The European Synchrotron

Welcome to the T7: Data reduction for scattering experiments

ESRF user meeting 2021, digital edition

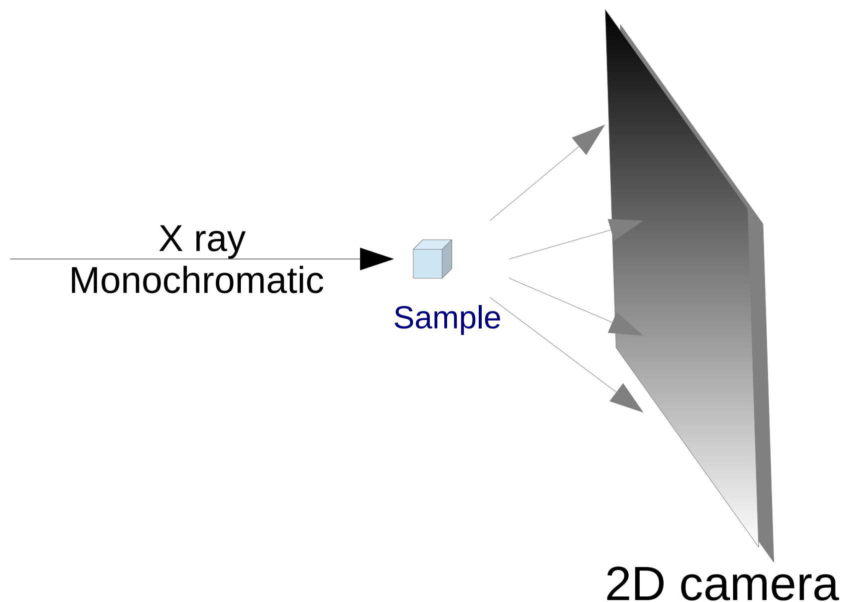
Data reduction tools for scattering experiments

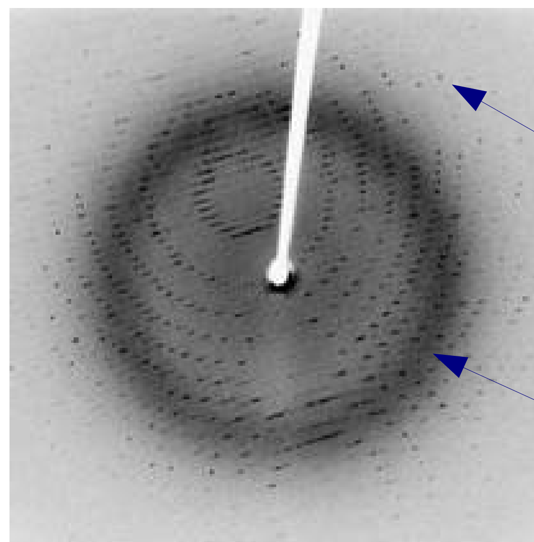
Jérôme Kieffer
Online data analysis @ ESRF

Layout

- **Power diffraction and scattering of X-Rays**
- **What is azimuthal integration of 2D detector data ?**
- **The need for faster data processing …**
- **… without compromising quality**
- **PyFAI:**
  - Ecosystem and user community
  - Within the *silx* collaboration
- **Conclusions**

X-ray scattering experiments





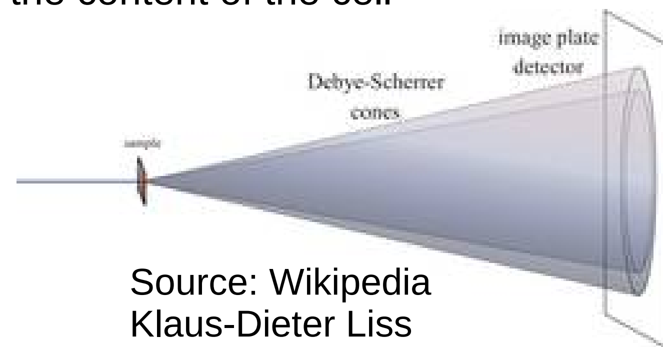
Source: Wikipedia
CC-BY-SA: Jeff Dahl

Bragg spots: diffraction from single crystal

Ice ring: diffraction from powder

- **Light is reflected as on mirrors:**
  - No energy change (elastic scattering)
  - Direction of diffracted beam depends on the crystalline cell and its orientation
  - Intensity of the diffracted beam depends on the the content of the cell

  → Bragg's Nobel price in 1915 $n\lambda = 2d \sin\theta$,
- **Multiple small crystals (powder)**
  - Isotropic cones gives ellipses when intersected by a flat detector



Source: Wikipedia
Klaus-Dieter Liss

Powder diffraction and small angle scattering

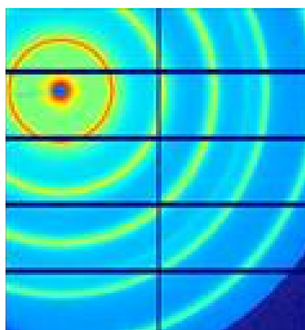
Application of powder diffraction:

- Phase identification (mapping)
- Crystallinity
- Lattice parameters
- Thermal expansion
- Phase transition
- Crystal structure
- Strain and crystallite size

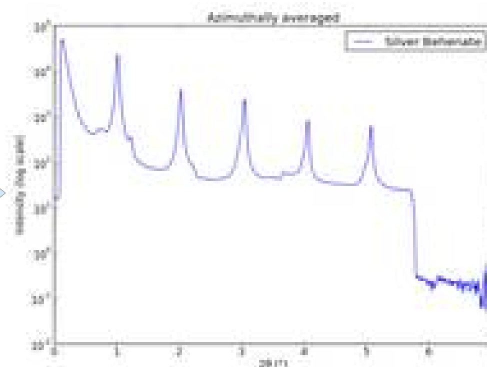
Application of small angle scattering

- Micro/nano-scale structure
- Particle shape
- Protein domains
- Protein folding
- Colloids

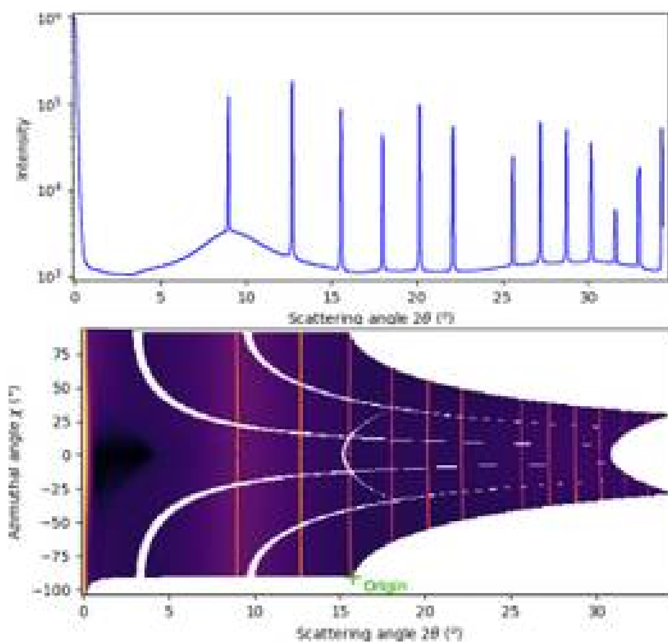
- **Both rely on the same transformation: 2D image → azimuthal average**

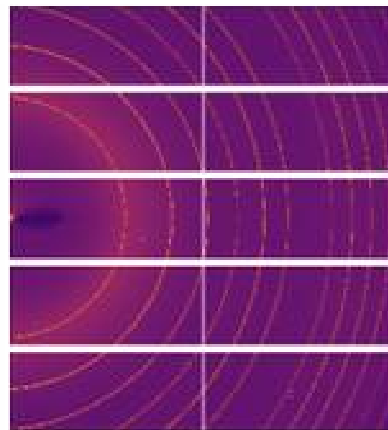


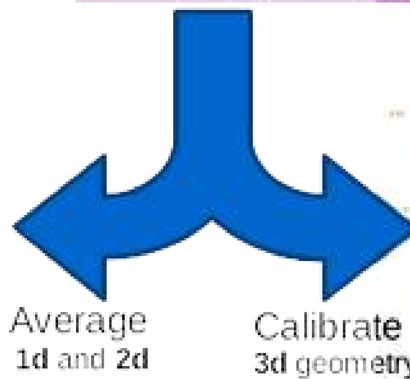
Azimuthal integration

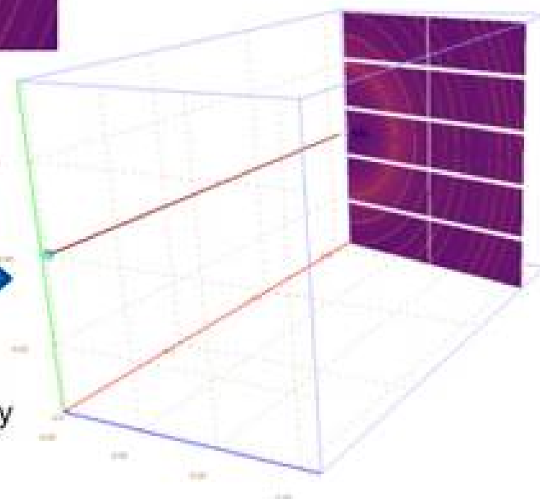


Fast Azimuthal Integration using Python









- **Why Python ?**
  - It is the main programming language used in science and at ESRF: Bliss, PyMca, …
- **But isn't Python slow ?**
  - Maybe … Python is just a convenient interface, what matters is written in C & compiled

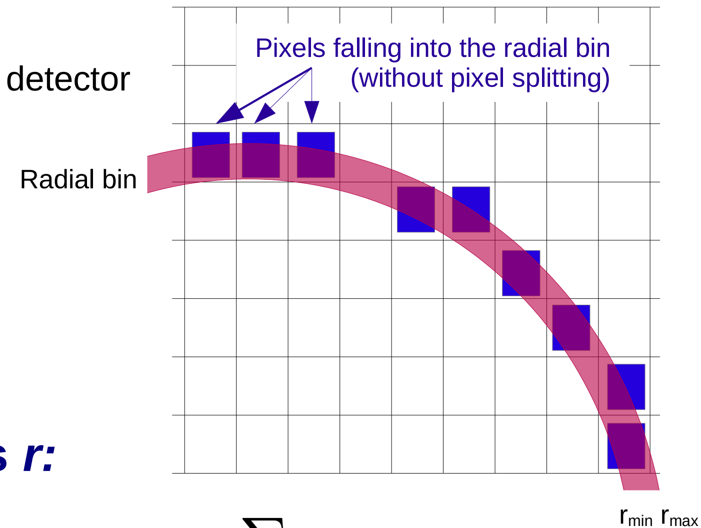
How it works

- **Pixel-wise corrections:**

$$I_{cor} = \frac{I_{raw} - I_{dark}}{F \cdot \Omega \cdot P \cdot A \cdot I_0} = \frac{signal}{normalization}$$

Where: I_0 is the incoming flux (pixel independent)

  - I_{raw} and I_{dark} are the signal measured from the detector
  - F is the flat-field correction
  - Ω is the solid angle for this pixel
  - P is the polarization factor
  - A is the parallax correction factor



- **Averaging over a bin defined by the radius *r*:**
  - Need for pixel splitting?
  - c_i being the fraction of the pixel i contributing to bin_r

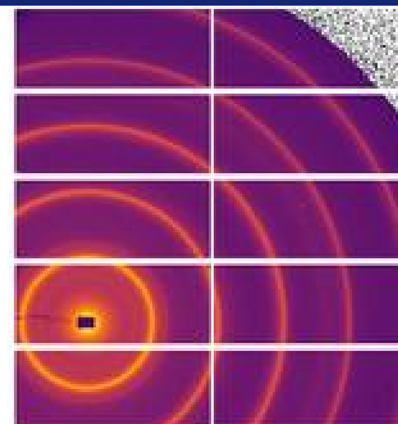
$$\langle I \rangle_r = \frac{\sum_{i \in bin_r} c_i \cdot signal_i}{\sum_{i \in bin_r} c_i \cdot normalization_i}$$

- **Associated uncertainty propagation:**
  - Assuming there is no correlation between pixels
  - Pixel splitting can create correlation between bins...

$$\sigma(\langle I \rangle_r) = \frac{\sqrt{\sum_{i \in bin_r} c_i^2 \cdot variance_i}}{\sum_{i \in bin_r} c_i \cdot normalization_i}$$

Math from Kieffer et al.; *J. Synch. Radiation* (2020)
https://doi.org/10.1107/S1600577520000776

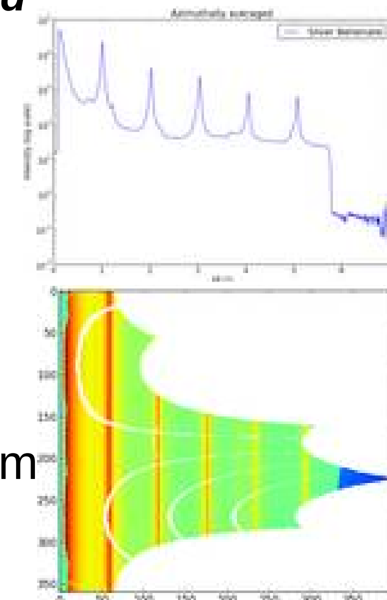
Concepts in PyFAI



- **Image**

  2D array of pixels as *numpy* array
  read using *silx, fabio, h5py,* ...

- **Azimuthal integrator: core object**
  - **powder diagram using *integrate1d***
  - **"cake" image, azimuthally regrouped using *integrate2d***



- **Detector**

  - **Calculates the pixel position (center and corners)**
  - **Calculates and stores the mask of invalid pixels.**

    → **saved as a HDF5 file**

- **Geometry**

  Position of the detector from the sample & incoming beam

  → **saved as *PONI*-file**

http://www.silx.org/doc/pyFAI/dev/geometry.html#detector-position

Geometry in pyFAI

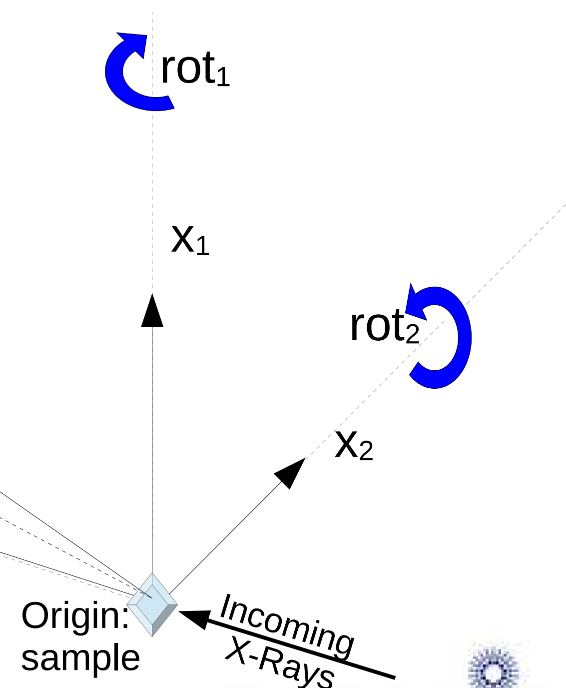
Parameters:
* 3 distances in meters: dist, $poni_1$, $poni_2$
* 3 rotations in radians: rot_1, rot_2, rot_3
+ wavelength || energy

} *PONI*-file

Area detector

From the sample's point of view, looking towards the detector :

↗ rot_1: moves detector → to the right
↗ rot_2: moves detector ↓ downwards
↗ rot_3: moves detector ↷ clockwise



d_1
d_2
d_3
Point Of Normal Incidence :
PONI = (P_1, P_2, P_3=0)
Beam center
Scattered beam
Distance
rot_3
x_3
2θ

Detector's origin:
lower left, looking from
the sample

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Calibration in pyFAI

- **Geometry is best determined from the analysis of a known reference sample**
- **This calibration step is preferred to measuring distances and beam center position**
  - The prerequisite is:
    - **detector geometry and mask,**
    - **calibrant (LaB_6, CeO_2, AgBh, …)**
    - **wavelength or energy used**
  - Only the position of the detector and the rotation needs to be refined:
    - **3 translations: dist, $poni_1$ and $poni_2$**
    - **3 rotations: rot_1, rot_2, rot_3**
- **It is divided into 4 major steps:**
  1) Extraction of groups of peaks
  2) Identification of peaks and groups of peaks belonging to same ring
  3) Least-squares refinement of the geometry parameters on peak position
  4) Validation by a human being of the geometry
- **PyFAI assumes this setup does not change during the experiment**

Tutorial 1:

http://www.silx.org/doc/pyFAI/dev/usage/cookbook/calib-gui/index.html

What happens during an integration

1) **Get the pixel coordinates from the detector, in meter.**

   There are 3 coordinates per pixel corner, and usually 4 corners per pixel.

   1Mpix image → 48 Mbyte !

2) **Offset the detector's origin to the PONI and rotate around the sample**

3) **Calculate the radial (2θ) and azimuthal (χ) positions of each corner**

4) **Assign each pixel to one or multiple bins.**

   If a look-up table is used, just store the fraction of the pixel.

   Then for each bin sum the content of all contributing pixels.

5) **Histogram bin position with associated intensities**

6) **Histogram bin position with associated normalizations (i.e. solid angle)**

7) **Return bin position and the ratio of sum of intensities / sum of norm.**

   → **Tutorial 2**

Example of simplified implementation in Python

Common initialization step:

In [1]:
```
import numpy
npt = 1024
y,x  = numpy.ogrid[-512:512,-512:512]
radius = (x*x+y*y)**0.5
rmax = radius.max()+0.1
data = numpy.random.random((1024,1024))
```

Naive approach integration using corona extraction with masks:

In [2]:
```
%%time
res_loop = numpy.zeros(npt)
for i in range(npt):
    rinf = rmax * i / npt
    rsup = rinf + rmax / npt
    mask = numpy.logical_and((rinf <= radius),(radius < rsup))
    res_loop[i] = data[mask].mean()
```

```
CPU times: user 1.04 s, sys: 0 ns, total: 1.04 s
Wall time: 1.04 s
```

Vectorized version using histograms:

In [3]:
```
%%time
count_of_pixels = numpy.histogram(radius, npt, range=[0,rmax] )[0]
sum_of_intensities = numpy.histogram(radius, npt, weights=data, range=[0,rmax])[0]
res_vec = sum_of_intensities / count_of_pixels
```

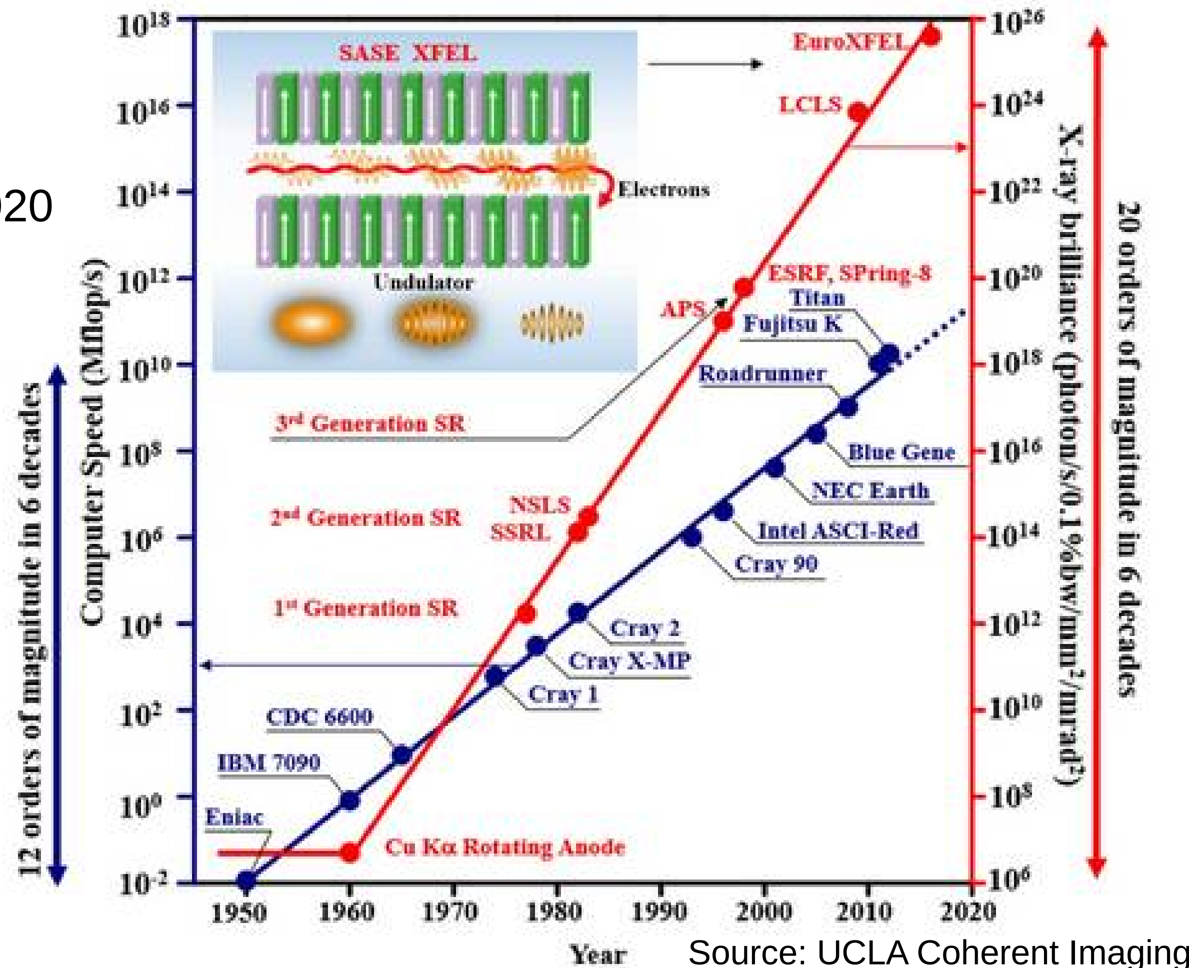
```
CPU times: user 19.5 ms, sys: 1.44 ms, total: 20.9 ms
Wall time: 19.4 ms
```

In [4]:
```
# Speed-up: 50x, validation:
numpy.allclose(res_loop, res_vec)
```

Out[4]: True

But speed does matters ...

- **New EBS source**
  - 50x brighter
  - User mode since 2020



Source: UCLA Coherent Imaging

- **Faster detectors**
  - Eiger2 detector (2-20 kHz)
  - Jungfrau detector (2 kHz)

→ Stream limited to 2 GB/s/detector !

The gap between computing and acquisition grows

- **Most other codes use the same algorithm based on histograms … … and reach the same speed:**
  - Fit2D written in Fortran
  - SPD written in C
  - Foxtrot written in Java

- **The algorithm needs to be changed !**
  - Histograms **cannot** easily/efficiently be parallelized !
  - Re-develop based on parallel algorithms
    → CSR sparse matrix dot product is many-core friendly
    Described in https://arxiv.org/abs/1412.6367v1

Look-up table integration using only Python

Using a Sparse matrix multiplication

Those multiplication can take advantage of parallel hardware unlike histogram which require costly *atomic* operations. This trick is called "scatter to gather" transformation in parallel programming.

In [5]:
```
%%time
from scipy.sparse import csc_matrix
positions = numpy.histogram(radius, npt, range=[0,rmax] )[1]
row = numpy.digitize(radius.ravel(), positions) - 1
size = row.size
col = numpy.arange(size)
dat = numpy.ones(size, dtype=float)
csr = csc_matrix((dat, (row, col)), shape = (npt, data.size))
print(csr.shape)
```

```
(1024, 1048576)
CPU times: user 60.5 ms, sys: 6.21 ms, total: 66.7 ms
Wall time: 69.7 ms
```

In [6]:
```
%%time
count_csr = csr.dot(numpy.ones(data.size))
sum_csr = csr.dot(data.ravel())
res_csr = sum_csr / count_csr
```

```
CPU times: user 3.11 ms, sys: 3.1 ms, total: 6.21 ms
Wall time: 4.69 ms
```

In [7]:
```
# Speed-up: 5x vs histograms, validation:
numpy.allclose(res_csr, res_vec)
```

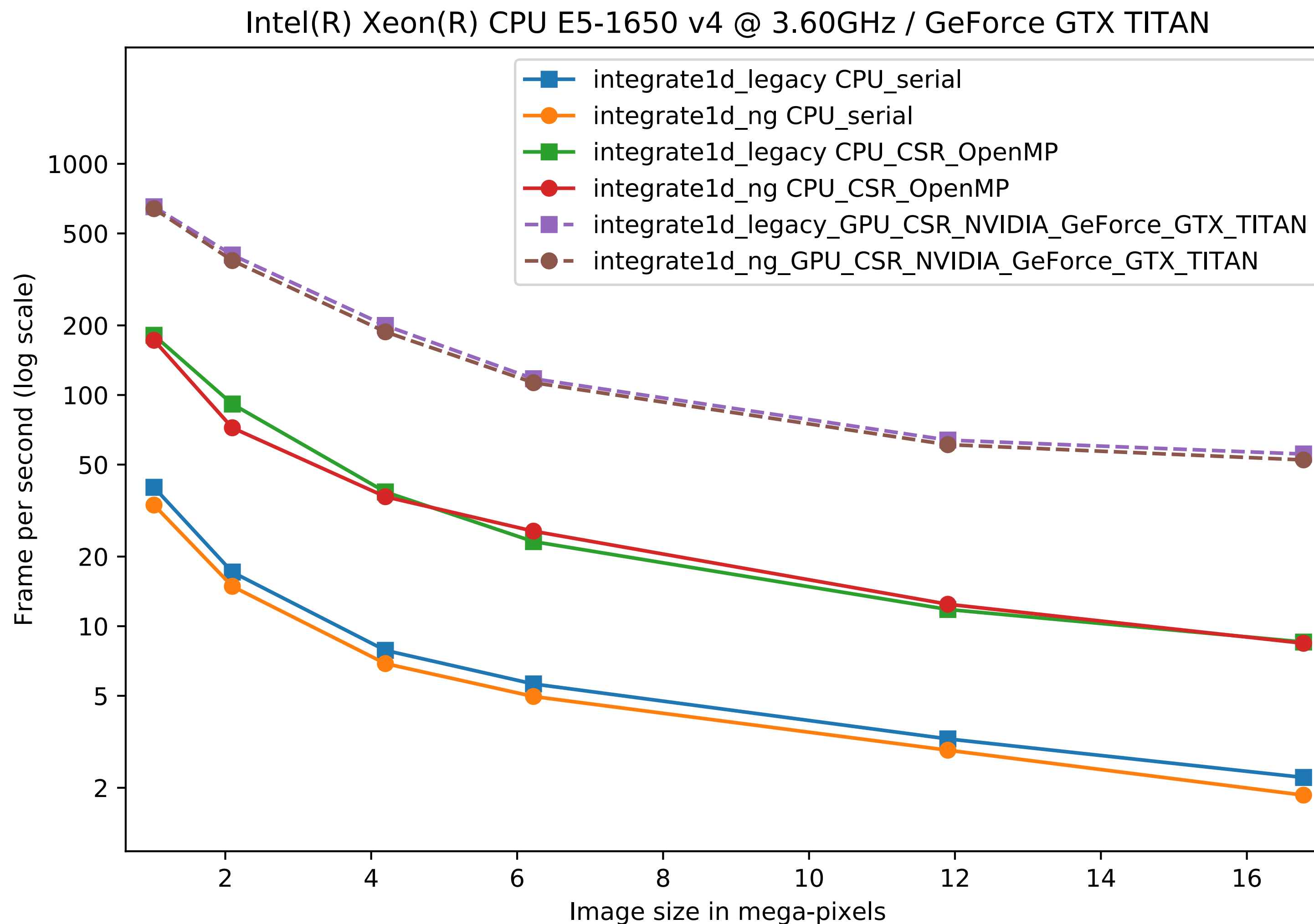
Out[7]: True

Sources of this demo available on:
https://gist.github.com/kif/ab37c61351d8238f90245b0afb56192e

Advantages of *histograms* vs *CSR* matrix multiplication

	Histograms	Sparse matrix multiplication
Pro	• **Easier to understand** • **Low memory consumption** • **Fast initialization**	• **Faster, even on a single core** • **Many-core friendly** – OpenMP and OpenCL
Con	• **Pretty slow** • **Hardly parallelizable**	• **Slower initialization** • **The sparse matrix can be large**
Rule of thumb:	< 5 frames	≥ 5 frames

Benchmark: Let’s speak about speed !

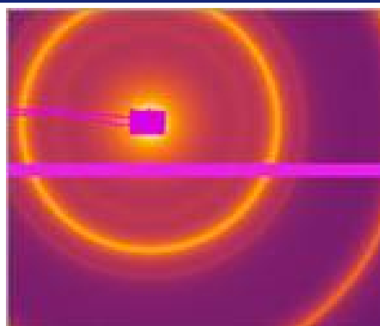


7 year old workstation with high-end graphics card

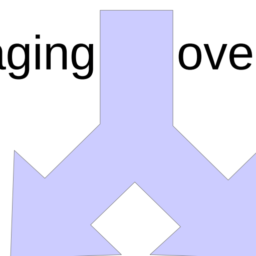
High frequency noise issue

Where pixel splitting comes back

Example with SAXS data integrated in 2D



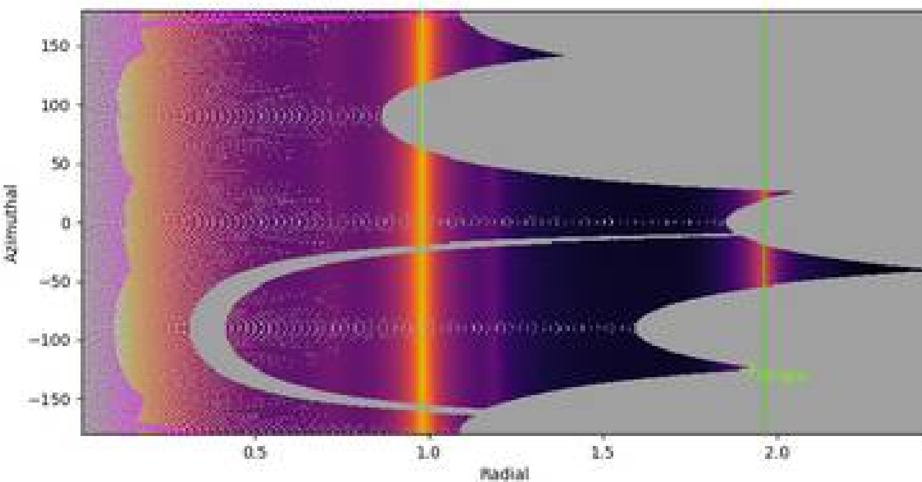
Pilatus 200k:
~500 x 400 pixels

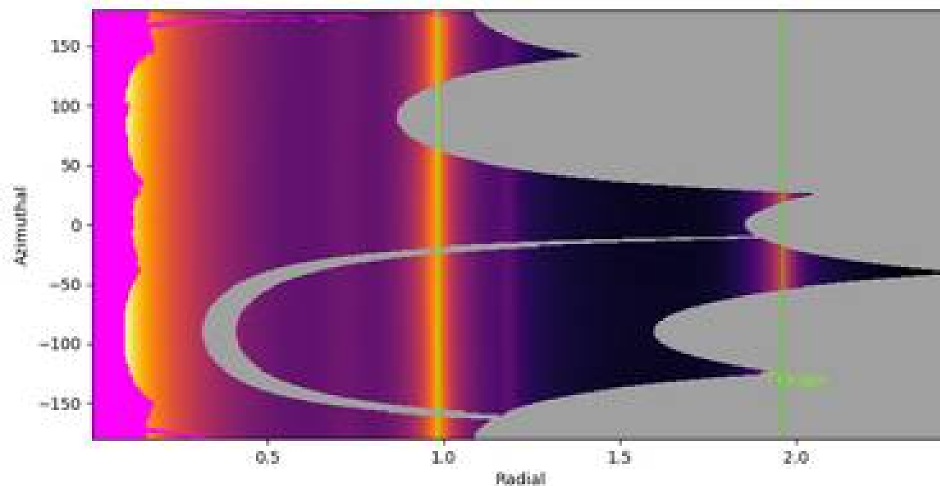


2D averaging over 512x360 bins

Without pixel splitting

With pixel splitting

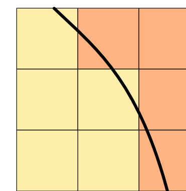




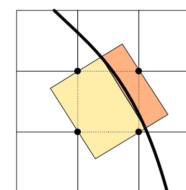
⚠ creates bin cross-correlation ⚠

Pixel splitting schemes available in pyFAI

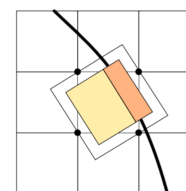
- **No pixel splitting: default histograms**
  - Each pixel contributes to a single bin of the result
  - No bin correlation but more noisy
  - The pixel has no surface: sharpest peaks



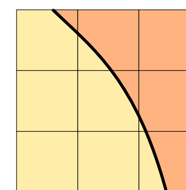
- **Bounding-box pixel splitting**
  - The smoothest integrated curve
  - Blurs a bit the signal



- **Pseudo pixel splitting**
  - Scale down the bounding box to the pixel area, before splitting.
  - Good cost/precision compromise, similar to FIT2D



- **Full pixel splitting**
  - Split each pixel as a polygon on the output bins.
  - Costly high-precision choice



Impact of pixel splitting on integration speed

- **Histogram based algorithms:**
  - Each pixel is split over the bins it covers.
  - The corner coordinates have to be calculated (4x slower initialization)
  - The slow down is function of the oversampling factor, for every image
- **Sparse matrix multiplication based algorithms**
  - The sparse matrix contains already the pixel splitting scheme
  - Longer initialization time related to the oversampling factor
  - There are *NO* performance penalty on the integration itself

All those consideration are independent of the programming language

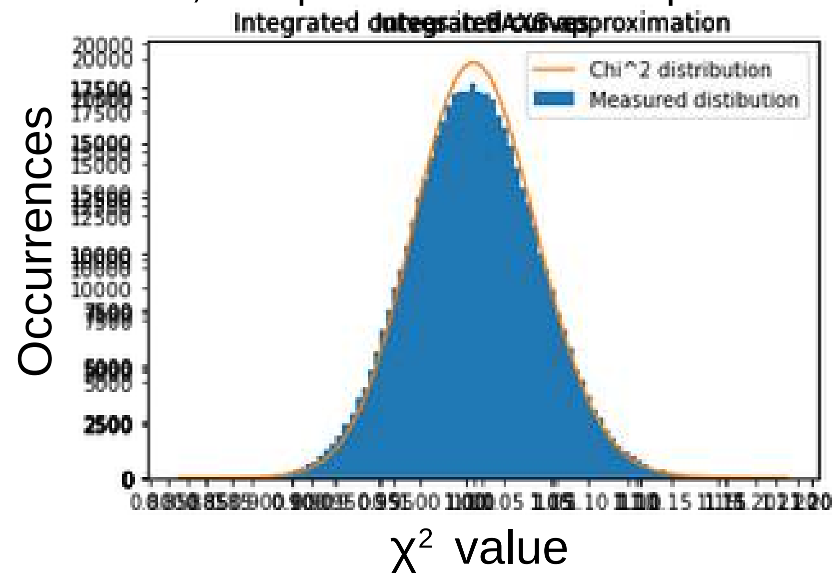
Nevertheless, Python which is interpreted is expected to be 1000x slower than:

- compiled code like C, C++, Fortran, ...
- JIT compiled code like Java, Julia or numba

Impact of averaging & pixel splitting on precision

- **Test case:**
  - SAXS-like data, 1000 frames with synthetic distribution, 5e5 pairs of curves compared.

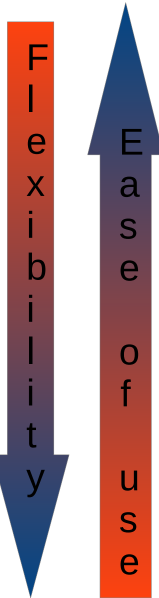
- **No splitting / No intensity correction**
- **No splitting / intensity correction prior int.**
- **No splitting / intensity correction while int.**
- **BBox splitting / intensity correction while…**
- **Full splitting / intensity correction while…**



- **This demonstrates that:**
  - Intensity correction needs to be performed together with integration, not before
    - **Fixed since PyFAI v0.20.0 (1d integration)**
  - Pixel splitting
    - **Actually creates bin-correlation**
    - **Affects precision of the propagated uncertainties**
- **Full demonstration at:** **http://www.silx.org/doc/pyFAI/0.20.0/usage/tutorial/Variance/Variance.html**

Layers in pyFAI

- **Applications level:**
  - GUI applications: **pyFAI-calib2, pyFAI-integrate, diff_map**
  - Scriptable applications:**pyFAI-average**, pyFAI-saxs, pyFAI-waxs, diff_tomo, ...



- **Python interface:**

  - Top level: azimuthal integrator
  - Mid level: calibrant, detector, geometry, calibration
  - Low level: rebinning/histogramming engines (Cython + OpenMP or OpenCL)

- **Question: how to define the right balance ?**

  It is up to you !

- Applications in **bold** will be demonstrated in the introduction tutorial.

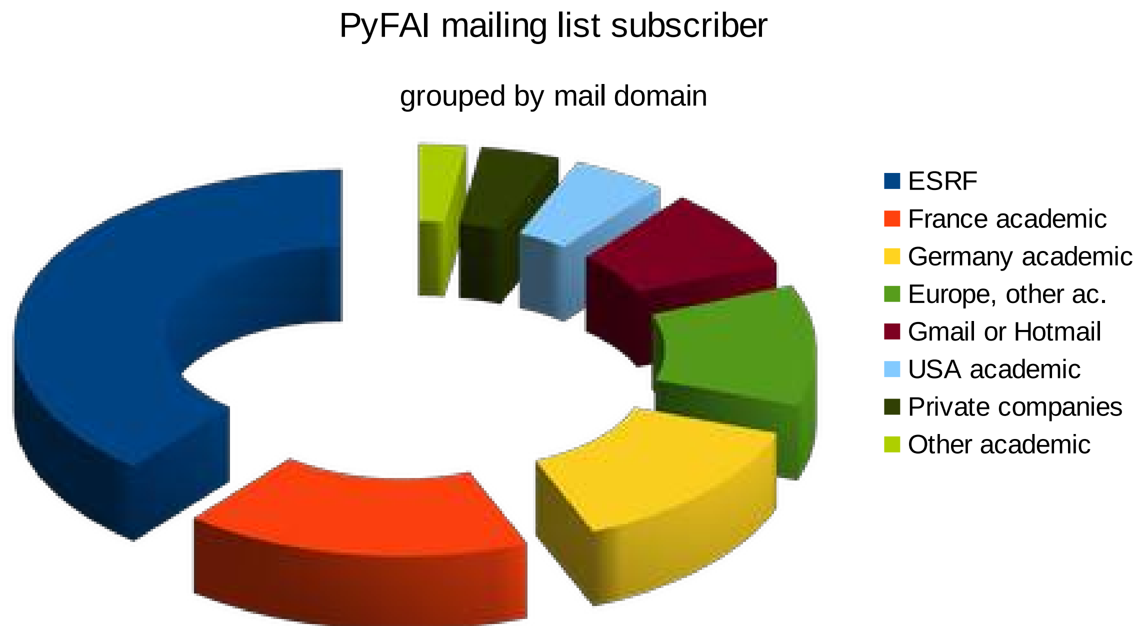
Silx & pyFAI

PyFAI is yet another azimuthal integration tool

- **Written in Python (compatible with ~~2.7, 3.5~~, 3.6, 3.7, 3.8 & 3.9)**
  - Free, fast and portable
  - MIT licensed: compatible with both science & business
  - Part of the *silx* collaboration on data analysis initiated by ESRF
  - Graphical user interface using Qt5
- **Open to collaboration**
  - About 20 direct contributors,
    - **Mainly from ESRF**
    - **Also from other synchrotrons and XFELs:**
      - Soleil, NSLS-II, Petra-III, Eu-XFEL
    - **Industrial contributions from Xenocs**
  - Used by > 50 other projects from all the largest X-ray sources in the world
    - EuXFEL, SLAC, ALS, APS, NSLS-II, Petra-III, Soleil, Diamond, SLS, Max-IV, …
- **Avoid compromises: no difficulty is hidden**
    - **science does not suffer approximations**

User community of pyFAI

- **PyFAI is used in most European and American synchrotons/FELs**



- **User support is provided via the mailing list: pyFAI@esrf.fr**
  - Archived on http://www.silx.org/lurker/list/pyfai.en.html
  - 142 people subscribed to the list 2021 (was 137; 132; 112)
  - limited activity (~1 thread/month)

http://www.silx.org/doc/pyFAI/dev/project.html#getting-help

Reasons to choose pyFAI

- **Faster than others**
  - First tool using sparse matrix multiplication to perform integration
  - All computation intensive kernels are ported to C, C++ or OpenCL
  - PyFAI is the only azimuthal integration tool benefiting from GPU
- **More versatile (hackable) than other**
  - Many integration space already exists ...
    - **you can add your own easily**
  - Its geometry is so generic it matches any configurations
    - **SAXS, WAXS, moving detectors …**
  - Most detectors are already defined
    - **Each detector can be adapted, and saved in a Nexus file**
  - It has a nice user interface thanks to Valentin !
- **Part of the *silx* collaboration**
  - Bus-count slightly larger than one !

silx-kit: join efforts, share the maintenance

Fork me on GitHub

silx

Scientific Library for eXperimentalists

Resources

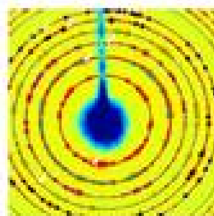
- silx on GitHub
- Wheels and source on PyPI
- Installation instructions

Documentation

- Latest release
- Nightly build
- v0.3.0
- v0.2.0
- v0.1.0

pyFAI

Fast Azimuthal Integration in Python



Resources

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FabIO

I/O library for images produced by 2D X-ray detector

Resources

- FabIO on GitHub
- Wheels and source on PyPI
- Installation instructions

Documentation

- Latest release
- Nightly build

silx-kit: Shared development around:

- **User interface**
  - Common interface to Qt and soon jupyter-lab
  - Common visualization widgets
- **GPU computing**
  - Common initialization
- **Scientific data analysis**
  - Multi-threaded implementation of core algorithms

Management of the *silx-kit* project

- **Public project hosted at github**

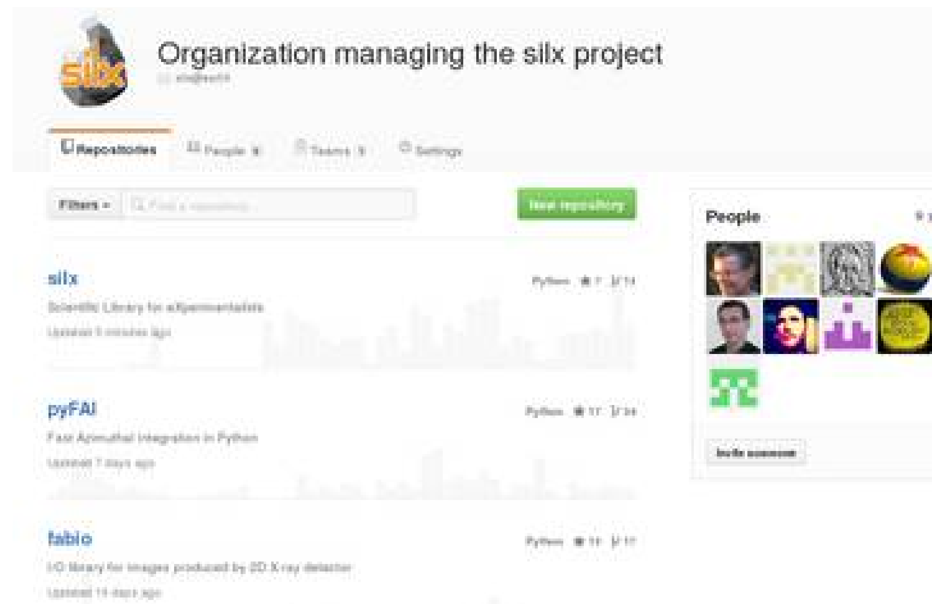
  https://github.com/silx-kit/silx

- **Continuous testing**

  Linux, Windows and macOS

- **Nightly builds**
  - Debian packages
- ~~**Weekly meetings**~~
- ~~**Quarterly releases**~~
- ~~**Code camps before release**~~
- **Continuous documentation**

  http://www.silx.org/doc/silx/



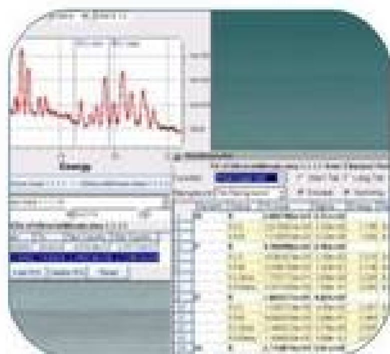
silx-kit project and the *silx* library

Was Pierre Knobel

Mainly Jérôme Kieffer

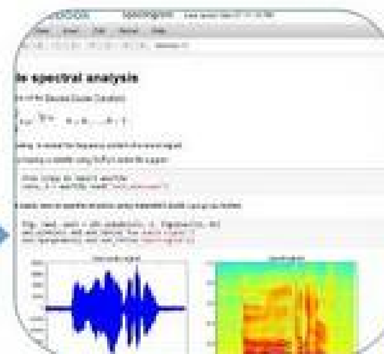
Mainly Loïc Huder

Online data analysis
e.g. PyFAI



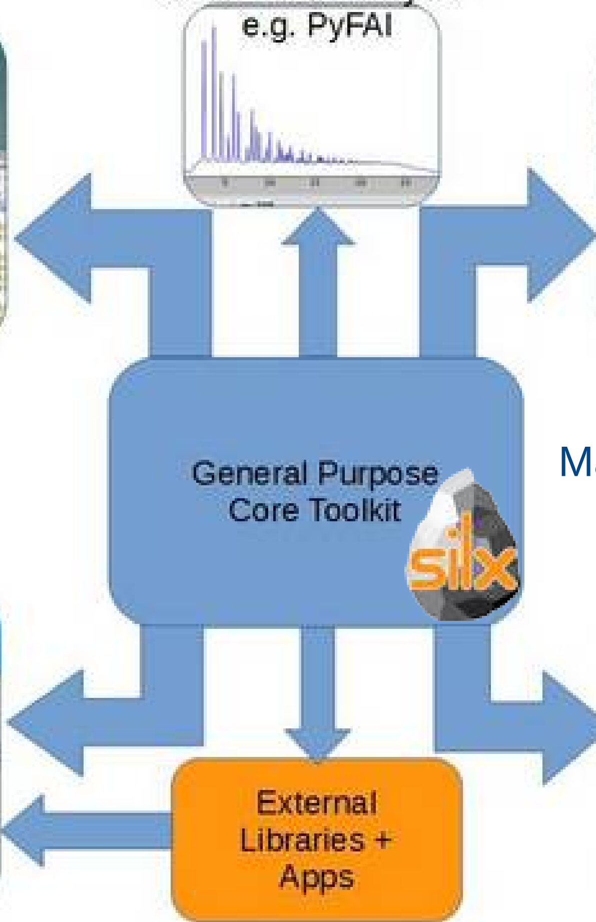
Standard Apps e.g.
PyMCA, PyDIF

… and Valentin Valls

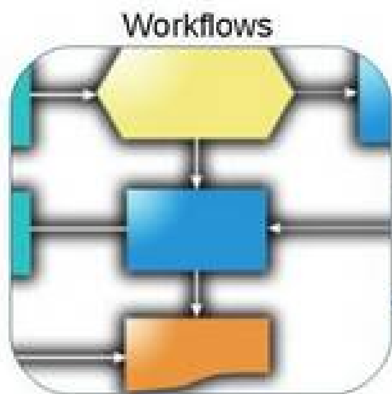


Ipython Notebook

Mainly Thomas Vincent



Workflows

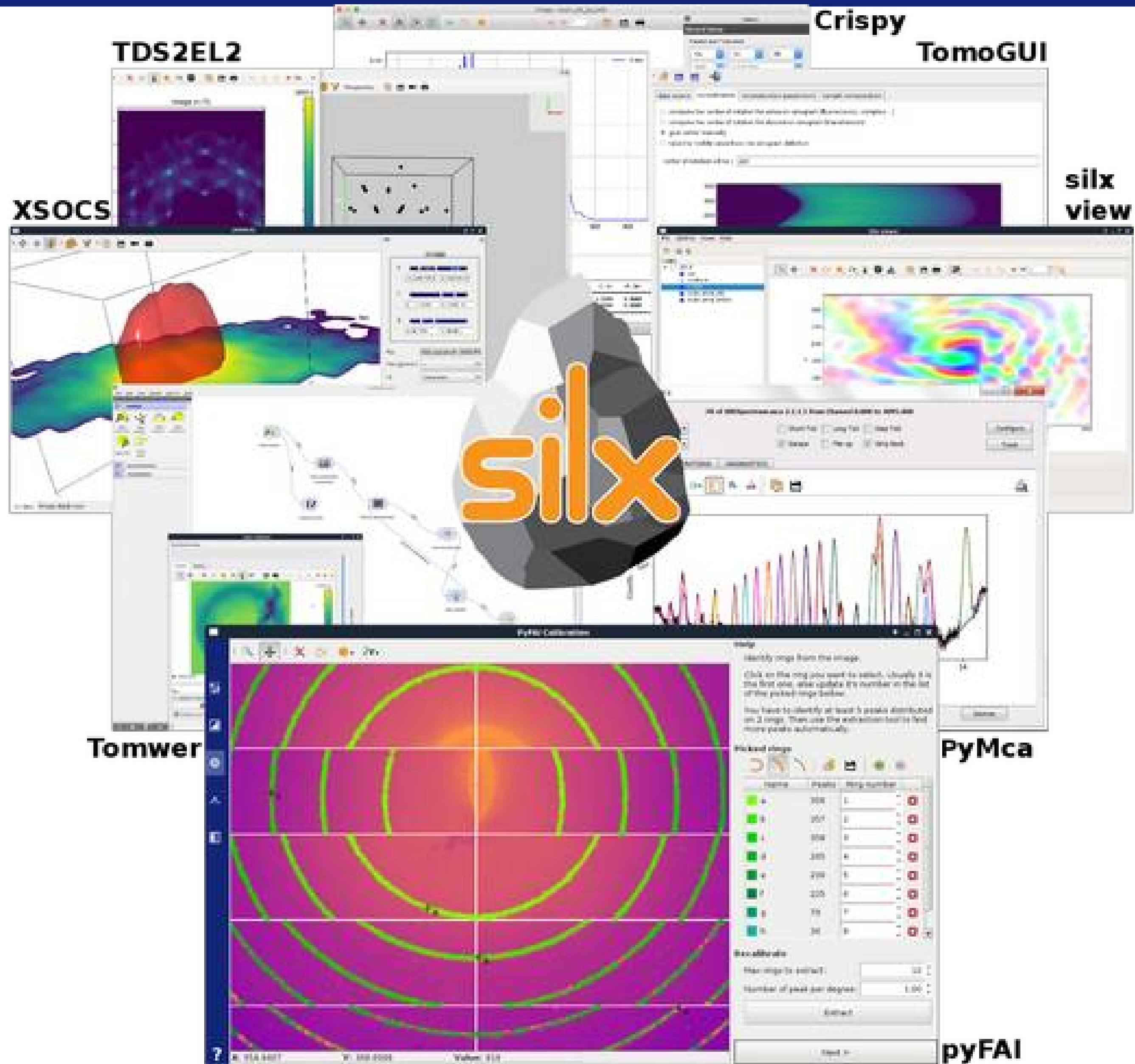


Mainly Henri Payno

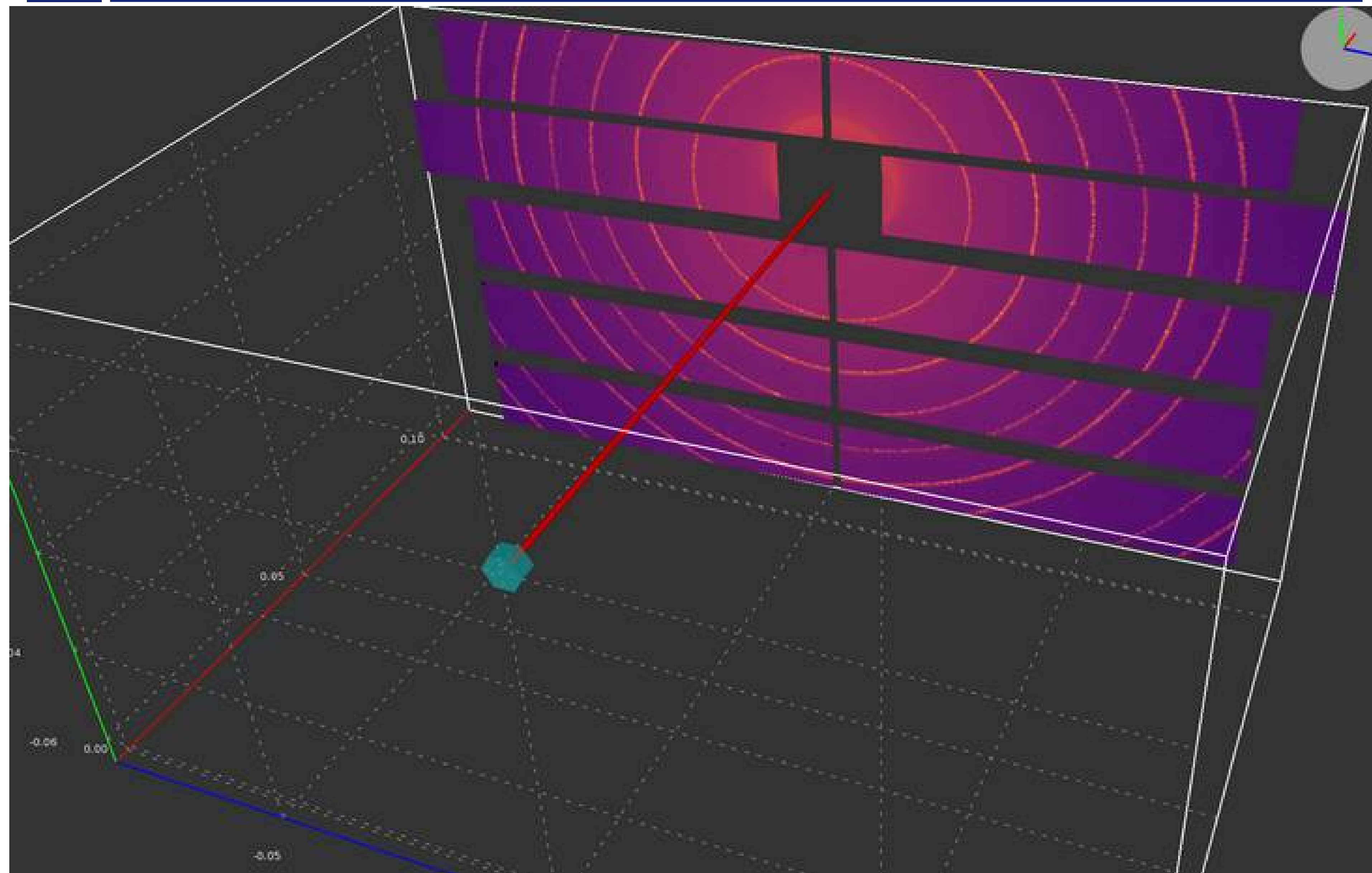
Extensions

Extension library
e.g. PyHST, ...

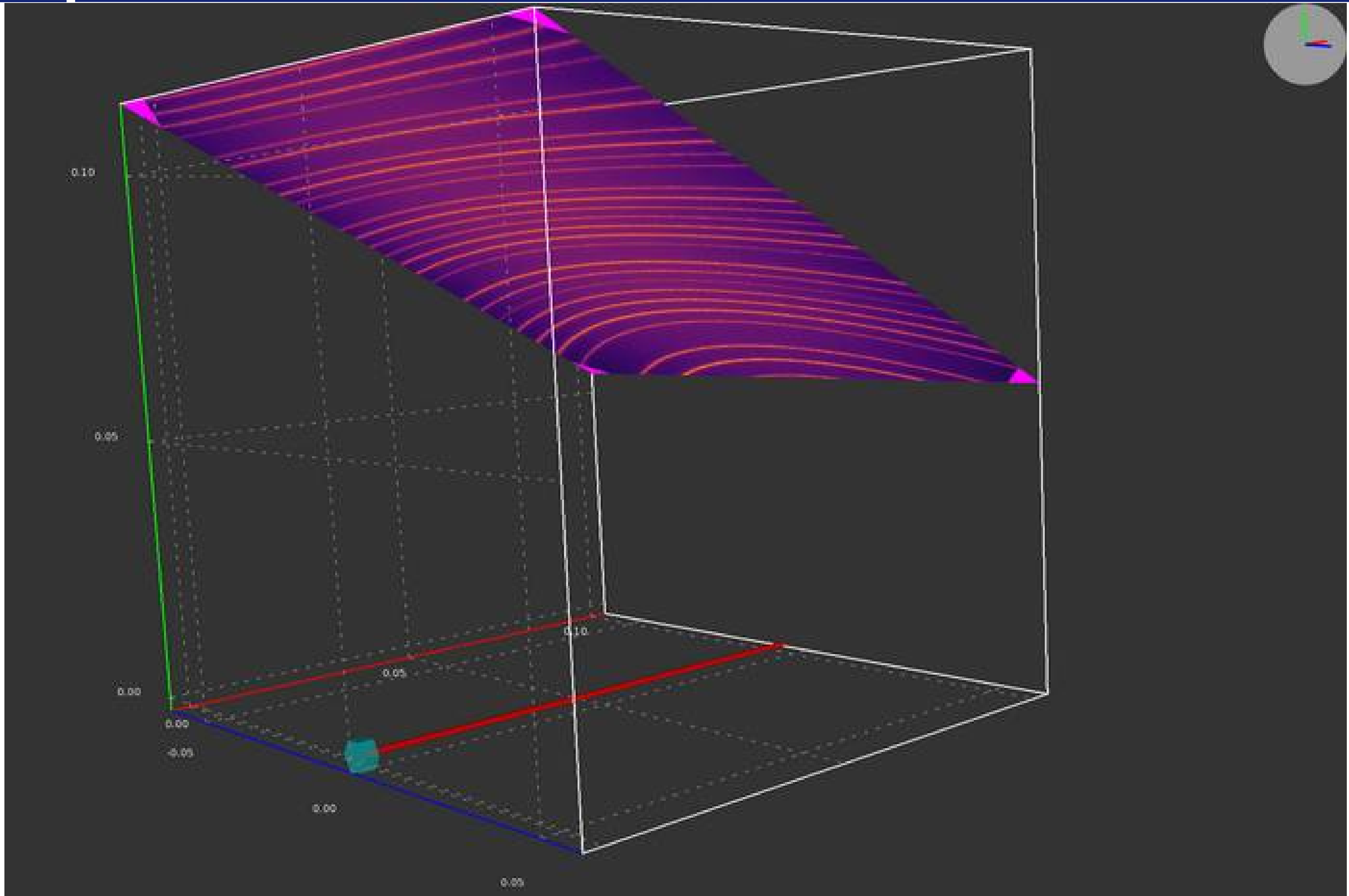
Outcome of the *silx* toolkit (2015-2018)



3D view of the diffraction setup



3D view of the diffraction setup



Calibration tools

PyFAI Calibration

Experiment settings
Mask
Peak picking
Geometry fitting
Cake & integration

Help

Identify rings from the image

Click on the ring you want to select. Usually it is the first one, else update it's number in the list of the picked rings bellow.

You have to identify at least 5 peaks distributed on 2 rings. Then use the extraction tool to find more peaks automatically.

Picked rings

Name	Peaks	Ring number
a	41	1
b	57	2
c	34	3

Extract more rings

Auto-extraction options

Amount of ring to extract: 5

Number of peak per degree: 1.00

Guess geometry from: Control points

Next >

PyFAI Calibration

Integration parameters

Radial unit: Scattering angle

Radial points: 1024

Azimuthal points: 360

Polarization factor

Pixel splitting: Bounding box

Display mask overlay

Integrate

Geometry

Save as PONI file...

Online help...

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  - Claudio Ferrero†
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  - Frederic Sulzmann
  - Guillaume Bonamis
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  - APS: Clemens Prescher
  - NSLS-II: scikit-beam project
  - ALS: Camera project
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  - LinkSCEEM-2 grant
    - **Dimitris Karkoulis**
    - **Giannis Ashiotis**
    - **Zubair Nawaz**

Questions ?

Installation procedure on MacOS

- **Download all data needed:**
  - `Download some diffraction data from:` `http://www.silx.org/pub/pyFAI/pyFAI_UM_2021/Eiger2_CeO2_75keV.h5`
  - `Download Python 3.8 from:` `https://www.python.org/ftp/python/3.8.7/python-3.8.7-macosx10.9.pkg`
- **Install Python 3.8**
  - Double click on the dmg file found in the `archive`
  - Drag-and-drop into the `Applications` folder
- **Install pyFAI into a virtual environment**
  - `python3.8 -m venv pyfai`
  - `source pyfai/bin/activate`
  - `pip install pyFAI[gui]`
- **Run the application of your choice:**
  - `pyFAI-calib2`
  - `pyFAI-integrate`
  - `pyFAI-benchmark`

Installation procedure on Windows

- **Download all data needed**
  - Download some diffraction data from: http://www.silx.org/pub/pyFAI/pyFAI_UM_2021/Eiger2_CeO2_75keV.h5
  - Download Python from https://www.python.org/ftp/python/3.8.6/python-3.8.6-amd64.exe
- **Install Python3.8**
  - Double click on the *.exe* file
  - Install `python` to the root of the system
- **Install pyFAI into a virtual environment**
  - `python3.8 -m venv pyfai`
  - `pyfai\bin\activate.bat`
  - `pip install pyFAI[gui]`
- **Run the application of your choice:**
  - `pyFAI-calib2`
  - `pyFAI-integrate`
  - `pyFAI-benchmark`

Installation procedure on Linux

- **Download all data needed**
  - `Download some diffraction data from:` `http://www.silx.org/pub/pyFAI/pyFAI_UM_2021/Eiger2_CeO2_75keV.h5`
- **Install Python 3.x (x≥6) and create a virtual environment**
  - Follow the procedure of your distribution to install python
  - `python3 -m venv pyfai`
  - `source pyfai/bin/activate`
- **Install pyFAI and the missing dependencies**
  - `pip install pyFAI[gui]`
- **Run the application of your choice:**
  - `pyFAI-calib2`
  - `pyFAI-integrate`
  - `pyFAI-benchmark`