Requirements Gathering and Tracking for Instrument Classes

7th Experiment Control Workshop

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Outline

- Re- Baselined ESS schedule and impact on ECP
- High level requirements and instruments
- BCG & TG3

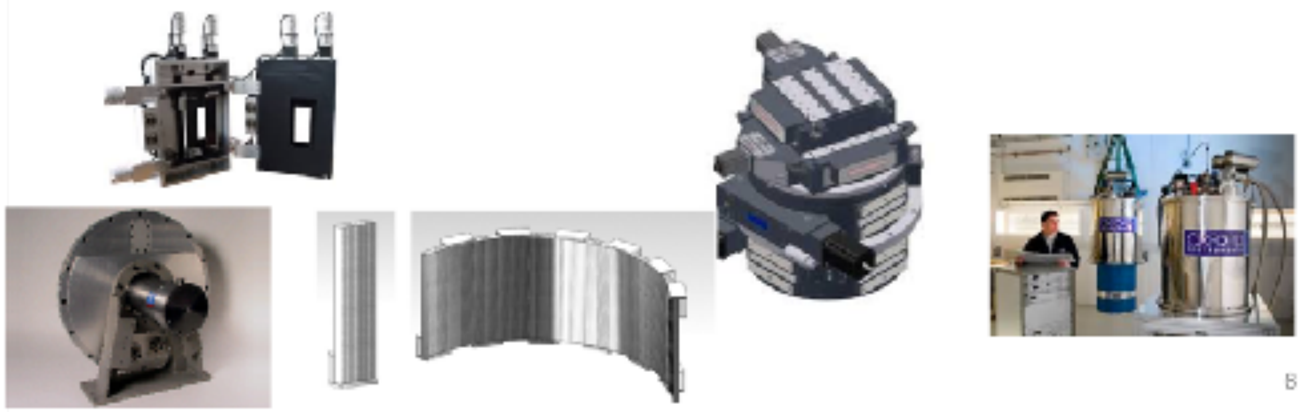
May 2015 …

Purpose of the workshop (s)

- This will be the first of a series
- Discuss requirements use cases and solutions
- Discuss system architecture & interfaces
- Discuss common goals
- Discuss modes of collaboration & working practices
- Define the experiment control system for ESS
- Feedback progress to stakeholders
- …

Experiment control project

- Key objective 1
  - Give scientists **useful** control of their experiment
- Key objective 2
  - Meet key objective 1



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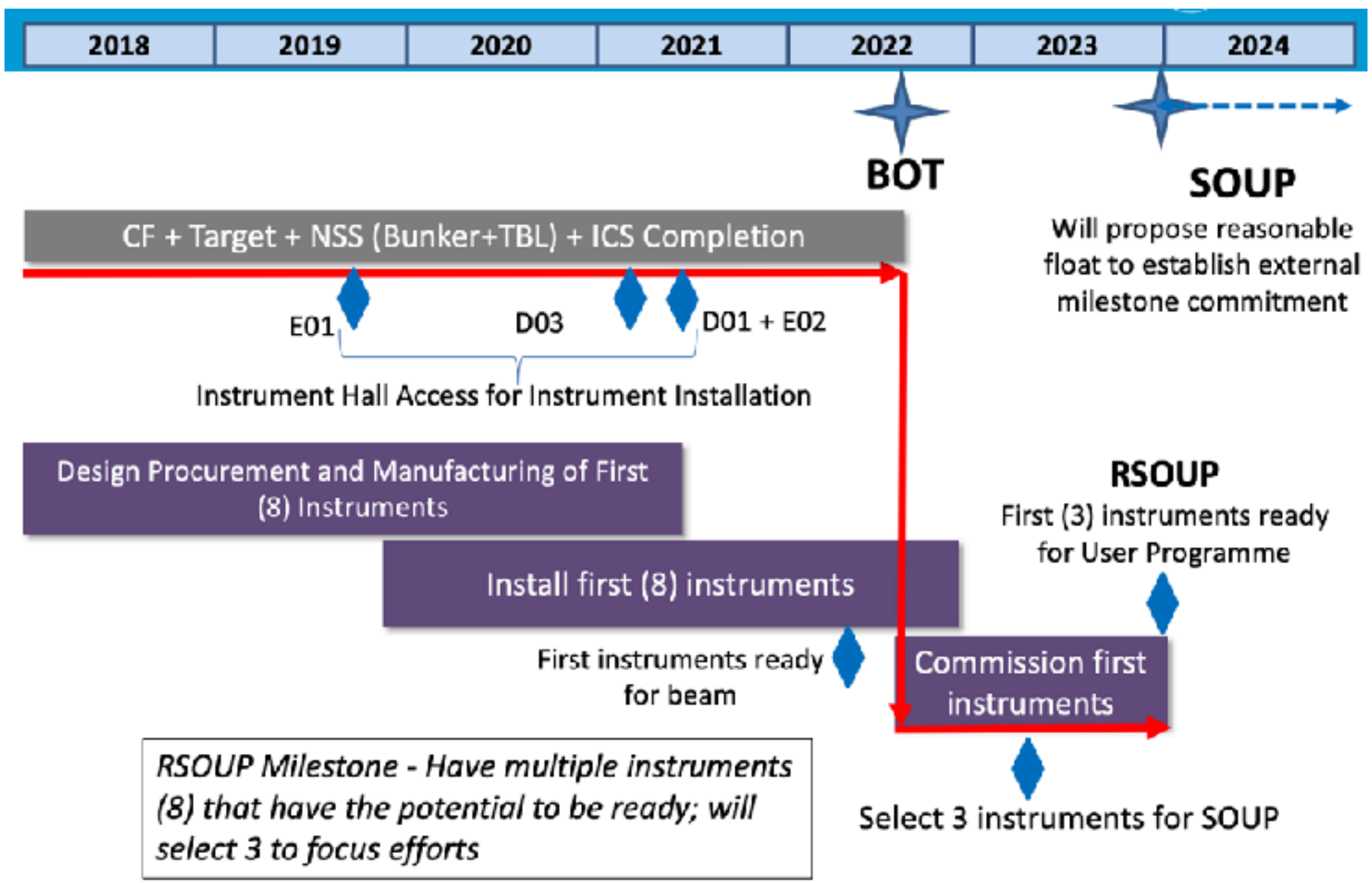
ESS Re-Baselined Schedule

- Un mitigable delays to civil construction triggered a schedule revision



Specifically for Instruments

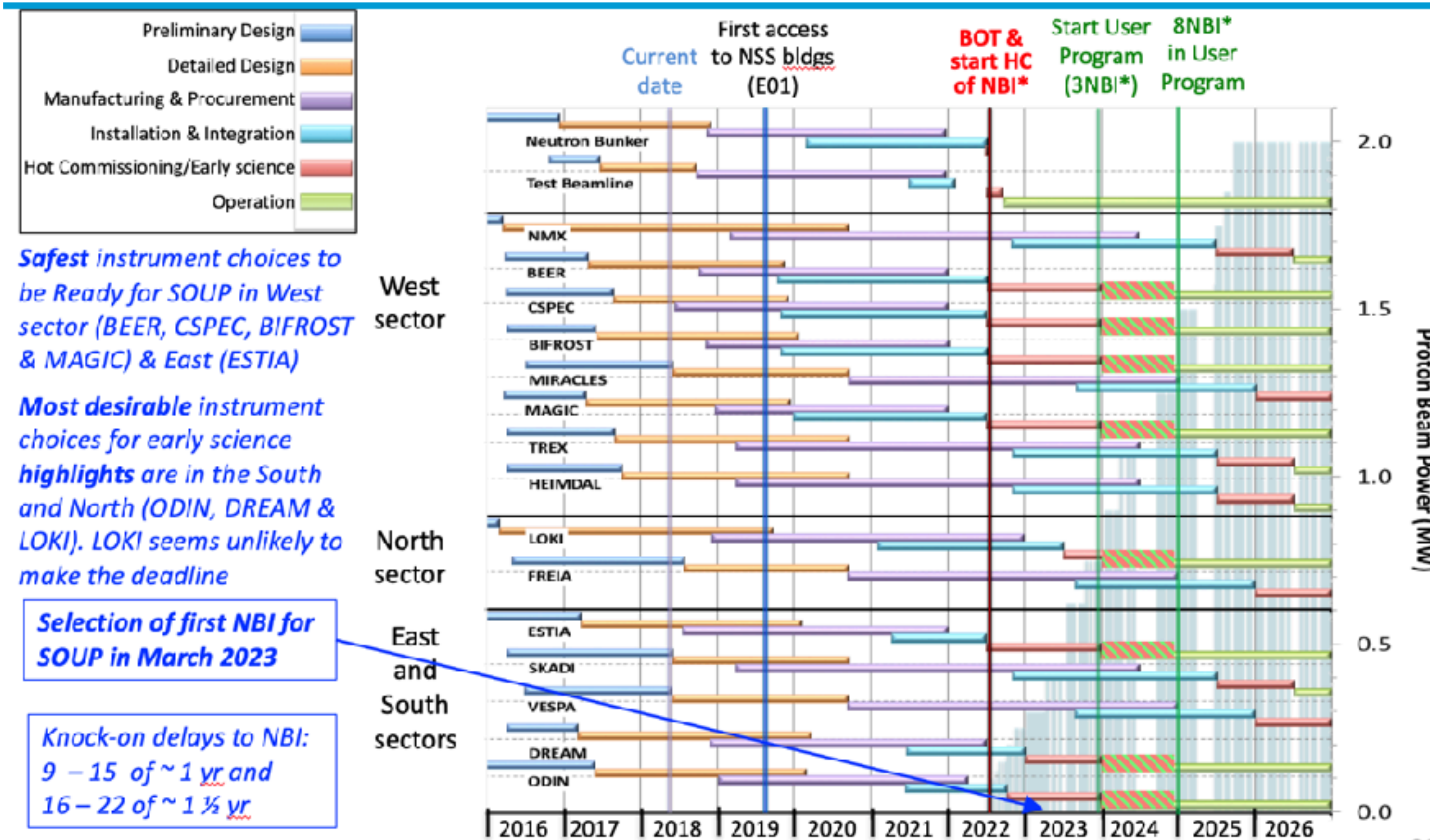
- Focus on 8 instruments for 2022
- Select 3/8 for SOUP starting late 2023 to mid 2024

__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



Requirements gathering

- A series of workshops in 2017
- Aimed at all instruments within a class
- Object to specify high level requirements for all DMSC scope
    1. Must have and nice to have
    2. For commissioning and user programme start
    3. Define milestones for delivery and acceptance criteria
- Item 1 - Some success, very high level needs collected
- Item 2 - Most instrument teams made a division
- Item 3 - Mostly failed to generate this information*

* Re- baselined schedule has generated a very different set of milestones

High level Controls requirements Diffraction instruments (not NMX)

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Instrument control

	DREAM			HEIMDAL			MAGIC			BEER		
M = Must, S = Should, N = Nice	M	S	N	M	S	N	M	S	N	M	S	N
Data Display												
Full detector area: (n-dimensional (nD): 2θ, d, Q, E, Intensity	X			X			X			X		
1D live histogram display: Integrated intensity over all detectors vs ToF)	X			X						X		
Save detector and 1D histogram images	X				X						X	
Region of interest (ROI) selection and readout of physical location of detector module	X			X			X			X		
Remote access to live detector data for users			X			X		X			X	
Remote access to live detector data for instrument team	X				X		X			X		
Incident beam spectrum		X			X		X			X		
Correction of the live detector data for distortions, efficiency, calibration,		X			X				X		X	
Plot of SEE parameters (field, temp) as a function of time		X		X				X		X		
Under the Hood												
All relevant EPICS information saved in NeXuS file	X			X			X			X		
sample, user, experiment information in NeXuS file	X			X			X			X		
Logbook of entire experiment including instrument configuration, beam status and SEE parameters	X				X		X			X		
CLI & GUI Interfaces												
Driving motors, setting limits, offsets	X			X			X			X		
Changing SEE parameters	X			X			X			X		
Reading SEE parameters	X			X			X			X		
Ability to script counting for time, monitor counts, proton charge	X			X			X			X		
Continuous measurements during sweeping of field, temperature, current		X		X			X			X		
Loops, if-then	X			X			X			X		
Script simulation		X			X		X			X		
Quick change of instrument setups (SEE, high/low resolutions, polarized/unpolarized neutrons)	X			X			X			X		

Instrument Live feedback				
Choppers frequency and position	X	X	X	X
Vacuum systems	X	X	X	X
Beam power monitor	X	X	X	X

Instrument specific control

Item	Must	Should	Nice
MAGIC: XYZ polarized measurements	X		
HEIMDAL: SANS detector position readout		X	
HEIMDAL: Imaging detector readout		X	
BEER: laser alignment and 3D scan to define sample coordination system	X		
BEER: Standalone mode for SEE (reading, changing parameters) off the beam for long term experiments	X		

Comments and questions from BEER:
"**Full detector area: (n-dimensional (nD): 2θ, d, Q, E, Intensity**": I missed ToF as one of the axis. For the BEER instrument in modulation setup ToF vs 2θ diagrams will be needed to see the possible overlap regions.
"**1D live histogram display: Integrated intensity over all detectors vs ToF**": If integrated over all detectors than it should be vs d not ToF. It would be good to have an option to select predefined part of the detector for live view. But it is probably the ROI option you explained next.
"**Region of interest (ROI) selection and readout of physical location of detector module**": It will be used just for data visualization? Or it can be used as selected region for the data reduction? For BEER it can help in the case of texture to analyze for example the intensity variation as a function of detector position within the selected ROI.
"**Remote access to live detector data for users**": It doesn't need to be exactly live data but user should be able to see what is currently measuring and what is the collected patterns and status of the instrument.
"**Driving motors, setting limits, offsets**": On BEER there will be hexapod and robot for positioning of the samples. It is necessary to set the position in the defined (sample based) coordinating system not as a set of positions for individual motors in the robot or hexapod piston.

High level Controls requirements Reflectometers

Item	Example	Must	Should	Must	Nice
Data Display					
live histogram display – X+Y vs. I	SNS/PSI	X			
live histogram display – X/Y + λ/ToF vs. I	SNS/PSI	X			
transformation of axes to Qz/pi-pf					X
save histogram images	SNS	X			
way to compare histograms			X		
selection, readout, cross-section of live	SNS/PSI		X		
ROI of histogram with integrated counts	SNS	X			
full spin-state integration (one histogram for +	SNS	X			
λ-normalization by function and measured		X			X
live binning and normalization to 1D-R(Q)			X	X	
fast live counter of ROI/full detector for			X		
Under the Hood					
all relevant EPICS information saved in		X			
sample, user, experiment information in		X			
store experiment planning info (runs			X	X	
Scripted Instrument Interface					
driving motors, setting limits, offsets		X			
changing SEE parameters		X	X		
reading SEE parameters		X			
counting for time, monitor, counts, charge		X			
counting for minimal statistic in R(Q)				X	X
simplified experiment planning (calculate slit	SNS/ILL		X	X	
countinuous driving while counting (sweep)					X
loops, if-then		X			
script simulation	MLZ			X	
quick change of instrument setups (polarizer,	SNS		X		
GUI Interface			X	X	
driving motors, setting limits, offsets		X	X		
changing SEE parameters			X		
reading SEE parameters			X		
counting for time, monitor, counts, charge		X	X		
counting for minimal statistic in R(Q)				X	
simplified experiment planning (calculate slit				X	
continuous driving while counting (sweep)					X
instrument calibration help (polarization	SNS	X		X	

Item	Already	Mus	Sho	Mus	Nice
Estia Selene guide segment		X			
Laser alignment and live	PSI			X	
Diverse alignment and		X!			X
FREIA liquid height control	ILL, ISIS	X			

Engineering diffraction

Item	Example	Must	Should	Must	Nice
Data Display					
2D live raw counts data for each detector	Stress-Spec.	X			
1D live histogram display: integrated intensity	Stress-Spec.	X			
1D live histogram of ROI with integrated	Takumi	X			
Correction of the live detector data for			X		
Incident beam spectrum		X			
Plot of SE parameters (temp, stress, position,	Stress-Spec.	X			
Visualization of the positioning system status			X		
Transformation of engineering SE parameters	Stress-Spec.	X			
Way to compare histograms (fix display of			X		
Save detector and 1D histogram images					X
Region of interest (ROI) selection		X			
Remote access to live data		X			
…					
Under the Hood		X			
All relevant EPICS information saved in		X			
Sample, user, experiment information in		X			
Logbook of entire experiment including		X			
Scripted Instrument Interface					
Driving motors, setting limits, offsets		X			
Changing SEE parameters		X			
Reading SEE parameters		X			
Counting for time, monitor, counts, charge		X			
Simplified experiment planning		X			
Continuous driving while counting (sweep)		X			
Loops, if-then		X			
Script simulation		X			
Quick change of instrument setups (SE, high/		X			
GUI Interface					
Driving motors, setting limits, offsets		X			
Changing SEE parameters		X			
Reading SEE parameters		X			
Counting for time, monitor, counts, charge		X			
Read of pre-measured 3D coordinates and	ENGIN-X	X			
Adjustment and visualization of positioning				X	
Quick change of instrument setups (SE, high/				X	
Simplified experiment planning (experiment		X			
Experiment simulation for multiplexing (predict				X	
Continuous driving while counting (sweep)		X			
Instrument Live feedback					
Choppers frequency and position		X			
Beam power monitor	Stress-Spec.	X			
SEE parameters	Stress-Spec			X	

Item	Already Implem	Mu st	Sh oul	Mu st	Nic e
Laser/Optical alignment of sample positions			X		
SE calibration procedure (deformation rig)				X	
Simple real-time data analysis (individual peak				X	

Imaging requirements

Basic Functions						
Calibration tools						
Parameters automatically from NICOS / hdf files		Yes	X			
(McStas integration into same workflow)		Yes		X		
Stitching with calibration option (reference sample options)		Yes	x			
Flux Normalization						
Normalization by monitors: the raw data (images) to monitors (Beam monitor counts in hdf file)		Yes	X			
Normalization to images ROI's	Muhrec, commercial		x			
General Tools (including, but not limited to…):						
WFM stitching (as 1D and 2D) as option before AND/OR after the normalization/analysis routines	In progress at V20/DMSC	Yes	X			
Simple conversion between TOF and lambda	JPARC, SNS, ISIS	Yes	X			
Conversion between attenuation coefficients and transmission	JPARC, SNS, ISIS, TUM, PSI	Yes	X			
General tools from image J as reference suite:						
Ability to process several image formats (single tiff, fit, txt, jpeg, etc)	ImageJ	Yes	X			
other mathematical operations: scaling, adding,…	ImageJ	Yes	X			
filtering, averaging (in all dimensions)	ImageJ	Yes	X			
histograms of ROIs	ImageJ	Yes	X			
data extraction from ROIs, line plots, z-plots	ImageJ	Yes	X			
binning (2D and 3D)	ImageJ	Yes	X			
ROI flexibility: ○specifically very flexible ROI tools (more than one)	ImageJ	Yes	X			
visualization tools (contrast, brightness…) available at selected processing step	ImageJ	Yes	X			
Re-sorting and re-naming (stroboscopic – phase – time sorting..)		Yes	X			
dynamic/automated ROI recognition tool…		Yes				x
Additional: running averages and interpolation tools in x-y-t		Yes	X			
Spatial image stitching (also workable for tomography)	ImageJ	Yes	X			

Common features

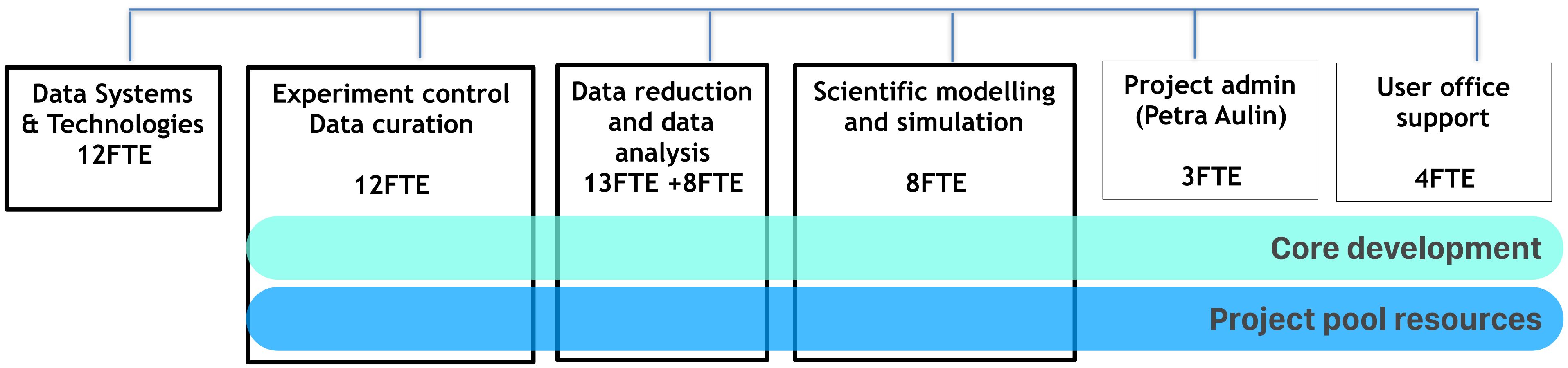
- Script interface
- GUI interface
- Set & Get instrument parameters
  - Choppers, Motion, SE
- Scanning and scripting.
- Fly scan
- Script testing
- Conditional operators
- Iterable operators
- Time, Proton Charge, Monitor counts

- Live view of detector data (TOF & derived units)
- Defining ROI on 2d detectors
- Data management – relevant variables saved in nexus
- Experiment planning

Feature that are expected …

- Everything works!
- Start / Stop DAQ
- Configure and switch configurations
- At ESS users will be able to control complex systems
  - Robots for example

DMSC service delivery for SOUP



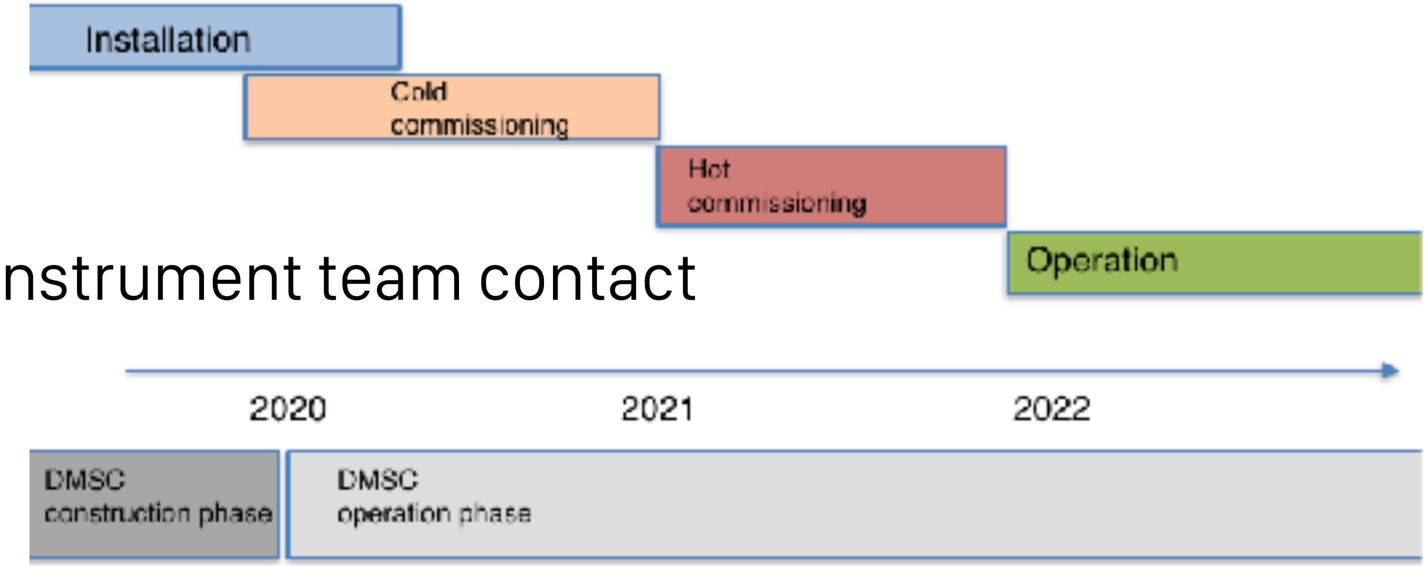
Development of a credible baseline provision for analysis, reduction and control

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

Delivery by 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



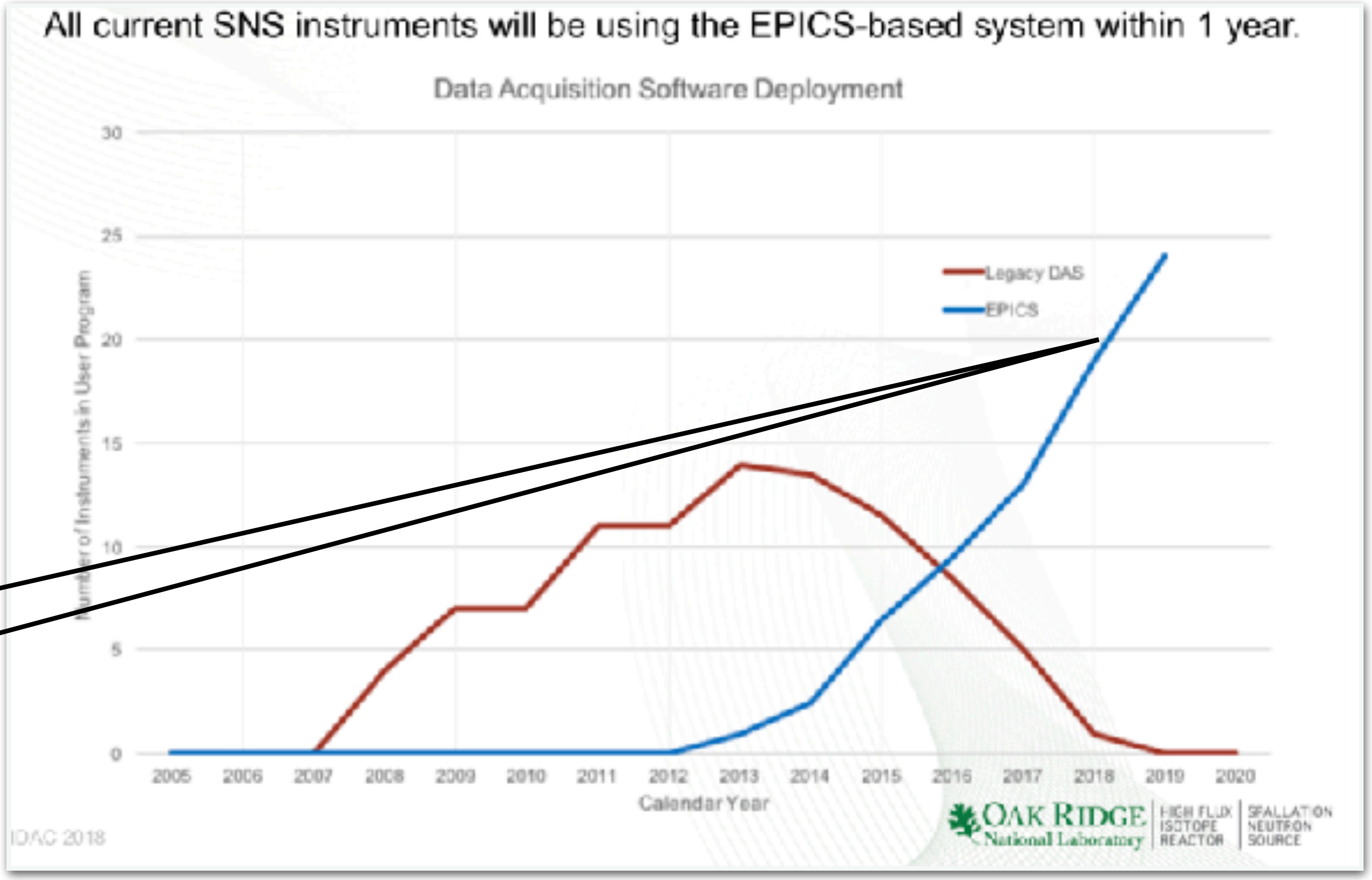
SNS example, Controls and DAQ

	DAQ software & hardware 2018	Controls integration & UI 2018
SNS	8FTE	7FTE
DMSC	4+4 (DAQ software)	3(UI)
ICS, NT, SAD	-	5 (Int)

SNS Migrated to an Epics based ECP

4 instruments commissioned per year

Instrument and **source** characteristics **understood**



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	15	16	15	13	9	9

Instrument example

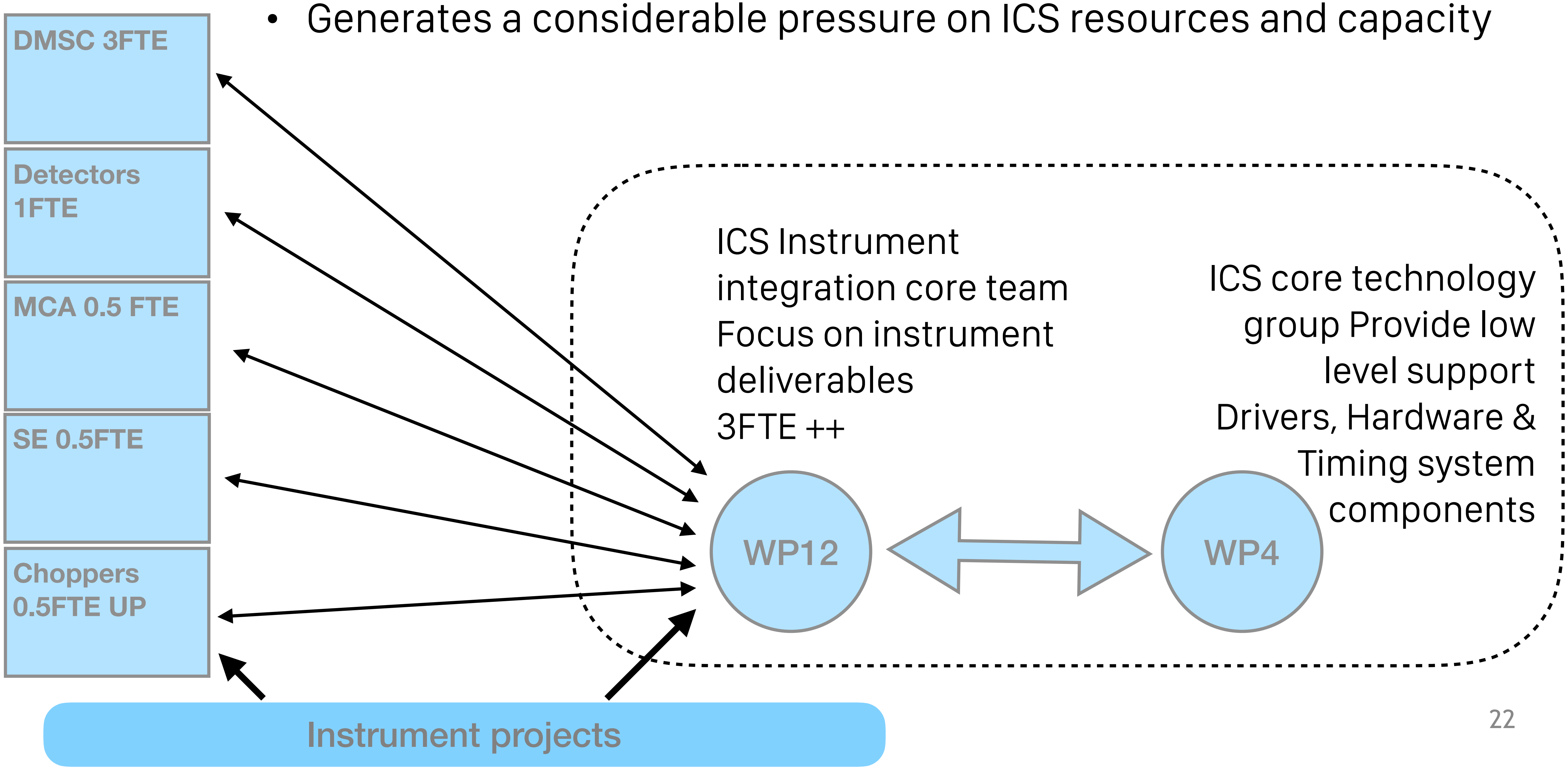
- Instrument data scientist is part of instrument team
  - PM for software delivery
  - Knowledge of both beam-line science & beam-line software
- Experiment control development split between
  - Controls
  - DAQ

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

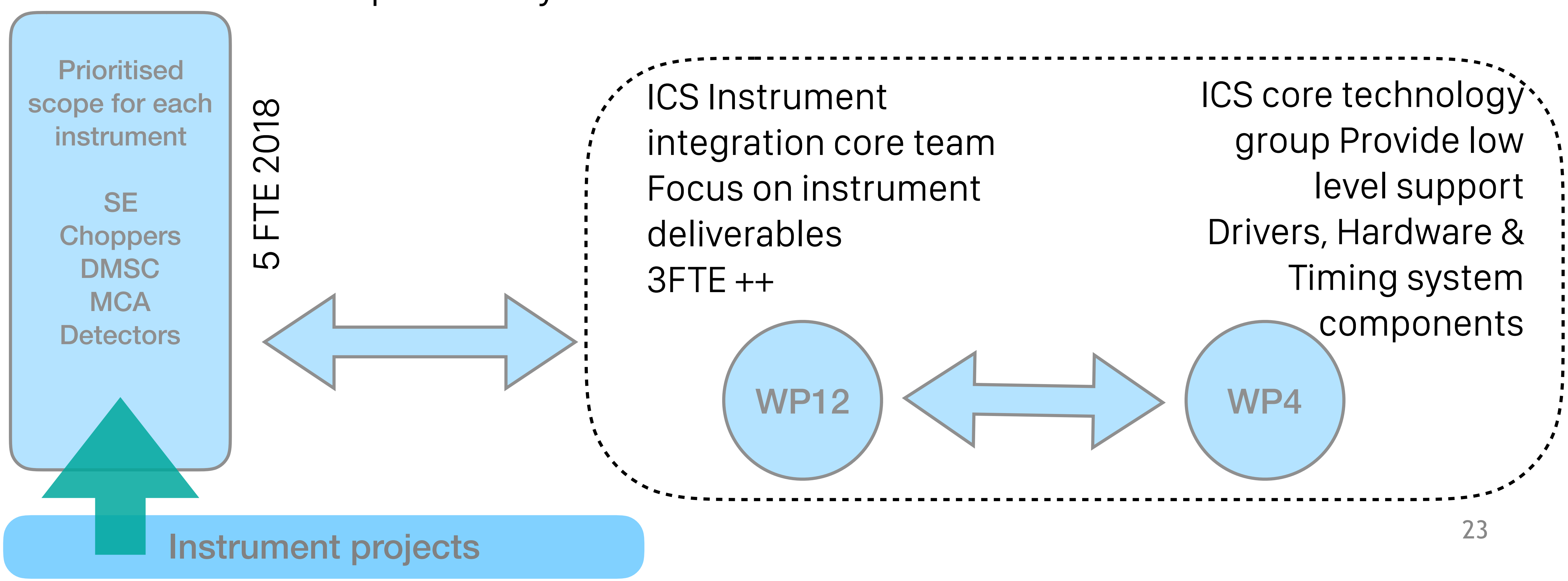
Pre 2018 Integration model

- Inefficient integration model
- Unclear interface for instrument teams
- No overall prioritisation of requirements
- Generates a considerable pressure on ICS resources and capacity



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



Toll gate 3 reviews

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- Review gateway between detailed design & procurement and installation.
- Post TG3 instrument systems are under CC
- ESS process involves
  - Sub Tg3s, Intermediate Design Reviews.
  - Is not one big meeting (there will be one big meeting)
- ICS DMSC will review documentation
- Flag aspects that would slow commissioning or excursions from standards.

Looking forwards

- Build functionality that enables commissioning* to proceed fast.

- Drill down into the requirements for the instruments that are the first 8.

- Beamline Controls Group has the scope and responsibility for delivery to instruments

*Cold commissioning, hot committing and early scientific commissioning