convert anything to a float ... or None if not applicable

`pyFAI.utils.gaussian(M, std)`

Return a Gaussian window of length M with standard-deviation std.

This differs from the scipy.signal.gaussian implementation as: - The default for sym=False (needed for gaussian filtering without shift) - This implementation is normalized

Parameters

- **M** – length of the windows (int)
- **std** – standatd deviation sigma

The FWHM is $2 * \text{numpy.sqrt}(2 * \text{numpy.pi}) * \text{std}$

`pyFAI.utils.gaussian_filter(input_img, sigma, mode='reflect', cval=0.0)`

2-dimensional Gaussian filter implemented with FFTw

Parameters

- **input_img** (*array-like*) – input array to filter
- **sigma** (*scalar or sequence of scalars*) – standard deviation for Gaussian kernel. The standard deviations of the Gaussian filter are given for each axis as a sequence, or as a single number, in which case it is equal for all axes.
- **mode** – {‘reflect’, ‘constant’, ‘nearest’, ‘mirror’, ‘wrap’}, optional The mode parameter determines how the array borders are handled, where cval is the value when mode is equal to ‘constant’. Default is ‘reflect’
- **cval** – scalar, optional Value to fill past edges of input if mode is ‘constant’. Default is 0.0

`pyFAI.utils.get_cl_file(filename)`

`pyFAI.utils.get_ui_file(filename)`

`pyFAI.utils.int_(val)`

Convert anything to an int ... or None if not applicable

pyFAI.utils.lazy_property

meant to be used for lazy evaluation of an object attribute. property should represent non-mutable data, as it replaces itself.

pyFAI.utils.maximum_position (*img*)

Same as `scipy.ndimage.measurements.maximum_position`: Find the position of the maximum of the values of the array.

Parameters *img* – 2-D image

Returns 2-tuple of int with the position of the maximum

pyFAI.utils.measure_offset (*img1, img2, method='numpy', withLog=False, withCorr=False*)

Measure the actual offset between 2 images :param *img1*: ndarray, first image :param *img2*: ndarray, second image, same shape as *img1* :param *withLog*: shall we return logs as well ? boolean :return: tuple of floats with the offsets

pyFAI.utils.readFloatFromKeyboard (*text, dictVar*)

Read float from the keyboard

Parameters

- **text** – string to be displayed
- **dictVar** – dict of this type: {1: [set_dist_min],3: [set_dist_min, set_dist_guess, set_dist_max]}

pyFAI.utils.relabel (*label, data, blurred, max_size=None*)

Relabel limits the number of region in the label array. They are ranked relatively to their `max(I0)-max(blur(I0))`

Parameters

- **label** – a label array coming out of `scipy.ndimage.measurement.label`
- **data** – an array containing the raw data
- **blurred** – an array containing the blurred data
- **max_size** – the max number of label wanted

:return array like label

pyFAI.utils.removeSaturatedPixel (*ds, threshold=0.1, minimum=None, maximum=None*)**Parameters**

- **ds** – a dataset as ndarray
- **threshold** – what is the upper limit? all pixel $> \max * (1 - \text{threshold})$ are discarded.
- **minimum** – minimum valid value (or True for auto-guess)
- **maximum** – maximum valid value

Returns another dataset

pyFAI.utils.shift (*input_img, shift_val*)

Shift an array like `scipy.ndimage.interpolation.shift(input_img, shift_val, mode="wrap", order=0)` but faster :param *input_img*: 2d numpy array :param *shift_val*: 2-tuple of integers :return: shifted image

pyFAI.utils.shiftFFT (*input_img, shift_val, method='fftw'*)

Do shift using FFTs Shift an array like `scipy.ndimage.interpolation.shift(input, shift, mode="wrap", order="infinity")` but faster :param *input_img*: 2d numpy array :param *shift_val*: 2-tuple of float :return: shifted image

`pyFAI.utils.str_(val)`
Convert anything to a string ... but None -> ""

`pyFAI.utils.timeit(func)`

`pyFAI.utils.unBinning(binnedArray, binsize, norm=True)`

Parameters

- **binnedArray** – input ndarray
- **binsize** – 2-tuple representing the size of the binning

Returns unBinned input ndarray

3.23 `gui_utils` Module

`gui_utils`

Module to handle matplotlib and the Qt backend

class `pyFAI.gui_utils.Event` (*width, height*)
Bases: object

Dummy class for dummy things

`pyFAI.gui_utils.maximize_fig` (*fig=None*)
Try to set the figure fullscreen

`pyFAI.gui_utils.update_fig` (*fig=None*)
Update a matplotlib figure with a Qt4 backend

Parameters `fig` – pylab figure

PROJECT STRUCTURE

PyFAI is a library to deal with diffraction images for data reduction. This chapter describes the project from the computer engineering point of view.

PyFAI is an open source project licensed under the GPL mainly written in Python (v2.6 or 2.7) and heavily relying on the python scientific ecosystem: numpy, scipy and matplotlib. It provides high performances image treatment thanks to cython and OpenCL... but only a C-compiler is needed to build that.

4.1 Programming language

PyFAI is a Python project but uses many programming languages:

- 14000 lines of Python (plus 4300 for the test)
- 8500 lines of Cython which are converted into ...
- 700000 lines of C, most of them generated by cython
- 3500 lines of OpenCL kernels

4.2 Repository:

The project is hosted by GitHub: <https://github.com/kif/pyFAI>

Which provides the [issue tracker](#) in addition to Git hosting. Collaboration is done via Pull-Requests in github's web interface:

Anybody can [fork the project](#) and adapt it to his own needs (people from CEA-saclay, Synchrotron Soleil or APS did it). If developments are useful to other, new developments can be merged into the main branch.

Noticeable scientific development based on pyFAI:

- “Dioptas” is a graphical user interface for calibrating and processing high pressure Xray diffraction experiment, developed by Clemens Perscher (APS, USA).
- “NanoPeakCell” allows the pre-treatment of serial crystallography written by Nicolas Coquelle (IBS, France)

4.3 Run dependencies

- Python2.6 or python2.7

- NumPy
- SciPy
- Matplotlib
- FabIO
- pyopencl (optional)
- fftw (optional)
- PyQt4 or PySide (for the graphical user interface)

4.4 Build dependencies:

In addition to the run dependencies, pyFAI needs a C compiler. There is an issue with MacOSX (v10.8 and 10.9) where the default compiler (Xcode5) switched from gcc 4.2 to clang (v<3.5) which dropped the support for OpenMP. Multiple solution exist, pick any of those:

- install a recent version of GCC (≥ 4.2)
- install Xcode6 (instead of Xcode5) which provides clang 3.5 (with OpenMP support)
- install pyFAI without OpenMP support using the `--no-openmp` flag.

C files are generated from cython source and distributed. Cython is only needed for developing new binary modules. If you want to generate your own C files, make sure your local cython version supports memory-views (available from Cython v0.17 and newer), unless your Cython files will not be compiled or used.

4.5 Building procedure

4.5.1 As most of the python projects:

```
python setup.py build install
```

There are few specific options to setup.py:

- `--no-cython`: do not use cython (even if present) and use the C source code provided by the development team
- `--no-openmp`: if you compiler lacks OpenMP support, like Xcode5 on MacOSX 10.9
- `--with-testimages`: build the source distribution including all test images. Download 200MB of test images to create a self consistent tar-ball.

4.6 Test suites

4.6.1 To run the test an internet connection is needed as 200MB of test images will be downloaded.

```
python setup.py build test
```

Setting the environment variable `http_proxy` can be necessary (depending on your network):

```
export http_proxy=http://proxy.site.org:3128
```

PyFAI comes with 26 test-suites (145 tests in total) representing a coverage of 60%. This ensures both non regression over time and ease the distribution under different platforms: pyFAI runs under linux, MacOSX and Windows (in each case in 32 and 64 bits)

Note that the test coverage tool does not count lines of Cython, nor those of OpenCL

Continuous integration is made by a home-made scripts which checks out the latest release and builds and runs the test every night. Nightly builds are available for debian6-64 bits in: <http://www.edna-site.org/pub/debian/binary/>

4.7 List of contributors in code

```
$ git log --pretty='%aN##s' | grep -v 'Merge pull' | grep -Po '^[^#]+' | sort | uniq -c | sort -rn
```

As of 09/2014:

- Jérôme Kieffer (ESRF)
- Aurore Deschildre (ESRF)
- Frédéric-Emmanuel Picca (Soleil)
- Giannis Ashiotis (ESRF)
- Dimitris Karkoulis (ESRF)
- Jon Wright (ESRF)
- Zubair Nawaz (Sesame)
- Amund Hov (ESRF)
- Dodogerstlin @github
- Gunthard Benecke (Desy)
- Gero Flucke (Desy)

4.8 List of other contributors (ideas or code)

- Peter Boesecke (geometry)
- Manuel Sanchez del Rio (histogramming)
- Armando Solé (masking widget + PyMca plugin)
- Sebastien Petitdemange (Lima plugin)

4.9 List of supporters

- LinkSCEEM project: porting to OpenCL
- ESRF ID11: Provided manpower in 2012 and 2013 and beamtime
- ESRF ID13: Provided manpower in 2012, 2013, 2014 and beamtime
- ESRF ID29: provided manpower in 2013 (MX-calibrate)
- ESRF ID02: provide manpower 2014

INDICES AND TABLES

- *genindex*
- *modindex*
- *search*

BIBLIOGRAPHY

- [SRI2012] PyFAI, a versatile library for azimuthal regrouping J. Kieffer & D. Karkoulis J. Phys.: Conf. Ser. 425 202012 <http://dx.doi.org/10.1088/1742-6596/425/20/202012>
- [EPDIC13] PyFAI: a Python library for high performance azimuthal integration on GPU J. Kieffer & J. P. Wright, Powder Diffraction / Volume 28 / Supplement S2 / September 2013, pp S339-S350 <http://dx.doi.org/10.1017/S0885715613000924>
- [FIT2D] Hammersley A. P., Svensson S. O., Hanfland M., Fitch A. N. and Hausermann D. 1996 High Press. Res. vol14 p235–248
- [SPD] Bösecke P. 2007 J. Appl. Cryst. vol40 s423–s427
- [EDNA] Incardona M. F., Bourenkov G. P., Levik K., Pieritz R. A., Popov A. N. and Svensson O. 2009 J. Synchrotron Rad. vol16 p872–879
- [PyMca] Solé V. A., Papillon E., Cotte M., Walter P. and Susini J. 2007 Spectrochim. Acta Part B vol vol62 p63 – 68
- [PyNX] Favre-Nicolin V., Coraux J., Richard M. I. and Renevier H. 2011 J. Appl. Cryst. vol44 p635–640
- [IPython] Pérez F and Granger B E 2007 Comput. Sci. Eng. vol9 p21–29 URL <http://ipython.org>
- [NumPy] Oliphant T E 2007 Comput. Sci. Eng. vol9 p10–20
- [Cython] Behnel S, Bradshaw R, Citro C, Dalcin L, Seljebotn D and Smith K 2011 Comput. Sci. Eng. vol13 p31 –39
- [OpenCL] Khronos OpenCL Working Group 2010 The OpenCL Specification, version 1.1 URL <http://www.khronos.org/registry/cl/specs/opencl-1.1.pdf>
- [FabIO] Sorensen H O, Knudsen E, Wright J, Kieffer J et al. 2007–2013 FabIO: I/O library for images produced by 2D X-ray detectors URL <http://fable.sf.net/>
- [Matplotlib] Hunter J D 2007 Comput. Sci. Eng. vol9 p90–95 ISSN 1521-9615
- [SciPy] Jones E, Oliphant T, Peterson P et al. 2001– SciPy: Open source scientific tools for Python URL <http://www.scipy.org/>
- [FFTw] Frigo M and Johnson S G 2005 Proceedings of the IEEE 93 p 216–231
- [LImA] The LIMA Project Update S. Petidmange, L. Claustre, A. Homs, R. Homs Regojo, E. Papillon Proceedings of ICALEPCS2013 <http://accelconf.web.cern.ch/AccelConf/ICALEPCS2013/html/auth1084.htm>
- [PyOpenCL] PyCUDA and PyOpenCL: A scripting-based approach to GPU run-time code generation Andreas Klöckner, Nicolas Pinto, Yunsup Lee, Bryan Catanzaro, Paul Ivanov, Ahmed Fasih, Parallel Computing Vol 38, 3, March 2012, Pages 157–174 <http://dx.doi.org/10.1016/j.parco.2011.09.001>
- [AMD] The American Mineralogist Crystal Structure Database. Downs, R.T. and Hall-Wallace, M. (2003) American Mineralogist 88, 247-250 <http://rruff.geo.arizona.edu/AMS/amcsd.php>

[COD] Crystallography Open Database: an open-access collection of crystal structures and platform for world-wide collaboration Saulius Grazulis et al. Nucl. Acids Res. (2012) 40 (D1): D420-D427. <http://dx.doi.org/10.1093/nar/gkr900> <http://www.crystallography.net/>

PYTHON MODULE INDEX

p

- pyFAI.__init__, ??
- pyFAI.azimuthalIntegrator, ??
- pyFAI.blob_detection, ??
- pyFAI.calibrant, ??
- pyFAI.calibration, ??
- pyFAI.detectors, ??
- pyFAI.distortion, ??
- pyFAI.geometry, ??
- pyFAI.geometryRefinement, ??
- pyFAI.gui_utils, ??
- pyFAI.integrate_widget, ??
- pyFAI.io, ??
- pyFAI.massif, ??
- pyFAI.ocl_azim, ??
- pyFAI.ocl_azim_csr, ??
- pyFAI.ocl_azim_csr_dis, ??
- pyFAI.ocl_azim_lut, ??
- pyFAI.opencl, ??
- pyFAI.peak_picker, ??
- pyFAI.spline, ??
- pyFAI.units, ??
- pyFAI.utils, ??
- pyFAI.worker, ??