SANS STAP
ESS, Lund
25-26 September 2019

SANS STAP members present: Anna Sokolova (ANSTO), Jonathan White (PSI), Daniel Clemens (HZB), Joao Cabral (Imperial College), William Heller (ORNL)
Chair: Charles Dewhurst (ILL)

Instrument teams: Loki, Skadi
Others: Reflectometry STAP members, ESS Staff

Meeting format:

- The autumn 2019 SANS STAP was held over 2 days and in person with all STAP members able to attend. This follows the spring 2019 meeting by video.
- Reflectometry (24-25 Sept.) and SANS (25-26 Sept.) STAPs were intentionally held at overlapping times and benefitted from some joint sessions including a general overview 'ESS Update' (K. Andersen) and 'Status and DMSC – SANS & Reflectometry' (J. Taylor). Other than these general update presentations there was little or no scientific or technical overlap or discussions between the SANS & Reflectometry STAPs. It could have been interesting to have more overlap and joint discussions.
- Brief but sufficient update reports were provided by the Loki and Skadi teams providing elements such as the status of design works, purchasing and critical technological tests and developments, e.g. detectors.
- The proposed move to arrange STAPs to be held directly before the SAC, with participation in the SAC by the STAP chair, is seen to be very positive and generally more useful.

General comments:

- It remains interesting and useful for the STAP to follow the ESS SANS instrument projects. That said, the STAP generally felt that there remain few technical or instrumentation issues that require their consideration. This is a good thing. The Loki and Skadi instruments are in different stages of advancement but all major technical choices have been made and the instrument projects are advancing well into their design and construction phases.
- The STAP would welcome more details on sample environments, data analysis and treatment next time.
- An 'ESS update' is always useful and well received. STAP members are not able to follow closely progress at ESS so a general update is always welcome. This kind of progress update is useful and tends to end up disseminated to the wider neutron community.

- The ESS project appears to be progressing well, 60% complete and 2019 representing a peak in construction activity. Accelerator commissioning underway, first instrument hall delivered, target installation underway and no major technical issues. The working hypothesis remains first beam on target and first instrument(s) commissioning in 2022 and ability to deliver some since in 2023. By the end of 2025 all 15 instruments should be commissioned.
- A 'DMSC update' is also well received and of general interest in terms of both preparation of readiness of the ESS suite of instruments but also in terms of common or similar software developments being carried out at other facilities.
- Instruments are foreseen to be staffed by 2 instrument scientist and 1 data scientist / 2 instruments. This corresponds to a healthy 2.5 people / instrument available for local contacting and importantly 0.5 people / instrument engaged directly in software for data treatment and analysis. This instrument-software-scientist model, i.e. a scientist with software interest and expertise working directly with the instruments, doing science but with software responsibilities, is generally seen by the STAP to be very positive and efficient model. Will it be a difficulty if data scientists are to report to two difference bosses (science division & scientific computing division)?
- The STAP are impressed by the work being carried out by DMSC and as to the future of online data visualisation, access to scientific data and efficient extraction of parameters in real time to drive experiments, e.g. the link between instrument control, Mantid and SAS view. If coupled with early science could be very impressive and be a unique selling point of a modern and powerful instrument suite. The DMSC are to be commended for developing such advanced tools and are 'ahead of their game'. However, online visualisation and advanced data tools already exist at many synchrotrons. The question was posed as to why it hasn't already appeared at existing neutron sources? Is it simply a question of resources allocated to scientific computing?
- Data reduction tools are critical for early scientific success of ESS and needs to be sorted out - it looks like this is being taken care of. Where do they expect to be with the level of data reduction on day one – how perfect do they expect to be? This should be thought about.

Early science:

A strategy for achieving early scientific success at ESS is being developed. It will be a crucial role of the instrument science teams to foster collaborations and bring users to ESS. This will be an extremely challenging and heavy load on the instrument scientists. That said, it should be recognised that instrument scientists cannot control when a user will deliver great science. This means that even in 'fishing' for high profile scientists, the instrument scientists and ESS are at their mercy to a large extent. Relationships need to be established now, doing experiments and collaboration elsewhere before bringing them to ESS. Thought

needs to be given as to what are the grand scientific challenges. It was noted that growing a new user community at a new facility such as ESS will be very difficult compared to growing a community around new capabilities at existing neutron sources. ORNL experienced this when they built SANS instruments having no existing user community. It's hard to convince established users from elsewhere to be patient with new instruments and facilities.

- Performance indicators shown for Loki and Skadi estimate neutron fluxes for the both instruments will be ~5x D22 (ILL) and 20 x SANS2D (ISIS). This is a significant gain in intensity over ISIS and 'incrementally transformative' over ILL for SANS. The intensity will, never the less, be impressive and when combined with the wide dynamic q-range offered by TOF and large detector area coverage should enable new science.
- Background calculations: It was noted that instrument background is a critical parameter in determining instrument performance. Shielding for radiological protection has been calculated but calculations for instrument background (difficult) have not been calculated yet but are in progress.
- The first ESS users need to go away with successful experiments and a highly positive impression of instrument performance and capabilities. If this is got wrong it is a sure-fire way for users not to return to ESS. Instead they will continue doing what they usually do and using neutrons at their favourite source. It is critical that instruments, sample environment and data treatment are fully commissioned and optimised before exposure to users.
- An expectation for a 'first scientific milestone' might be can we trust the instruments, calibration, standards and correctness
- There was much discussion on:
    - Early publishable experiments beyond calibration and testing. Part of hot commissioning process.
    - End 2023, start real user programme. Start with people who know the techniques. Not new users. A graded approach to increase to full user programme.
    - How to open the user programme. Call and selection of proposals.
    - How to engage early users.
    - Use the local science community to engage with commissioning experiments.
    - Need collaborative groups to do new 'fancy science' resulting in publications and press releases.
    - Focus on things that are scientifically interesting but not necessarily technically challenging. Fancy science is not always dependent on fancy sample environments.
    - Complimentary experiments e.g. x-ray (MaxIV next door) very important. Much more stimulus with MaxIV e.g. Joint beam time proposals for SAXS & SANS.
    - Early science cases need to feed requirements in to software for data treatment and analysis.
- ESS has begun a series of science colloquia with Max IV.

- ESS instrument teams are working on a series of detailed instrument papers describing the instruments being built and their expected performance. A single big paper described the entire instrument suite is in advanced stages of preparation and publication in Nuc. Inst. Meth. A.

Instruments:

The Loki and Skadi instrument projects are both showing excellent progress, detailed design work and readiness for tender, purchasing and fabrication of major components. Both instrument teams should be congratulated.

Loki:

The Loki project has entered procurement of major components and is (intentionally) in an advanced stage of the project being one of the first 3 instruments to come on line at ESS. Designs are almost finished and all major technological choices made. The instrument project is in excellent shape.

There has been excellent progress and technological tests, experiments and understanding the response of the complex boron-tube detector assemblies. This has been extremely well appreciated and should continue. The detector performance appears to be excellent, although complicated. With time, effort and understating this should be ok and ultimately an excellent detector solution.

- The time schedule for the project needs to be respected and kept under control - in the hands of the in-kind partner, ISIS.
- While individual components are inspected / tested for compliance, time and testing will be required integrated into a system.
- Purchasing / fabrication. Much of the instrument to be built by AVS (Spain) (Collimation and detector vessel). These components have been ordered with detailed designs made by AVS. Design reviews to come.
- Detector system in advanced conceptual design. Pre-amplifiers will be at the detector with the main electronics outside of the detector tank. Many cables coming out.

Skadi:

The Skadi instrument project is also progressing well. The conceptual design and technological choices have all been made. The Skadi project is ready to launch calls for tender for many of the main components. This is on hold at the present time awaiting the TA (technical annex), i.e. technical documents relating to a call for tender have been approved but finances have not yet been approved (ESS/Germany/France). During this effective 'pause' of the instrument project the STAP urge that the Skadi team are kept together and fear that key people might be moved to other projects. It is critical that the project does not lose momentum.

The SONDE detector technology for Skadi looks highly impressive in terms of efficiency, count rate, resolution and modularity. The EU funded SONDE project itself is considered to be a success. The STAP urge thorough testing of the SONDE detector concept and not only the testing of individual modules but aslo assemblies of modules to form a large area detector. In this way various aspects of the detector bank can be understood such as parallax effects but also issues such as detector cooling. Individual detector modules generate ~7W of heat while a full detector bank is estimate to generate ~ 1.5kW of heat. The STAP are concerned about the cooling requirements for this detector and urge urgent and convincing calculations and prototype tests of the proposed air-cooling system. The 'donut' vacuum detector cover between the inside air-pressure detector chamber and the detector tank vacuum is also of concern in terms of the real-world stresses the cover has to withstand and also in terms of maintenance aspects of removing the cover for detector module repair.

The VSANS option (qmin < 1e-4 Angs-1) for Skadi was discussed and its development and approach seems reasonable allowing large samples of up to 30 x 30 mm. At the STAP's request the suitability of Skadi for GISANS measurements has been considered. The detector geometries (front detector central aperture) allow specularly reflected incident beams up to 0.4 degrees. This seems reasonable to allow for GISANS measurements on Skadi.