ESS Diffraction STAP - Questions for 24th April 2020 Meeting

ESS presentation (Andrew Jackson)

Welcome to Andrew Jackson.

Re-organisation, common projects, construction noted.

What is latest ESS timeline? (we usually have it included in the ESS presentation)

- The baseline schedule has not changed. We are working to a June 2022 Beam-on-target date. I will add the latest master schedule to my presentation.

What are expected Covid delays to milestone dates like SOUP?

- We are just now starting the exercise to develop a new baseline schedule, taking into account both existing project delays and also the additional ones from COVID. The SAC, PAC and Council will all consider these questions and we expect a formal change to the project schedule by the end of this year. In the instruments' case, we are concerned that such delays will put pressure on the time available for hot commissioning. It is already rather short given the tandem commissioning of the source and instruments, so any thoughts from the STAP on this question would be appreciated.

DREAM

What are current and expected future Covid delays? Any critical aspects? Will these affect instrument start date?

Congratulations to Mikhail on ESS staff position from mid-2021 – any effects on DREAM plans?

TG3 in 12/20 on track? Many packages to be checked that month!

20-sample cryofurnace looks a great development but ambitious/expensive? What are min/max T?

Collimator progress? Will it be needed for above cryofurnace?

Simulations of detectors are useful but how about real testing on neutron beams, as raised in the last STAP report? Not much time before detector procurement in Q3 2020. Lack of detector testing is potentially a serious risk for the whole Diffraction suite.

Please elaborate on the chopper installation / bunker problem – speeding up manufacturing by the Jülich chopper group by four months may be over-ambitious. If parts have to be installed after bunker is closed, does this delay SOUP? What would be the impact if accessing bunkers after closure is not possible?

External funding for SANS detector is welcome but will there be time and resources to develop this in parallel with the main instrument programme? 'simultaneous PDF and polarized SANS' is rather far from the principal high resolution PND focus of DREAM, and potentially overlaps with HEIMDAL case.

MAGIC

What are current and expected future Covid delays? Any critical aspects? Will these affect 2023 instrument start date(s)?

Good that VAT arrangements with PSI sorted.

ICEB meetings are a positive development. (Would they like a STAP representative?)

As for DREAM, is neutron-testing of detector elements a critical task?

Consequences of guide redesign on instrument performance? Does this affect 10/19 proposed increase of bender field? Is it complex and risky to spread the guide manufacture over 4 different lots and tenders?

What is the currently foreseen timeline on building the xyz setup? Is it too complex with 3 different labs involved?

HEIMDAL

What are current and expected future Covid delays? Any critical aspects? Will these affect instrument start date?

TA's 'In Review' (as shown in table) or fully approved?

Progress on costings for Change of Scope request? And related neutronics calculations, NBOA, cold guide and shielding? Too many changes? By what date will the change of scope request have to be submitted to still be meaningful? Are the preparations on track for this?

Same detector testing questions as for DREAM and MAGIC.

ESS Polarisation

Welcome to Hal Lee.

Thank you. Glad to join the ESS at this exciting time.

"It is planned that the work package will be funded …" What does this mean – is there a concrete, agreed-upon budget?

The work package is being developed in the next 6 months. A concrete, detail budget will be determined in this process. We will go for approval of the work package in October/November (after the Polarisation Workshop on 21-22 September). At that point, a concrete, agreed-upon budget and schedule will be set.

Is polarisation a high priority for non-dedicated instruments? Data collection/analysis, support facilities, sample environments etc. are likely to be more important to early users of many instruments e.g. DREAM.

During the scope setting of the respective instruments, ESS explicitly considered a centralised project and removed scope, which could be centralised, from the individual instrument construction project. The effective transfer of polarisation into a centralised project ensures polarisation remains a high priority and proceeds in a coordinated manner, while at the same time allowing instrument teams to focus on the neutronics performance and the associated data processing, sample environment in conjunction with the SE group and related infrastructure for operation.

The selection of instruments into the polarisation work package came from discussions with the 15 approved instrument's teams on the benefit and plusibility of having polarisation capability. The need to start proceeding with the polarisation upgrade project in parallel and separately came from experiences and feedbacks from facilities worldwide. The administrative design to carry out the project separately with no change to any instrument scopes is to ensure the instrument teams stay focused on their respective current scopes.

We have been very careful in devising the polarisation upgrade process to prevent diverting the focus of any instrument teams including DREAM team from their current scopes: (1) a separate Centralised Polarisation Support has been established in the Neutron Technologies Division to plan and carry out the polarisation upgrade; (2) no change to any current instrument scopes. Note that other than MAGiC and ESTIA, instruments do not have polarisation in their respective current scopes; (3) we emphasise coordinating with instrument teams to ensure minimum impact on the instrument design and construction processes while ensuring a seamless upgrade process and a smooth future operation.

With these measures in place, we are confident that polarisation upgrade will be carried out in a timely manner while having no impact on current instrument schedule.

Would it be better/more cost effective to ensure that MAGIC and ESTIA work well as polarised instruments from Day 1, with developments on other instruments deprioritised?

From my detailed discussions with the MAGiC and ESTIA teams about the polarisation setup, I have complete confidence in their ability and in-scope resources to fully construct their respective instruments to be the best-in-performance among their peers. It would add no benefit

to either MAGiC or ESTIA by deprioritising polarisation development on other instruments, especially in light of the arrangement that polarisation upgrade runs separately from any instrument scope.

On the other hand, the need to proceed with the upgrade project now has come from experiences and feedbacks from facilities worldwide: Once an instrument enters the user programme, the process to upgrade for polarisation would require unacceptable disruptions and risk to the user programme. As a consequence, taking a delayed polarisation upgrade path is the main reason for many lost opportunities. In fact, a delayed upgrade is only possible when an instrument has been operating for about 10 years. Retrofitting, even when an instrument had initially put in best-effort measures for later upgrade, has proven to be more costly and often has to make more compromises in performance and useability.

We recognise that Europe has a large and active polarised neutron user community and a long and fruitful tradition of polarised neutron instrumentation. If the ESS were to follow an delayed upgrade process that has been proven to be ineffective and that results in years of inadequate polarised neutron capability at the ESS, the user community will not be well-served and damage to its scientific reputation will be profound and prolonged.

For polarisation to succeed at the ESS, we have taken the crucial step of proceeding with the upgrade project now while carefully devising the process to be carried out separately, to ensure instrument teams staying focused on their respective current scopes so that there is no impact on any instrument schedule.

DMSC

Focus on DREAM and ODIN data treatment noted positively.

How does development of EasyDiffraction relate to and interface with existing diffraction analysis software such as JANA, GSAS and Fullprof that users will wish to use?

How are ESS developments of Fullprof progressing?

Until now easyDiffraction has only been interfaced to CrysPy (from LLB), the main reasons being that it is a Python library and that we have good connections to the developer behind (and the MAGIC team). Moreover, CrysPy has functionality needed for MAGIC (e.g. local susceptibility approach for 1d and 2d data) that are not available from FullProf. The next library to interface will be CrysFML, which is the library underpinning FullProf. CrysFML is open source, whereas FullProf is not. ILL is currently working on Python bindings for CrysFML and it is the outcome from that development we will use for easyDiffraction. It is the aim that any library interfaced to easyDiffraction will be accessible from a unified Python scripting interface (incl. Jupyter notebooks) and from GUI.

We will ensure that appropriate line profiles for the ESS instruments are implemented in CrysFML and hence FullProf. Thus, users will be able to use CrysFML from both easyDiffraction and FullProf and CrysPy from easyDiffraction.

Other libraries / software can be interfaced, e.g. GSAS-II, Jana, CCTBX and diffpy. We would like to interface those and specifically consider GSAS-II as a good test case for testing the suitability of easyDiffraction to interface to other libraries. However, at this point in time we do not have concrete plans to do so, and these tasks will have to be prioritized against other tasks in the future. We also hope that other will take on the tasks of interfacing other libraries and would be happy to support such external contributions. Even if GSAS-II and Jana2006 (and FullProf/CrysFML for that matter) are not interfaced to easyDiffraction and the associated Python interface, we intend to make them available as is for users on the ESS remote analysis service and reach out to the developers of those packages and encourage them to implement ESS specific functionality (e.g. line profiles). This is also our current thinking for Maud that is critical for engineering diffraction.

Apart from ensuring that appropriate line profiles are available in CrysFML, we (ESS) are not planning to do development of CrysFML /FullProf. We focus on the interfaces, whereas ILL focuses on the fundamentals of CrysFML and FullProf. For instance, CrysFML has been put under version control on GitLab as part of this work.

SAD

Good 8T magnet (MAGIC) progress noted.

A: Thank You!

Plan B for DREAM 20-sample cryofurnace?

A: Indeed the specs in the recent CTV for the cryofurnace are worth asking for but quite technically ambitious. If we don't get a satisfactory result for the tender it is worth thinking about a plan b, which could either be something much simpler or scaling back a just bit in ambition. Which one is best depends on the results of the tender, but it might be worth sketching out a simple solution that would work for first science. The latter could start using a standard wet (orange) cryostat and an (ILL-type) furnace noting that both systems are already part of the SE priorities for DREAM.

PE cells <4K, ease of changing P,T?

A: We are currently pursuing a high-performance CCR-based cryostat based on the ILL design which indeed would limit the base temperature to T>5K, these should reduce cooldown time from 7 hours to 4 hours. Pressure and temperature can be changed fully remotely, however, experience shows cold compression introduces high strain into sample. Correspondingly, best diffraction data are achieved by warming/compressing/cooling routes. For lower temperature, we will have clamp and DAC-devices, that are compatible with standard cryostats. However, these will be limited in pressure due to lower force capability (to retain compatibility with ø50mm cryostat bore). We will also procure a gas loader suitable for both PE and DAC.