# PyFAI user meeting
# NoBugs 2024 satellite meeting

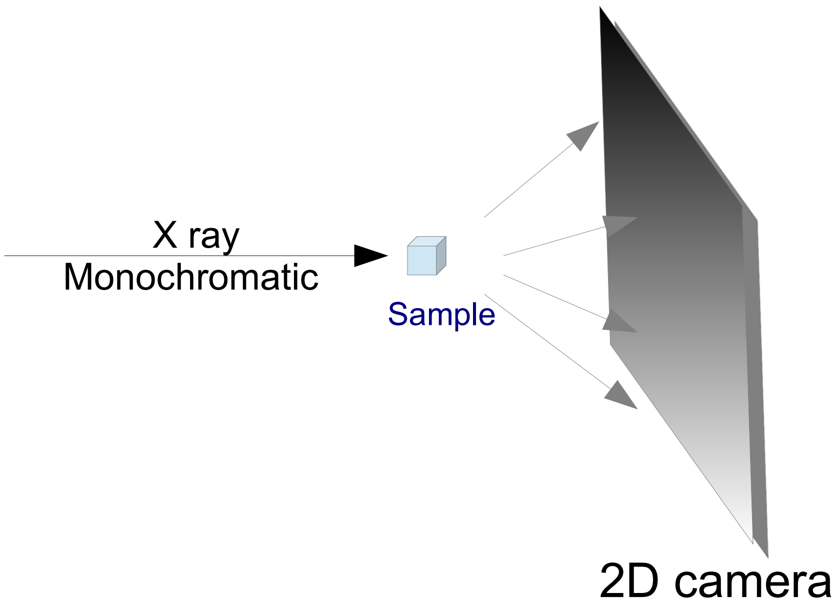
Jérôme Kieffer*
Edgar Gutierrez-Fernandez
Maciej Jankowski

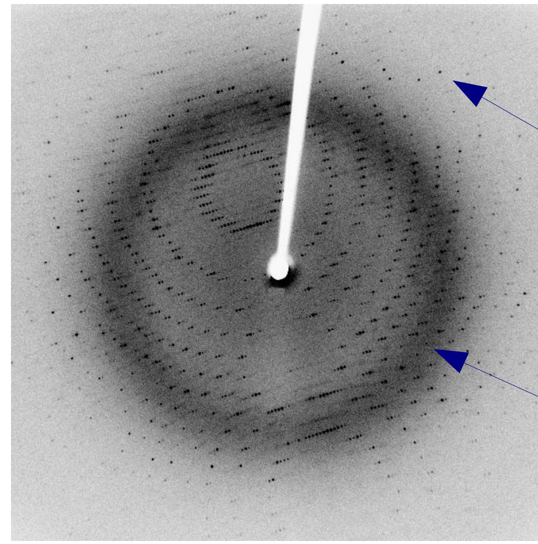
Algorithms & scientific Data Analysis

# 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: latest news**
- **Conclusions**

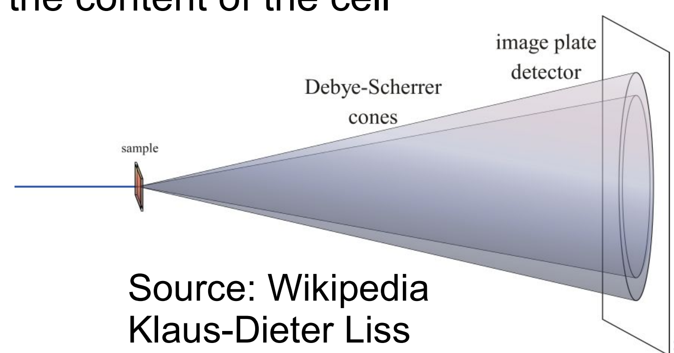
# X-ray scattering experiments




Source: Wikipedia
CC-BY-SA: Jeff Dahl

- **Light is reflected on crystallites 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

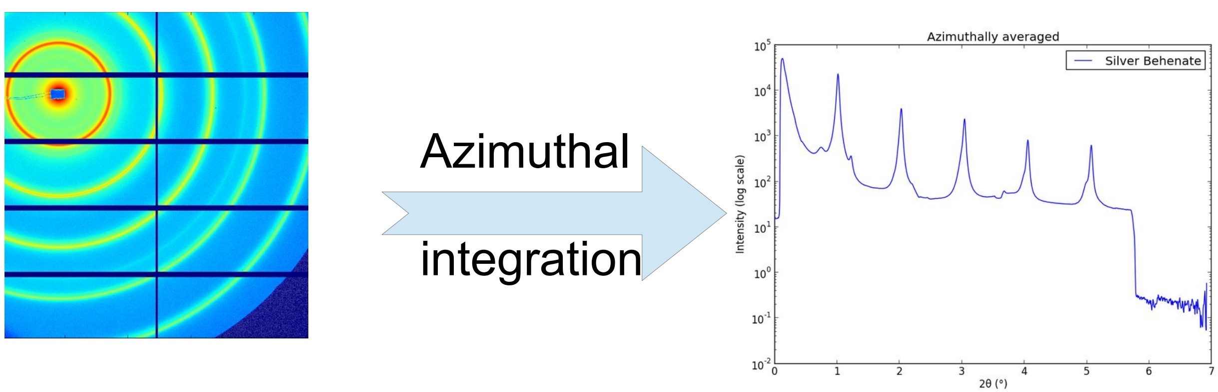
**Application of powder diffraction:**

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

**Application of small angle scattering**

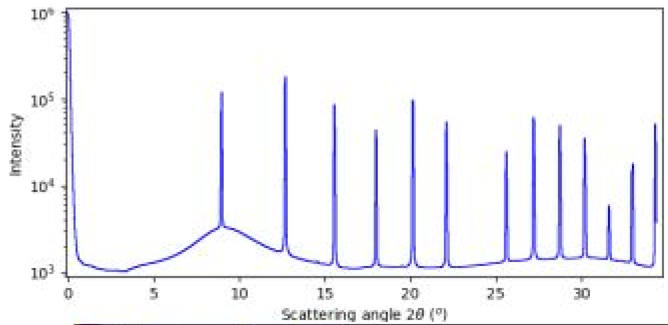
- Micro/nano-scale structure
- Particle shape
- Protein domains
- Protein folding
- Colloids
- Fiber orientation

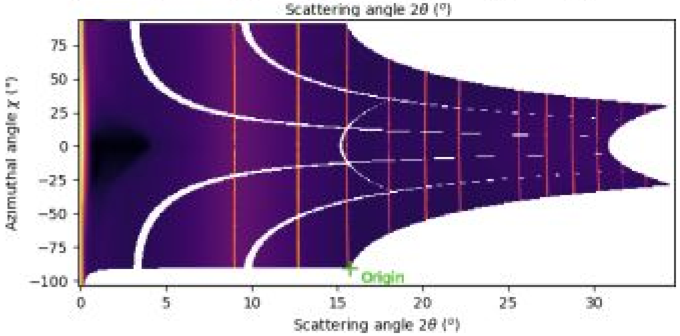
- **Both rely on the same transformation: 2D image → azimuthal average**

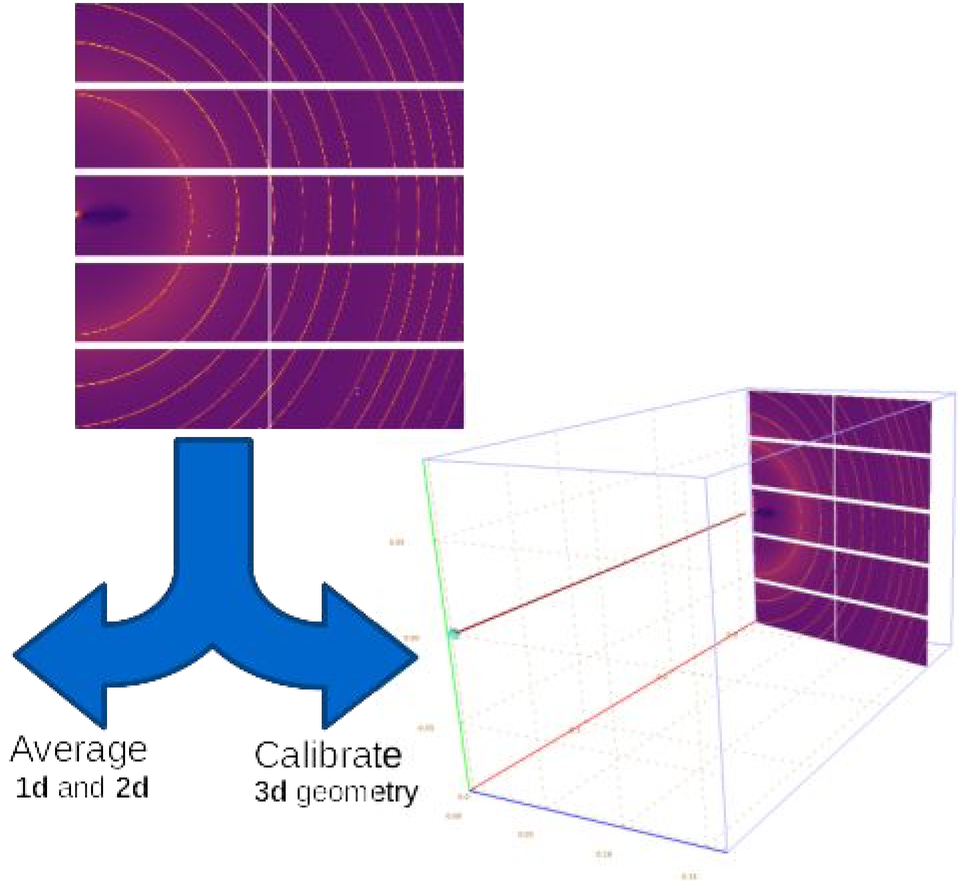


# Fast Azimuthal Integration using Python

PyFAI
Fast Azimuthal Integration




- **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

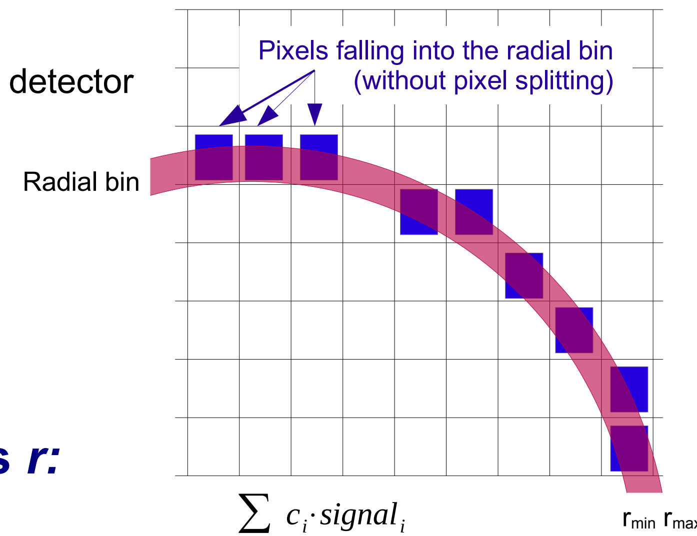
# How it works

- **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...

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

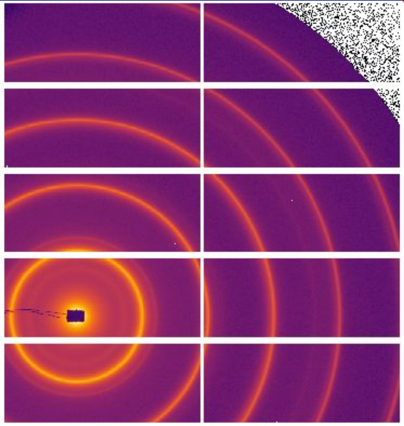
$$\sigma(\langle I \rangle_r) = \frac{\sqrt{\sum_{i \in bin_r} c_i^2 \cdot variance_i}}{\sum_{i \in bin_r} c_i \cdot normalization_i}$$

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

# Many different tools exist …

| Name | License | Institute | Language | Last release |
|---|---|---|---|---|
| PyFAI | MIT | ESRF | Python | 2024 |
| FIT2D | MIT | ESRF | Fortran | 2016 |
| XRDUA | GPL | U. Antwerp | IDL | 2021 |
| Dawn | EPL | Diamond | Java | 2024 |
| DataSqueeze | $$$ | U. Pens. | Java | 2023 |
| Foxtrot | Free | Soleil | Java | 2023 |
| Maud | Free | U. Trento | Java | 2023 |
| GSAS-II | Free | APS | Python | 2023 |
| Scikit-beam | BSD | BNL | Python | 2023 |
| AzInt | MIT | MaxIV | Python | 2023 |
| SaxsDog | GPL | U.Graz | Python | 2022 |

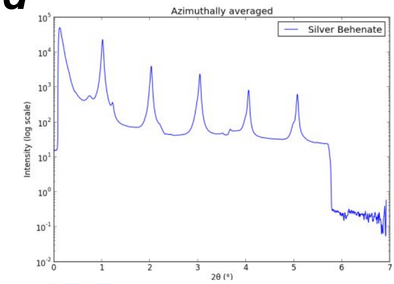
# Concepts in PyFAI

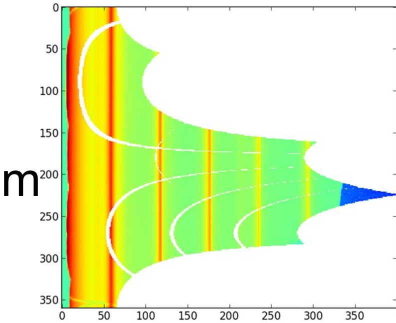


- **Image**

  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:

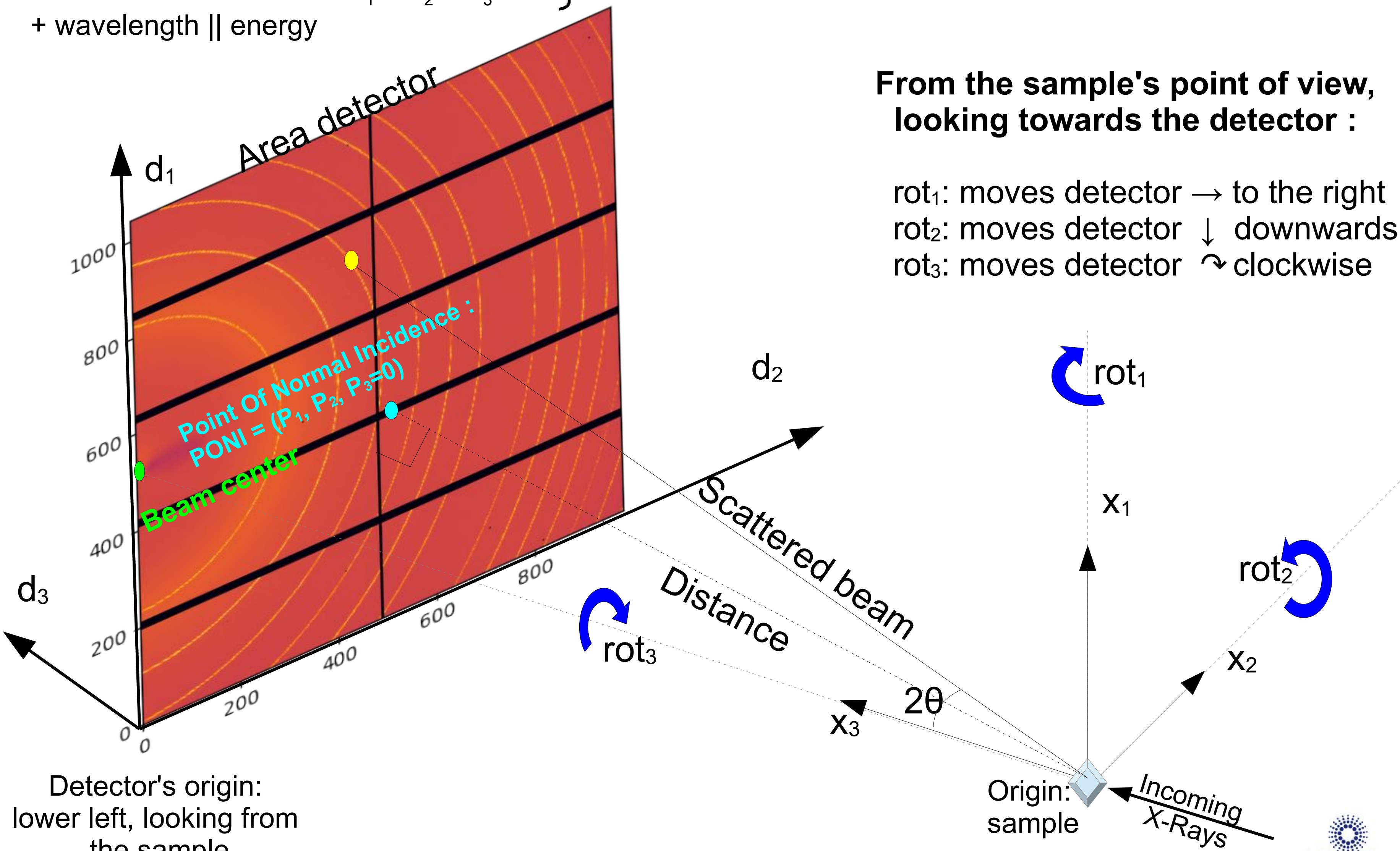
* 3 distances in meters: dist, $poni_1$, $poni_2$
* 3 rotations in radians: $rot_1$, $rot_2$, $rot_3$

} *PONI*-file

+ wavelength || energy

**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



# 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**

# 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 ($2\theta$) and azimuthal ($\chi$) 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.**

# Example of simplified implementation in Python

## Common initialization step:

In [1]:
```python
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]:
```python
%%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]:
```python
%%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
```

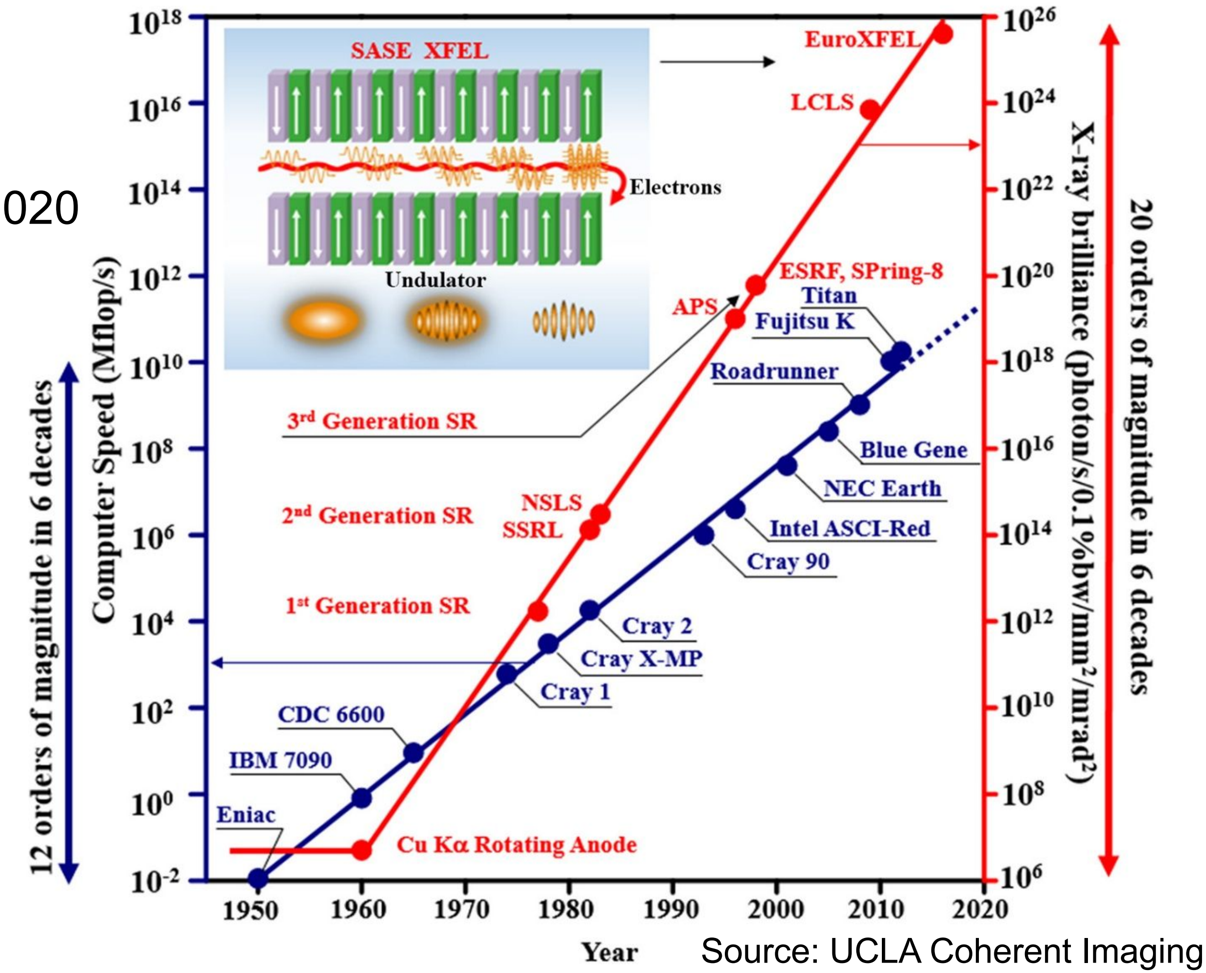
```
CPU times: user 19.5 ms, sys: 1.44 ms, total: 20.9 ms
Wall time: 19.4 ms
```

In [4]:
```python
# 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 (2014)
  - Several projects copied this idea:
    - **Saxsdog https://arxiv.org/abs/2007.02022 (2020),**
    - **MatFRAIA https://doi.org/10.1107/S1600577522008232 (2022)**

# 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)
```

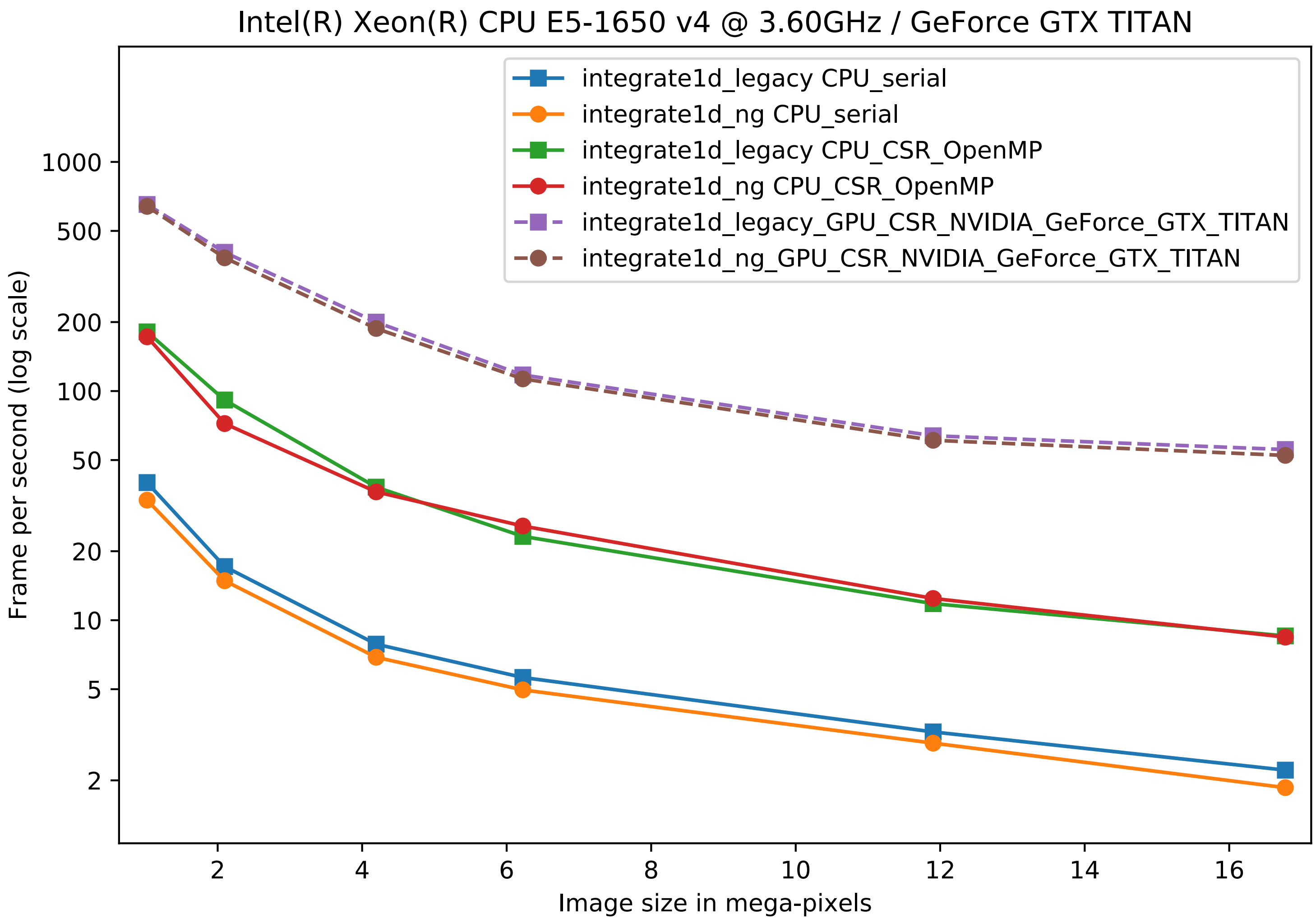
Out[7]: True

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

# Advantages of *histograms* vs matrix multiplication

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

# Benchmark: Let's speak about speed !



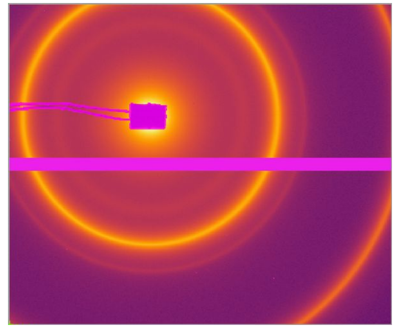

6-year-old workstation: CPU from 2016, GPU from 2013

# Moiré effect

## High frequency noise issue

Where pixel splitting comes back

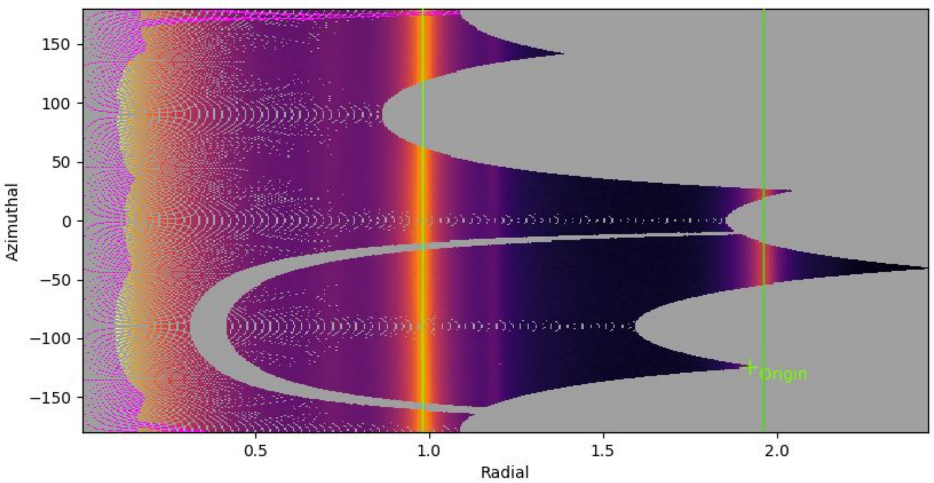
# Example with SAXS data integrated in 2D



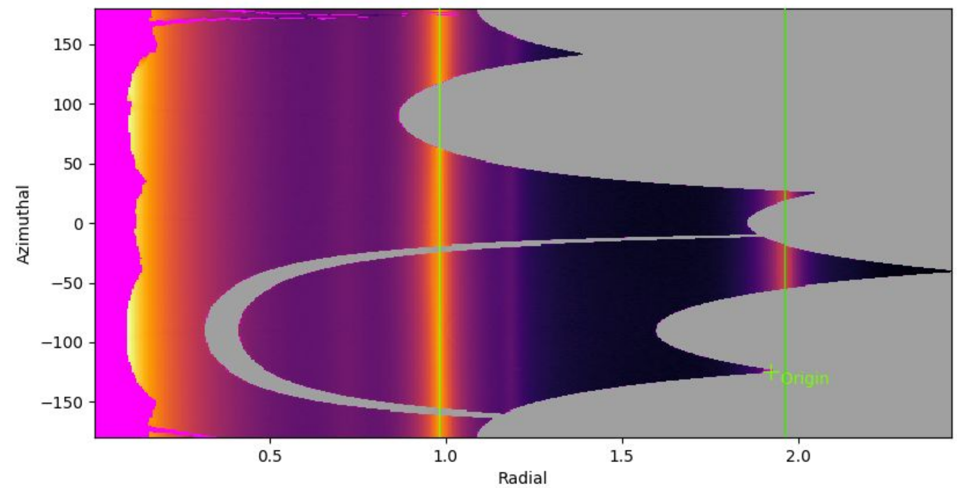
Pilatus 200k:
~500 x 400 pixels

2D averaging over 512x360 bins

Without pixel splitting



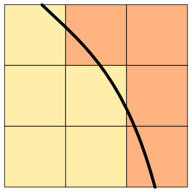

With pixel splitting



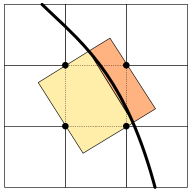

creates bin cross-correlation

# Pixel splitting schemes available in pyFAI

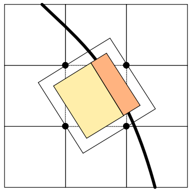
- **No pixel splitting: default histograms**
  - Each pixel contributes to a single bin of the result
  - No bin correlation but noisy
  - The pixel has no surface: sharpest peaks



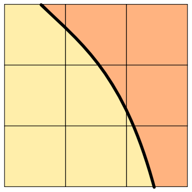
- **Bounding-box pixel splitting**
  - The smoothest integrated curve
  - Blurs a bit the signal



- **Pseudo pixel splitting (deprecated)**
  - 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

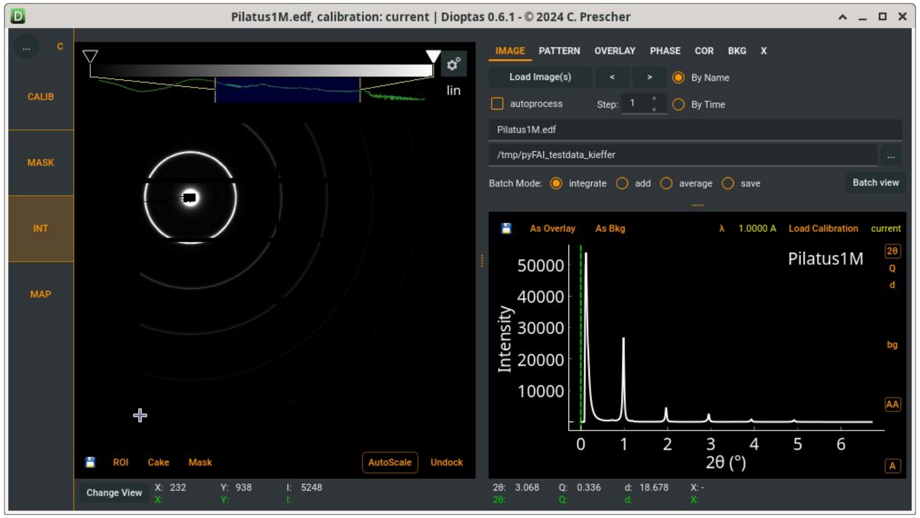
# Latest news from pyFAI (2022)

- **High speed *sigma-clipping***
  - Enforce normal distribution in every azimuthal bin :
    - **Remove single crystal contribution from powder diffraction**
    - **Several error models: *poissonian, azimuthal, hybrid***
  - Enables:
    - **Single crystal frame compression (2x-20x, lossy compression)**
    - **Peak-finding: 250 Hz / GPU**
  - Sponsored by serial crystallography (ESRF ID29, MX)
    - **Kieffer & al. (2024) J.Appl.Cryst** *accepted*

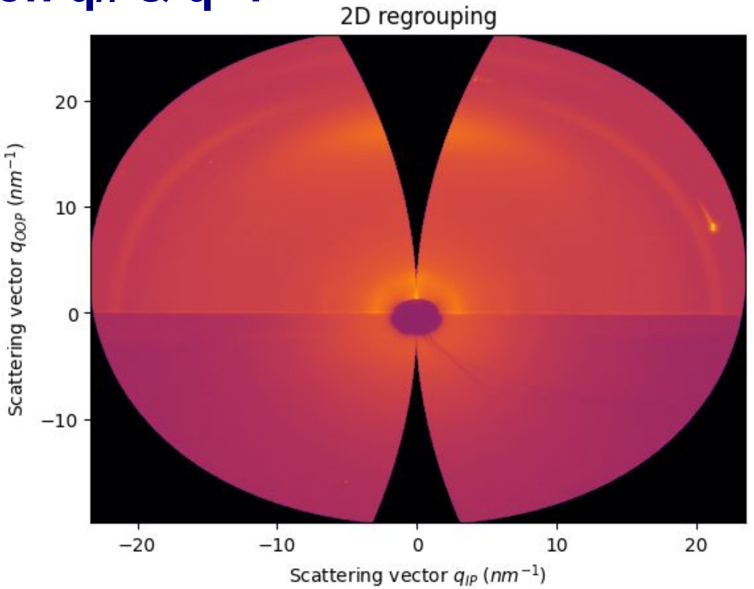
- **Square out all integration engines:**
  - Any type of integration: 1d (averaging) and 2d (caking)
  - Any type of pixel-splitting: without, bounding-box or full splitting
  - Any type of algorithm: histogram or sparse matrix multiplication
  - Any type of implementation: Python, Cython (C++) and OpenCL (GPU)

# Latest news from pyFAI (2023)

- **Orientation management**
  - Allows to flip the detector V/H
  - Compatibility with Dioptas
  - New orientation tag:
    - PyFAI's default is **3**
    - Dioptas's default is **2**



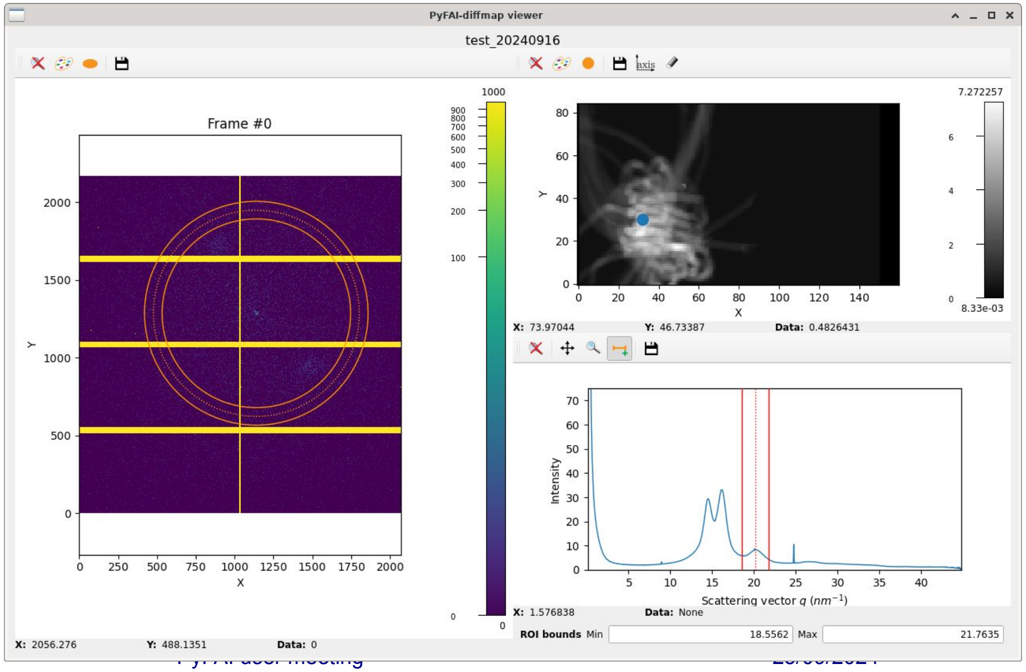

- **Grazing incidence representation q// & q┴:**
  - Thanks to Edgar



# Latest news from pyFAI (2024)

- **Ewoks integration**
  - Lot of improvement in the `worker`
  - Tutorial tomorrow morning by Wout & Loïc

- **Mapping**
  - Visualization tool thanks to Loïc & Edgar



# Acknowledgments

- **Algorithm & Data Analysis group**
  - Edgar Gutierrez-Fernandez
  - Maciej Jankowski
  - V. Armando Sole
  - Vincent Favre-Nicolin

- **Data analysis unit colleagues:**
  - Valentin Valls
  - Loïc Huder
  - Thomas Vincent
  - Claudio Ferrero†

- **Other synchrotron/labs**
  - Soleil: Fred Picca
  - Clemens Prescher (Dioptas)
  - Sesame: Philipp Hans
  - NSLS-II, ALS, APS, ...

- **LinkSCEEM-2 grant**
  - Dimitris Karkoulis
  - Giannis Ashiotis
  - Zubair Nawaz

- **ESRF Beamlines:**
  - BM01, BM02, ID02, ID11, ID13, ID15a, ID15b, ID21, ID22, ID23, BM26, ID27, ID28, BM29, ID29, ID30, ID31 ...

# Questions ?