LoKI STAP Update

Instrument progress
23rd October 2023

PRESENTED BY THE LOKI TEAM

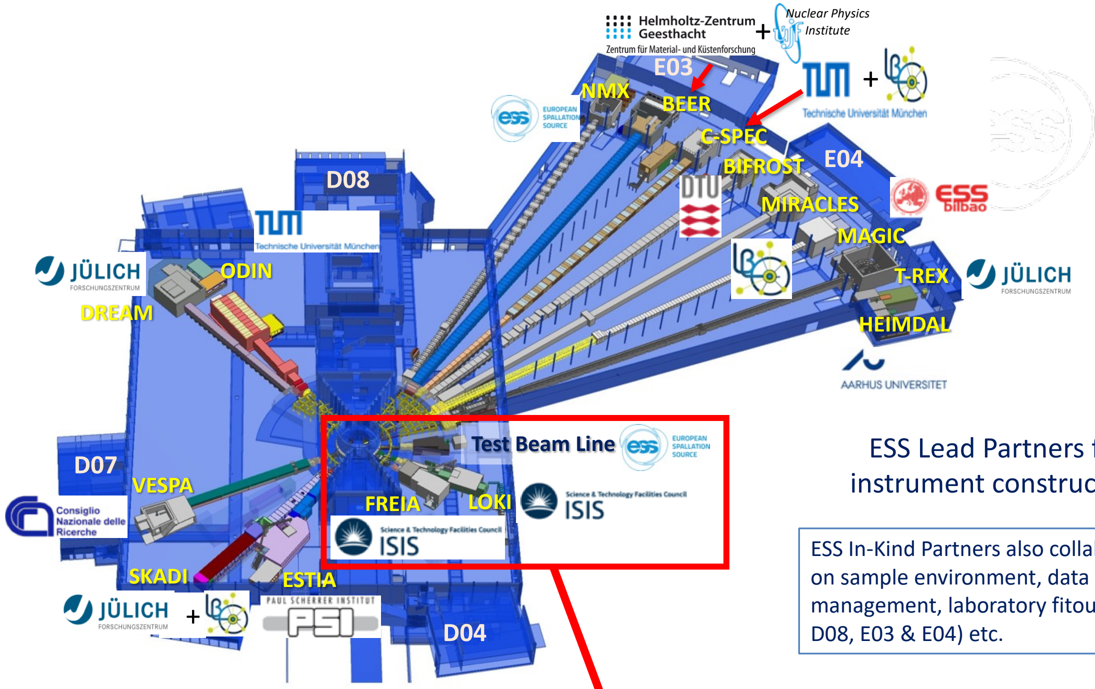
LoKI team

Lead engineer :	Jim Nightingale
(ISIS lead detector scientist :	Davide Raspino)
Installation package leader :	Clara Lopez
Instrument technician :	Dennis Vedelgart
Instrument scientist :	Judith Houston
Instrument data scientist :	Wojciech Potrzebowski
Instrument associate :	***recruitment underway*** *(ETA: Jan 2024)*
Commissioning scientist (in-kind) :	***recruitment to begin*** *(ETA: Q1 2024)*

As well as continuous support from various technical teams at ISIS and ESS

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

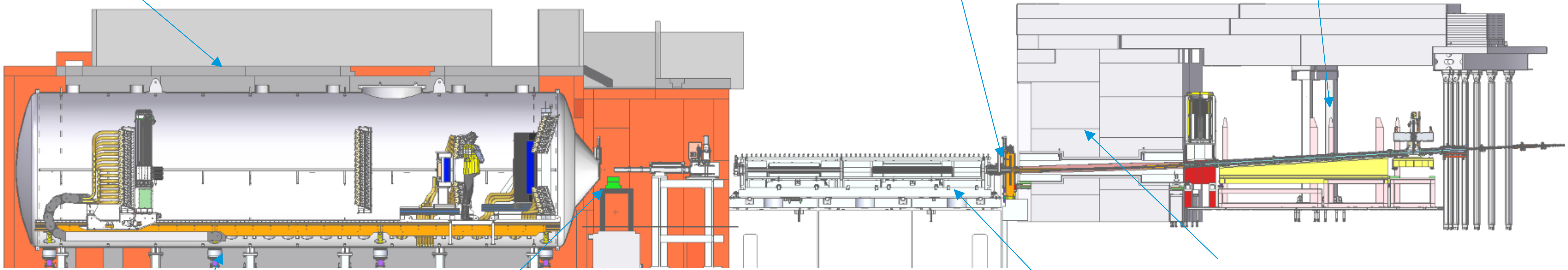
Updates since we sent out the report

Detectors
Vessel, **mechanical frames and 18 modules** installed
Almost all detector components delivered to ESS, awaiting beamstop mechanism

Utilities
Electrical services and utilities being installed
PSS under detailed design
Network under detailed design

Chopper 2
Installed

In-bunker
ALL components on site, delays due to access, starting imminently



BWI
Insert installed

Cave Shielding
- Steel is installed
- Concrete roof is installed

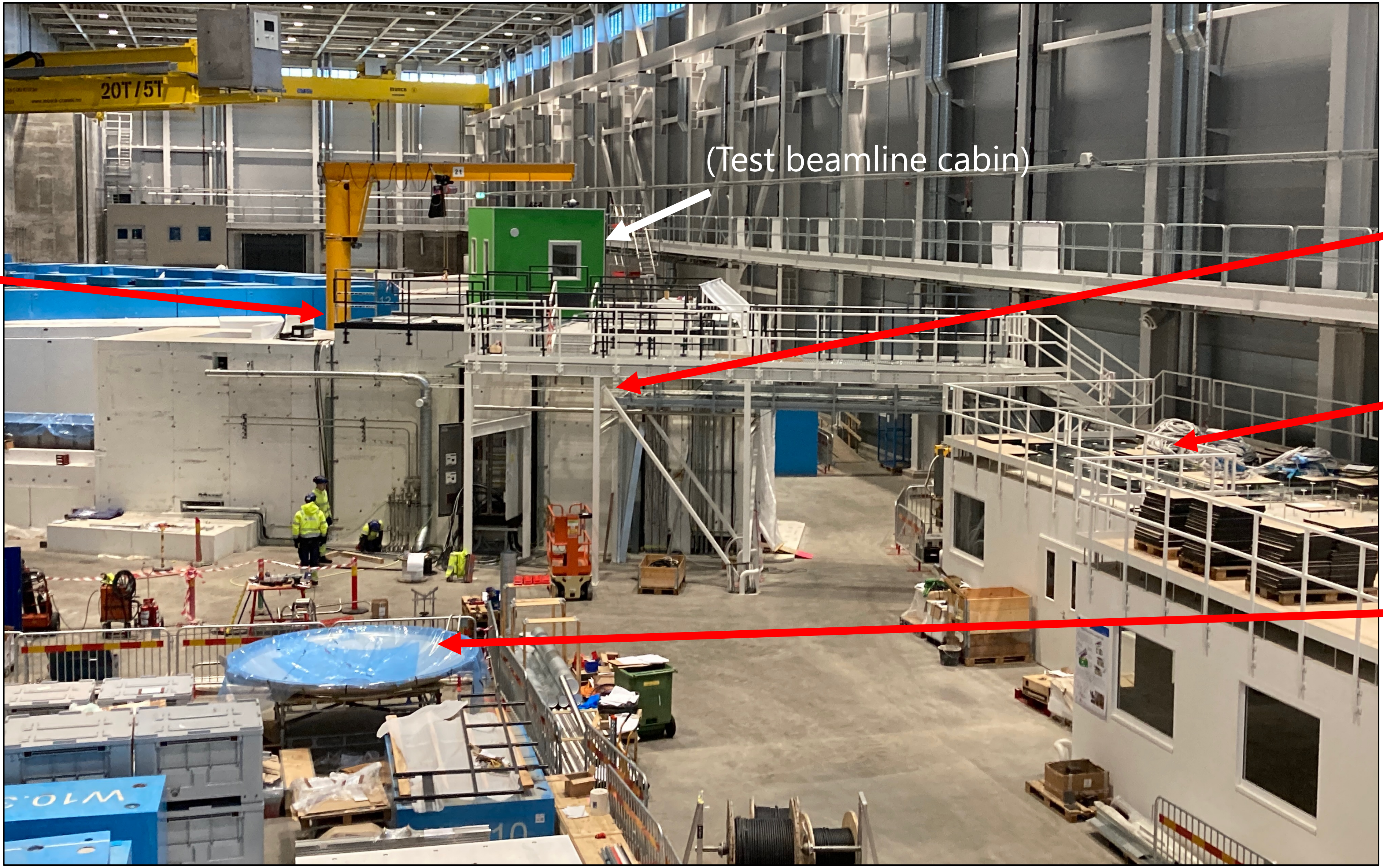
Sample Area
- Stack awaiting installation
- Snout system awaiting installation
- Utilities, etc currently being installed

Beam monitors
- First 2 monitors awaiting testing at ISIS TS1
- Other 3 monitors awaiting final assembly

Bunker-to-cave
- Collimation tank installed
- Motion control group fixing issue with the translation stage – **delaying guide installation**

Installations in the last 6 months

Cave roof & railings



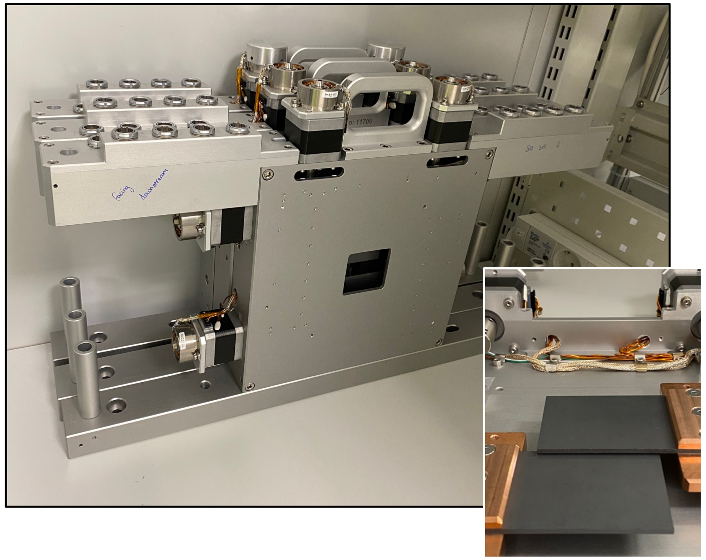
Cable raceways and piping

Detector cables

Rear of the tank open for detector installation

Installations in the last 6 months

Bunker-to-cave



- Chopper 2 and Collimation vessel installed
- Selector 1 motion issues delaying installation
- Slit sets tested, blades installed and awaiting installation (after selectors)

Installations in the last 6 months

Sample area

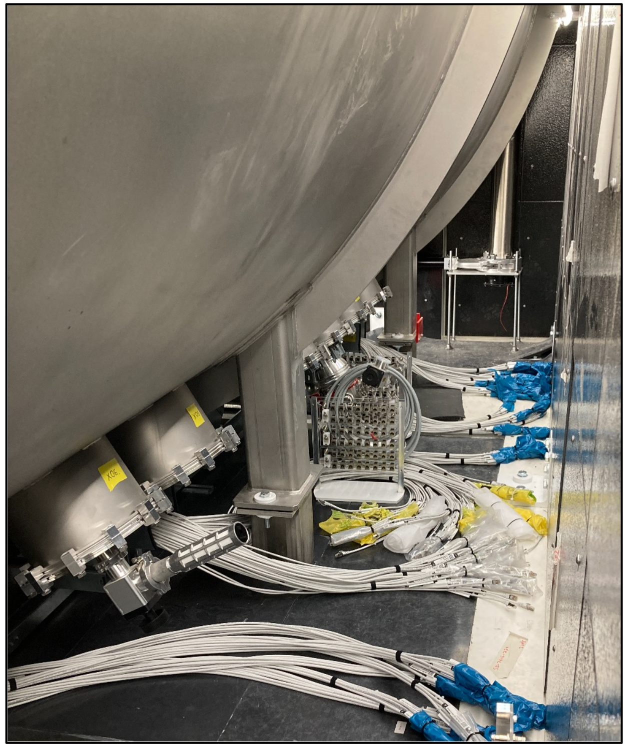
Huge amount of infrastructure being installed including false floor, electrical, utilites.

Detector update

On-site progress

- Delivery of most of the day 1 detector modules
- Delivery of all detector mechanics
- Delivery of most of the electronics for the full coverage

- Massive amount of work laying the detector cables by ESS CEP team

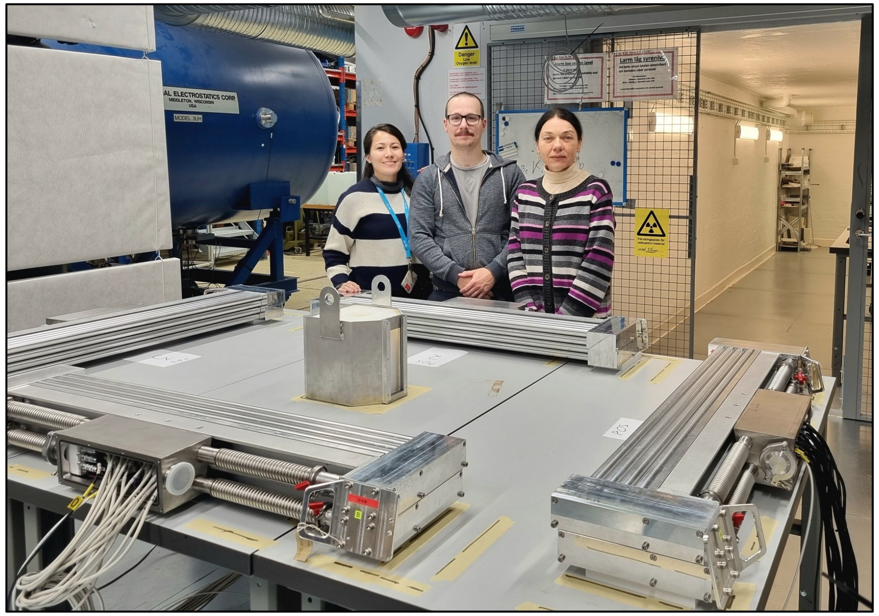


- In-tank installations progressing well…

Detector update

Updates since we sent out the report

Testing the modules with neutrons at the radiation testing facility at Lund University – first 18 modules tested



Thanks to the ESS detector group:

- Nathaly De La Rosa
- Nicholai Mauritzson
- Irina Stefanescu

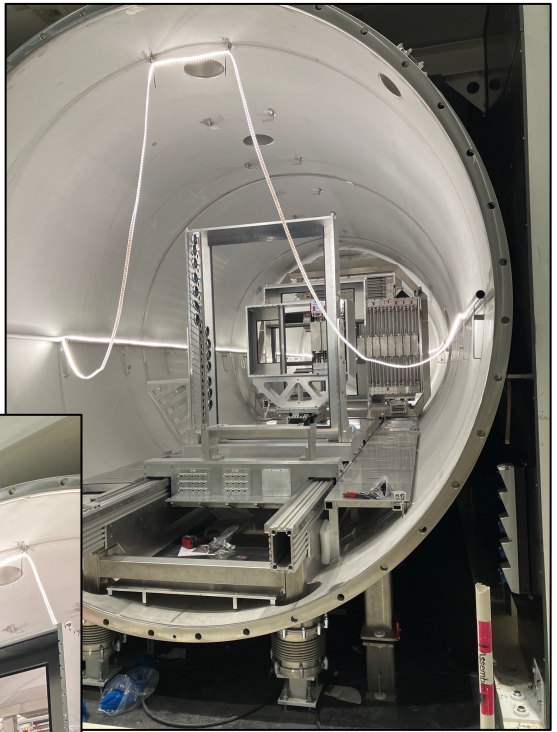
Detector update (new)

Updates since we sent out the report

All 3 carriage now in the detector vessel

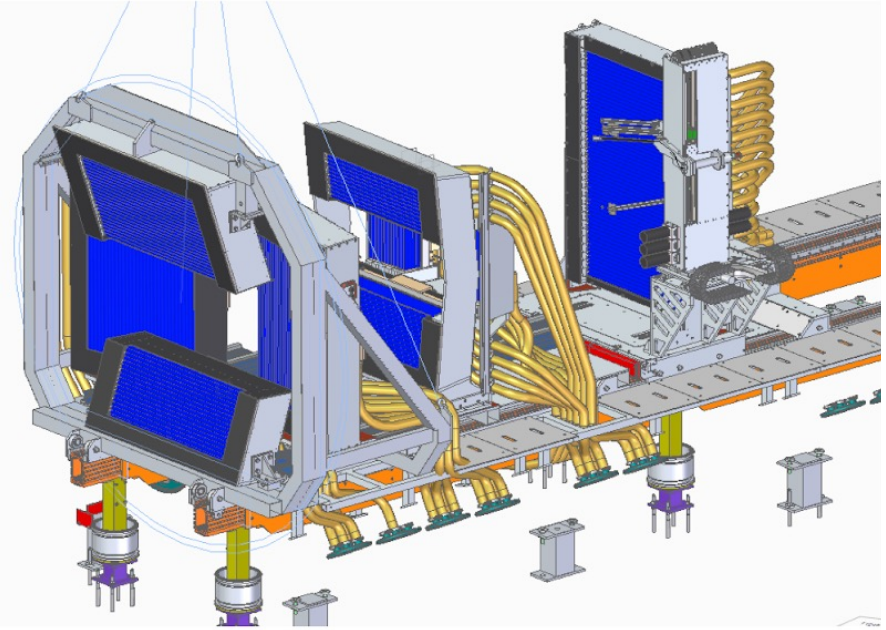


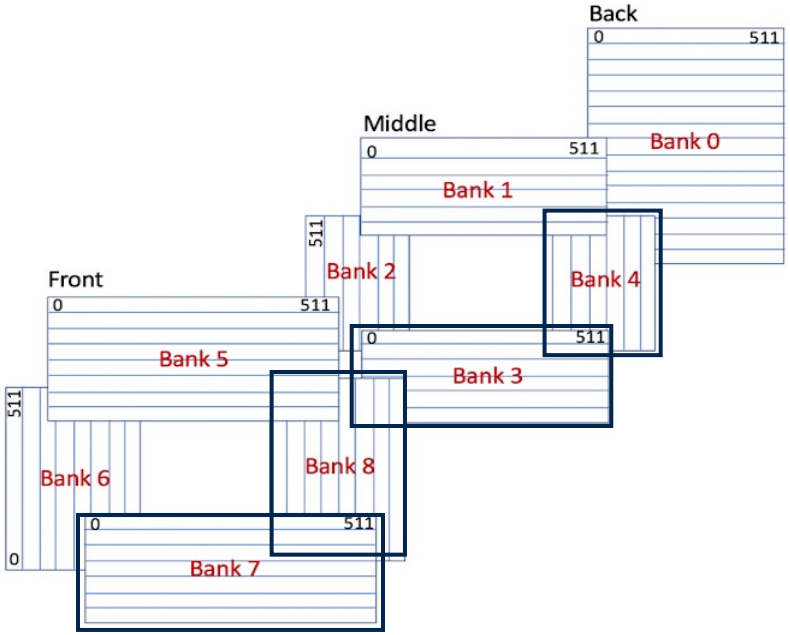




Detector Upgrade

- All cables and mechanical structures are at ISIS, only waiting for the tubes from PTI (USA).
- Electronics already at ESS
- External cables from detector vessel to racks already in place
- On target to made January 2025 delivery.

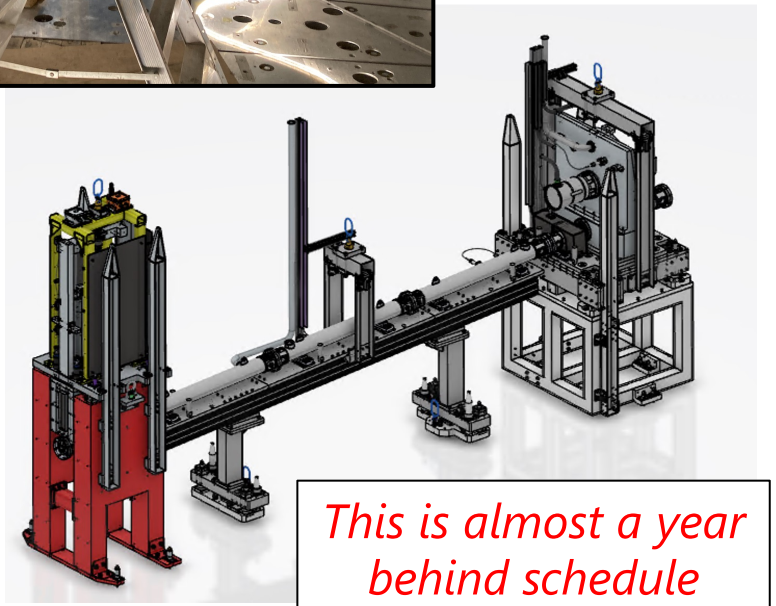




Installations planned for the next 6 months

In bunker components (starting almost immediately)

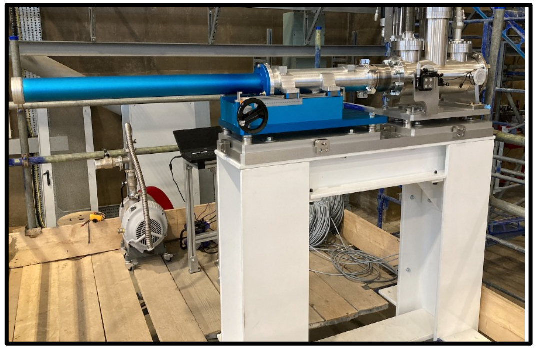
- Chopper 1
- Heavy shutter
- Guides
- Monitor 1



This is almost a year behind schedule

Remaining out-of-bunker components

- Selectors/slit sets
- Guides
- **Remaining** detector modules
- Sample area components
- Door and roof



Other progress

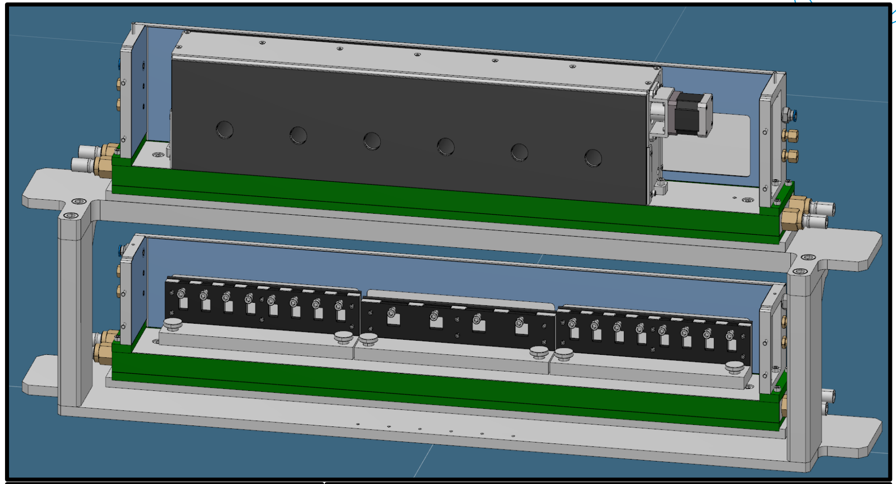
- TG3 (design) documentation submitted by ISIS
- All TG4 (final manufacture) documentation submitted by ISIS (except door & roof, which is also almost complete)
- Raised flooring contract placed by ISIS, design complete and currently in manufacture
- Major issues remaining:
  - Selector motion failure delaying the installation of the inner collimation components <u>including the guides</u>.
  - Beamstop mechanism still at ISIS, awaiting commissioning, delayed by extremely limited motion resource at ISIS
  - Still waiting full and final access to the in-bunker area, partial access limiting installation
- Outstanding deliveries: door and roof, beam stop, monitors and raised floor
- Current installation complete date is **summer 2024**

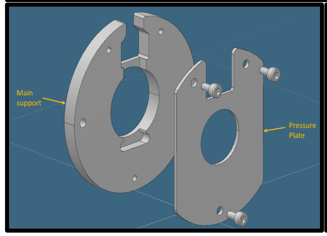
2

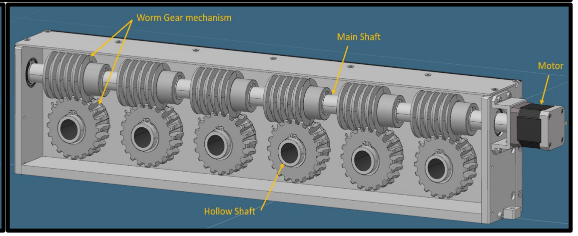
Sample environment

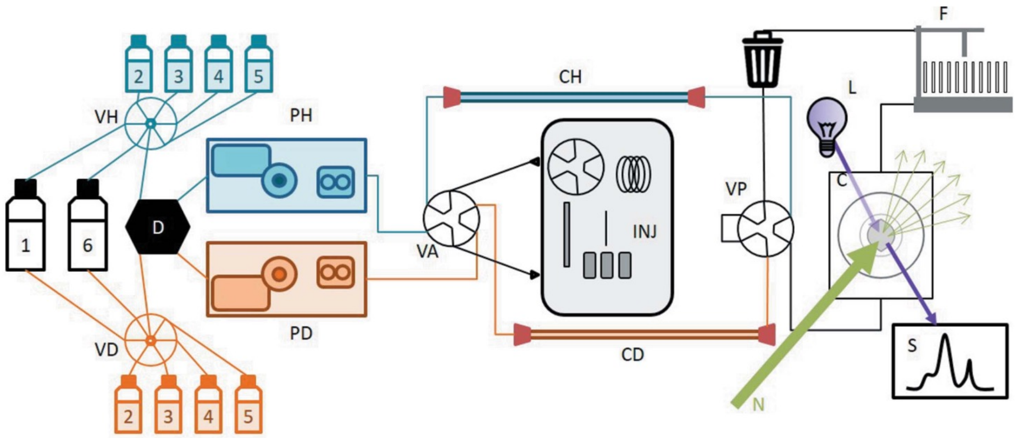
General sample environment updates

- **Thermostated cell holder** and **rotating cell holder** awaiting the arrival of the instrument associate (Jan 2024), before resuming production and assembly.
- **Rheometer** integration is underway and making progress (ESS pool equipment). Sub-pulse project with Uppsala on-going with ISIS
- **Size-exclusion chromatography** set-up ordered, working with ISIS and ILL on the set-up and integration.
- **NURF (in situ spectrometers and continuous flow cell)** cell prototyped and devices integrated.



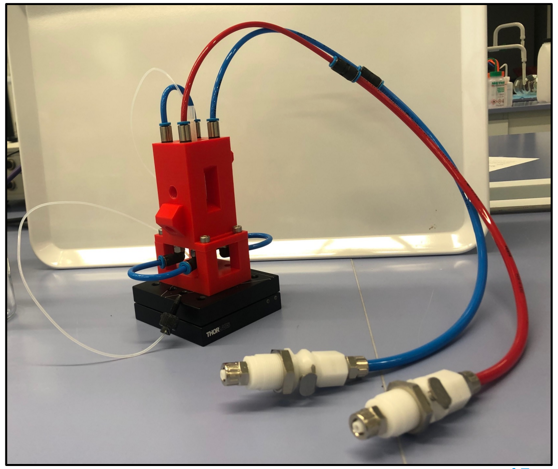






(a)

Ann Martel's SEC set-up (J. Appl. Cryst. (2023). 56)



Sample environments

Priority	Sample Environment System (SES)	Phase	Date Needed	Status
1	Thermostated sample changer for quartz cuvettes	HC	**Q1 2024**	**IA will lead the procurement and assembly as first task**
1	Cell tumblers/rotating sample holders	HC	**Q1 2024**	**IA will lead the procurement and assembly as first task**
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	Q4 2023	**Integration almost finished, including manufacture of cell holder**
2	**NEW: Size Exclusion Chromatography**	**ES**	**Q4 2023**	**Ordered, replicating ILL set-up**
2	Rheometer	ES	Q1 2023	Anton Paar - still 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 2024	ESS to purchase
4	Dismountable 'sandwich'-style cells (ESS)	ES	Q4 2023	Designs exist. Just to be sent for manufacture
4	Warm Bore Cryomagnet 2.5T	SOUP	Q1 2027	**Contract underway, design complete**
4	Stress/stretching rig (ESS)	SOUP	Q1 2027	ESS colaboration(s) to develop different rigs
4	Cryostat – dilution fridge less than 1K	SOUP	Q1 2027	
4	Cryostat wet	SOUP	Q1 2027	

Changes from last update

3

Early Science

Early science workshops

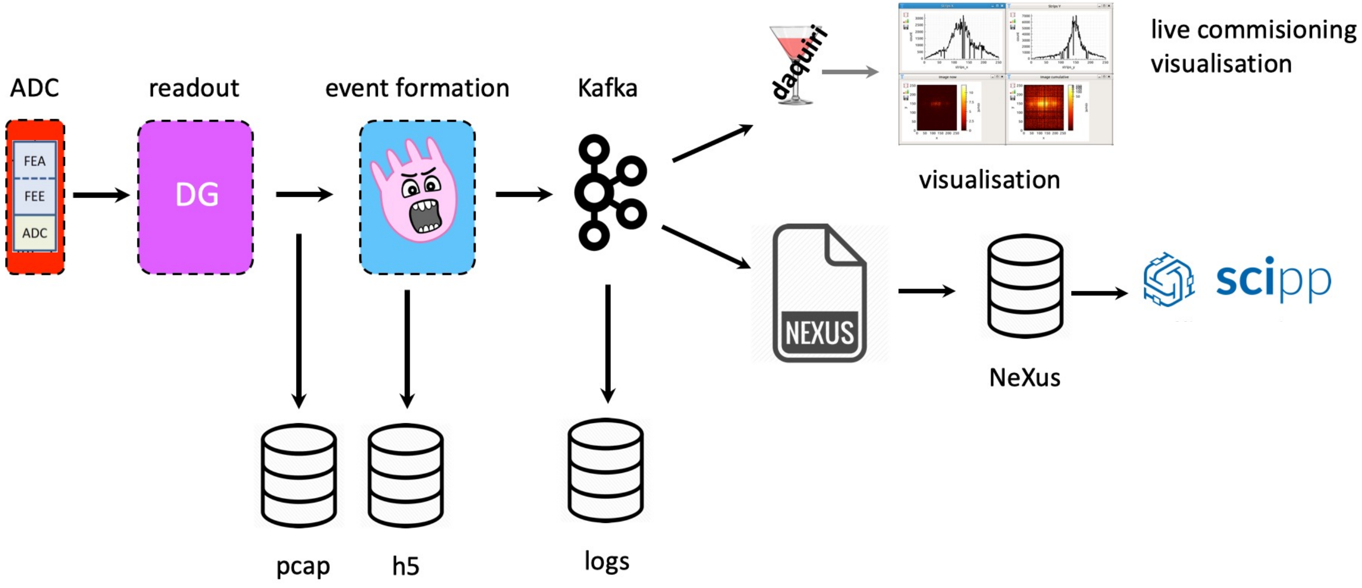
- Plan to have the first three “Early Science” workshops for LOKI, DREAM and ODIN in 2024.
- Workshops are meant to (re-)introduce the early instrument capabilities to the user community, discuss potential early science with an impact, and if we find additional ambitious projects that may require developments in sample environment or scientific support
- For LOKI: Satellite workshop to ECIS to be held in Copenhagen in Sepetember 2024. Exact details will be provided in the coming months.

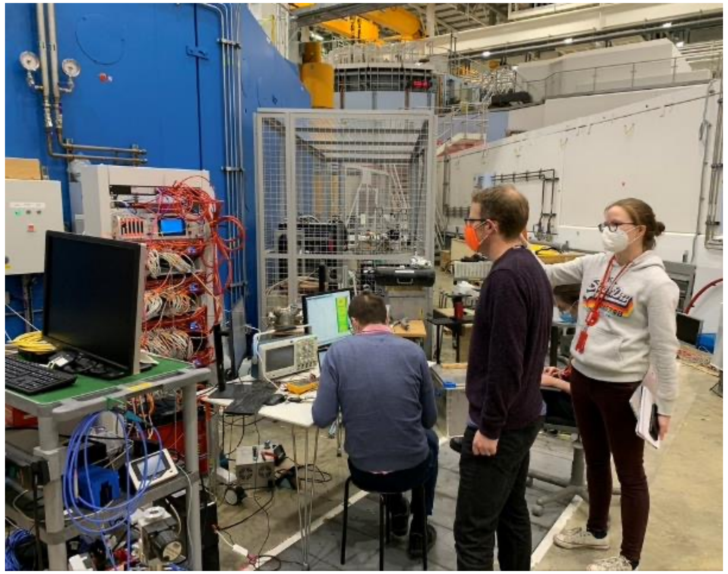
4

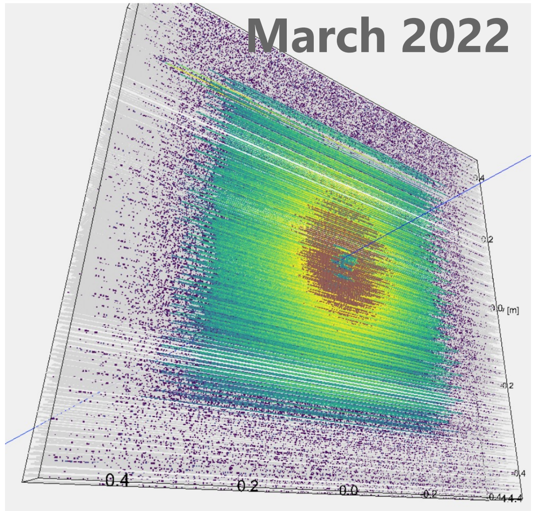
Detector Tests & Data Reduction Progress

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.







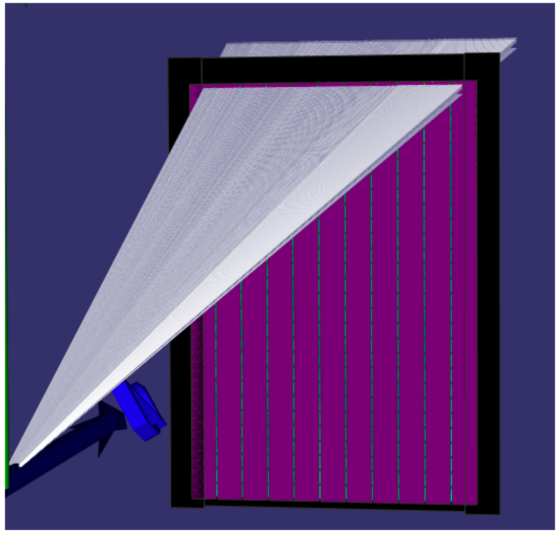
NeXus file displayed in scipp

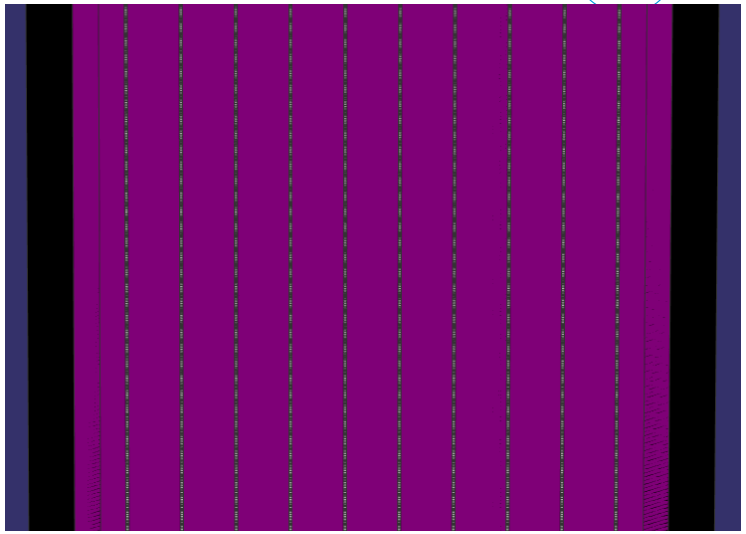
Sample measured:

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

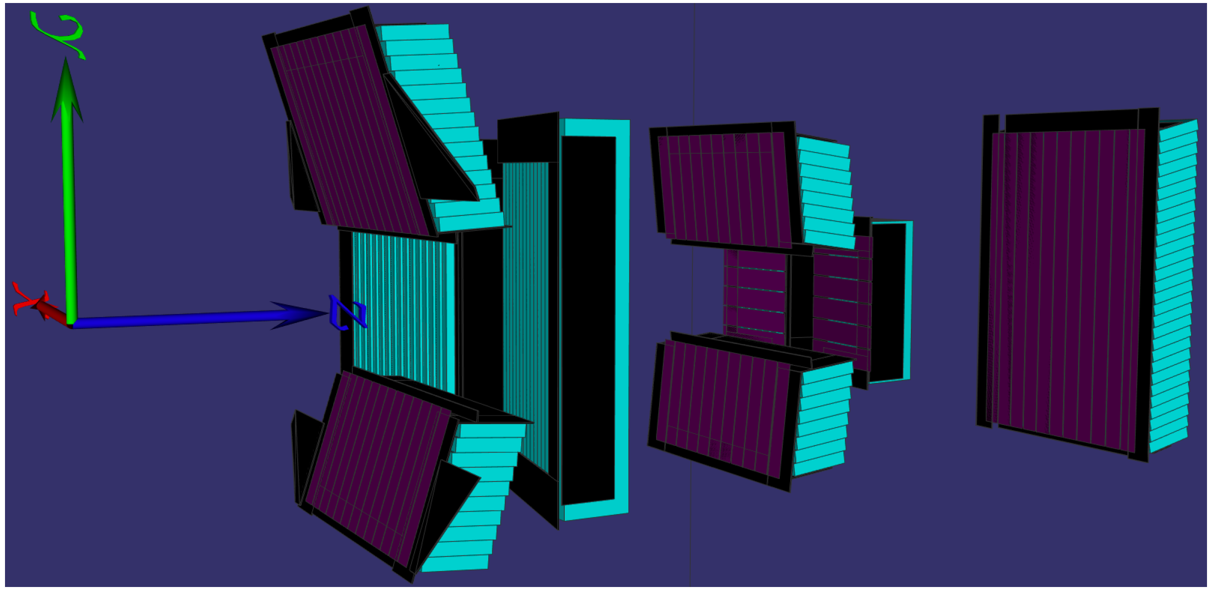
Detector simulations

Geantinos aimed at the detector model
with the calibration mask





- Robust workflow for creating position correction masks
- Robust workflow to create simulations of standard samples, flood source, etc
- Easy definition of custom calibration mask geometry for all detector banks (few parameters + slit pattern)
- Code is now (or soon to be) available in GitHub repository where automated testing has been implemented

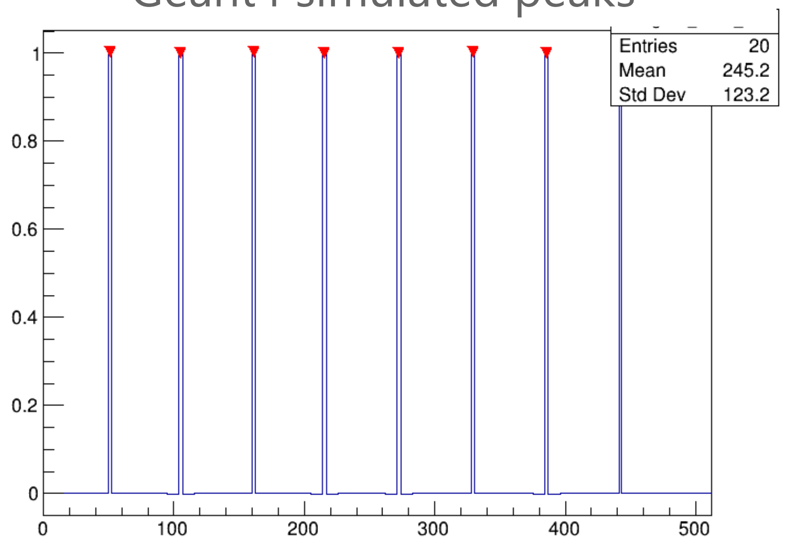


Work of Milán Klausz (Hungary)

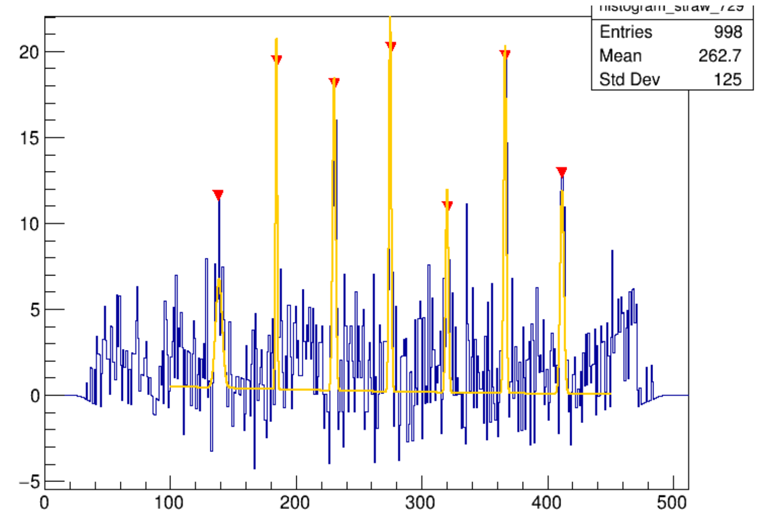
Position calibration

- Position calibration data is generated by place a mask with narrow slits
- For challenging noisy peaks algorithmically approximated
- The difference between simulated and measured peaks is calculated, and a polynomial relationship is fitted.
- The result is used by Event Formation Unit in order to generate position-corrected NeXus files.
- For the LoKI detector tests, the demultiplexing and position correction was originally performed at ISIS by Davide Raspino, but **can now be replicated by code written by ECDC in preparation for hot commissioning**.

Geant4 simulated peaks



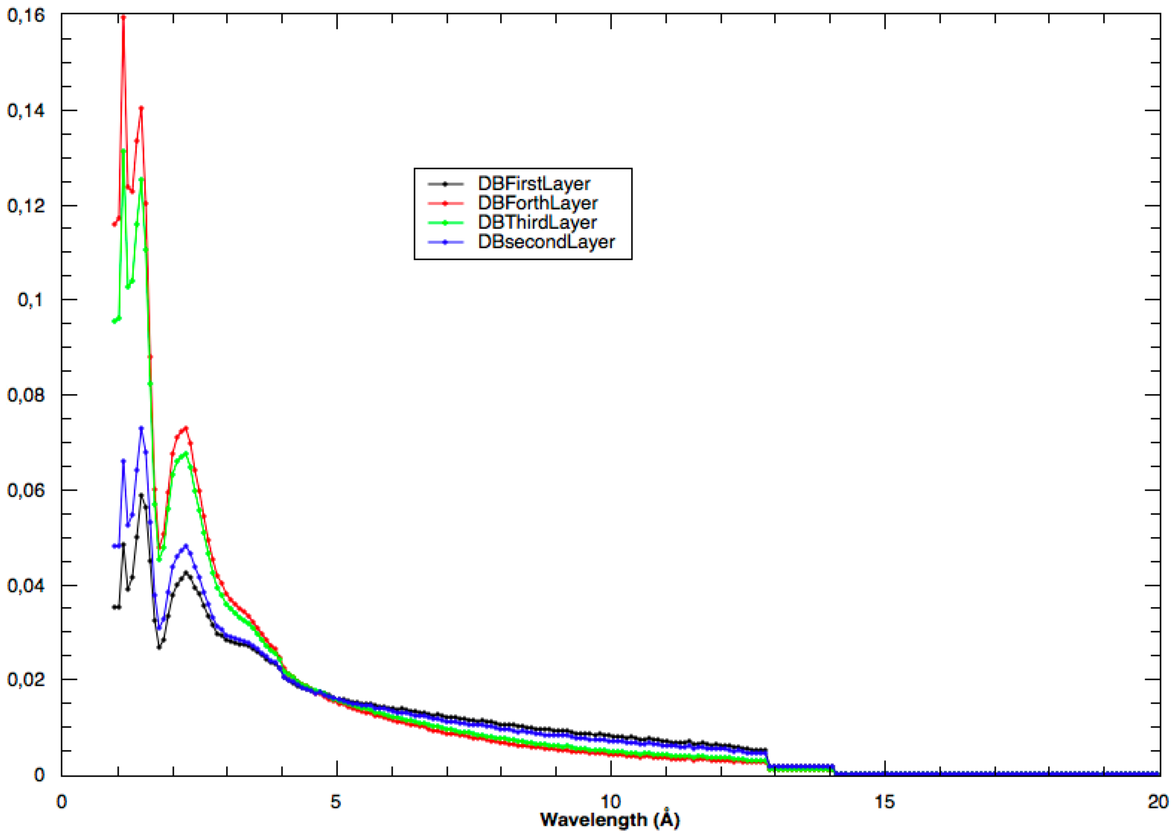
Measured peaks (naturally worse towards the back of the detector)



Data from March 2023 STAP report

Data reduction of the LoKI test data

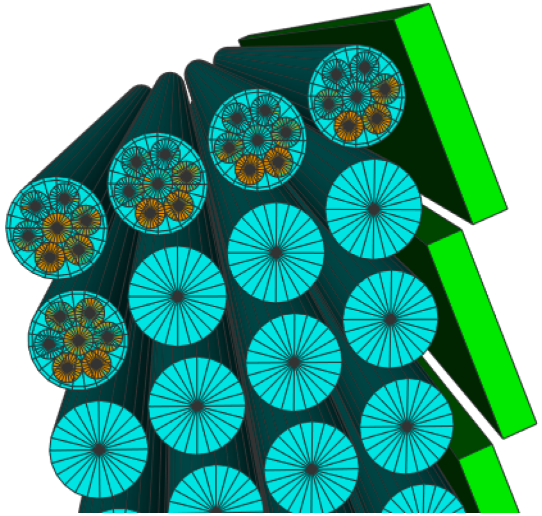
- As expected we observed: a hardening of the direct neutron beam as we go through the panel of detector straws, due to self-screening from one layer of straws to another.
- To account for this effect, we need to create a "direct-beam function" (D(λ)) that changes through the depth of the detector
- D(λ) is the **relative efficiency of the main detector** (or detector straws) **compared to the incident beam monitor as a function of wavelength**. D(λ) allows us to cross-normalise the incident spectrum to that of the empty beam (without sample) is seen on the main detector.

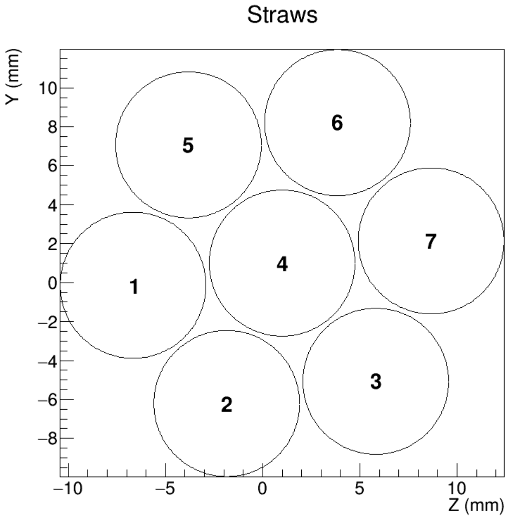


Query over "layers"

One challenge for us has been to decide to what resolution we should be generating the D(λ), e.g. per each straw (difficult with poor statistics), per each "straw layer" (consider 7 straws in each of 4 tube layers = 28 layers), grouping the straw layers in logical geometrical layers (= 11/12 layers), or per each tube layer (= 4 layers).

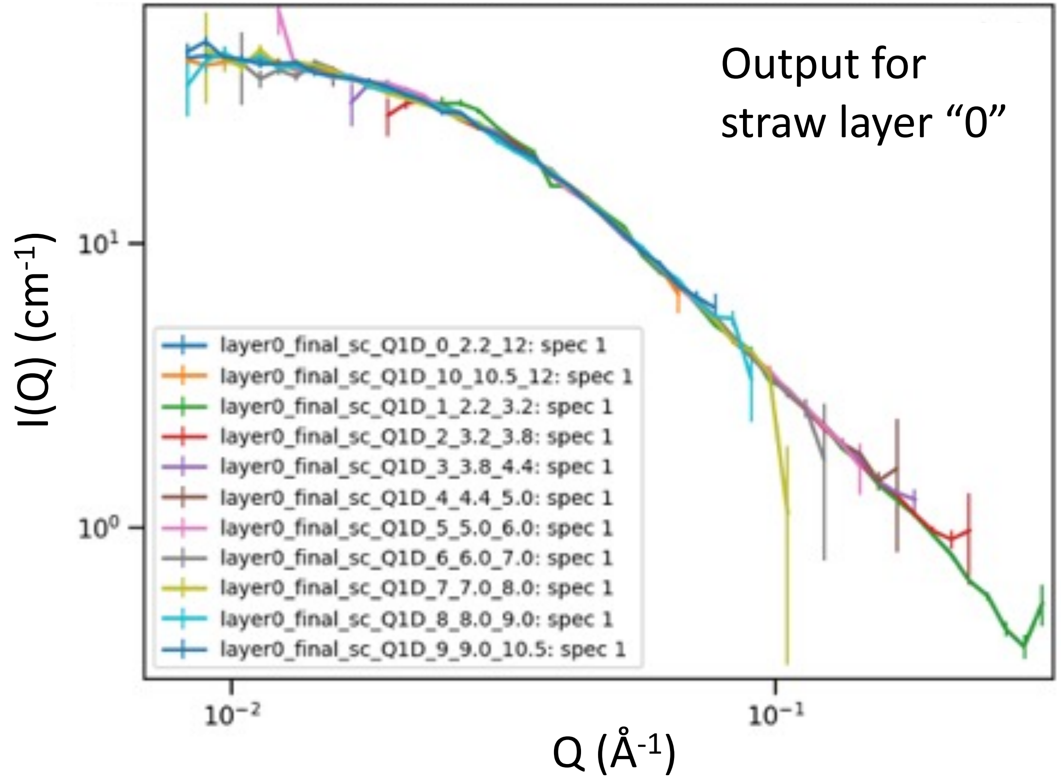
Currently, we are still working with the **28 layers approach** (so all straw number 0 in Tube layer 1 are one "layer").





Direct Beam Function

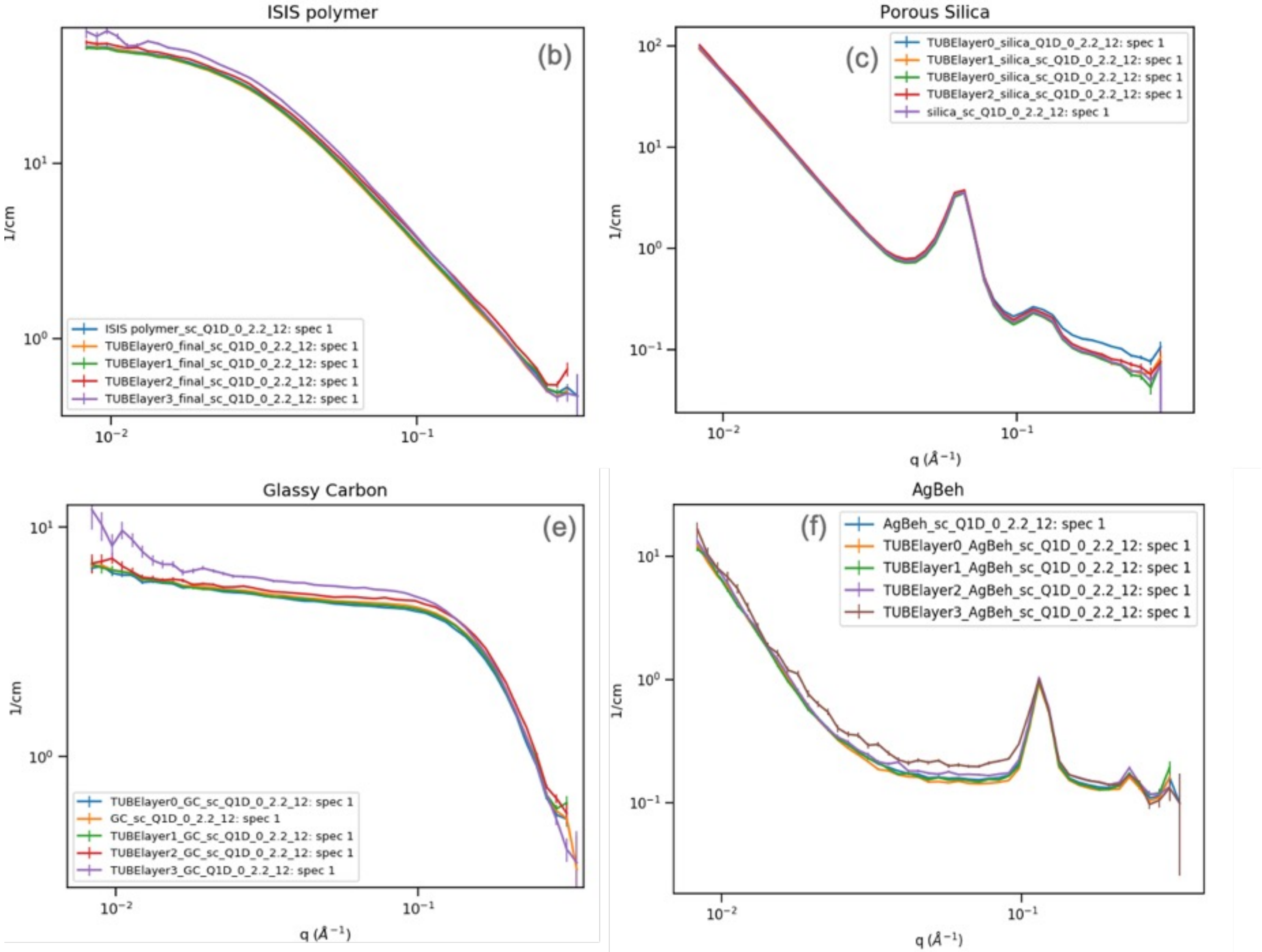
- I(Q) is generated by the reduction of 6 to 12 wavelength bands which are then compared to I(Q) from the full wavelength range. The process is iterated until the correction converges to a nearly flat polynomial.
- We then iterate and correct the wavelength adjustment profile, until the wavelength sufficiently overlaps. The final step simply scales the D(λ) to correct for the overall absolute intensity.
- Start with a simulation of a flat scattering from Geant4. This simulation helpfully picks up any straw-to-straw variability and provides a "master" file in which we can save the new D(λ) functions.
- The generated D(λ) for each layer is then applied to all the straws in the relevant layer of the master file (i.e. original flat simulation).

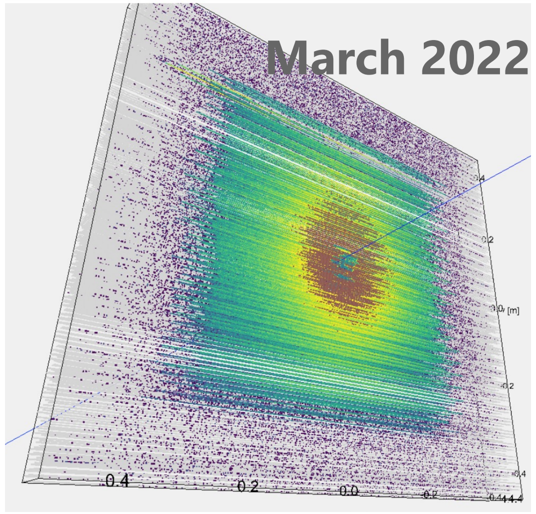


After many iterations we are considering 28 layers (so all straw number 0 in Tube layer 1 are one "layer")

Detector Tests on Larmor (ISIS, UK)

Data reduction in Mantid (demonstrated before) is being transferred to SCIPP





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

Data from previous report

5
DMSC Updates

WOJCIECH POTRZEBOWSKI

SANS data processing pipeline

Current status for LOKI

Experiment control → Stream events & meta data → Data reduction & visualization → Data analysis → Data management

• Baseline version • Use case at Ymir • NURF setup	• Full chain tested • Detector calibration scripts • Meta data	• Basic workflow • Pipelining • Direct beam • TOF Resolution	• Basic functionality • TOF Resolution • New release	• Basic functionality • Automation and integration • Meta data

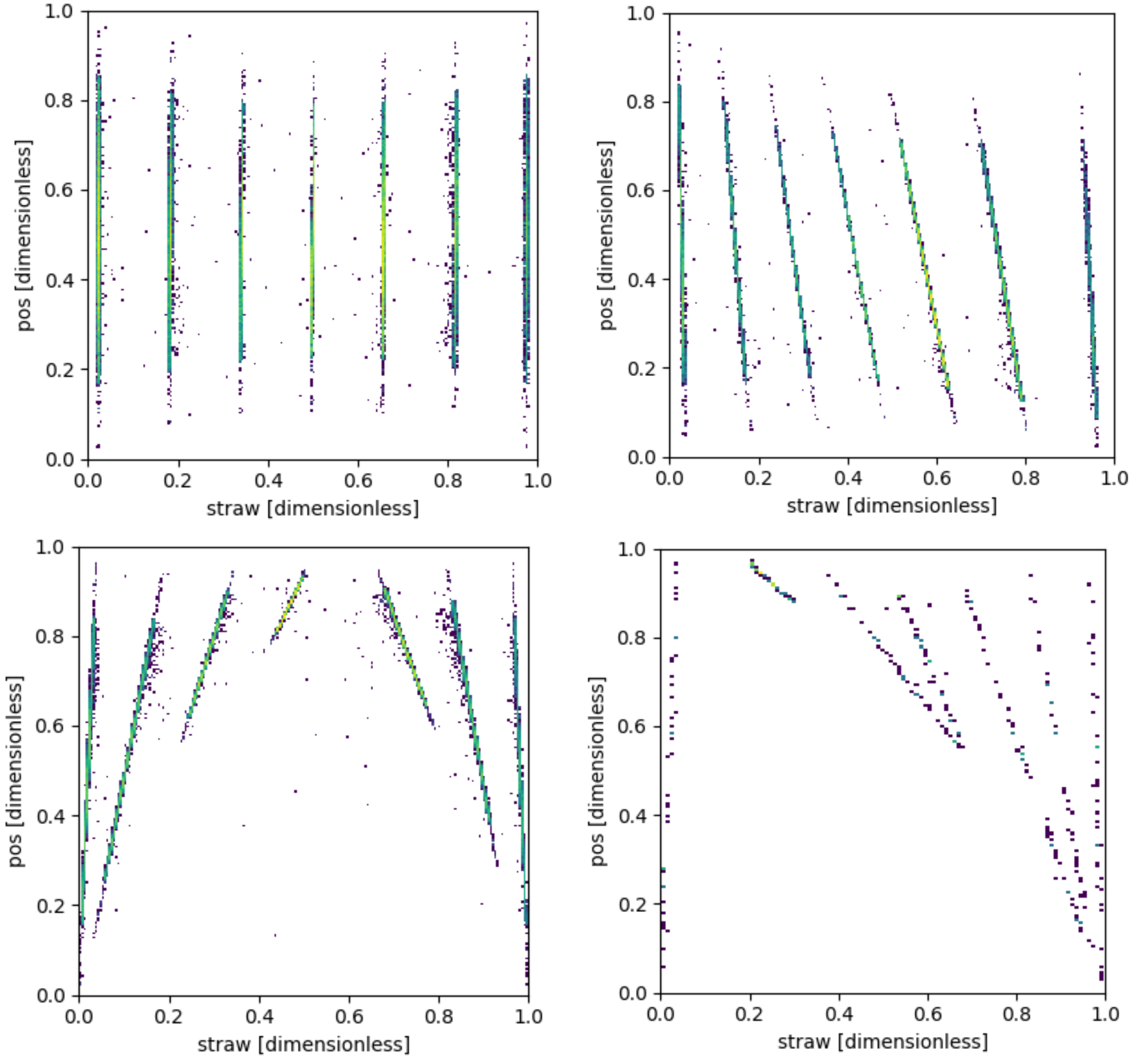
Completed
Work in Progress

+ User office software, DST requirement (storage, VISA)

Detector calibration

Straw/position callibration

- Data from LOKI detector test analyzed wrt straw and position determination
- Majority of cases straightforward
- Exploring procedures for identyifing “doggy” straw/tubes
- Possible masking and corrections discussed with ECDC
- Work on proof-of-concept on DREAM (which likely can be adapted to LOKI)

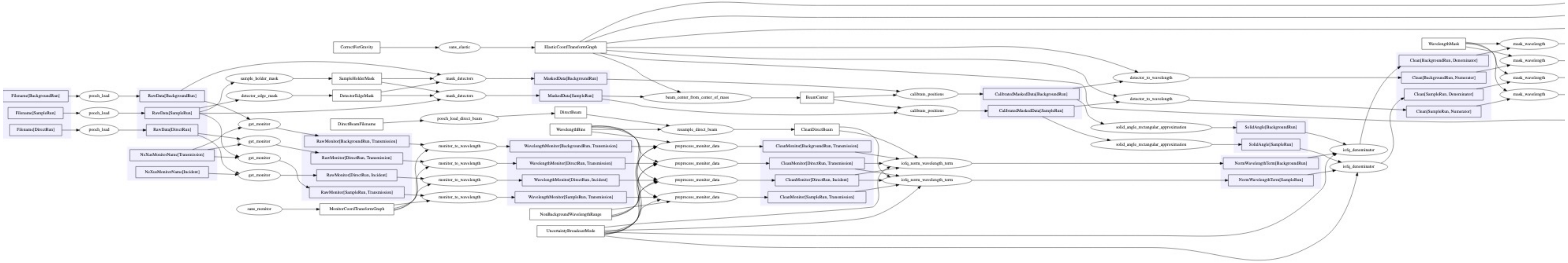


Data reduction

High level Scipp developments

sciline

- Framework for writing, testing, and maintaining complex data analysis workflows
- Easier to develop code for repetitive tasks (e.g. wavelength slicing, meta-data filtering)
- Easier integration with future GUI
- Auto-generated workflow graphs

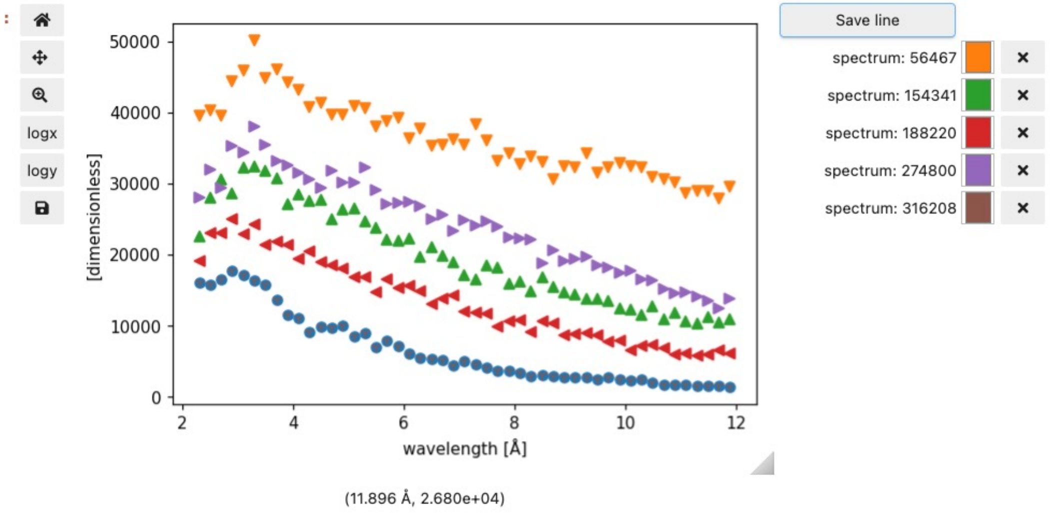


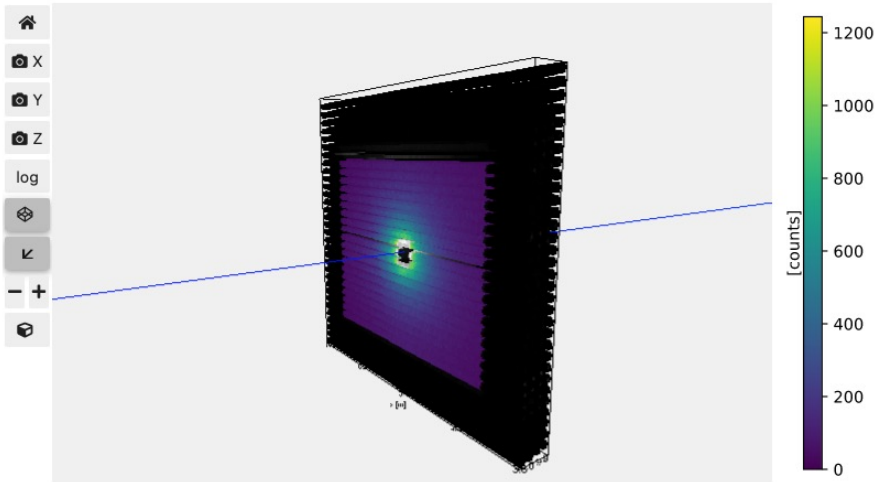
https://scipp.github.io/sciline/index.html
https://scipp.github.io/esssans/

Data reduction

Direct beam function

- Development of direct beam iteration functionality in Scipp
- Adapted data reduction pipeline in Scipp to use Mantid direct beam file
- Benchmarking Scipp results with Mantid
  - Per layer-defined direct beam function
  - Step-by-step comparisons
  - Mask and monitors exactly as in Mantid





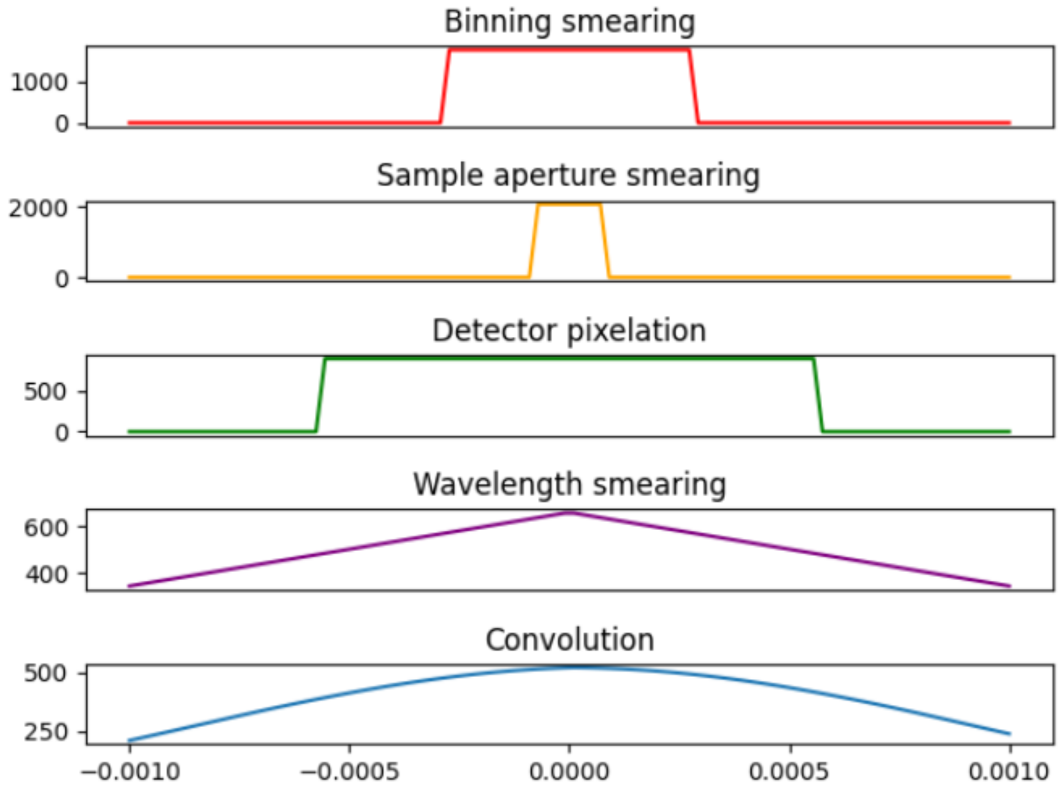
Data reduction (+ data analysis)

TOF resolution

- Demonstrated that SasView can read in arbitrary resolution function
- Developed kernel convolution (aka GRASP) functionality in Python
- Working on Scipp implementation

TODO:

- Save to CanSAS format
- Demo for CanSAS working group



Data analysis

SasView 6.0.0-alpha release

- Orientation viewer available
- Corfunc perspective refactored
- Simultaneous fitting allows for a weighting scheme
- Preferences panel with display and plotting options
- Improved label handling on plots
- Residuals plots refactored
- PDB reader refactored
- Wedge slicer added
- Sasdata package separated
- Custom Model writing tutorial