uf-TS/PDF Software Meeting 2

Dean Keeble

20th July, 2023

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Agenda

1. Welcome
2. Review of previous meeting
3. Update from Dean
4. Discussion of sample database options
5. Pre-visit computer access
6. November experiment logistics
7. AOB

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Review of Previous Meeting - Actions

1. Collect a blank data collection into our pre-visit session so that we can familiarise ourselves with the offline file formats (Karen + HED team)
2. ✅ Finalise the design of the detector geometry and distribute the drawings when available (Karen + HED team)
3. ✅ Build a multigeometry in pyfai to simulate data according to the finalised drawings (Phil)

4. ⏸️ Define the dependencies required in a python environment for it to be useable within EXtra-metro (Thomas, Luca?)
5. ⏸️ Confirm an environment can be built which contains both pyFAI and PDFgetX3 and the deps specified above (Dean)
6. ✅ Confirm the impact that "gaps" have on PDFgetX3: what value should they take? can they be masked? what impact should we expect? (Dean)

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7. ✅ Is it possible to do a better job mitigating the characteristic features seen close to gaps with data which are not azimuthally symmetric? (Dean)
8. ✅ It was mentioned that DAMNIT runs on SQLite, meaning we can't write from EXtra-metro processing but we can read. Draw out a data schematic for the various collections we'll use (Dean)
9. Convert these schematics to toy/psuedo context files (Dean)

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Update from Dean

- Gaps & detector geometry
- Overall schematic and context files
- Gap mitigation

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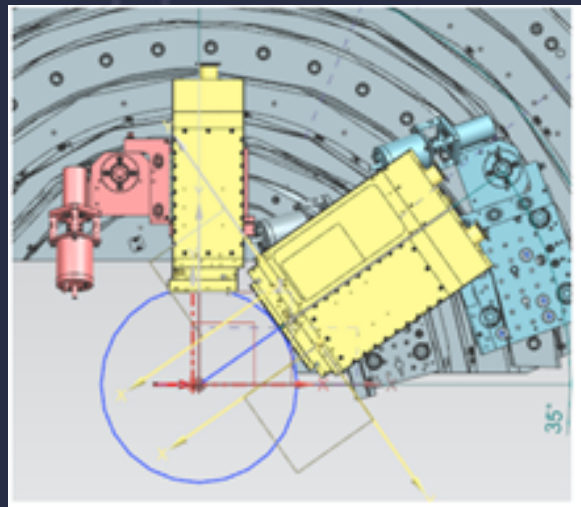
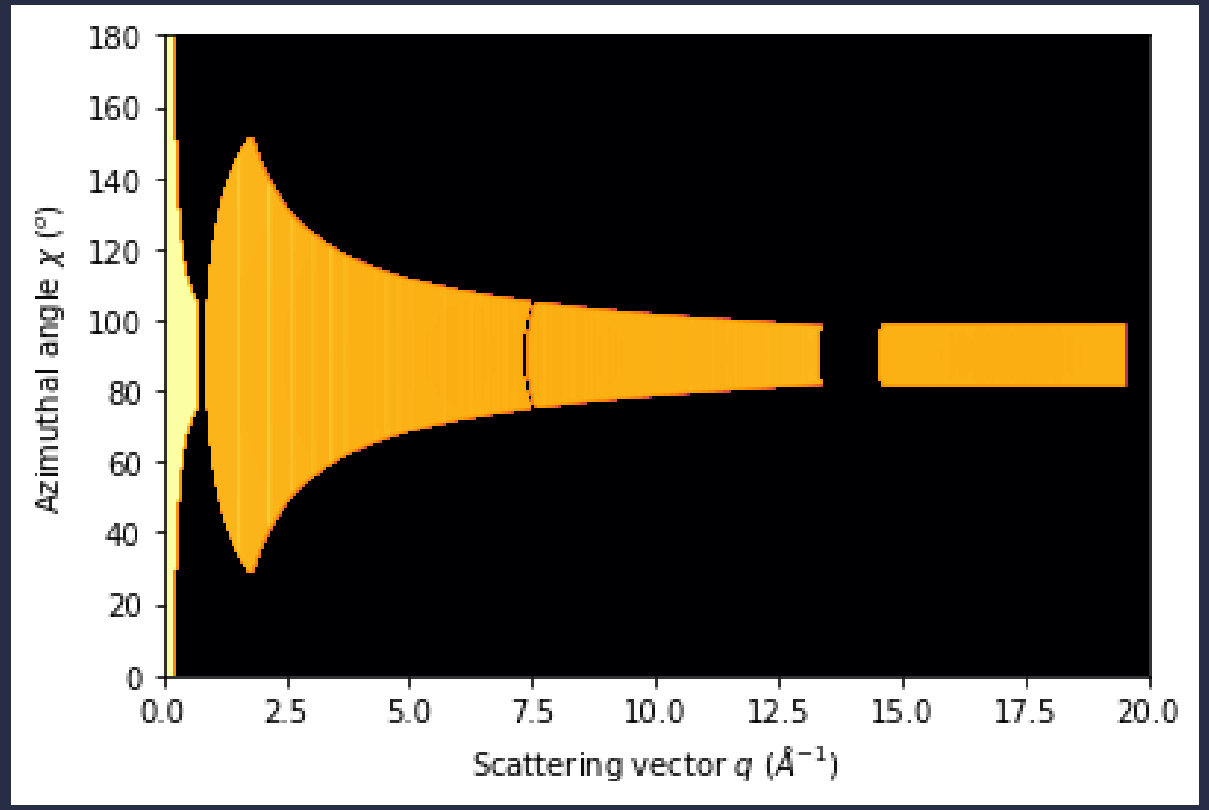
PDFGetX3 and detector gaps



4 x Jungfrau Detectors
77x38mm² (75µm pixels)

For comparison:
Perkin Elmer on XPDF (I15-1)
150µm pixels
Sample to detector ~ 200mm

	2θ centre (°)	L2 (mm)	Δ2θ (°)	ΔQ (Å⁻¹)
Detector 1 (Pair)	35 (variable)	130 (fixed)	4.4–65.6	0.93–13.2
Detector 2	~90 (variable)	130 (variable)	67–110	13.4–19.9
Detector (low angle)	~3.9 (fixed)	~1500	2.4–5.4	0.5–1.1
				(24keV X-rays)



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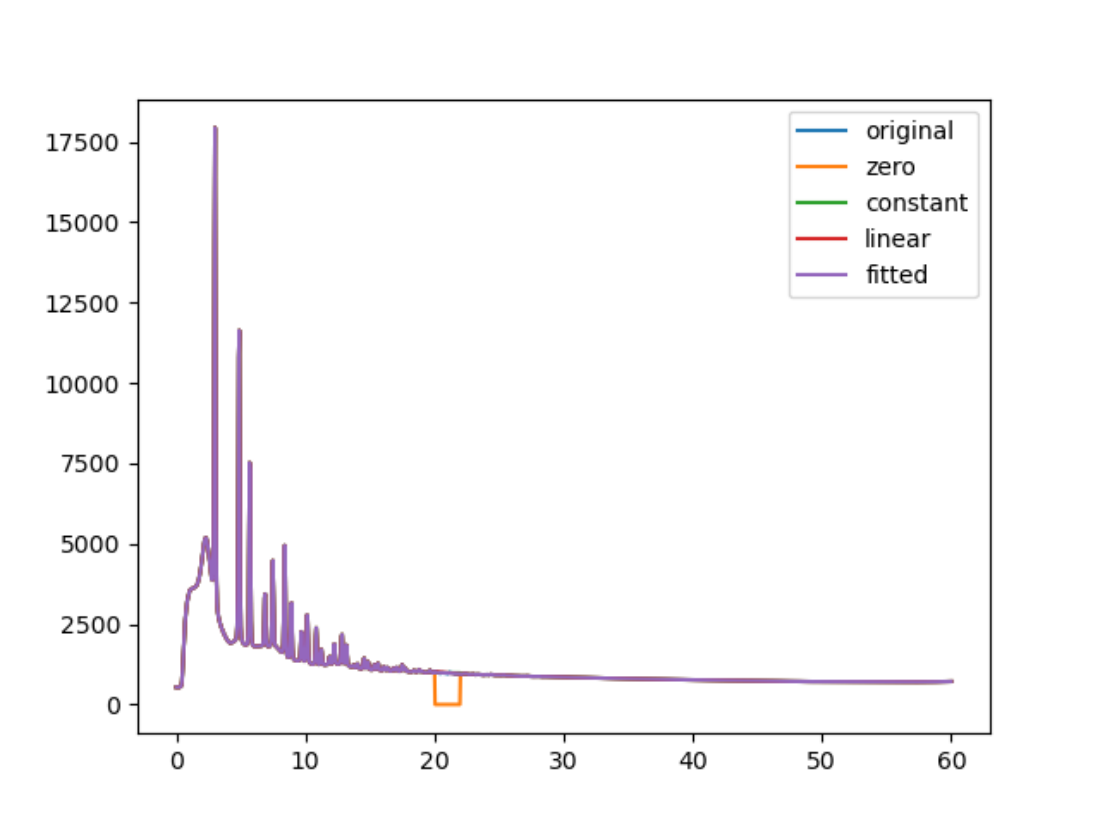

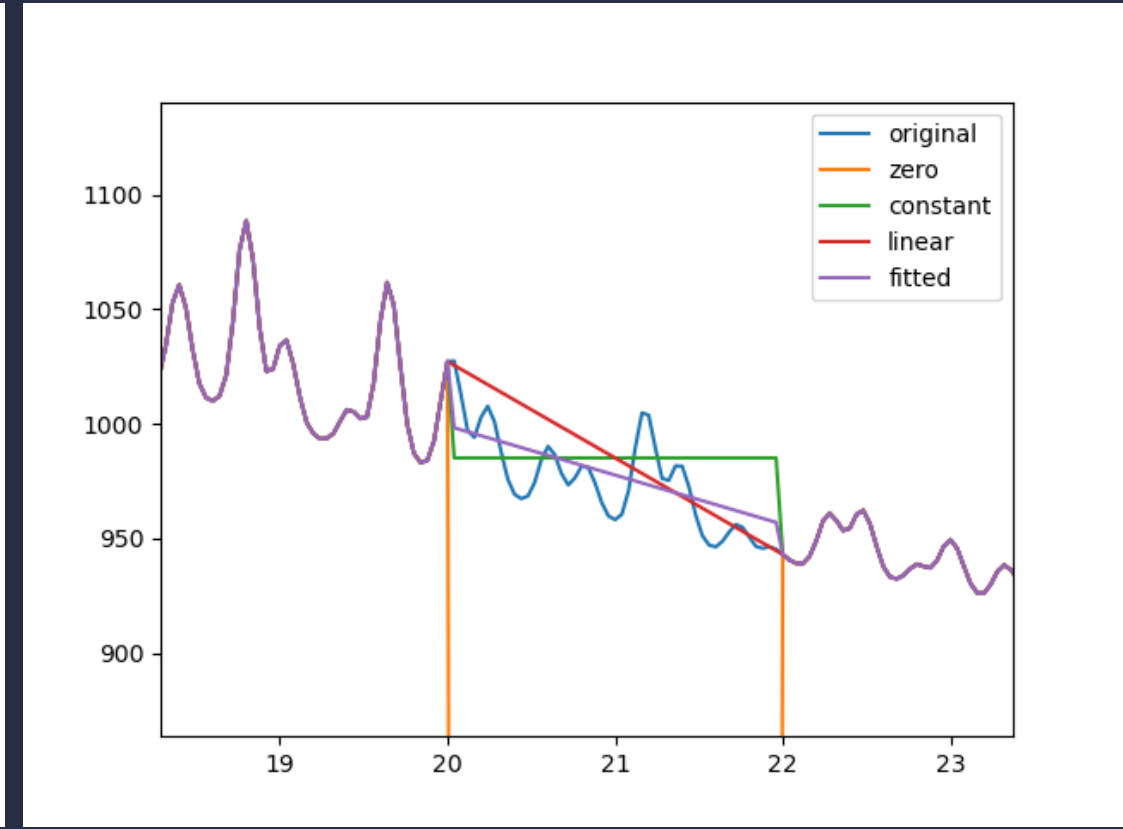

gap is roughly 13.5 - 14.8

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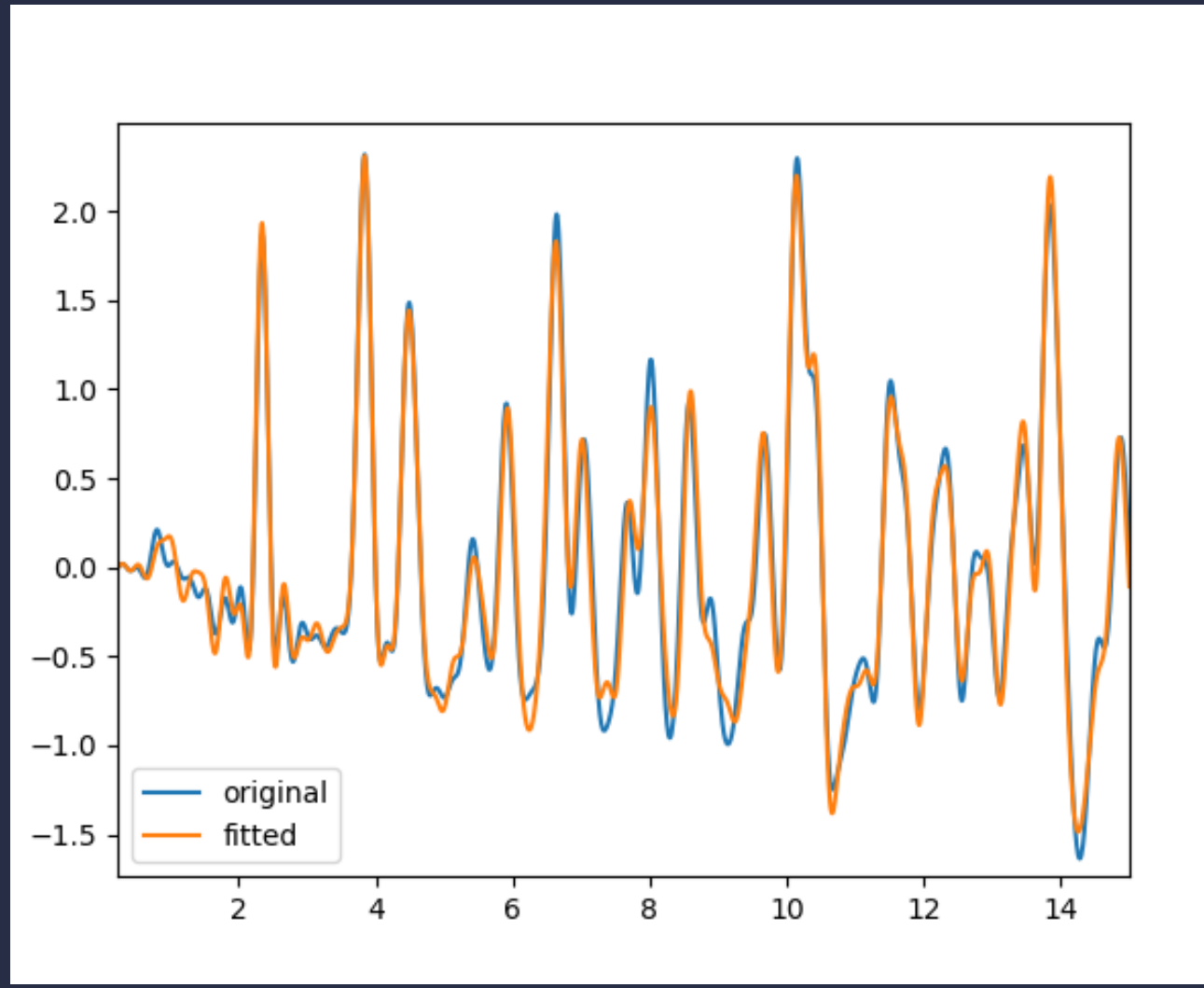
Does anyone have any concerns about this approach?



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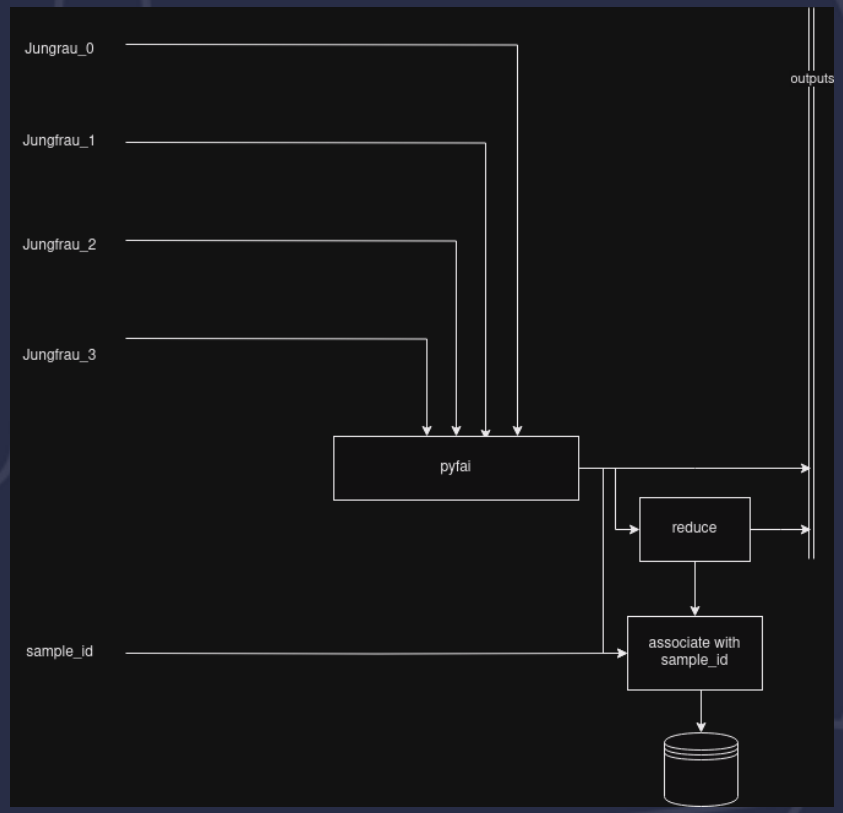
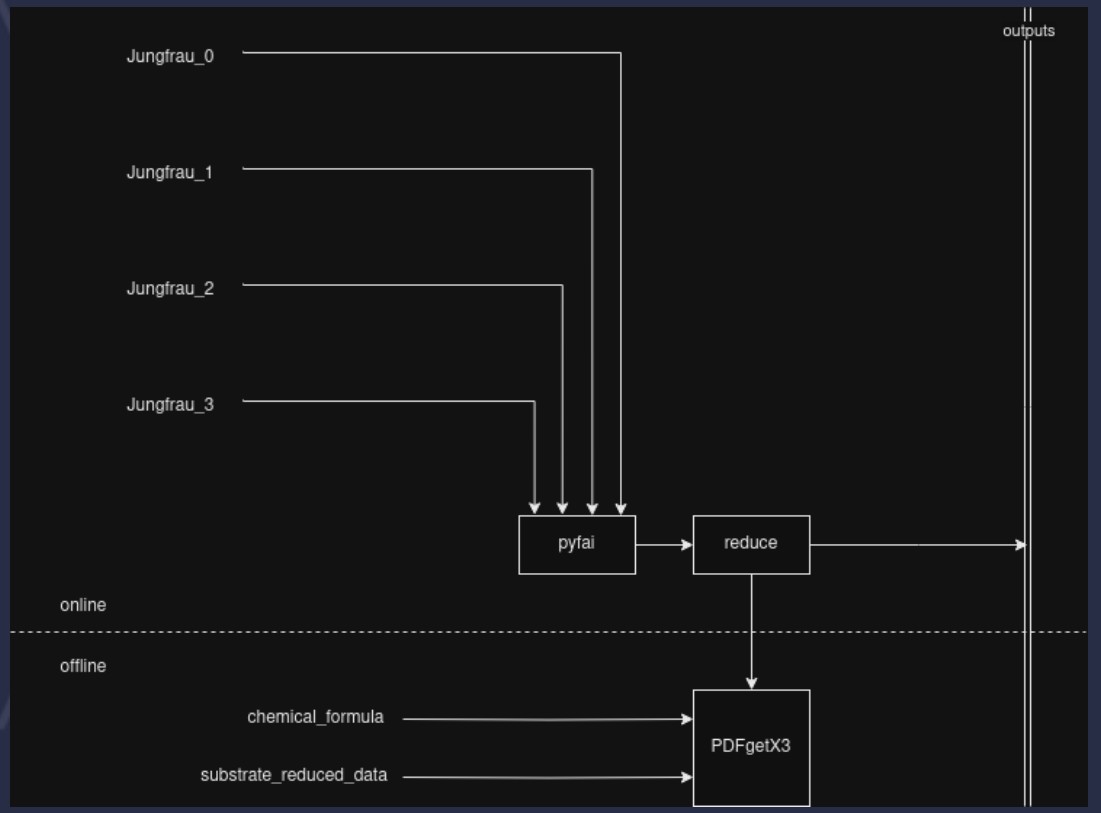
Overall schematic and context files

Following the example online, we have schematics for our two types of data collection





Points to note 1:

- *calibration* at EuXFEL is the process of taking the raw signal from the detector and making an image out of it
    - ➡️ I will endeavour (and probably fail) to refer to pyfai geometry calibration as *geometry calibration*
- we don't need to worry about *calibration*

Points to note 2:

- EuXFEL have *online* and *offline* processing
- Online processing is performed on streams of data on the ONC cluster within seconds
    - ONC cluster has no access to internet
    - Proposal directory *is* mounted on ONC
- Offline processing is performed on data saved to disk and takes place ~15 minutes after the data collection

Summary of the schematics

- We'll be able to see 1D scattering data within seconds as we can do this online
- Currently the DA team are proposing we perform the PDFGetX3 step *offline*

  How critical is instantaneous PDFGetX3-ing?

Gap mitigation

This is where the signal is not azimuthally symmetric, and a sudden radial change in the range of contributing pixels leads to discontinuities in the integrated signal

- More of an issue with large azimuthal coverage
- More soluable issue with large azimuthal coverage

Database Options

For anything to happen automatically, we need some metadata about the sample:

- Composition (so we can pipe this in to PDFGetX3)
- Substrate (so we can figure out which run to use as a background)

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Database Options

Various solutions we can look at

- emailing of sample info to nominated person
- shared google spreadsheet
- a simple web app with a database backend

Thoughts, suggestions, alternatives?

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Pre-visit computer access

Typically users get access to computer system 1 month before visit, but this can be increased for specific users upon request

Who wants to be added to this list?

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November experiment logistics

- Monday 13th November - on-site preparation begins
- Thursday 16th November - set up and alignment
- Friday 17th November - experiment begins

Who from this group plans to attend?

Any Other Business

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