DMSC report for SANS STAP (Oct 2021)

The main purpose of this report is to provide overview of activities related to software developments for LoKI. The report is divided into 4 parts:

- DMSC deliverables
- Instrument control and NeXus data format
- Data reduction
- Data analysis

DMSC deliverables

The main goal of defining these deliverables is to test the entire DMSC software stack and interfaces between ESS sites in Lund and Copenhagen, such that we are ready for performing commissioning and early science activities. While a set of user stories (tasks) have been defined with the LoKI instrument in mind, they are to large extent generic and are thus also relevant for other beamlines. Effort has also been made to link the user stories with network infrastructure that is currently being implemented at ESS in Lund for test beamline (YMIR). Some elements, e.g. delivering drivers for specific sample environment, have been deliberately excluded from this exercise to keep it coherent. The anticipated outcome will be a frequently updated page on confluence and/or JIRA where status of different user stories will be monitored and ESS/DMSC dependencies will be checked. Discussion on drafted deliverables has already identified few requirements for stakeholders and provided better overview of the current status of tasks. From the Instrument Data Scientist's perspective it has also improved interaction with different stakeholders.

Instrument control and NeXus data format

As reported in the STAP meeting in April 2021, the ECDC group has been working on the NICOS interface for LoKI. The basic functionality that has been implemented so far includes experiment setup, instrument interaction, script editor and sample setup (Fig. 1). As of July 2021 it was concluded that baseline level was reached. The baseline version will continue to be developed.

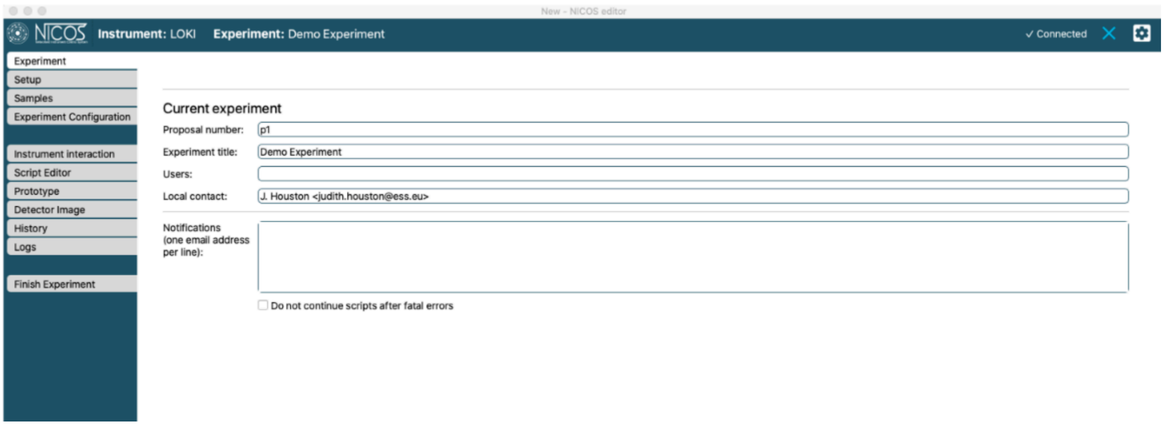

Fig. 1. LoKI interface in NICOS

The creation of a NeXus data file template that will contain LoKI specific data and geometry information is in progress. The file will, among other things, contain information about detectors, choppers, slits, monitors and the sample environment. A plot of the pixel coordinates for the nine LoKI detector panels stored in the NeXus file geometry is shown in Fig. 2.

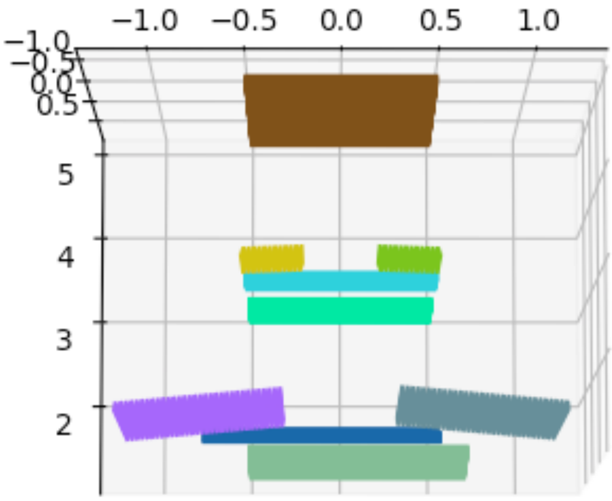

Fig. 2. 3D representation of the LoKI detector geometry which is stored in the NeXus file.

Data reduction

Scipp is the data reduction framework actively developed at DMSC. The Scipp framework now contains different subprojects/repositories serving different purposes (Fig. 3). *scipp* covers core functionality (data structure, operations and backend calculations), *scippneutron* includes neutron specific functions, while *ess* and *ess-notebooks* contain python code and notebooks specific to ESS instruments or techniques (e.g. sans or loki folders).

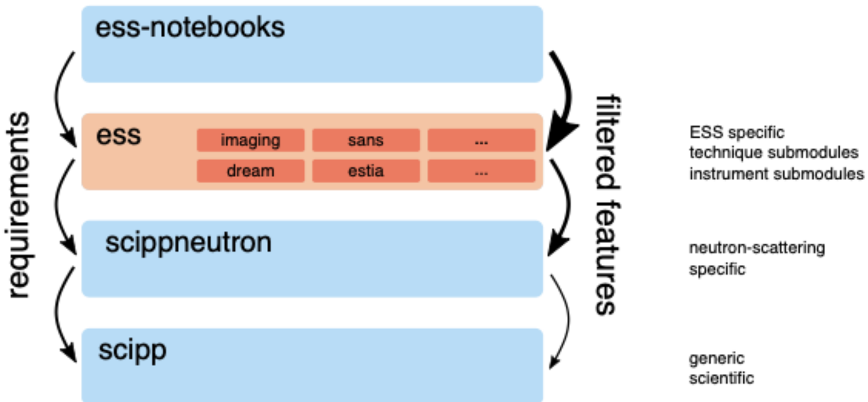

Figure 3. Scipp framework structure

Currently we are working on adding LoKI specific code into *ess* and ess-notebooks repositories based on new and previous developments. An important feature of this work is the ability to test individual modules/functionalities in order to be able to reproduce results. The work on developing testing modules is two-fold, firstly providing set of basic functions to reduce McStas simulated data for LoKI and SANS2D and secondly to reduce real experimental SANS2D data using an entire data reduction workflow (with geometry transformations, more complex normalization, etc.). As a part of adding code to scipp repositories, the results from scipp has been compared with Mantid results. While the comparisons are in the good agreement for simplified workflows (simulated SANS2D and LoKI data sets) and when Mantid is used directly from the script, a difference is observed for reduction of SANS2D experimental data when using ISIS interface from Mantid workbench and scipp (Fig. 4).

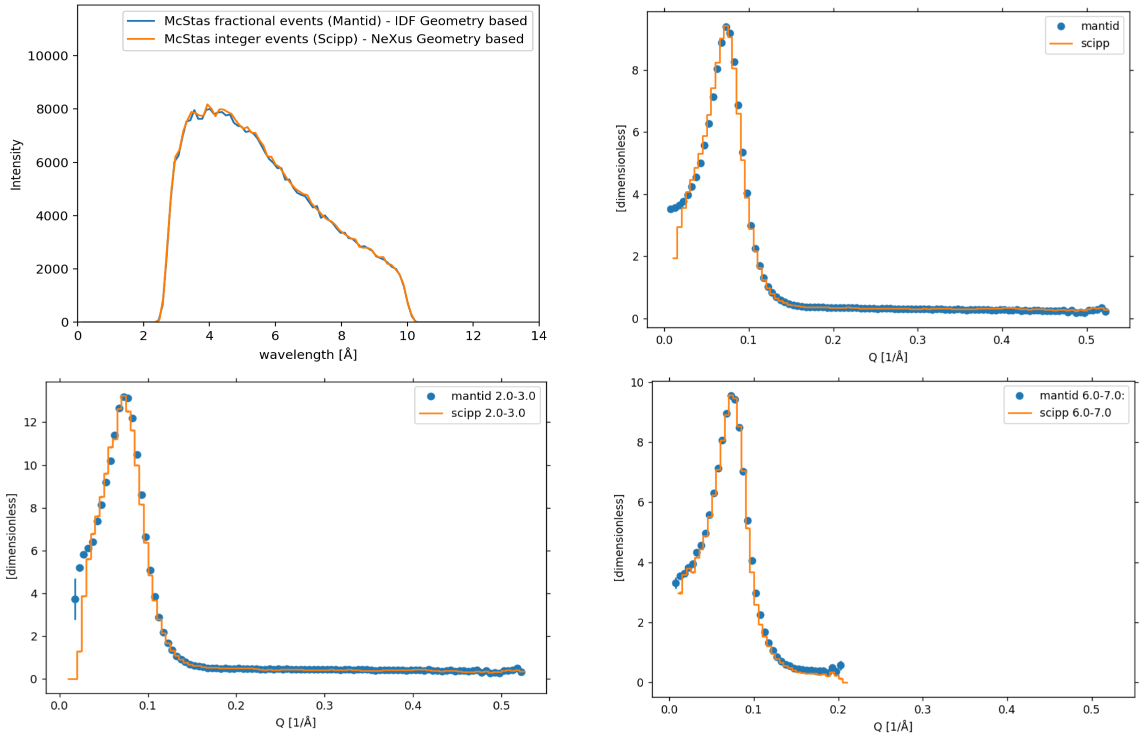

Figure 4. Top-left panel presents results from TOF to λ conversion of McStas data for LoKI beamline using scipp and Mantid script. Remaining panels presents reduction of SANS2D experimental data using scipp and Mantid workbench for full range (top-right) and wavelength bands (bottom panels).

The source of these differences is currently being investigated both on the scipp and Mantid side, and - even though it is a rather slow process - it helps to better understand the effect of different parameters to the reduction process.

Jupyter-notebook is recommended for running scipp as a user. However, it has also been recognized that it typically requires certain knowledge of Python code and questions have been raised whether it can provide adequate interfaces for performing tasks during hot commissioning and user operation. Late August, DMSC held a workshop that gathered instrument scientists, instrument data scientists and scipp developers to discuss GUI interfaces and to give the developers the opportunity to demonstrate different approaches to (graphical) user interfaces based on jupyter-notebook. These potential approaches start from pure jupyter-notebook, notebook with graphical widgets (scipp-widgets) and a web browser based addon to notebooks (voila package) as illustrated in Figure 5.

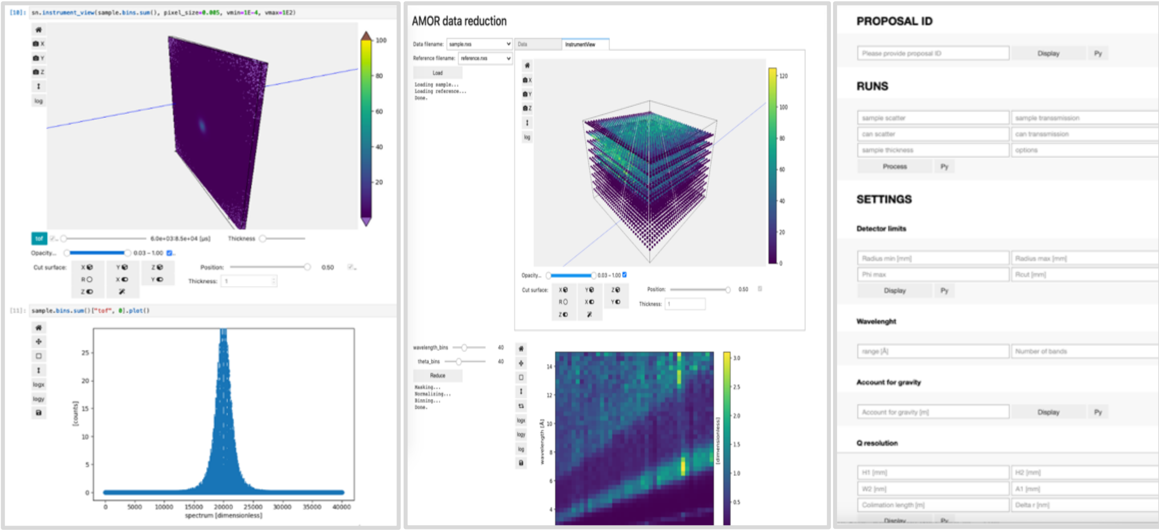

Figure 5. Different approaches for user interfaces based on jupyter-notebooks. Left panel - pure notebook with native plotting from scipp, middle panel - voila interface to data reduction notebook for AMOR instrument at PSI, right panel - scipp widgets input fields for SANS interface.

The feedback from the workshop has been collected and used to develop a strategy for developing GUIs.

Data analysis

ESS continues to be involved in developing, maintaining and managing SasView. In the last half year the SasView community held two hackathons (on-line code camps). The first one was focused primarily on functionality and the other on computational infrastructure. SasView 5.0.4 was released in April 2021 and apart from various bug fixes provides new functionality such as slicers, slider bars on plots for selecting the q-range for fitting, and improved manipulation with loaded datasets. The current efforts are devoted to next release, which among other improvements will feature a refactored generic scattering calculator accounting for magnetic contribution (Fig. 6). This work has been primarily done by Robert Bourne (summer student at STFC) and from the feedback received from magnetic SANS expert users is an important contribution to the field. This functionality will be particularly useful for the magnetic experiments on the SKADI instrument.

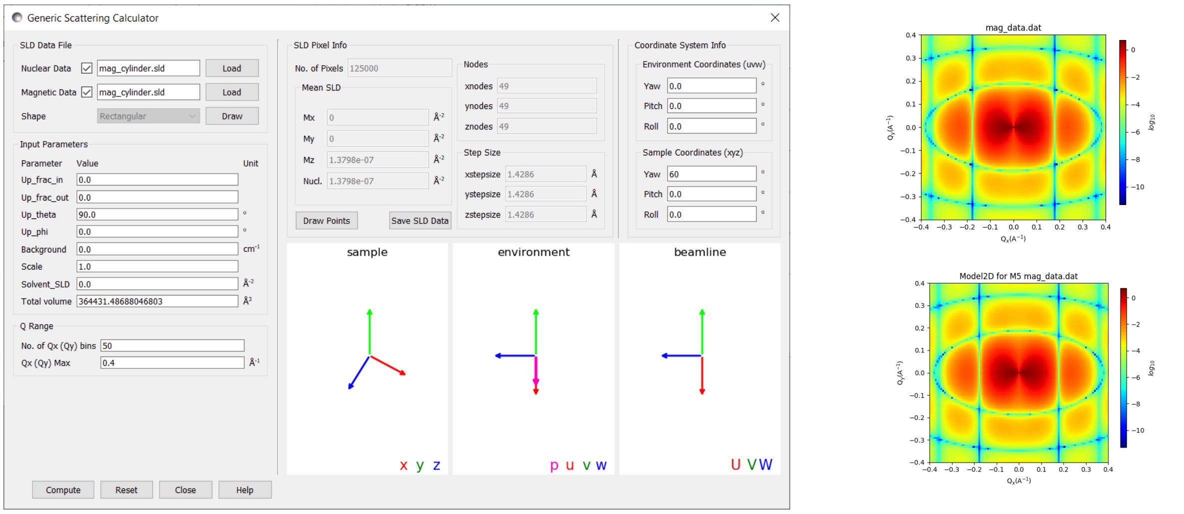

Figure 6. Result for calculating scattering pattern from magnetic cylinder obtained using Generic Scattering Calculator from SasView.

Correct description of TOF resolution function is important for proper treatment of SANS data at ESS. At the dedicated CanSAS meeting (organized by Judith Houston, Wojciech Potrzebowski and Andrew Jackson) a few action items were identified. One of these involves implementing resolution functions in SasView. However, this requires some resources that are currently limited within the SasView developer team, as developers to large extent focus on fixing “bugs” and maintaining infrastructure. This, and the fact that SasView has also been receiving more attention from universities and other facilities, triggered discussion within SasView management team about managing such sub-projects. Short and long term solutions have been investigated.