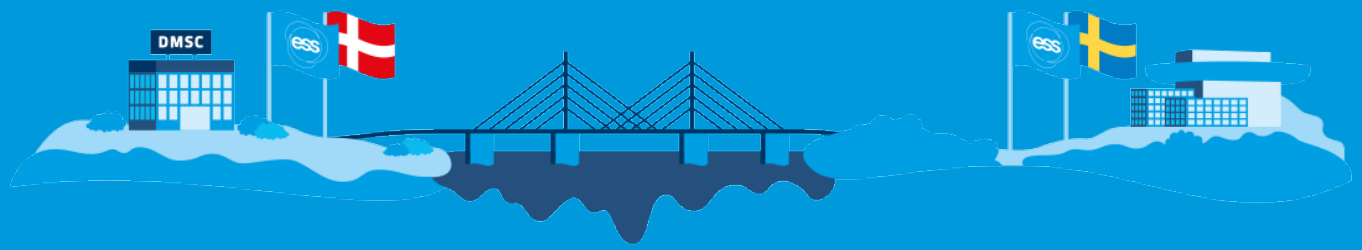
LoKI: The data perspective

DMSC–IDS contribution

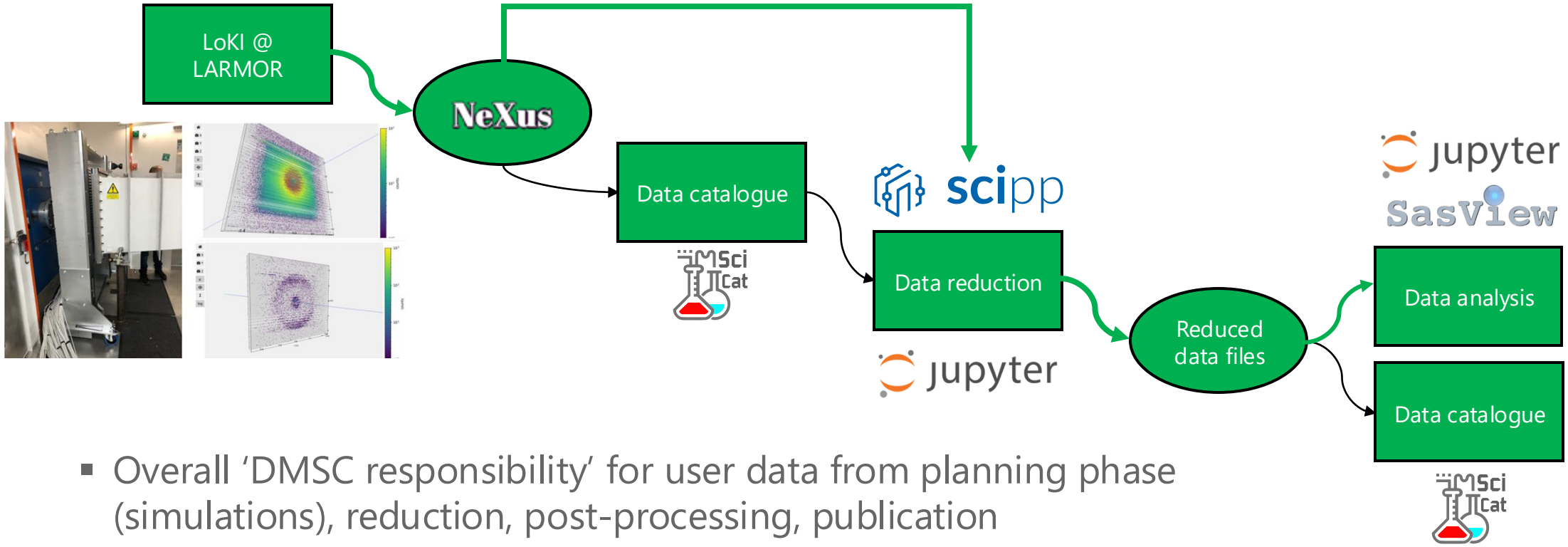
PRESENTED BY OLIVER HAMMOND

2025-09-11



Overview

General data pipeline



- Overall 'DMSC responsibility' for user data from planning phase (simulations), reduction, post-processing, publication
- **Focus on cold commissioning test cases**

Cold commissioning planning

Initial phase

- Early involvement with instrument team, ECDC, etc, in defining cold commissioning test plan documentation:
  - Sample area systems
    - ESS-5758591
  - Detector motion system
    - ESS-5601102
  - Collimation system
    - ESS-5601101
  - Detector & Beam monitor system
    - ESS-5758315

Cold commissioning

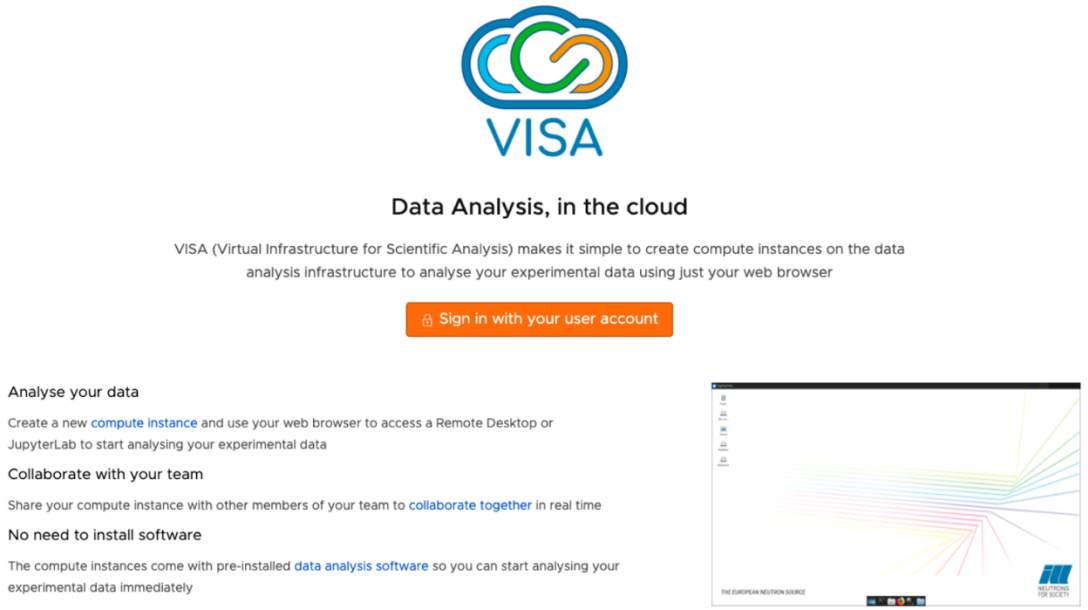
Testing and reporting involvement

- Physically present at all tests
- Responsible for data-orientated test cases and review for:
  - Chopper system
    - ESS-5759105
  - Sample area systems
    - ESS-5769853
  - Detector motion system
    - ESS-5767051
  - Collimation system
    - ESS-5769855
  - Detector & Beam monitor system
    - ESS-5818477

General approach for CC testing

From a data point of view

- Using, where possible, **a representative workflow:**

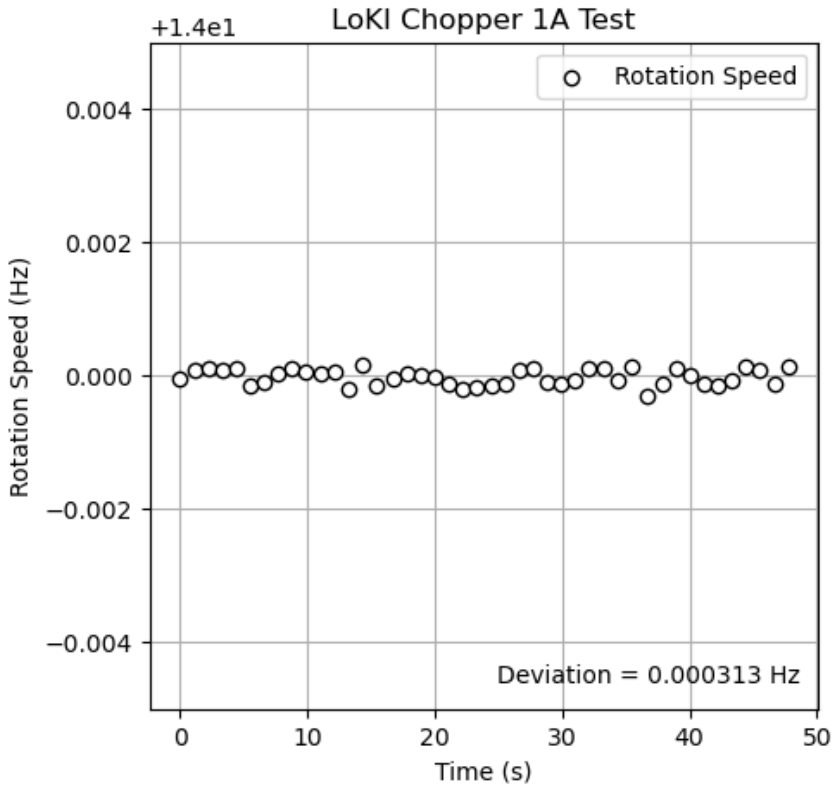


- **VISA instances** (provided by DST @ DMSC)
- **LoKI proposal 051657 – dedicated to commissioning activities**

i. Chopper system

ESS-5759105

- Passed all test cases for data acquisition
- Singular punch list item (6) to clarify for HC:
  - “Follow up on how fit is implemented in NICOS for chopper phasing”
- Example LoKI BWC (Band Width Chopper) rotation data (right) from a LoKI NeXuS file
  - It spins! But also proves a lot of functioning systems:
    - Part of proposal system
    - Written to hdf-format file
    - Saved in the generated file structure
    - Accessed on VISA (authorisation, virtualization, etc)



ii. Detector motion system

ESS-5767051

- Passed all test cases for data acquisition with a punch list item:

- NIT-206 and ECDC-4437
  - Important issue noted with filewriter crashing resulting in corrupted files that could not be opened (051657_00000055.hdf)
  - Being checked with a fix in PR
  - Tested at recent ILL detector tests for NMX

  - Reliable filewriting critical for all instruments

iii. Collimation system

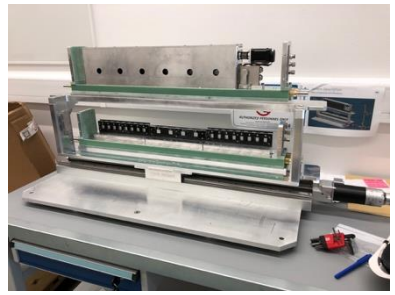
ESS-5769855

- Passed all test cases for data acquisition with only a single minor note:
  - There was a temporary issue with the DK filewriting server at the time of the test, preventing writing
  - Motor positions were nevertheless captured accurately through the test
  - If we wish to have a definitive file showing the motion of each system, we will simply repeat the tests with fixed filewriting.

iv. Sample area systems

ESS-5769853

- All cases were recorded as **failed** due to a few missing components during the test, namely, sample stack z axis motion and a functioning sample position macro in NICOS.
- Sample position offset was missing during the test, but 'sample_position_z' was subsequently added to NICOS and the NeXuS file: NIT-233
- Regarding the sample changer NICOS and NeXuS discrepancies, requirements are:
  - Sample changer position mapping data is needed (ultimately this will come from HC, but placeholders would have been sufficient for the test) NIT-220
  - *cf* punch list item 16; a NICOS 'sample changer macro' should allow a user to script samples to be run at pre-set named positions, and write these sample position to the NeXuS file for the changer environment NIT-221
    - Naming convention needs to be discussed and decided, ie. AT, BT, CT … XT (top row), AB–XB (bottom row), or similar
    - Needs to be responsive to flexibility of the design
    - Logging simple motor position readouts is deemed insufficient

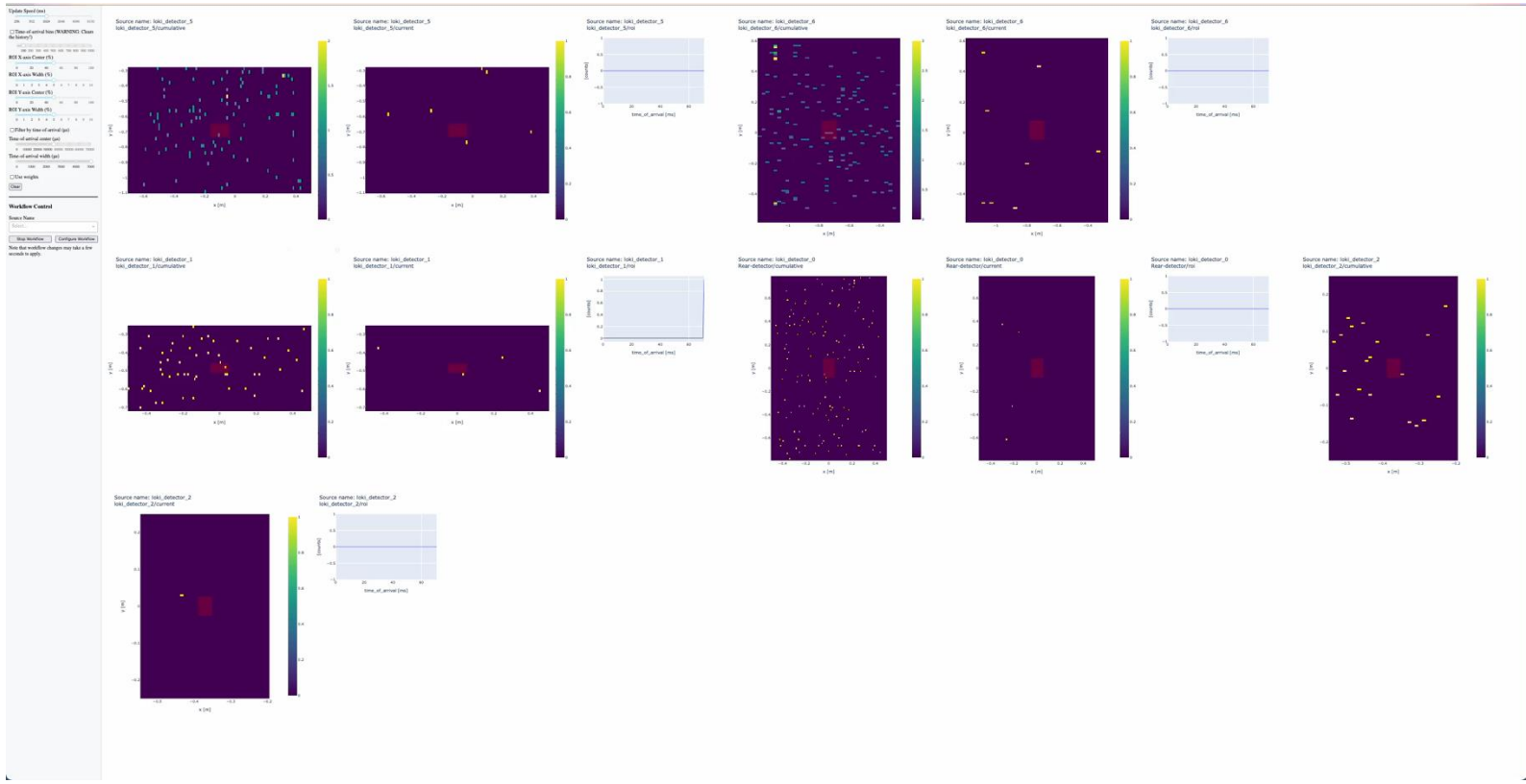


v. Detector and beam monitor systems

ESS-5818477, test case 2: Live Display of Neutron Data

- Excluding beam monitors (now deferred scope)
- Live display worked in NICOS implementation (JustBinIt)
- Live display worked in DMSC implementation (Scipp Live dashboard)

- Random stopping issue observed for JustBinIt counting: NIT-318
- NIT-315 : Counts should start/stop in connection with measurements (also pertinent to Scipp Live view)
- Count rate display is available, but hidden under inspection menu for device: NIT-316



v. Detector and beam monitor systems

ESS-5818477, test case 3: Storage of Neutron Events

- Excluding beam monitors (now deferred scope)

- Test case 3.1: Compared EFU readout from Grafana (~6 cps)…
- To those written to file 051657_0000084.hdf

  between 07:19:08.624 – 07:38:18.733 (6697 events; 5.87 cps)

- ‘Good enough’ – but exploring a suggestion to build tools to examine this on a more precise basis to ensure events aren’t being dropped: NIT-317

v. Detector and beam monitor systems

ESS-5818477, test case 4&5: Instrument and Timing/Source metadata

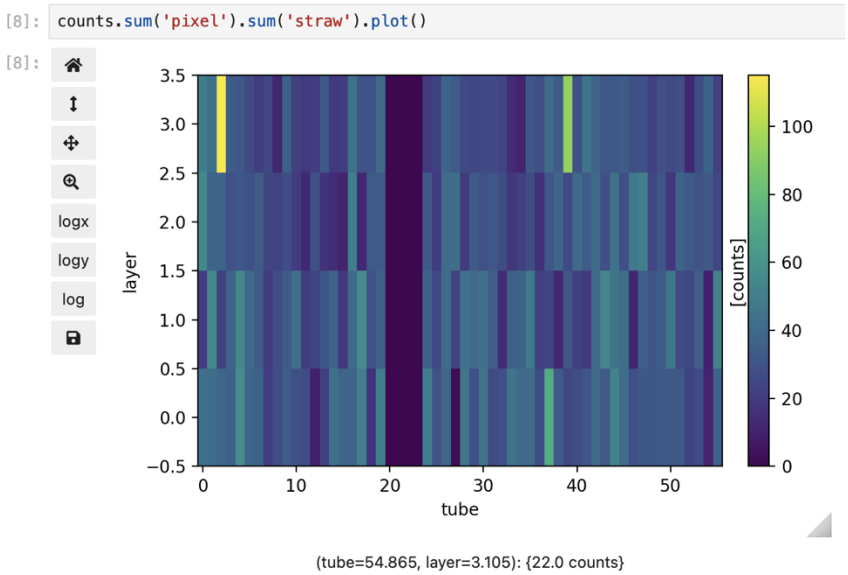
- Excluding beam monitors (now deferred scope)
- 4.1, detector positions written to file: Fail
  - The NeXuS file definition specifically for bank_0 (the only mobile bank) was modified to a transformation chain with motor position dependency and a linear offset, as highlighted previously: NIT-209
    - Strictly speaking, detector positions are not written to file, but enough information is provided for this to be calculated during reduction in Scipp.
      - Is this a requirement?
- 5.1, Proton pulse information written to file: Fail
- 5.2, Target status information writen to file: Fail
  - Issue (undiagnosed during the test), possibly credentials/network config, for connection from TN to NiN to transfer accelerator PVs.
  - Vital to fix, must be robust: NIT-327

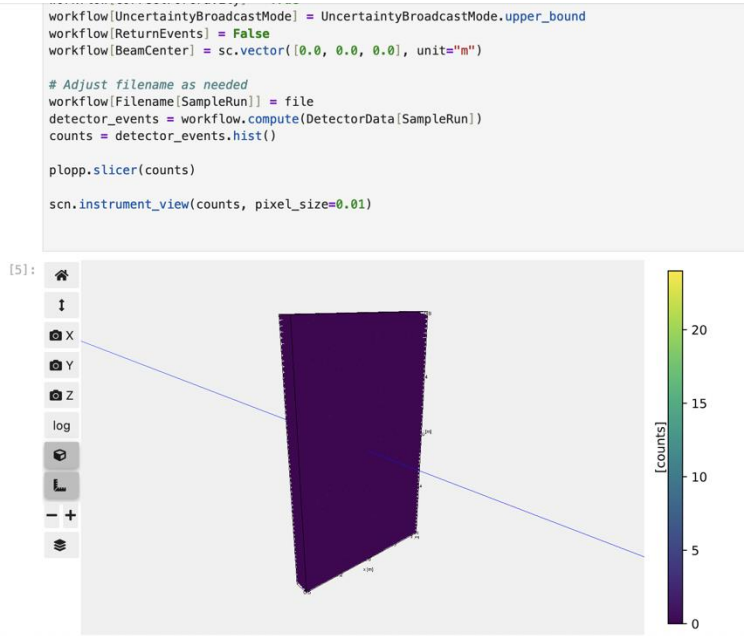
v. Detector and beam monitor systems

ESS-5818477, test case 6: Data Processing

- Excluding beam monitors (now deferred scope)

- 6.1, Data file listed in SciCat: Pass, “Immediate” = 11 seconds.
- 6.2, Stored data file can be loaded in VISA Jupyter notebook: Pass
- 6.3, Detector data plotted in VISA Jupyter notebook: Pass



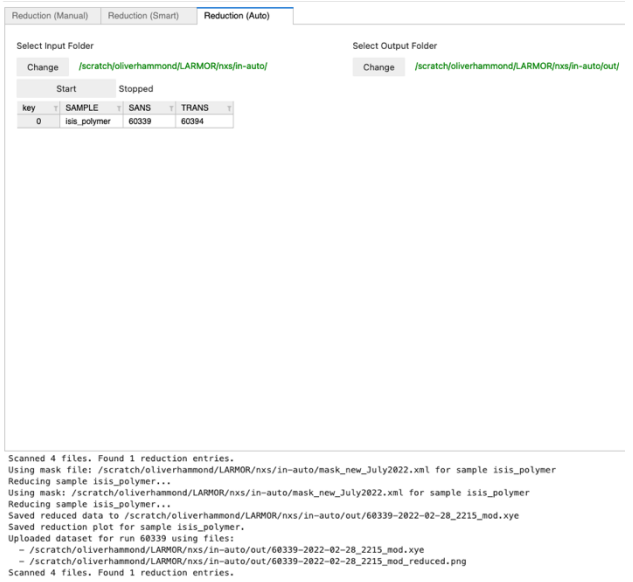


v. Detector and beam monitor systems

ESS-5818477, test case 6: Data Processing

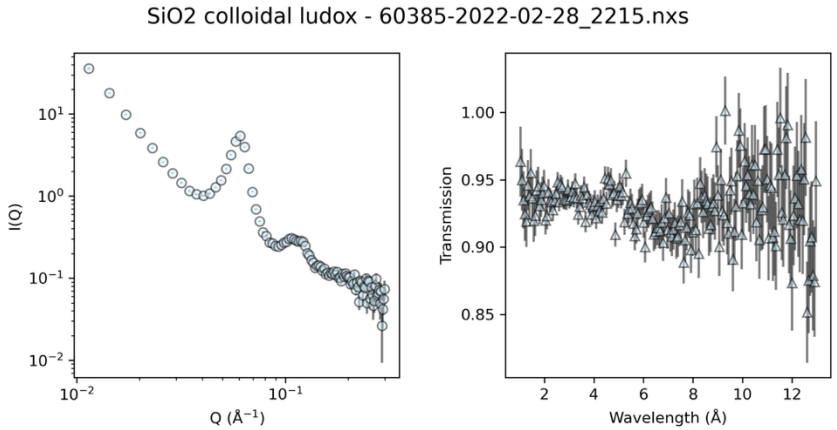
- Excluding beam monitors (now deferred scope)

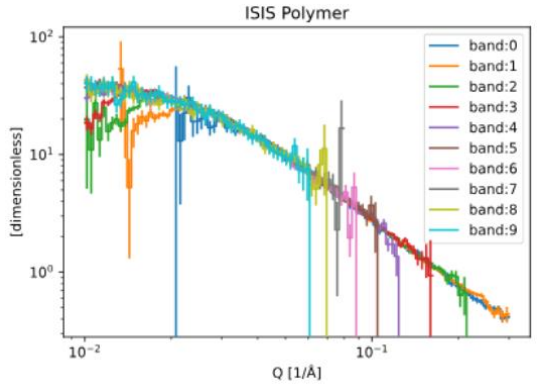
- 6.5 & 6.6, Synthetic test data can be loaded, plotted and reduced: N/A
  - Less focus on synthetic testing to date
  - Will revisit the state of LoKI–McStas in the next period for multi-detector reduction
- 6.7 & 6.8, Larmor test data can be loaded, plotted and reduced: Pass
  - Preliminary work on GUI widgets for auto-reduction

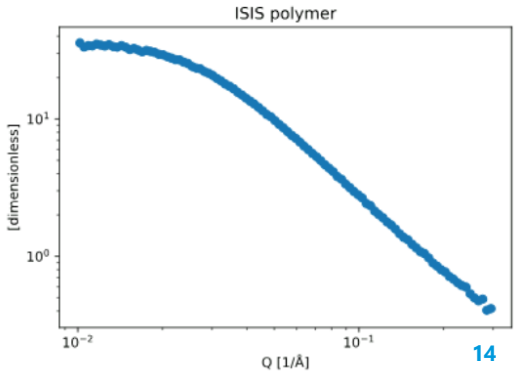



```
#log bins
workflow[QBins] = sc.geomspace('Q', 0.01, 0.3, 101, unit='1/angstrom')
da = workflow.compute(BackgroundSubtractedIofQ)
da.plot(norm="log", title="ISIS polymer", scale={'Q': 'log'})

#save output
da.coords['Q'] = sc.midpoints(da.coords['Q'])
sxye.save_xye(fname='ISIS-polymer-i.xye', da=da)
da.plot(norm="log", title="ISIS polymer", scale={'Q':'log'})
```

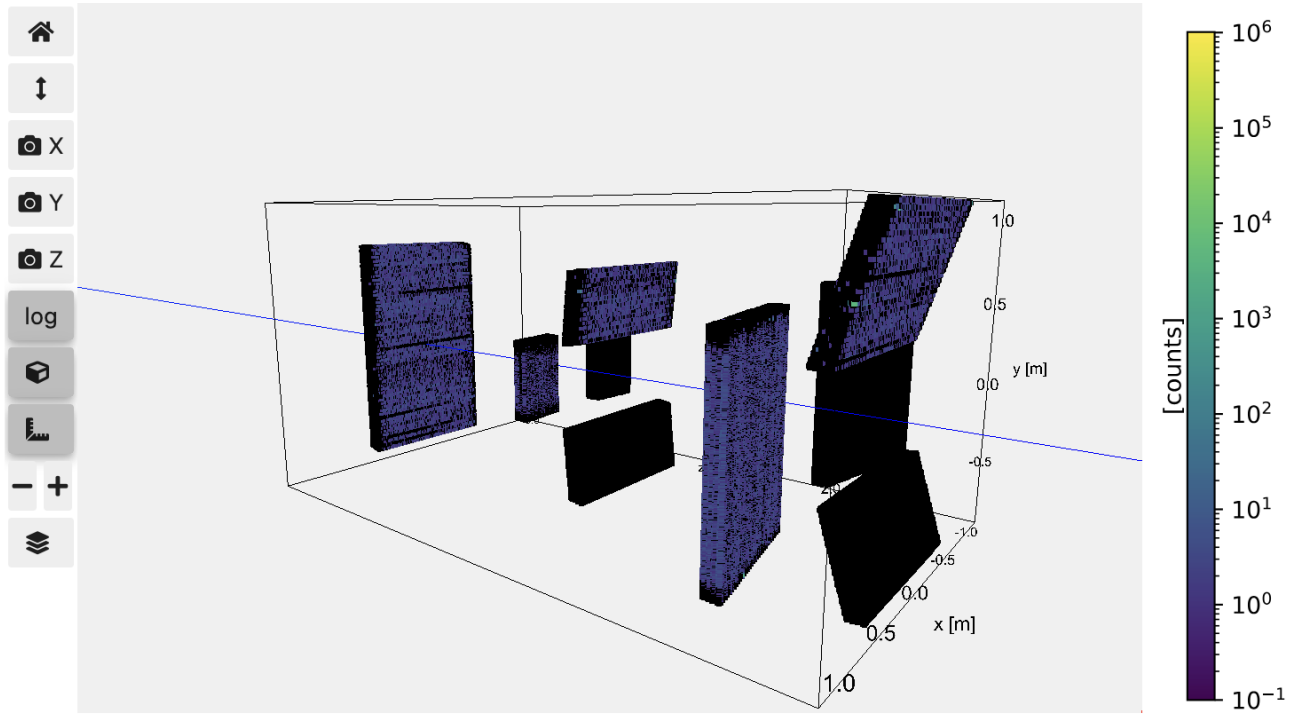






Summary

- DMSC systems post-ECDC are in an excellent position and ready for HC



Thank you for your attention!

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