



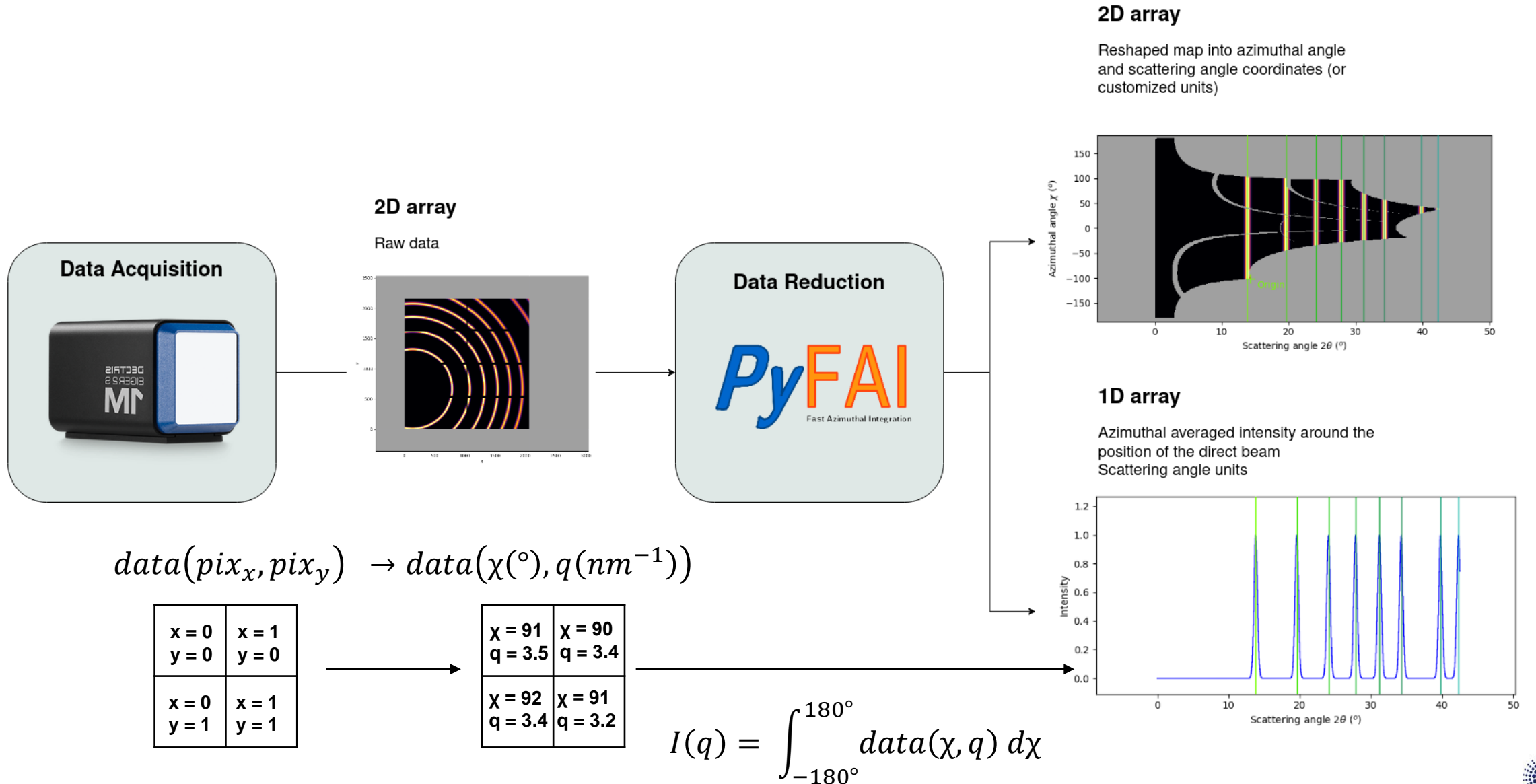
# NoBUGS 2024 PyFAI satellite

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Edgar Gutierrez Fernandez

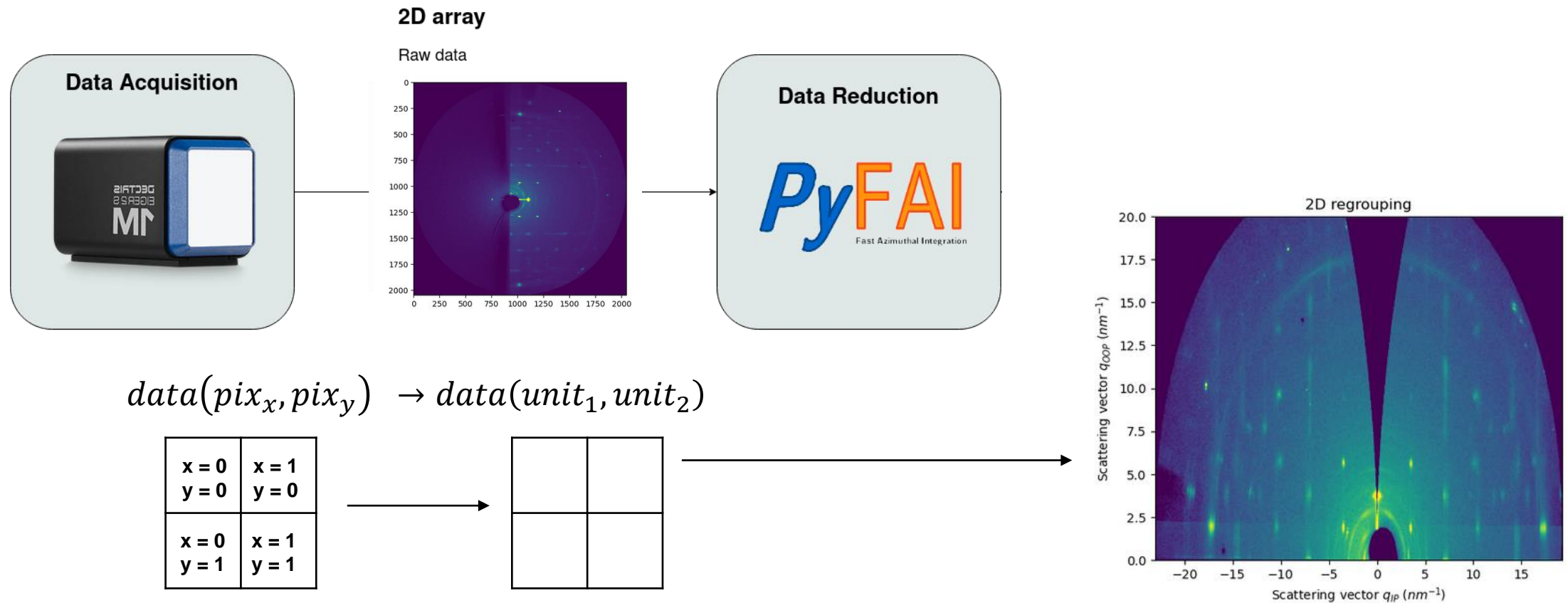
PIONEERING SYNCHROTRON  
SCIENCE



# Single frame pipeline in pyFAI: standard azimuthal integration

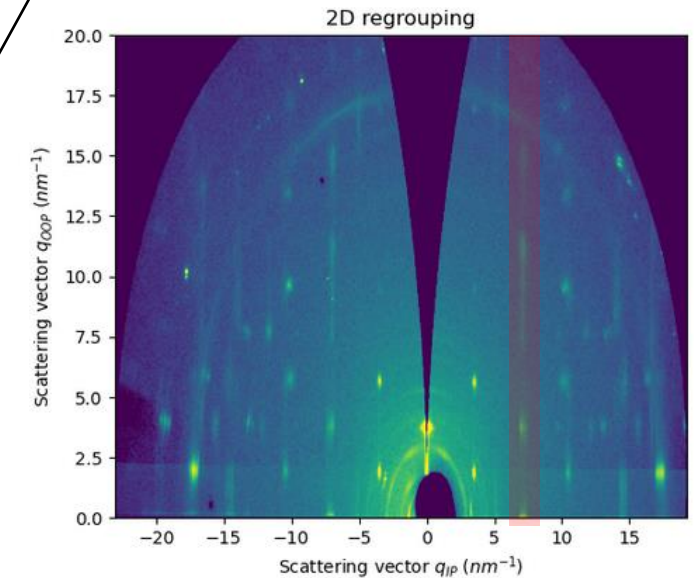
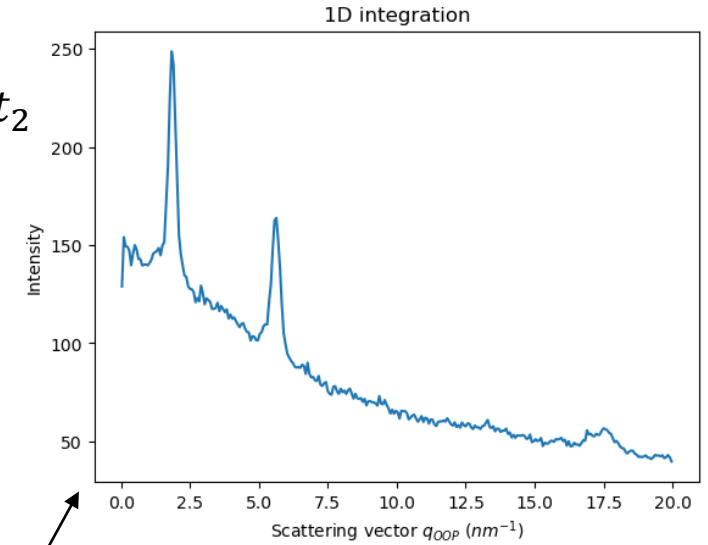
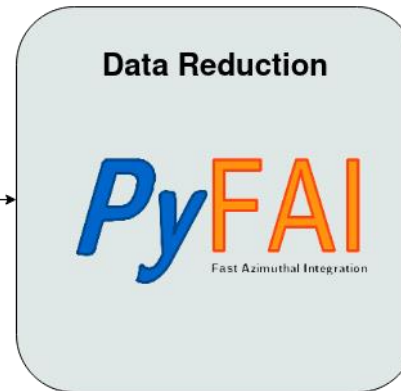
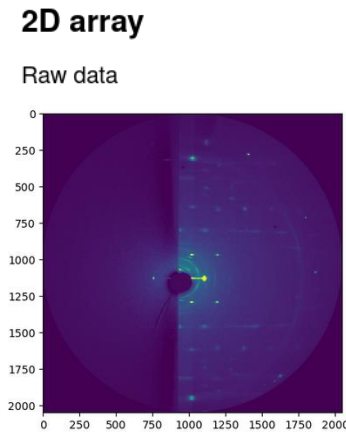


# Single frame pipeline in pyFAI: generic data integration



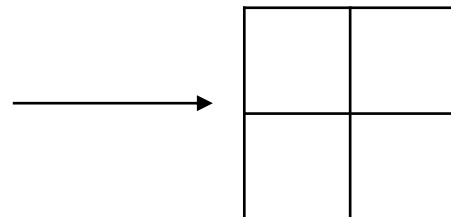
# Single frame pipeline in pyFAI: generic data integration

$$I(\text{unit}_1) = \int_a^b \text{data}(\text{unit}_1, \text{unit}_2) d\text{unit}_2$$



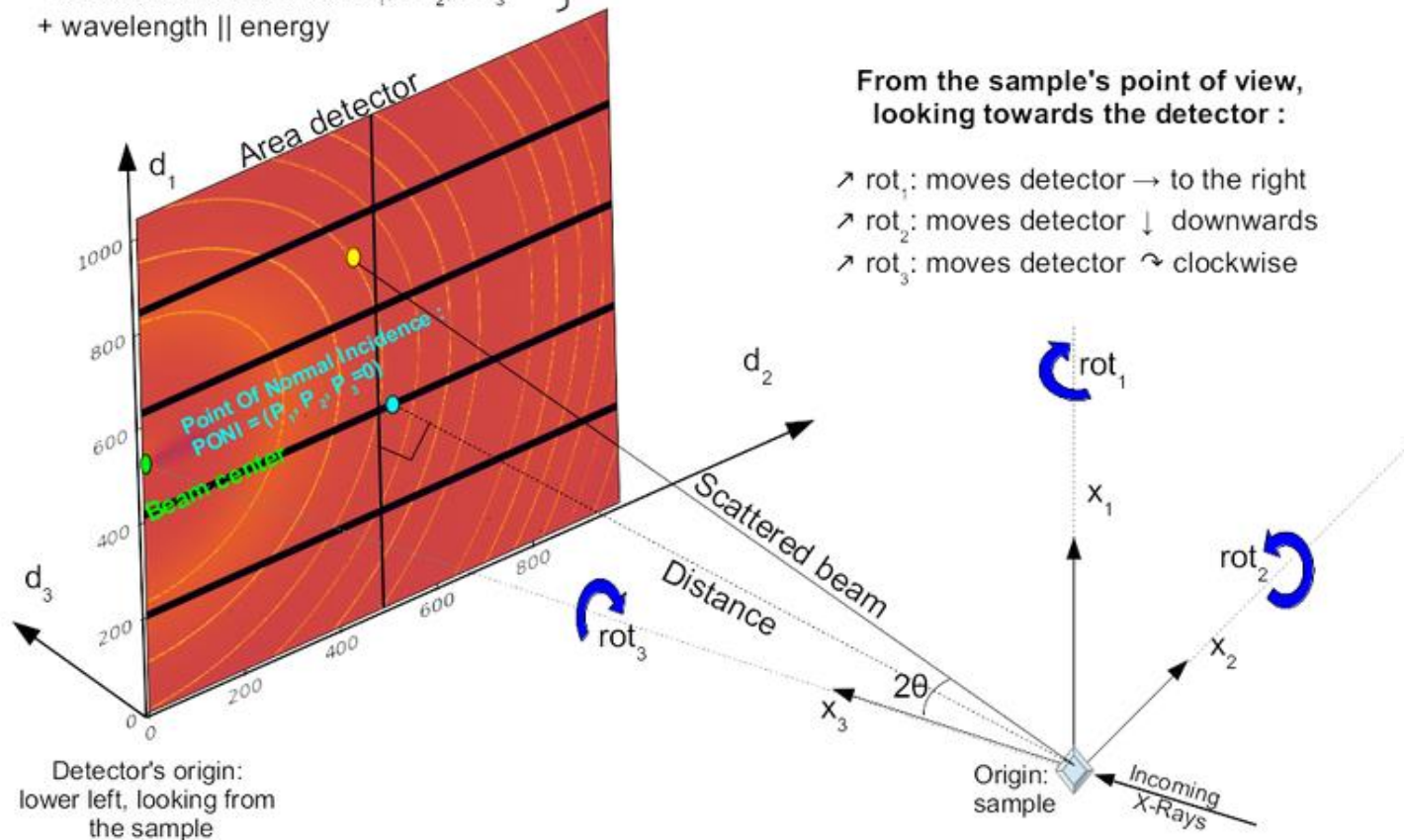
$$\text{data}(\text{pix}_x, \text{pix}_y) \rightarrow \text{data}(\text{unit}_1, \text{unit}_2)$$

x = 0	x = 1
y = 0	y = 0
x = 0	x = 1
y = 1	y = 1



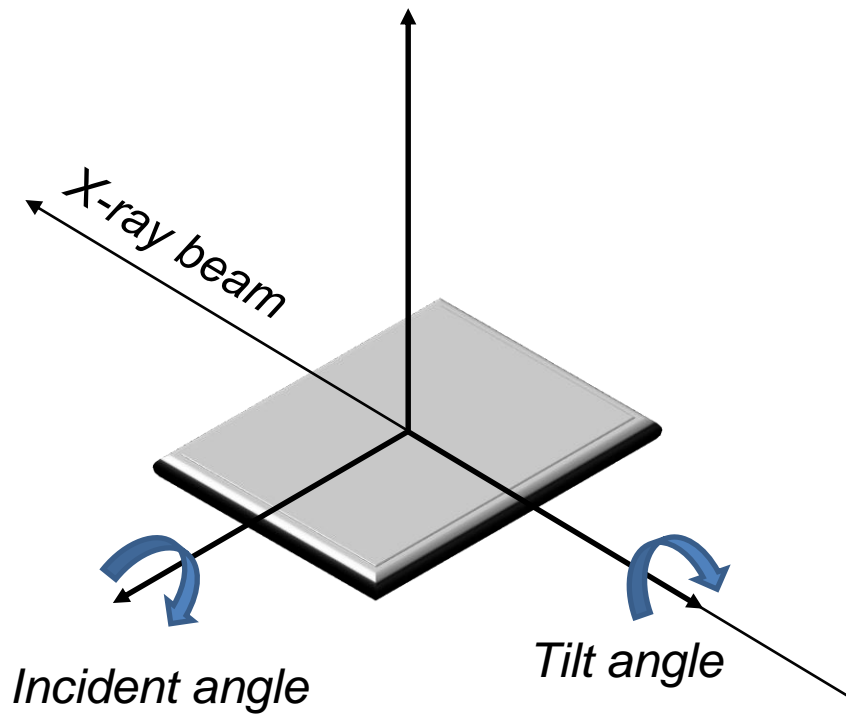
Parameters:

- \* 3 distances in meters:  $\text{dist}$ ,  $\text{poni}_1$ ,  $\text{poni}_2$
  - \* 3 rotations in radians:  $\text{rot}_1$ ,  $\text{rot}_2$ ,  $\text{rot}_3$
- + wavelength || energy
- } *PONI*-file



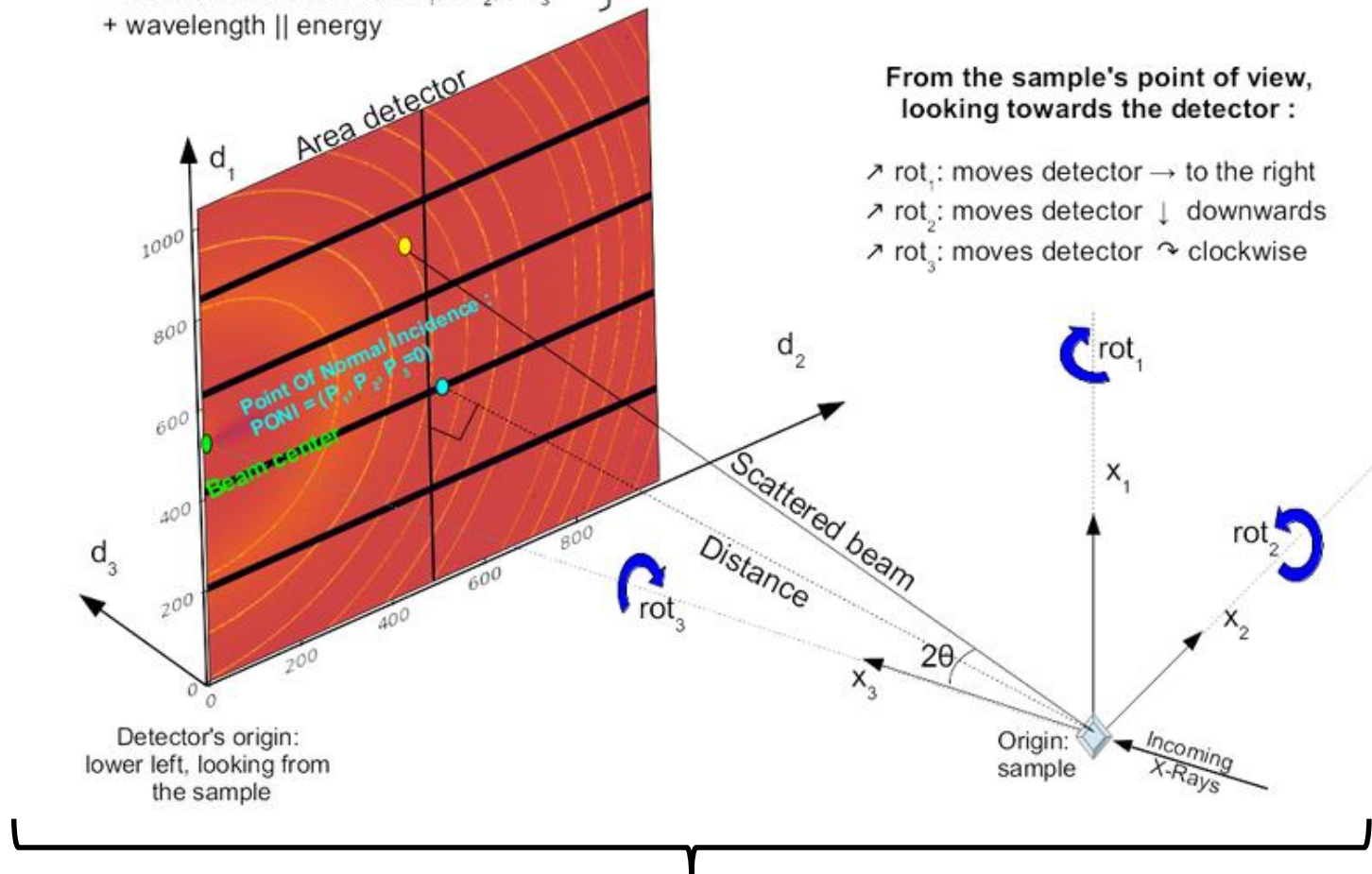
From the sample's point of view,  
looking towards the detector :

- ↗  $\text{rot}_1$ : moves detector → to the right
- ↘  $\text{rot}_2$ : moves detector ↓ downwards
- ↻  $\text{rot}_3$ : moves detector ↻ clockwise



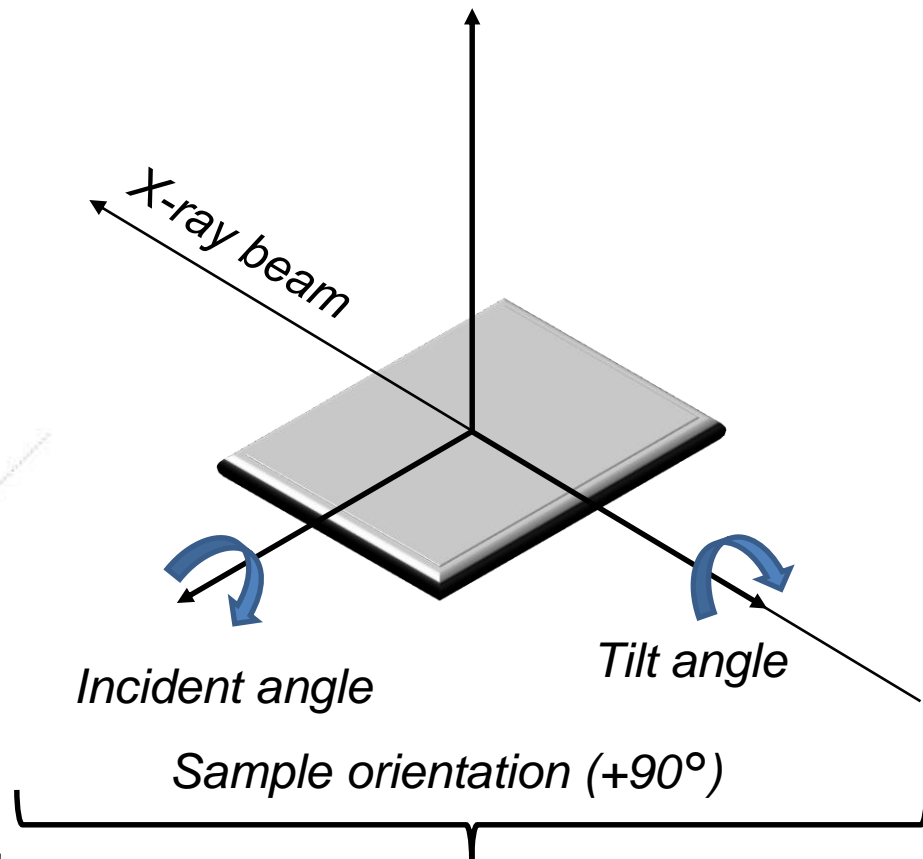
Parameters:

- \* 3 distances in meters:  $dist, poni_1, poni_2$  } *PONI*-file
- \* 3 rotations in radians:  $rot_1, rot_2, rot_3$
- + wavelength || energy



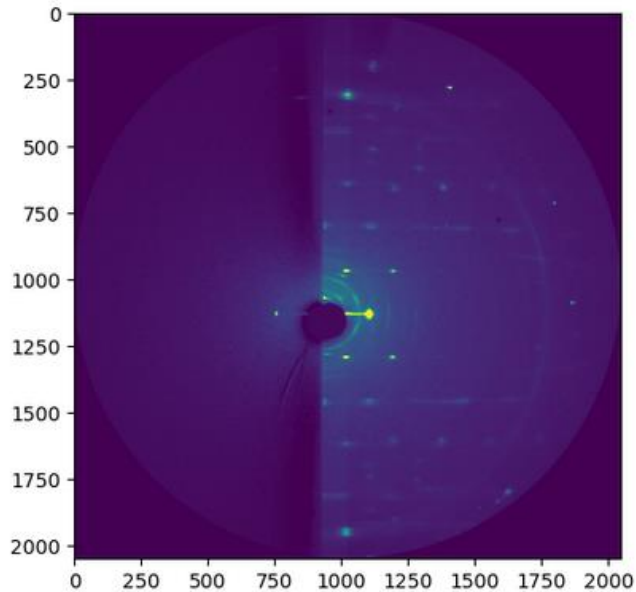
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Units

Geometry (.poni file)



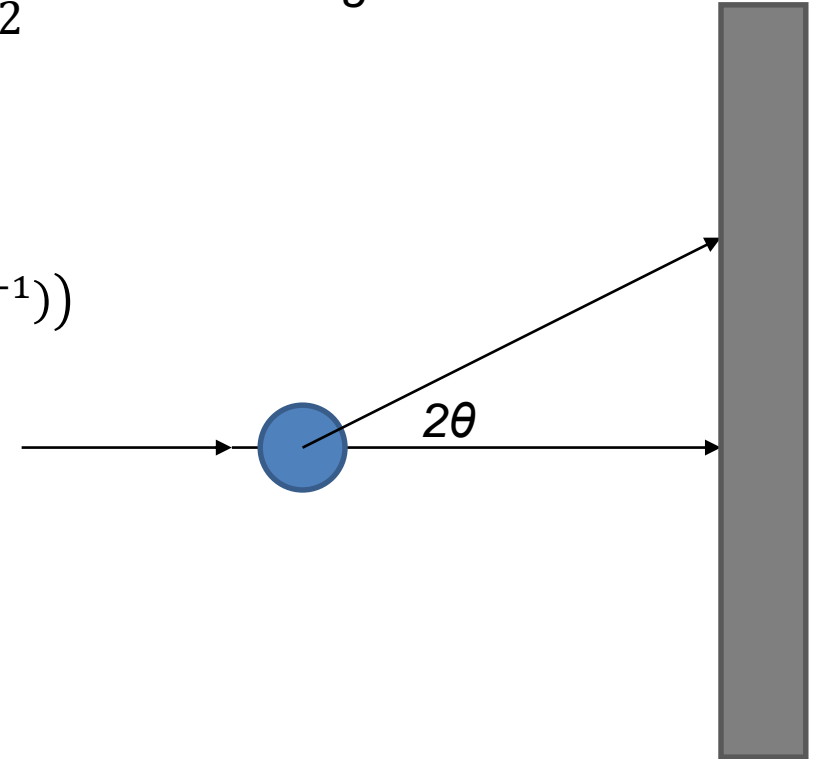
Bragg Law

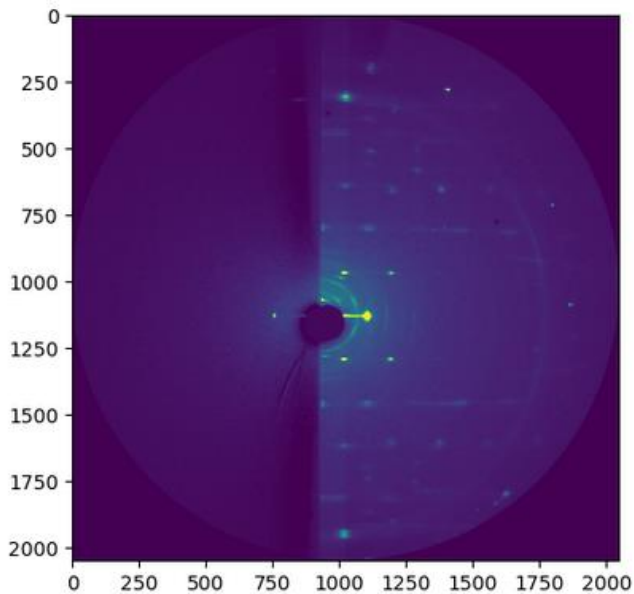
$$|\mathbf{q}| = \frac{4\pi}{\lambda} \sin \frac{2\theta}{2}$$

Scattering angle

$$data(pix_x, pix_y) \rightarrow data(\chi(^{\circ}), q(nm^{-1}))$$

$$I(q) = \int_{-180^{\circ}}^{180^{\circ}} data(\chi, q) d\chi$$





Bragg Law

$$|\mathbf{q}| = \frac{4\pi}{\lambda} \sin \frac{2\theta}{2}$$

Scattering angle

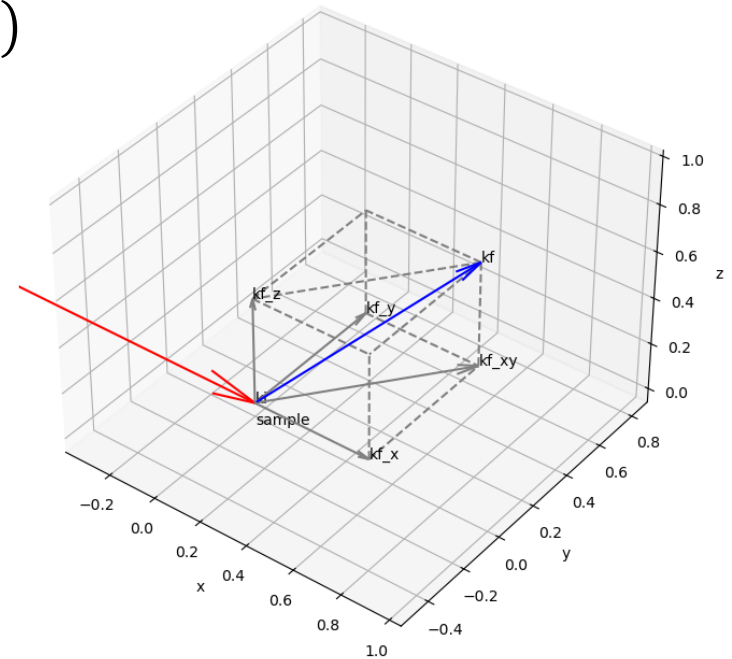
$$q_x = f(\text{pix}_x, \text{pix}_y, \text{incident}, \text{tilt})$$

$$q_y = f(\text{pix}_x, \text{pix}_y, \text{incident}, \text{tilt})$$

$$q_z = f(\text{pix}_x, \text{pix}_y, \text{incident}, \text{tilt})$$

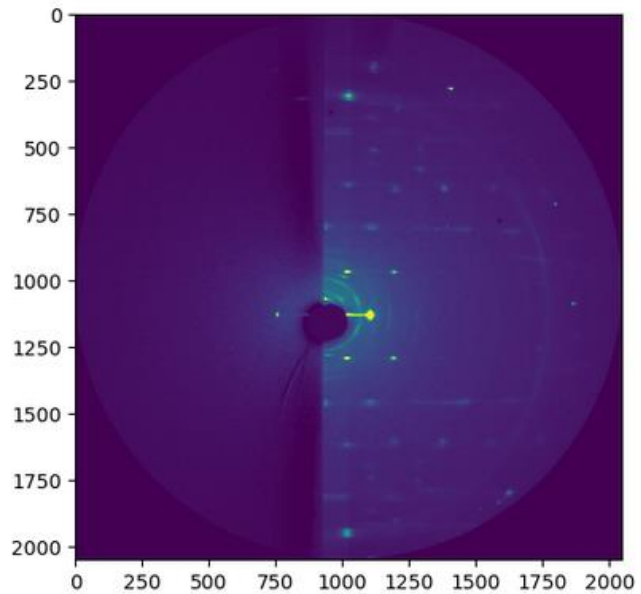
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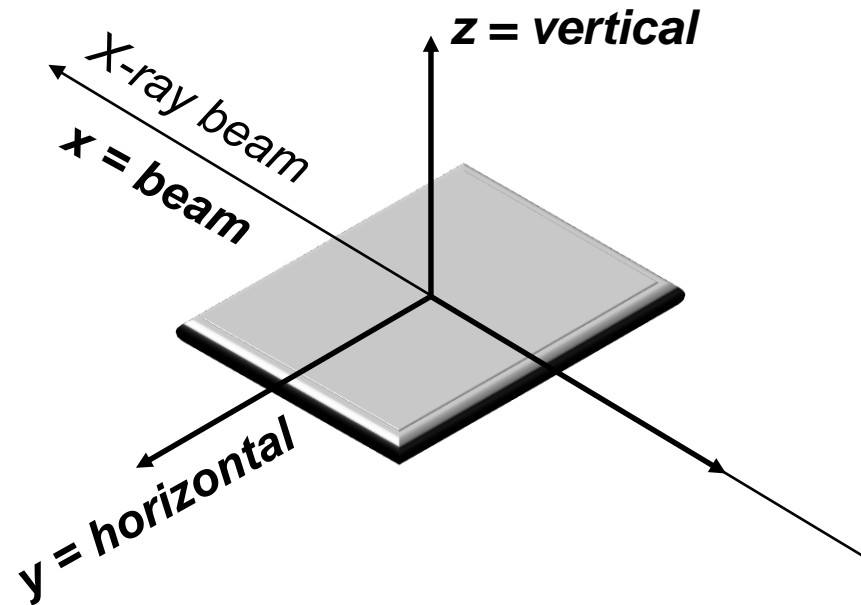




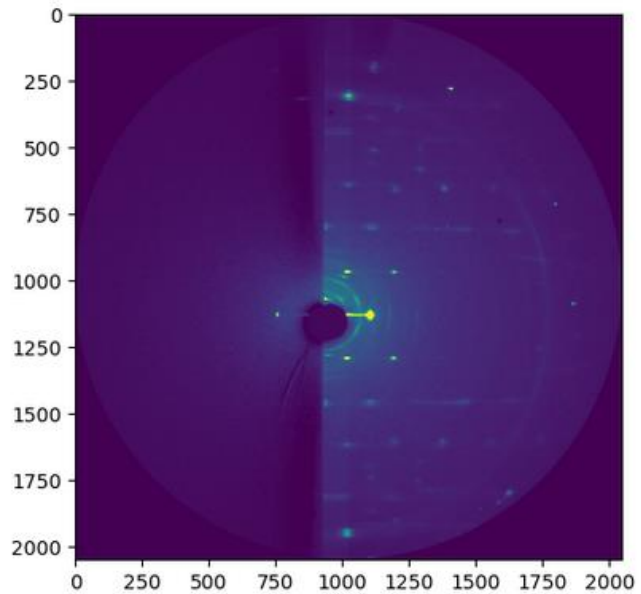
$$data(pix_x, pix_y) \rightarrow data(\chi(^{\circ}), q(nm^{-1})) \rightarrow data\left(\sqrt{q_x^2 + q_y^2}, q_z\right) = data(q_{IP}, q_{OOP})$$



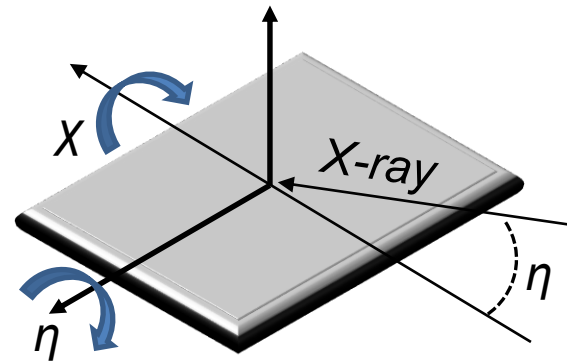
$$q_{IP} = \sqrt{q_x^2 + q_y^2} \quad q_{OOP} = q_z$$



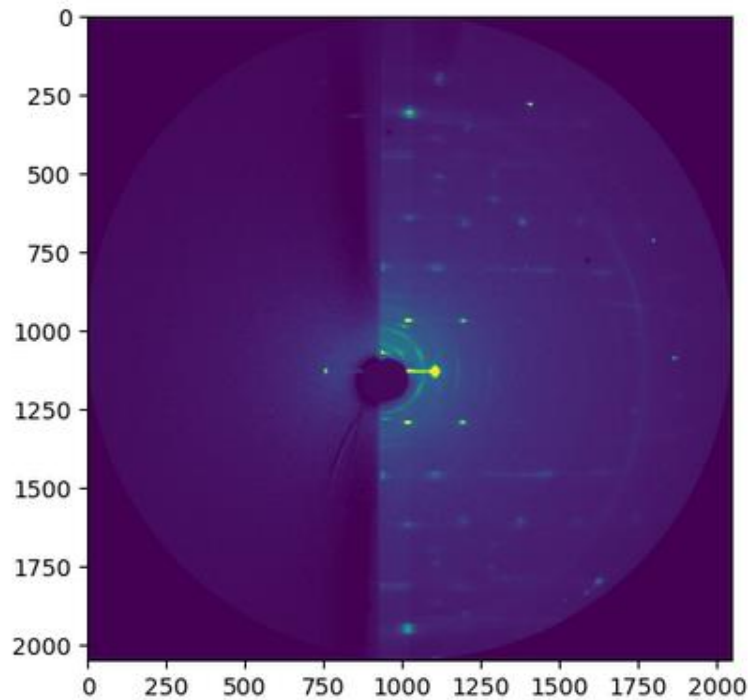
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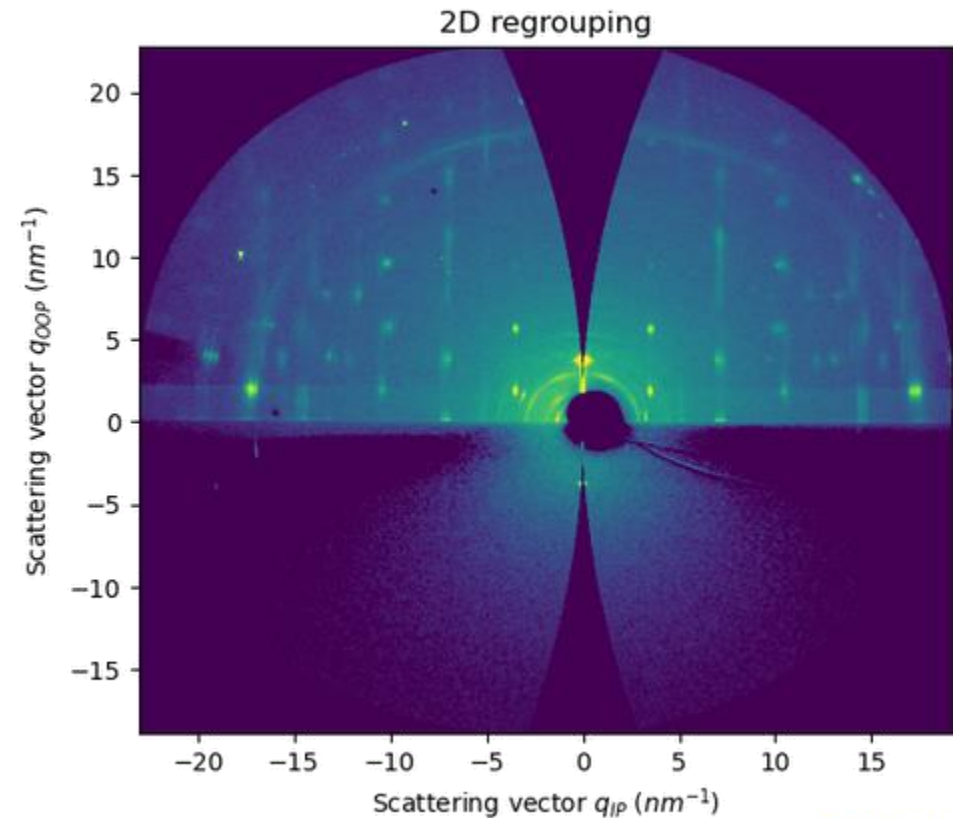
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## 1) Instantiate the units

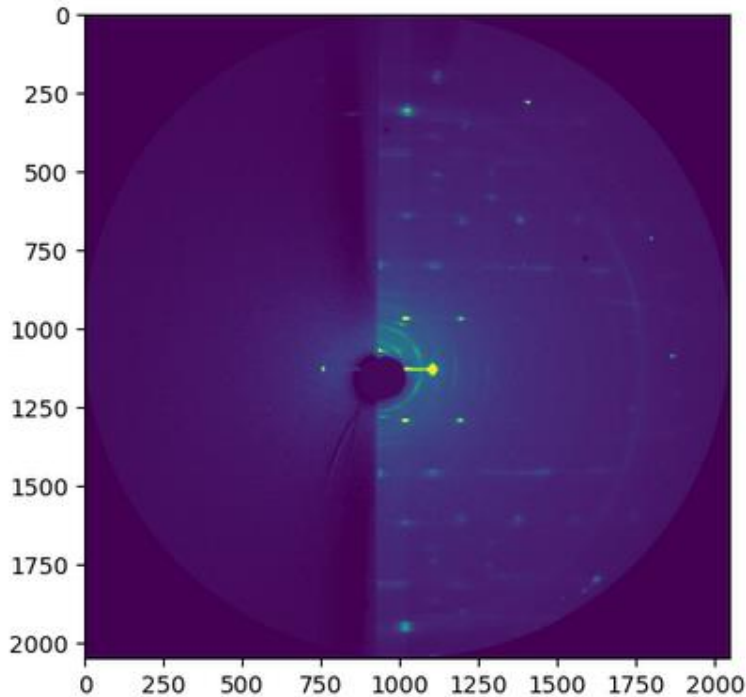
- `from pyFAI.units import get_unit_fiber`
- `qip = get_unit_fiber(name='qip_nm^-1', incident_angle=0.12, tilt_angle=0.0, sample_orientation=2)`
- `qoop = get_unit_fiber(name='qoop_nm^-1', incident_angle=0.12, tilt_angle=0.0, sample_orientation=2)`

## 2) Integrate using different units and a method without pixel splitting

- `units = (qip,qoop)`
- `method = ("no", "csr", "cython")`
- `res2d_gi = ai.integrate2d(data=data, npt_rad=1000, npt_azim=1000, unit=units, method=method)`

## 3) Plot the results:

- `from pyFAI.gui.jupyter import plot2d`
- `plot2d(res2d_gi)`



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