SAXS Documentation

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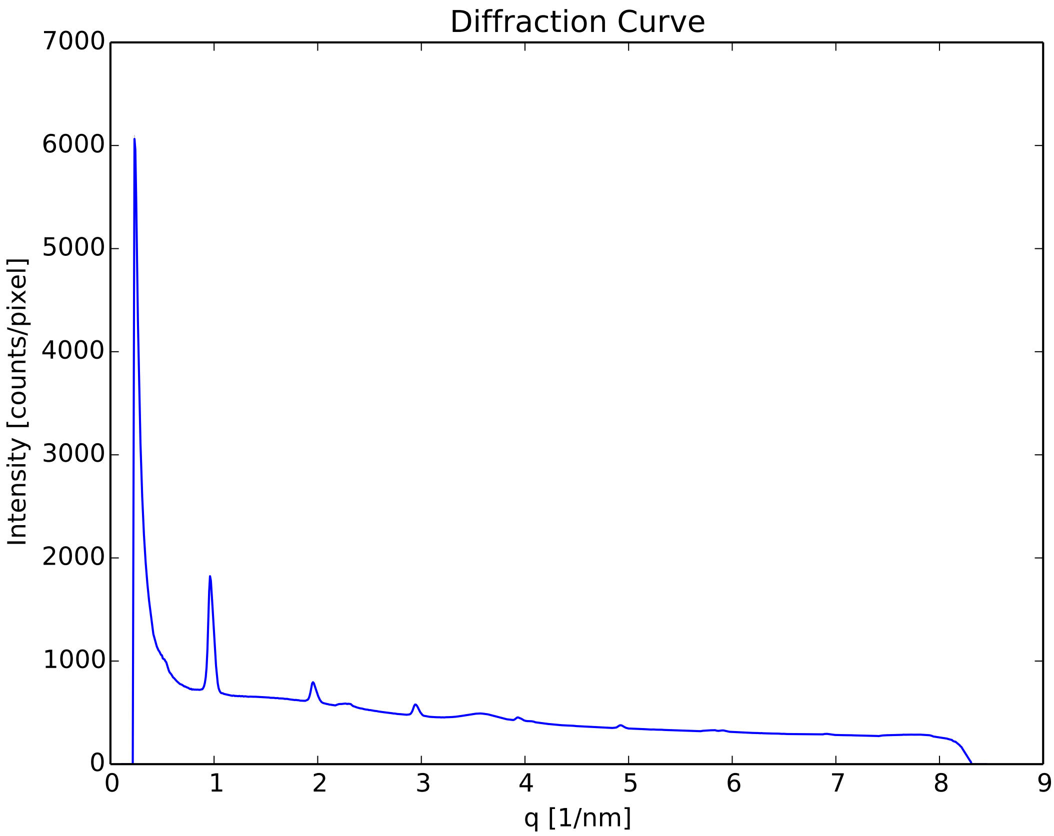
The SAXS Python package implements analysis tools for Small Angle X-Ray Scattering (SAXS) data analysis. The first and most important one is to efficiently integrate 2d sensor data to an angle dependent diffraction curve.



The SAXS module consists of a Python library and 3 command line tools: *The Saxsdog*, *Plotchi* and *The Converter*

CHAPTER

ONE

INSTALL

The SAXS Package is distributes as a Python package. So in order to use it, you need a Python system installed. It depends on following Python modules that don't come with the standard Python:

```
numpy scipy matplotlib jsonschema bitarray watchdog sphinxcontrib-programoutput\
 sphinxcontrib-programscreenshot pyzmq
```

they are all available through "pip" so the command:

```
>>pip numpy scipy matplotlib jsonschema bitarray watchdog sphinxcontrib-programoutput\
 sphinxcontrib-programscreenshot pyzmq
```

Should get all the modules. For Windows, use the Anaconda Python distribution which includes pip.

The code can be obtained on github: https://github.com/ChristianMeisenbichler/SAXS where you would also find a "Download Zip" button. After unpacking or cloning with git you end up with a directory called "SAXS" containing the files. Go there, and type into the command line:

```
python setup.py install
```

This installs the Python module where it is found by Python, creates the command line tools and installs them on the system. Where that is, depends on the Python installation. The setup script will also try to satisfy all the dependencies by downloading and installing them.

CHAPTER TWO

THE TOOLS

2.1 The Saxsdog

The saxsdog is a script that converts directories with images to curves. It can use multiple threads and watch the file system for changes.

For Help on the usage type:

```
$ saxsdog --help
Traceback (most recent call last):
  File "/usr/local/bin/saxsdog", line 9, in <module>
    load_entry_point('SAXS==0', 'console_scripts', 'saxsdog')()
  File "/usr/local/lib/python2.7/dist-packages/SAXS-0-py2.7.egg/SAXS/saxsdoglib.py", line 76, in s
    (options, args)=saxsdogparseopt()
  File "/usr/local/lib/python2.7/dist-packages/SAXS-0-py2.7.egg/SAXS/saxsdoglib.py", line 43, in s
    help="Servermode.")
  File "/usr/lib/python2.7/optparse.py", line 1021, in add_option
    self._check_conflict(option)
  File "/usr/lib/python2.7/optparse.py", line 996, in _check_conflict
    option)
optparse.OptionConflictError: option -S/--servermode: conflicting option string(s): -S
```

The calibration file must be a valid *root*

2.2 The Converter

The converter extracts information from the calibration.txt generated by fit2d and adds them to a SAXS.calibration configuration file. (*root*)

```
$ saxsconverter  --help
Usage: saxsconverter [options] calibration.txt ouput.json

Options:
  -h, --help            show this help message and exit
  -t FILE, --template=FILE
                        Path to calibration file which serves as template.
```

If there is a target file and it is a valid *root*, the parsed values are added or updated in place.

2.3 Plotchi

The tool “plotchi” plots a list of ”.chi”-files:

```
$ plotchi  --help
Usage: plotchi [options] CHIFILE [List of more ".chi" files]

Options:
  -h, --help            show this help message and exit
  -o FILE, --out=FILE   Write the plot to FILE. The format is derived from the
                        suffix, e.g. '.svg','.pdf'.
  -c, --compare         Compare datasets to first one.
  -l, --log             Use log scale.
  -n, --no-legend       Hide legend.
  -t TITLE, --title=TITLE
                        Give plot title.
  -s N, --skip=N        Skip first N points.
  -k N, --clip=N        Clip last N points.
  -x TYPE, --xaxsistype=TYPE
                        Select type of X axis scale, might be
                        [linear|log|symlog]
  -y TYPE, --yaxsistype=TYPE
                        Select type of Y axis scale, might be
                        [linear|log|symlog]
```

2.4 Saxsdmerge

This tool adresses a very specific problem only applicable under our groups needs.

```
$ saxsdmerge   --help
Usage: saxsdmerge [options] iMPicture/dir peakinteg.log datalogger.log

Options:
  -h, --help            show this help message and exit
  -t SEC, --timeoffset=SEC
                        Time offset between logging time and time in
                        imagedata.
  -1, --syncfirst       Sync time by taking the time difference between first
                        shutter action and first image.
  -o FILE, --outfile=FILE
                        Write merged dataset to this file. Format is derived
                        from the extesion.(.csv|.json|.hdf)
  -i FILE, --imagedata=FILE
                         Load image data from previously stored file
                        (imgdata.pkl).
  -b, --batch           Batch mode (no plot).
  -c, --includechi      Include radial intensity data (.chi) in hdf.
  -l FILE, --mergedlogfile=FILE
                        Write merged dataset to this file. The format is
                        derived from the extesion.(.csv|.json|.hdf)
  -f, --includetif      Include  all image data in hdf.
```

What it does is the following: It merges the two log files by interpolating the missing data in the joined table of the the 1 sec interval data logger and the shutter log. The interpolation method takes the closest previous entry. The two logfiles are presumed to have the same clock. This data is then merged with the data extracted from the image headers and written to a output file as a Table. As the image time stamps are from a different clock which might have a significant offset, the `-1` and `-t` options allow for dealing with that. In order to check if the time synchronization is reasonable, the tool displays a graph with the shutter times and the exposure times from the images.

CHAPTER

THREE

THE CALIBRATION FILE

The `SAXS.calibration` class and the saxsdog tool accepts a input file with the calibration data. This input file is written as a JSON file. This is a common syntax to express structured data as text. You might want to read a bit about it before moving on.

3.1 Calibration file Reference

The '*' signifies a required Field.

The SAXS configuration file specifies the parameters of a SAXS sensor calibration. It is written in the JSON format which governs the general syntax.

Type object

Contains *Title*, *Tilt**, *BeamCenter**, *DedectorDistanceMM**, *Imagesize**, *MaskFile**, *Oversampling**, *PixelSizeMicroM**, *PixelPerRadialElement**, *Wavelength**, *PolarizationCorrection*

Required True

JSON Path

- *#*

Example JSON:

```
{
  "PixelSizeMicroM": [
    172.0
  ],
  "Imagesize": [
    1043,
    981
  ],
  "PixelPerRadialElement": 1,
  "Tilt": {
    "TiltRotDeg": 0,
    "TiltAngleDeg": 0
  },
  "MaskFile": "AAA_integ.msk",
  "Oversampling": 3,
  "Wavelength": 1.54,
  "BeamCenter": [
    800.0,
    400.0
  ],
  "DedectorDistanceMM": 1000.0
}
```

3.1.1 Title

Type string

Required False

JSON Path

- *#* ['*Title*']

Example JSON:

```
{"Title": ""}
```

3.1.2 Tilt

The sensor, usually is not perfectly perpenticular to the ray direction. The tilt angle can be specified by giving the following paramters.

Type object

Contains *TiltRotDeg**, *TiltAngleDeg**

Required True

JSON Path

- *#* ['*Tilt*']

Example JSON:

```
{"Tilt": {"TiltRotDeg": 0,"TiltAngleDeg": 0}}
```

3.1.3 TiltRotDeg

This gives the angel of the tilt direction.

Type number in degree

Required True

Default 0

JSON Path

- *#* ['*Tilt*']['*TiltRotDeg*']

Example JSON:

```
{"TiltRotDeg": 0}
```

3.1.4 TiltAngleDeg

This gives the angle between the ray direction and the normal to the sensor plane.

Type number in degree

Required True

Default 0

JSON Path

- *#* ['*Tilt*']['*TiltAngleDeg*']

Example JSON:

```
{"TiltAngleDeg": 0}
```

3.1.5 BeamCenter

Gives the beam center in pixel coorinates.

Type array(2) items: number number

Required True

Default [800.0, 400.0]

JSON Path

- *#* ['*BeamCenter*']

Example JSON:

```
{"BeamCenter": [800.0,400.0]}
```

3.1.6 DedectorDistanceMM

Distance between diffraction center and sensor.

Type number in Millimeters

Required True

Default 1000.0

JSON Path

- *#* ['*DedectorDistanceMM*']

Example JSON:

```
{"DedectorDistanceMM": 1000.0}
```

3.1.7 Imagesize

Size of sensor image in pixel.

Type array(2) items: number number

Required True

Default [1043, 981]

JSON Path

- *#* ['*Imagesize*']

Example JSON:

```
{"Imagesize": [1043,981]}
```

3.1.8 MaskFile

Path of Maskfile

Type string

Required True

Default AAA_integ.msk

JSON Path

- *#* ['*MaskFile*']

Example JSON:

```
{"MaskFile": "AAA_integ.msk"}
```

3.1.9 Oversampling

Oversampling factor for radial integration. The higher, the longer the setup but the higher the accuracy. More then 3 is probably overkill.

Type number

Required True

Default 3

JSON Path

- *#* ['*Oversampling*']

Example JSON:

```
{"Oversampling": 3}
```

3.1.10 PixelSizeMicroM

The pixel size on the sensor.

Type array(2) items: number

Required True

Default [172.0]

JSON Path

- *#* ['*PixelSizeMicroM*']

Example JSON:

```
{"PixelSizeMicroM": [172.0]}
```

3.1.11 PixelPerRadialElement

Expresses the width of a radial step in terms of pixels. '1' means $\delta R \approx 1$ *PixelSizeMicroM*.

Type number

Required True

Default 1

JSON Path

- *#* ['*PixelPerRadialElement*']

Example JSON:

```
{"PixelPerRadialElement": 1}
```

3.1.12 Wavelength

Refined wavelength.

Type number in Angstrom

Required True

Default 1.54

JSON Path

- *#* ['*Wavelength*']

Example JSON:

```
{"Wavelength": 1.54}
```

3.1.13 PolarizationCorrection

The scattering direction id dependend on the light polarization. This may be acconted for with the polarization correction.

Type object

Contains *Fraction**, *Angle**

Required False

Default OrderedDict([(u'Fraction', 0.95), (u'Angle', 0)])

JSON Path

- *#* ['*PolarizationCorrection*']

Example JSON:

```
{"PolarizationCorrection": {"Angle": 0.0,"Fraction": 0.95}}
```

3.1.14 Fraction

Fraction of light polarized in the given (*Angle*) direction.

Type number

Required True

Default 0.95

JSON Path

- *#* ['*PolarizationCorrection*']['*Fraction*']

Example JSON:

```
{"Fraction": 0.95}
```

3.1.15 Angle

Angle of the polarization plane.

Type number in degree

Required True

Default 0.0

JSON Path

- *#* ['*PolarizationCorrection*'\]['*Angle*']

Example JSON:

```
{"Angle": 0.0}
```

CHAPTER

FOUR

THE TECHNOLOGY

4.1 Integration as Matrix-Vector Multiplication

Every SAXS image $\mathbf{p}$ is a list of pixels that have an intensity value. This 2d array might as well be addressed as a vector with all the pixels addressable with one index $\mathbf{p}_i$.

The integration over pixels that are within a certain radial interval is in any case a weighted sum of some of the pixels.

This weighted sum is a scalar product with another vector containing the weight factors. As only the pixels in a radius interval are counted, most of these factors are 0.

$$r = \mathbf{c} \cdot \mathbf{p}$$

As we intend to do all the radial intervals at once, we write it as a matrix vector product.

$$\mathbf{r} = \mathbf{X} \cdot \mathbf{p}$$

The columns are the weight factors for the i^{th} radial element. Rearranged in the order of the image, this looks like the ring element relevant for the radial Point.

This matrix would be quite big as it has the dimensions len($\mathbf{r}$)*len($\mathbf{p}$). Fortunately most of the entries are 0 and we can use a sparse matrix representation which uses only about ~len($\mathbf{p}$) of memory, as every pixel is counted only once, or, as we will see, about once.

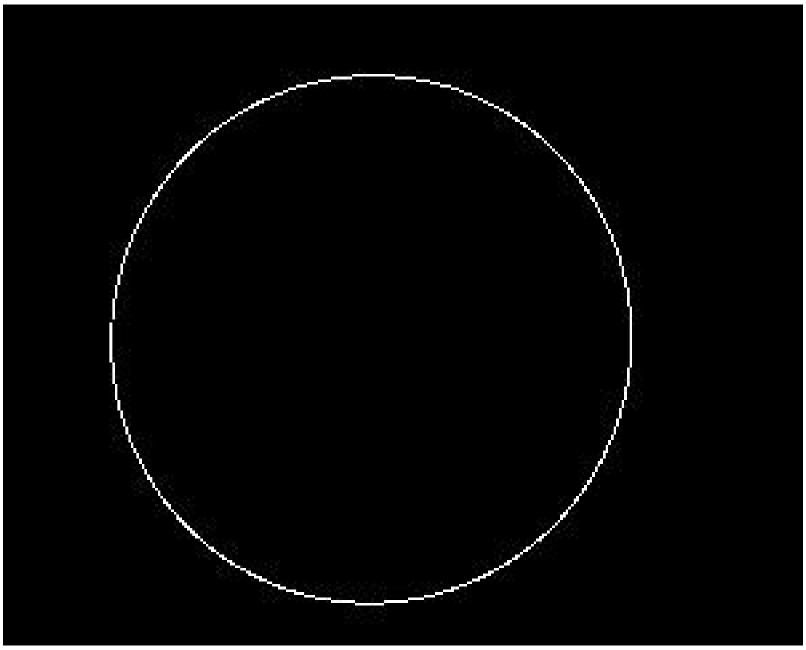


Figure 4.1: The vector $\mathbf{c}$ displayed as image.

Figure *CircleNoAA* Shows the data of such a matrix column.

4.2 Over sampling

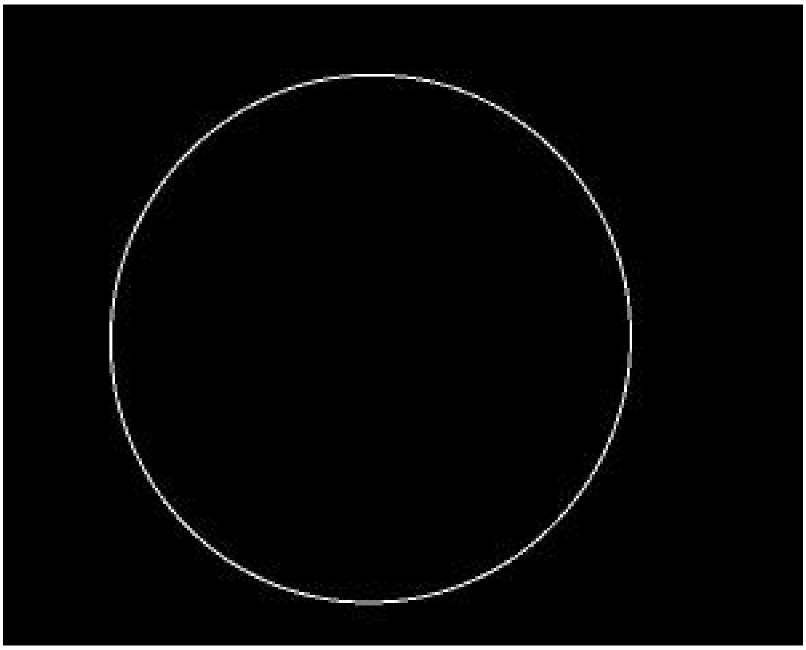


Figure 4.2: Ring with anti aliasing / over sampling.

A pixel might lie on the border of two radial intervals, making it unclear to which one it should be added. By only choosing the nearest one, one may get artifacts in the resulting curve especially when only few pixels contribute. So, how could we calculate to which fraction a pixel should account to one radial interval?

The idea here is to use an algorithm comparable to anti aliasing in computer graphics. We will divide a much larger picture into the radial intervals and down sample it to the real pixels. Which results in nicely balanced factors for the border pixels that add up nicely over joining intervals such that the intensity is conserved. If one looks closer at image *Ring with anti aliasing / over sampling.* , one sees that the ring has soft edges. Quite as it would have through anti aliasing.

4.3 The Geometry

The plane of the sensor is not perfectly normal to the beam. So in order to calculate witch pixel is on witch cone in the diffracted light, we need to express the geometry somehow.

Every pixel has the polar coordinates r, ϕ with the projected diffraction center in the origin. For each pixel (P) the triangle S,C,P (Sample, Center, Pixel, θ, β, γ) can be fully expressed with the law of cosines.

l is the distance the light travels from the diffraction center to the sensor.

$$l^2 = d^2 + r^2 - 2dr\cos(\pi/2 + \alpha)$$

r is the radial coordinate of the pixel P.

$$r^2 = l^2 + d^2 - 2ld\cos(\theta)$$

from these two formulas the diffraction angle (here) θ can be computed.

$$\theta = \arccos(-r^2 - l^2 - d^2 2ld)$$

α comes from the following relation in figure *Angle between two planes.*

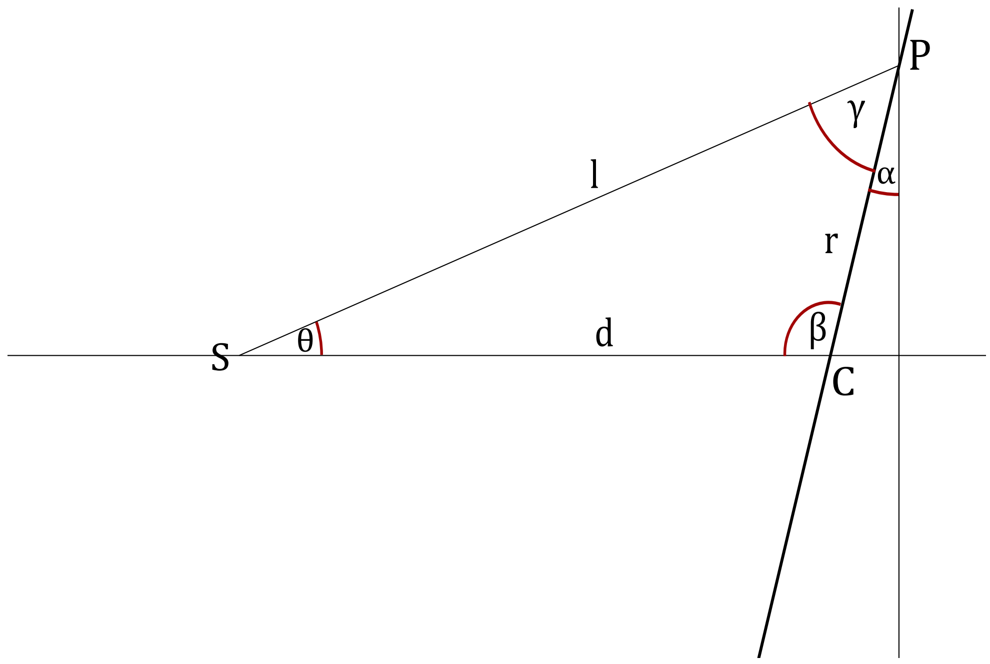


Figure 4.3: The SCP triangle.

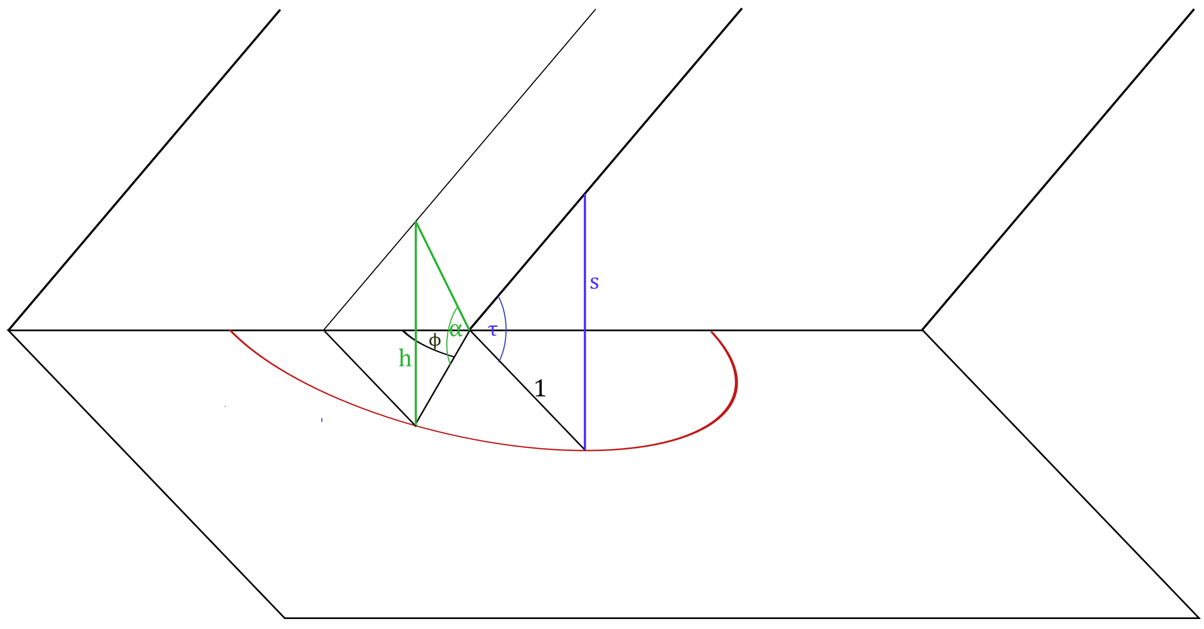


Figure 4.4: Angle between two planes.

The angle between the sensor plane and the normal plane to the ray is given by τ. The slope s derived from τ is

$$s = \sin(\tau)$$

On the (red) unit circle in the plane of the sensor the distance to the plane normal to the ray is expressed as

$$h = \sin(\phi)s$$

The angle α is therefore:

$$\alpha = \arcsin(\sin(\tau)\sin(\phi))$$

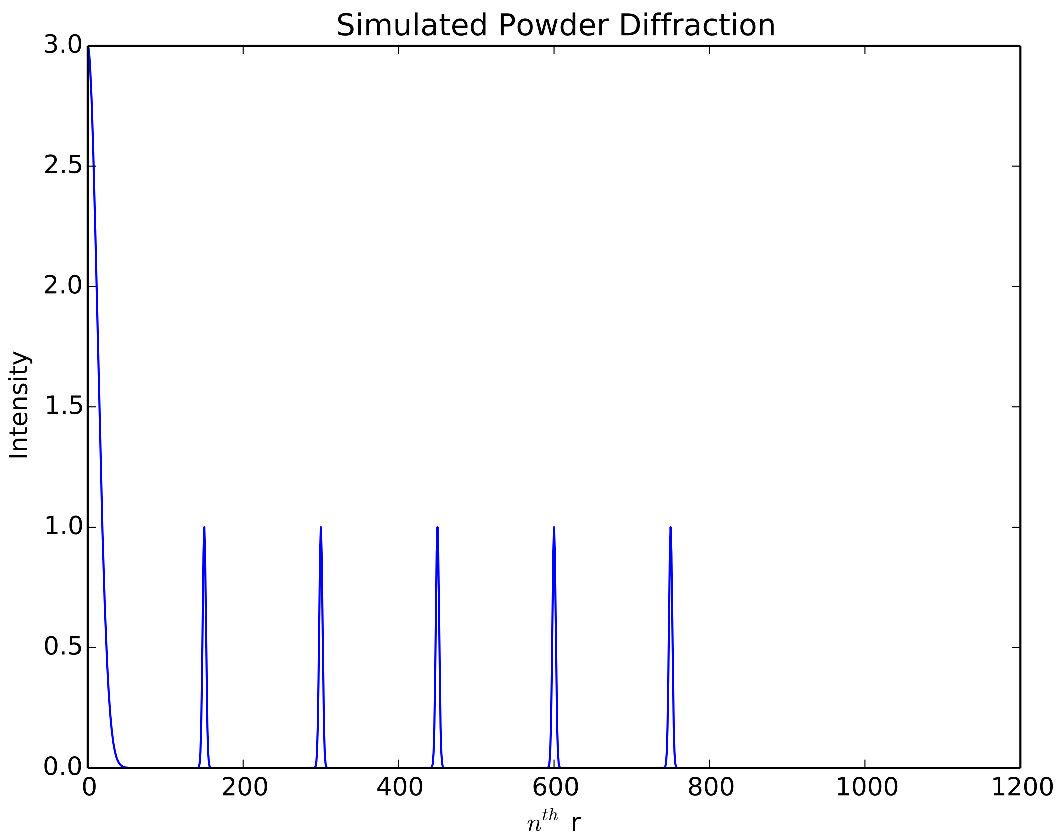
in Python code this is `SAXS.calc_theta()`:

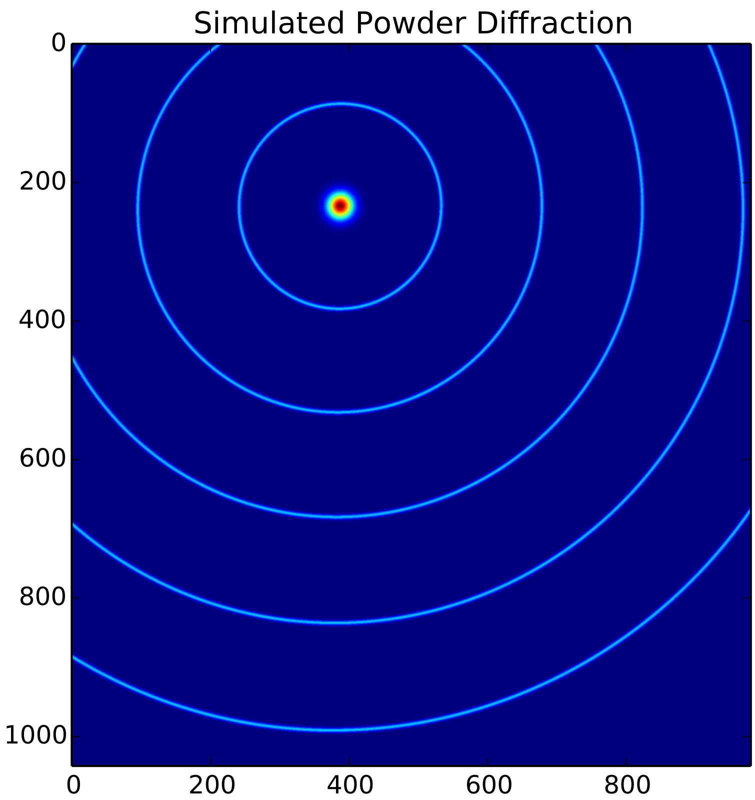
```
def calc_theta(r,theta,d,tilt,tiltdir):
    alpha=np.arcsin(np.sin(tilt)*np.sin(theta+tiltdir))
    lsquared=d**2 +r**2 -2*d*r*np.cos(np.pi/2+alpha)
    return np.arccos(-(r**2-lsquared-d**2)/(2*np.sqrt(lsquared)*d))
```

This angle θ then is calculated for every sub pixel in the sensor. This number then can be rescaled and rounded to the nearest integer in order to get unique integer labels for all the pixels. This labels are the index of the radial interval.

4.3.1 Tilt Angle Correction Test

To check if the tilt angle correction is working, lets create some fake calibration data, with the following peaks in the diffraction curve:





This was done with this configuration file:

```
{
    "PixelPerRadialElement": 1,
    "Imagesize": [
        1043,
        981
    ],
    "Tilt": {
        "TiltAngleDeg": -10,
        "TiltRotDeg": 73.569
    },
    "MaskFile": "emptymask.tif",
    "PixelSizeMicroM": [
        172.0,
        172.0
    ],
    "Wavelength": 1.54,
    "DedectorDistanceMM": 1031.657,
    "BeamCenter": [
        808.37,
        387.772
    ],
    "Oversampling": 2
}
```

Which amounts to a large tilt, lets see what Fit2d makes of it

```
INFO: SOLUTION 2
INFO: Best fit beam centre (X/Y mm) =    66.78356      138.9544
INFO: Best fit beam centre (X/Y pixels) =    388.2765      807.8745
INFO: Cone  1 best fit 2 theta angle (degrees) =   1.392646
```

```
INFO: Cone  2 best fit 2 theta angle (degrees) =   2.780810
INFO: Cone  3 best fit 2 theta angle (degrees) =   4.168858
INFO: Cone  4 best fit 2 theta angle (degrees) =   5.556975
INFO: Cone  5 best fit 2 theta angle (degrees) =   6.944765
INFO: Best fit angle of tilt plane rotation (degrees) =   73.59509
INFO: Best fit angle of tilt (degrees) =  -10.00601
INFO: Estimated coordinate radial position error (mm) =  0.7136476E-02
INFO: Estimated coordinate radial position error (X pixels) =  0.4149114E-01
```

Seems OK.

4.4 Polarization Correction

The polarization correction is expected to be small at small angles, but it is deemed important.

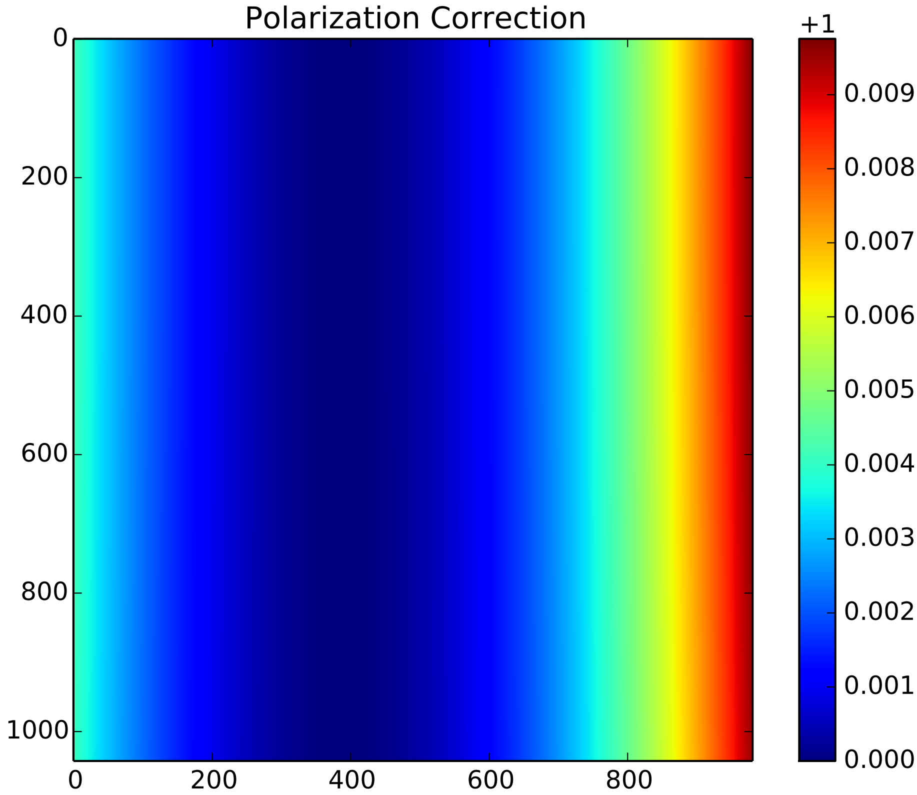
$$I_{cor} = I_j \left[P(1 - (sin(\phi)sin(2\theta))^2)(1 - P)(1 - (cos(\phi)sin(2\theta))^2) \right]$$

where ϕ is the azimuthal angle on the detector surface (defined here clockwise, 0 at 12 o'clock) 2θ the scattering angle, and P the fraction of incident radiation polarized in the horizontal plane (azimuthal angle of 90°) The polarization correction is configured by two parameters in *PolarizationCorrection*. Its factors are included in the integration matrix (operator).

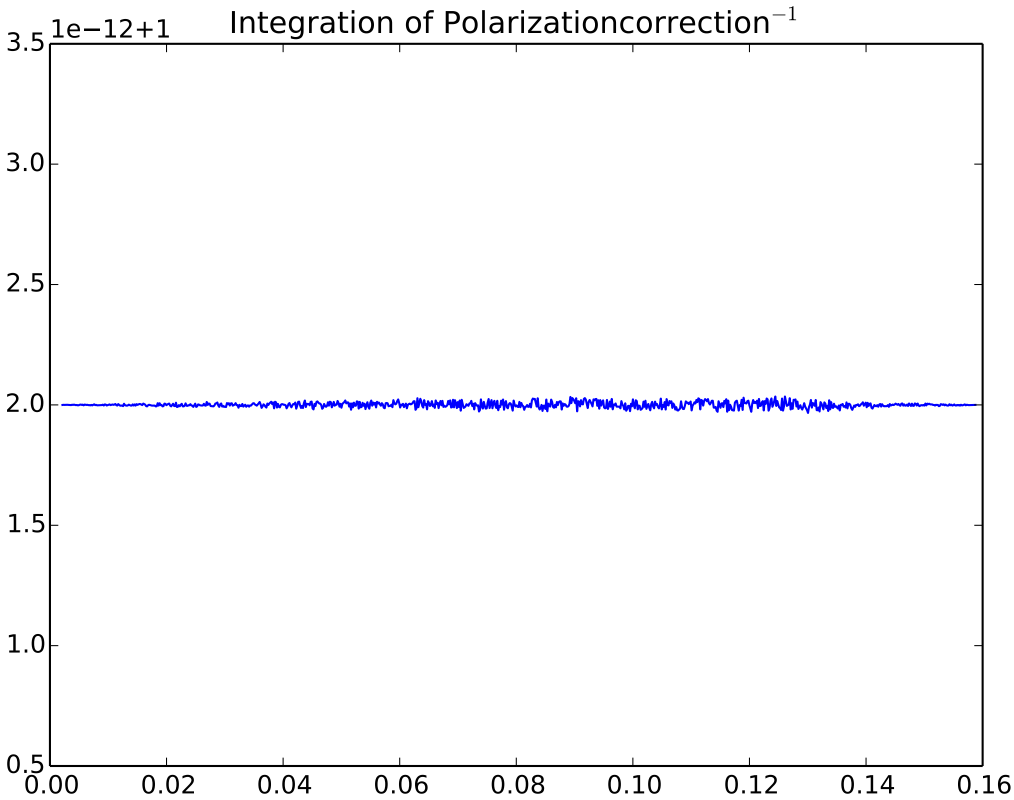
This input:

```
{
    "PixelPerRadialElement": 1,
    "Imagesize": [
        1043,
        981
    ],
    "Tilt": {
        "TiltAngleDeg": -0.56,
        "TiltRotDeg": 73.569
    },
    "MaskFile": "../data/AAA_integ.msk",
    "PolarizationCorrection": {
        "Angle": 0,
        "Fraction":1
    },
    "Oversampling": 2,
    "Wavelength": 1.54,
    "DedectorDistanceMM": 1031.657,
    "BeamCenter": [
        808.37,
        387.772
    ],
    "PixelSizeMicroM": [
        172.0,
        172.0
    ]
}
```

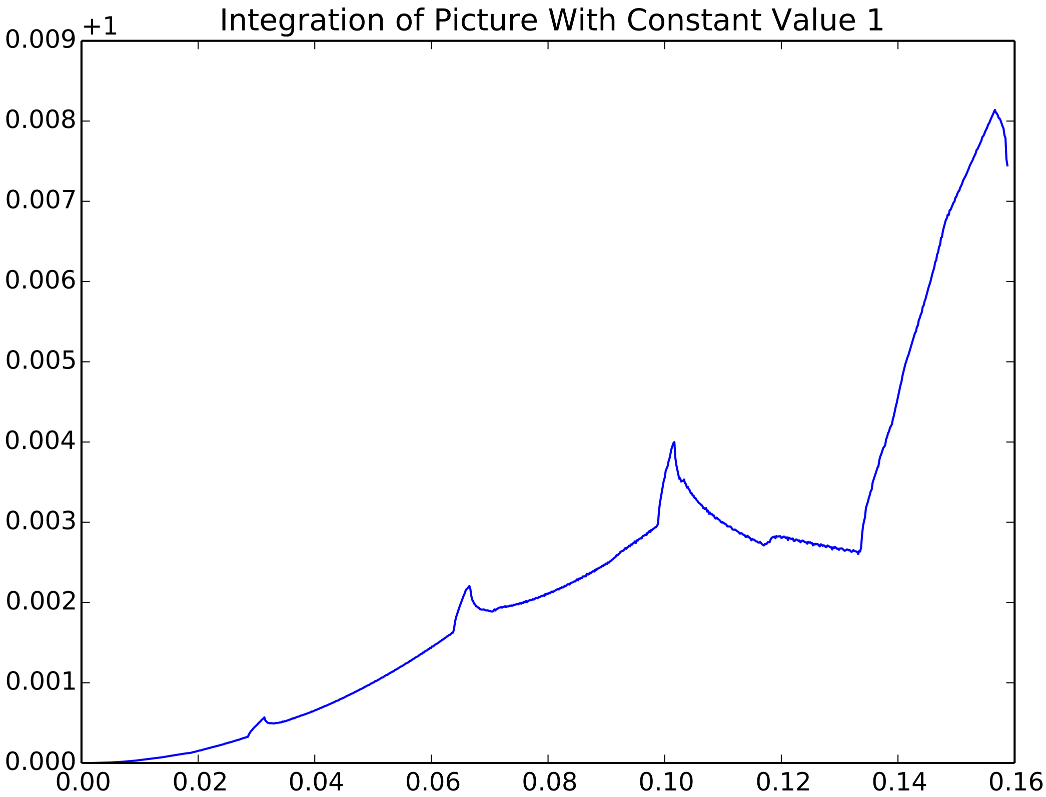
Gives:



If the correction factors are all correctly in the algorithm, the integration of an image containing $1/I_{corr}$ should give constant 1.0.



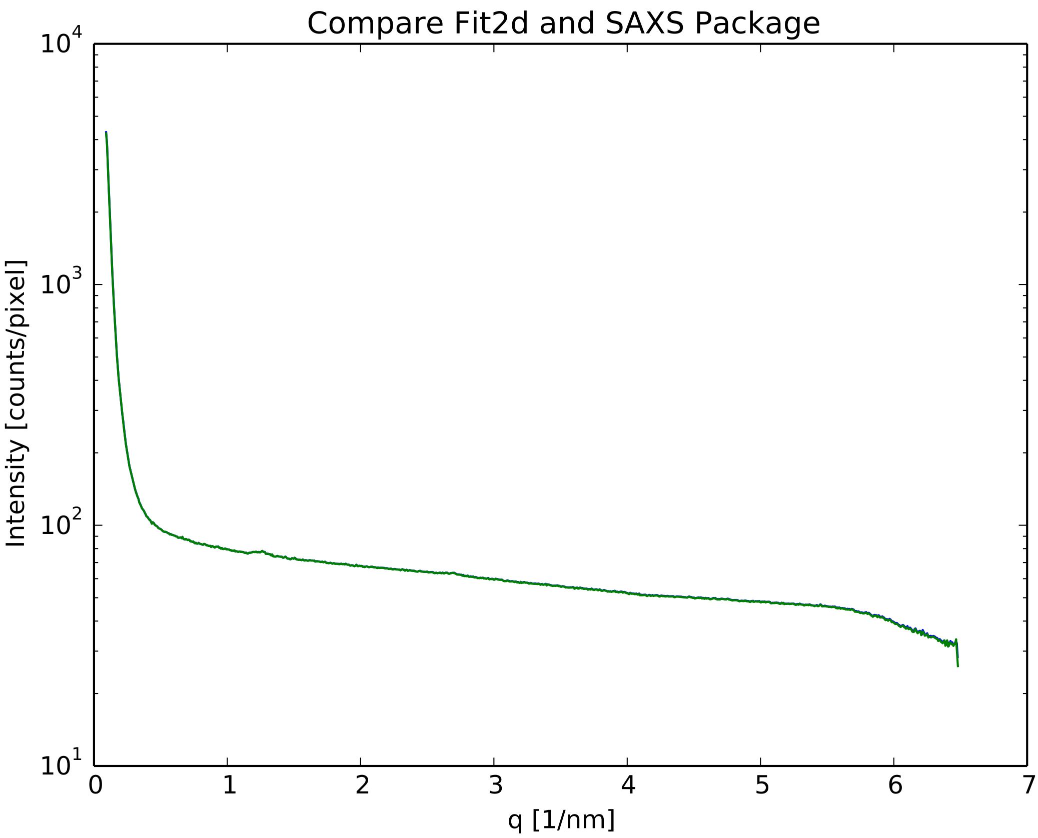
Just for checking: integrating a picture with only ones gives something different:



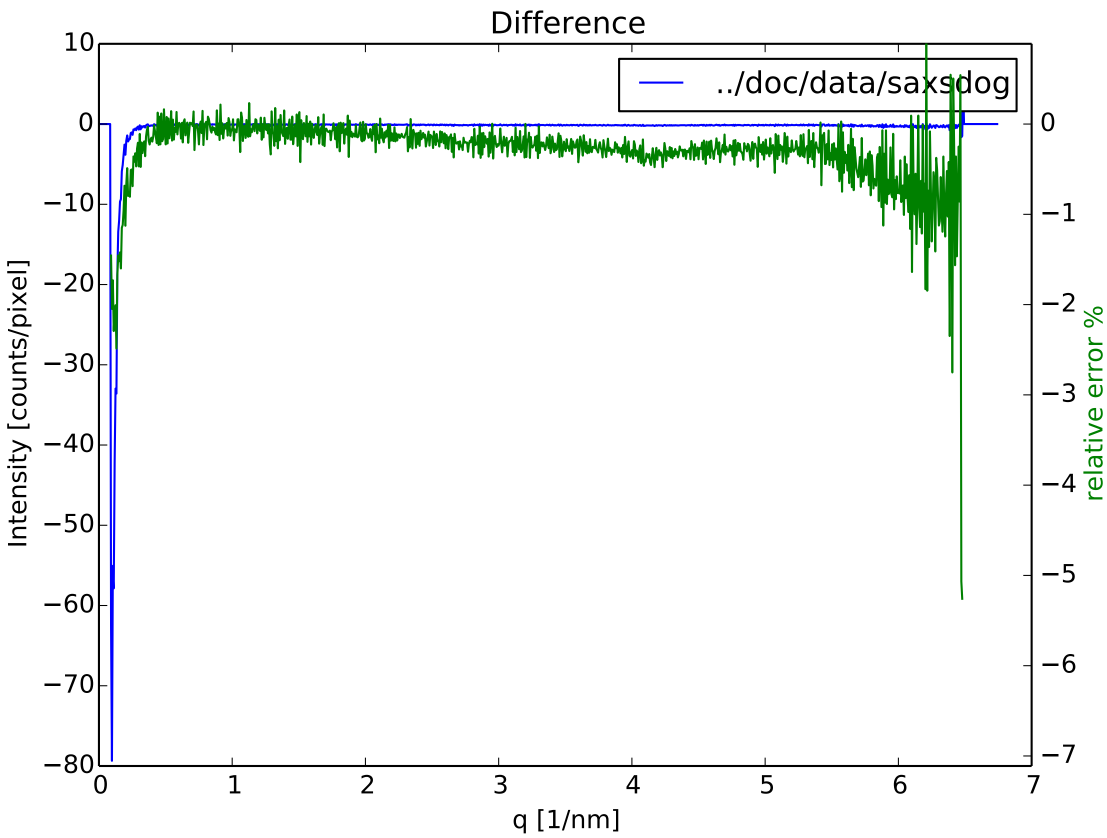
This are the wiggles that come from the polarization correction pattern

4.5 Compare With Fit2d

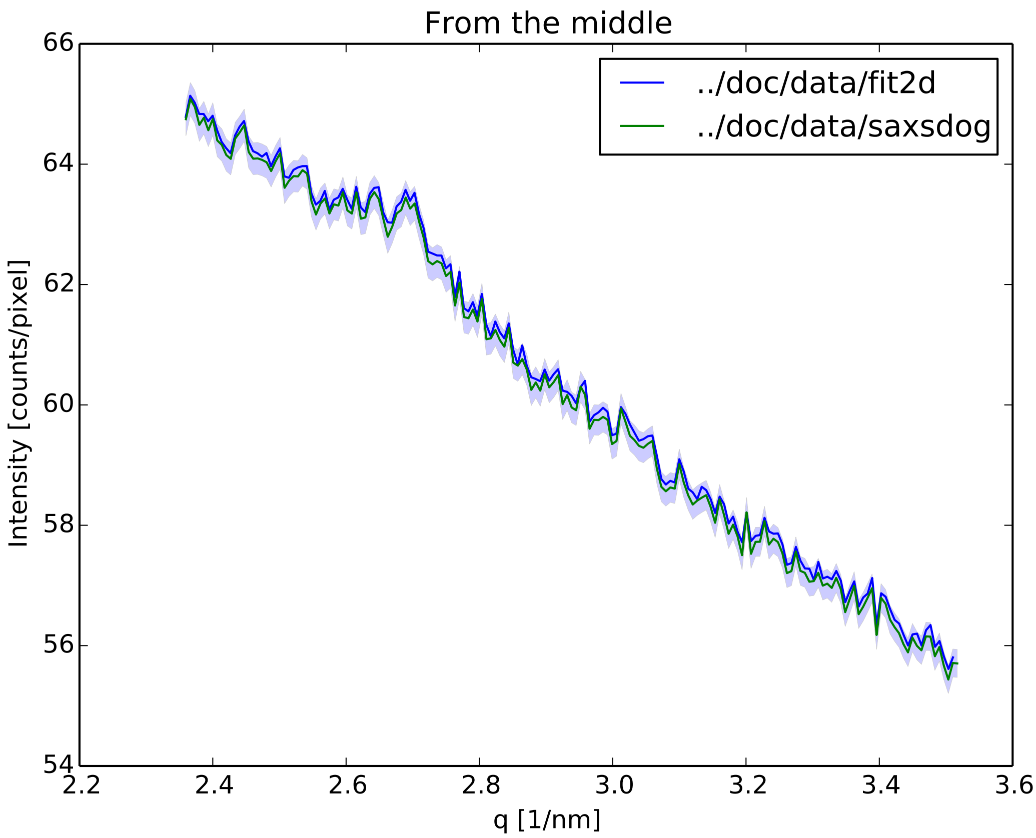
The program fit2d, which this package aims to partly replace, is the standard, so we better include a comparison plot here:

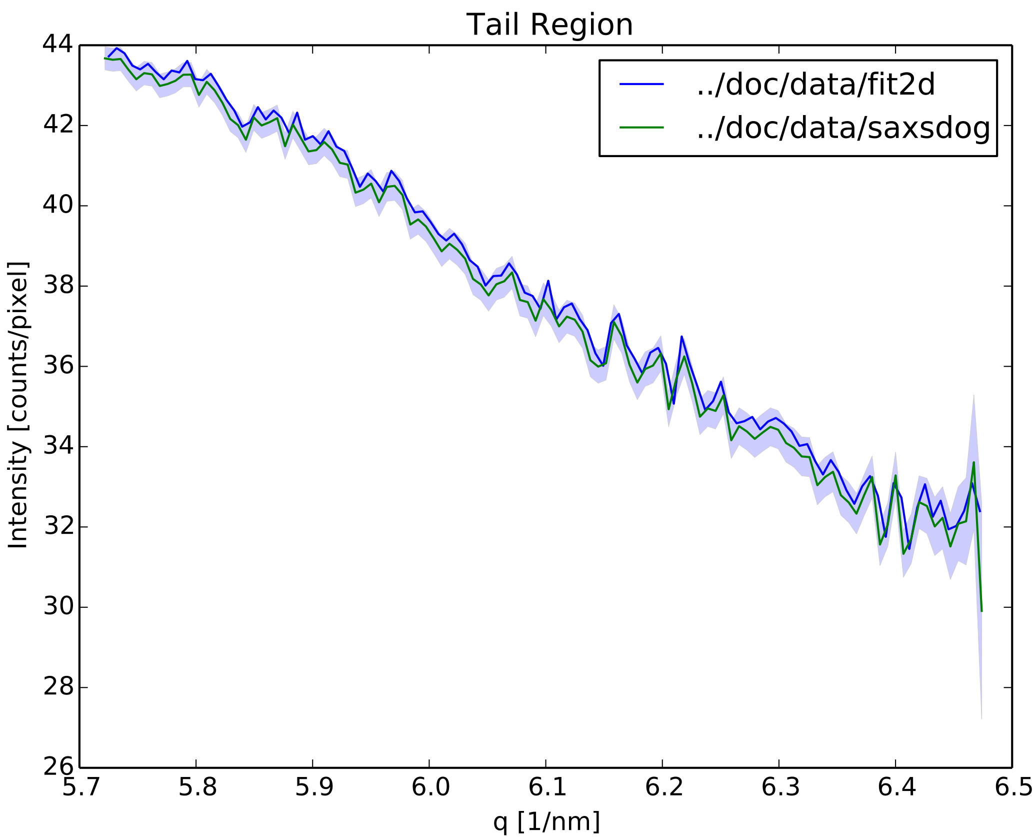


Okay, this doesn't show much but if we plot the difference:

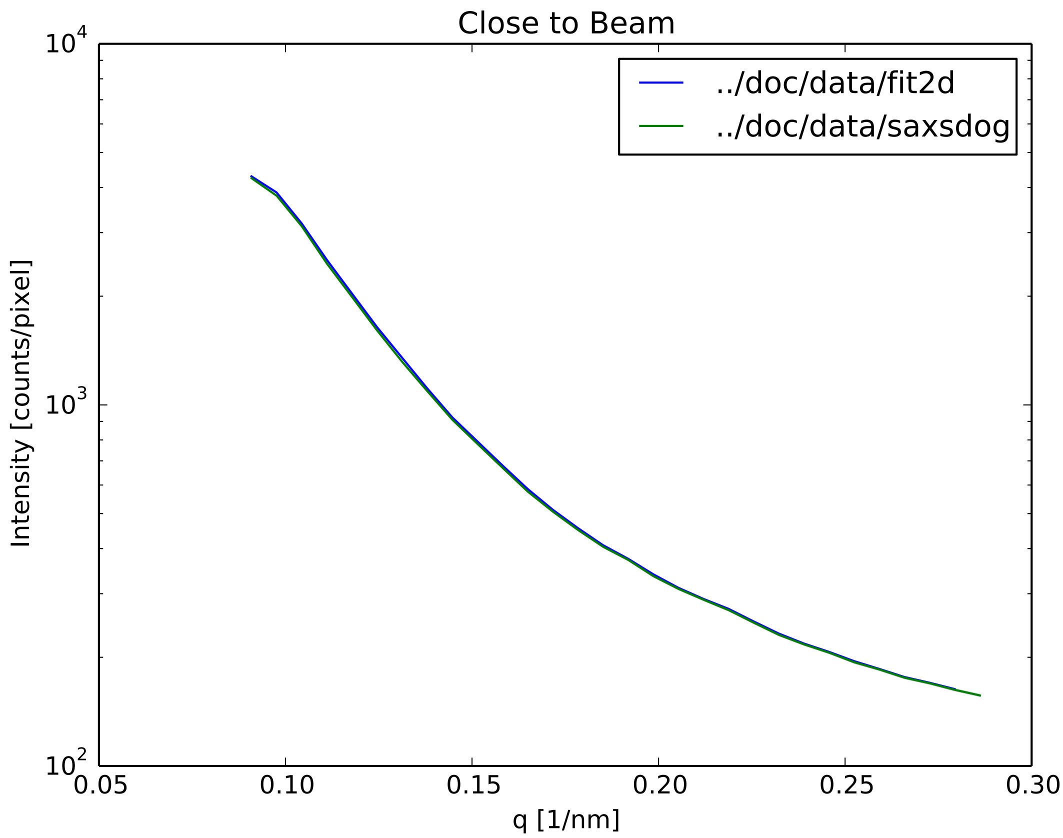


Still looks okay.





In the tail region the blue halo (Poisson error) signifies that there are not enough counts to make good statistics.



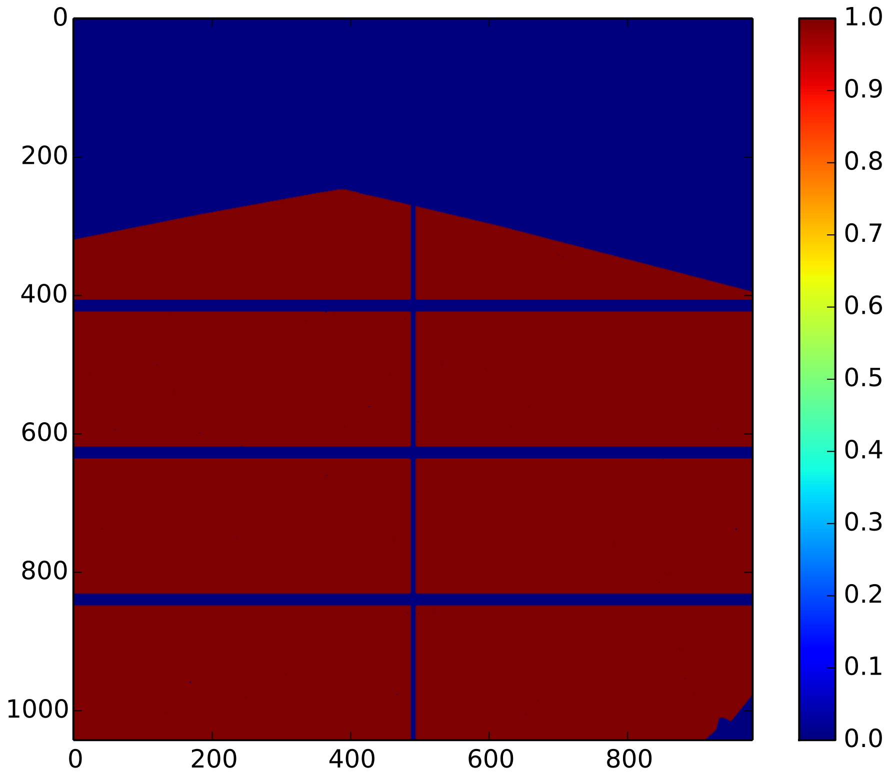
4.6 Integrating a Constant Image With Masked Values

This test shows that nothing wrong happens at mask borders. For those we want to integrate an image that is one everywhere except for the masked regions

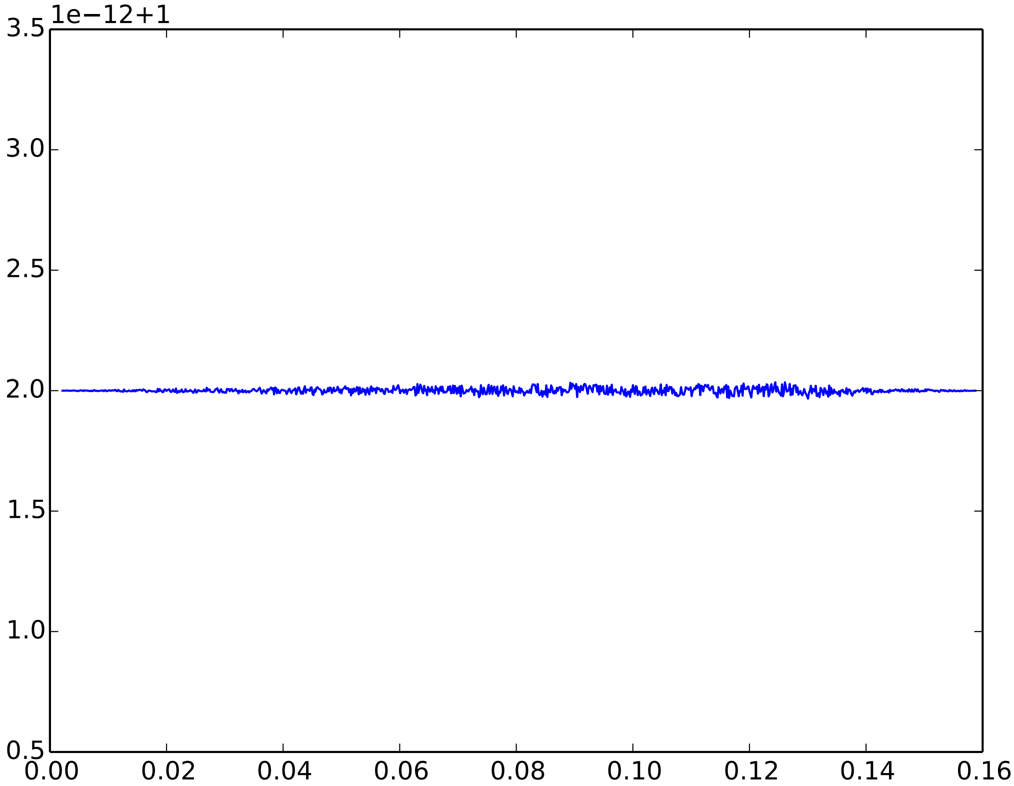
We use the following calibration without Polarization correction and mask:

```
{
    "PixelPerRadialElement": 1,
    "Imagesize": [
        1043,
        981
    ],
    "Tilt": {
        "TiltAngleDeg": -0.56,
        "TiltRotDeg": 73.569
    },
    "MaskFile": "../data/AAA_integ.msk",
    "PixelSizeMicroM": [
        172.0,
        172.0
    ],
    "Wavelength": 1.54,
    "DedectorDistanceMM": 1031.657,
    "BeamCenter": [
        808.37,
        387.772
    ],
    "Oversampling": 2
}
```

The image we are going to integrate is exactly the array the `SAXS.openmask()` returns:



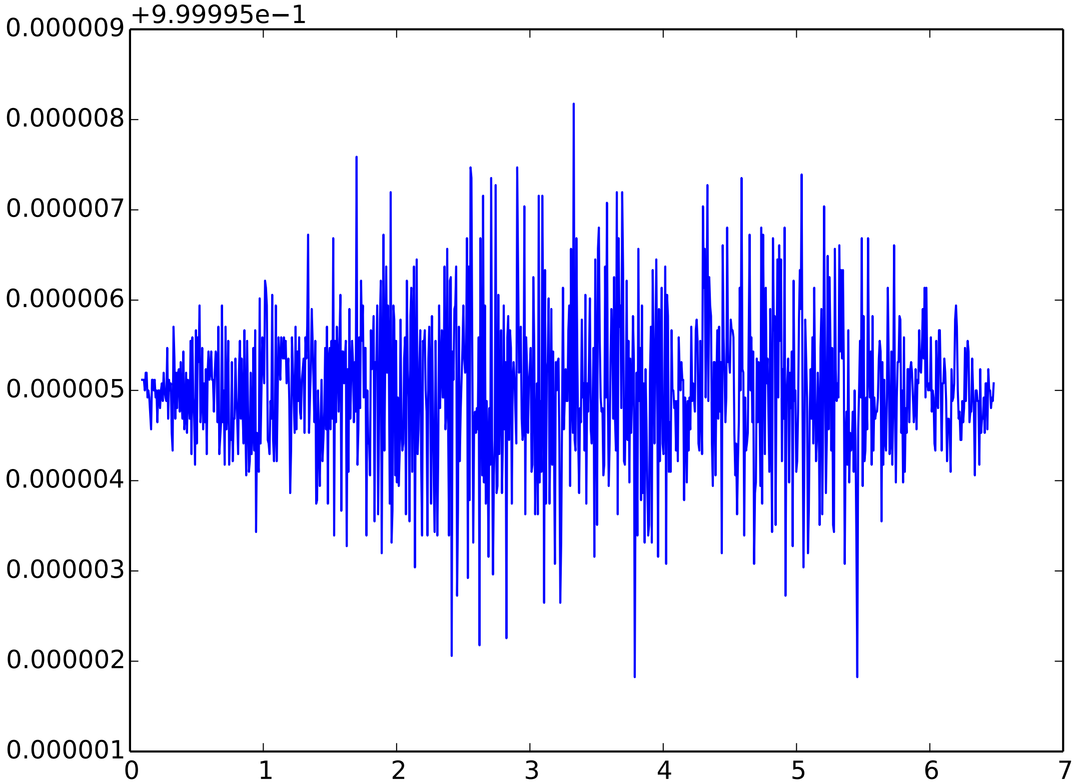
The result is constant 1 (where the intensity is not 0), save 2e-12.



Doing the same with Fit2d,

```
$ fit2d -svar\#IN=mask.tif -dim2000x2000 -svar\#OUT=data/const.chi -mac../data/AAA_integ_Pilatus1M

                                 --------------------------------
                                 PROGRAM   FIT2D   Version: V12.081
                                 ________________________________

            Copyright 1987-2005 Andy Hammersley / ESRF (hammersley@esrf.fr)

FIT2D: 2-D Detector Calibration/Correction; File re-formatting; 2-D Fitting

                                 YOU CAN ALWAYS ENTER:    ?
...
```

results in something similar, just with less precision, about 10e-7. Probably because of single precision arithmetics.



4.7 Statistics

4.7.1 Poisson Statistics

The most important error is the statistical fluctuation that stems from the randomness of the scattering events. Counts of such events follow the Poison distribution. Such, the error (σ) is $\sqrt{n}$ for a count of n. The result of which is, that the relative error $\frac{\sqrt{n}}{n}$ rapidly gets small for larger counts.

Each Pixel in the SAXS sensor counts the number of events, and thus follows the Poisson statistics. The error of a sum of pixels is calculated as.

$$\sigma_{sum} = \sqrt{\sum_i \sigma_i^2}$$

which means here

$$\sigma_{sum} = \sqrt{\sum_i n_i}$$

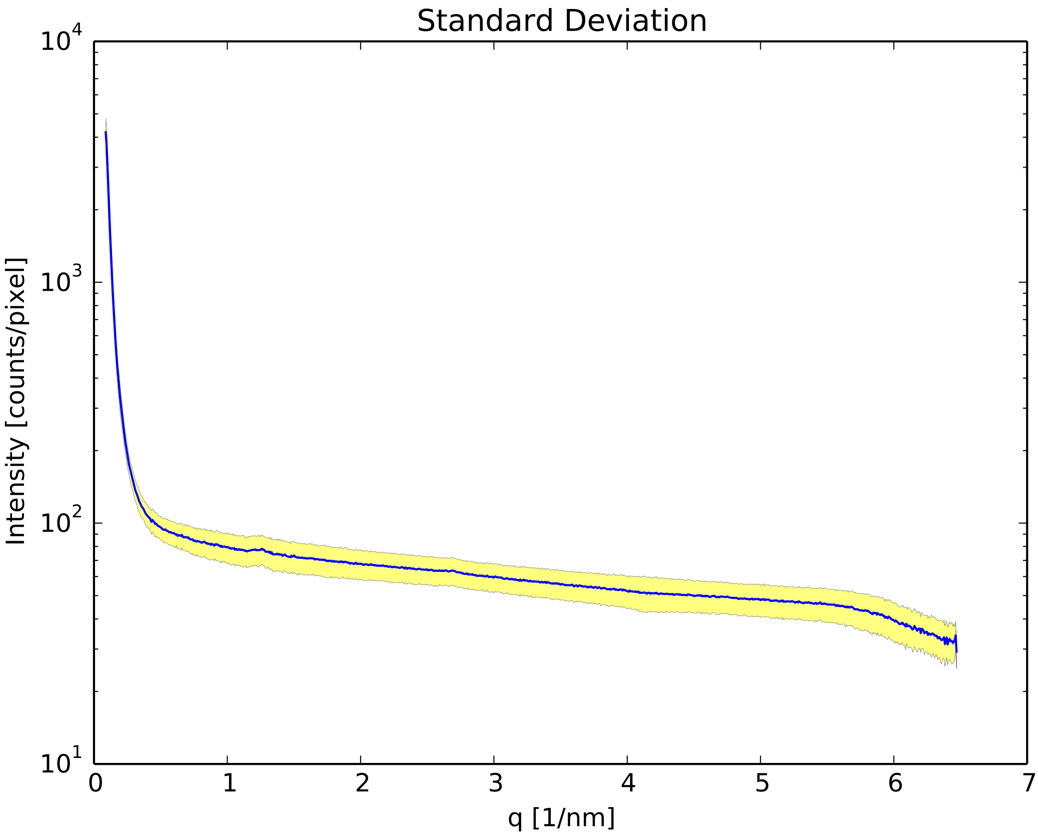
Rescaled over the number of pixels (P) in the sum this gives:

$$\sigma_{sum} = \frac{\sqrt{\sum_{i=1}^{P} n_i}}{P}$$

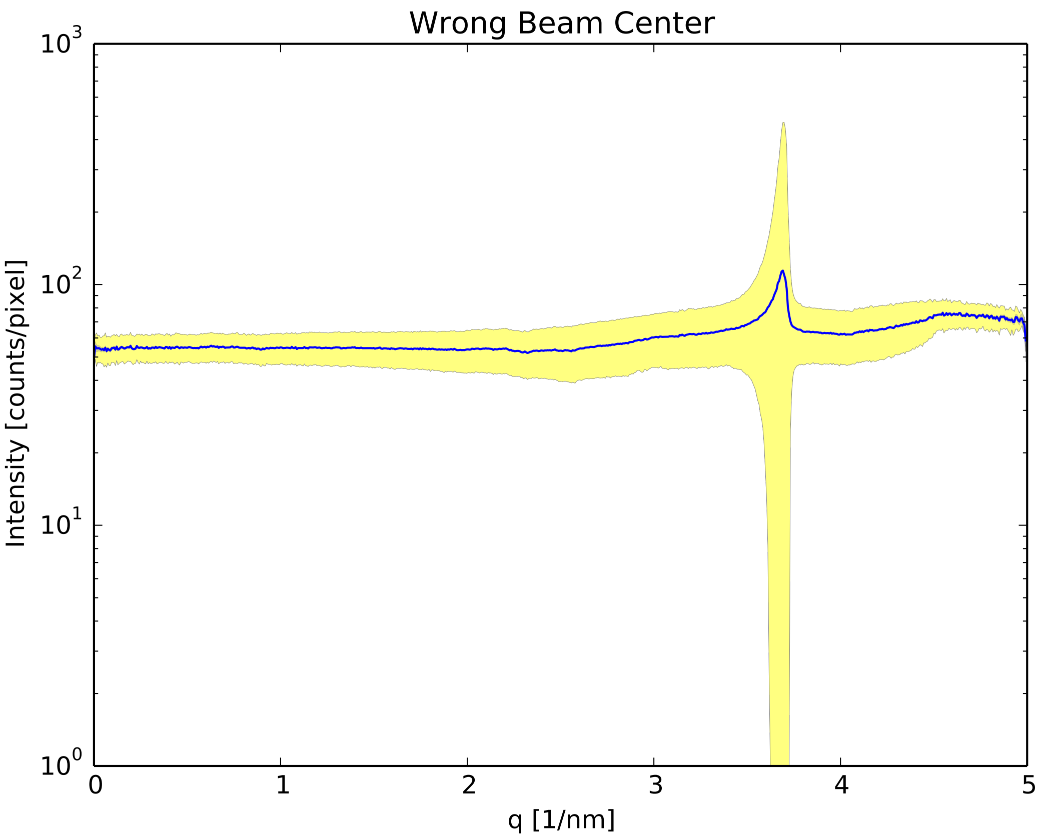
The `SAXS.calibration.plot()` method of the `SAXS.calibration` class will give you the Poisson error along with the standard deviation. So for regions, where the total number of counts is too small, you can see if there is a significant error. This might occur, if too few pixels are used for a data point or the intensity is just to small.

4.7.2 Standard Deviation

The standard deviation of the mean that is taken through the integration is not as such particularly useful to estimate the error of the resulting intensities because there are quite a few things that produce an angle dependence. In an optimal case, if the angle dependence can be corrected with the Polarization correction, the standard deviation of the integration might be very small. In an ordinary case the standard deviation gives you a measure of how spread the intensities within a radius interval are.



The standard deviation is bright yellow and the Poison error is blueisch



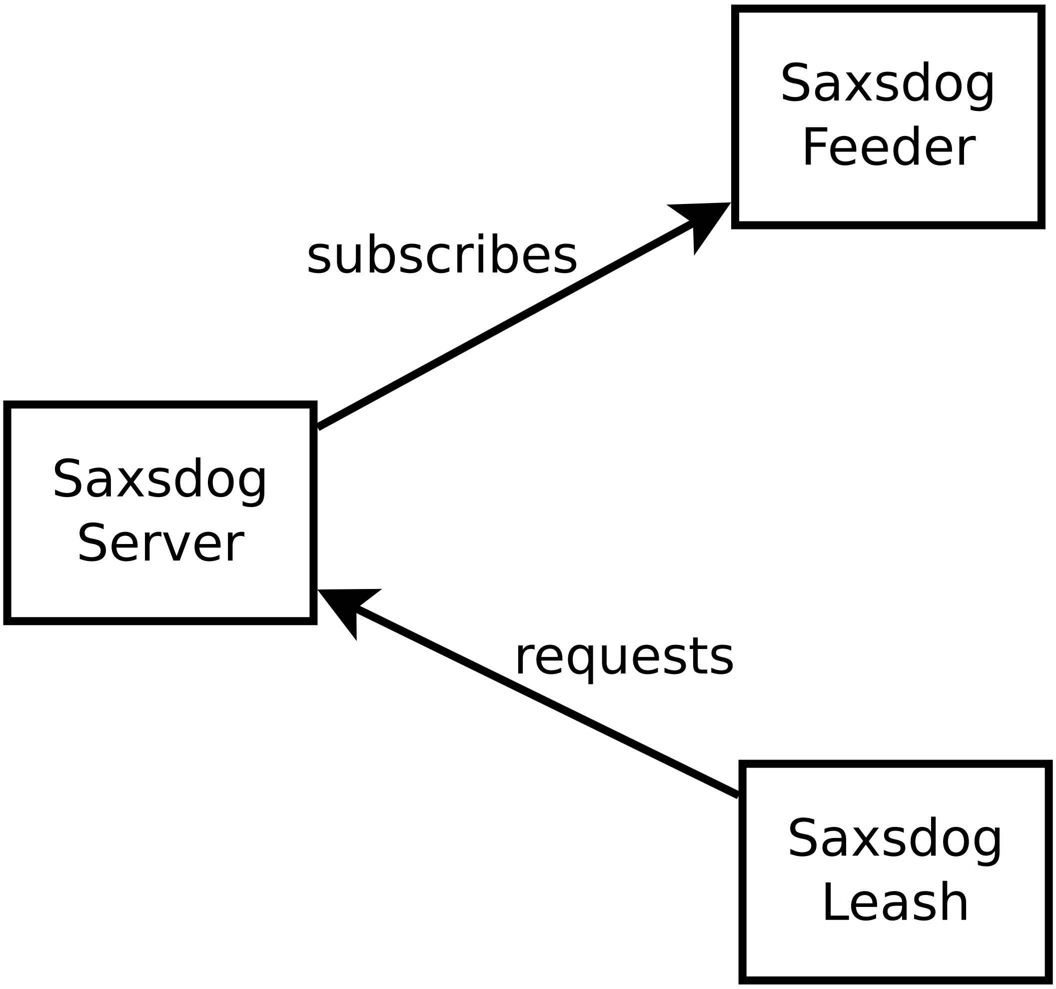
If the calibration is wrong you will for example see in the standard deviation. Like in this example. Here the beam center is wrong.

CHAPTER

FIVE

THE SAXSDOG NETWORK

The network may consist of 3 different services. The “Saxsdog Server” does the image processing. The “Saxs Feeder” publishes new file Events and the “Saxs Leash” controls an configures the server.



5.1 The SAXSNetwork configuration

The Saxsdog Server and the Saxsleash have a common configuration file, which tells them how to connect with each other and which also includes a shared secret for authentication. If you want two computers to connect via the Saxsleash you need to have a copy of the file on each of them.

To create such a configuration, use the command:

```
$ saxsnetconf
```

It will ask for the Feeder URL and for the Saxsdog Server URL. Then it will generate a random secret and save the file in file in `$Home/.saxdognetwork`. You will have to copy the file to the other computers you need to allow to connect to your network. The secret must be the same on all of them.

```
{
   "Server":"tcp://hostname:port",
   "Feeder":"tcp://hostname:port",
   "Secret":"Some large random string."
}
```

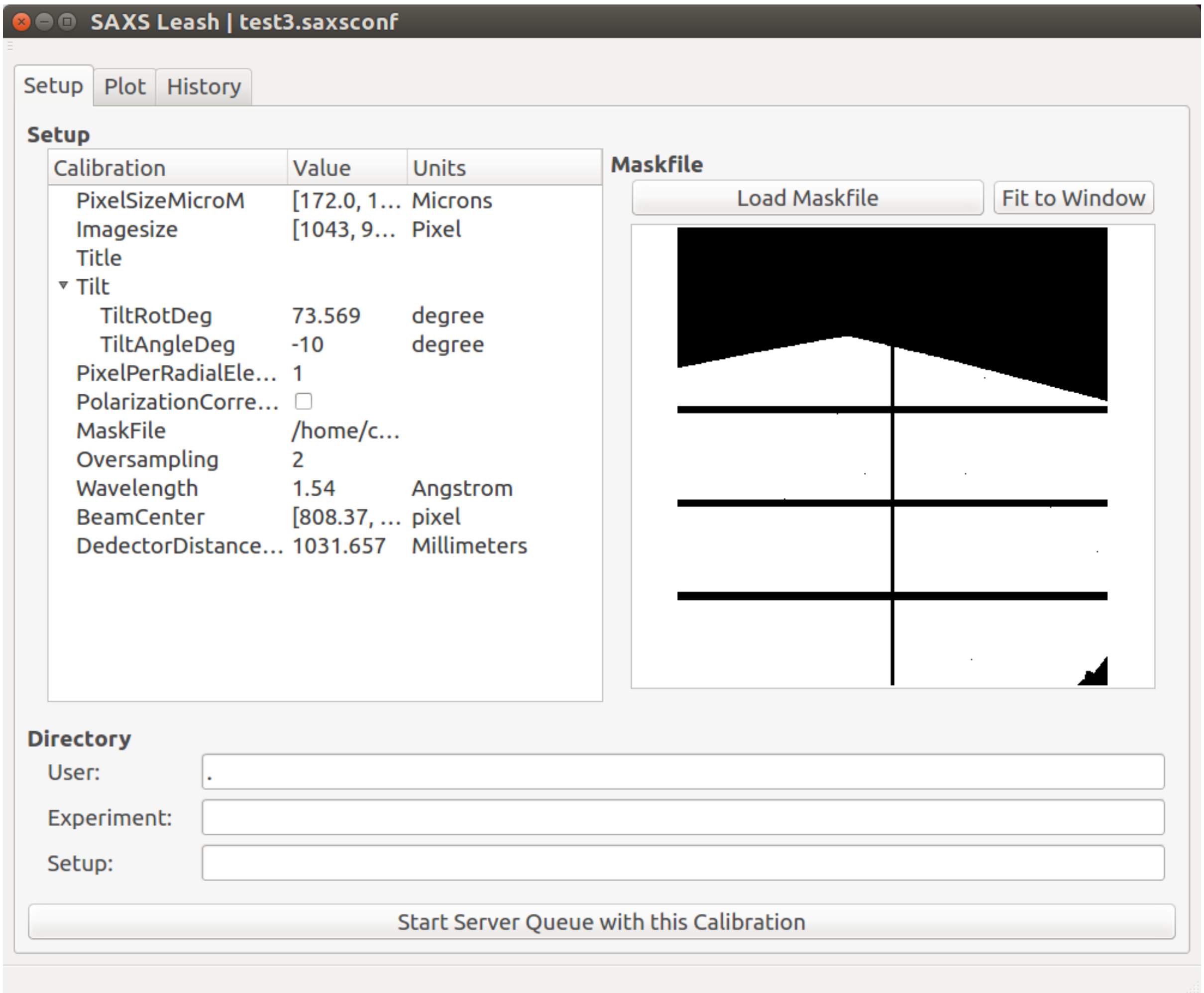
The authentication is done by hashing the request and the secret including a time stamp. The time stamp is checked if it lies within 900 seconds of the servers time.

5.2 The Saxsdog Server

The Saxdog Server is the program that is started on the processing computer (node). It may subscribe to a "new file" event service.

```
$ saxsdogserver --help
Usage: saxsdogserver [options] basedir

Options:
  -h, --help            show this help message and exit
  -p port, --port=port  Port to offer command service. Default is 7777.
  -t THREADS, --threads=THREADS
                        Number of concurrent processes.
  -f tcp://hostname:port, --feeder=tcp://hostname:port
                        Specify the URL of the new file event service (Saxsdog
                        Feeder)
  -w, --watch           Watch directory for changes, using file system events
                        recursively for all sub directories.
  -o OUTDIR, --out=OUTDIR
                        Specify output directory. Default is './out'.
  -i, --inplace         Files are written, in place, in the directory of the
                        image.
```

5.3 The Saxs Leash



The Leash Program is a GUI to load calibrations into the Saxdog Server and monitor the processing of the data. It provides a calibration editor, as mask preview and basic data import from *saxsconverter*.

The main window has 3 tab cards. The first is for setting up the server, the second to review the currently processed data and the third for basic statistics. The command to launch it is.

```
leash
```

5.4 Saxs Leash Commandline

The "Saxs Leash" client can issue the commands for the Saxsdog Server.

```
$ saxsleash --help
Usage: saxsleash close|abort|new|get|plot|plotdata|readdir|stat [options] [arguments]

Options:
  -h, --help            show this help message and exit
  -S tcp://HOSTNAME:PORT, --server=tcp://HOSTNAME:PORT
                        URL of "Saxsdog Server"
  -s N, --skip=N        plot: Skip first N points.
  -k N, --clip=N        plot: Clip last N points.
  -x TYPE, --xaxistype=TYPE
                        plot: Select type of X axis scale, might be
                        [linear|log|symlog]
```

```
  -y TYPE, --yaxistype=TYPE
                        plot: Select type of Y axis scale, might be
                        [linear|log|symlog]
```

Most of the command line options are about the `plot` command, but in order to visualize the processed data, one has to send the commands to setup a calibration.

5.4.1 New

```
$ saxsleash new cal.json data/AAA_integ.msk data/
```

The `new` command loads a calibration and starts the queue to receive new files. It requires 3 arguments:

1. Calibration file. as in *The Calibration File*,
2. mask file,
3. directory where the image files are or are going to be.

If there is a queue running, this command will abort the other one and replace it. One server can have only one queue at a time.

5.4.2 Plot

```
$ saxsleash plot
```

The `plot` command will grab the next image and show a plot of the result in a window. This command will be repeated until the user interrupts it with `Ctrl-C`.

5.4.3 Close

```
$ saxsleash close
```

Closes the queue. Which means, the server will process what is left in the queue but ignore all new files.

5.4.4 Abort

```
$ saxsleash abort
```

The `abort` command will close the queue and stop all data processing processes. It will only wait for each process to finish the picture they started before. The remaining pictures in the queue are ignored.

5.4.5 Stat

```
$ saxsleash stat
```

Return basic statistics data about the processes.

5.4.6 Read Dir

```
$ saxsleash readdir
```

This command will put all the images in the configured directory into the queue. This is useful to reprocess pictures.

5.5 The Saxsdog Network Protocol

5.5.1 The Saxsdog Server

The saxdog server can watch for filesystem events for himself or subscribe to a zmq service, the Saxsdog Feeder, that publishes new file names. The server can process the new images acording to one calibration. The server may only have one calibration at a time, it is not designed to be used by multiple users at the same time.

5.5.2 The Saxsdog Feeder

The "Saxsdog Feeder" service offers file events for subscription. It sould not do anny buffering or preselection, just send a new message when any new file was copied and is ready for processing. Also when a file is overwritten: Send a message. It should however, only send this event, when the file is completly written to the file system.

New file events are composed of the following message:

```
{
   "command":"new file",
   "argument":"/Path/to/file/"
}
```

The service must be a ZeroMQ `zmq.PUP` socket. This code is a simulation of the messages:

```
import zmq
import random
import sys
import time
import os
import json
from optparse import OptionParser

def startfeeder():
    parser = OptionParser()
    usage = "usage: %prog [options]  "
    parser = OptionParser(usage)
    parser.add_option("-p", "--port", dest="port",
                      help="Port to offer file changes service", metavar="port",default="")
    parser.add_option("-d", "--dir", dest="dir",
                      help="Directory to monitor", metavar="dir",default=".")
    (options, args) = parser.parse_args(args=None, values=None)



    context = zmq.Context()
    socket = context.socket(zmq.PUB)
    if options.port=="":
        conf=json.load(open(os.path.expanduser("~"+os.sep+".saxsdognetwork")))
        port=conf['Feeder'].split(':')[-1]
    else:
        port=options.port
    print "conecting:","tcp://*:%s" % port
    socket.bind("tcp://*:%s" % port)

    fileslist=[]
    if len(args)>0 and options.dir==".":
        dirtosearch =args[0]
    else:
        dirtosearch =options.dir
    for path, subdirs, files in os.walk(dirtosearch):
                for name in files:
                    if name.endswith('tif'):
```

```
                    fileslist.append( os.path.join(path, name))
    messageobj={"command":"new file","argument":""}
    while True:
        for file in fileslist:
            messageobj['argument']=file
            message=json.dumps(messageobj)
            socket.send(message)
            time.sleep(.01)


if __name__ == '__main__':
    startfeeder()
```

5.5.3 The Saxsdog Leash

The Saxsdog Leash is a user-facing controll interface. There, the user should enter new calibrations and specify the data directories connected to it. During the processing, it shows a graph of one of the current images.

It may send the following commands:

Close

Request:


```
{
  "command":"close queue",
  "time":1404979588.715198,
  "sign":"Signature generated for request"
}
```


Answer:


```
{
"result":"queue closed",
"data":{
   "stat": {
      "time interval": 0.8776118755340576,
      "queue length": 0,
      "frames per sec": 10.25510279760422,
       "images processed": 235, "pics": 9
      }
   }
}
```


Abort

Request:


```
{
   "command":"abort queue",
   "time":1404979588.715198,
   "sign":"Signature generated for request"
}
```


Answer:


```
{
   "result":"queue stopped emptied and closed",
   "data":{
      "stat": {
```

```
            "time interval": 0.8776118755340576,
            "queue length": 0,
            "frames per sec": 10.25510279760422,
            "images processed": 235,
            "pics": 9
        }
    }
}
```


New

Request:


```
{
    "command":"new queue",
    "argument":{
        "directory":"directory of data to take into account",
        "calibration":{},
        "maskbin":""
    },
"time":1404979588.715198,
"sign":"Signature generated for request"
}
```


Answer:


```
{ "result":"new queue",
  "data":{
         }

}
```


Plot

Request:


```
{   "command":"send plot",
    "time":1404979588.715198,
    "sign":"Signature generated for request"
}
```


Answer:


```
{
 "result":"plot data",
 "data":{
   "filename":"/name/.tiv" ,
   "stat": {
          "time interval": 0.8776118755340576,
          "queue length": 0,
          "frames per sec": 10.25510279760422,
          "images processed": 235,
          "pics": 9
          },
   "array":[[0],[0],[0]]
   }
}
```

Readdir

This puts all existing files in the queue directory into the queue again

Request:

```
{
   "command":"readdir",
   "time":1404979588.715198,
   "sign":"Signature generated for request"

}
```

Answer:

```
{
   "result":"directory refilled queue",
   "data":{
      "stat": {
         "time interval": 0.8776118755340576,
         "queue length": 0,
         "frames per sec": 10.25510279760422,
         "images processed": 235, "pics": 9
      }
   }
}
```

Stat

Get basic processing statistics.

Request:

```
{  "command":"stat","argument":{},
   "time":1404979588.715198,
   "sign":"Signature generated for request"}
```

Answer:

```
{
"data": {
   "stat": {
      "time interval": 711.6886098384857,
      "queue length": 0,
      "frames per sec": 9.972057866165134,
      "images processed": 7332,
      "pics": 7097
      }
    },
"result": "stat"
}
```

Error

In case of error in the Saxsdog Server it will return an error message:

```
{
"result":"Error",
"data":{"Error":"Error message"}
}
```

5.5.4 Request Schema

The '*' signifies a required Field.

Schema for requests from Saxs Leash to Saxs Server

Type object

Contains *command**, *argument*, *sign*, *time*

Required True

JSON Path

- *#*

Example JSON:

```
{"command": "close"}
```

command

Type string

values `[u'close', u'abort', u'new', u'get', u'plot', u'plotdata', u'readdir', u'stat']`

Required True

JSON Path

- *#* ['*command*']

Example JSON:

```
{"command": "close"}
```

argument

Type object

Contains *directory*, *calibration*

Required False

JSON Path

- *#* ['*argument*']

Example JSON:

```
{"argument": {}}
```

directory

Directory this queue is going to use. New files in other directories are going to be ignored.

Type string

Required False

JSON Path

- *#* ['*argument*']['*directory*']

Example JSON:

```
{"directory": ""}
```

calibration

Calibrarion data according to *The Calibration File*

Type object

Contains /

Required False

JSON Path

- *#* [’*argument*‘][’*calibration*‘]

Example JSON:

```
{"calibration": {}}
```

sign

Signature of request

Type string

Required False

JSON Path

- *#* [’*sign*‘]

Example JSON:

```
{"sign": ""}
```

time

time in seconds (pythons time.time())

Type number

Required False

JSON Path

- *#* [’*time*‘]

Example JSON:

```
{"time": 0}
```

5.5.5 Response Schema

The ‘*‘ signifies a required Field.

Schema for requests from Saxs Leash to Saxs Server

Type object

Contains *result**, *data**

Required True

JSON Path

- *#*

Example JSON:

```
{"data": {},"result": ""}
```

result

Type string

Required True

JSON Path

- *#* ['*result*']

Example JSON:

```
{"result": ""}
```

data

Type object

Contains *cal*, *Error*, *directory*, *stat*, *filename*, *array*

Required True

JSON Path

- *#* ['*data*']

Example JSON:

```
{"data": {}}
```

cal

Type object

Required False

JSON Path

- *#* ['*data*']['*cal*']

Example JSON:

```
{"cal": null}
```

Error

type object

Required False

JSON Path

- *#* ['*data*']['*Error*']

Example JSON:

```
{"Error": {}}
```

directory

Type string

Required False

JSON Path

- *#* ['*data*']['*directory*']

Example JSON:

```
{"directory": ""}
```

stat

type object

Contains *queue length*, *images processed*, *time interval*, *frames per sec*, *pics*

Required False

JSON Path

- *#* ['*data*']['*stat*']

Example JSON:

```
{"stat": {}}
```

queue length

Type integer

Required False

JSON Path

- *#* ['*data*']['*stat*']['*queue length*']

Example JSON:

```
{"queue length": 0}
```

images processed

Type integer

Required False

JSON Path

- *#* ['*data*']['*stat*']['*images processed*']

Example JSON:

```
{"images processed": 0}
```

time interval

Type number

Required False

JSON Path

- *#* ['*data*']['*stat*']['*time interval*']

Example JSON:

```
{"time interval": 0}
```

frames per sec

Type number

Required False

JSON Path

- *#* ['*data*']['*stat*']['*frames per sec*']

Example JSON:

```
{"frames per sec": 0}
```

pics

Type integer

Required False

JSON Path

- *#* ['*data*']['*stat*']['*pics*']

Example JSON:

```
{"pics": 0}
```

filename

Type string

Required False

JSON Path

- *#* ['*data*']['*filename*']

Example JSON:

```
{"filename": ""}
```

array

Type array() items: array

Required False

JSON Path

- *#* ['*data*']['*array*']

Example JSON:

```
{"array": null}
```

CHAPTER SIX

SAXS MODULE API

class `SAXS.calibration` (*config*)

This class represents a calibration for SAXS diffraction. After initialization, the `integrate()` method can compute the radial intensity very fast.

Parameters **config** (*string*) – is the path to the *root*:

`integrate` (*image*)

Integrate a picture.

Parameters **image** (*numpy.array(dim=2)*) – Sensor image to integrate as 2d *NumPy* array

Returns Returns Angle and intensity vector as a tuple (angle,intensity)

`integratechi` (*image*, *path*)

Integrate and save to file in "chi" format.

Parameters

- **image** (*np.array()*) – Image to integrate as numpy array
- **path** (*string*) – Path to save the file to

Returns Scattering curve data as numpy array

`integrateerror` (*image*)

Integrates an image and computes error estimates.

Parameters **image** (*np.array()*) – Image to integrate as numpy array

Returns The intensity the standard deviation and the Poisson statistics error in a numpy array.

`plot` (*image*, *outputfile=''*, *startplotat=0*, *fig=None*)

Plot integrated function for image in argument.

Parameters

- **image** (*numpy.array(dim=2)*) – Sensor image to integrate as 2d *NumPy* array
- **outputfile** (*string*) – File to write plot to. Might be any image format supported by matplotlib.
- **startplotat** (*integer*) – radial point from which to start the plot

`SAXS.calc_theta` (*r*, *phi*, *d*, *tilt*, *tiltdir*)

Calculates the difraction angle from pixel coordinates. It does work when called with arrays. See *The Geometry*

Parameters

- **r** (*float*) – Distance to beamcenter.
- **phi** (*float*) – Angle[rad] from polar sensor plane coordinates.
- **d** (*float*) – distance to difraction center.
- **tilt** (*float*) – Angle[rad] of sensor plane tilt.

- **tiltdir** (*float*) – Angle[rad] of direction of tilt.

Returns theta

SAXS.**scalemat** (*Xsize*, *Ysize*, *ov*)

Computes a scaling projection for use in computing the pixel weights for integration

Parameters

- **Xsize** (*int*) – Picture size in X direction.
- **Ysize** (*int*) – Picture size in Ydirection.
- **ov** (*int*) – Number of oversampling ticks in x ynd y direction
- **corr** (*array*) – Polarizationn an other correction factors

Returns sparce matrix toing the scaling

SAXS.**openmask** (*config*)

Open the mask file especialy the *.msk file. Unfortunately there is no library module for msk files available also no documentation. So, for the msk file, we have a very brittle hack it works for our sensor. Nevermind any other resolution or size.

Parameters **config** (*object*) – Calibration config object.

Returns Mask as logical numpy array.

SAXS.**convert** ()

This implements the functionality oft *The Converter*. It parses the commandline options and converts the Fit2d info file to the JSON data used by the SAXS.callibration class.

SAXS.**saxsdog** ()

This implements the functionality of *The Saxsdog*

class SAXS.**imagequeue** (*Cal*, *options*, *args*)

This class keeps a queue of images which may be worked on in threads.

Parameters

- **Cal** (*SAXS.calibration*) – The SAXS Calibration to use for the processing
- **options** (*optparser*) – The object with the comandline options of the saxsdog
- **args** (*list*) – List of command line options

fillqueuewithexistingfiles ()

Fill the queue with the list of images that is already there.

start ()

Start threads and directory observer.

class SAXS.**Server** (*conf*)

class to manage a saxsdog server

SAXS.**initcommand** (*options*, *arg*, *conf*)

Interface for issuing leash commands

SAXS.**validateResponse** (*message*)

Validate response from saxsdog server against the schema.

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