LoKI Progress Update
March 2023

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1 Overview

The progress of the LoKI project remains good, with manufacturing and testing complete for almost all major components. Everything other than detectors, cave roof, and door and roof hatch are now at the ESS, undergoing or awaiting installation. Detector data processing has also significantly progressed since the last STAP update. In this report, we outline the progress on engineering matters and address progress on the action items raised by the STAP in October 2022.

2 Engineering

2.1 Instrument overview

The progress of all the major instrument components is summarized in the figure below.

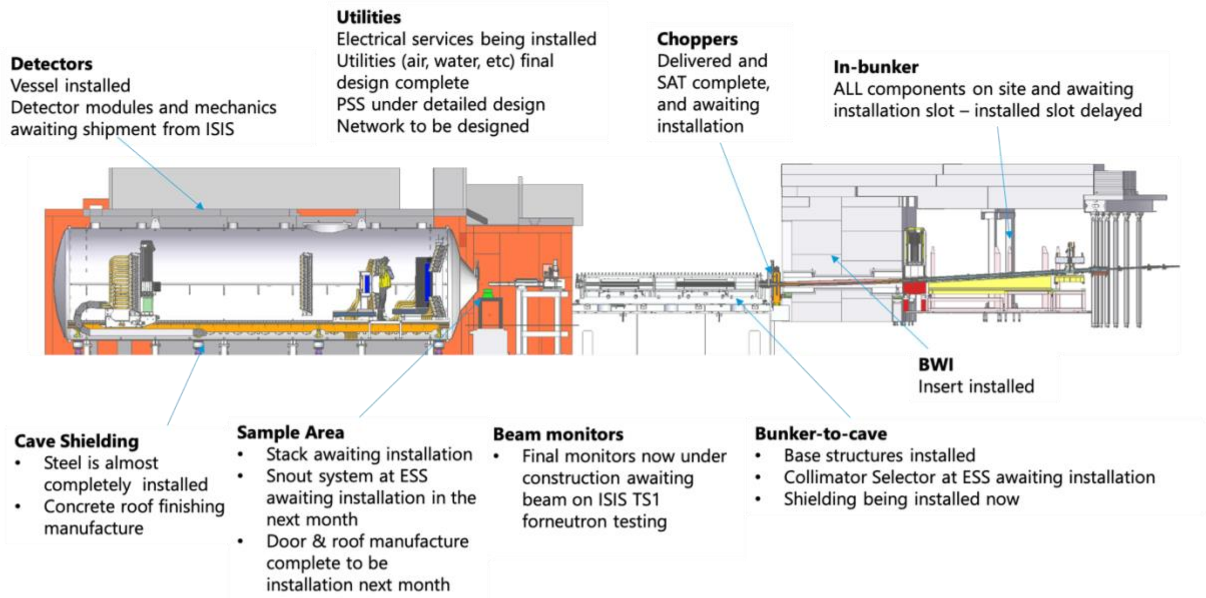


Figure 1 *Overview of the LoKI engineering status*

2.2 Installations in the last 6 months

Figure 2 shows the instrument as of the 12th March. Notable additions since last STAP include the crane, good lifts, cave shielding, sliding door for accessing the tank, and a lot of cable routing infrastructure.

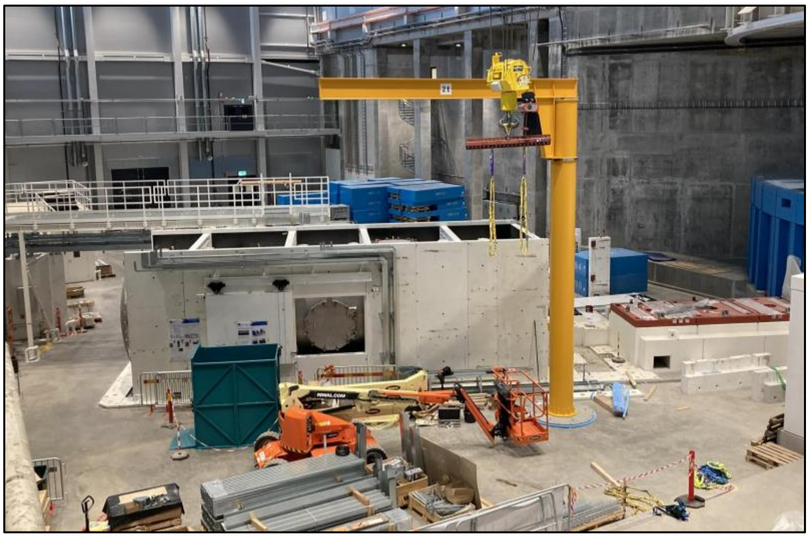


Figure 2 *Picture of the LoKI as of March 2023. Recent progress: remaining instrument cave structure, the good lifts, local crane, and cable routing infrastructure.*

2.3 Upcoming installations

2.3.1 Sample area

The wall and roof around the sample area will be installed in the coming days, in preparation for the arrival and installation of the sample area door and roof hatch (to be installed by the suppliers).

2.3.2 Collimation

During installation of the collimation shielding blocks there was a relatively small collision with the block and the base support for the vessel, bending the steel rods that should allow for future realignment. Rework of these pieces is underway, and has relatively little impact on the schedule. Once these pieces are complete, the collimation vessel and shielding will be installed.

2.3.3 Cave roof

The cave roof is undergoing manufacture, we expect its arrival in roughly 2 months. The roof will be immediately installed to allow key installations of electrical services, racks, and vacuum pumps.

2.3.4 In-bunker area

The LoKI in-bunker final installation slot has shifted slightly due to delays from target installation activities, and to better accommodate the long instrument installations (optimising the overall schedule for the instruments). Our current slot will be in June/July 2023. Therefore, we expect most of the installation to be underway by September 2023, after the electrical and utilities are installed.

2.3.5 Detectors

At the end of 2022, members of the ESS DG visited ISIS to learn how to build, test and repair a detector module. During this process a vacuum seal O-ring was found to have cracks. Therefore, it was decided to replace all vacuum O-rings with a better alternative. This process is complete, and now the final pre-build of the modules in the detector frames with the detector hosing is underway, and going well.

Final electrical testing is also required for the beamstop mechanism before the entire assembly will be sent to ESS.

Detector upgrade status: ESS and ISIS agreed on an approach in order to reduce risk, to either side, due to the potential inflation of the hardware costs. This was successfully managed by the ISIS team, who, as of two weeks ago, had the final signoff to place all hardware orders. The new projected delivery of modules to ESS is August 2025, with installation proceeding as soon as ESS resource is available at the time.

2.3.6 Sample environment

The overview of the LoKI sample environment is shown in the table below (the changes since the last STAP are shown in green). Good progress has been made from the perspective of integration. With the integration (phase 1) of the rheometer and fluorescence spectrometer is almost complete. ESS Sample Activities Division is also currently undergoing a recruitment for a soft matter sample environment engineer.

Sample Environment System	**Phase**	**Status**
Thermostated sample changer for quartz cuvettes	HC	Detailed design complete – starting to reach out to manufacturers
Cell tumblers/rotating sample holders	HC	Detailed design complete – starting to reach out to manufacturers
Flow cell (including HPLC pumps)	HC	Jasco HPLC integrated
In situ techniques, as spectrometer attachments to the flow-through cell	ES	Fluorescence spectrometer integration progressing well Issues with UV/Vis device
Rheometer	ES	Anton Paar undergoing integration at ESS. Progressing well with control through NICOS
Stopped-flow cell	ES	In-kind device from Estonia (Biologic) progressing with integration
Individually thermostated cuvette rack	ES	Prototype exists and integrated at ESS
Goniometer(s)	ES	ESS to purchase 2023
Dismountable 'sandwich'-style cells (ESS)	ES	Designs exist. Just to be sent for manufacture
Warm Bore Cryomagnet 2.5T	ES	ESS procurement underway
Stress/stretching rig (ESS)	ES	ESS collaboration(s) to develop different rigs

Plan for the next in-person meeting in October 2023: ECDC, sample environment and the LoKI team hope to set-up a sample environment (e.g. rheometer or, if possible, the LoKI cell holder) on YMIR (the prototype instrument owned by ECDC), where we would like to "live demo" the integration, as well as instrument control software NICOS for LoKI.

3 Detector Tests and Data Reduction Progress

3.1 Position Calibration

For the LoKI detector tests, the demultiplexing and position correction was performed at ISIS by Davide Raspino. To generate data, we place a mask with narrow slits directly in front of the detector panel, and then measure the scattering from an isotropic scatterer (e.g. Vanadium). For each straw in the detector, the measured peaks in neutron events are compared to simulated peaks, and a correction polynomial is fitted. The ECDC group is currently helping us adapt Davide's script so the instrument team can use it for instrument commissioning.

Simulated peaks (left in **Figure 3**) are clear and easily defined. Measured data is much noisier, particularly towards the rear of the panel (right in **Figure 3**), and, therefore, it is much harder to identify the peaks. For these values, we approximate with the ROOT function ShowPeaks and then refine it with a multi-gaussian fit. The difference between simulated and measured peaks is calculated, and a polynomial relationship is fitted. This is then saved to a json file in the expected format for the Event Formation Unit, in order to generate position-corrected NeXus files.

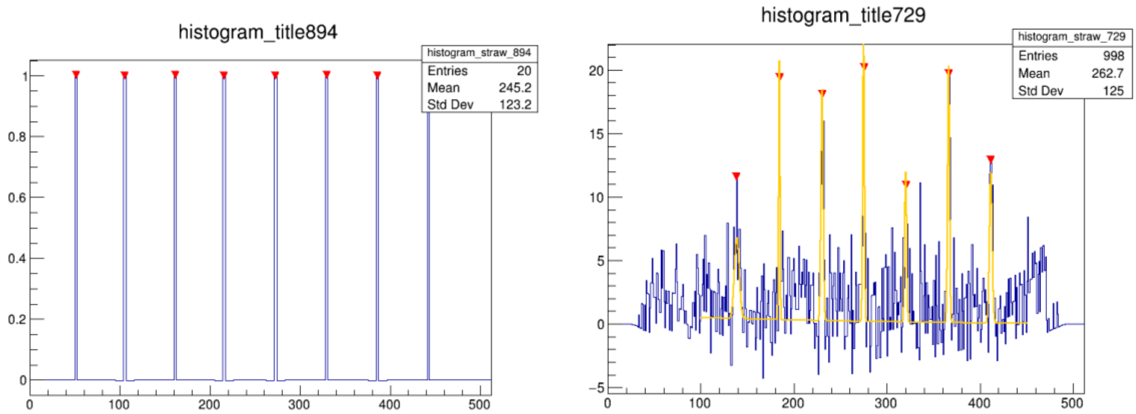


Figure 3 *(left) Simulated peaks along one straw. (right) Actual peaks measured along one straw towards the back of the detector with poor statistics.*

3.2 Progress in Mantid

The processing and analysis of the data from the detector tests in 2022 is now well underway. Position corrected data in NeXuS files (as described in Section 3.1), have now been generated directly from the ESS software stack. The repeat measurements of each have been successfully combined to generate workable, raw time-of-flight transmission and sans data for each of the samples measured.

As expected, we observe 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.

A reminder that 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) seen on the main detector. A full description can be found in the SANS reduction document we previously sent to the STAP for review (attached again for reference). Unfortunately, it is difficult to experimentally measure a good D(λ), as it is hard (impossible) to precisely attenuate the beam the same amount at all wavelengths. Also for LoKI, with the direct beam we can only fully illuminate a few straws in the detector. Therefore, we need to empirically fine-tune D(λ) across the whole detector with iterative reductions at different λ for a standard sample, in this case partially-deuterated solid polystyrene standard.

Key to this process is to consider wavelength overlap plots, in which I(Q) is split into 6 to 12 wavelength bands which are then compared to I(Q) from the full wavelength range, as shown in Figure 4a. By averaging these ratios over a sliding Q range a correction polynomial for D(λ) is generated. The process is iterated until the correction converges to a nearly flat polynomial. The sliding Q range in the comparisons avoids regions of Q where the background correction is large, or the elastic scattering is small.

Building on script from Richard Heenan, we are starting 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. 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 working with the 28 layers approach (so all straw number 0 in Tube layer 1 are one “layer”), but we can hopefully simplify this later.

The current status of the data correction is shown in **Figure 4**. As mentioned, to generate the D(λ) file. we have grouped “like straws” in each layer of tubes as their own layer (so 28 effective layers). In order to create the correction, we are doing a full wavelength range reduction over all the straws in each defined “layer”. We then iterate and correct the wavelength adjustment profile, until the wavelength sufficiently overlap. The final step simply scales the D(λ) to correct for the overall absolute intensity. For example, the output for one straw layer is shown in **Figure 4**a. 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).

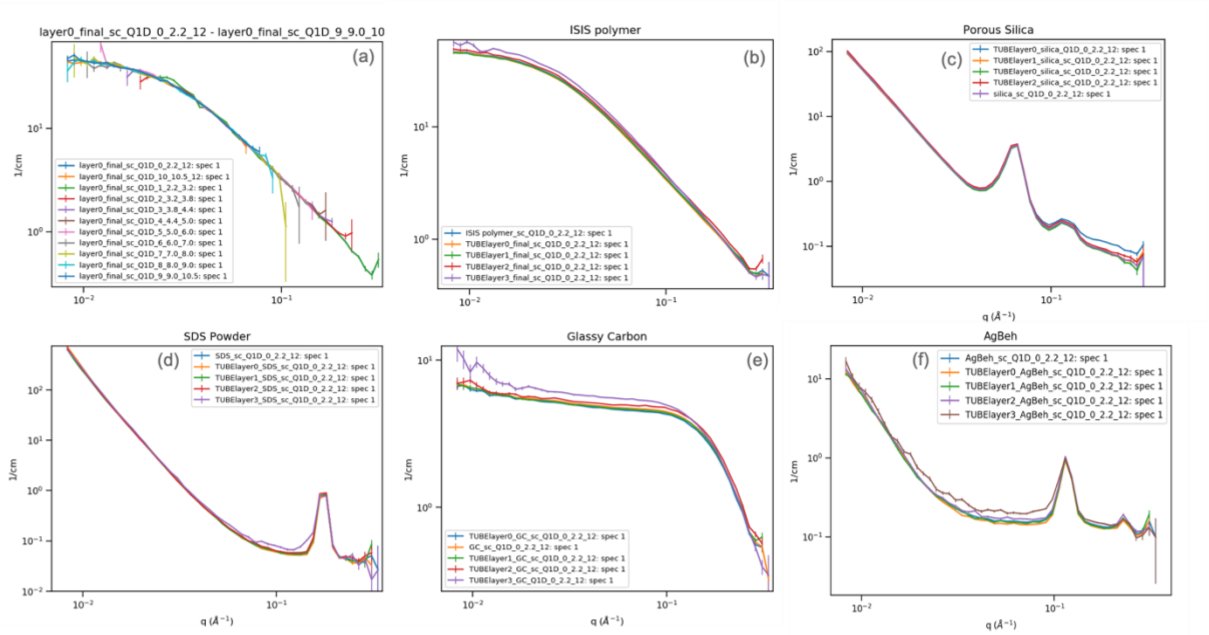


Figure 4 *Reduced SANS data from the LoKI detector test. (a) Example wavelength overlap plot of the ISIS polymer standard for one layer of straws (out of 28). (b-f) Reduced data using the DB correction function. The detector data in each has been split into the four tubes layers – to illustrate (i) the current methodology works well for layer 0-2. Layer 3 is clearly out in each case, however this is not surprising, given we need to adjust rerun now the masks have been finally sorted. (b) ISIS standard polymer of partially-deuterated solid polystyrene, (c) Porous silica, (d) deuterated SDS powder, (e) glassy carbon and (f) AgBeh.*

Our first check has been to confirm the reductions of each of the 28 layers overlap. Many, many bugs are being found, and oftentimes issues are found with masking (described below). We have then used this correction file to reduction the other data collected at the test (AgBeh, glassy carbon, etc), Figure 4c-f. To simplify, we have just plotted the reductions as a function of the four tube layers (0-3). It is clear, that tube layer 3 (the back layer), still needs adjustment, but we are confident this can be corrected (issues only found this week). As work is continuing on optimising the current script by Judith, and analysing the output, while Wojciech is simultaneously working with the scipp developers to replicate the output, building on their prototype for SANS2D data and earlier LoKI detector test data (from 2019).

Challenges:

- Poor statistics in the position calibration mask runs, meant that some of the straws towards the rear of the detector may not be accurately corrected – so need to be masked out.

- The beamstop on the Larmor instrument was unfortunately off-centre (relatively unavoidable given we couldn't directly read out detector images when we were setting up). This means that we have quite a lot of straight-through beam hitting the detector. This (a) caused issues with the calibration mask data as the position of at least one calibration peak was getting lost in the direct beam, and (b) potentially exaggerates any background we can expect on these detectors.
- Identifying dodgy straws/pixels and masking in general is painful, particularly on Mantid, which isn't optimised for these detectors. We practically need to check straw by straw if there is a fault that needs to be masked. Hopefully, this will be improved with SCIPP visualisation.

Plan for the next in-person meeting in October 2023: Details of efficiency corrections, resolution functions, including the current status and challenges, will be discussed with the STAP committee.

3.3 Progress in SCIPP

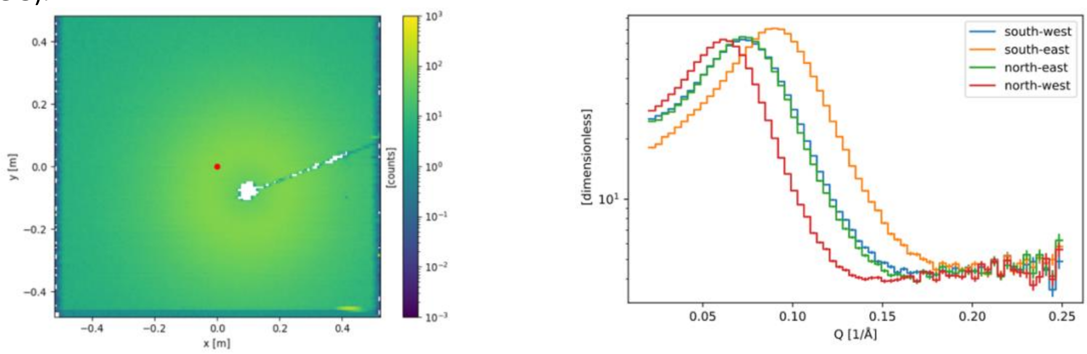
Main activities within data reduction in scipp included developing Beam Centre Finder algorithm and a generic description of TOF resolution function. In addition to that, the requirements for updating direct beam iteration scripts and streamlining multiple runs based on metadata parameters have been discussed with scipp developers' team and are planned for the future.

The Beam Centre Finder algorithm uses a combination of a centre-of-mass calculation and an iterative refinement on a computed scattering cross-section to find the centre of the scattering pattern.

The detailed procedure to determine the location of the beam centre is greatly inspired by Mantid functionality and is the following:

1. Obtain an initial guess by computing the centre-of-mass of the pixels, weighted by the counts on each pixel
2. Based on that initial guess, divide the panel into 4 quadrants
3. Compute $I(Q)$ inside each quadrant and compute the residual difference between all 4 quadrants
4. Iteratively move the centre position and repeat 2. and 3. until all 4 $I(Q)$ curves lie on top of each other

The implementation of the algorithm has been validated on SANS2D and LoKI detector test data (**Figure 5**).



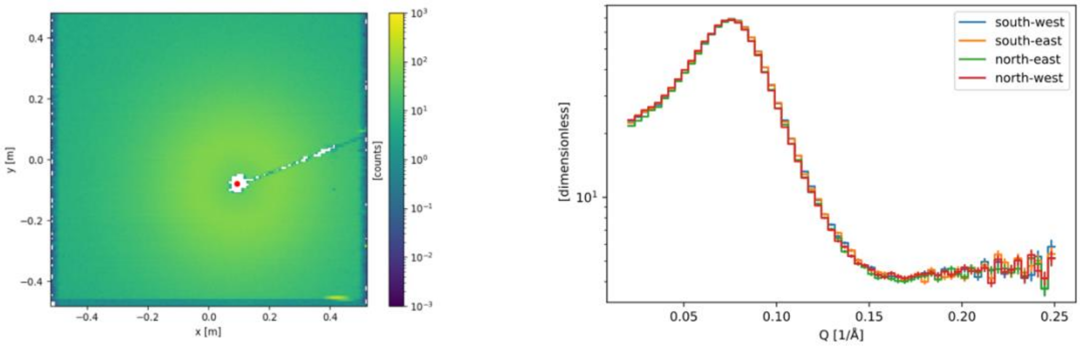


***Figure 5** Beam centre finder algorithm on SANS2D data. Top: the initial position of the centre (left) marked by the red dot at x = y = 0, and the corresponding intensity functions in all four quadrants (right). Bottom: the position of the beam centre (left) and the corresponding intensity functions (right) upon algorithm convergence.*

In the course of developing beam centre finder algorithm, a few improvements have been made to the existing data reduction code. Upcoming work will involve carrying out an extensive benchmark on available SANS2D data, as well as reducing the LoKI detector test data using scipp.

On a generic resolution description note, a prototype of the code that gives access to individual terms in the resolution function has been developed, and there is ongoing work on applying similar routines to GRASP to perform numerical convolution of these terms. The aspirational deadline to conclude this work (together with integration with SasView) is CanSAS meeting in October.

Plan for the next in-person meeting in October 2023: Live demo of scipp.

4 Other Software Activities

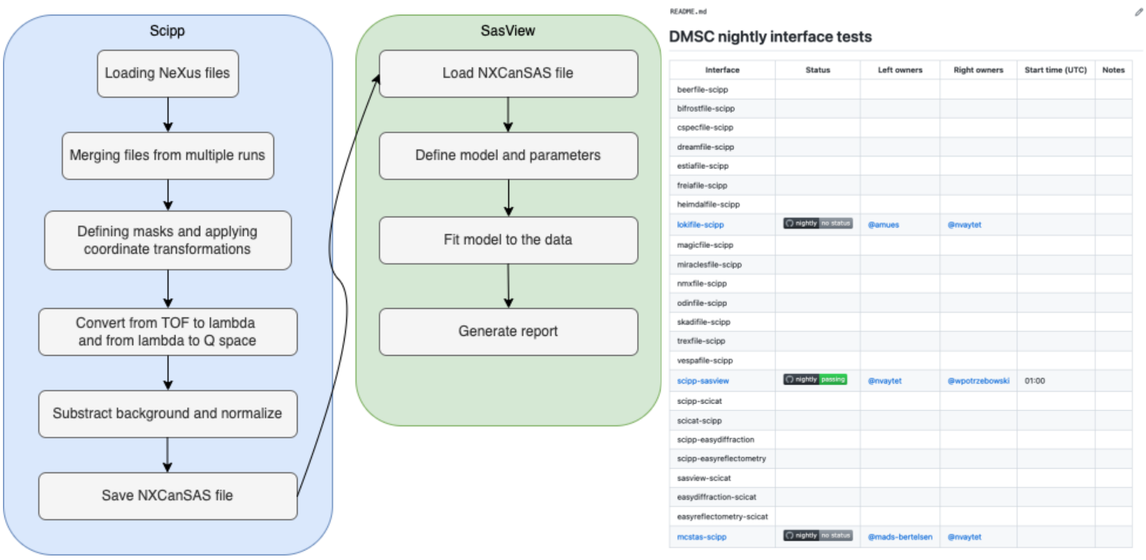
4.1 Testing interfaces across DMSC software stack

While each individual software component developed at DMSC has its own set of automatic tests, they assure consistency within a single software tool rather than connections with up or downstream dependencies. One can easily imagine that for example a change in data reduction output may have consequences on how the file is read by the data analysis software.

Over the last few months, efforts continued to integrate different services across the DMSC software stack. In particular, at the interface between data reduction and data analysis for SANS, we have set-up a job that runs every night and performs the following (Figure 6):

- reads in Nexus files containing experimental data
- runs the reduction workflow with scipp that computes I(Q)
- writes the I(Q) result to a NXCanSAS file
- loads the NXCanSAS file into SasView
- performs a fit to the I(Q) and makes sure that the fit parameters have not changed.

The automated job runs on GitHub actions, and is available at https://github.com/dmsc-nightly/scipp-sasview



Interface	Status	Left owners	Right owners	Start time (UTC)	Notes
beerfile-scipp					
bifrostfile-scipp					
cspecfile-scipp					
dreamfile-scipp					
estiafile-scipp					
freiafile-scipp					
heimdalfile-scipp					
lokifile-scipp	nightly no status	@amues	@nvaytet		
magicfile-scipp					
miraclesfile-scipp					
nmxfile-scipp					
odinfile-scipp					
skadifile-scipp					
trexfile-scipp					
vespafile-scipp					
scipp-sasview	nightly passing	@nvaytet	@wpotrzebowski	01:00	
scipp-scicat					
scicat-scipp					
scipp-easydiffraction					
scipp-easyreflectometry					
sasview-scicat					
easydiffraction-scicat					
easyreflectometry-scicat					
mcstas-scipp	nightly no status	@mads-bertelsen	@nvaytet		

Figure 6 *Steps in scipp and sasview interface automatically tested on daily basis.*

We are planning to continue adding new tests for services/interfaces to the continuous integration framework at https://github.com/dmsc-nightly.

4.2 Data analysis

After a successful code camp in October (Figure 7), a release candidate for SasView 5.0.6 was released. Based on the feedback gathered from developers and users there is ongoing work to release a full version. The new version fixes a number of issues reported in earlier versions of 5.0.x. Of particular note, the failure of the program to start when installing on a new system. The speed with which the program starts up has also been improved. The paracrystalline models, which have been labelled as "under review" since 2018, have been checked and corrected (bcc and fcc) and the documentation completely reworked (bcc, fcc, and sc). Elsewhere, plots now properly support custom data names in the legend, the LM optimizer failing to run on GPUs or when the starting value of a parameter is outside the min/max range has been fixed, a problem with the intermittent blanking of plots has also been fixed, a number of defaults have been changed to be more reasonable, and a number of other issues in the documentation have been corrected and/or updated.

There is also ongoing work on SasView publication and updating road map (https://github.com/SasView/documents/pull/3/). We expect to finish work on the road map in the coming months and present it to the wider community.

In April we will also hold a second edition of the Magnetic SANS workshop aimed at further defining requirements for SasView. We hope to be able to better define cases like: sector cut options for anisotropic data, decoupling magnetic from non-magnetic form-factors, interoperable formats that can be combined with SasView.

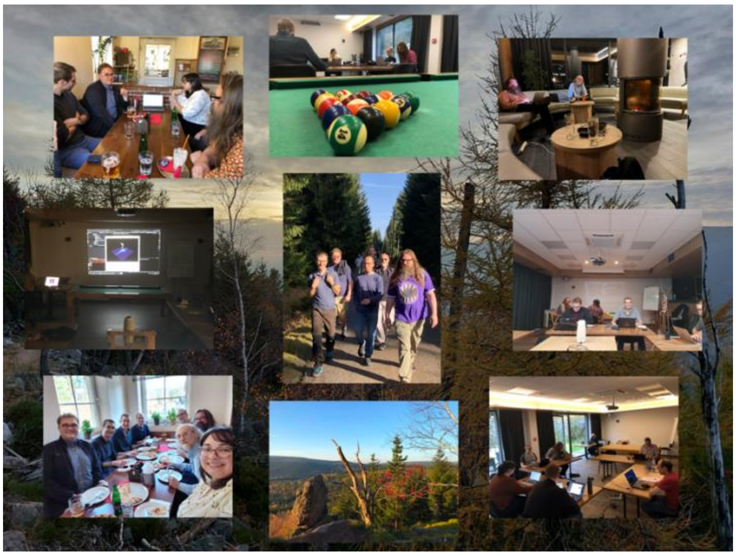


Figure 7 *Pictures from SasView Camp held in Poland in October 2022*

4.3 Education and outreach.

A number of teaching and outreach activities were conducted over the course of the past few months. LoKI instrument team was heavily involved in Swedness school, where PhD students from Sweden came for a week-long school on small angle scattering. The content of the course included lectures and practical sessions. For the hands-on sessions, students worked with data reduction in scipp and data analysis in SasView.

As a part of the PANOSC project Kinanti Aliyah Hantiyana worked together with Wojciech Potrzebowski on developing an e-learning course on “Publication guidelines for biomolecular small-angle scattering”. The course is now available online at https://e-learning.pan-training.eu/moodle/course/view.php?id=120 (requires login) and features teaching material, quizzes, and checklists (**Figure 8**). We plan to present this work at BSR14 meeting and IUCr congress (abstract submitted).

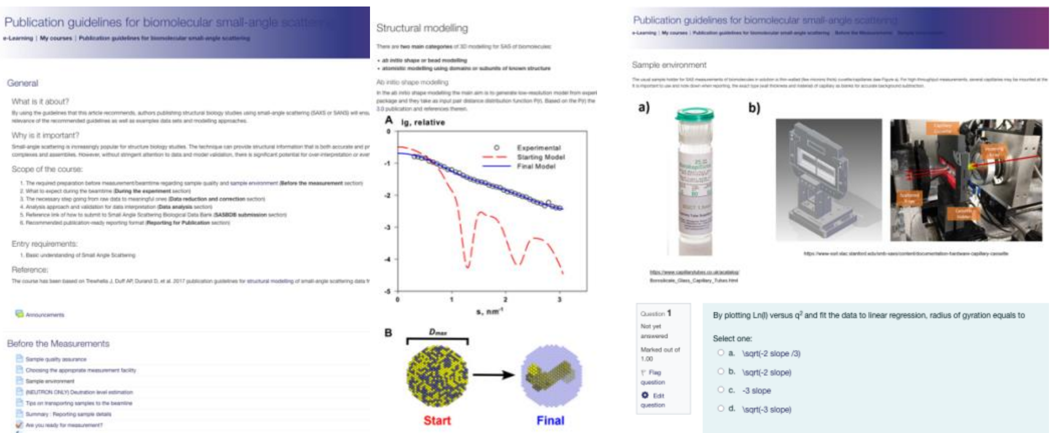


Figure 8 *Screenshots from the e-learning course on Publication guidelines for biomolecular small-angle scattering.*

Wojciech Potrzebowski is also involved in organizing FASEM school (French and Swedish School on Life sciences), which will cover different aspects of scattering experiments and modeling, however, Judith Houston is involved in organizing 25th anniversary CanSAS meeting.

It is also worth mentioning that SANS instrument teams started regular meetings with corresponding SAXS teams at MAXIV. The main topics so far included data processing pipelines and samples environment.