EUROPEAN SPALLATION SOURCE

DMSC STAP SEPTEMBER 2018

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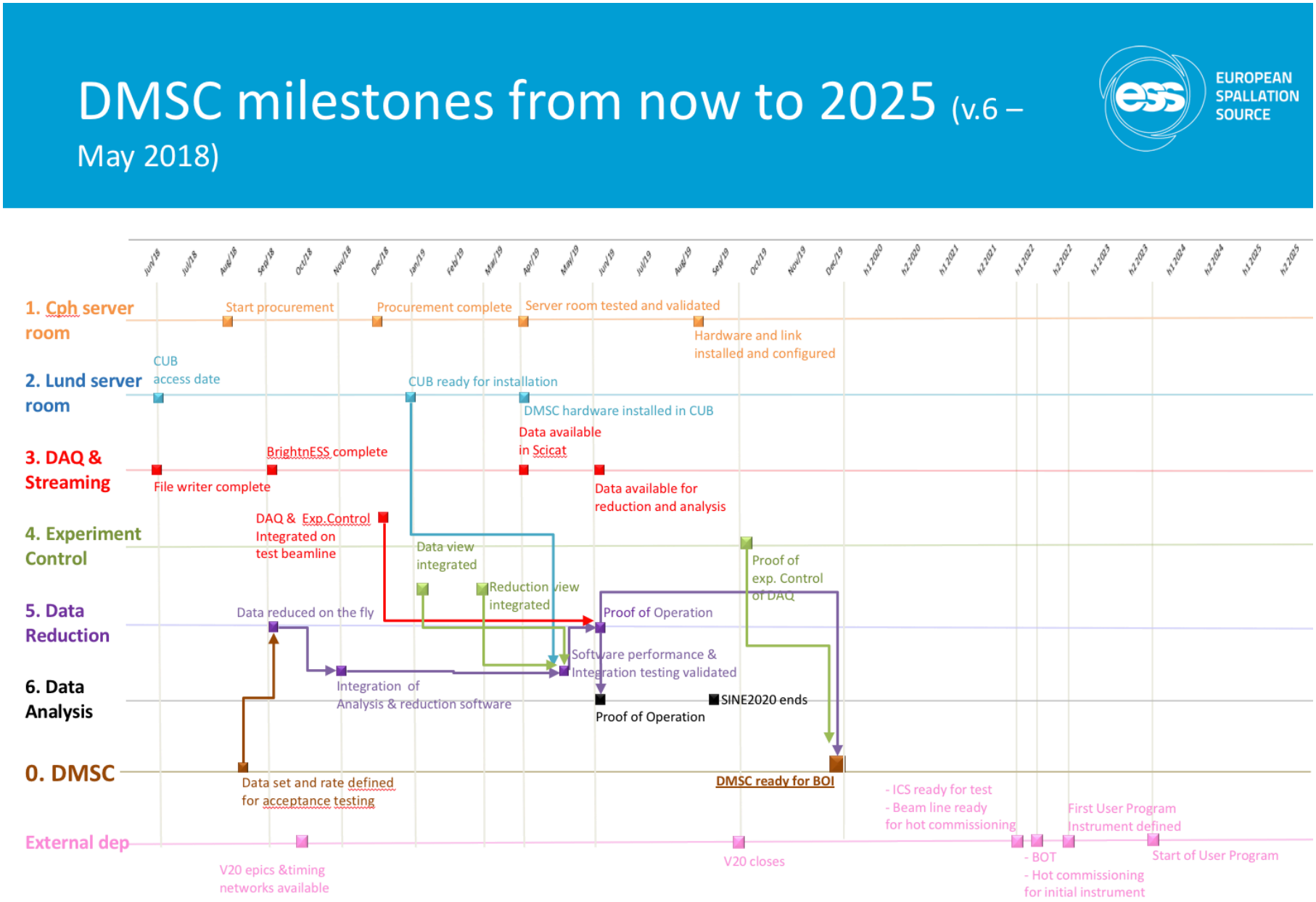
1. CHARGE

General advice and comments on our progress, plans, key technologies and risks.

We ask the STAP for specific comments on the following:

- To comment on a paper prepared on request of the DK Ministry of Research outlining the operational model for DMSC.
- To comment and advise on the DMSC strategy for diffraction software, specifically we would appreciate the STAP's advice on strategies to curate existing packages that are viewed as essential for Rietveld refinement.
- We would like to cross check with existing facilities that the estimates made for hardware provisioning at DMSC are credible.
- Comment on the DMSC suggested review process for Toll Gate 3 (detailed design to procurement & install project milestone) and specifically advice regarding the installation of beam line diagnostics (neutron beam monitors to assist commissioning and operations).

2. TIMELINE AND MILESTONES



Date	Row	Title	Definition of Readyness	Risks	Mitigation	SL
2018-08	0	Data set and rate for acceptance test defined	Data set and rate for acceptance test is well defined but may still need to be generated. Candidates are SANS2D modified to have flux expected from LoKI, or LoKI instrument model data, and test beamline for low flux. Called <INSTR> in other milestones.	Risk of defining an incorrect instrument - liked to the overall instrument schedule		
2018-09	5a	Data reduction on the fly	Data can be reduced on the fly for <INSTR> for acceptance test but only low flux			2
2018-08	1a	CPH Server room - Start procurement	The procurement approval form is signed			
2018-12	1a	CPH Server room - Procurement completed	Contract(s) have been signed			
2019-04	1a	CPH Server room tested and validated	Installations complete, handed over and validated			

2019-09	1a	Hardware and link installed and configured	Simple sync of files between CPH server room and Lund have been demonstrated	Relying on DEIC,SUNET and NORDUNET. Bandwidth at site.	Test link earlier as a pre-prototype.	
2018-06	2a	CUB access date	Access to the physical premises	CF risk	Other infrastructure at ESS in Lund (ICS or NSS lab).	0
2019-01	2a	CUB Ready for Installation of hardware	Access to racks with power and cooling			0
2019-04	2a	DMSC hardware installed in CUB	Event formation machines and storage servers installed and ready for deployment			0
2018-12	3b	DAQ & Exp, Control - integrated on test beamline	Can run experiment entirely from NICOS with control of detectors and file writing	ICS timing not functioning. Reactor not available.	Postprocessing the data. Wait for reactor available.	0

2018-11	5b	Integration of Analysis & Reduction Software	Data can be reduced and analyzed on the fly for limited flux for instrument(s) chosen for acceptance test	Delay in Mantid streaming reduced data.	Add resources	3
2018-06	3a	File writer complete	Can reproduce target NeXus format from streamed data.	In-kind risk.	Knowledge transfer to DMSC.	0
2018-03	3a	NeXus file definition ready				0
2018-08	3a	BrightnESS complete	Deliverables submitted			
2019-04	3a	Data available in Scicat	Metadata from scan at Utgård or v20 appear in SciCat shortly after experiment.	in-kind delay.	add resources	0
2018-10	5a	Data reduction of test workflow available from nexus files.	Data reduction works from nexus file data.	New format of instrument definition not implemented in Mantid.	Add resources.	1

2019-10	4a	Proof of experiment control of DAQ	Final version for construction phase with some amount of robustness.			0
2019-05	5b	Software performance and integration testing validated	1. Data can be reduced and analyzed on the fly for expected flux of <INSTR> when in full operation 2. post batch processing can be performed on CPH cluster			2
2019-06	5a	Proof of operation (reduction)	1. Data can be reduced on the fly for expected flux of <INSTR> when in full operation. Data are received from DAQ & Streaming system. 2. Data can be post rereduced on cluster 3. Need to be able to define the scaling parameter for the architecture rather than actually physically demonstrate	We need to be able to scale.		2
2019-06	6a	Proof of operation (analysis)	1. Data can be analyzed on the fly for flux of <INSTR> when in full operation. Data received from Mantid, which in turn receives data from DAQ & Streaming system. 2. Post batch processing can be performed on cluster			2
2019-09	6a	SINE2020 ends	End of EU funded collaboration			

2019-02	5b	Data view integrated	Data on detector can be live-visualized with EC (Widget from Mantid)			0
2019-03	5b	Reduction view integrated	Reduced data can be live-visualized with EC (Widget from Mantid)	Takes long time to implement for all instruments.	Define use cases and initial instruments.	1
2019-12-31	0	DMSC Ready for Beam on Instruments (BOI)	Data collection, reduction & visualisation chain working L1			1
2022-07-01	Ex	BOT	Beam On target milestone	Date will be affected by any delay in CF/Target/ accelerator / Bunker		
2023/12/15	Ex	Start of User programme	Start of User programme for three instruments	Date will be affected by delays from sub projects		
2022/12/01	Ex	First user programme instruments defined	The point where the first three instruments to enter the user programme is defined following 12m will focus on these instruments	Initial first instruments may not provide a balanced initial user programme		

2022-3-28	Ex	ICS ready for Test Beam Line ready for Hot-Commissioning (L1)	Date shifted by 18m. MS signifies when ICS integration for the Test Beamline is finished. Also possibly is linked to the transfer to init ops funding for ICS	Available recourses unknown and schedule unknown as of 4/2018		
2022-07-01	Ex	Start of Hot commissioning for initial instruments	NSS schedule 4.1 has 4 instruments that could be ready for hot commissioning at the BOT date			

3. HOW HAVE THE RECOMMENDATIONS FROM STAP APRIL 2018 BEEN HANDLED?

Organizational structure for beam-line controls	Who	Notes
Have an appropriate number of ICS staff, directly under the responsibility of NSS to facilitate the prioritization of tasks and to join the effort of providing an adequate level of control software and hardware integration to allow full operability on the instruments from day one of Operation	Tobias Richter	Tobias Richter has been appointed project leader for BCG. That group has been put in charge of prioritizing and monitoring the ICS delivery of scope for NSS. Milestones have been extracted and consolidated from NSS plans. ICS has increased the effort for the control system integration and recent progress has been good.

Server room	Who	Notes
Getting Lund data center operational ASAP as a short-term ability to preform all functions here while the DK server room is not in place	Jonathan Taylor	Status update on Lund server room and mitigation if not ready. CUB server room is planned for access in mid 2018. Tender for buildout is with procurement, budget is secured pending a CF cost transfer, It is likely that there will be a shortfall that will be mitigated by descope of the initial number of enclosures installed, and the groups responsible for funding enclosures. The mitigation for the CUB not being available for the DMSC completion of construction schedule is to use alternate areas at ESS in Lund.
Determine a clear plan for what provisional hardware platforms are to be deployed over the next 5 years in Copenhagen	Jonathan Taylor	Hardware requirements discussion have started with ECDC and DAM, who have supplied the high-level requirements for infrastructure in Lund and in Copenhagen. There is agreement on the high-level architecture that will be provisioned and the technologies / and or partners for some key aspects have been identified. Detailed design of the systems is still required to progress. There is a process in place for this.
Decide on starting the build the server room in COBIS or to use co-located facility - URGENT	Jonathan Taylor	Development of a document describing the high-level requirements and costs for the DK infrastructure was completed, Discussions with identified COLO partners were held. The decision was made with to process with a tender process for a design and build contract to deliver a server room in Cobis. The budget (1.2M euro) is secured for this process.
End-to-end testing between Lund and Copenhagen as soon as possible!	Jonathan Taylor	The key partners have been identified - SUNET (SWE), DEIC (DK) and NordUNET. Works needs to progress to finalise a contract for provisioning a connection between Lund and Cobis. Access to the research network needs to be clarified in both Lund and Copenhagen. DEIC are connecting Cobis to the DK research network. Clarifying the schedule for the connection with the key stakeholders is a priority.

Installation and Commissioning phase for instruments	Who	Notes
Include Calibration Procedures to the requirements for the commissioning plans	Jonathan Taylor	talk with LOKI and DREAM on how they will calibrate detectors. Ongoing discussion with instrument partners and the detector group.
Recruit the Data Scientists as soon as possible in 2020	Thomas Holm Rod	look at instrument schedule and write descriptions and start think of names that could be relevant and talk with the instrument teams. Write specification for the first 8 instruments and run it by the instrument teams. I have started thinking. Some suitable candidates applied for open position.
Make detailed plans, including core activities common to all instruments, for the period end of construction through steady state operations		have it ready by September 2018 STAP. (1 slide per group)
Have clear criteria for acceptance (functionality and reliability) for SL0, SL1 (parts of SL2) agreed between DMSC and instrument teams, for • control • calibration • commissioning • initial user operations	Jonathan Taylor	Discuss with instrument teams at IKON and feedback info to STAP. SL deliverables have been communicated with instrument teams and also reviewed in May 2018. No stakeholders were surprised that the DMSC will stage capability in such a way. We need to develop the plan that delivers the higher-level service that we will deliver post SOUP

Aspire to have a general look and feel independently of instrument (UX)	Tobias Richter Thomas Holm Rod	Not urgent. Something to have in place in 2019 maybe. Tobias Richter: NICOS workshop on UX is planned for early 2019. Thomas Holm Rod: This is not easy for data processing software because we are not in full control of fits development.
Start training on the software ecosystem sooner than later, for current instrument scientists and other interested scientists		This is part of the training plan from 2020 and onwards. Thomas Holm Rod: SasView and MuhRec tutorials have been given at summer schools. SasView 5 will be presented at SasView user meeting (workshop) at SAS2018 and MuhRec was presented at dedicated workshop WCNR-18.

Advanced Data Analysis and Modelling	**Who**	**Notes**
Carefully manage instrument team- and User community- expectations of longer-term analysis and modelling provision	Thomas Holm Rod	Ongoing. Expectations are being managed

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4. WHAT HAS HAPPENED SINCE STAP APRIL 2018

4.1 High level project activities

The management and planning activities for the first half of 2018 focussed on the review of the re-baselined schedule held in May 2018. From the perspective of DMSC a resourced loaded plan was developed in line with the proposal for the NSS re-baseline, that at a high level, aims to deliver 3 instruments into a user programme in Q4 2023 / Q1 2024.

The review committee was positive about the proposal and suggested that a staged commissioning plan be developed that allowed an expert user programme to start as soon as possible after beam on target (July 2022).

The re-baselined schedule was endorsed by the June 2018 council meeting and is now the schedule the project is working to. As of Sept 2018 the overall project is 45% complete.

From Q2 2018 the toll gate three review process has started for the instrument projects in NSS. The TG3 review is the instrument project gateway between detailed design and procurement and installation. Post TG3 the instrument designs will be under change control.

The TG3 process is critical for DMSC as it defines key instrument components that impact directly DMSC scope. Detector readout and chopper cascade design and diagnostics will be reviewed by DMSC staff for compliance with standards for technologies and also for data processing and commissioning.

A considerable effort has been made since the last stap meeting to progress the DK server requirements and strategy. Largely this has been successful. A decision on the DK server room is made and a tender process initiated with ESS procurement. The schedule for delivery is not thought to impact the DMSC completion of construction and certainly not the ESS operations schedule.

4.2 Q1 activities

Staff from DMSC and NID attended the yearly Mantid user workshop and Mantid developer meeting held at the Spallation Neutron Source in Oak Ridge National Laboratory. This meeting sets the medium-term user priorities for the Mantid software project, and as a core partner for the project ESS requirements are presented. The developer meeting is an essential face to face meeting for all developers of Mantid, Simon

Heybrock presented the development led by ESS that improved framework performance and allows reactor-based instruments to use the Mantid framework in a sustainable way.

Jonathan Taylor Chaired a review of the scientific software at the ORNL neutron sources. The purpose of the review was to evaluate progress made at ORNL against a plan set in by the last triannual DOE review to ensure scientific software capabilities match the needs of the user community.

During Q1 a full integration test was carried out at the V20 test beamline at BERII. The test saw successful integration and control of multiple chopper axis and acquisition of timestamped chopper meta data and timestamped detector data from two neutron beam monitors. The test validated the operation of the ESS DAQ system and highlighted areas for future work to fully understand the ESS distributed timing network.

DMSC organised a BrightnESS WP5 meeting discuss work needed to transition into the final phase of the very successful BrigtnESS work package and to ensure that all deliverables are completed.
Considerable effort has been made to better define the detector readout interface to DMSC and to agree a roll out schedule for test readout hardware.
Staff from the experiment control and data curation group were involved in multiple visits to detector test facilities to collaborate with the ESS detector group with development readout and data visualisation functionality for detector commissioning.

DMSC staff were involved in the preparation of two key EU proposals. The Photon and Neutron Open Science Cloud (PaNOSC) is a proposal which aims to leverage the European Open science cloud to enable facility users to efficient collect and analysis data. PaNOSC is part of the much wider European Open Science Cloud initiative. NMIStar is an EU proposal that provides networking joint research activities and very importantly funding for transnational access for European neutron users. DMSC are proposed to lead the joint research activity for NMIStar which aims to provide sustainable software for neutron data analysis, (with a focus on powder and single crystal diffraction) and research novel uses of emerging tech like VR and AR for neutron instrument control.

Thomas Rod hosted a user experience workshop for DMSC staff and in-kind partners. This workshop focused on the often-overlooked area of ensuring software applications provide a positive user experience. Whilst the most obvious area is in the design of user interfaces (either graphical or command line) the workshop also considered development in areas that ensure good user experience can provided in a tested and maintainable way.

The Data Reduction Analysis and Modelling group initiated a collaboration with PSI and ISIS, working together to improve pipeline performance and functionality of inelastic neutron scattering data analysis software for magnetic excitations in strongly correlated electron systems.

4.3 Q2 activities

The management and administration group along with the data systems and technology group have complied the data and written a report to outline the strategy for deployment and placement of DMSC hardware systems in Denmark. This work precedes the construction phase of the DMSC data centre and outlines the long-term costs for ESS.

The DST group have been in discussion with both DEIC (Danish E-Infrastructure Consortium) and representatives of the GEANT infrastructure to connect the DMSC to the European research network and also to link the two ESS sites together over a managed link.

DST have been working with colleagues in ICS to develop the specification for the ESS site data centre which will be located in the H01.

The BeamLine Controls group led by Tobias Richter was setup to create a single entity to develop the scope for instrument and experiment control in an integrated manner. The working group comprises of colleagues from DMSC, ICS Neutron technology division and the scientific activities division who collectively hold the scope for the full stack Neutron instrument control at ESS.

The experiment control in-kind work package at PSI in Switzerland have successfully simulated the AMOR instrument using the ESS control stack technology. A test has been completed on AMOR that successfully showed the control stack worked. Ongoing work is underway to convert AMOR to the ESS experiment control solution for user operations at SINQ.

A number of DMSC staff attended the Brightness closeout meeting Brussels, Tobias Richter presented the results from WP5 of Brightness which has delivered the core components of the ESS Data Acquisition (DAQ) system.

A number of DMSC staff attended the Sine2020 general assembly meeting in Palma Italy. Progress of the WP10 was presented by Thomas Holm-Rod, who had organised a WP10 satellite software development workshop. The workshop ran over three days (lunch-to-lunch) and had participants from all involved facilities (with the exception of LLB) and was a good opportunity for coordinate across facilities and sharing knowledge. Software discussed were BornAgain, SasView, Mantid, MuhRec, and MDANSE and although not part of WP10, also SpinW and nsxtools. Many other topics of relevance for the scientific computing groups were also discussed, e.g. Jupyter notebooks and GUI testing. to discuss development of SASView and Bornagain.

The DSMC hosted an Engineering diffraction software workshop to discuss requirements and solutions for the engineering diffraction science area and the BEER instrument at ESS. The workshop was attended by instrument and software specialists from ISIS, Los Alamos, SNS, JPARC and PSI. The workshop output forms the high-level requirements for DSMC scope in the area of engineering diffraction.

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DMSC hosted a small meeting with the core developer of GSASII, one of the major Rietveld refinement packages used in neutron powder diffraction, with the objective of clarifying the requirements needed to ensure that GSASII is a sustainable software framework and available for use in the future at ESS.