Reflectometry STAP Report: Software

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Since the previous STAP, Andrew McCluskey has taken up the role of Instrument Data Scientist (IDS) for ESTIA. This role aims to liaise between the DMSC and the instrument teams to ensure that reflectometry data processing, reduction and analysis (the entire data workflow) at ESS is successful and accurate. Andrew will work closely with the software teams at DMSC and the instrument teams from ESTIA and to some extent also FREIA.

I. DATA REDUCTION AND CONTROLS UPDATE

The AMOR instrument at the SINQ neutron source is being used as a model for the ESTIA design and has recently been equipped with a double Selene guide system similar to that planned for ESTIA. The similarity between the instruments makes AMOR a useful test environment for a range of ESS technologies, recently this has included the prototype multi-blade detector (Figure 1) that will be used for both ESTIA and FREIA and associated data infrastructure. Therefore, in collaboration with the scientists at AMOR, it was determined that this instrument offers a useful opportunity to test the components ESS-DMSC data stack.

To this aim, the IDS has begun to collaborate with the AMOR team and the `scipp` development team to implement a `scipp`-based live data reduction workflow. This included capturing data as it is collected, and presenting it, in a reduced form to the user during data collection. The code associated with this is currently in the testing and development phase and is written flexibly so that it is easily adaptable for use at both ESTIA and FREIA, as well as AMOR.

Following testing of the data reduction package at the DMSC infrastructure, the workflow will be deployed at AMOR before summer 2021. This will allow for the successes and failures of this project to be discussed at the late 2021 STAP meeting. Furthermore, a detailed document describing the physics of the reduction processes being used and detailed documentation to accompany the code will be made available to the STAP at that time.

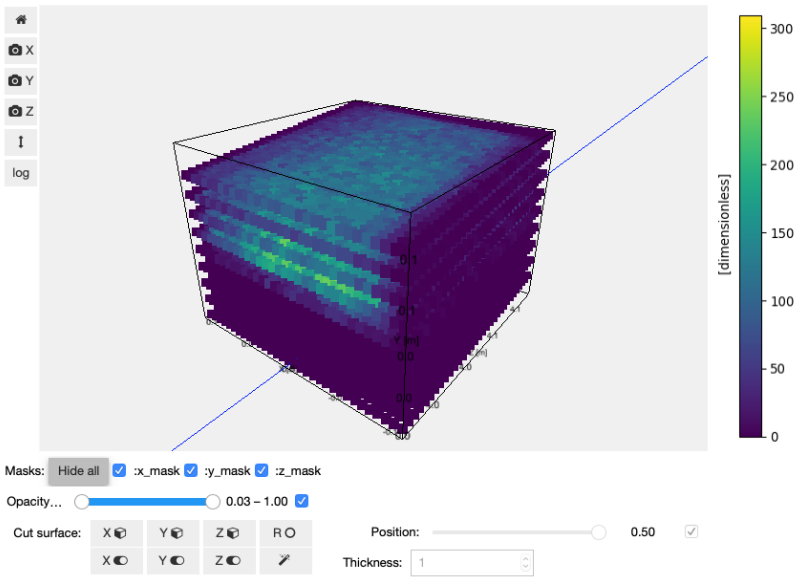

FIG. 1. The `instrument_view` of the multi-blade detector installed at AMOR, during data collection from a multi-layer battery material.

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The instrument control software that will be used throughout the ESS project is NICOS, overseen by the Experiment Control and Data Curation (ECDC) group. This is the same as the control software currently in place at the AMOR instrument. Therefore, the experience of the AMOR project discussed above will be used to inform instrument control and feedback from reduction.

The WFM test experiment paper was published in December [1]. Since this experiment, work has continued on WFM data reduction, primarily focusing on the first-8 instruments (of which ODIN and DREAM will utilise WFM), with a number of other publications in preparation.

II. REPLY TO THE PREVIOUS STAP REPORT

A. DMSC communication

It is important that timely and accurate information regarding instrumentation details is communicated and this ownership of this falls to the IDS. In reference to the specific points raised:

- *Details about detector signals*: The detector signals (as in the event formation units) will be general across all instruments (and therefore outside of the purview of the IDS). However, the specifics of the data that is received by `scipp` will be instrument-specific and for reflectometry is closely linked to the reduction project at AMOR that is discussed above.
- *Control of and data acquisition from sample environments*: The ECDC group is in close interaction with the sample environment group, to ensure that sample environments can be controlled and data obtained with them stored.
- *Expectations for GUI's and scripting for experiment control*: The NICOS interface means that some scripting will be necessary for experiment control. However, the ECDC group will work closely with the instrument teams to ensure this is as user-friendly as possible.

To ensure close communication between the DMSC and the instrument teams, Andrew has biweekly meetings with Tom Arnold (as the instrument class coordinator) and regularly as necessary with the teams from ESTIA and AMOR (in particular, related to the reduction project discussed above). In 2022, when the ESTIA project moves to ESS-Lund, Andrew will regularly visit Lund and work closely with Alessandra Luchini during installation and commissioning.

B. `scipp` position paper

The comments from the STAP on the `scipp` position paper have been very useful in informing our approach to data reduction with `scipp`. In response to the particular points raised:

- *Will ESTIA be supported by scipp during ESTIA's hot commissioning phase?*: Yes, `scipp`-based reflectometry reduction is currently being prototyped at AMOR (see above), given the similarity of the two instruments similar code can be used at ESTIA.
- *Many reflectometry users feel more comfortable with a GUI, while others with scripts, e.g., Jupyter notebooks. The STAP believes an options for script-based, e.g., Jupyter notebooks, and GUI's are required for our community. Reflectometry should have representation at the '21 GUI strategy meeting.*: The DMSC is in the process of planning a GUI workshop focused on data reduction so that we can better understand the requirements of the user base. Robert Jacobs has agreed to participate in this workshop, which will take place in the summer.
- *An emerging interest is application of continuous wave techniques to reflectometry data acquired at a pulsed source. This interest requires a continuously variable instrument/detector geometry, e.g., movements of the goniometer and detector in small discrete steps numbering a few hundred during data acquisition, i.e., implement motor scans during data acquisition. Scipp should accommodate variable instrument/detector geometry during a measurement.*: The flexibility of `scipp` means that this can be accommodated (indeed, reflectometry reduction code in development is considerate of this), by methods such as event-filtering.
- *scipp should accommodate a wide variety of sample environment, which is often custom-built off-site or commercially purchased by the soft matter community*: `scipp` is not responsible for instrument control, however, it is important `scipp` is reactive to data that is tagged with sample environment metadata. This is an important consideration in the development of reflectometry reduction code.

- *A neutron event should include information about time of flight, position in the detector, and the states of all components of the instrument and ancillary (sample environment) equipment*: This is an important consideration, however, not strictly the remit of `scipp` which will reduce the data once measured. However, we are in close contact with the ECDC group to ensure that this data is captured and available to `scipp` as necessary.
- *Scipp should accommodate "kinetic" experiments which modulate sample environment at high frequencies, e.g., much greater than the neutron source frequency. This requires fast acting software to calculate the state of the sample environment and or instrument at the time when the detected neutron was at the sample or at special locations in the instrument, e.g., locations containing components which change state with time like spin flippers*: Again while this is important to consider, the main role of `scipp` is data reduction. The capture of information from aspects such as the sample environment is outside of the role of `scipp` and will be handled by the data acquisition / instrument control software based on NICOS/EPICS. However, as mentioned above the data that is available to `scipp` can then be processed with this information, using tools like event filtering.

C. ESS view on BornAgain

Before going on to address the specific comments regarding BornAgain, we will address the concern of the STAP regarding the vision for reflectometry data analysis at ESS and the role BornAgain will have in this.

> *The STAP is concerned about the future commitment of the ESS to implement and maintain the BornAgain platform. Our understanding is the in-kind contribution terminates in a year. If the contribution is not renewed, then what happens to the platform? The STAP recommends that a transition plan be developed now in the case the contribution is not continued. What is being transitioned, how will it be implemented and maintained? The STAP is not convinced there is strategic alignment of the ESS and JCNS-MLZ for realization of the BornAgain platform. We encourage all stakeholders to proactively develop and implement a vision for reflectometry data analysis at the ESS.*

This is very good advice. We have started to discuss the transition and ongoing maintenance of BornAgain and to develop a vision for reflectometry analysis software at ESS. One of the current main objectives is to develop a coherent plan for reflectometry analysis at ESS, and we will share this with the STAP at the late-2021 meeting. To the best of our knowledge the JCNS-MLZ is committed to the long-term maintenance of the BornAgain platform, and the IDS is now working closely with the BornAgain team, both to steer the development and to facilitate future co-development or transition to ESS by learning the framework in detail. This has included the development of a tutorial showing how Bayesian sampling can be achieved in BornAgain (available in `likelihood.pdf`), which is currently being integrated into the BornAgain webpages. Additionally, we are in close communication with ISIS regarding the formalisation of facility support for their RasCal project.

Now to address the specific comments regarding the BornAgain community:

- *The JCNS-MLZ team should lead the charge to engage the scattering science community on what the worthy goal should be and develop a strategic plan (a flow chart would be helpful) to achieve the goal:* The BornAgain development team agree on the "worthy goal" for BornAgain to support reflectometry, off-specular scattering and GISAS in a unified framework and on an absolute scale.
- *The JCNS-MLZ team is committed to develop a transparent architecture for the code to achieve the goal. This step should involve considerable engagement of the community and inclusion of a science expert in scattering theory on the JCNS-MLZ team:* The BornAgain team are working closely with the IDS to ensure the accuracy of the BornAgain package. Furthermore, as part of the work of ORSO the accuracy of BornAgain is now compared with other popular reflectometry analysis packages (`https://github.com/reflectivity/analysis/actions/runs/739426180`).
- *Develop a proactive plan to solicit community feedback, and to connect "the enabling capability" to the community who benefits from it, i.e., promote the tool. (An opportunity to engage the Open Reflectometry Standards Organization, ORSO?)*: The appointed IDS is a founding member of ORSO and is actively engaged with the BornAgain developers, offering usability improvements (such as tutorial notebooks) and by evangelising on the benefits of BornAgain within the reflectometry community.
- *Many neutron scattering experiments benefit from complementarity of X-ray scattering (e.g. L.J. Collins-McIntyre, et al., EPL 115, 27006 (2016) – https://iopscience.iop.org/article/10.1209/0295-5075/115/27006/meta. Embrace the X-ray community; leverage it to make a better and more widely used product.*: The role of BornAgain as a GISAXS analysis software will aid adoption in the X-ray reflectometry community. BornAgain includes support for X-ray reflectometry already.

- *The STAP had the impression that the JCNS-MLZ team did not understand that theory exists to calculate S(Q) self-consistently (e.g., without fitted scale factors for specular vs. off-specular scattering) (It should be noted that we were running late and Wuttke had another meeting, so he was not in a position to offer clarity.) Our primary concern is that fundamentally the scattering calculations must be done correctly before attention is focused on user interfaces (we acknowledge the user interface is important). Thus, we recommend hiring a scattering science expert to work with the computer scientists. We further recommend world-experts such as S. Sinha, V. Holy, M.K. Sanyal, M. Tolan. . . , review the evolving BornAgain platform.*: Joachim has investigated this and asked for the included document (`IntensityScale.pdf`) to be shared with the STAP to confirm the handling of this within BornAgain. Moreover, as mentioned previously there is close interaction between the IDS and the BornAgain developers.

- *We acknowledge that details of an instrument will influence the calculation, yet these details can be posited and incorporated into the code now as opposed to waiting until an instrument is built. In fact, this step may also be instructive to the instrument team in order to anticipate problems or to optimize measurement protocols prior to commissioning.*: The AMOR project (discussed above) will provide substantial opportunity to investigate the integration of instrumental factors into the analysis process. Additionally, this will become a priority for the ESTIA instrument during the installation/cold commissioning phase in preparation for hot commissioning/validation.

III. BORNAGAIN UPDATE

The following update is taken from communication with Joachim Wuttke. The basic update for BornAgain progress is as follows:

- Unexpected departure of a long-standing developer, Gennady Pospelov.
- Departure of physicist Randolf Beerwerth.
- New team members starting in April and May.
- Version 1.19 is released. It brought many bug fixes, simplified and unified Python examples, and a new, versatile importer for reflectometry data.
- Current focus is on internal consolidation. This will also help new developers to familiarize themselves with the codebase.

Further to this, the following goals have been outlines for the next six months (this final under ESS in-kind support):

- Fitting
  - Translate differential evolution code from SciPy to an independent C++ library
  - Provide Python scripting example for simultaneous fit of several data sets
  - Provide Python scripting example for data scaling
  - Provide Python scripting example for visualizing likelihood vs parameter
- SLDs from materials library
  - Rewrite library xsection
  - SLD from chemical formula and density
  - SLD from molar SLD and molar volume
  - wavelength-dependent SLD and absorption
- Sample models:
  - Support repeating multilayers
  - Extend GUI layer editor
  - Rewrite parameter distribution handling

[1] O. Löhmann, L. Silvi, P. M. Kadletz, N. Vaytet, O. Arnold, M. D. Jones, J. Nilsson, M. Hart, T. Richter, R. v. Klitzing, A. J. Jackson, T. Arnold, and R. Woracek, Wavelength frame multiplication for reflectometry at long-pulse neutron sources, Review of Scientific Instruments **91**, 125111 (2020).