



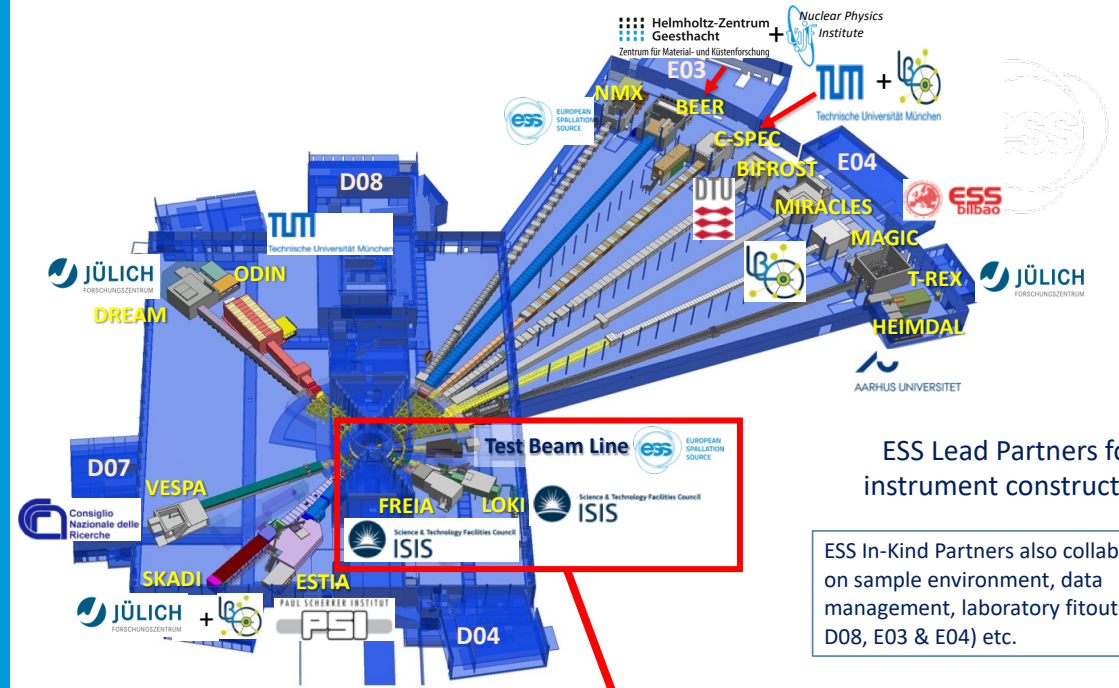
LoKI STAP Update

Instrument progress
24th October 2022

PRESENTED BY THE LOKI TEAM

1

Installation activities



ESS Lead Partners for instrument construction

ESS In-Kind Partners also collaborate on sample environment, data management, laboratory fitout (D04, D08, E03 & E04) etc.



LoKI Status Overview



Detectors

Vessel installed
Detector modules and mechanics awaiting shipment from ISIS

Utilities

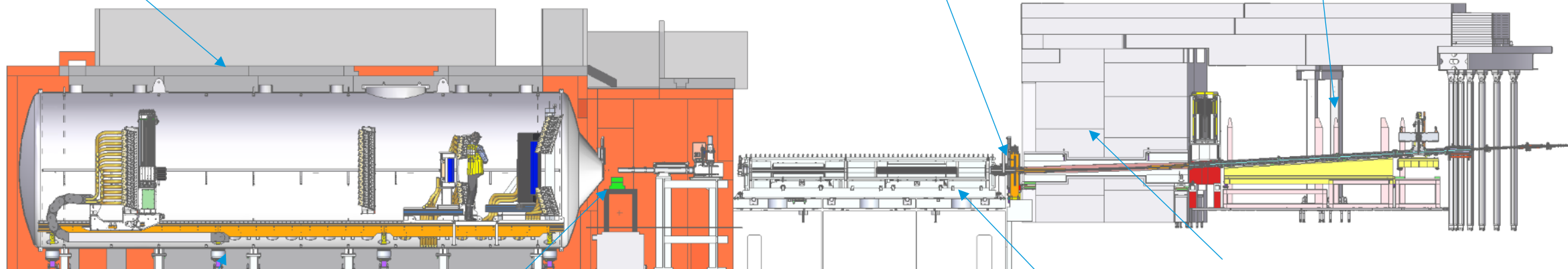
Electrical services being installed
Utilities (air, water, etc) nearing final design
PSS under detailed design
Network to be designed

Choppers

Delivered and SAT complete, and awaiting installation

In-bunker

ALL components on site and awaiting installation slot



BWI

Insert installed

Cave Shielding

- Steel is currently being installed
- Concrete roof in procurement

Sample Area

- Stack awaiting installation
- Snout system being shipped to ESS
- Door & roof manufacture almost complete

Beam monitors

- Finalised preamp electronics - final monitors now under construction
- Undergoing final neutron testing

Bunker-to-cave

- Base structures installed
- Collimator Selector being shipped to ESS now
- Shielding on site and awaiting installation

Installations in the last 6 months

B₄C lining in the tank nose cone

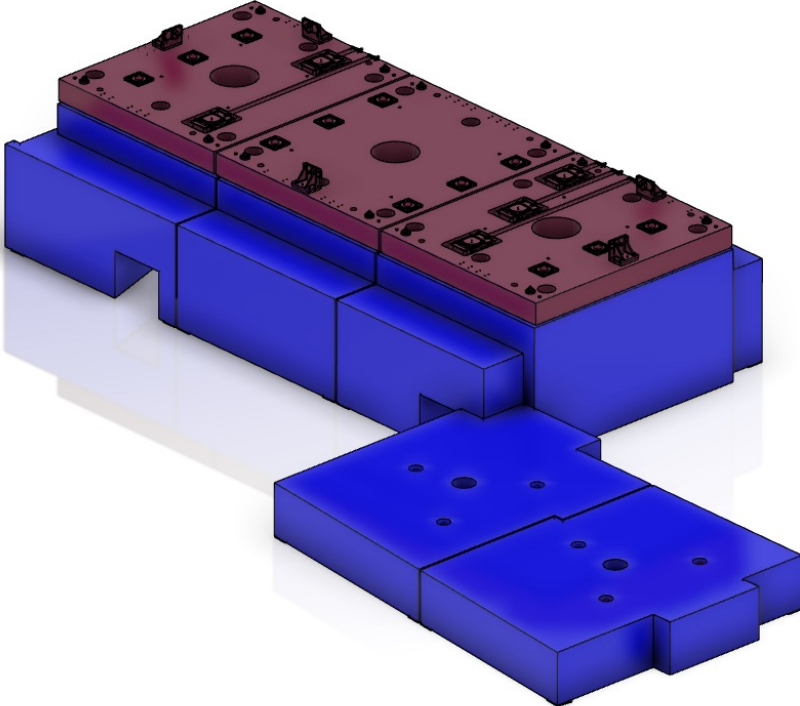


External fixtures on the vacuum tank complete



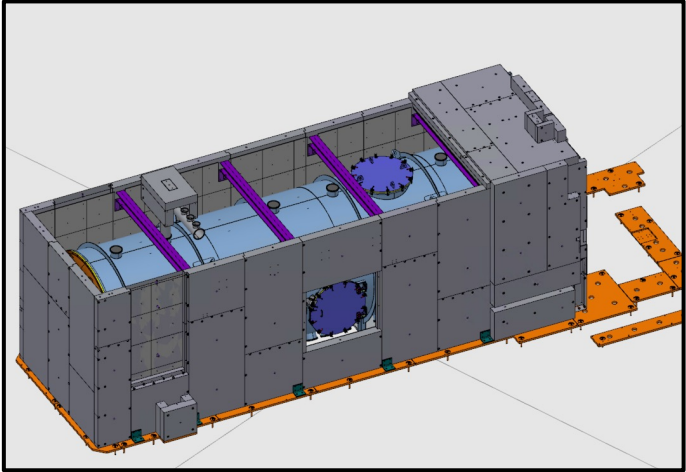
Installations in the last 6 months

Alignment baseplates for collimation and sample stack installed



Installations in the last 6 months

Cave walls



Installations in the last 6 months

Raceways and other infrastructure for electrical and detector cabling



Installations planned for the next 6 months

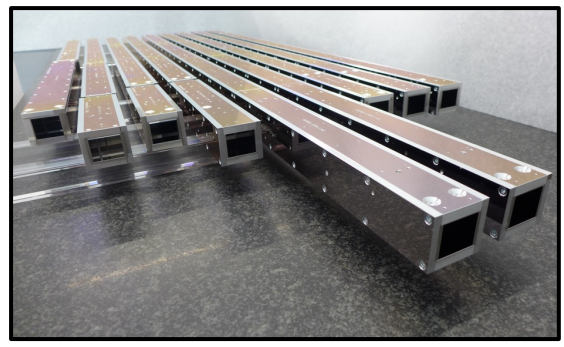
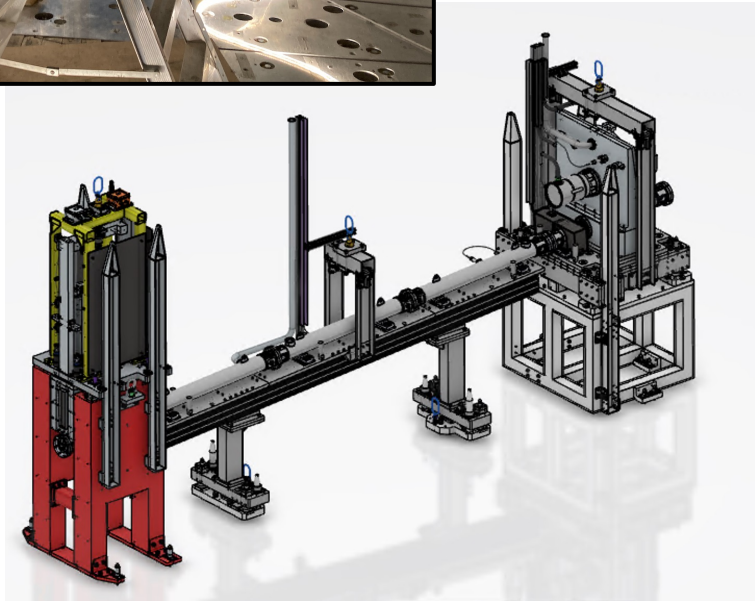
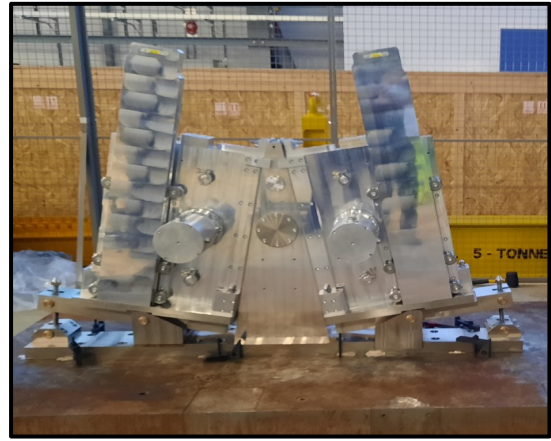
In bunker components (expect access beginning of 2023)



- Including:
- Chopper 1
 - Heavy shutter
 - Guides
 - Monitor 1

Including:

- Bunker-to-cave shielding
- Collimation
- Guides
- Chopper 2





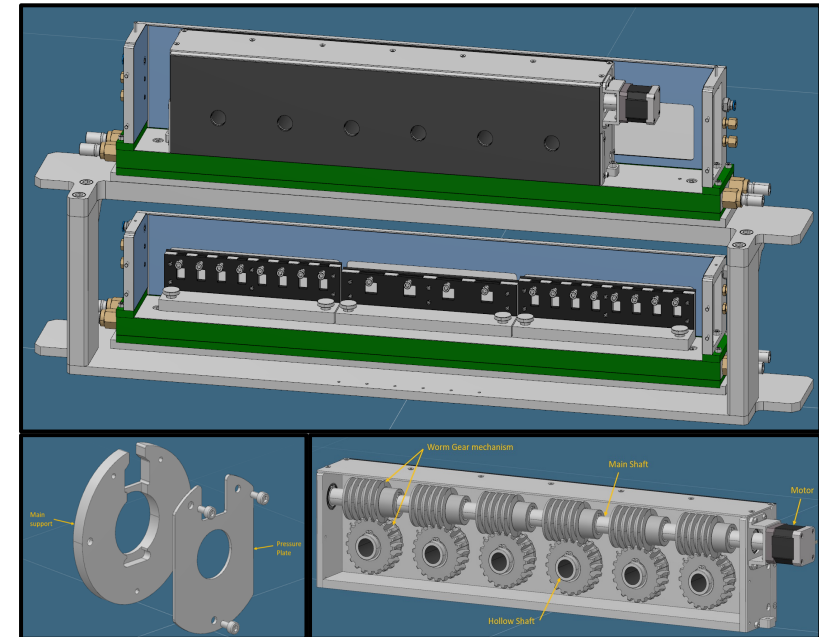
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Sample environment

General sample environment updates



- **Thermostated cell holder** and **rotating cell holder** drawings for manufacture currently under review before being sent to manufacturer.
- **Descoping of permanent skid** (isolated cooling water). 2 locations for placement of temporary skid identified. Place on roof if permanent skid is required in the future.
- **Rheometer** integration is underway and making progress.



Sample environments



| Priority | Sample Environment System (SES) | Phase | Date Needed* | Status |
|----------|--|-------|--------------|---|
| 1 | Thermostated sample changer for quartz cuvettes | HC | Q1 2023 | Detailed design almost complete - based on ISIS set-up |
| 1 | Cell tumblers/rotating sample holders | HC | Q1 2023 | Detailed design almost complete |
| 1 | Flow cell (including HPLC pumps) | HC | Q3 2022 | Jasco HPLC integrated |
| 2 | In situ techniques, as spectrometer attachments to the flow-through cell | ES | Q2 2023 | Direct purchase (Ocean Insights). Integration underway |
| 2 | Rheometer | ES | Q1 2023 | Anton Paar undergoing integration at ESS |
| 3 | Stopped-flow cell | ES | Q3 2023 | In-kind device from Estonia (Biologic) undergoing testing at ESS |
| 4 | Individually thermostated cuvette rack | ES | Q2 2023 | Prototype exists and integrated at ESS |
| 4 | Goniometer(s) | ES | Q1 2023 | ESS to purchase early 2023 |
| 4 | Dismountable 'sandwich'-style cells (ESS) | ES | Q2 2023 | Designs exist. Just to be sent for manufacture |
| 4 | Warm Bore Cryomagnet 2.5T | ES | Q2 2023 | ESS procurement underway |
| 4 | Stress/stretching rig (ESS) | ES | Q1 2023 | ESS collaboration(s) to develop different rigs |
| 4 | Cryostat – dilution fridge less than 1K | ES | | |
| 4 | Cryostat wet | ES | Q4 2022 | |



Additional projects

NURF

in situ fluorescence, UV/vis absorption, densimetry on a continuous flow cell

- Integration of hardware on-going
- Data streamlining in NeXus and SCIPP (Gudrun Lotze and Cedric Dicko)

Microfluidics

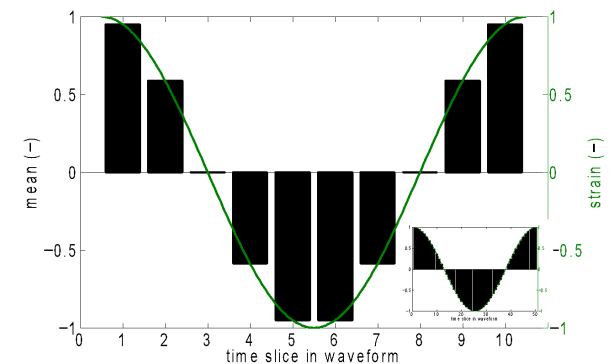
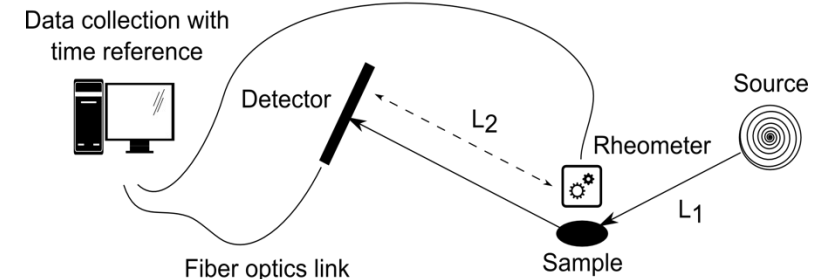
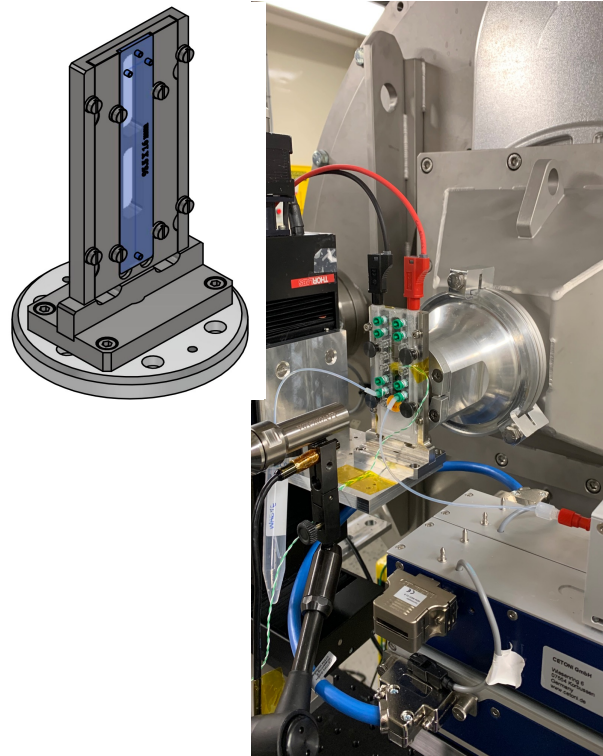
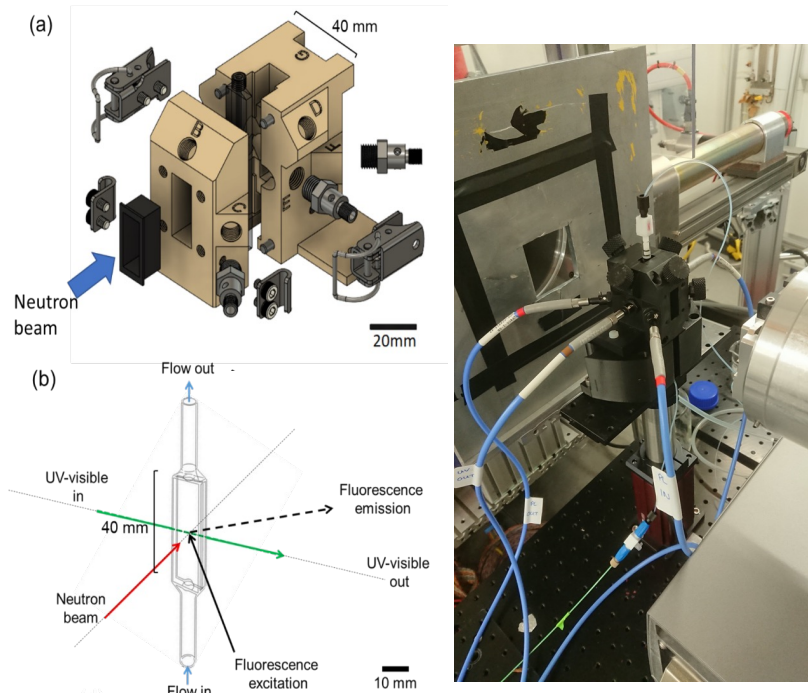
novel flow-SANS sample environment

- Chip holder in manufacture
- Beamtime proposal to study lipid nanoparticles under flow
- SREss3 project with Federica Sebastiani (Malmö)

Neutron data mining on sub-ms timescale

The detection/scattering time of the neutrons will be linked to external stimuli from sample environment, e.g. rheometry

- Collaboration with ISIS (Sarah Rogers) & Uppsala (Max Wolff)
- PhD student just started, data scientist to be hired next year

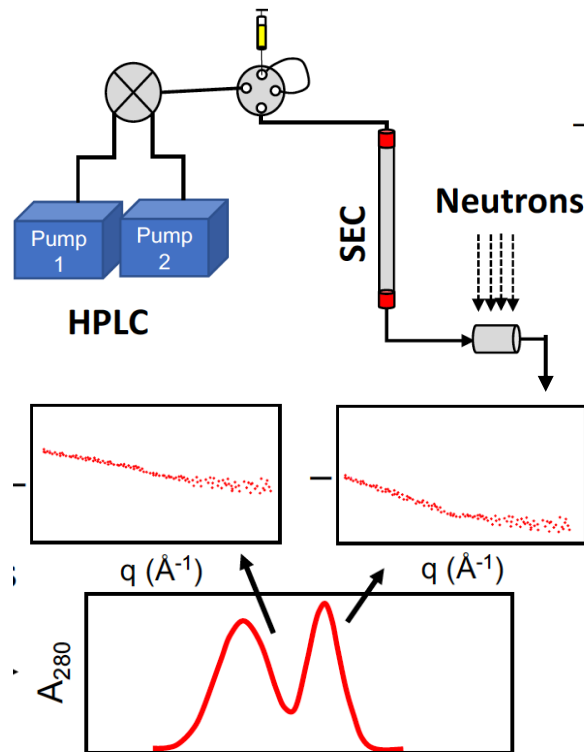


Grants applied for...

SEC-SANS

In situ size-exclusion chromatography set-up

- VR grant submitted with Lund University (Ingemar Andre)
- Industrial collaboration with WREN pharmaceuticals

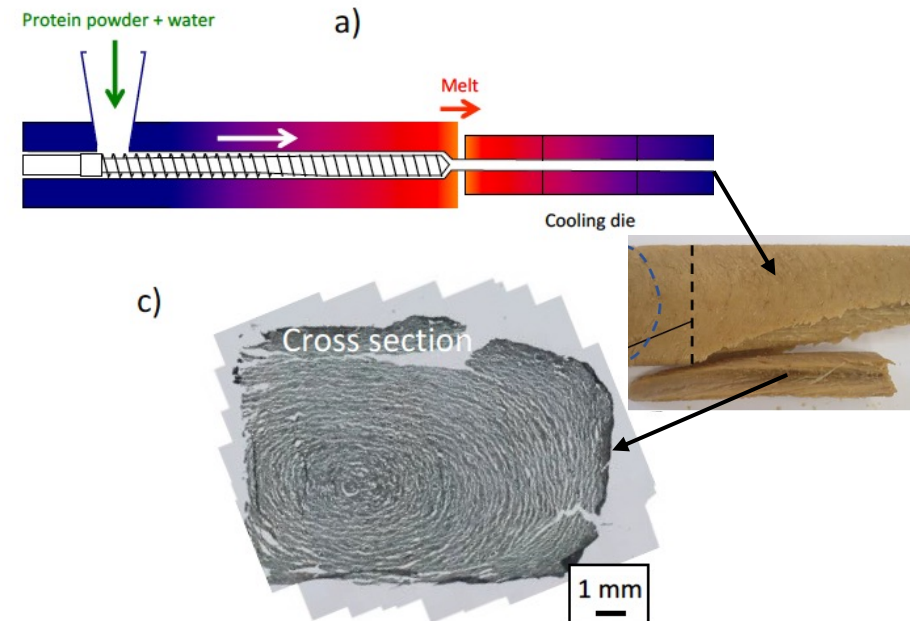


Contact: Wojciech (& Judith)

In situ extruder set-up

For in situ SAXS/SANS studies for food processing

- VR grant submitted with Lund University (Niklas Lóren)
- Industrial collaboration with Lantmännen and Orkla



Contact: Judith



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Challenges & Delays



Challenges & Delays

Global supply chain issues have affected Loki:

- Concrete roof will not be delivered until March 23
- Cables (motion and detector) delayed until spring 23

The installation schedule has been updated to reflect this – further delays will directly delay installation.

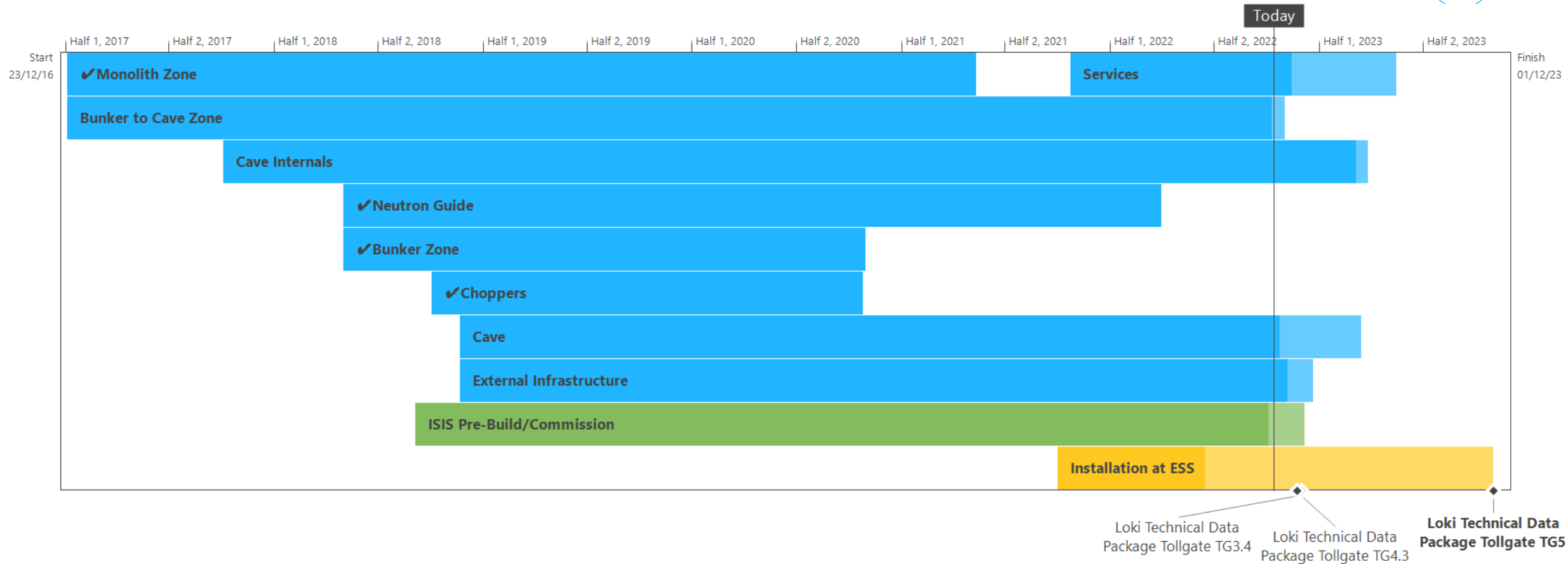
ESS's access dates to in-bunker slipped to Dec 2022 (earliest...)

ESS installation delayed due to limited resource and other ESS priorities.

Remaining ESS design scope to be completed: CUP, PSS, network...

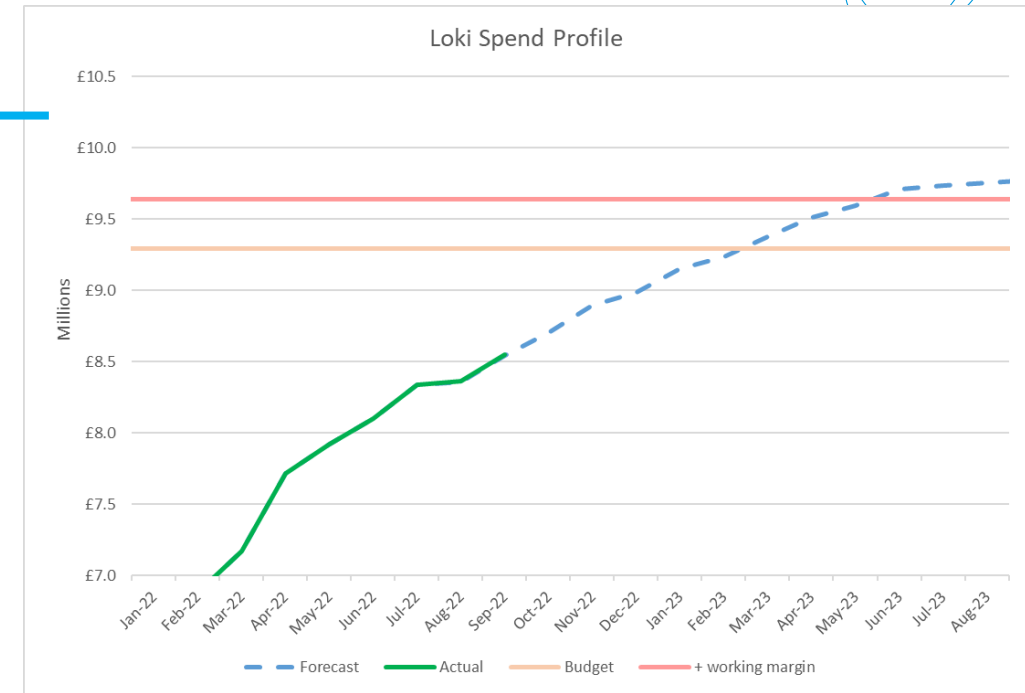
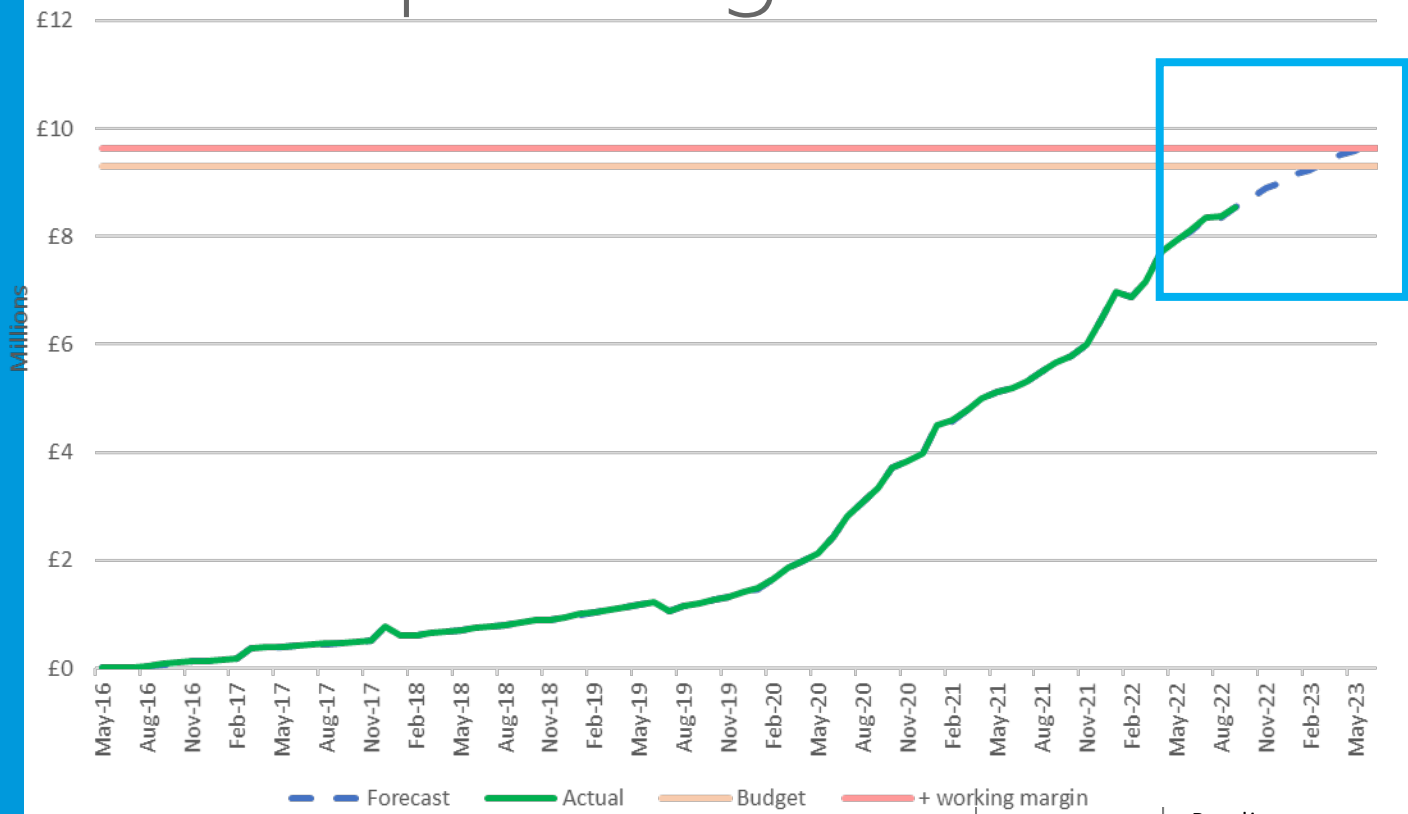
→ All Loki components will to be delivered to ESS by Q1 2023.
Detectors are critical path.

LoKI Schedule

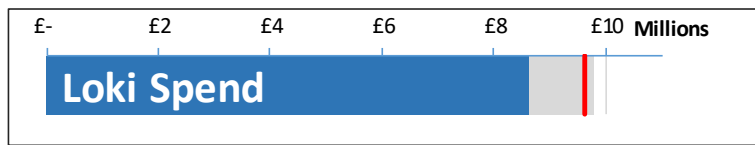


- TG5 has moved 6 months since last STAP. Partly due to late deliveries from ISIS. Mostly due to generation of a realistic installation schedule.
- Increased confidence in delivery date

LoKI Spending Overview



| | | Baseline | Working Margin | Baseline date | |
|-------------|---------------|-------------|----------------|---------------|--------------------------|
| LoKi | Budget | £ 9,636,529 | £ 9,292,529 | £ 344,000 | 16/04/21 |
| | EAC | £ 9,774,551 | | | |
| | Spend to date | £ 8,619,674 | | | |



%Spend of Forecast: **88%**
 EAC vs Budget: **1.4%**

Procurements remaining:

- External flooring
- Cave Guard rails
- AC and extract hood for sample area



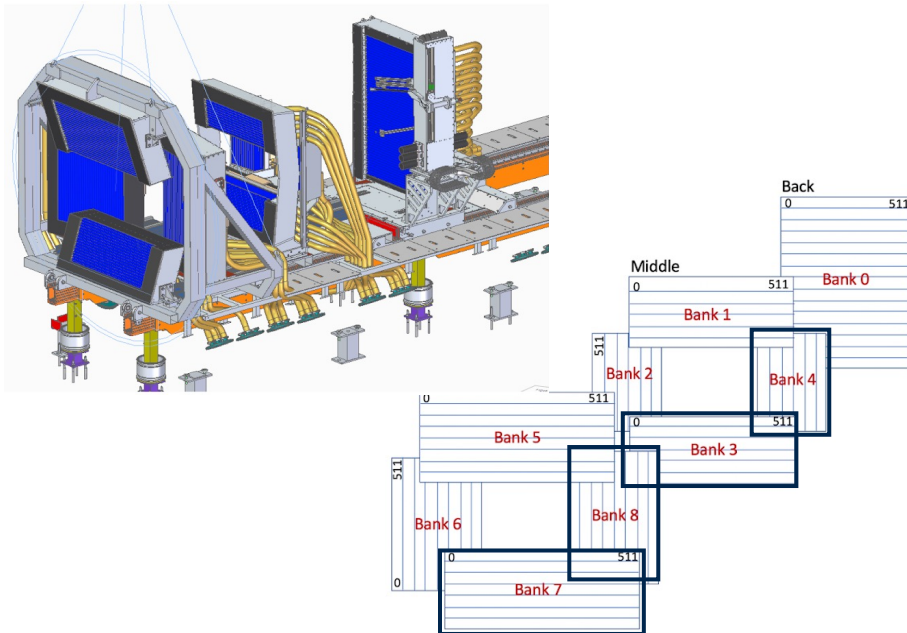
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Detectors

Detector update

Detector upgrade

- Provisional green light on the detector upgrade
- Proposals under review at ESS and ISIS
- Anticipate being ready for installation at the beginning of 2025.
- Thanks a lot to the SANS STAP and SAC for their support



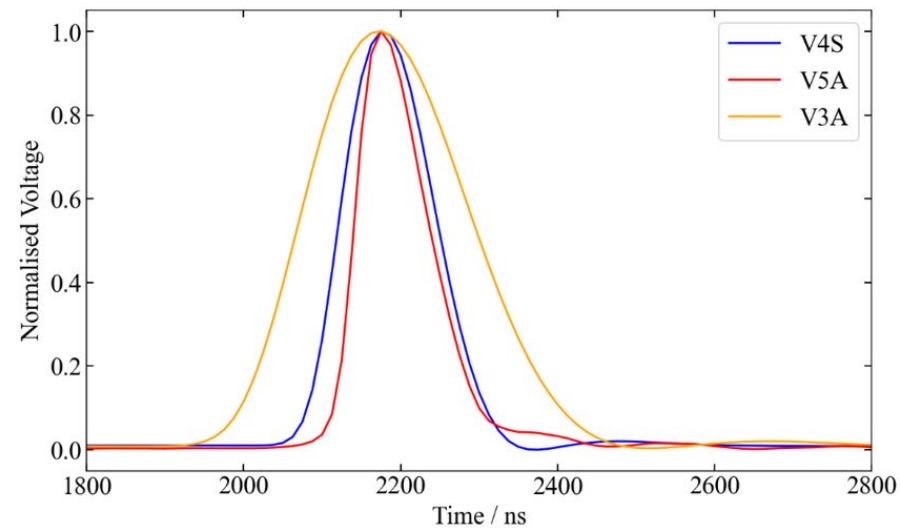
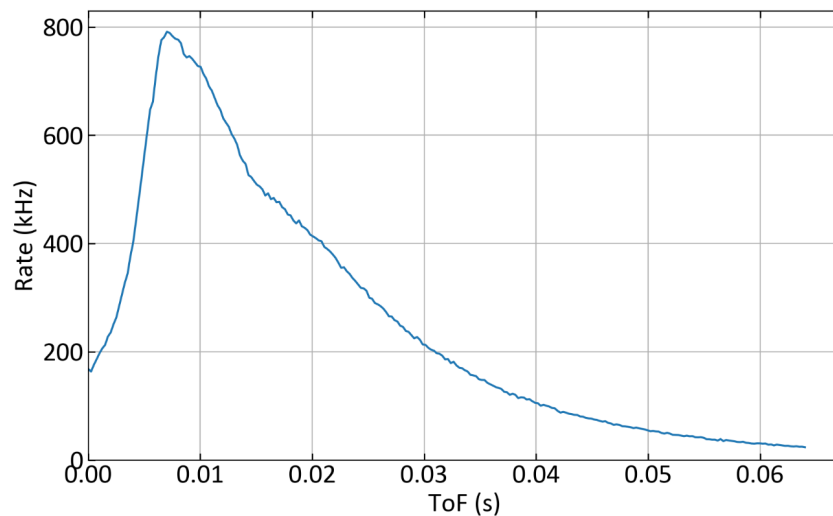
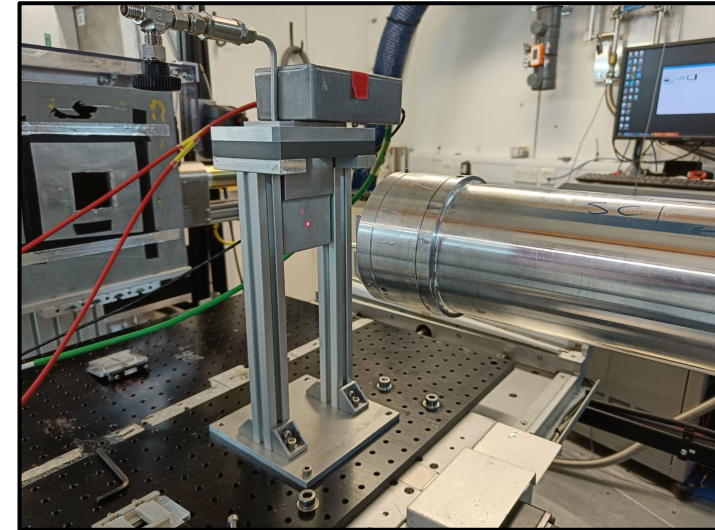
Detector delivery & Installation

- Rear detector and half of the mid-detector tested and in boxes ready for shipment. Testing of the front detector half-way through
- Trained the ESS detector group to test the detectors after the shipment and during the commissioning
- Detector Mechanics wiring currently underway
- Beam-stop assembly and testing in Q1 2023
- Cable procurement started. Slight lead-time risk to installation
- Detector delivery expected to ESS Q1 2023



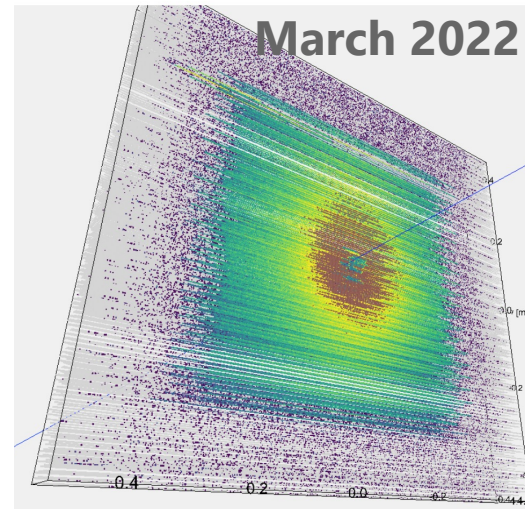
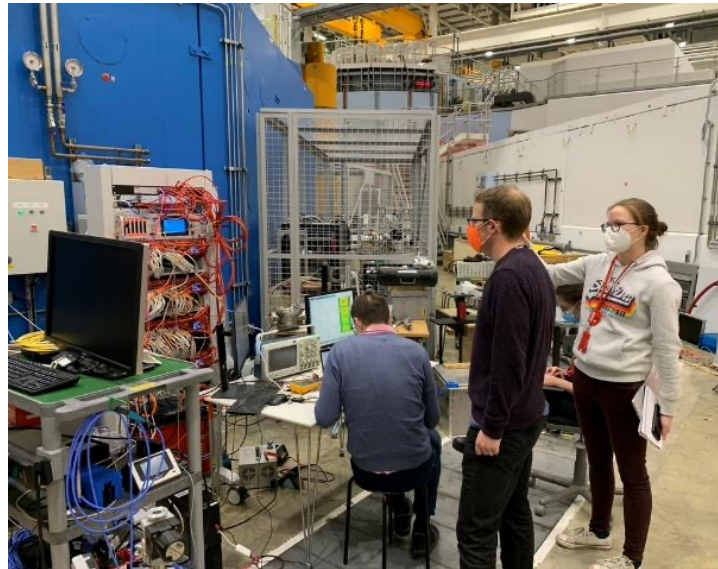
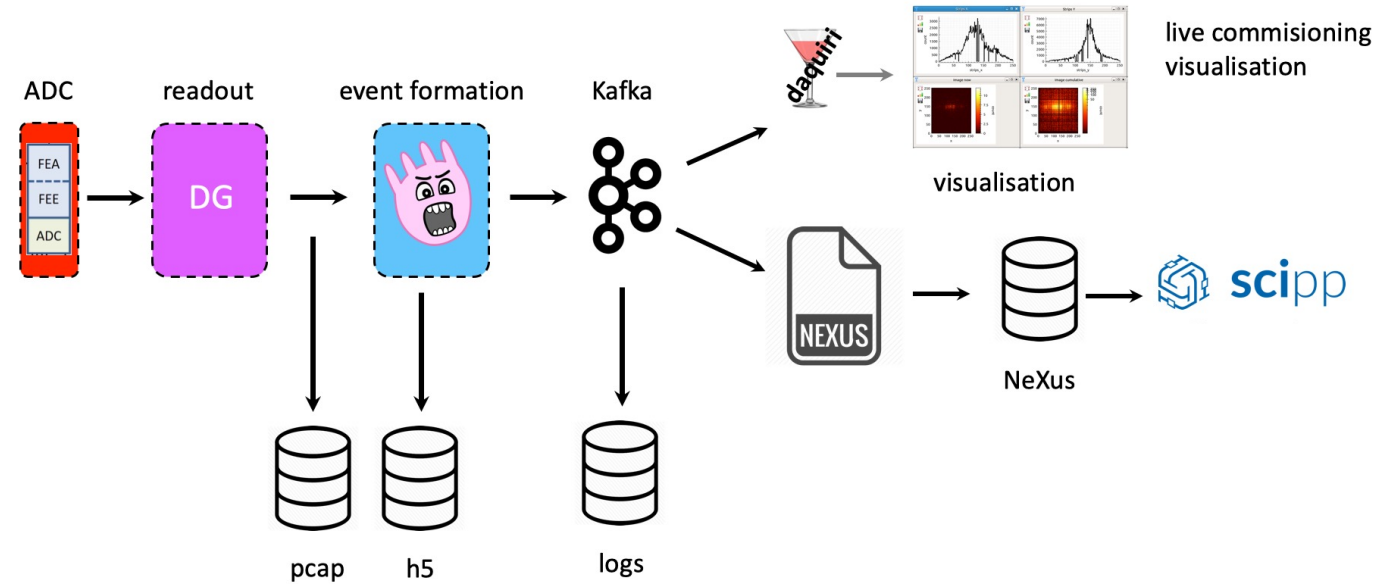
Monitors update

- In-bunker monitor built
- Finalised preamp electronics to speed up the signal and increase the rate-capability. Boards for the chopper monitor already produced
- HT boards in manufacture
- High rate test of the monitors performed on Larmor up to 700 kHz



Final Detector Test on Larmor – where are we? –

Collected calibration data on the LoKI rear detector using the **full ESS software stack**:
Excellent test for HC.



NeXus file displayed in scipp

- Sample measured:
1. Cd stripped mask
 2. Silver behenate
 3. SDS powder
 4. empty beam
 5. blocked beam
 6. ISIS standard polymer
 7. Silica particles
 8. Vanadium

Detector testing



Where are we? Not as far as we want to be...

- Richard Heenan has officially properly retired. He kindly still answers emails but won't be doing any further coding etc.
- Judith is working in Mantid (building on Richard's scripts) giving a baseline for Wojciech's work in SCIPP
- Progress so far:
 - Data is finally correctly loadable in SCIPP and Mantid without issues
 - Issues with NeXus file generation took a while to sort. Problems due to spurious TOF when beam current dropped during a measurement
 - Davide's tube calibration to remove the demultiplexing effect applied at the EFU stage to create "corrected" raw NeXus files (all files reprocessed) - ~130 files
 - All SANS and TRANS raw detector and monitor files now sorted: checked with simple data reduction (Mantid), and summed correctly in Mantid and SCIPP
 - Straw calibration script rerun in Mantid (no major improvements noted yet)
 - Masks created and dodgy tubes identified (tedious process for this reduced detector size)
 - Simple data reduction with monitors

Detector testing

Where next?

Mantid:

- Beam centre finder
- Direct beam iteration script starting from the simulation of the Larmor instrument set-up with flat background in Geant4

SCIPP:

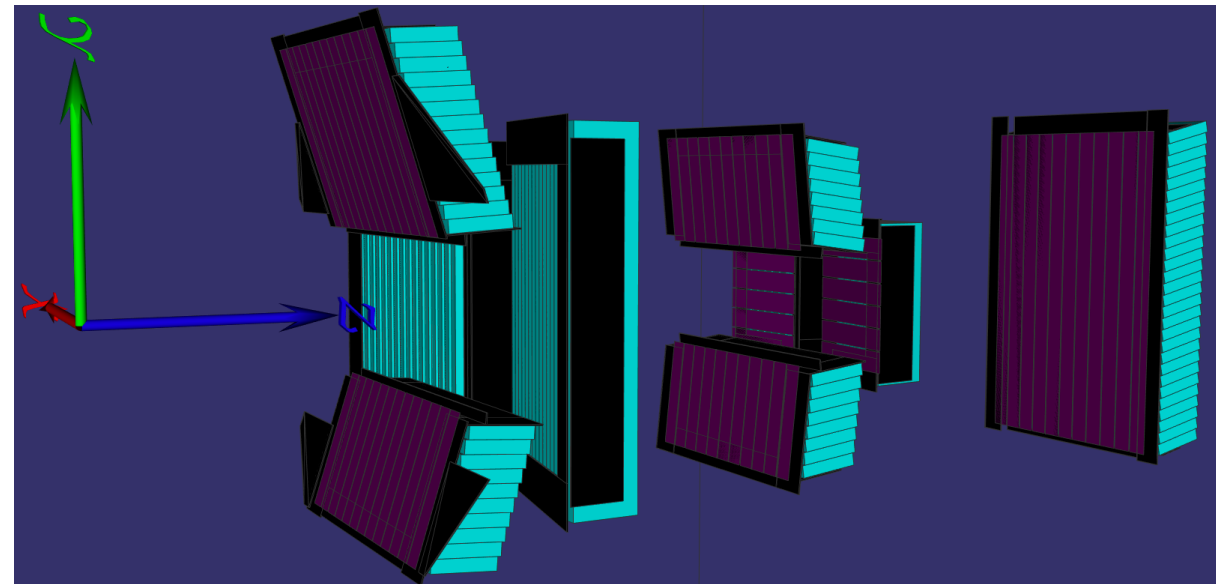
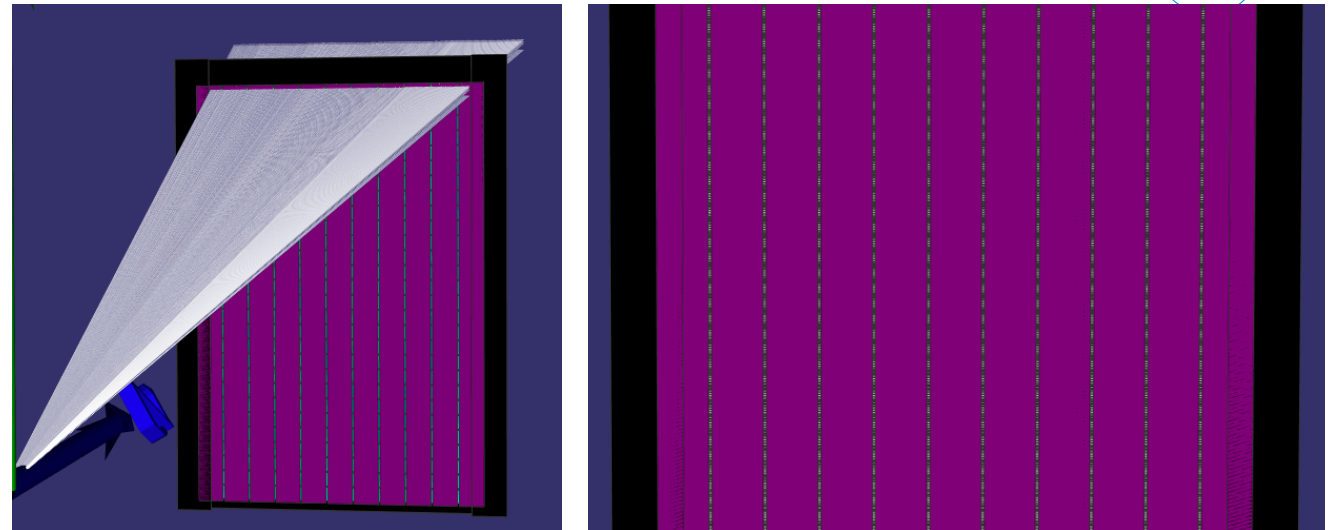
- Gradual conversion of Mantid scripts to SCIPP (direct beam, beam centre finder)
- Running full data reduction in SCIPP (based on earlier developed workflow).
- Updating SCIPP documentation currently referring to SANS2D data with data from the test

Detector simulations

Geantinos aimed at the detector model
with the calibration mask



- Work of Milán Klausz (Hungary)
- Migrate Geant4 related code to the new GitHub repository where automated testing has been implemented
- Documentation & tidying the code
- Easy definition of custom calibration mask geometry for all detector banks (few parameters + slit pattern)
- Create databank for the LOKI detector banks with high statistics (various samples, and instrument settings)





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Any questions
here?

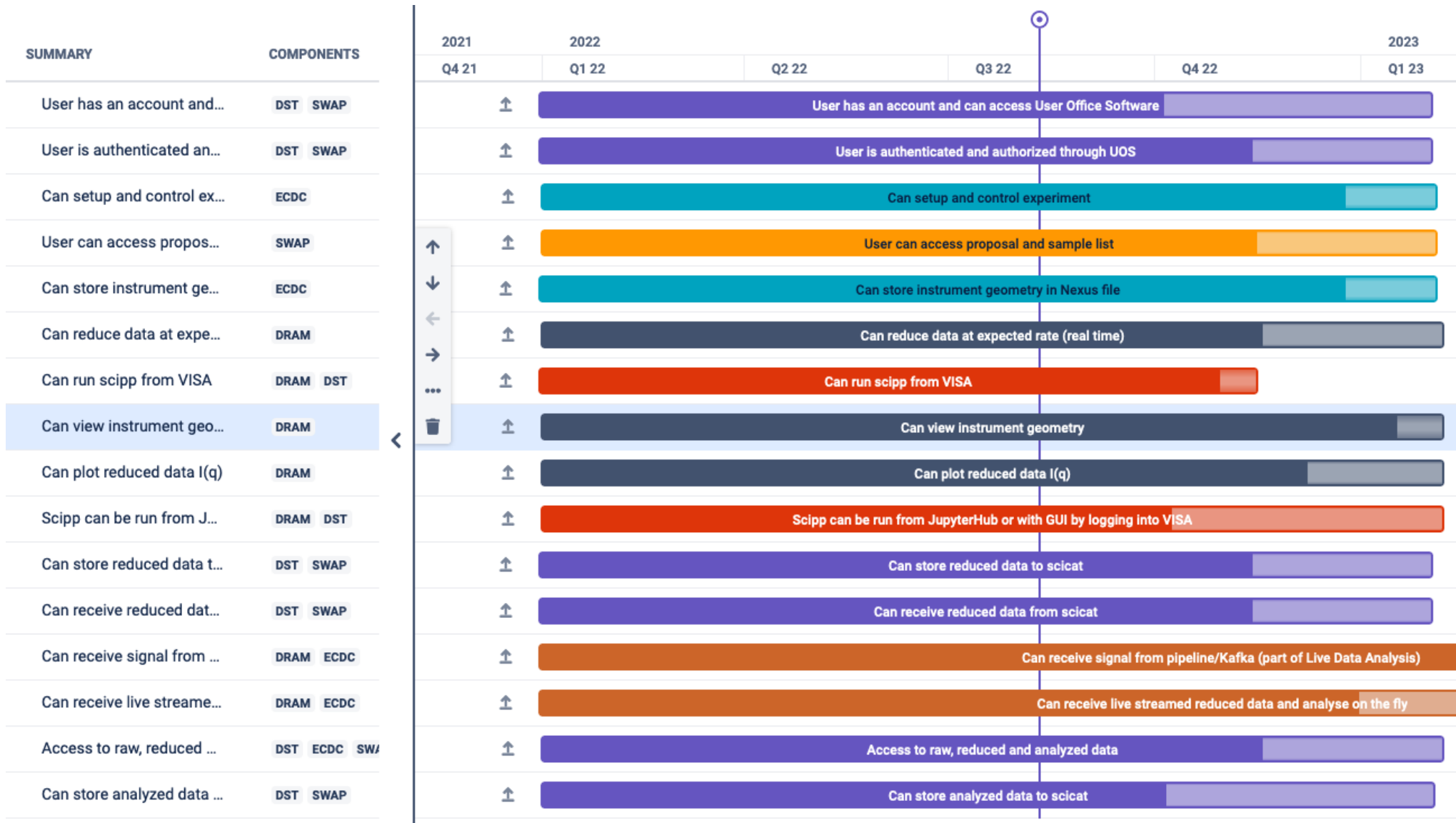


Software/IDS update

1. DMSC software and infrastructure ready for Hot Commissioning
2. Data reduction:
 - General SCIPP update
 - SANS related activities
3. Data analysis:
 - General SasView update
 - Magnetic SANS workshop
 - Generic resolution description and other activities

Presented by Wojciech Potrzebowski

DMSC software and infrastructure ready for HC





Continuous integration of full DMSC stack

Edit Add comment Assign More Start Progress Done

Details

| | | | |
|--------------|---|-------------|------------------------------|
| Type: | Epic | Status: | TO DO (View Workflow) |
| Priority: | Medium | Resolution: | Unresolved |
| Component/s: | None | | |
| Labels: | None | | |
| Epic Name: | Continuous integration of full DMSC stack | | |

Description

Develop infrastructure for running continuous integration of different software tools to make sure entire pipeline works.

Take a look at <https://snakemake.readthedocs.io/en/stable/>

Experiment with simple workflow using SANS2D data example in scipp and pass it to sasview script.

- 1) Deploy scipp and sasview using conda
- 2) Run data reduction on SANS
- 3) Store reduced data into file
- 4) Pick-up file in sasview and do some simple analysis
- 5) Compare obtained results with ground truth

Data reduction

General scipp update (selected items)

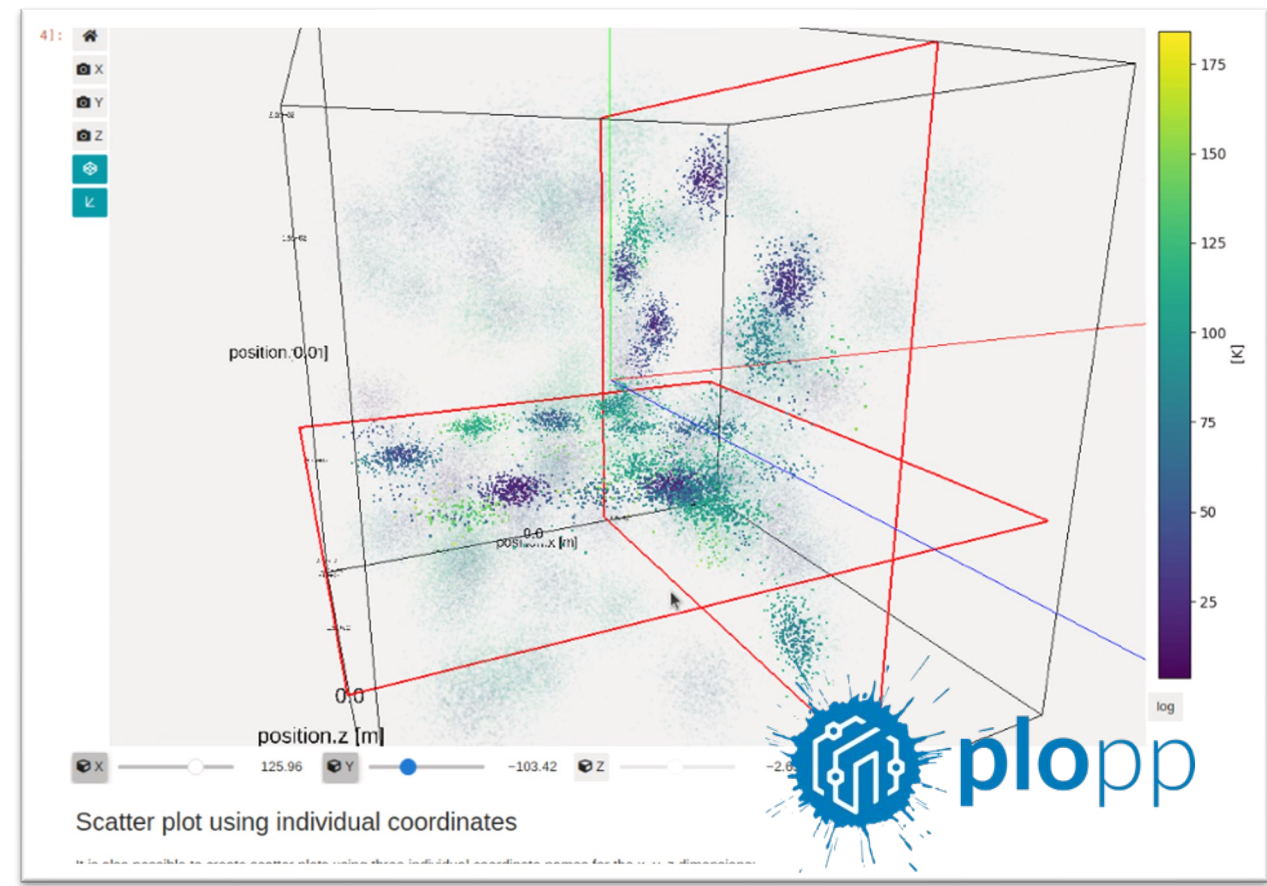
Scippnexus:

- Link between the HDF5-based NeXus Data Format and SCIPP
- Simplified loading of additional data/metadata, e.g., NURF data.
- Easier integration with ECDC software

Plopp:

- New data visualization framework
- More reliable plotting of event and histogram data
- More flexibility for future developments

Improved usability of event filtering (polarized and stroboscopic (VR project) data treatment)



Data reduction

SANS specific activities

Saving reduced data to the file:

- NXCanSAS format
- Can be read by SasView

Generic resolution function:

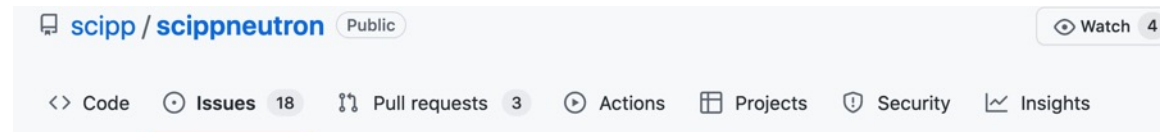
- Easy access to individual terms
- Saving to NXCanSAS file

Beam centre finder

Processing of LOKI detector test data:

- Batch script for the quick overview of data
- Merging runs
- Direct beam iterations (to do, earlier version)

Coordinating polarized SANS activities with DREAM



Saving reduced SANS data to NXCanSAS file #373

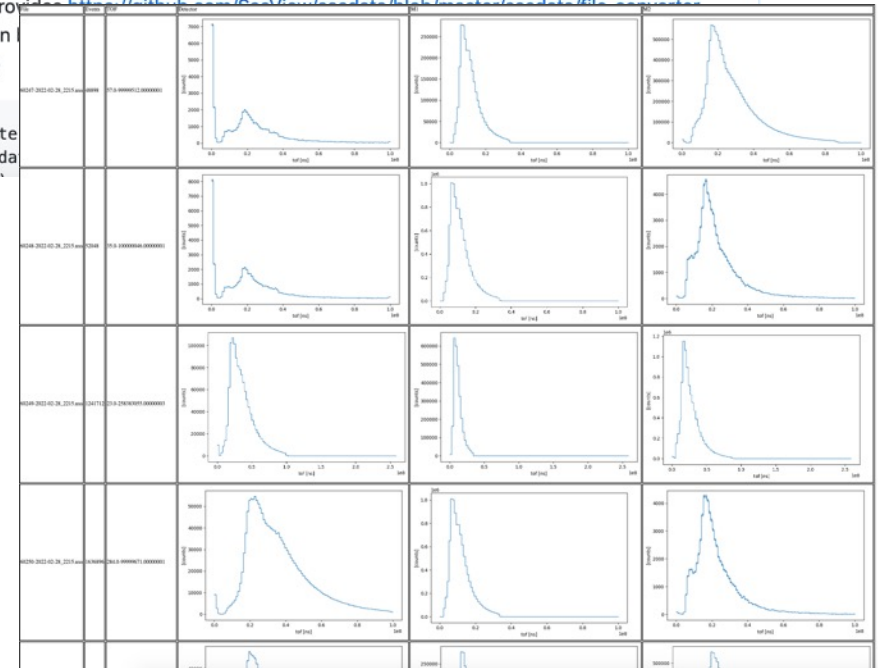
Open wpotrzebowski opened this issue 5 days ago · 3 comments

wpotrzebowski commented 5 days ago

Current implementations of SANS data reduction workflows don't store reduced data to the file. I've explored some options and it seems that at minimum support to NXCanSAS file needs to be provided.

sasdata (part of SasView) provides `nxcan_sas_writer.py`, which can do the work (see [https://github.com/SciTools/sasdata/blob/master/sasdata/nxcan_sas_writer.py](#) for more details). The following code can do the work

```
from sasdata.file_converter import nxcan_sas_writer
from sasdata.data_loader import DataLoader
```



Data Analysis

General SasView updates

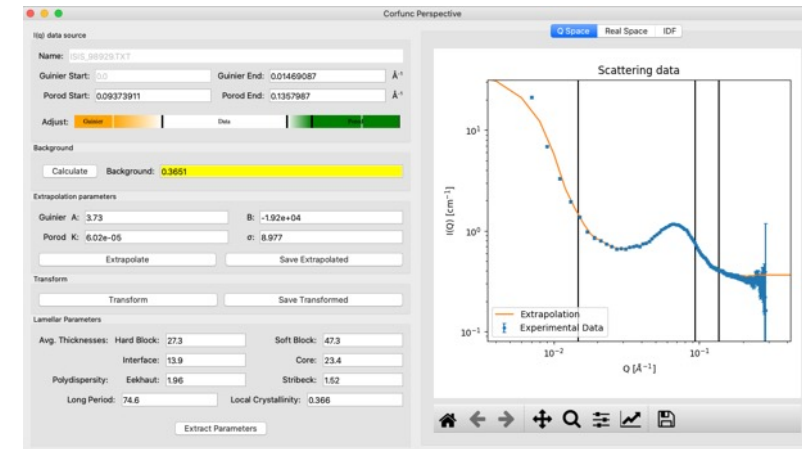
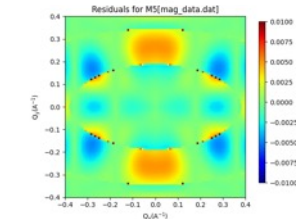
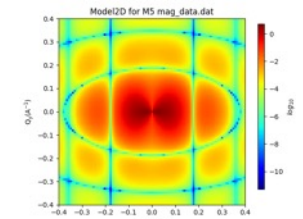
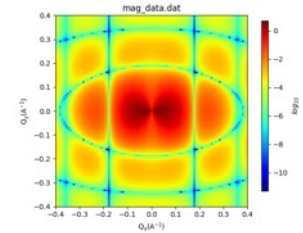
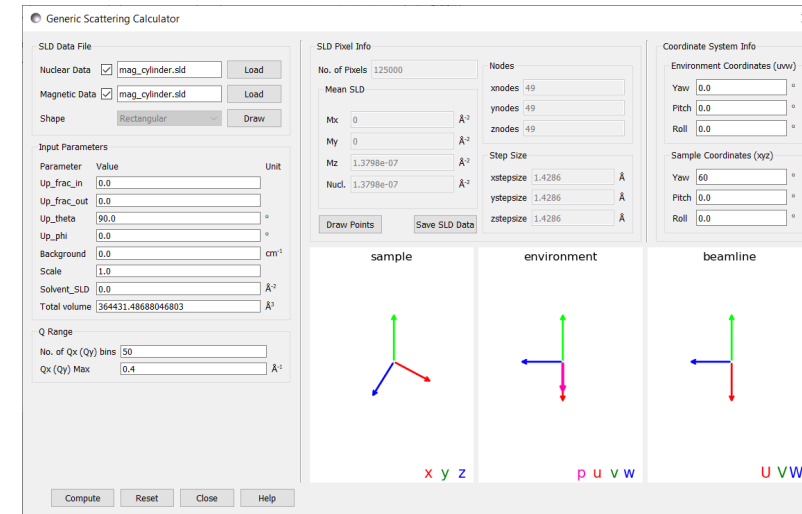
SasView 5.0.5 is out:

- Refactored Generic Scattering Calculator, support for magnetic/polarized SANS
- Available on conda-forge
- New models on marketplace

On-going projects:

- Refactoring correlation function
- Refactoring P(R) inversion)
- SAXS/SANS co-refinement
- Magnetic workflows upgrades
- Improved scripting interface

Code camp (Oct 25th to Nov 1st)



Magnetic SANS workshop

2-day workshop in June 13-14 2022 at LINXS (Lund)

Questions addressed:

“What are you currently missing regarding data analysis and simulation to optimally process your data?”

“Which in-house developed functions and workflows are you using because public software packages do not yet provide them?”

Defined issues/requirements:

<https://github.com/SasView/sasview/wiki/DevNotes>
[Projects](#) [magsans](#)

Followed-up by SasView training for new contributors at ESS



Generic resolution description

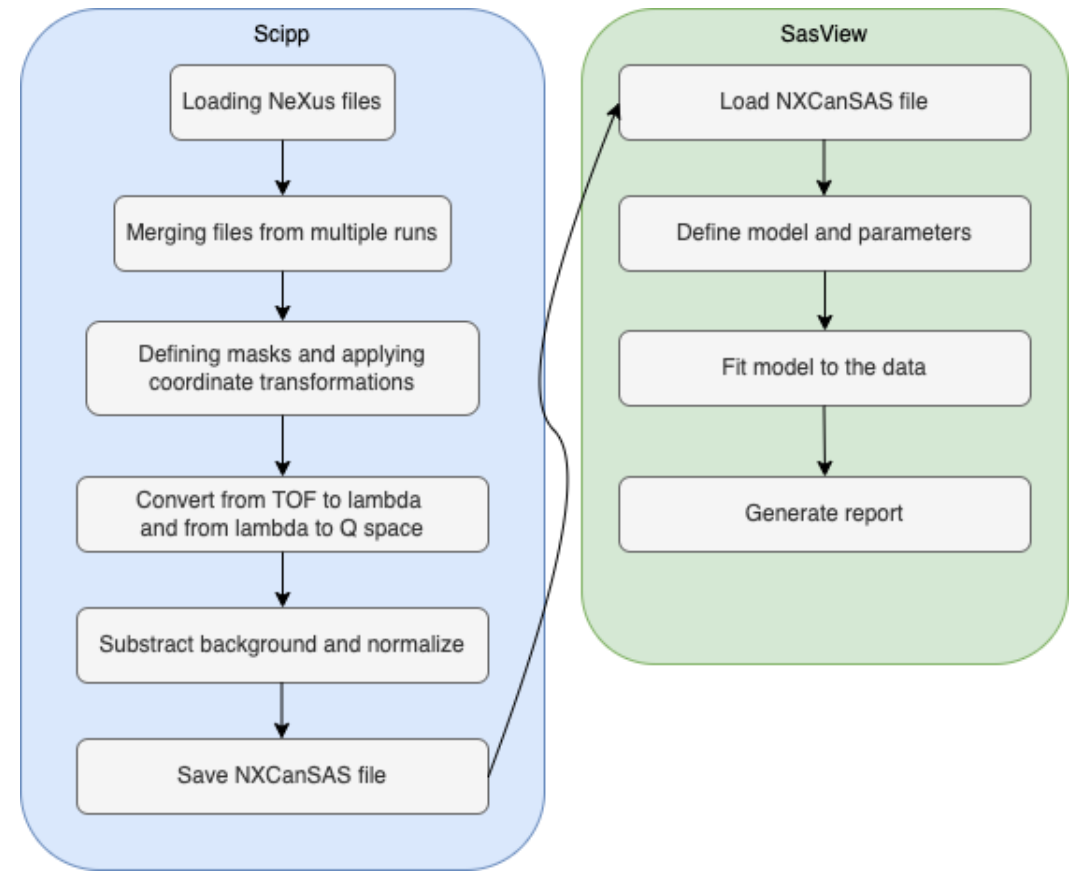
and other ESS related activities

Resolution function:

- Backbone functionality in scipp: access to individual resolution terms and saving to NXCanSAS files
- Proof-of-concept for point based resolution function in SasView
- Presented at ORSO and CanSAS meetings

Other:

- Integration with SciCat and SASBDB
- Multiple scattering calculator
- Autonomous experiments/machine learning





Extra slides

Data pipeline/workflow

