EuXFEL Processing Update

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Processing Meeting 12th April 2023

Agenda:

- uf-TS/PDF processing requirements

- EuXFEL processing capabilities

- Discussion of best processing route

- Downstream analysis

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Summary of Discussion

Aim for automation as much as possible

- Use PDFGetX3 for processing

- One EuXEFL processing framework called EXtra-metro seems very suitable

- Some questions remain on best way to handle sample metadata

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EXtra-metro

- Operates on streams of data

- Allows for the description of processing graphs using a context, so a graph such as
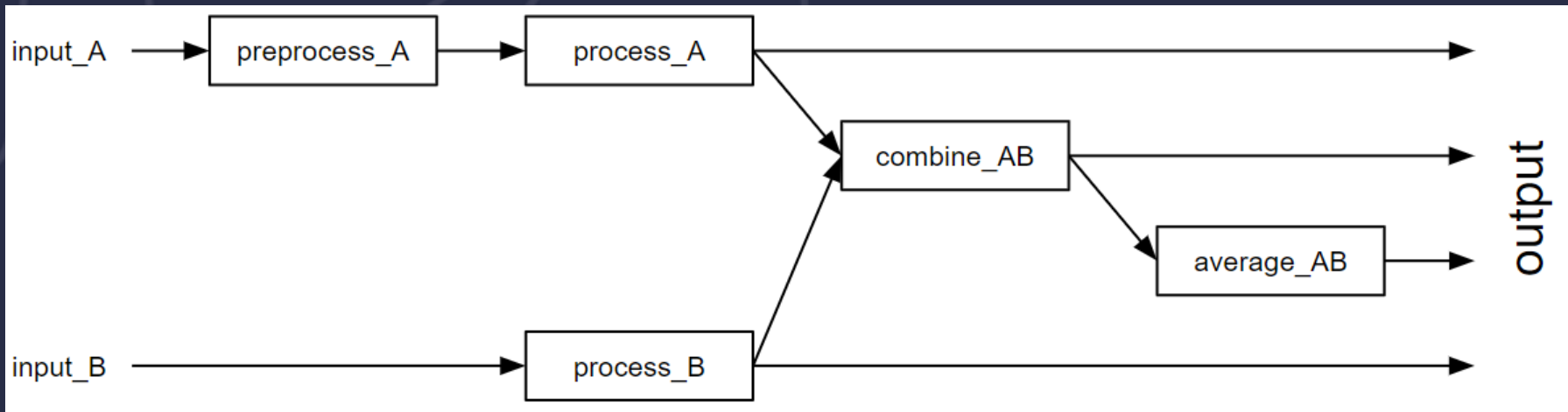
```python
import numpy as np
import xarray as xr
from my_analysis_library import correct_background

# Do background correction for input A, add custom axes to A and B,
# calculate the interpolated quotient and average it.

@View.Compute
def preprocess_A(data: 'input_A'):
    # Correct background for input A.
    return correct_background(data)

@View.Vector
def process_A(data: 'preprocess_A'):
    # Add calibration axis specific for A.
    return xr.DataArray(data, dims=['position'],
                        coords={'position': np.linspace(0, 1, len(data)))

@View.Vector
def process_B(data: 'preprocess_B'):
    # Add calibration axis specific for B.
    return xr.DataArray(data, dims=['position'],
                        coords={'position': np.linspace(0, 1, len(data)))

@View.Vector
def combine_AB(data_A: 'process_A', data_B: 'process_B'):
    # Calculate interpolated quotient.
    common_axis = np.linspace(0, 1, min(len(data_A), len(data_B)))
    return data_A.interp(position=common_axis) / data_B.interp(position=common_axis)

@View.Vector_MovingAverage(N=20)
def average_AB(AB: 'combine_AB'):
    return AB
```
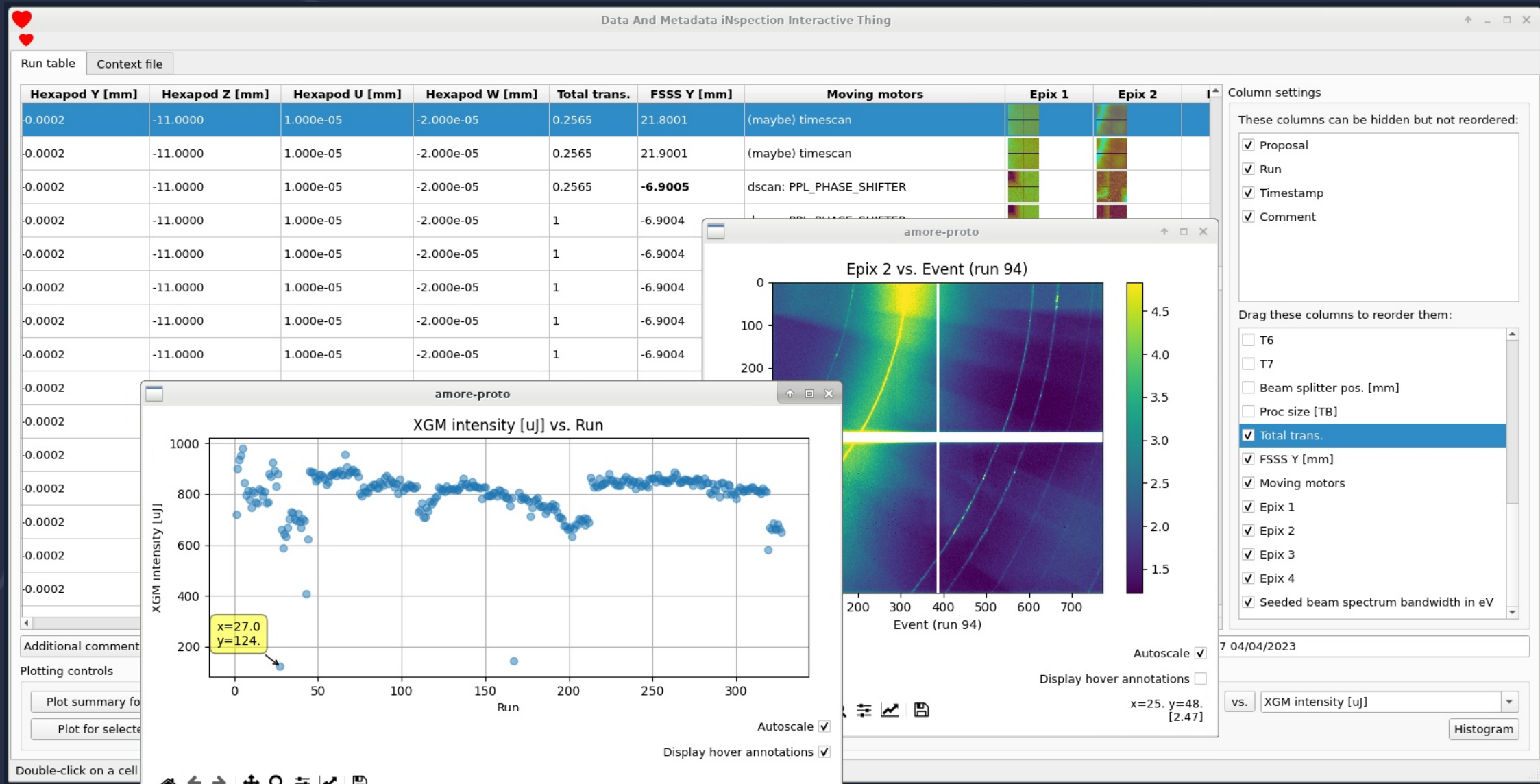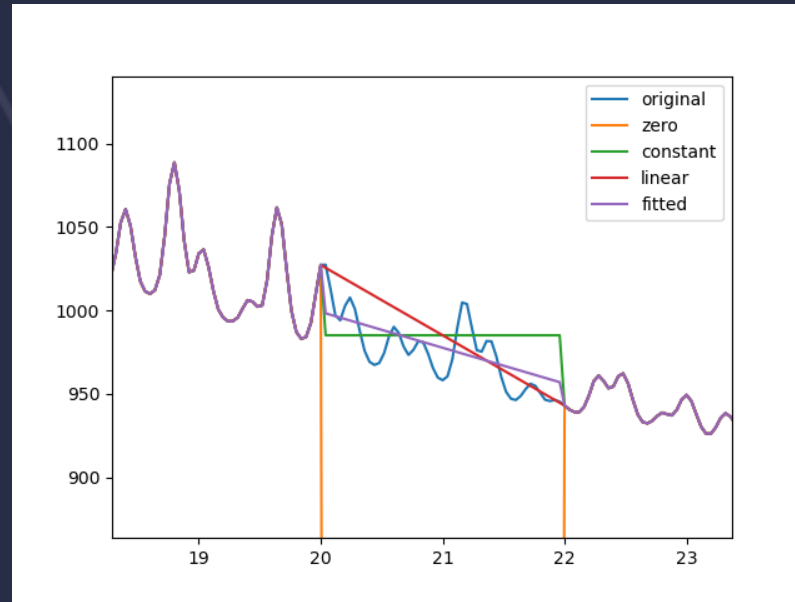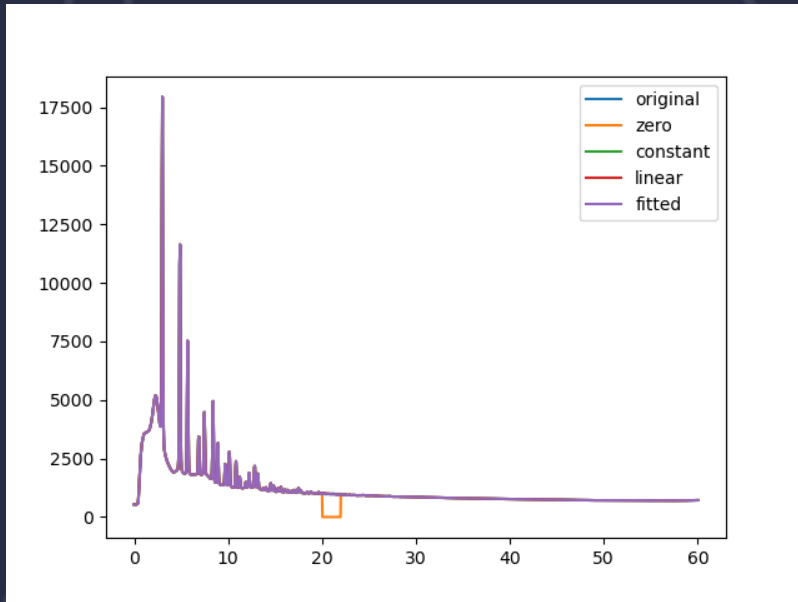
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- These context files present an ideal language in which to discuss our processing needs in pure python

- Work is currently underway to describe our processing specifications (in some cases just using pseudo-code) in this format

- Aim to reuse code blocks for processing of accumulated data and reprocessing

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Run table | Context file

Hexapod Y [mm]	Hexapod Z [mm]	Hexapod U [mm]	Hexapod W [mm]	Total trans.	FSSS Y [mm]	Moving motors	Epix 1	Epix 2	
-0.0002	-11.0000	1.000e-05	-2.000e-05	0.2565	21.8001	(maybe) timescan			
-0.0002	-11.0000	1.000e-05	-2.000e-05	0.2565	21.9001	(maybe) timescan			
-0.0002	-11.0000	1.000e-05	-2.000e-05	0.2565	**-6.9005**	dscan: PPL_PHASE_SHIFTER			
-0.0002	-11.0000	1.000e-05	-2.000e-05	1	-6.9004	dscan: PPL_PHASE_SHIFTER			
-0.0002	-11.0000	1.000e-05	-2.000e-05	1	-6.9004				
-0.0002	-11.0000	1.000e-05	-2.000e-05	1	-6.9004				
-0.0002	-11.0000	1.000e-05	-2.000e-05	1	-6.9004				
-0.0002	-11.0000	1.000e-05	-2.000e-05	1	-6.9004				
-0.0002									
-0.0002									
-0.0002									
-0.0002									
-0.0002									
-0.0002									

Additional comment

Plotting controls

Plot summary fo

Plot for selecte

Double-click on a cell

Column settings

These columns can be hidden but not reordered:

☑ Proposal
☑ Run
☑ Timestamp
☑ Comment

Drag these columns to reorder them:

☐ T6
☐ T7
☐ Beam splitter pos. [mm]
☐ Proc size [TB]
☑ Total trans.
☑ FSSS Y [mm]
☑ Moving motors
☑ Epix 1
☑ Epix 2
☑ Epix 3
☑ Epix 4
☑ Seeded beam spectrum bandwidth in eV

7 04/04/2023

vs. | XGM intensity [uJ]

Histogram

amore-proto

Epix 2 vs. Event (run 94)

Event (run 94)

Autoscale ☑

Display hover annotations ☐

x=25. y=48.
[2.47]

amore-proto

XGM intensity [uJ] vs. Run

XGM intensity [uJ]

x=27.0
y=124.

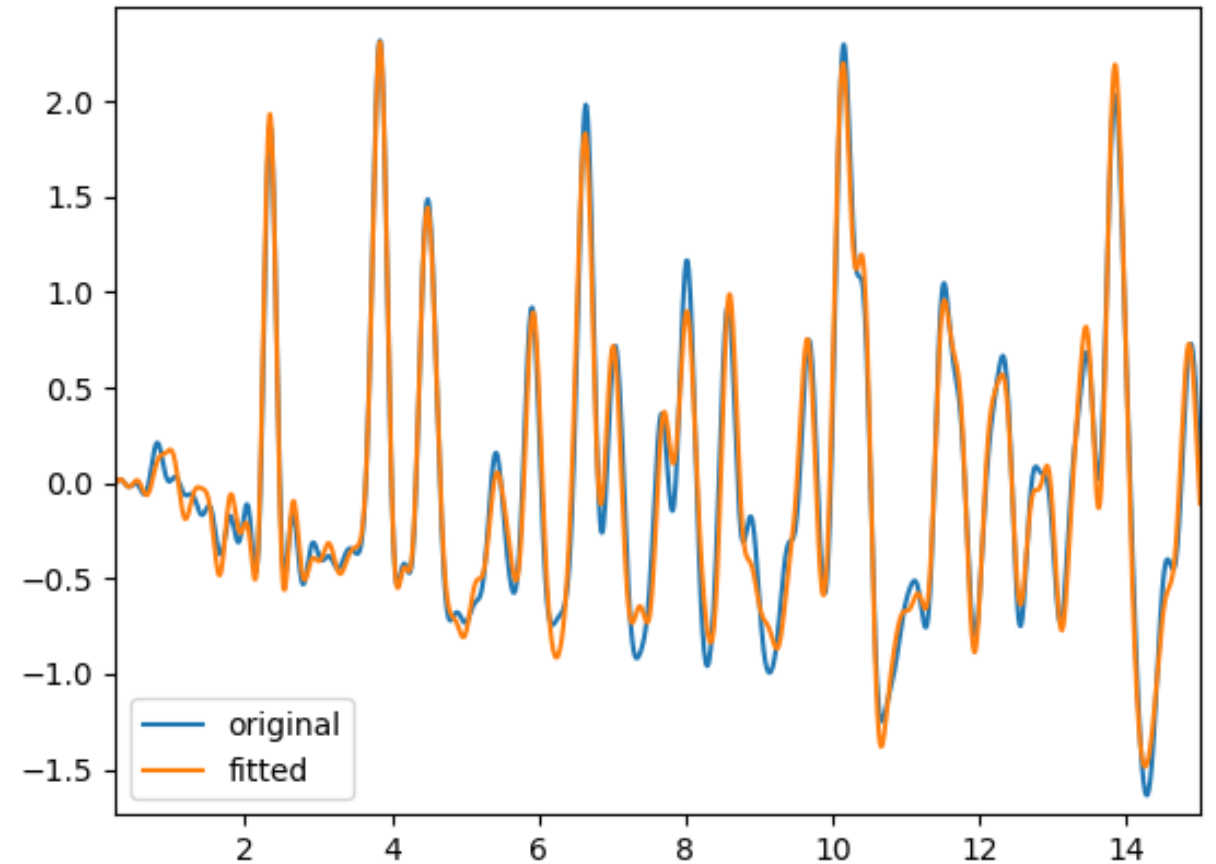Run

Autoscale ☑

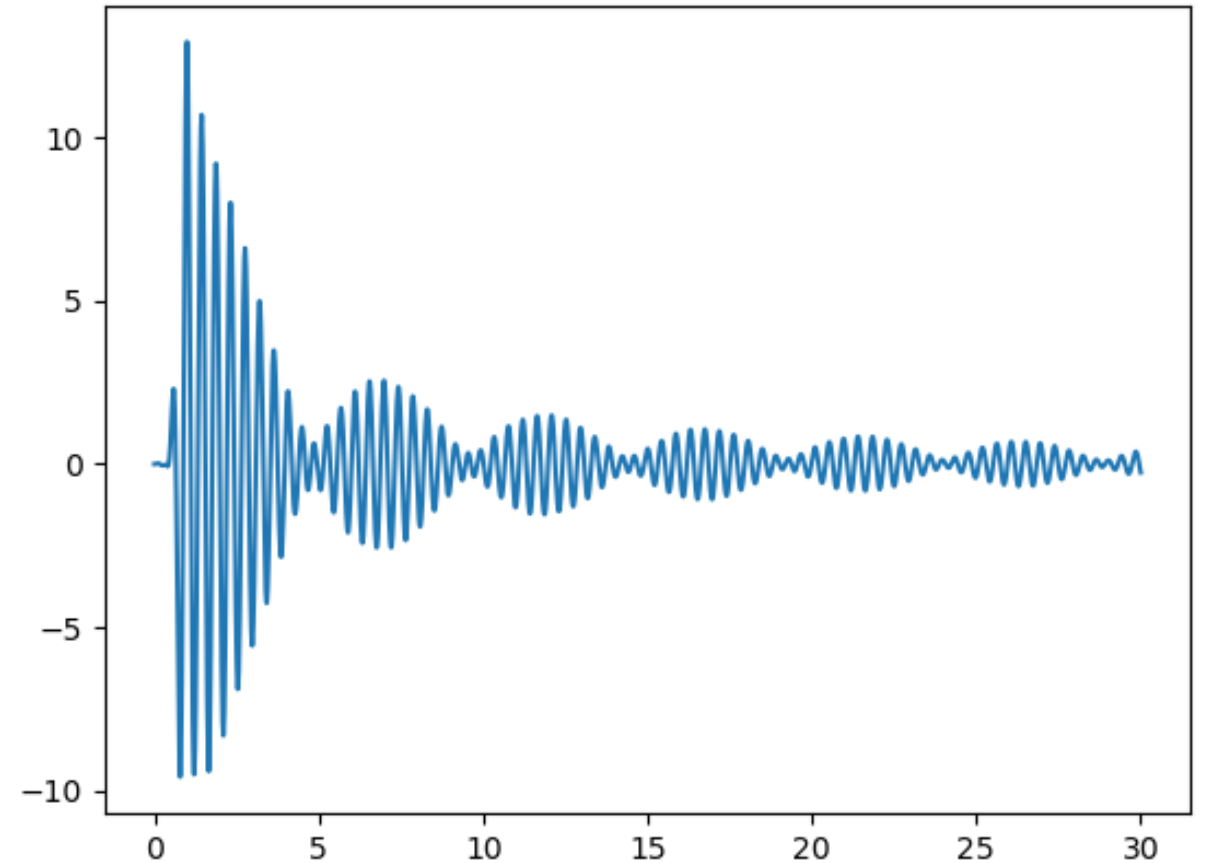Display hover annotations ☑

PDFGetX3 and detector gaps

The exact detector geometry is yet to be finalised, but processing should be prepared for incomplete data

- Some simple linear fitting gives the best match to the original data

- Can also attempt to optimise gap placement relative to expected sample features

Summary

- Discussions have been ongoing

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