DMSC STAP - September 2019
Project Update

Jonathan Taylor

Welcome & Charge

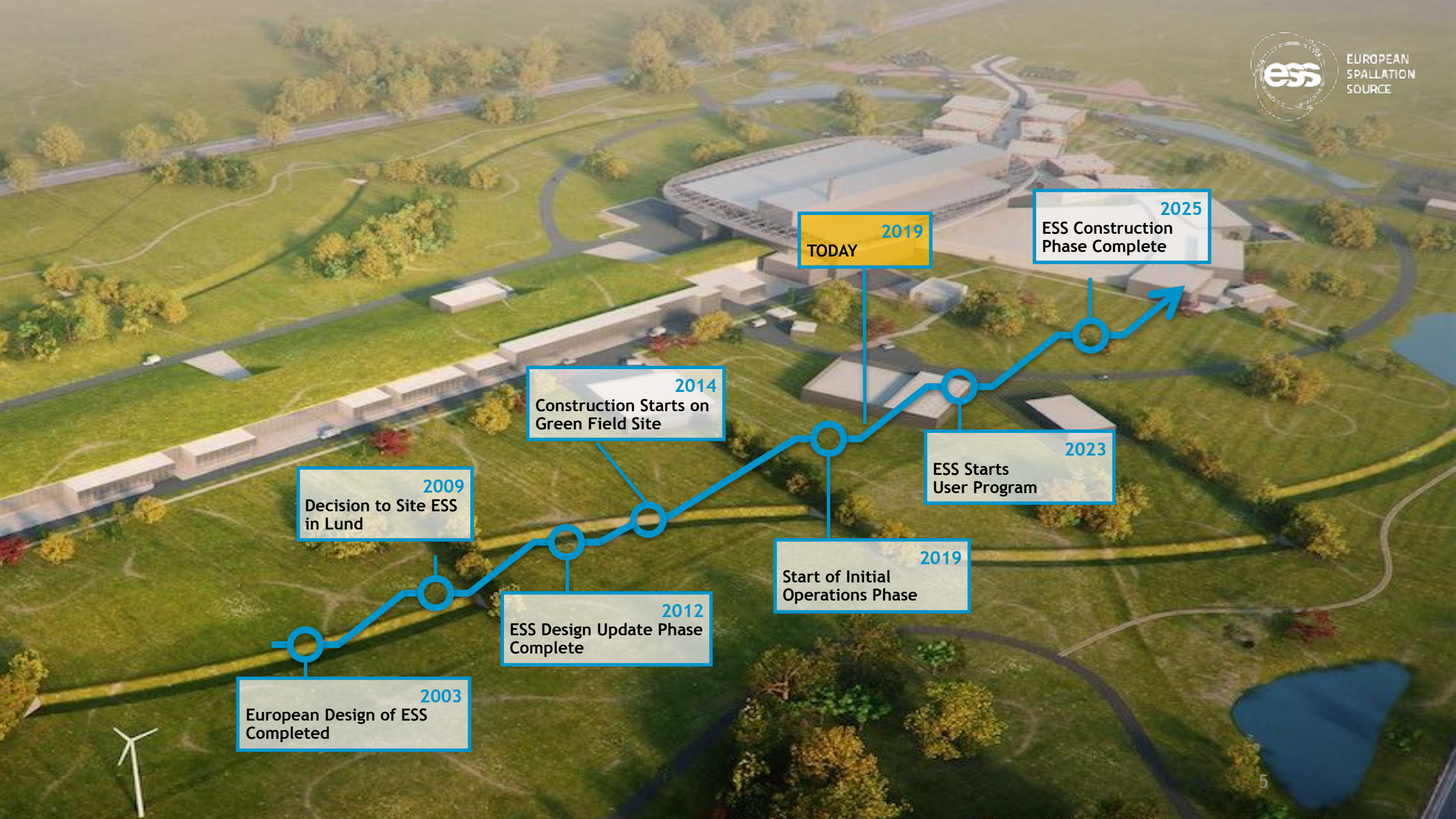
- Charge :
- Provide feedback, advice and recommendations on the progress of DMSC in respect of our planning, key technologies and risks.
- We request:
- Advice and recommendations on how we can ensure the new organisational structure of the science and technical directorate will have a positive impact on scientific computing at ESS.
- An evaluation of our resource request the initial operations period (2019 - 2025) for staff effort and capital investment.
- Advice and recommendation regarding our strategy for milestone planning for 2020-2025.
- Evaluation of our current level of completeness against our construction scope and advice / recommendation on how to best progress with instrument specific development and commissioning.

Summary

- ESS project update
- Initial Operations planning and budget
- BCT update
- Reorganisation for installation and cold Commissioning Phase
- DMSC status

ESS status

EUROPEAN SPALLATION SOURCE


EUROPEAN SPALLATION SOURCE
2003
European Design of ESS Completed
2009
Decision to Site ESS in Lund
2012
ESS Design Update Phase Complete
2014
Construction Starts on Green Field Site
2019
TODAY
2019
Start of Initial Operations Phase
2023
ESS Starts User Program
2025
ESS Construction Phase Complete

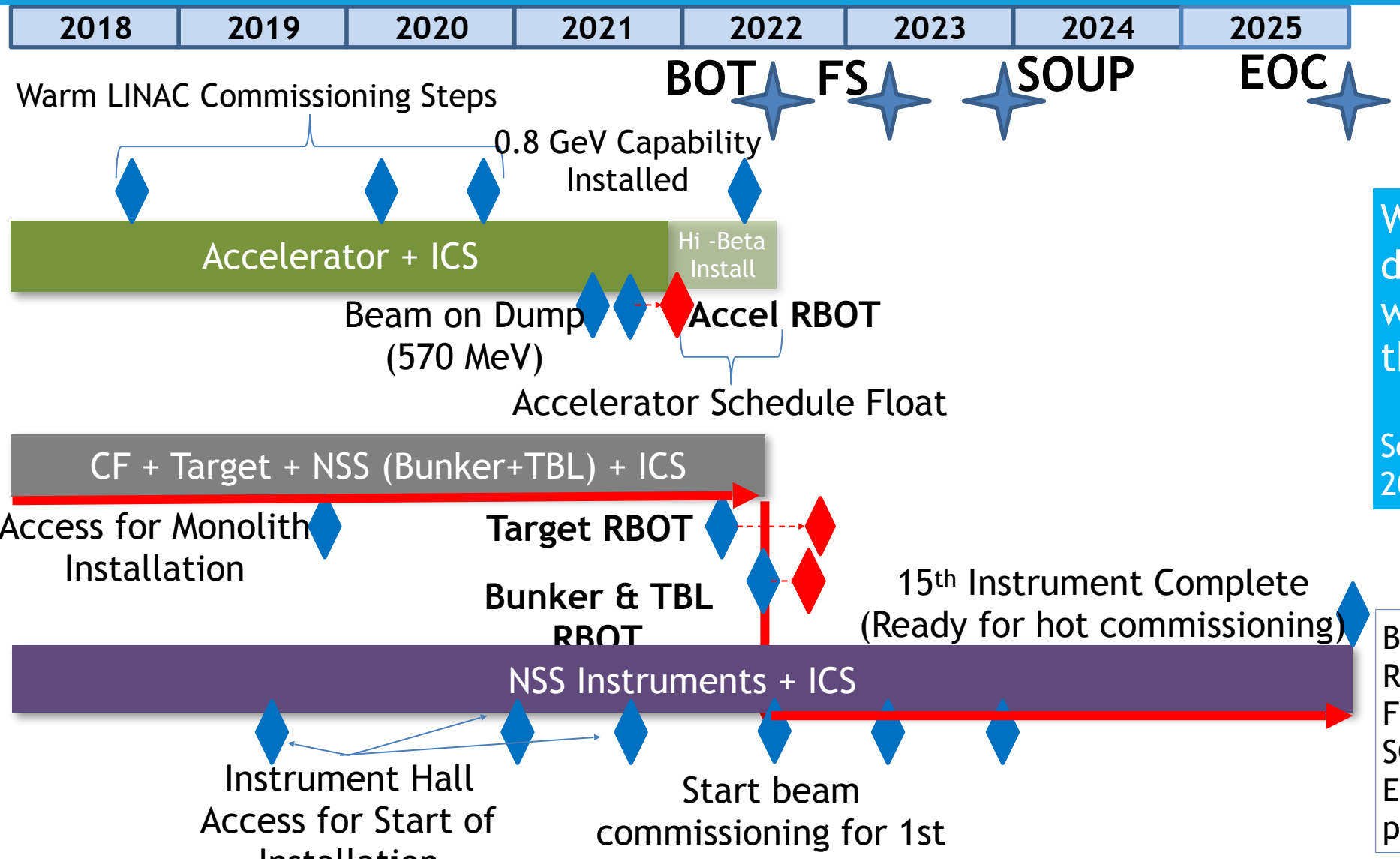
ESS update

- Project is 60% complete
- Currently tracking the 2018 baseline
  - Some delays 3-6m possible on BOT

- Initial operations has begun:
  - Accelerator installation making rapid progress
  - Ion source and LEBT commissioned
  - MEBT installed
  - DTL received and being integrated
  - RFQ delayed, but final components expected this week
  - Cryo-test stand permit received

- Project contingency is low
- Initial operations funding expected to be 810M
- Organisational structure changing to address installation and integration.

The ESS Critical Path

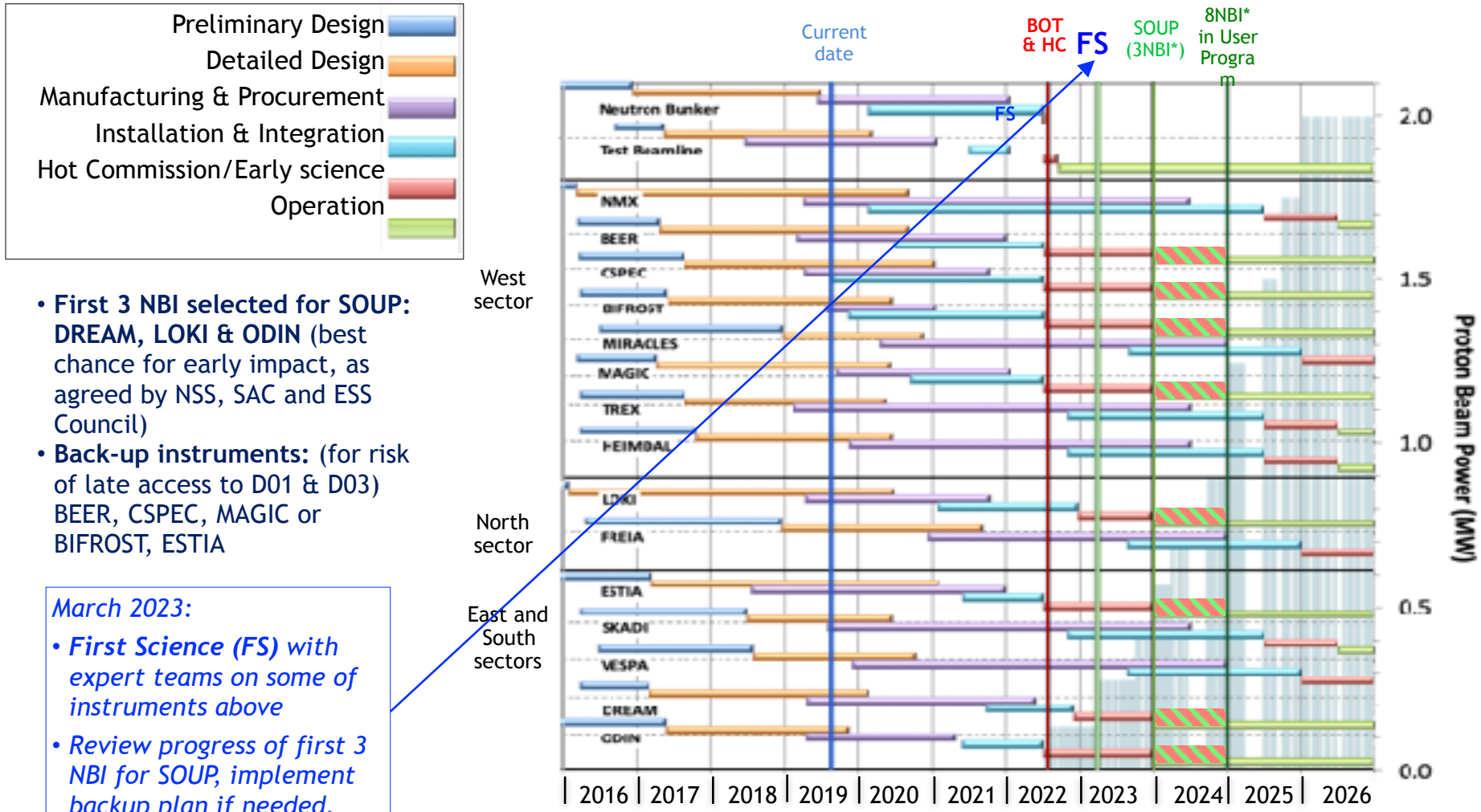


We are focused on delivering First Science with three instruments by the end of 2023

Schedule date (no float) is March 2023

BOT - Beam on Target
RBOT - Ready for Beam on Target
FS - First Science
SOUP - Start of User Programme
EOC - End of Construction project

Baseline schedule for Neutron Beam Instruments
(NSS MS V4.2)



- **First 3 NBI selected for SOUP: DREAM, LOKI & ODIN** (best chance for early impact, as agreed by NSS, SAC and ESS Council)
- **Back-up instruments:** (for risk of late access to D01 & D03) BEER, CSPEC, MAGIC or BIFROST, ESTIA

March 2023:

- ***First Science (FS)** with expert teams on some of instruments above*
- *Review progress of first 3 NBI for SOUP, implement backup plan if needed.*

* NBI = Neutron Beam Instrument

NSS major non instrument IK work packages: (total value 20.3 M€)

		CBV (k€)	
Science and Technology Facilities Council	Detector Readout	2,500	
Science and Technology Facilities Council	Data Reduction and Experiment Control	1,586	
Science and Technology Facilities Council	Data Streaming Infrastructure	1,296	
Science and Technology Facilities Council	User Laboratory equipment	1,000	
Forschungszentrum Jülich	Data Analysis & Modelling (FZJ)	791	
Paul Scherrer Institute	Experimental Control Software	749	
Helmholtz-Zentrum Geesthacht	Am-CLD demonstrator detector	572	supply & services agreement
Paul Scherrer Institute	Data Curation (Adara - Data Cataloguing)	554	
Forschungszentrum Jülich	Test Package for Linear Motion Technology	511	work package complete
National Research Council of Italy	GEM Detectors	500	work package complete
Paul Scherrer Institute	Data Analysis & Modelling for Imaging	471	
Forschungszentrum Jülich	Robotics Sample Changer Platform	466	
Forschungszentrum Jülich	Standardised High speed choppers	460	supply & services agreement
The University of Tartu	Gas Handling Systems	400	work package complete
The University of Bergen	DEMAX - Macromolecular Crystallisation	305	work package complete
Forschungszentrum Jülich	Choppers control system integration	300	supply & services agreement
The University of Tartu	Laser-Neutron Pump-Probe Experiments	196	work package complete
Roskilde University	Peltier Temperature Control Sample Platforms	171	work package complete
	sub-total value (k€)	**13,328**	

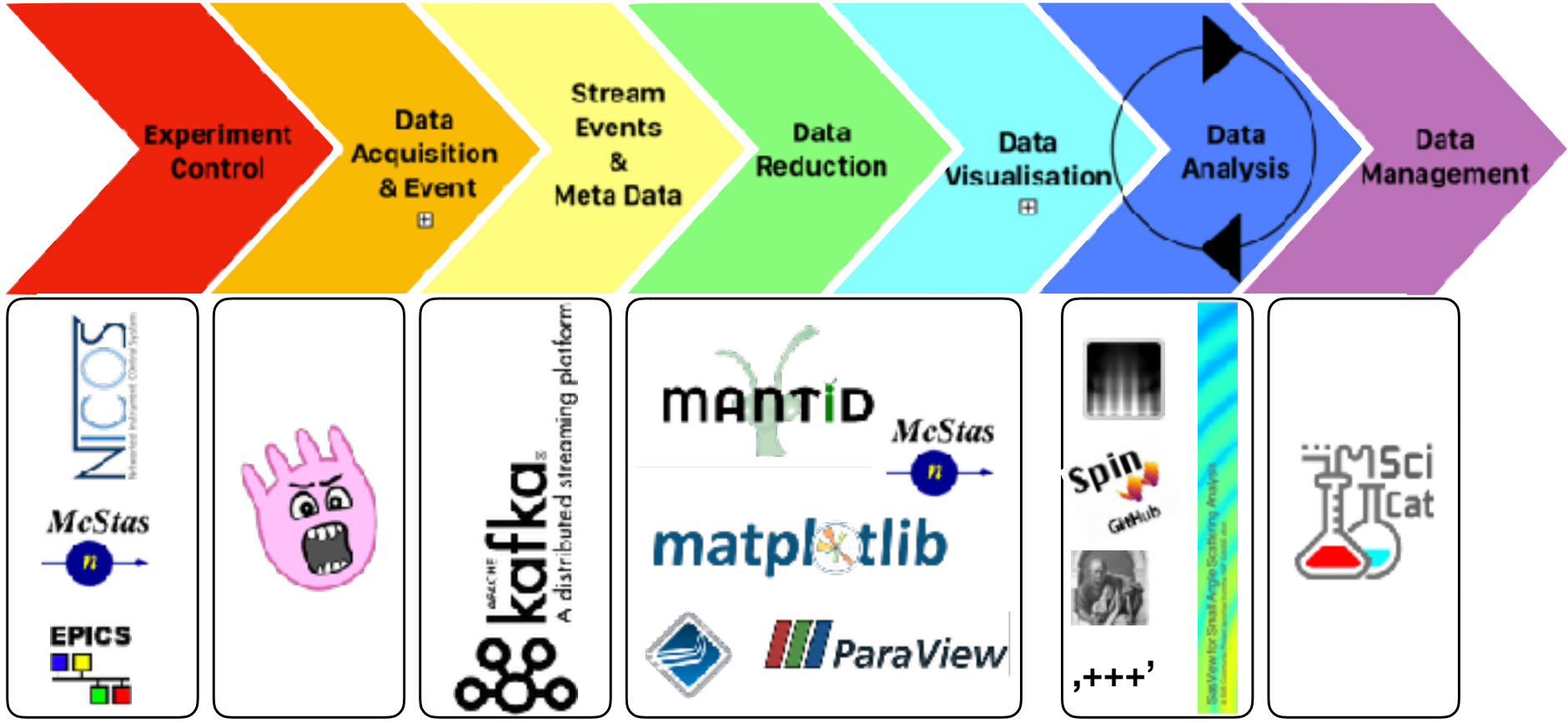
- DMSC inkind (Red)
- DMSC inkind Ends 2021 (q1)

Current total value (including planned work) = 20.3 M €

Sept 2019

Scientific Computing Pipeline

- Neutron Instruments Division 15x Instrument projects
- Detector group
- Motion Control & Automation
- Chopper Group
- Scientific Activities Division
- Integrated Controls System Division
- Accelerator



DMSC Construction phase & Initial Ops Phase

- 2019 Prioreties
  - Complete DMSC construction phase.
  - Begin Installation in E buildings / site (Science directorate objective)
    - Network & testing Comms rooms -> CUB Server room
  - Start user office development after Demax prototype
  - Develop instrument specific project plans and coordinate with instrument installation planning

Schedule I

2013 2014 2015 2016 2017 2018 2019

Construction Funding -20.2M
Development of core technologies and capabilities. DMSC ready for BOI

DMSC Scope setting
5M moved to
Initial Operations

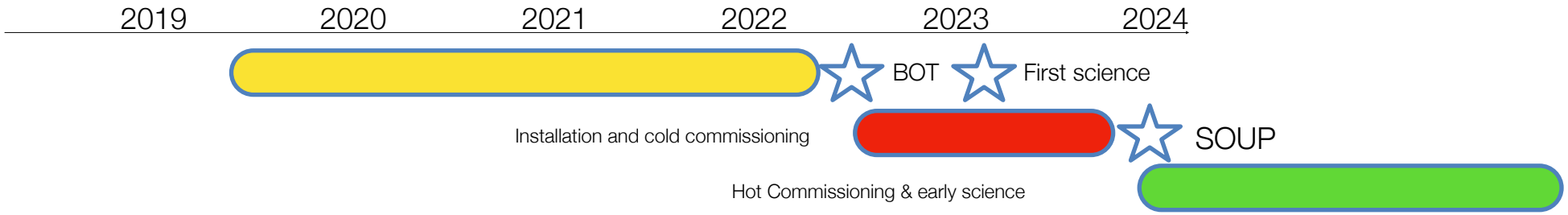
ESS re-baseline
First Science 2023

SINE2020 WP10

Brightness Wp4 4.5M

STFC, PSI, Julich In-kind - Data reduction controls & analysis

Schedule II



DMSC end of construction activities
Baseline architecture and software ready

ESS infrastructure installed
H01 server room & network

DMSC construction InKind for core data reduction & analysis

Deliver deferred scope from construction

Instrument projects Focus on first 8 instrume
Commissioning systems along with ins
Development of Instrument & techn

ort and development

Training activities
Users and Staff

nissioning and early
ence support

Instrument projects Instruments 9- 15
Commissioning systems along with installation
Development of Instrument & technique specific Control, reduction & analysis.

Considerable coordinated effort & planning required for installation, integration & commissioning.

2020 onwards Milestone strategy

Integration of DMSC activities with Instrument Construction.

- Generic Milestone list generated.
  - Motion, Choppers, detectors
  - Covers the installation requirements and upstream dependencies

- Schedule will be centrally developed & Managed by NSS planning team and fed into P6

- Requirements from DMSC on instruments developed.

- Points of contact were to be instrument data scientists.
  - DMSC point of contacts depend on hiring and STAP advice.

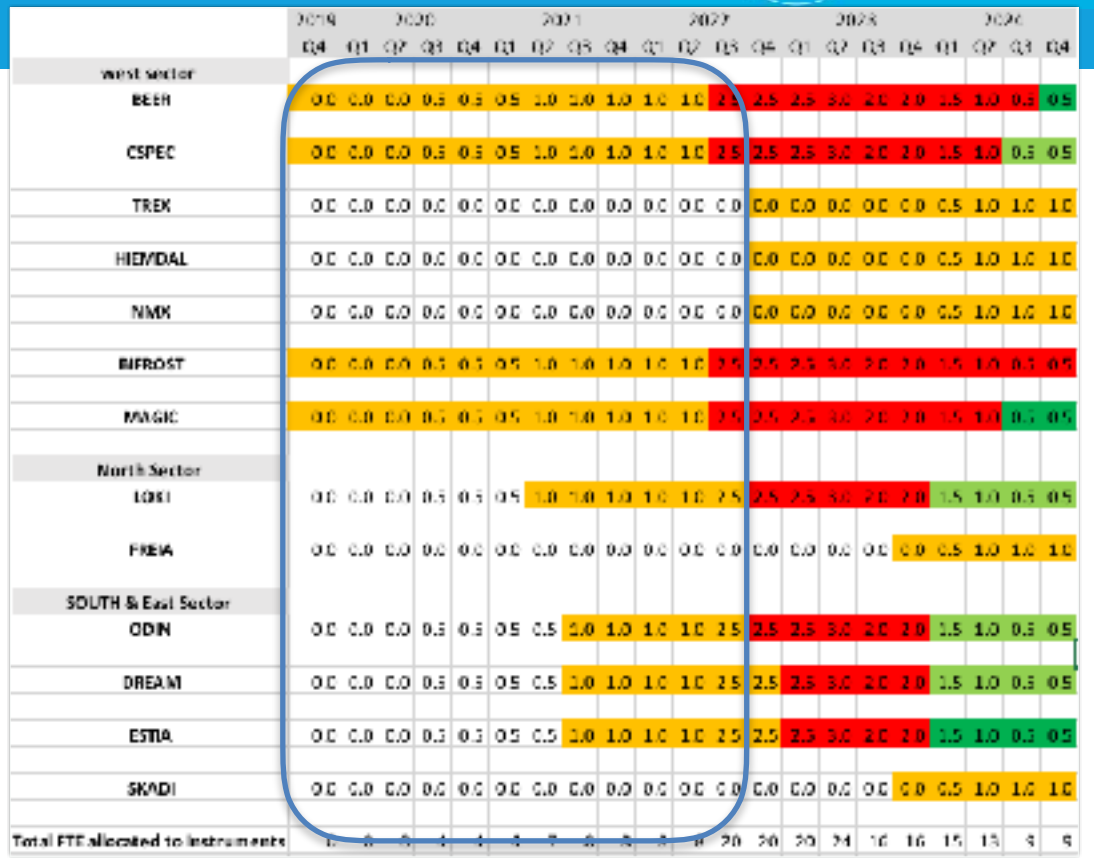
Surveyed positions for	
	Chopper axis positions
	Guide geometry & alignment
	sample position
	detector panel positions / offsets of active area for surveyed positions
	individual pixel / voxel locations can be derived
	Monitor positions
	Surveyed L1 and L2 flightpaths
	geometry co-ordinates to follow mantid convention with z as beam direction - thus R,T,P will work directly
	Pre calibrations either lab or part of cold commissioning
	Chopper axis geometry and slit positions from lab tests
	Motor calibration of steps / mm and sense - (part of cold commissioning of motion axis)
	Chopper geometry pre calibration

Overview on staff resources required to meet SOUP schedule

- Scientific computing scope delivered from DMSC
  - 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

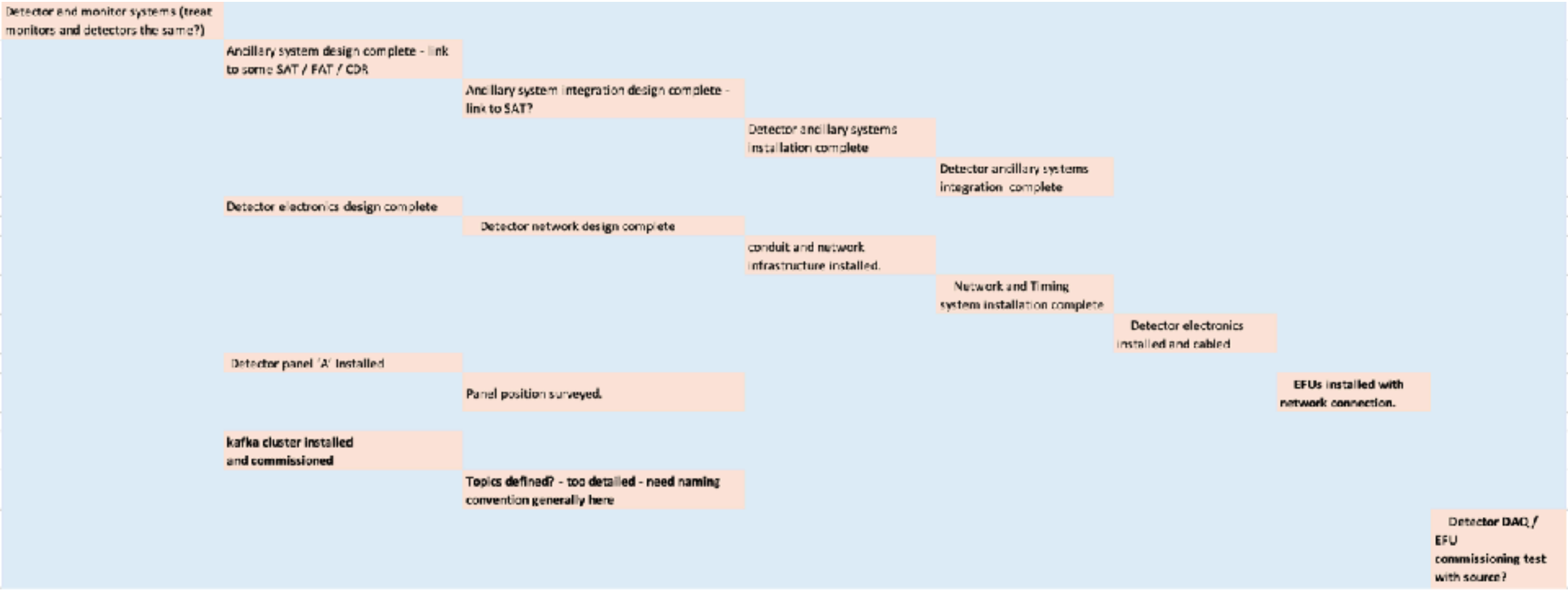
- Instrument data scientists hired 2020



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	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

Generic milestones (just for detectors)

Coordination of milestones with installation schedule made by central planning team.



Instrument requirements refresh

- Information to be held on the instrument confluence pages
- https://confluence.esss.lu.se/pages/viewpage.action?pageId=311646930

Current planned staff resources

- Deferred scope from 2016 front loaded
- All instrument specific development

	2020	2021	2022	2023	2024	2025
TOTAL FTE ex Admin & Mangament	39.5	40.75	44	47	47	48
DRAM	15.5	15.75	18	20	20	21
ECDC	11	12	13	14	14	14
SWAP	5	5	5	5	5	5
DST	8	8	8	8	8	8
Instruments in construction	4	9	6	7	7	3
Hot Commisioning /Early Science at EOY	0	0	6	8	0	4
Instruments User programme at EOY	0	0	0	0	8	8
	4	9	12	15	15	15
staff per instrument	9.875	4.52777778	3.66666667	3.13333333	3.13333333	3.2
	Staff cost per year					
	2020	2021	2022	2023	2024	2025
	4977	5134.5	5544	5922	5922	6048
deferal FTE	10.5	6.75	5			
defreal value	1323	850.5	630			

Initial operations funding

- ‘Instrument specific development’ for all scope moved into initial operations period 2019 -2025.
- Capital investment for instrument computing (including for instrument control cabins)
- Sum of staff resources is
  - Per instrument scheduled at ~20py effort for each instrument including hot commissioning for instru. 1-8.
  - 7.5 py for installation
  - Total across division (to include core development maintenance / support - xx
- 12 hires scheduled for 2020 to include
  - Instrument data scientists
  - Additional effort for ECDC
  - Additional effort for SWAP - already moved from original plan of hiring in 2019

DMSC Structure & planned staff for 20 - 23

	Data Systems & Technologies	Experiment control Data curation	Scientific Web Applications	DRAM(s)	Project admin (Petra Aulin)
	5 staff 1 PaNOSC	6 Staff 1 PaNOSC 5 FTE IK	3 Staff (1/5) 1 ©	10 Staff 1 PaNOSC 5.5 FTE IK	3 Staff
2023 SOUP 3 Instruments	8FTE	14FTE	5FTE	15 FTE (20FTE inc Planned Simulation)	3 staff

Development of a credible baseline provision for analysis, reduction and control
Next generation analysis provision remains the overall objective for ESS

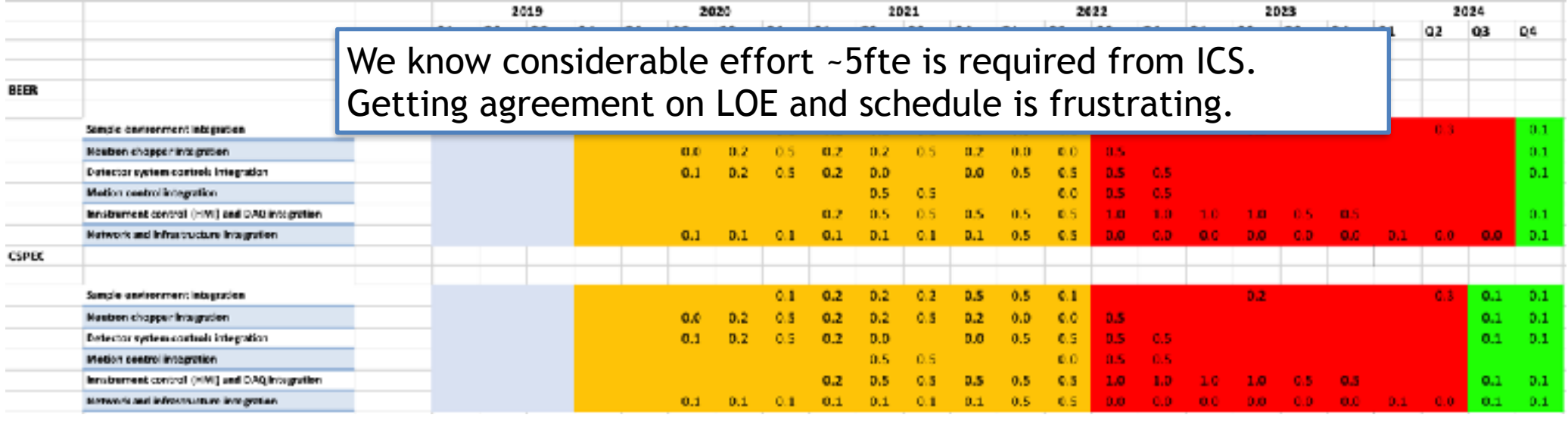
- SL 0 - Control of instruments and acquisition of data, archive and curation of collected data
- SL 1 - Framework for manual data reduction, Data analysis packages manual operation
- SL 2 - Automated reduction workflows, automated analysis - experiment control feedback
- SL 3 - Data Analysis Service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

Beam Line Controls team

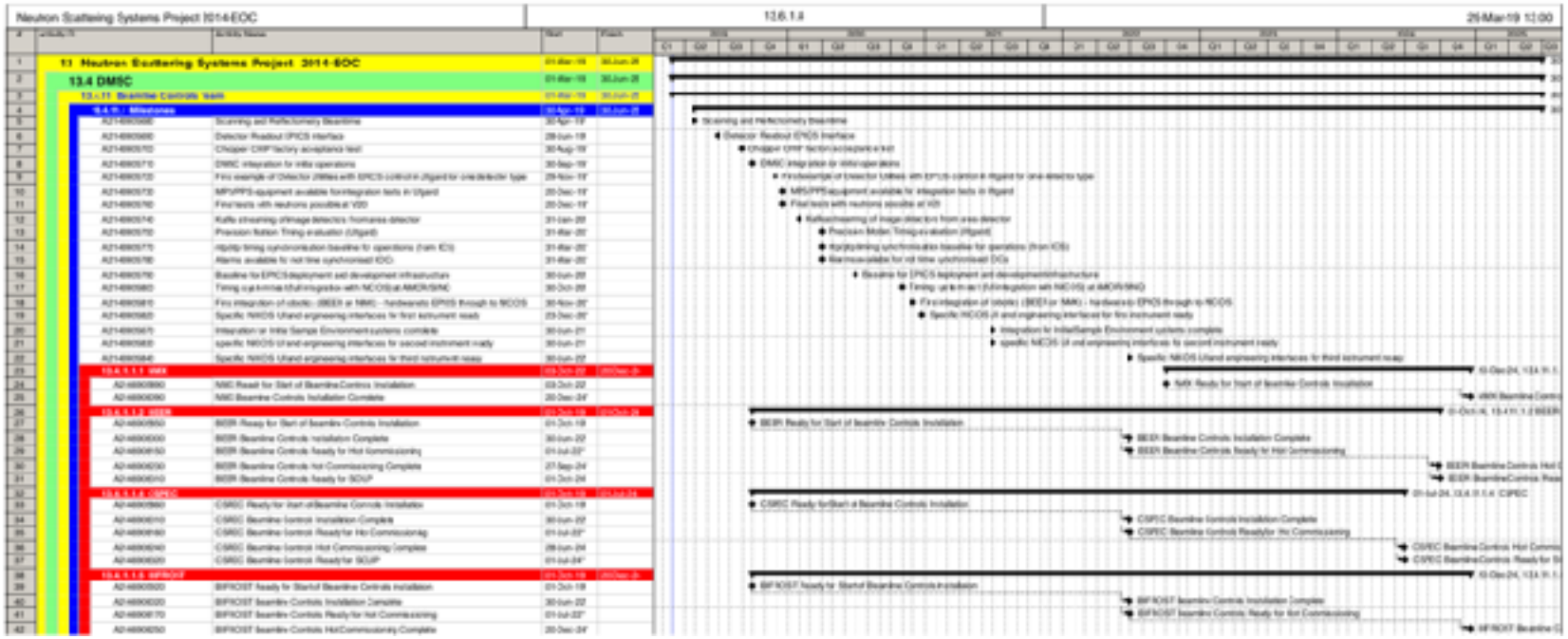
- Staff matrixed from NSS & ICS
- Provide a single entity for communication, prioritisation and delivery
- Led by NSS
- NSS owns scope and controls activities
- Resources requirements reviewed regularly
- This is not a service delivery model for ICS

- Requires careful planning to match instrument installation to match available LOE.
- Awaiting formal agreement from ICS on this delivery model for instrument integration
- 10 FTE required 2019 6FTE allocated
- 20 —>23 increases to around 13 FTE for any quarter

We know considerable effort ~5fte is required from ICS.
Getting agreement on LOE and schedule is frustrating.



BCT II

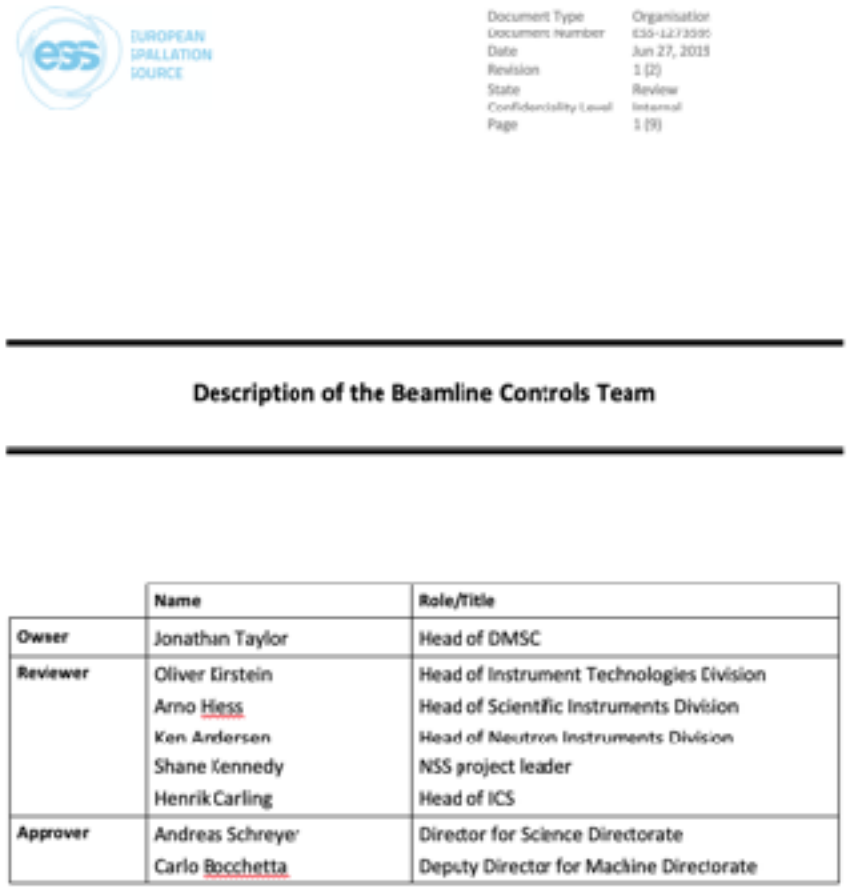


- Detailed P6 plan from now until TG5
- Covers Instrument specific controls and core technology development.
- Aligned with the current NSS baseline

- NSS plan is not at sufficient level of detail for ICS to plan provisioning resource

BCT Current Status

- Awaiting comment and / or approval of the steering document
- BCT works effectively in-spite of intransigence of ICS management.
- Status could be resolved as part of the re-organisation



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State	Review
Confidentiality Level	Internal
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Description of the Beamline Controls Team

	Name	Role/Title
Owner	Jonathan Taylor	Head of DMSC
Reviewer	Oliver Kirstein	Head of Instrument Technologies Division
	Arno Hiess	Head of Scientific Instruments Division
	Ken Andersen	Head of Neutron Instruments Division
	Shane Kennedy	NSS project leader
	Henrik Carling	Head of ICS
Approver	Andreas Schreyer	Director for Science Directorate
	Carlo Bocchetta	Deputy Director for Machine Directorate

Desired outcome

Focus on organisational priorities

(Build the facility AND ESS' operational capacity)

Agile decision-making process

Better integration and coordination using common processes

Achieve First Science 2023

NSS Project work packages *(Essential for first science)*:

- Neutron bunker: BOT
- Test beamline: BOT
- All Neutron Instruments (15): each Tollgate 5 (Hot commissioning)
- NSS Infrastructure (electrical and services): Tollgate 5 on 3 instruments
- Common guide shielding: Tollgate 5 on 3 instruments
- Common slow choppers: Tollgate 5 on 3 instruments
- Detectors: Completion and acceptance of detectors for CSPEC, ESTIA; and Tollgate 5 on 3 instruments
- DAQ and Beamline Controls: Tollgate 5 on 3 instruments
- Safety and Licensing: obtain license to operate facility

Scope that remains with the Science Directorate until onset of Hot Commissioning (TG5):

- *Scientific Advocacy and Programme Development*
- *Prepare for First Science and Start of User Program*
- *Scientific Activities including User Program*
- *DMSC activities not related to Data Acquisition*
- *Sample Environment Equipment: first science (or SOUP) on 8 instruments*
- *MCA systems*
- *Laboratory Facilities*

Summary of Concepts

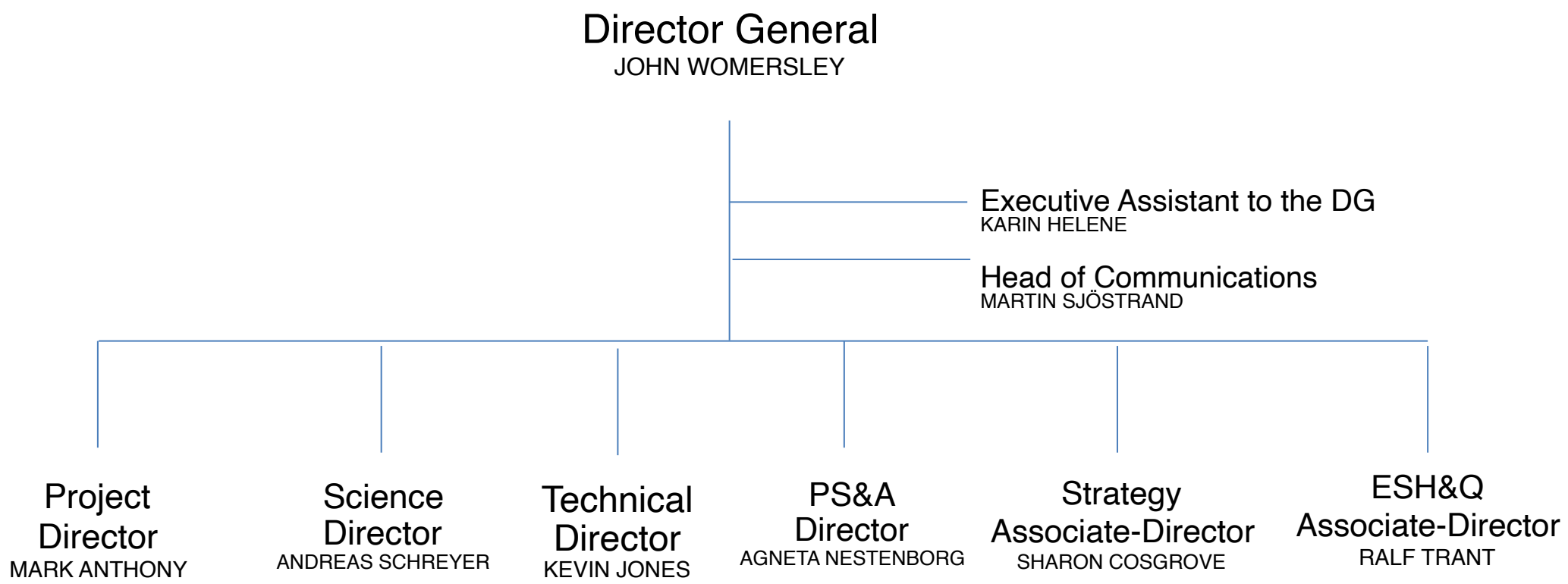
- Project, installation and integration is moved into a single organisational unit

- Key concepts.
  - Some SD staff move into TD Line management - SK and KJ
  - Some SD staff move into Installation and Field Support Line MA
  - Some SD staff remain in SD Line AS

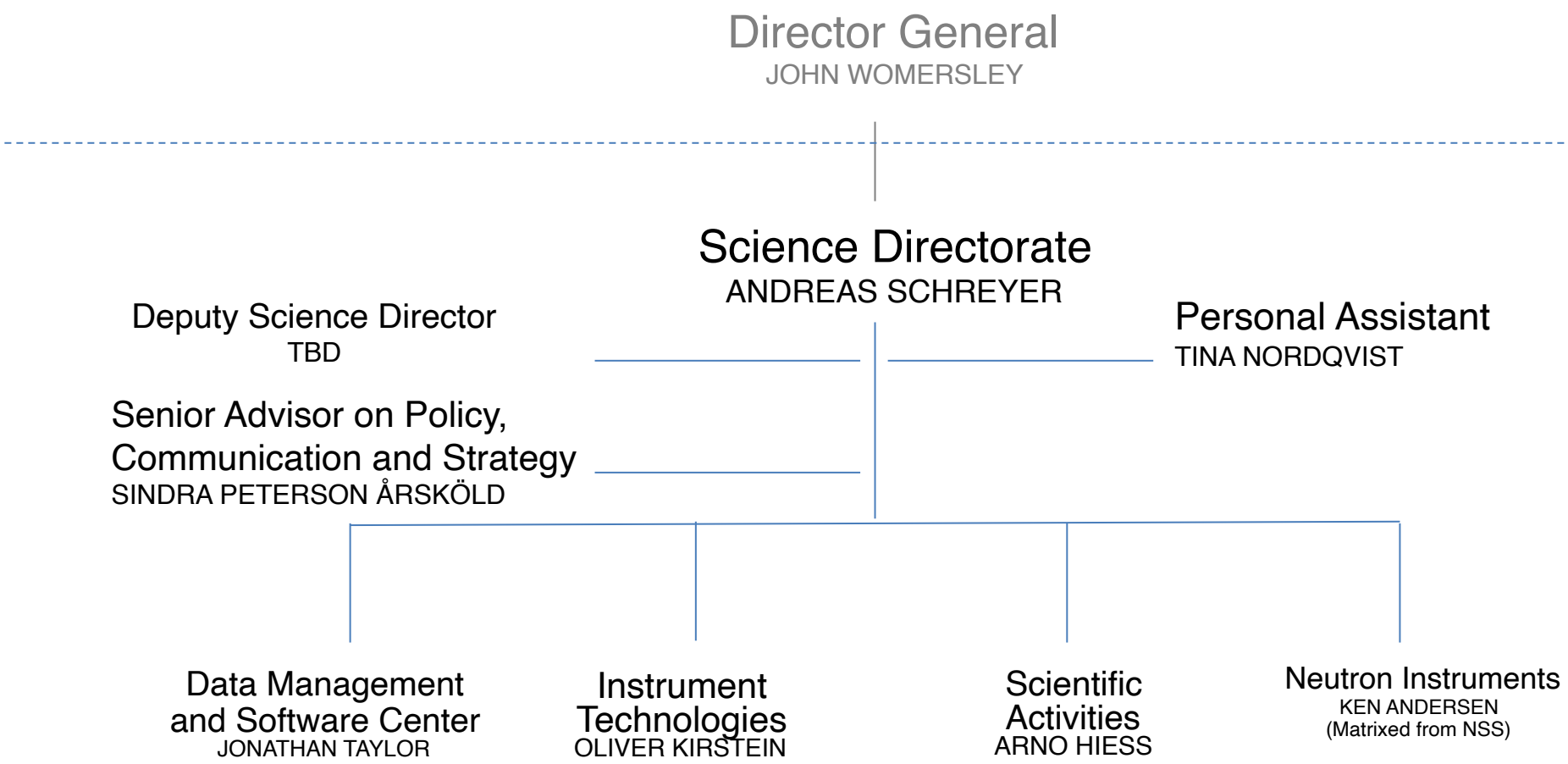
- Scope and responsibility transfers back to SD at TG5 for 3 instruments.
  - Coincides with BOT

Future organization negotiated and agreed:

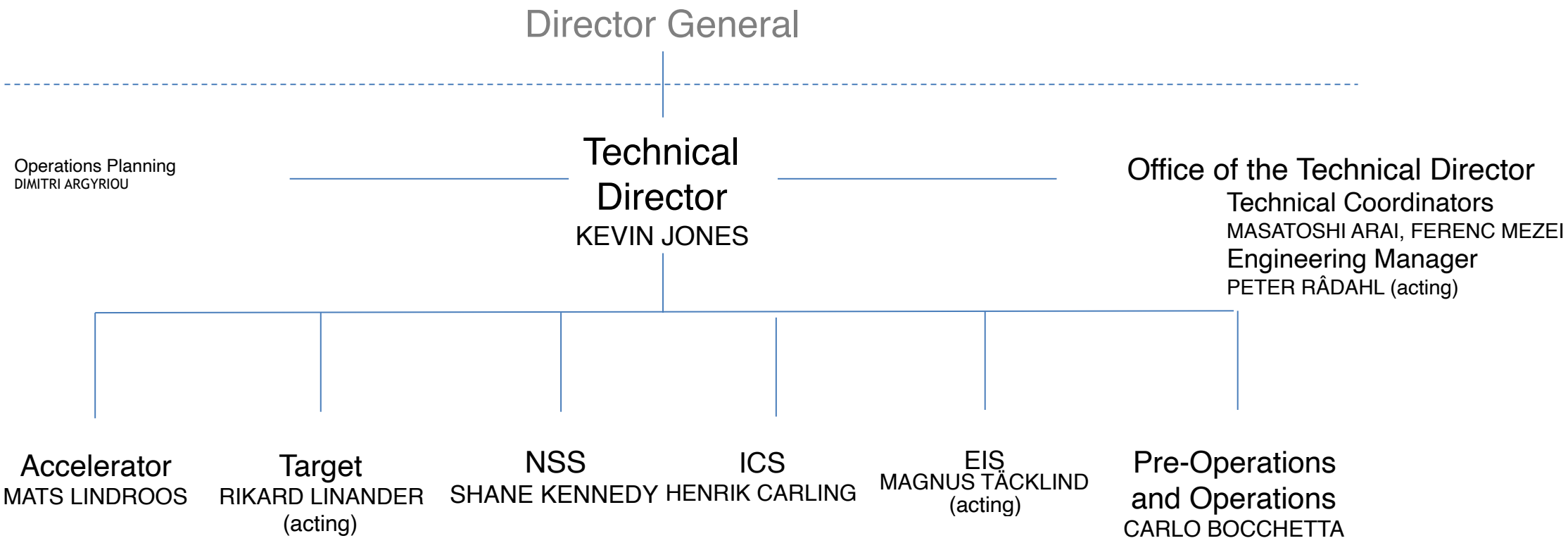
ESS Executive Team



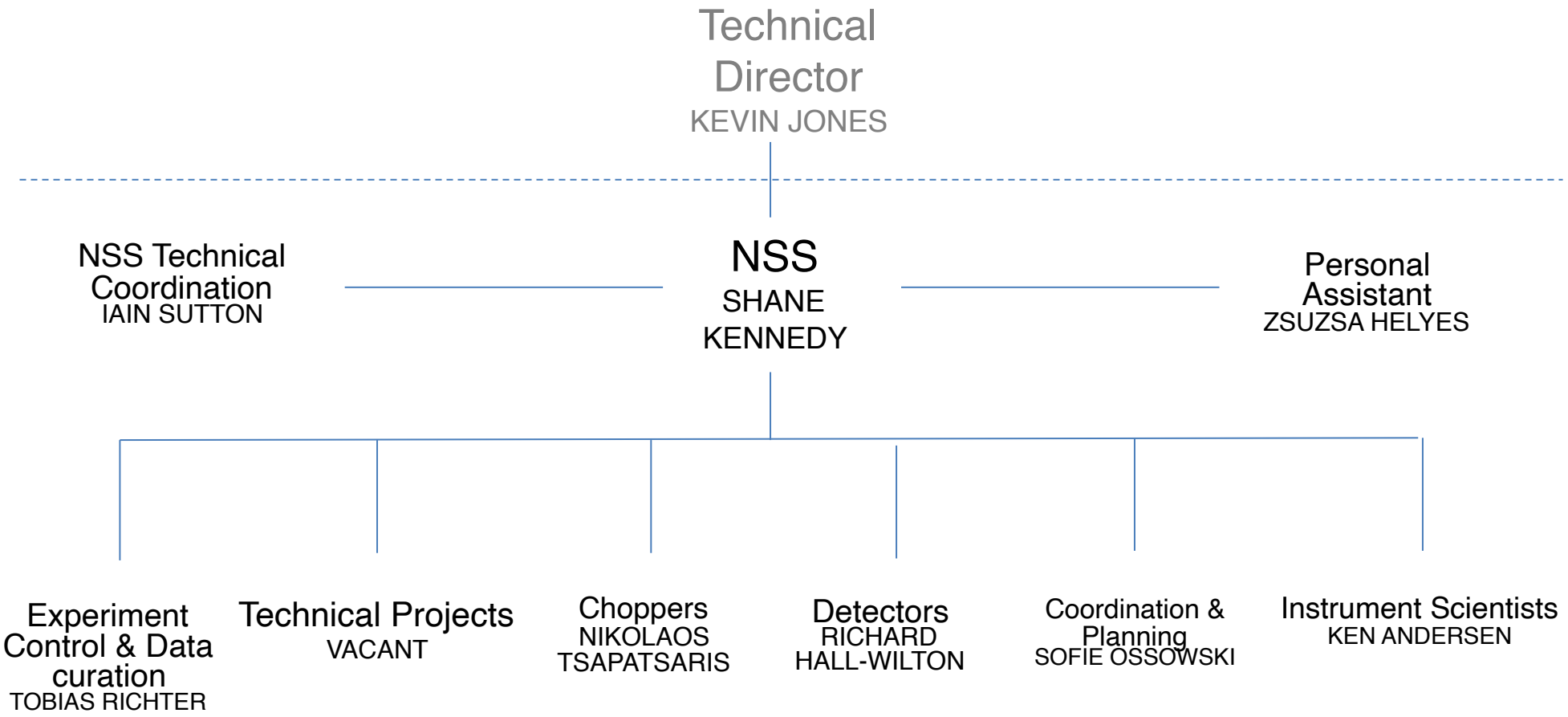
Future organization to negotiate
Science Directorate (overview)



Future organization negotiated and agreed:
ESS Technical Directorate



Future organization to negotiate
NSS



DMSC update

- Huge amount of progress has been made in the last 6m.

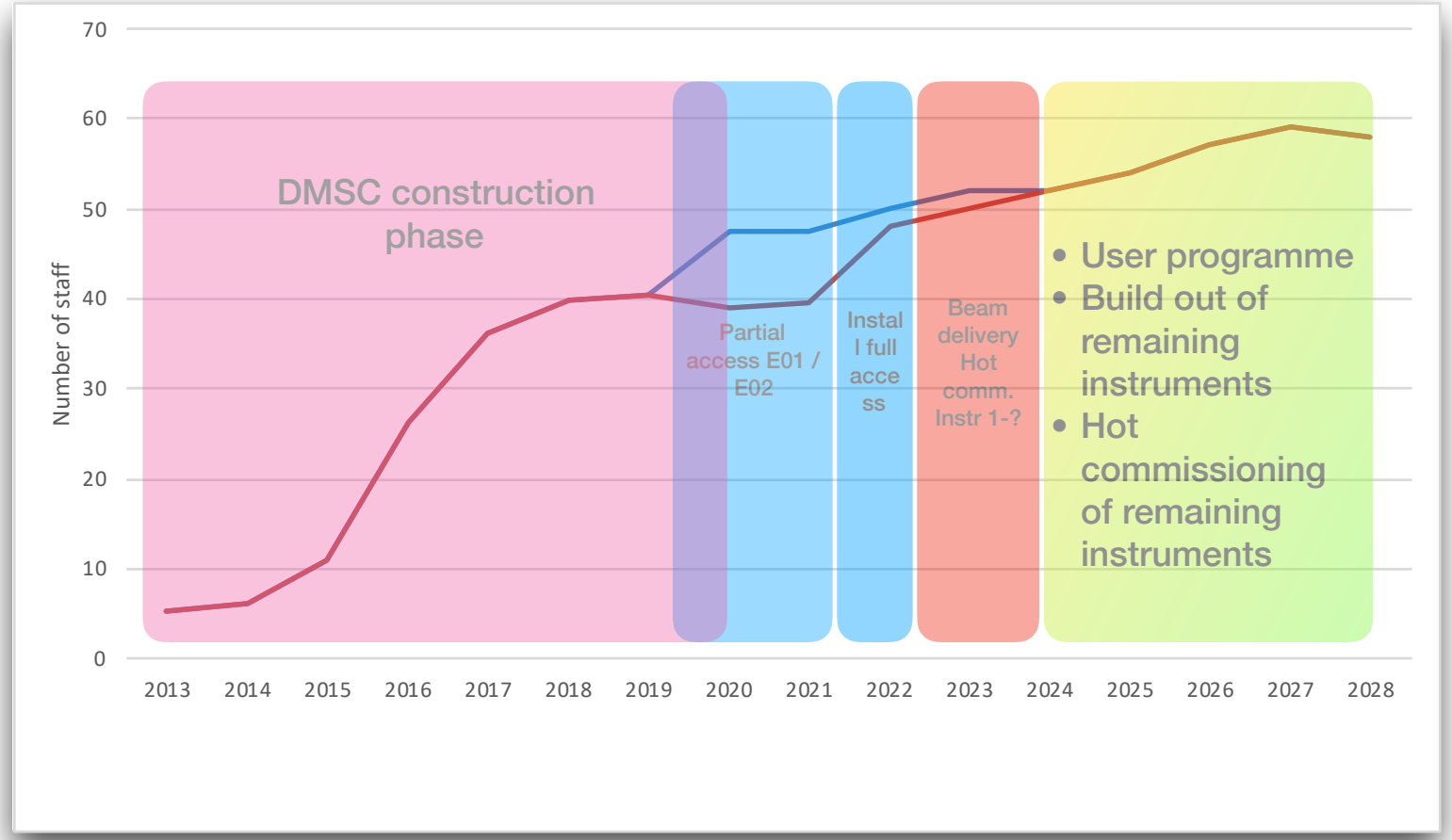
- BCT & data pipeline verified on V20
- Utgaard test area now a ‘virtual beam-line’
- Spectrum scale testing
- User office development started
- Development of
  - Imaging software
  - Diffraction software
  - Data reduction & visualisation development of SCI++
- Server room build completed
- Link in place (pending some tests)

Any questions?

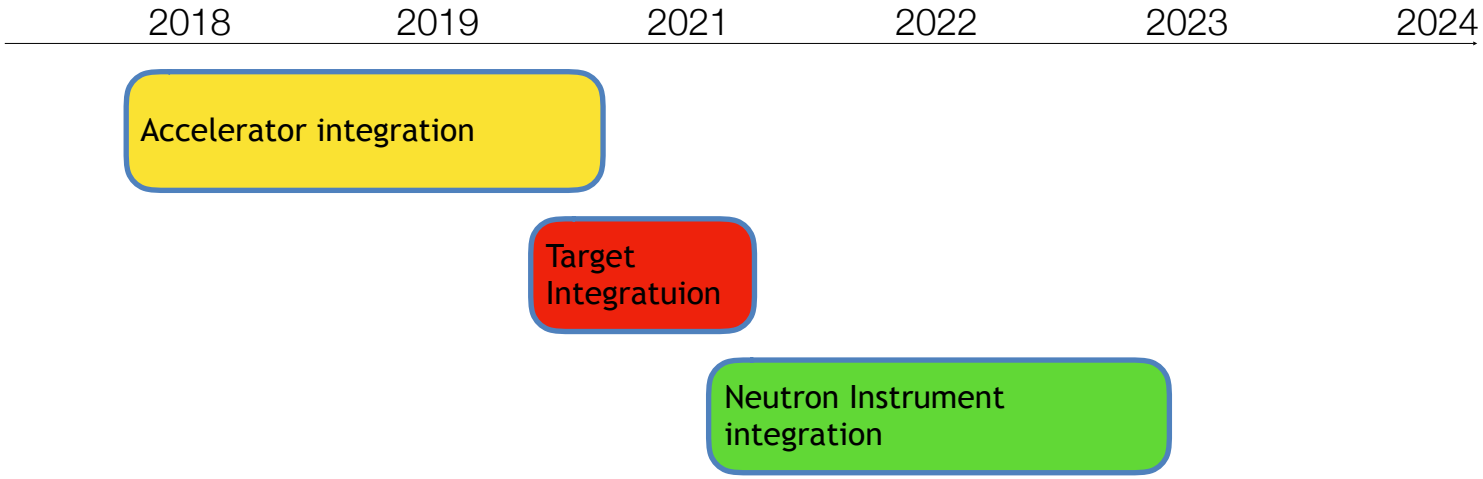
DMSC staff profile and ESS high level plan

- **DMSC scope Service level 0 - essential for operations**
  1. Detector readout linked with Detector group
  2. Experiment control linked with ICS
  3. Data acquisition linked with #1 & 2
  4. data management

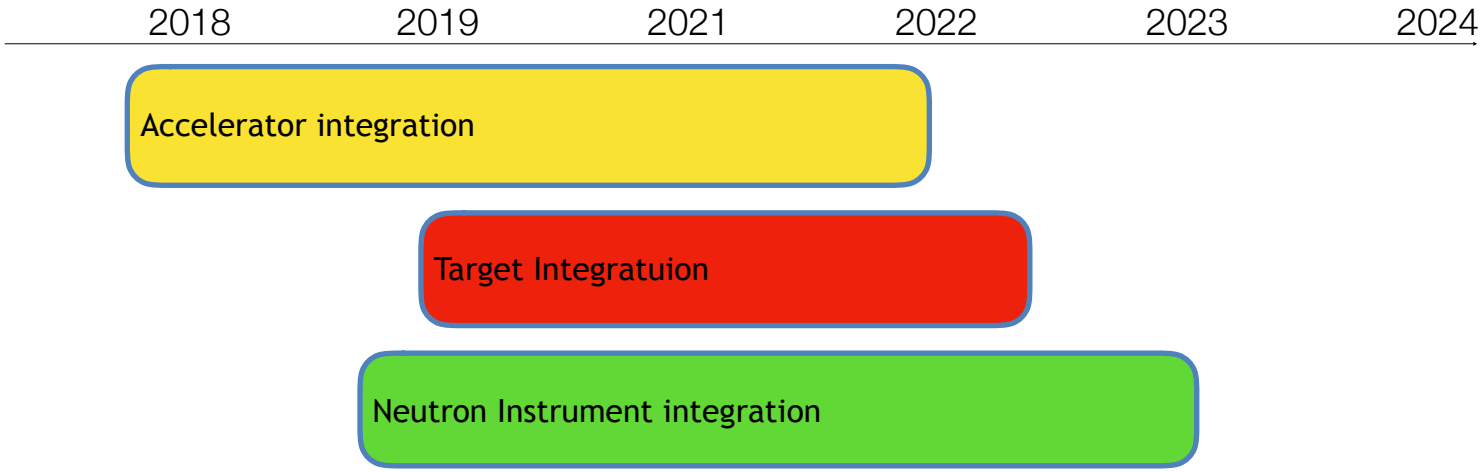
- **DMSC scope Service level 1 - essential for science delivery**
  1. Data reduction (SL 2 fully automatic)
  2. Data analysis (SL 2 fully automatic for standard runs)
  3. Simulation and modelling - essential for impact.



Integrated Controls System



Original ESS integration strategy
Based on linear progression (and expectation from ICS)
Organisation expected a service delivery model



Current requirements from key stakeholders for integration requires a parallel approach.

ICS under considerable pressure
80% of activities directed toward Accelerator

Neutron technology staffing initial operations

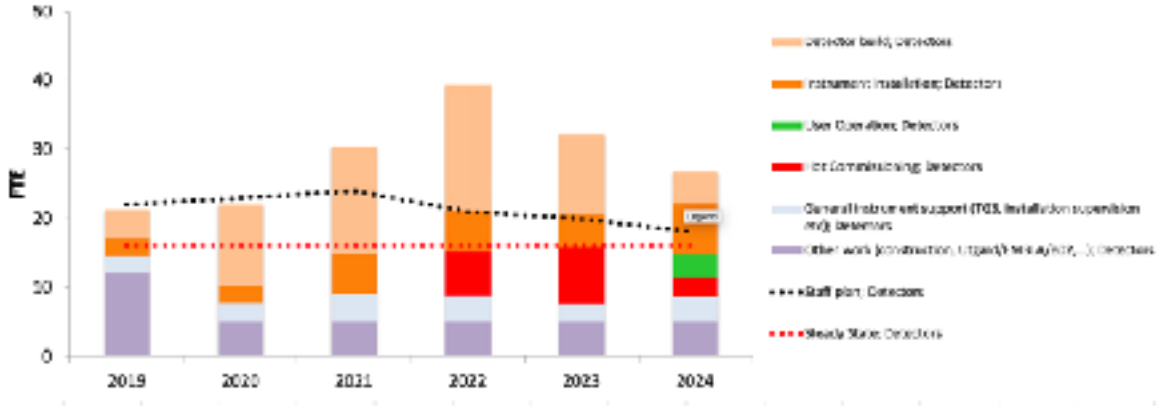
Neutron technologies

All aspects considered i.e. detector construction

Matched to Install schedule

Matched to installation LOE estimates.

Hot commissioning resources covered by ESS initial operations budget



Neutron Detector Group LOE

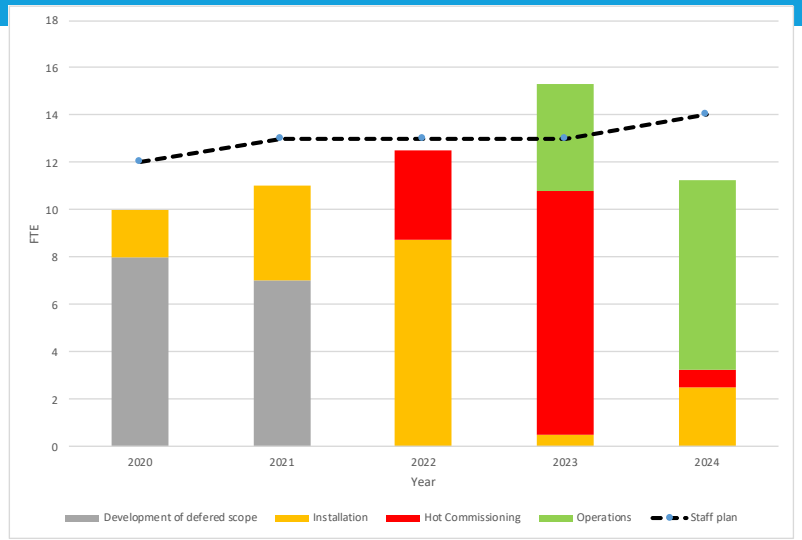
			2019				2020				2021				2022				2023				2024			
			Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
West Sector	BEER																									
		Optics&Shield	0.1	0.1	0.1	0.0	0.5	0.5	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.5
		Detectors	0.1	0.1	0.1	0.0	0.5	0.5	0.5	1.0	1.0	1.0	1.0	2.0	2.0	2.0	2.0	2.0	2.0	2.0	2.0	2.0	2.0	1.0	1.0	0.5
		Choppers	0.1	0.1	0.1	0.4	0.8	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.5	0.8
		MCA	0.1	0.1	0.1	0.3	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	0.5	0.5
	CSPEC																									
		Optics&Shield	0.1	0.1	0.1	0.0	0.5	0.5	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.5	0.5
		Detectors	0.1	0.1	0.1	0.0	0.0	0.5	0.5	1.0	1.0	1.0	2.0	2.0	2.0	2.0	2.0	2.0	2.0	2.0	2.0	1.0	1.0	1.0	1.0	0.5
		Choppers	0.1	0.1	0.1	0.8	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.5	0.8	0.5
		MCA	0.1	0.1	0.1	0.3	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	0.5	0.5

Resources for installation & commissioning

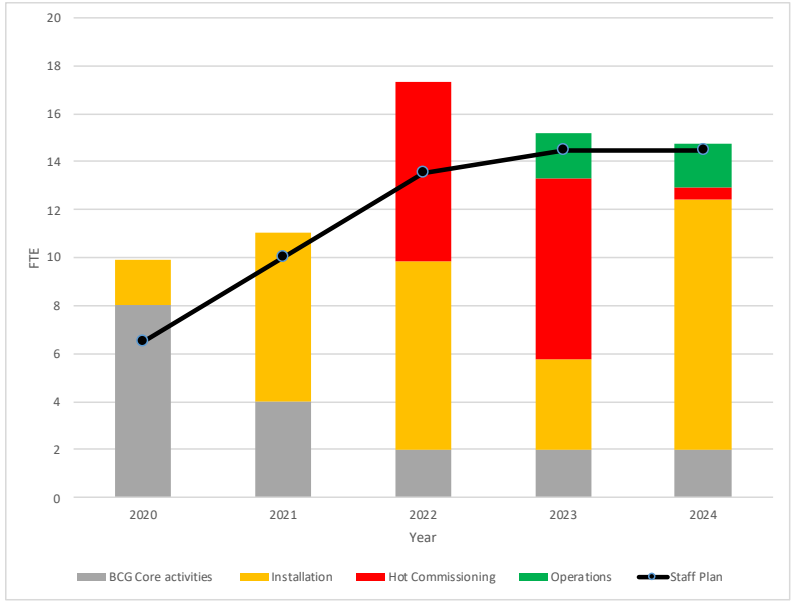
- 2 scientists for each Instrument

- 0.5 Instrument data scientist from DMSC
- Data reduction and analysis from DMSC
- Beamline controls team matrixed from NSS and ICS
- Staffing seems aligned with other facilities

- Changes in staff profile will effect project



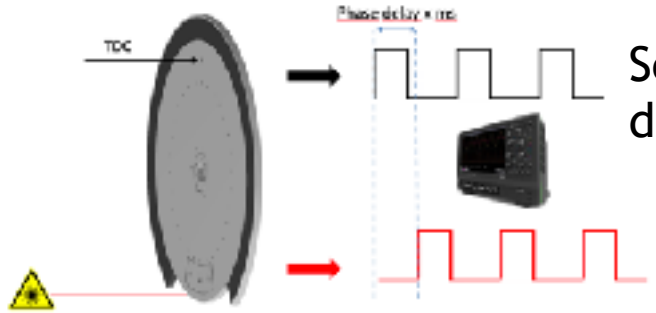
Staffing from DMSC covering data reduction and analysis Including Instrument Data Scientist



Staffing required for Beamline controls Assuming an slight uplift in ICS staff NSS staff allocated as per staff plan for NT and DMSC for controls and DAQ

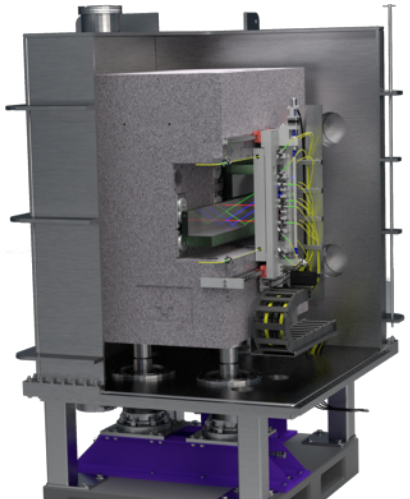
Commissioning

- Cold commission and integrate key components during installation.
- Scope, resources and framework are defined to execute.
  - BeamLine Controls Team
  - NT groups
  - Chopper group SAT includes calibration of axis geometry
- Instrument teams resources pre - builds and significant prototyping projects
  - Minimising / Mitigating future delays
- Hot commissioning plans are being developed, and reviewed at TG3
- Workshops with instruments teams to maintain schedule alignment, priorities and tasks.



Schematic of chopper disc laser alignment

Selene Guide prototype Build at PSI and fully integrated into control system



Construction of R106 where STFC will pre-build LOKI and FRIEA

Commissioning - Calibration

Considerable complexity for ESS Instruments with multiple axis chopper systems

Detector Geometry is challenging

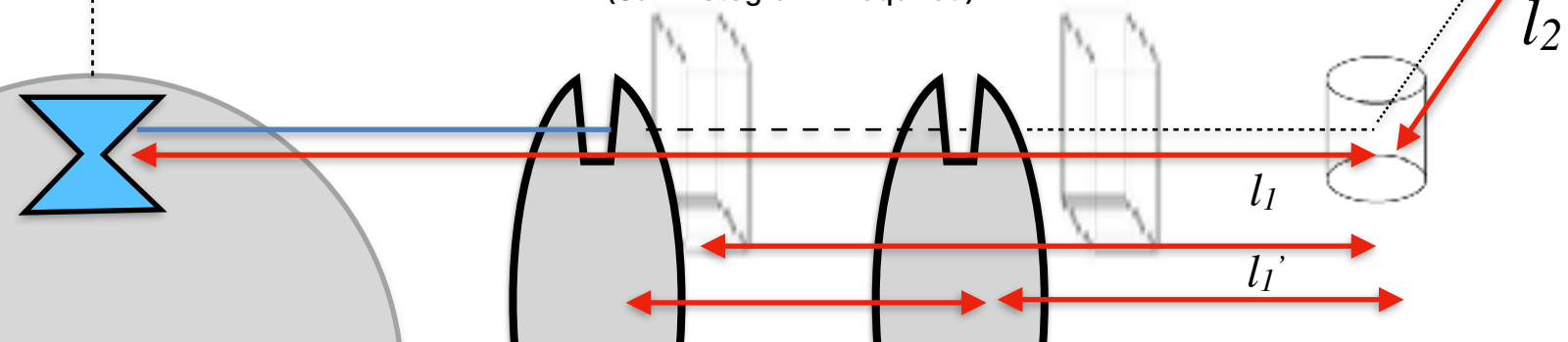
A number of methods of defining T_0 will be available

Calibration of chopper cascade will be aided by diagnostics

Neutron monitor project led by ESS

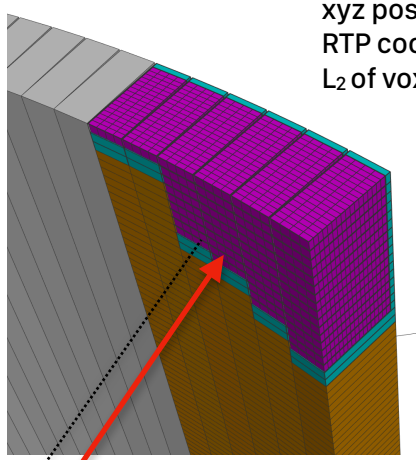
Monitor List mode DAQ
offsets from Wall clock
:01
:02
...
+ ID
(Can histogram if required)

Wall clock time proton pulse
11:10
Proton Pulse ID



Detector List mode DAQ
offsets from Wall clock
:05
:06
...
+Pixel ID

xyz position
RTP coordinates
L_2 of voxel



$$\lambda = \frac{h}{p} = \frac{h \,.\, tof}{m_N \,.\, L_{tot}} = 2d\sin\theta$$

$$tof = t - t_0$$

$$L_{tot} = L_1 + L_2$$

Calibration required for:
Motion axis
chopper offsets and transmission
Flight paths
Detector voxel / pixel positions

Challenges for Hot Commissioning

- Normalisation of individual frames of data.
  - Each frame is extracted from a different region of the pulse
- Defining T_0 and T_0 for each frame
- Target segment and moderator coupling
- Current activities aimed understanding these key complexities