

DMSC STAP

Report of the ESS DMSC Science and Technical Advisory Panel (Draft)

28 October 2024 - remote

STAP Members Participating: Stuart Campbell (BNL), Garrett Granroth (ORNL), Toby Perring (Chair - STFC), Andrew Richards (Imperial College London), Anna Sokolova (ANSTO). Apologies: Paolo Mutti (ILL).

Report

The meeting was only scheduled as a short Zoom meeting, as the on-site long meetings of the DMSC STAP are scheduled for the April round of STAP meetings.

Demonstrations of extent of readiness for hot commissioning from instruments

At the previous (in-person) meeting, the STAP emphasised the importance of demonstrated readiness in advance of beam-on-target and hot commissioning, which is expected in late 2025. Consequently, the entire meeting was devoted to presentations by the Instrument Data Scientists (IDSs) of the data collection and reduction of the Tranche-1 instruments (DREAM, LOKI, ODIN, BIFROST and NMX) and ESTIA, largely as real-time demonstrations. Typically, these included:

- proposal creation and coupled data location created on the data server for the particular 'experiment';
- opening of a VISA session (virtual machine for a particular user on the compute server).
- Jupyter notebooks used to perform data reduction.
- running analysis codes (such as SASview for SANS, MuhRec to produce tomograms, EasyDiffraction for powder diffraction analysis).

The STAP was impressed by these demonstrations, and they gave confidence in the good state of approaching readiness for beam on target (BOT). The STAP wants to congratulate the DMSC staff for all their work. The demonstrations collectively exercised most of the components of end-to-end requirements for instrument operation and data collection and reduction. To pick one example, we had a real-time demonstration of controlling the YMIR test station (set up to perform tomography using light) using NICOS for instrument control, then collecting transmission data from multiple orientations of a test sample, building a tomogram using the MuhRec software, and real-time slicing-and-dicing of the image data that had just been collected. We also wish especially to remark on the presentation of LOKI by Oliver Hammond, appointed IDS for IDS only a few weeks previously but was already very much on top of the job, and Celine Durniak, IDS for DREAM, who was unable to be

present but had nevertheless followed the spirit of the STAP request by making a video recording of her live demonstration for us to see at the meeting.

As the DMSC STAP meeting was scheduled as a half-day on-line meeting only, time constraints prevented the truly deep-dives into each of the instruments that the DMSC would have really liked in order to give detailed technical advice, and there are areas that are not yet ready on any one instrument e.g. integration with SciCat for LOKI, and calibration and commissioning scripts are a work in progress on ODIN. The STAP looks forward to updated end-to-end demonstrations with time for deep dives in the longer in-person STAP meeting scheduled in April 2025. This particularly applies to NMX and ESTIA, as the STAP meeting was running out of time, and we could have only short slide presentations with no real-time demonstrations from those instruments.

Interaction with instrument teams

The interaction between IDSs and instrument teams seems to have significantly improved over the past few STAPs. For example, the Spectroscopy division is trying out workflows with their IDS. However, we would like to emphasise that while currently the instrument teams will be rightly occupied with the hardware installation and cold commissioning of their instruments, it is essential that they are fully fluent with the data visualisation and reduction framework, scipp, so they can work alongside the IDSs in the hot commissioning of their instruments. The STAP suggests Python and scipp training for all instrument team members, and interactive working with the IDSs at monthly intervals (not the three-monthly intervals suggested during the STAP meeting). It is essential that there is close engagement during the planning and creation of applications and scripts for interpreting commissioning data, so that only the 'unknown unknowns' are a surprise when neutrons arrive. Accordingly, at the next STAP meeting, the STAP would like to have a report on the status of readiness of commissioning and calibration scripts for each of the Tranche-1 instruments.

Holistic analysis of bottlenecks

At the next STAP we would like to see an analysis of other bottlenecks in the end-to-end data flow. For example, the VISA system: it is one thing to see isolated instrument demonstrations, but another to have an analysis of stress-testing the compute cluster with all instruments operating.

Data centre server room in Denmark: Moving the DMSC server room to a new location remains a high priority. While the DMSC office has been relocated to DTU (c. 15 km north of central Copenhagen) since March 2024, the servers remain in their original central Copenhagen location, where the lease has been extended to the end of 2026. However, relocation well before then is essential, otherwise the move will be close to coinciding with the start of user science – with the corresponding reputational risk with the community if there are problems.

DTU is developing a proposal for relocation at the campus in mid-2026. There is still a lack of a proposal for a location at the Lund site. The current risk has now been classified by the

ESS/DMSC as 'medium' rather than 'high' (as at the previous STAP). However, the current plan is for there to be just a one-week data buffer on the Lund site, and at that on servers in a temporary location. The risk mitigation therefore appears fragile.

Detectors: The STAP was pleased to have the presentation about detectors as part of the common STAP meeting. What would be useful in the April 2025 DMSC STAP is to have status reports of the detectors and their integration into the data acquisition for each of the specific instruments in Tranche-1 and ESTIA. As part of assessing the end-to-end readiness for hot commissioning this will be important for the STAP.