

DMSC STAP

Report of ESS DMSC *Science and Technical Advisory Panel*, December 2015

Meeting Dates: 7 and 8 December 2015, Copenhagen

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1. General Comments

Presentations about the work in the previous eight months indicated that good progress has been made in most areas. One overall measure has been the progress in hiring. Not only has the DMSC been able to recruit in most of the key areas, the quality of the new personnel is exceptional. Several issues, raised at the previous meeting, had been addressed (Report March 2015). Nevertheless, we highlight below some points that need further attention. Most of the current large challenges are recognised at the DMSC and we feel that they should be noted as part of the overall ESS project management – the DMSC will be crucial to the scientific operation and eventual success of ESS.

As an example of good progress, the Data Systems group has introduced excellent management of priorities. There would be a clear benefit from a similar system being used across the DMSC with appropriate tasks.

The establishment of a laboratory in Lund for tests of hardware and software will be very helpful. We look forward to hearing about tests from that system. They should also consider coupling the test station with a McStas simulation to get closer to a real day 1 instrument.

The DMSC has been making excellent progress in securing in-kind partners. The partnerships with STFC and PSI should meet much of the requirements. In order to secure the remainder of the in-kind contributions, the DMSC should consider novel collaborations that may involve partners contributing to new areas, and to creating work packages that span different tasks. Investigating these opportunities is important, as some obvious possible partners will have reached their limits of in-kind work.

There is generally a good awareness of risks but a common register of risks and sharing procedures for mitigation of the risks across different groups at ESS would be advantageous. In this respect, we recommend that there be liaison between the DMSC STAP and other relevant advisory panels. As a minimum sharing of reports would be helpful but meeting with some representatives of other groups would be beneficial and some particular cases are identified below.

2. Recommendations

Detectors - The DMSC needs a date for a definition of the interface for detectors. The alternative is that the DMSC should define an appropriate hardware and software but there are clear advantages for this to be done in connection with the detector and controls groups. As resources, provided by short term external funds are now available, it is particularly important that this activity does not suffer delays. Otherwise, these added personnel may no longer be available. We recommend that the present report be discussed by the STAP for detectors.

Data Policy - The DMSC STAP welcomes the policy document but identifies that there is an anomaly in requiring a proposal for access to archived data. A general trend that original data must be publicly accessible would not be met although such a procedure may be appropriate for use of computational resources or access to reduced data. Defining a licence agreement for re-use of publicly accessible data may be better. The concept of indefinite storage should be defined.

Project Management & Integration - DMSC is in a phase that development and production of software necessarily starts now but many other aspects of the instruments are not yet in production. It will be necessary to address the possibility that staff may be lost before commissioning. This concern relates particularly to staff engaged on externally funded projects or work made on time-limited in-kind contributions. Changes in schedule of other aspects of the ESS project need to be considered as regards their impact on the definition and delivery of appropriate software by the DMSC.

Instrument and scientific software requirements - There is a good initiative with a questionnaire to instrument groups. In order to create the best and modern analysis some focussed small workshops would be helpful and direct interactions with relevant visionary users would be advantageous. The mission of ESS is to be more than the source of neutrons and the delivery of science is key to success. This mission needs to be reiterated clearly in order to drive prioritisation and to create an appropriate budget. Plans, perhaps with external funding, to exploit fully event mode data acquisition in connection with models that include time as well as structure and dynamic behaviour of materials should be made.

User Office Software - This should exploit existing software and databases. It will probably be necessary to recruit a specialist in databases eventually. The scope of what can realistically be delivered needs to be defined. We do not recommend development of an entirely new system, for example using ERP, if that can be avoided.

3. Organisation of the work of the STAP

The STAP felt that it would be helpful to have focussed and concise presentations of ideas for future meetings. Circulation of short summaries with key issues before a meeting could give a more effective discussion. Information about revised staffing and work plans would be useful for the next meeting.

Liaison and information from other relevant STAP would be helpful. For example, we recommend that the present report is discussed by the Detector STAP and we welcome their feedback.

Appendix: Further Detailed Comments

During the course of the discussion at the STAP, there were some further comments relating to details that we note below:

- 1) The overall intensity on samples will vary on a pulse-by-pulse basis and the pulse shape may vary on a pulse-by-pulse basis. This may result either from how the proton beam is rastered across the target or from time dependent moderator effects. While this needs to be investigated further, the need for good beam line monitors is identified. From a software perspective, it may be useful to talk to the XFEL people as their incident beam profile varies considerably from pulse to pulse.
- 2) The instrument data group has a good handle on the SANS beam line. We expect that it will be ready for day 1 operation.
- 3) Good progress has been made on planning for the reflectometer. The test station is crucial for the design of systems for instruments with multiple motors.
- 4) As resources for software development are restricted and the requirements are demanding, work should be prioritised so that the instrument software with greatest impact on scientific output is completed and optimized first. Some instruments may need to rely on the instrument staff acting as the interface to the users during the years of initial start-up. For example, macromolecular crystallography cannot be supported to the same level as at synchrotron facilities where there are large co-operative activities and multiple beam lines.
- 5) Decisions will be needed concerning choices of analysis software that can be developed and supported, such as for powder diffraction (FullProf, GSAS, etc) and for reflectometry. Consultations with users and instrument scientists will be needed in these and other areas.
- 6) Epics V4 and 0MQ are the two possible platforms for streaming the data. Initial evaluation is going well and we look forward to a report on the choice.