ESS Project and DMSC update

DMSC stap Meeting September 2018

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www.europeanspallationsource.se

19-20 September 2018

Data Management and Software Centre

EUROPEAN SPALLATION SOURCE

Provide world leading scientific software and scientific computing support for neutron scattering at ESS

- Construction budget 20M euro
- Staff 2018 27 + 8
- Staff 2028 60

Scientific Software development.

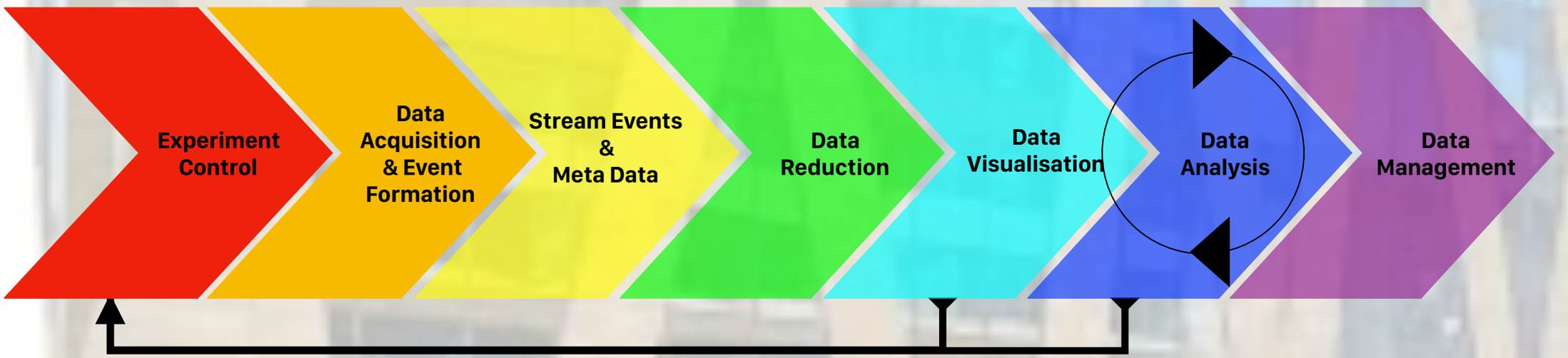
- Experiment control
- Data acquisition system
- Data reduction, analysis & modelling

Data centre operations.

- Dual location - Lund & Copenhagen
- Data management and curation

User programme support

- Instrument Data scientists
- User office software
- Remote access to data and software tools



Outline

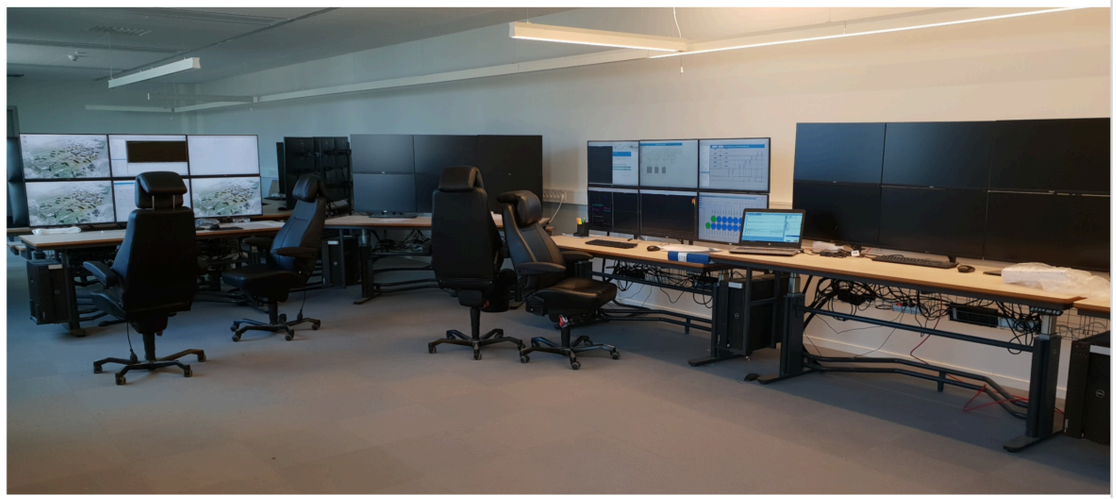
- ESS update
- Re- Baselined ESS schedule & review may 2018
- DMSC progress update
- Toll Gate III process & DMSC involvement
- Beamline Controls Group. BCG
- Copenhagen Server room update
- Photon and Neutron Open Science Cloud project
- Diffraction RoadMap development

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 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 appreciates 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.

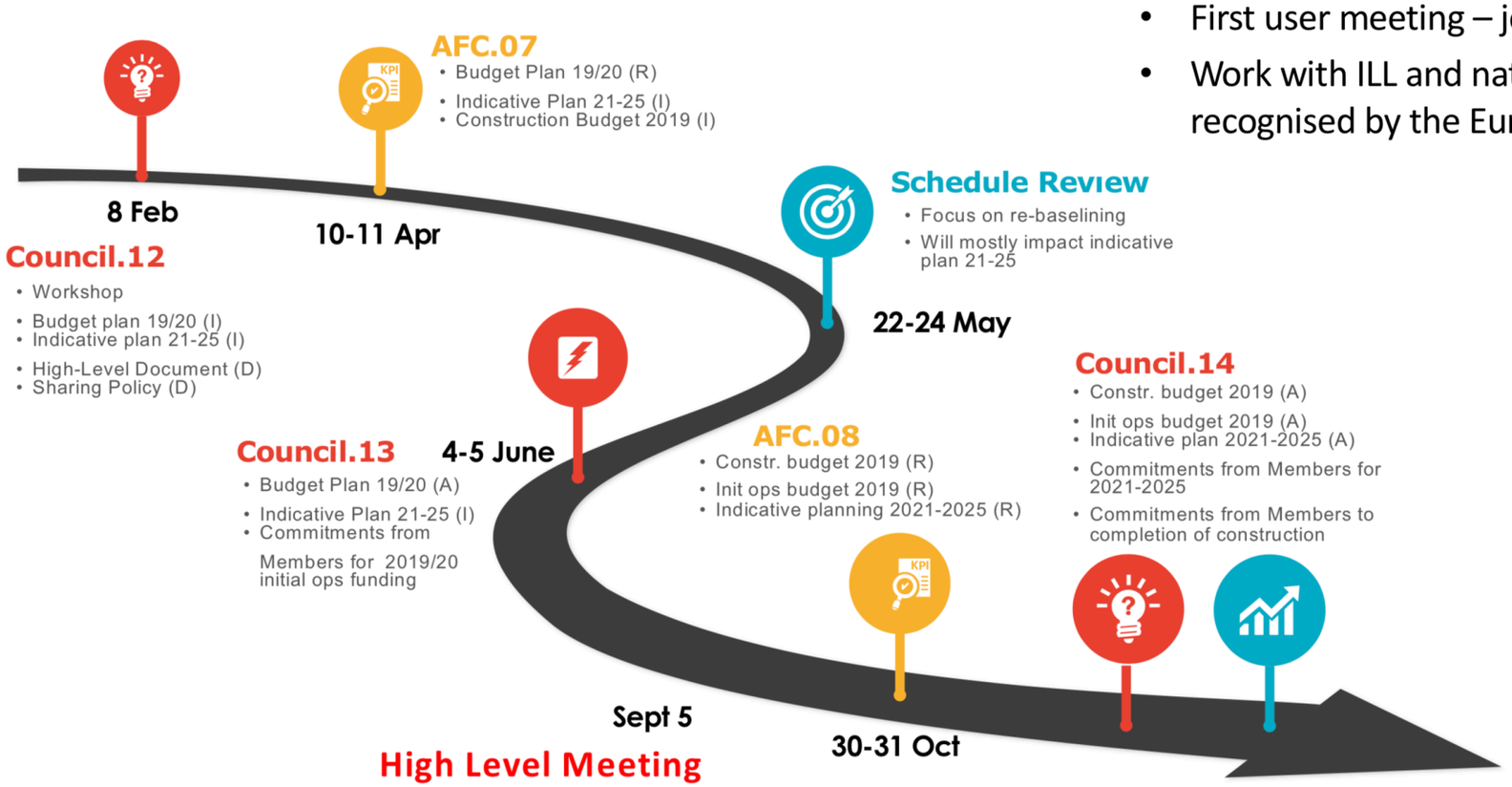
ESS update project 45% complete

EUROPEAN SPALLATION SOURCE



In progress

- Submit to SSM the application for the trial operations of the Warm Linac
- Start of commissioning of ion source and LEBT, local control room operational — Sept
- Complete manufacturing and Factory Acceptance Tests of Moderator plug, Cryo-Moderator System and Cryoplant.
- All instruments start Tollgate 3 process and begun procurement
- Move ESS Lund organisation to site
- A detailed plan for first two years (2019 & 2020) of Initial Operations
- Secure Spain as an ERIC member and finalise all remaining in kind agreements (UK, DE…)
- First user meeting – joint with ILL — Oct 10-12
- Work with ILL and national sources to establish a neutron initiative recognised by the European commission in their planning for FP9 — Kick-off this week



ESS Re Baseline

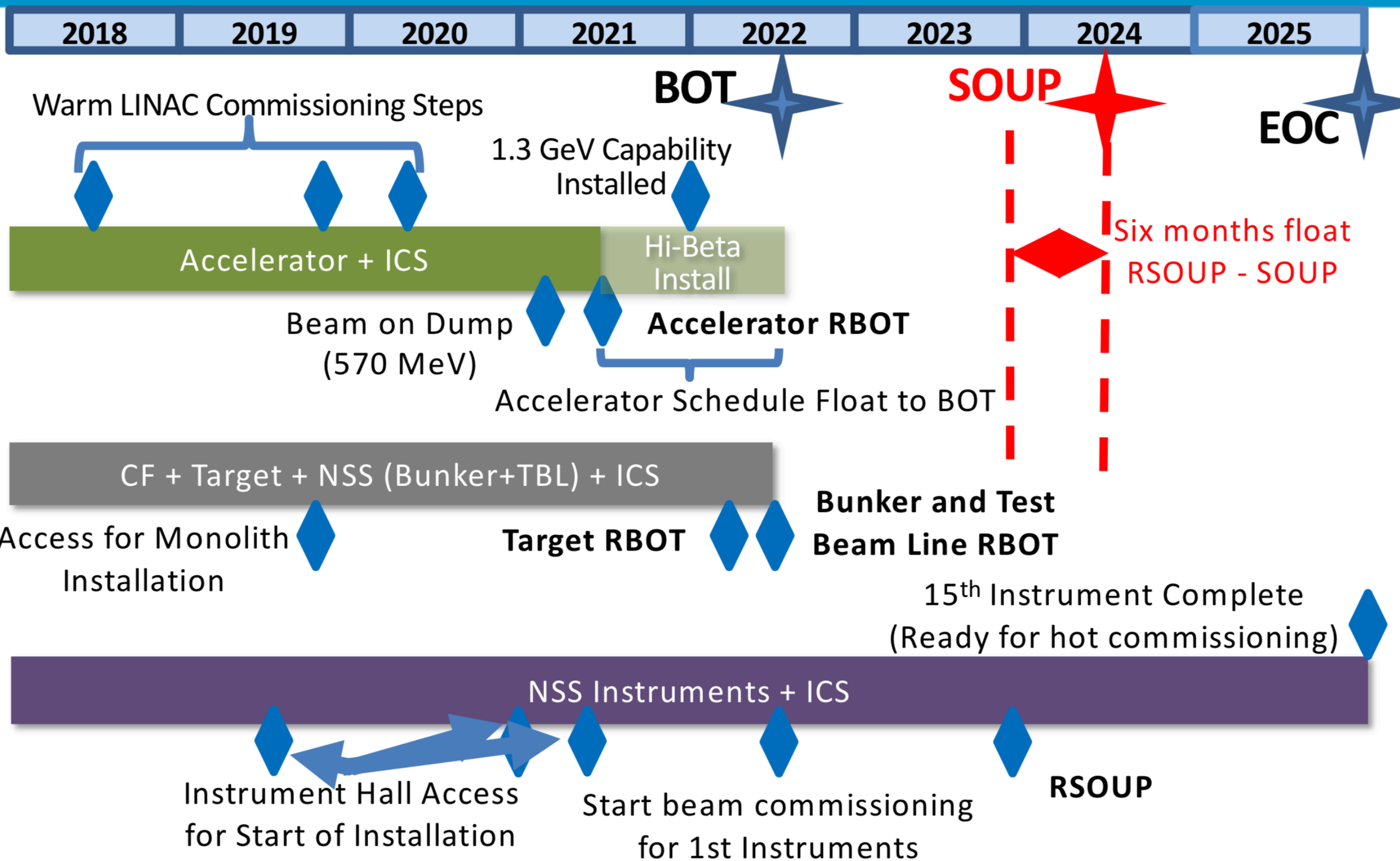
- Extensive planning in first Quarter from all parts of ESS

- How to mitigate the 24m delay to access and BOT???

- Re-baselined Schedule reviewed in May 2018

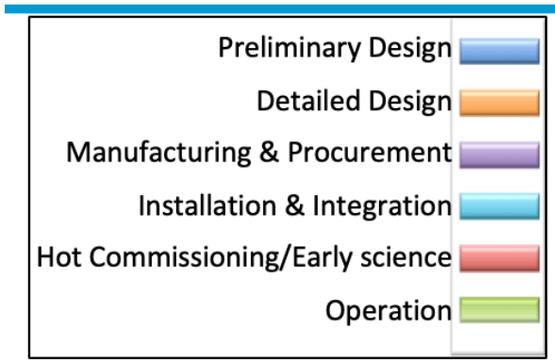
- Re-baselined review accepted by Council June 2018

RB Schedule 4m delay in User programme



Specifically for Instruments

- Focus on 8 instruments for 2022
- Select 3/8 for SOUP starting late 2023 to mid 2024

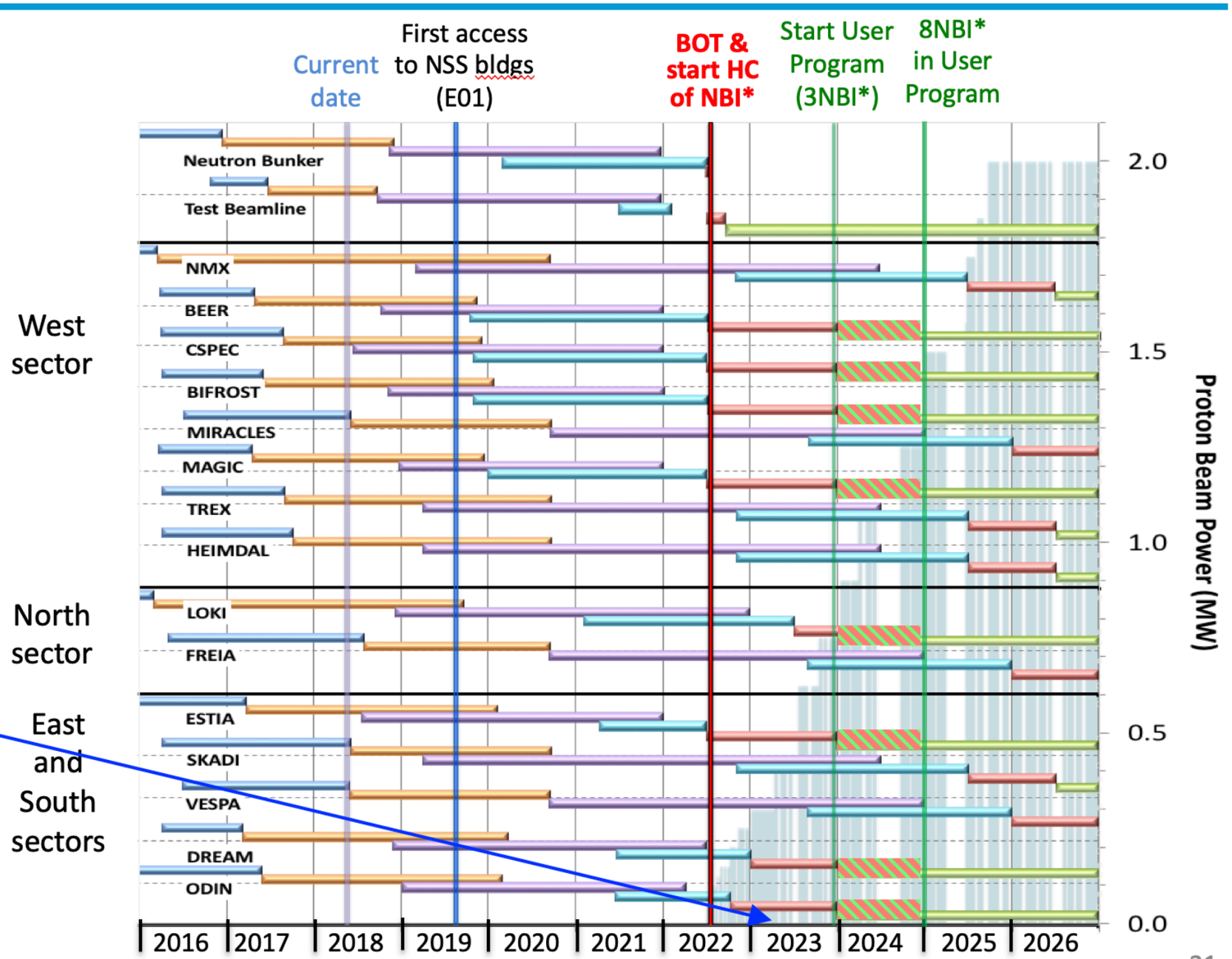


Safest *instrument choices to be Ready for SOUP in West sector (BEER, CSPEC, BIFROST & MAGIC) & East (ESTIA)*

Most desirable *instrument choices for early science* ***highlights*** *are in the South and North (ODIN, DREAM & LOKI). LOKI seems unlikely to make the deadline*

Selection of first NBI for SOUP in March 2023

Knock-on delays to NBI:
9 – 15 of ~ 1 yr and
16 – 22 of ~ 1 ½ yr



Review outcome

Working with the ESS Council, ESS Management should develop a tiered instrument commissioning schedule which will achieve meaningful science (to be defined) starting six months after BOT. Definitions of the interim user-related commissioning milestones should be clearly defined (i.e., Early Science, User-Assisted Commissioning), which lead up to the full SOUP. The commissioning schedule can be incorporated in the ESS baseline when completed. This recommendation would preclude the need to move the SOUP milestone to June 2024 at this time.

Review outcome 2

Propose to follow the recommendations of the panel and

- manage aggressively to the current schedule which defines SOUP as the start of a **full, peer-reviewed-access user programme with three fully commissioned instruments by December 2023**
- note there is no float in this date, but rather than adding additional float now, we propose **at a future date to scale back the definition of SOUP if needed.**
  - The modified definition would keep the same date but reduce the level of commissioning promised:
  - Open three instruments to users by December 2023, but allow that the users may be ‘experienced users,’ and allow that the instruments may not have all capabilities fully commissioned

Review 3 – ESS response and plan

Propose to follow the recommendations of the panel and

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  - The modified definition would keep the same date but reduce the level of commissioning promised:
  - Open three instruments to users by December 2023, but allow that the users may be 'experienced users,' and allow that the instruments may not have all capabilities fully commissioned
- Management also suggests we follow the spirit of the recommendation to develop an additional, externally communicated plan for the **start of early science** involving the SAC based on the early science success strategy communicated to Council
- Early science would come maybe 6 months after BOT, i.e. **early 2023** (zero float) for the first instruments assuming that accelerator and target commissioning goes well

DMSC input to the Re-baseline

- What rate can instruments can credibly be commissioned.

- Can DMSC support that activity and be confident that the schedule can be maintained.

- What activities are essential to deliver a commissioned instrument suit.

- How long will this process take in beam days.

- I presented the plan during the last STAP.

Installation and Commissioning

SNS commissioning plan documentation taken as a guide.

We assume instrument team consists of 2 scientists + 0.5 Instrument data scientist (from DMSC)

Considerable cold commissioning work will be undertaken during the installation phase of components

Complex instrument systems commissioned into control system and verified as installed
Work performed by both ICS and NSS beam-line controls group

Phase 1 Commission and verify beam-line components

Estimate from all ESS contributing groups 2.5-4.5 FTE + core team key staff
1-2 FTE ICS, 1-2 ECDC, 0.5 FTE DST, Staff from ICS and NT core as required
30 days BOT

Phase 2 Verification of source and beam-line performance

Estimate from all ESS contributing groups 2-3 FTE + Core team
1 ECDC, 1.5 DRAM, Staff from ICS and NT core as required
20 - 30 days BOT

Phase 3 Commissioning experiments

1 FTE + Core team
1 .5- DRAM
1+ SE support + engineering support
50 days BOT

Required ~110 days BOT

Provisional Accelerator ramp-up 2022- 2023
~200 days available

Phase 1 Commissioning

30 days BOT
2 DMSC FTE + 2.5 instrument FTE

Timing system verification

- Time-stamping accuracy and jitter
- Delay compensation accuracy (per beam line)
- Machine synchronisation

Target and moderator data verification

- Moderator state
- Moderator temperature

Shutter verification

- Light shutter
- Heavy shutter

Chopper axis verification

- Cold commissioning component during installation
- Hot Commissioning on instrument

Beam-line mechanical components commissioning and verification

- Slits, attenuators, motion stages (including monitors)

(Cold commissioning performed during install)

Vacuum system verification

Monitor commissioning and verification

Detectors commissioning and verification

- High Voltage control
- Slow controls & gas system
- Pulse Height spectrum
- Fibre connection test - instrument positions —> CUB

Data Acquisition

- Verification that DAQ receives data from all sources
- Data file verification Lund
- Data file verification Cph
- verification of DAQ operating modes - counting in 1st -2nd... frames
- Efficacy of soft vetos from time-stamped data

Detector evaluation and calibration

- Event formation performance
- Position calibration

Phase 2 Verification of performance

Verification of source performance & data processing

- Measurement and verification of source spectrum
- Normalisation by current
- Normalisation by monitor
- Verification of beam raster characteristics
- Ion sorce fluctuation evaluation
- Moderator performance check
- Performance verification for each target segment

Measurement and verification of guide performance

- Beam profile at sample position
- Measurement and verification of incident flux
- Calibration and alignment of guides and beam-line components

Verification of beam line performance

- Beam-line operation in various accelerator operating modes
- Flux on sample
- Signal / Background evaluation

Verification of chopper cascade

- Transmission
- Bandwidth
- Resolution
- Operating mode WFM / RRM

Verification of instrument resolution

- Standard sample measurements

30 days BOT
3 DMSC FTE + 2.5 instrument FTE

Phase 3 Commissioning experiments

50 days BOT
1.5 DMSC FTE + 2.5 instrument FTE

Scientific test and validation

Data processing and data analysis workflow verification

- Data reduction workflow verification
  - WFM stitching
  - Image processing
  - SANS data reduction to 1D I vs Q & 2D Qx,Qy
- Data analysis verification
  - Diffraction peak heights (in WFM mode)
  - SANS model fitting of standard sample
  - Volume Reconstruction and validation

Calibration procedure

Early science programme with expert friendly users

Overview on resources required to meet SOUP schedule

- Only DMSC scope considered here
  - ICS are vital to a lot of commissioning activities
  - NSS will operate a beam line controls group
- For the initial instruments and first two open bunker periods only
- Two DMSC groups **100% utilised** in 2022 against our current initial operations plan

- SOUP instruments allocated extra resources at UP start

- Instrument data scientists hired 2020

	2019		2020			2021				2022				2023				2024			
	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
west sector																					
BEER	0.0	0.0	0.0	0.5	0.5	0.5	1.0	1.0	1.0	1.0	1.0	2.5	2.5	2.5	3.0	2.0	2.0	1.5	1.0	0.5	0.5
CSPEC	0.0	0.0	0.0	0.5	0.5	0.5	1.0	1.0	1.0	1.0	1.0	2.5	2.5	2.5	3.0	2.0	2.0	1.5	1.0	0.5	0.5
TREX	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.5	1.0	1.0	1.0
HIEMDAL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.5	1.0	1.0	1.0
NMX	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.5	1.0	1.0	1.0
BIFROST	0.0	0.0	0.0	0.5	0.5	0.5	1.0	1.0	1.0	1.0	1.0	2.5	2.5	2.5	3.0	2.0	2.0	1.5	1.0	0.5	0.5
MAGIC	0.0	0.0	0.0	0.5	0.5	0.5	1.0	1.0	1.0	1.0	1.0	2.5	2.5	2.5	3.0	2.0	2.0	1.5	1.0	0.5	0.5
North Sector																					
LOKI	0.0	0.0	0.0	0.5	0.5	0.5	1.0	1.0	1.0	1.0	1.0	2.5	2.5	2.5	3.0	2.0	2.0	1.5	1.0	0.5	0.5
FREIA	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.5	1.0	1.0	1.0
SOUTH & East Sector																					
ODIN	0.0	0.0	0.0	0.5	0.5	0.5	0.5	1.0	1.0	1.0	1.0	2.5	2.5	2.5	3.0	2.0	2.0	1.5	1.0	0.5	0.5
DREAM	0.0	0.0	0.0	0.5	0.5	0.5	0.5	1.0	1.0	1.0	1.0	2.5	2.5	2.5	3.0	2.0	2.0	1.5	1.0	0.5	0.5
ESTIA	0.0	0.0	0.0	0.5	0.5	0.5	0.5	1.0	1.0	1.0	1.0	2.5	2.5	2.5	3.0	2.0	2.0	1.5	1.0	0.5	0.5
SKADI	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.5	1.0	1.0	1.0
Total FTE allocated to instruments	0	0	0	4	4	4	7	8	8	8	8	20	20	20	24	16	16	15	13	9	9

Instrument example

- Instrument data scientist is part of instrument team
  - PM for software delivery
  - Knowledge of both beam-line science & beam-line software
- Experiment control development split between
  - Controls
  - DAQ

Role	2019		2020			2021				2022				2023				2024			
	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
ECDC control	C	C	C	C	C		0	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5						
ECDC DAQ	C	C	C	C	C							0.5	0.5	0.5	0.5	0.5	0.5				
RAG ID Sci				0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5
RAG reduction	C	C	C	C	C						0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5		
RAG Analysis	C	C	C	C	C										0.5	0.5	0.5	0.5	0.5		
DST										0.5	0.5	0.5	0.5	0.5	0						
Total				0.5	0.5	0.5	0.5	1	1	1.5	2	2.5	2.5	2.5	2.5	2	2	1.5	1.5	0.5	0.5

C - Allocated to core development

Progress highlights

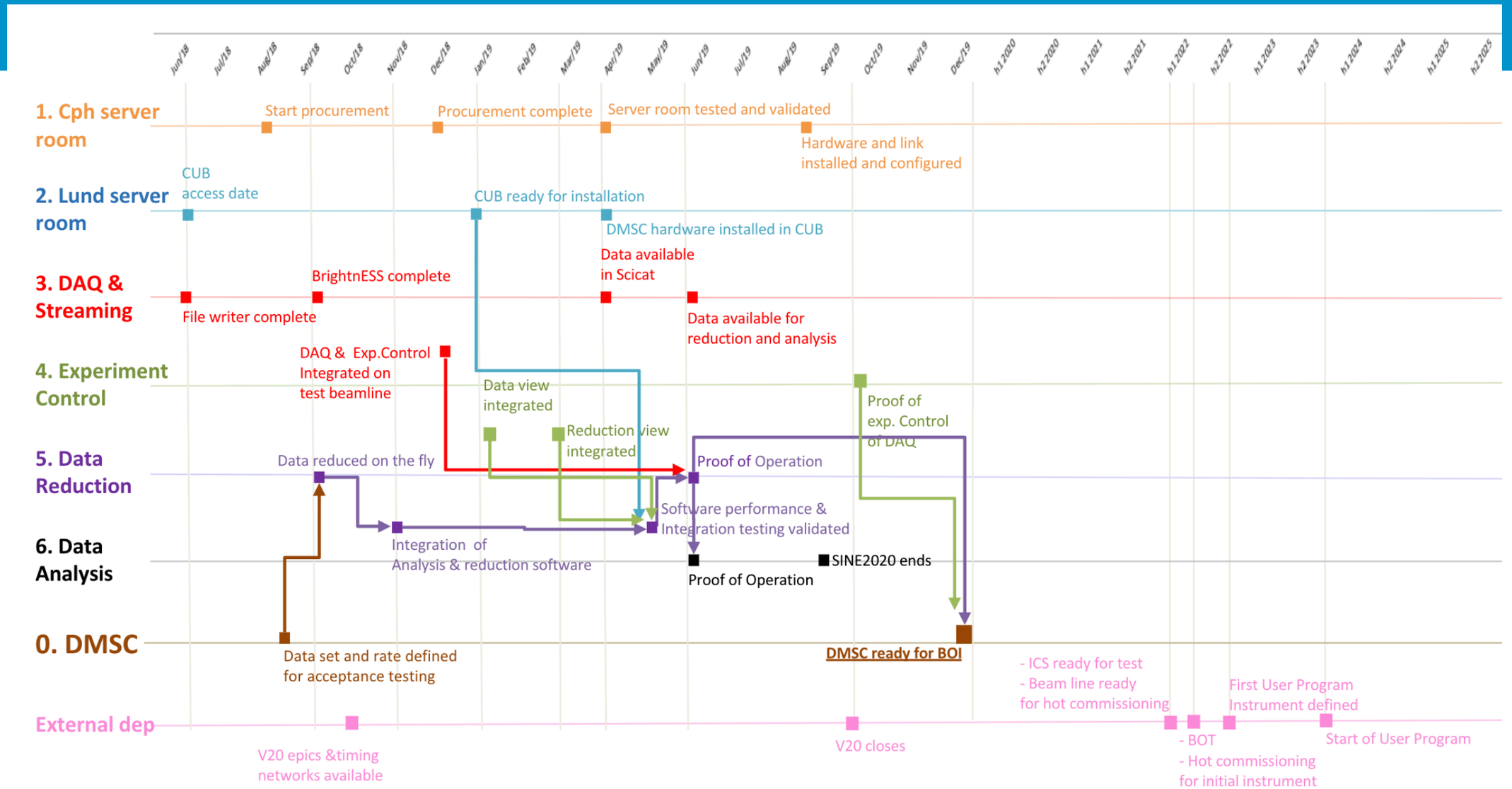
- DMSC – DG collaboration / integration
- BCG
- PaNOSC project
- Mantid development progress

- Excellent progress on Data analysis
  - including considerable community engagement & acceptance.

Key stakeholder engagement

- DK ministry requested a paper on DMSC operations
- How should we maximise impact
- Visitors to DMSC
  - Users - How many users currently visit to perform data analysis at existing facilities
  - Should ESS offer this as part of the access mechanism
- Data analysis as a service
  - What level of the ESS user programme Can / Should DMSC support.

Milestones to 2020 & planning



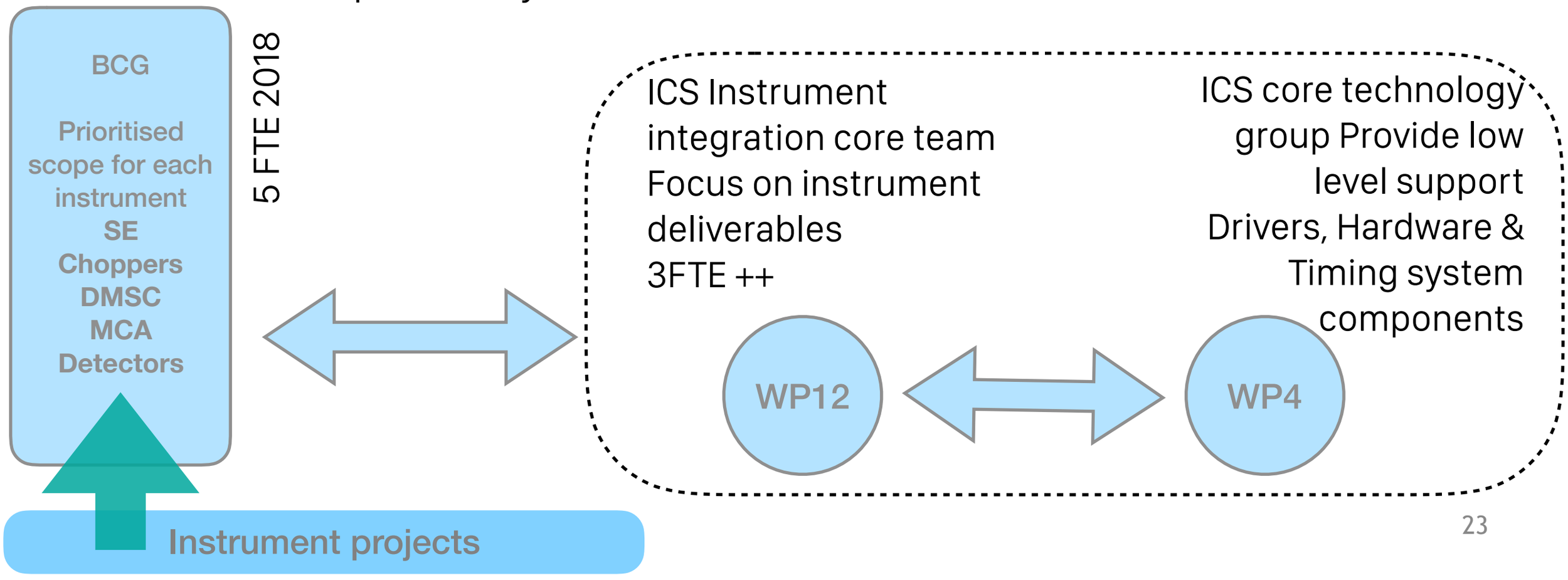
- Schedule on track
- 1 external dependency for CUB (with credible mitigation on risk)
- Largest uncertainty – Cph server room progressing into procurement
- BiMonthly project control meetings tracking P6 and updating plan, risks and priorities.
- Steering committees in place on key projects. Both in house and unkind

2018 - BOT - SOUP …

- Finish core technology development
  - On schedule.
- Develop project structure and milestones for 2020 onwards
  - Instrument project structure maturing
  - Critical focus on first 8 instruments
  - Deliver functionality for first 8 instruments 2020 - BOT
  - Start hot commissioning
  - Deliver SL1 and SL2 for hot commissioning and SOUP
  - Develop strategy for implementing SL3 & 4
    - Deliver expected scientific computing impact and capability
  - Support operations and remaining construction

NSS BCG ICS integration

- BCG is a matrixed group
- Agreed with ICS and NSS
- In line with existing Large Scale Facilities
- Consolidation of planning and prioritisation
- Authority over development direction and project priorities
- Beneficial and complimentary to ICS



2018 - BOT - SOUP ...

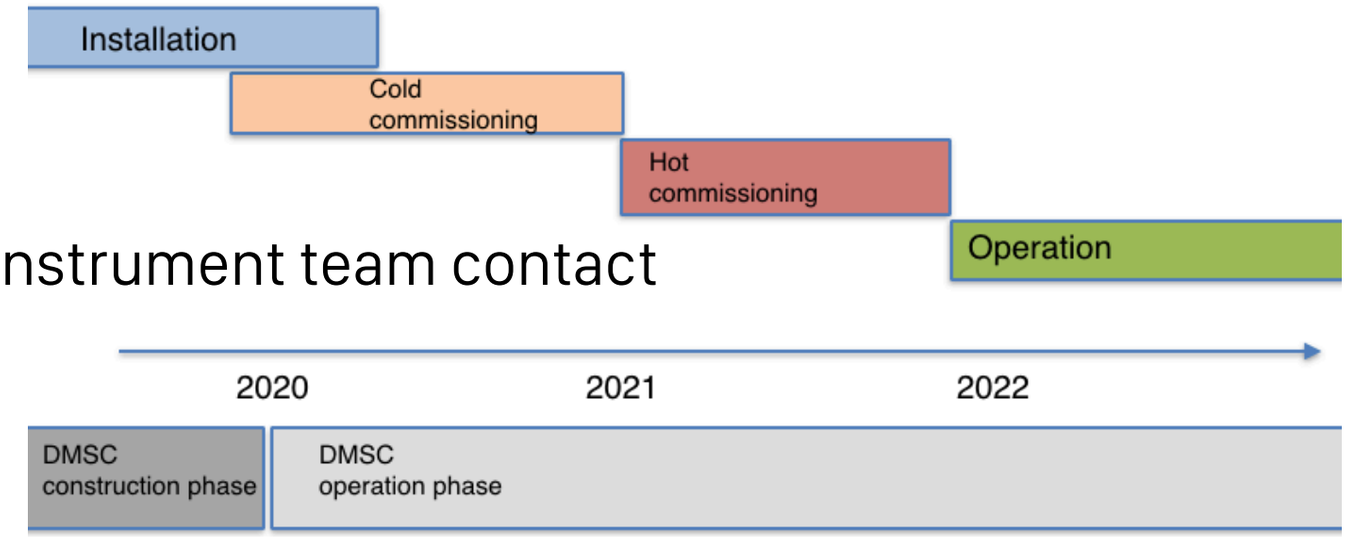
Development of a credible baseline provision for analysis, reduction and control

Next generation analysis provision remains the overall objective for ESS

- SL 0 - Control of instruments and acquisition of data, archive and curation of collected data
- SL 1 - Framework for manual data reduction, Data analysis packages manual operation
- SL 2 - Automated reduction workflows, automated analysis - experiment control feedback
- SL 3 - Support for advanced analysis and simulation

Instrument Software projects

- Requirements summary document for 2017 workshops at ESS-0148155
- Scientific software Scope will be delivered with project management
- 1 instrument 1 project
- **PM** at DMSC - The instrument data Scientist
- **Sponsor** HO DSMC
- **Customer** NSS project lead
- **Project scientist** - Lead scientist or Instrument team contact
- Start date
  - Definition phase pre 2018
  - After ESS re-baseline
- End date: instrument in UP



Progress.

- High level requirements gathered.
- For day one operations requirements are agreed and credible.
- Milestones and post 2020 plan maturing
  - Tightly coupled with instrument schedules
  - Install and cold commissioning aligned with buildout
  - Instrument projects feed into commissioning plan
  - Success will depend upon keeping to standards
  - **Focus on first 8 instruments**
  - Developing plan is priority for Q3-4 2018
  - PM recruitment starts in 2019 Q2
  - Projects start when resources become available 2019*
  - Develop commissioning plan and staging beyond ‘simple’ operation

- Schedule workshops 2019 – Couple instrument projects to DMSC projects

* Scope deferred to operations phase on 2016
  Staff profile remains as planned – possible risk due to hiring slowdown

Generic instrument Milestones for instrument projects 2020 - BOT

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	Project	Control	DAQ	Reduction	Analysis
MS1	Software project definition start	Chopper Cold integration	DAQ integration starts	Workflows defined	Development roadmap
MS2	Software project definiion end	Motion Cold integration	Detector prototype ready for integration	Instrument definition proto	Development complete
MS3		Sample environment Cold integration	Monitor ready for integration	MPI workflow developed	pipeline integration complete
MS4			DAQ integration ends	MPI Live workflow developed	
MS5				Data visualisation developed	

Next steps …

- We have the major milestones BOT, RSOUP etc
- Workshops to define project schedule post TG3
- At this stage the instrument project schedules are not well enough defined to generate credible milestones.
  - For installation & commissioning

Toll Gate III

- Project gateway between detailed design and procurement
- Post TG3 instruments are under change control
- To keep schedule staged TG3s are envisaged
  - CTV – Call for Tender Verification
  - IDR – Intermediate design reviews
  - Sub TG3 – Sub systems CDR
  - Full TG3 instrument progressed

- DMSC will review Detector integration, DAQ, data reduction feasibility and commissioning plan

TG3 meetings 2018 and 2019

EUROPEAN SPALLATION SOURCE

2018-19	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec	Jan	Feb	Mar	Apr	May	Jun	Jul
LOKI																			
SKADI																			
ESTIA																			
FREIA																			
NMX																			
MAGIC																			
HEIMDAL																			
DREAM																			
BEER																			
ODIN																			
CSPEC																			
BIFROST																			
MIRACLES																			
T-REX																			
VESPA																			

31

DMSC STAP 24-25

23

Council-12

IKON14

SE STAP

12-13

ICB10

SAC20

13

Re-Baselining Review

Council-13

IKON15

DMSC STAP 19-20

ICB11

SAC21

Council-14

IKON16

DMSC STAP 10-11

ICB12

SAC22

STAP

TG2 ongoing/passed

IDR

TG3 intermediate/final

Beamline Diagnostics

- Not all instrument teams are convinced on the need for beam monitors near choppers

- ESS proposes a common monitor project & essential monitors

- High level requirements generated

- Resources are an issue

Progress

- Joint TG3 review process DMSC and Detector group

- Beamline diagnostics requirements developed
  - Do we need diagnostics for hot commissioning 100+ choppers?
  - Are diagnostics essential for hot commissioning and data reduction?

Copenhagen Server room progress

- Requirements and high level architecture defined and agreed
- Requirements for compute well underway
- Colocation partners were not confident on delivery
- Build server room in Cobis
- Procurement started
- Budget covers
  - Buildout of room infrastructure
  - power and cooling for 130kW
  - Utilities
  - Initial enclosures
- Will cover requirements unto 2026 given current expected power ramp and re-baselined instrument schedule.

DMSC infrastructure

- Lund – CPH link a priority for Q3 2018
- Availability of systems under evaluation
- User experience and core technologies under review
  - Remote access
  - File system

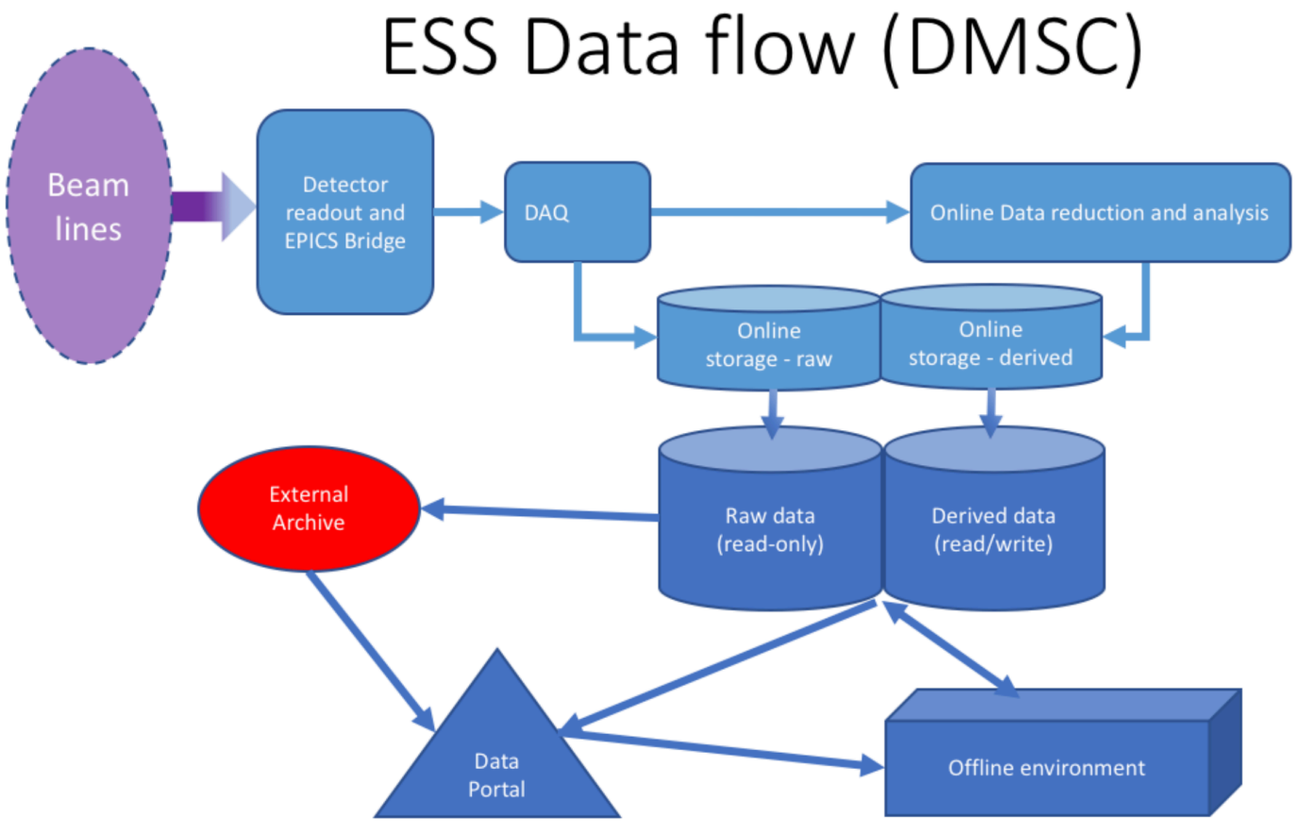


Figure 1: Simplified representation of selected components of the data flow. The blue and teal shapes represent systems and services operated by the DMSC. See section 3.1 for details.

Table 2 Storage requirements – storage produced per year

Year	2019	2023	2025	2028	2035
Storage for online/live experiment data	0.0 PB	0.6 PB	7.4 PB	17 PB	22 PB
Storage for User services	0.0 PB	0.1 PB	0.6 PB	1.5 PB	3.4 PB
Storage for off-line environment	0.0 PB	1.1 PB	12 PB	30 PB	41 PB
Storage for ESS projects	0.2 PB	0.7 PB	1.2 PB	1.3 PB	1.5 PB
Storage for operational infrastructure	0.1 PB	0.1 PB	0.2 PB	0.2 PB	0.3 PB

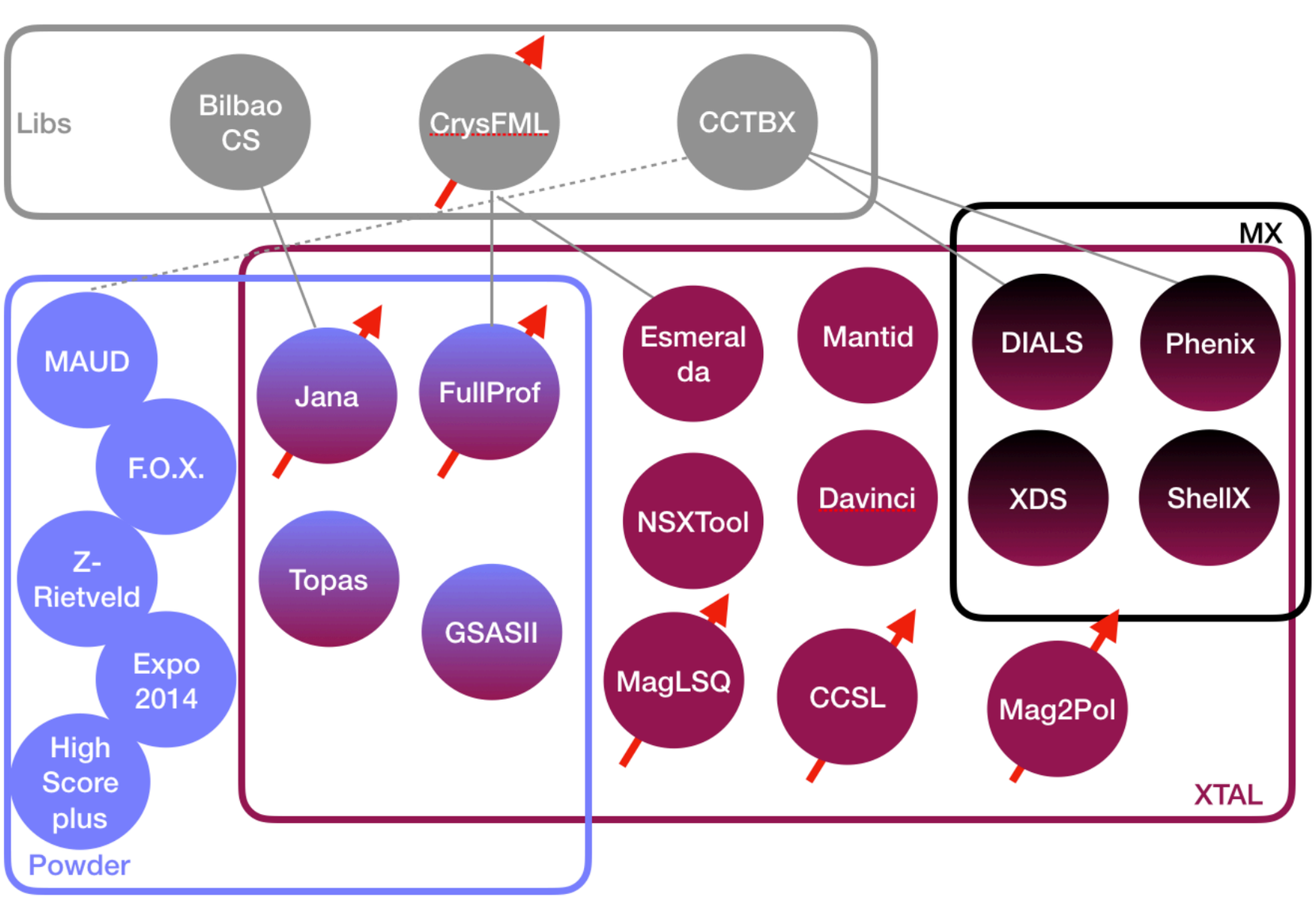
Diffraction Software Roadmap

- NMIStar – Rejected
- NMI* JRA 135 pm for powder and stall diffraction
  - Framework development and sustainability of existing tools to SINE2020 standards.
- Initial tasks were to develop roadmap
  - ESS is committed to undertake the first step
- Define medium term requirements

- The landscape is large
  - Many single points of failure exist

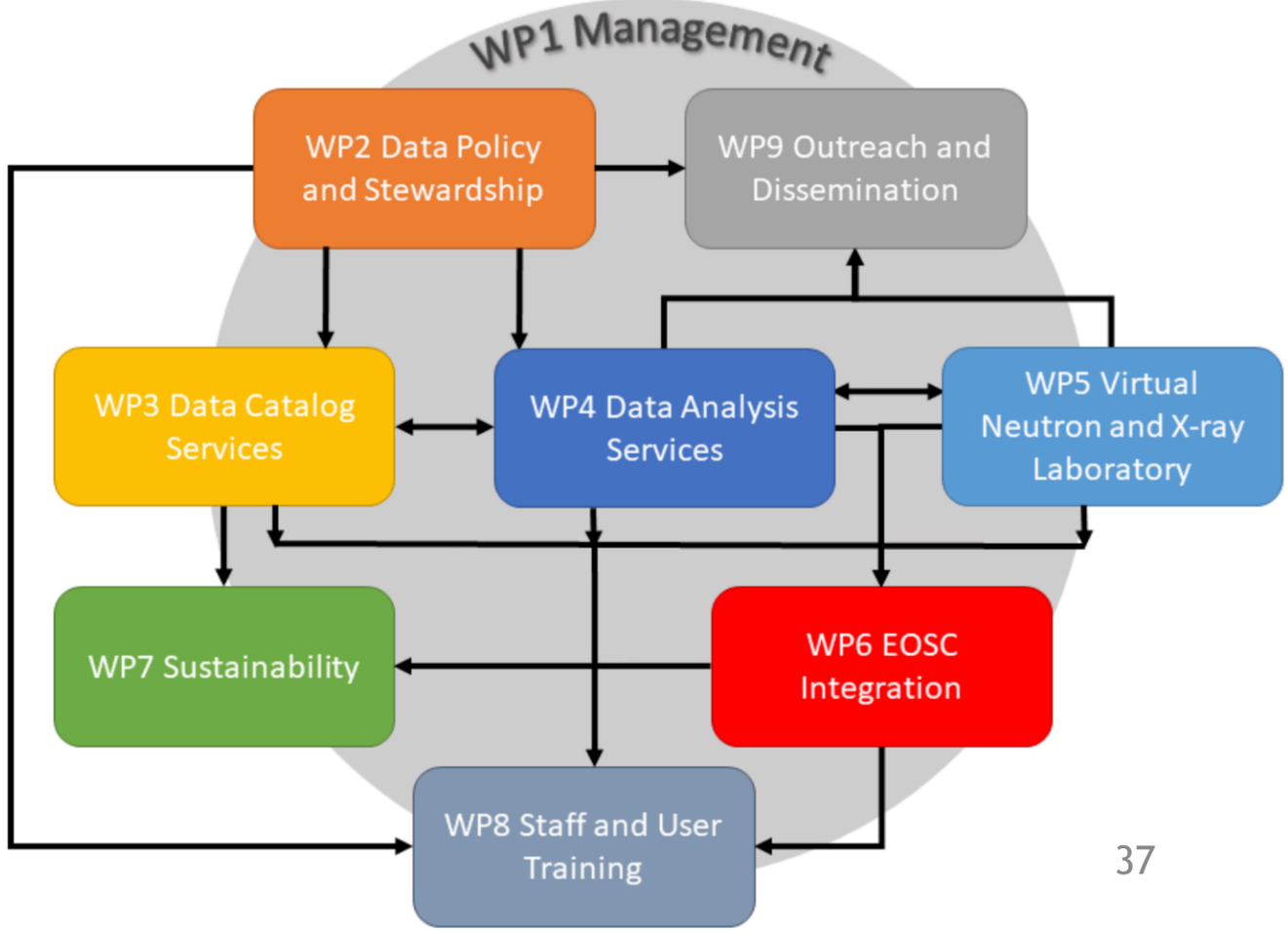
Diffraction Software landscape 2018

- ESS aims to lead a roadmap towards sustainability
- Current landscape assessed wrt sustainability



- PaNOSC proposal funded. Work starts January 2019
- ILL, ESRF, ESS, EUXFEL,ELI, CERIC
- Photon and neutron specific open science cloud
- Data management and analysis services
- ESS allocation 2M euro
  - Data management & curation
  - Policies and governance
  - Analysis
  - E-Learning
- DMSC leads
  - WP3 - Data catalogues
  - WP8 - User training

3.1 Work plan -Work packages, deliverables



Any questions?