ESS Spectroscopy STAP

April 2023

PASCALE DEEN
SENIOR SCIENTIST, EUROPEAN SPALLATION SOURCE

RESPONSIBLE FOR SPECTROSCOPY
SECOND SCIENTIST: CSPEC

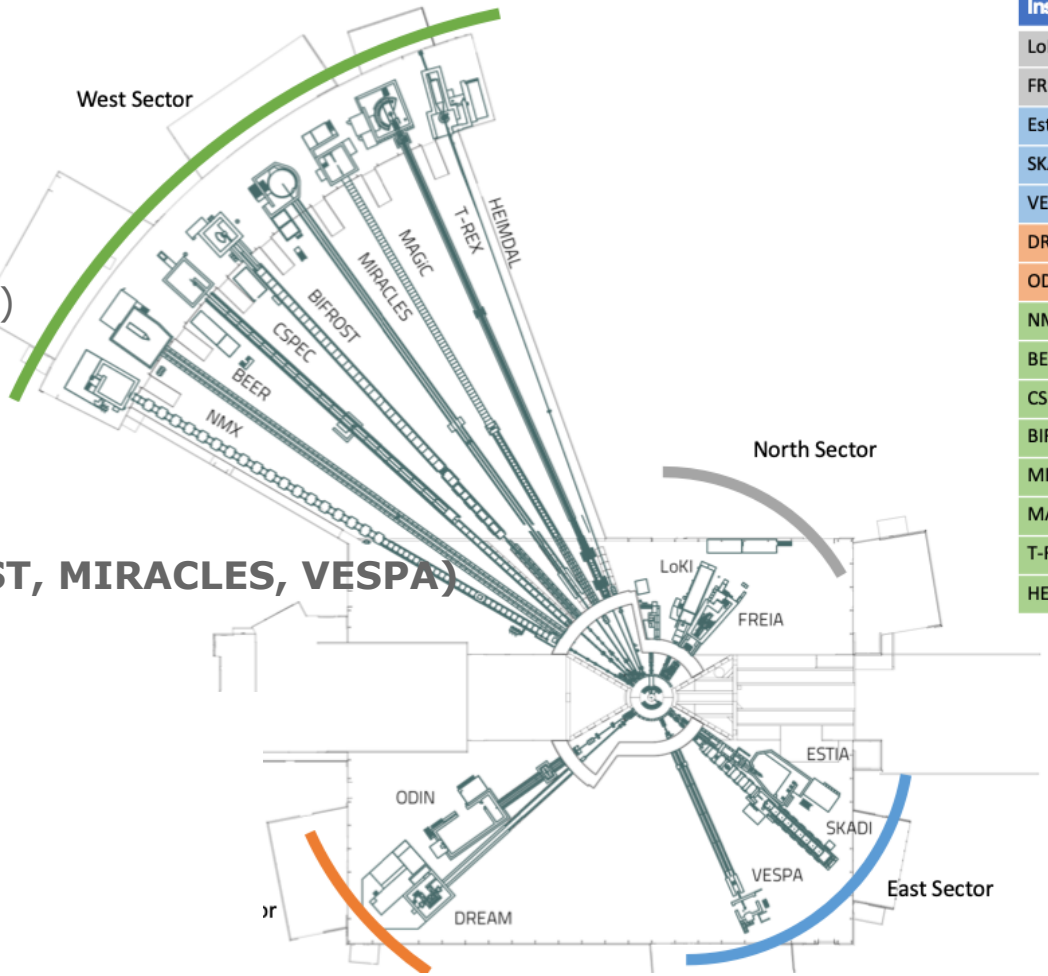
Neutron Instruments

Andersen, K. H.; Argyriou, D. N.; Jackson, A. J. et al. The Instrument Suite of the European Spallation Source. *Nuclear Instruments and Methods in Physics Research Section A:* **2020**, *957*, 163402. https://doi.org/10.1016/j.nima.2020.163402.

15 instruments + Test Beamline

Diffractometers (DREAM, MAGiC, HEIMDAL)
SANS (LoKI, SKADI)
Reflectometers (Estia, FREIA)
Imaging (ODIN)
Engineering Diffraction (BEER)
Macromolecular Crystallography (NMX)
Spectrometers (CSPEC, T-REX, BIFROST, MIRACLES, VESPA)

Reach 22 in near future
Reach 42 eventually



Instrument	Beamport
LoKI	N7
FREIA	N5
Estia	E2
SKADI	E3
VESPA	E7
DREAM	S3
ODIN	S2
NMX	W1
BEER	W2
CSPEC	W3
BIFROST	W4
MIRACLES	W5
MAGIC	W6
T-REX	W7
HEIMDAL	W8

Spectroscopy

5 Instruments

General-purpose chopper spectrometers

CSPEC: Cold chopper spectrometer
Lead scientist: Daria Noferini (ESS)
Second scientist: Pascale Deen (ESS)
IK partners: TUM (50%), LLB (50%)

T-REX: Bispectral chopper spectrometer
Lead scientist: Christian Franz (FZJ)
IK partners: FZJ (75%), CNR (25%)

Crystal-analyser instruments

BIFROST: Extreme environment spectrometer
Lead scientist: Rasmus Toft-Petersen (DTU)
IK partners: DK (24%), PSI (28%), LLB (21%), IFE (24%), Wigner (3%)

VESPA: Vibrational spectroscopy
Lead scientist: xxx (CNR)
IK partners: CNR (75%), ISIS (25%)

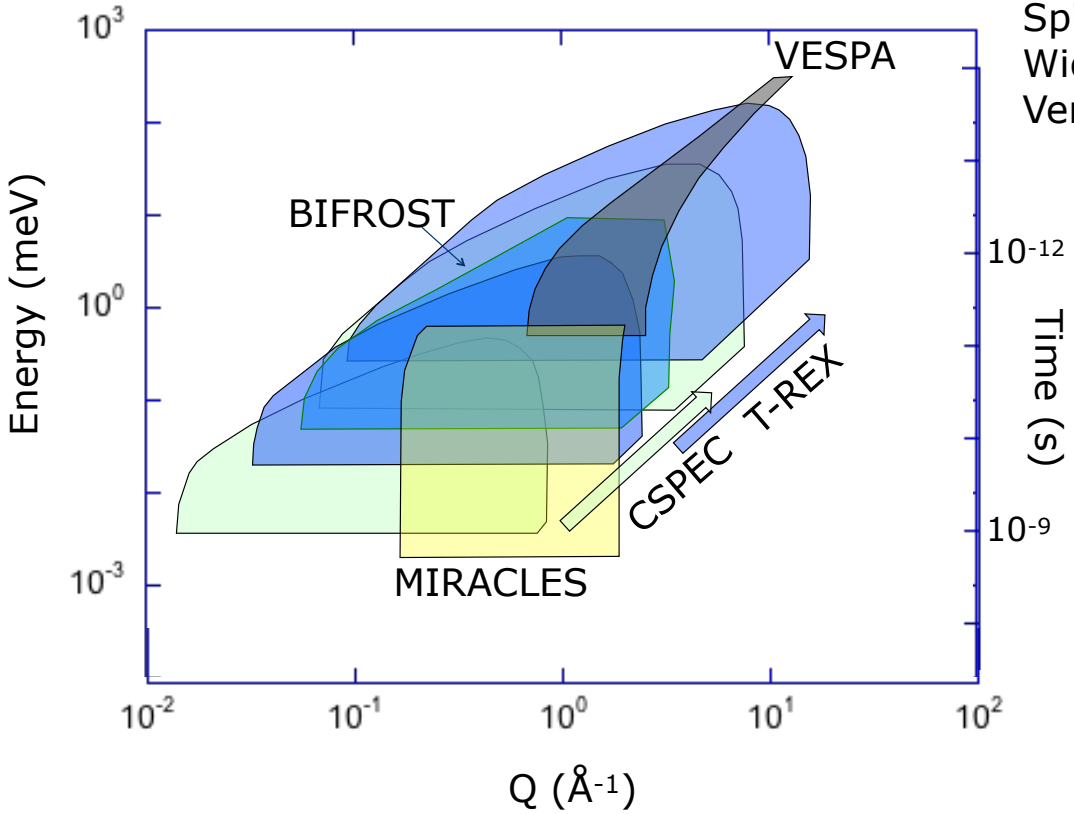
MIRACLES: Backscattering spectroscopy
Lead scientist: Felix Villacorta (ESS-Bilbao)
IK partners: ESS-Bilbao, KU

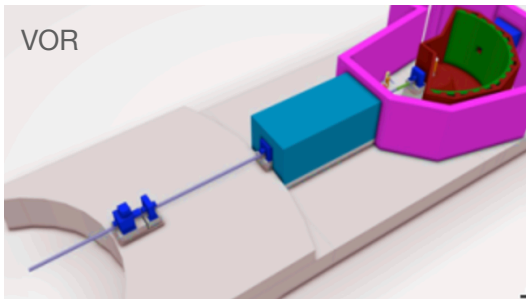
On-site

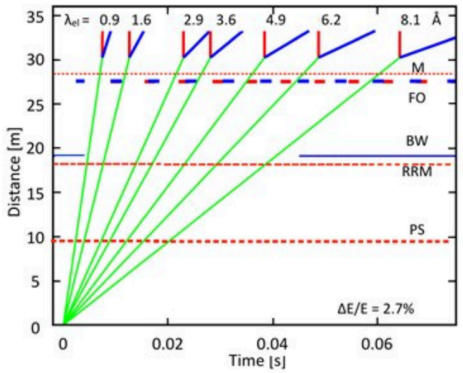
Spectroscopy Kinematic Range

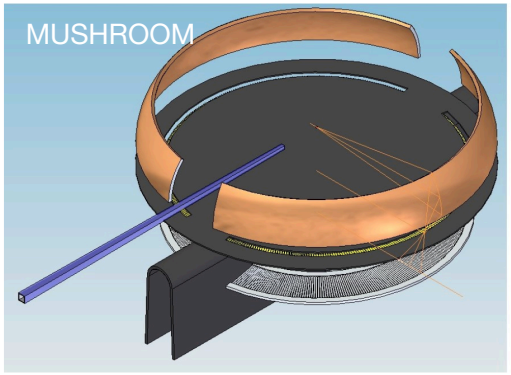
Extend instrument suite:

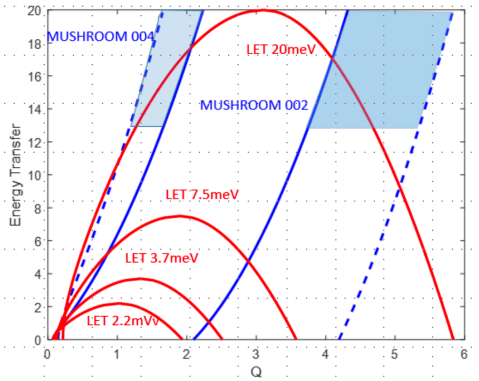
- Spin echo (high resolution or wide angle).
- Wide bandwidth spectroscopy (~ 9 Å, 1x1cm^2): Direct: VOR
- Very fast spectroscopy: Indirect: Prismatic: MUSHROOM











ESS Priorities and Timelines

ESS Beam on Target (BOT) = May 2025
Instrument TG5: current estimate (TG5 = end of construction of instrument)

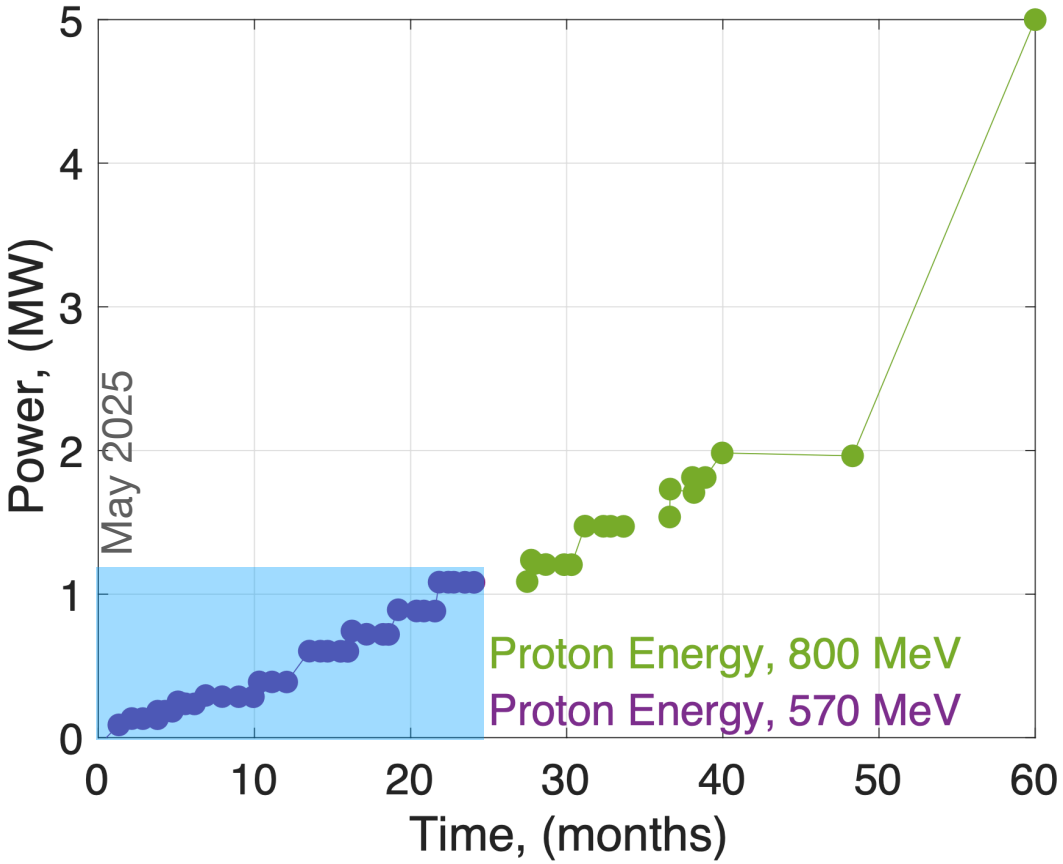
Tranche 1	Loki May 24	Odin Dec 23	Bifrost June 24	ESTIA Sept 24	Test Beam Line	DREAM July 24
Tranche 2	Magic Mar 25	NMX Apr 25	CSPEC Nov 25	SKADI Aug 25		
Tranche 3	FREIA May 26	T-REX July 26	MIRACLES Dec 25	HEIMDAL Feb 26	VESPA June 26	

Add 6-9 months for Safety Readiness Review
TG5 (IK partner)
SAR (ESS, includes PSS - Personal Safety System) System Acceptance Review (Nov 24 for Tranche 1 instrument)
SRR (ESS) Safety readiness review (April 25 for Tranche 1 instrument)
HC = Hot commissioning.

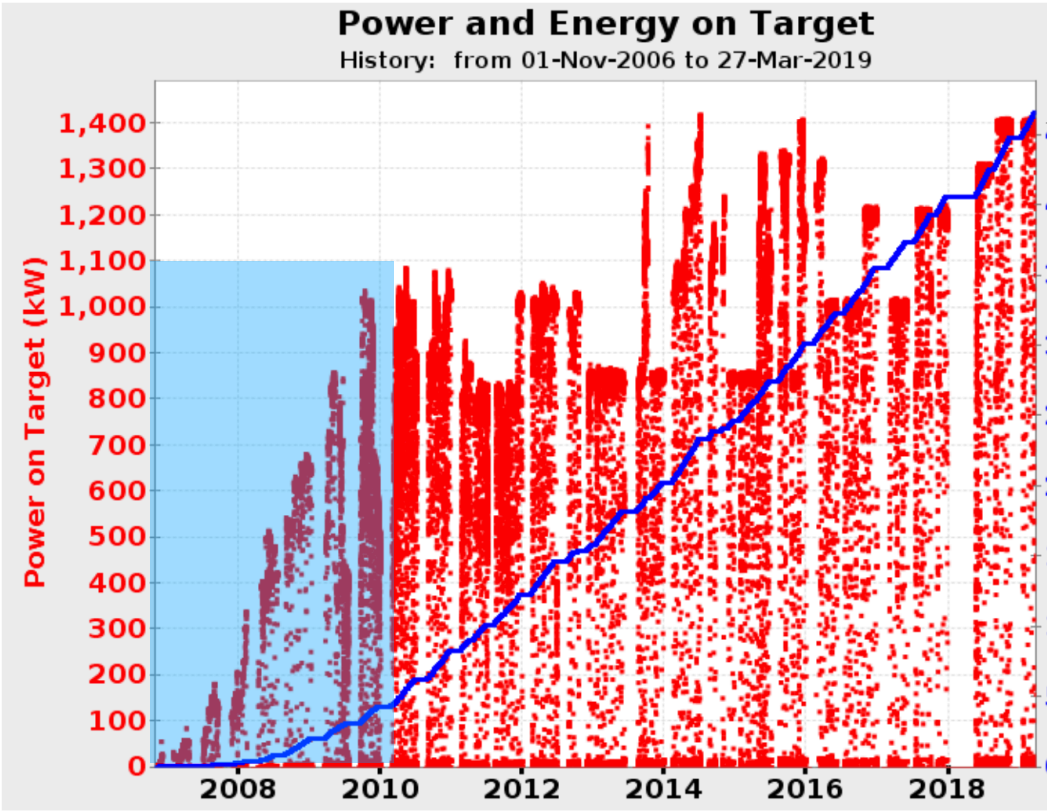
Between TG5 and SRR, there is 6-9months until SRR / start of HC. This includes PSS finalisation but also various documentation and submissions / reviews for SAR & SRR.

Current anticipated ramp up.

ESS



SNS TS1



Spectroscopy RISKS
As presented to ESS by instrument teams

Top Individual Risks (all rated 10 or above)

Index	Global ID	Risk Title	Risk Rating	Category	Owner	CHNG
0	TRX-07	Detector performance requirements may not be met	25	quality	Detector Group (ESS)	steady
1	CSP-04	CAVE costs	25	cost	CSPEC/LLB	steady
2	TRX-14	Mulit-Grid Detector not ready for hot commisioning	25	schedule	Detector Group	steady
4	TRX-10	Increasing costs of materials (Experimental cave)	20	cost	Andrea Oreccini (CNR)	steady
5	CSP-02	Detector delivery	20	schedule	ESS	steady
6	TRX-09	Increasing costs of materials (Beamline shielding)	20	cost	Andrea Oreccini (CNR)	steady
8	VSP-03	Experimental Cave/Spectrometer integration	20	schedule	R.Senesi	increase
11	CSP-01	Staffing resources	16	schedule	CSPEC/LLB	decrease
12	CSP-03	Detector tank costs	16	cost	CSPEC/LLB	decrease
14	VSP-06	HOPG tiles availability	16	schedule	R.Senesi	decrease
23	VSP-02	Budget+contingency Vs scope	15	cost	R.Senesi	decrease
27	CSP-05	Installation resources	15	schedule	CSPEC	steady
28	CSP-07	Chopper delivery	15	schedule	CSPEC	steady
31	BFR-18	Software development delayed	12	quality	Rasmus/Greg	steady
35	VSP-08	Detector modules cost overrun	12	cost	G.Gorini	steady
36	BFR-09	Software development mismatched to user requirements	12	quality	Rasmus/Greg	steady
50	MRC-09	Cave design	12	schedule	Félix J Villacorta	steady
56	TRX-15	Guide suppliers working at capacity	10	cost	Marcel Serwe (FZJ)	decrease
61	MRC-04	Delayed delivery and technical challenges of fast choppers	10	quality	Félix J Villacorta	steady

STAP Agenda

Day 1

09:45 → 10:00 **Coffee**

10:00 → 10:20 **Welcome and introduction: Overview and charge**

Overview of charge

Convener: Pascale Deen (European Spallation Source ERIC)

10:20 → 11:05 **BIFROST**

11:05 → 11:50 **CSPEC**

11:50 → 12:35 **Data analysis considerations for Bifrost and CSPEC**

Convener: Gregory Tucker (European Spallation Source ERIC)

12:35 → 13:35 **Lunch**

13:35 → 14:20 **Detector technology (inclusive of monitors)**

Convener: Kevin Fissum (European Spallation Source ERIC)

14:20 → 14:50 **Overview of ESS Project**

Conveners: Giovanna Fragneto (European Spallation Source ERIC), Pascale Deen (European Spallation Source ERIC)

14:50 → 15:35 **TREX**

Day 2

08:30 → 09:15 **MIRACLES**

09:15 → 10:00 **Sample environment for spectroscopy**

Conveners: Caroline Curfs (European Spallation Source ERIC), Monika Hartl (European Spallation Source ERIC)

10:00 → 10:30 **Polarisation analysis considerations**

Convener: Wai Tung (Hal) Lee (ESS)

10:30 → 10:45 **Coffee**

10:45 → 11:20 **ECDC: Integration of spectroscopy instruments**

Convener: Tobias Richter (European Spallation Source ERIC)

11:20 → 12:00 **NICOS: with the example from Bifrost (choppers) (or LOKI**

Convener: Matt Clarke (European Spallation Source ERIC)

12:00 → 13:00 **Lunch**

13:00 → 13:45 **VESPA**

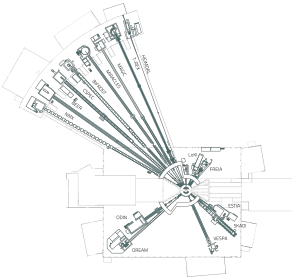
13:45 → 14:30 **Closed session**

14:30 → 15:00 **Comments from STAP to spectroscopy teams and ESS**

- Overview of instruments: Instrument scientist.
- Detector technologies: Kevin Fissum.
- Sample environment: Caroline Curfs (Materials Engineering and Solid State Physics) and Monika Hartl (Chemistry and Life Science).
- DMSC: Tobias Richter (Experimental control and data curation, Matt Clark (NICOS), Greg Tucker (Instrument Data Scientist)
- Polarisation analysis: Wai Tung Lee (Hal).

DMSC: Integrated data pipeline

Strategy for sustainable software



ISIS | TUM, PSI | MLZ, ORNL? | PSI, MAX IV, …

UOS | EPICS, NICOS, kafka | scipp | Technique specific | SciCat, NeXus

User office software → Experiment control → Stream events & meta data → Data reduction & visualization → Data analysis → FAIR Data management

- Tobias Richter (ECDC)
- Matt Clark (NICOS)
- Greg Tucker (IDS)

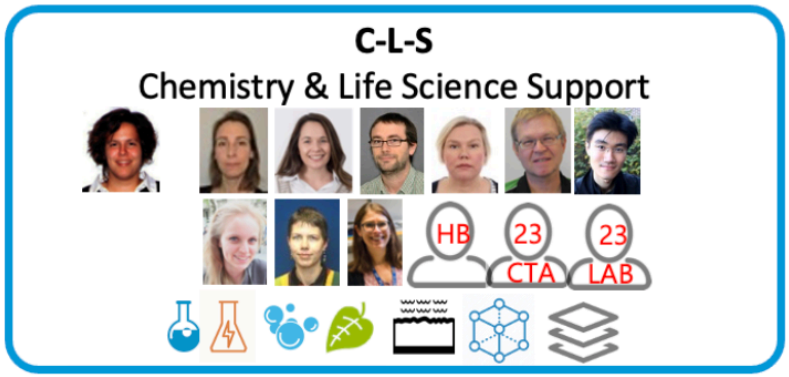
Focus on sustainability & usability

- **Standardize** where feasible
- **Collaborate** and promote collaborations
- Modern & **best practice** software eng.
- Be serious about **user experience**
- Be as ready as possible; **test**, **test**, **…**

Technique	Software	Collaborators
SANS	SasView	NIST, ISIS, ILL, DLS, SNS
Reflectometry	BornAgain / easyRefl.	FZJ (ISIS), ORSO
Diffraction	CrysFML, CrysPy, easyDiff.	ILL, LLB
Spectroscopy	Mantid, SpinW, PACE, Dave, LAMP, easySpec	ISIS
Imaging	MuhRec / KipTool / TOFlib	PSI
MX	SCIPP, DIALS?, PHENIX	LU, STFC, DLS

Sample environment

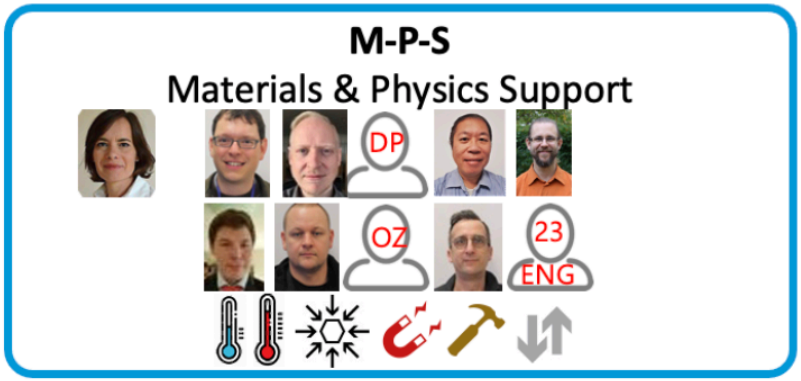
Monika Hartl



ensures Chemistry, Life Science, Soft Matter and Biology support

- provide deuteration, chemistry, life science, crystallisation services
- install, operate, calibrate, maintain sample env. for phys. chemistry, fluid control, surfaces, interfaces
- ensure sample management e.g. receive, handle, ship, characterise, synthesize, condition, mount, orient, align samples)
- operate deuteration, chemistry, LS labs & workshops
- develop, procure, refurbish, integrate and commission new equipment
- ensure method development
- provide neutron guide characterisation & simulations

Caroline Curfs



ensures Materials Engineering and Solid State Physics support

- provide services for materials engineering, quantum materials and physics
- install, operate, calibrate maintain sample env. for low-T, high-T, high-p, fields B E; mech. Processing
- ensure liquid helium cycle for user programme as well as mechanical and control integration of sample environment systems
- operate materials eng. lab and T-B-p SE workshops
- develop, procure, refurbish, integrate and commission new equipment
- ensure method development
- ensure the neutron polarisation function

Charge:
Construction and completion of instruments

1. **Are the instrument teams moving ahead as expected and are there any notable instrumental areas that the instrument teams are overlooking ?**

2. The ^{10}B multigrid detectors remain foreseen for T-REX, however development is currently on-hold while a delivery plan is put in place. T-REX is foreseen to come online in 2027. **Is the timeline for TREX consistent with community expectations and requirements or is there a need to accelerate progress ?**

3. **Are the solutions proposed for instrument monitors suitable?**

4. The instrument control, to data acquisition and data analysis chain is presented. **Is the STAP confident that the DMSC chain will enable both commissioning and first science on the spectroscopy instruments?**

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6. Polarisation analysis. The first 4 spectroscopy instruments have future proofed their engineering design to enable polarisation analysis. There is also some work on going to develop the details of polarisation and analysis components, although limited at this moment in time. **At which point would the STAP foresee further dedication to PA on the spectroscopy instruments?**

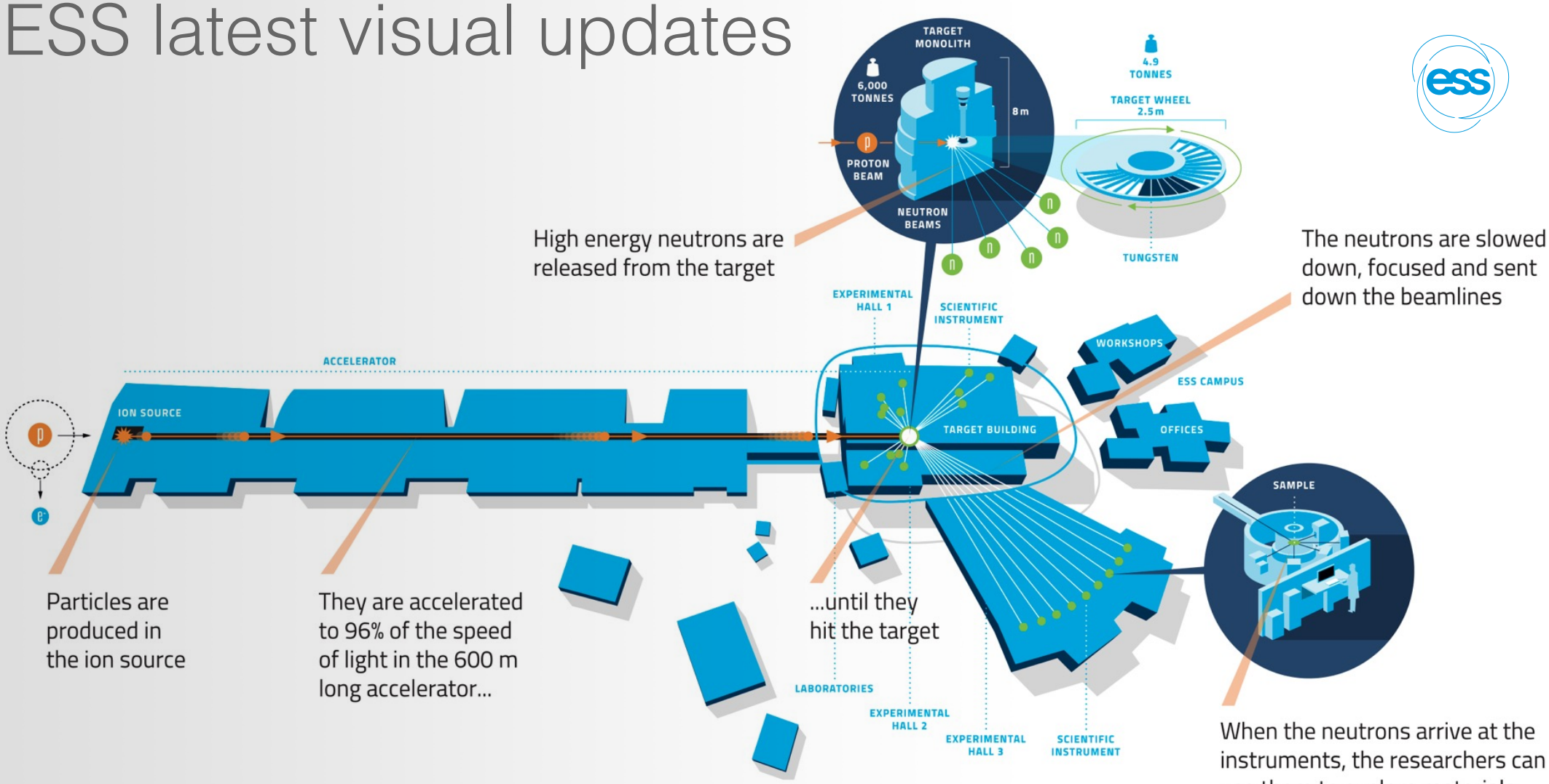
Charge:
First science & beyond

7. First science is the period after instrument commissioning and before user operation. The instruments will be available to perform experiments that will show case the various capabilities. **What would the STAP vision for first science be in terms of collaboration between instruments groups and friendly users? How do we determine who performs the first science experiments?**

8. **What is the role of the test beamline for first science?**

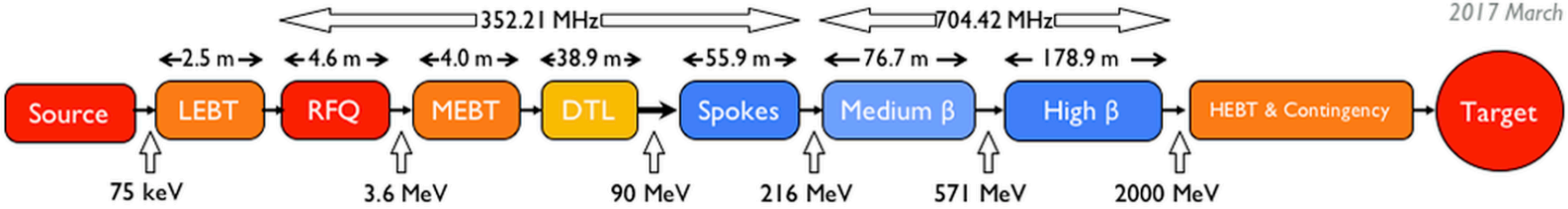
9. **There will shortly be a call for the next 7 instruments (15-22). An obvious current gap is a spin-echo instrument, what further instruments should we focus on?**

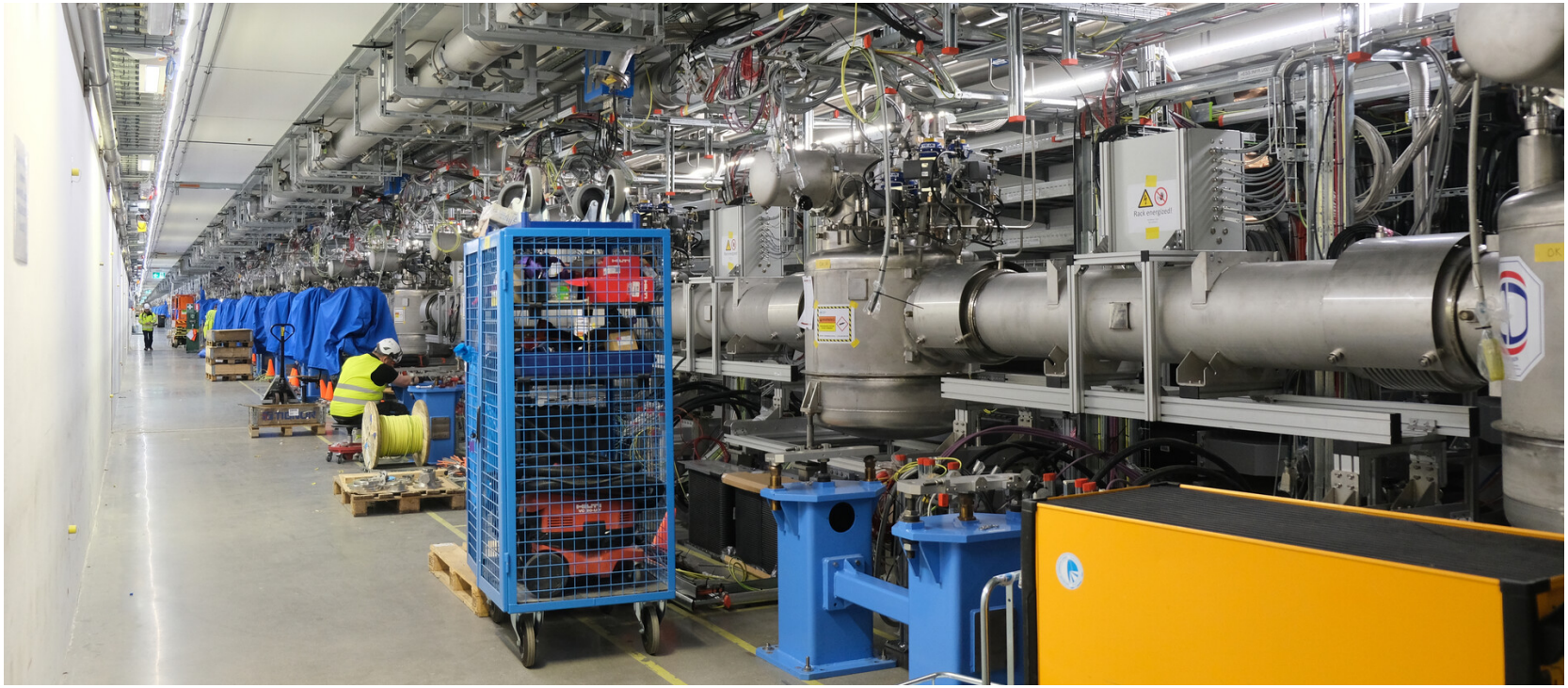
ESS latest visual updates



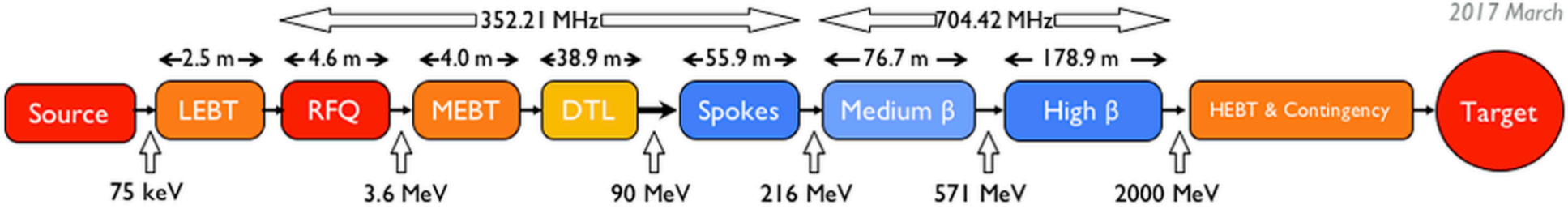
Linear Accelerator

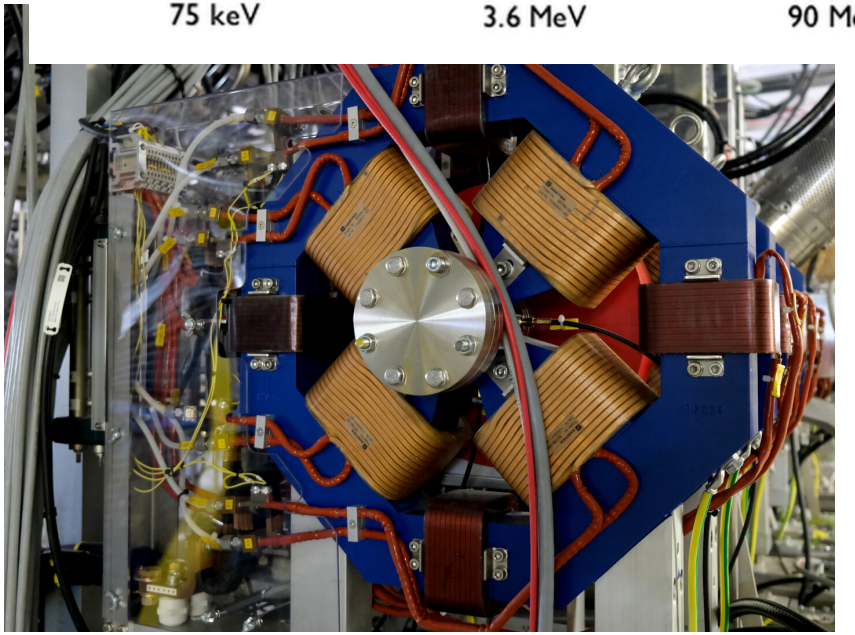
~ 600 m

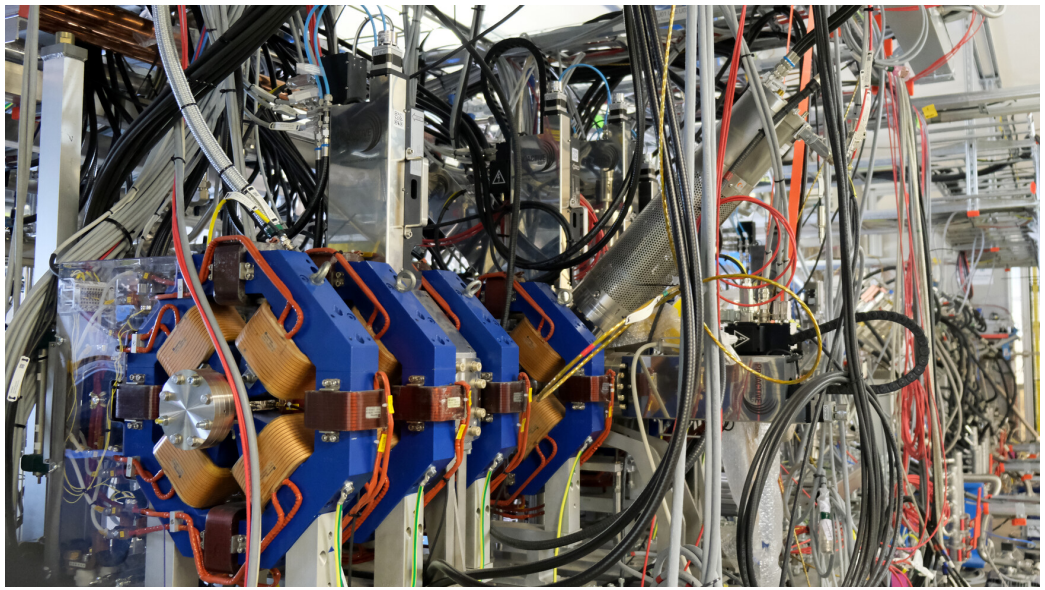




Accelerator

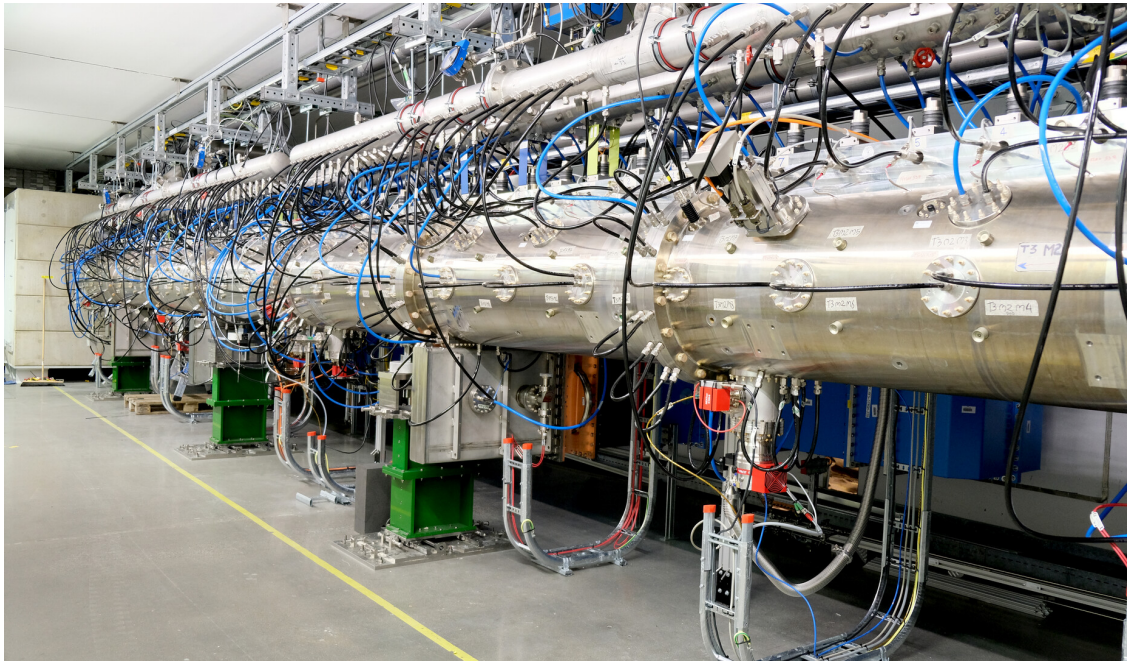




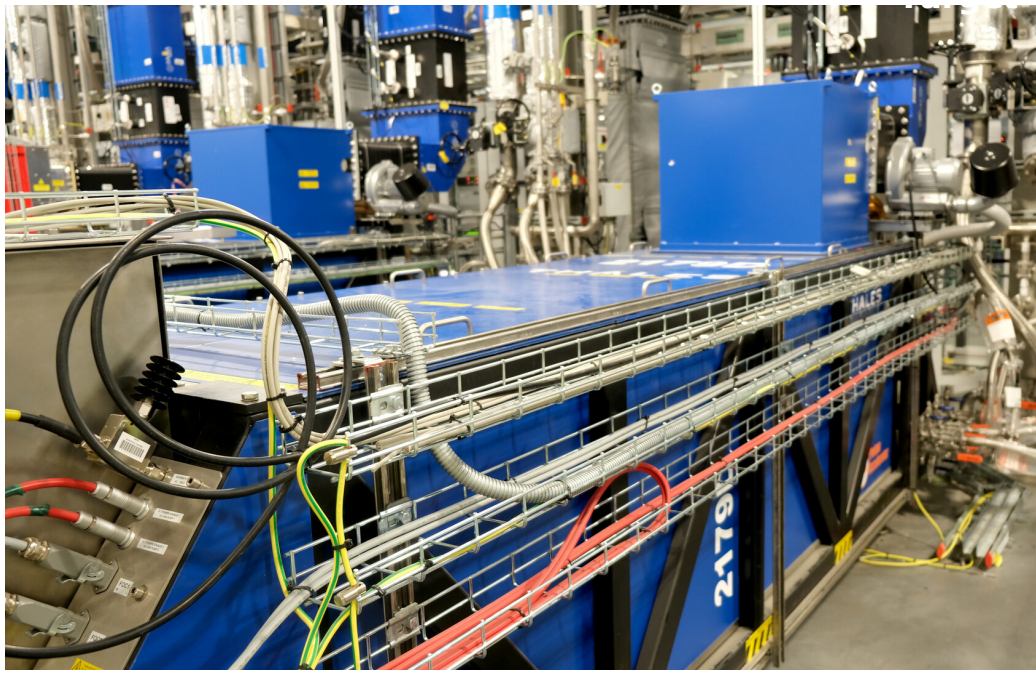


MEBT

Linear Accelerator

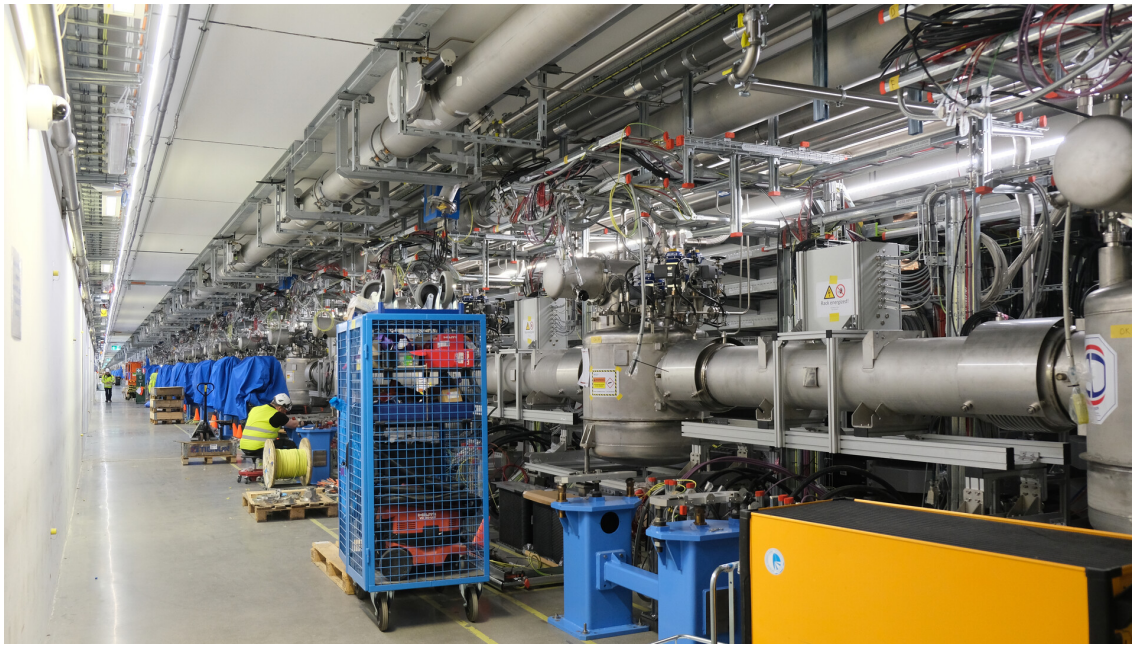


DTL



Klystron

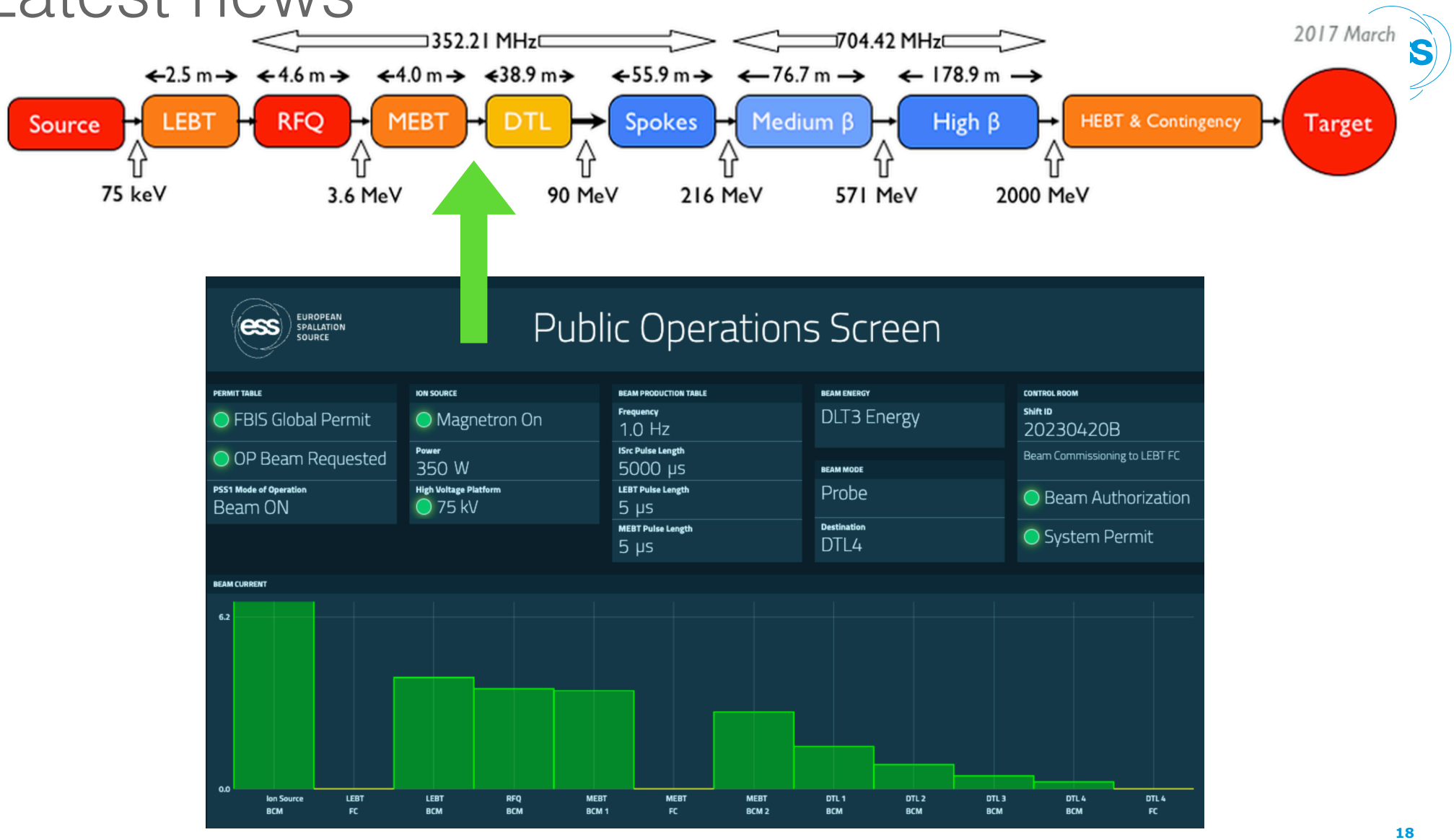
Linear Accelerator



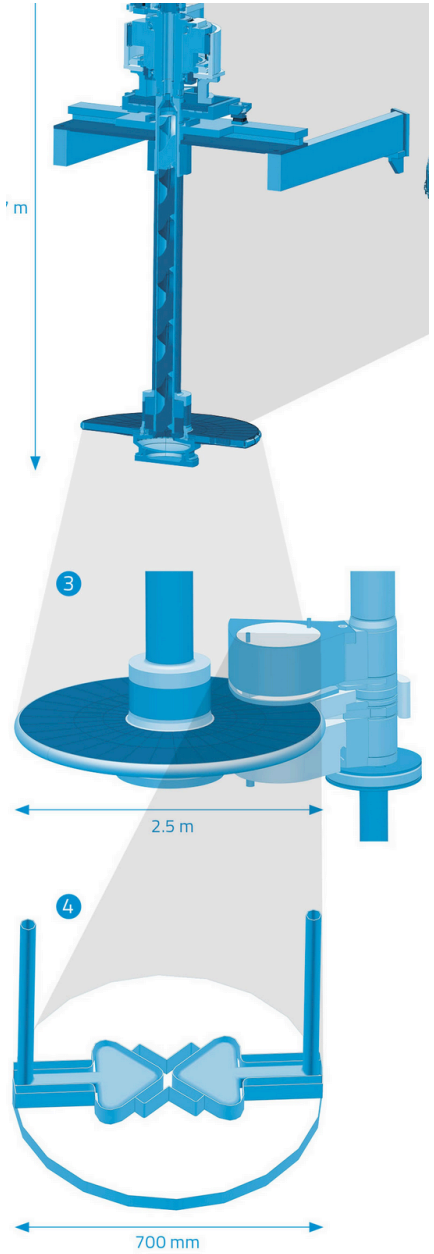
Cryo Systems for superconducting linac components

Cryomodule

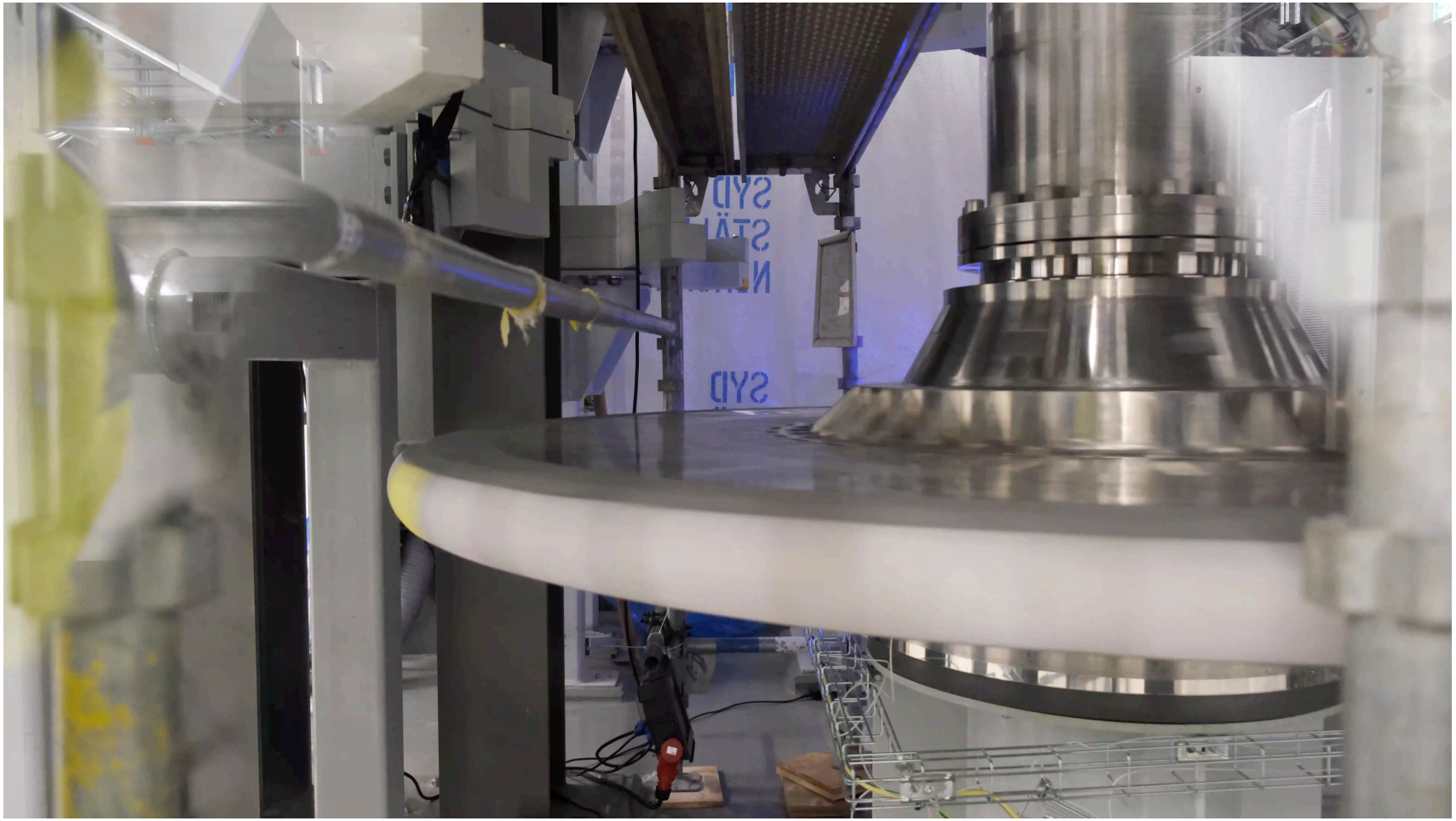
Latest news


2017 March
352.21 MHz
704.42 MHz
2.5 m
4.6 m
4.0 m
38.9 m
55.9 m
76.7 m
178.9 m
Source
LEBT
RFQ
MEBT
DTL
Spokes
Medium β
High β
HEBT & Contingency
Target
75 keV
3.6 MeV
90 MeV
216 MeV
571 MeV
2000 MeV
EUROPEAN SPALLATION SOURCE
Public Operations Screen
PERMIT TABLE
FBIS Global Permit
OP Beam Requested
PSS1 Mode of Operation
Beam ON
ION SOURCE
Magnetron On
Power
350 W
High Voltage Platform
75 kV
BEAM PRODUCTION TABLE
Frequency
1.0 Hz
ISrc Pulse Length
5000 µs
LEBT Pulse Length
5 µs
MEBT Pulse Length
5 µs
BEAM ENERGY
DLT3 Energy
BEAM MODE
Probe
Destination
DTL4
CONTROL ROOM
Shift ID
20230420B
Beam Commissioning to LEBT FC
Beam Authorization
System Permit
BEAM CURRENT
6.2
0.0
Ion Source BCM
LEBT FC
LEBT BCM
RFQ BCM
MEBT BCM 1
MEBT FC
MEBT BCM 2
DTL 1 BCM
DTL 2 BCM
DTL 3 BCM
DTL 4 BCM
DTL 4 FC

Moderator and Moderator Assembly

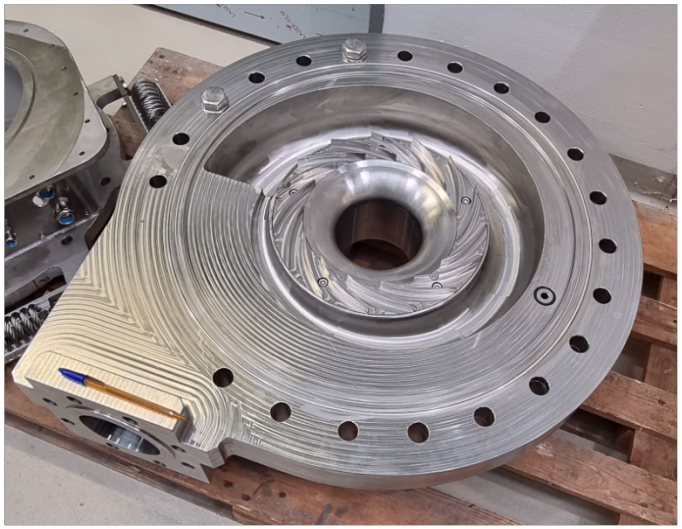


Target Wheel



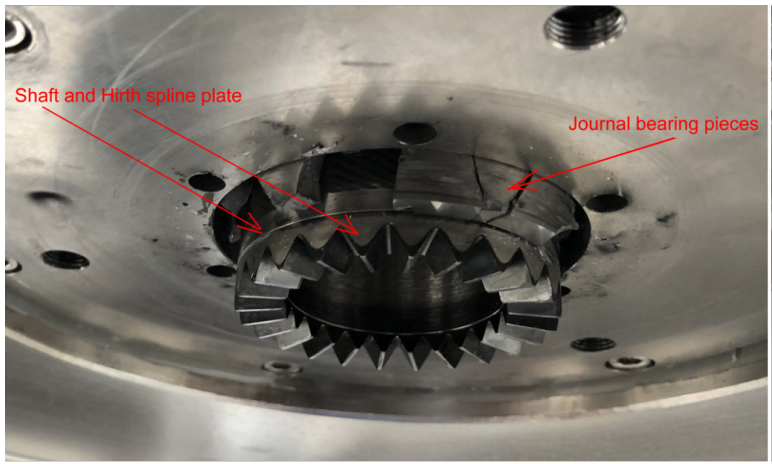
Damage to helium circulator

Helium circulator assembly

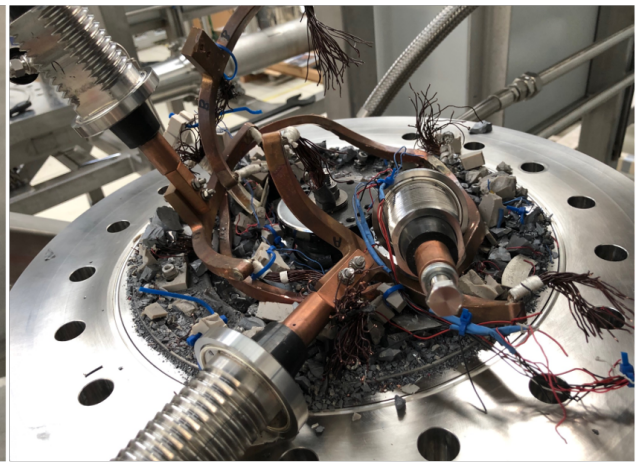


Volute

Impeller

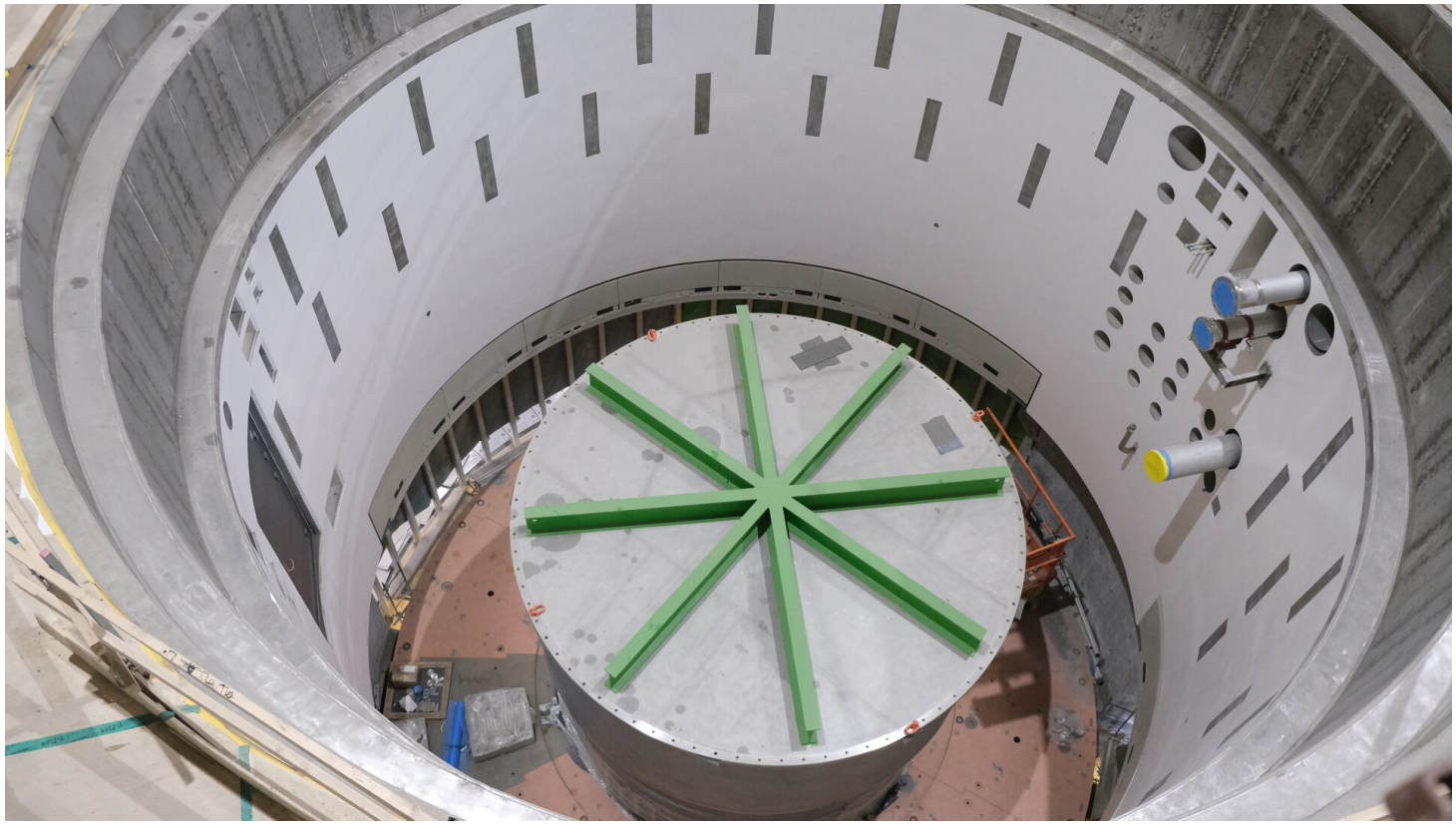


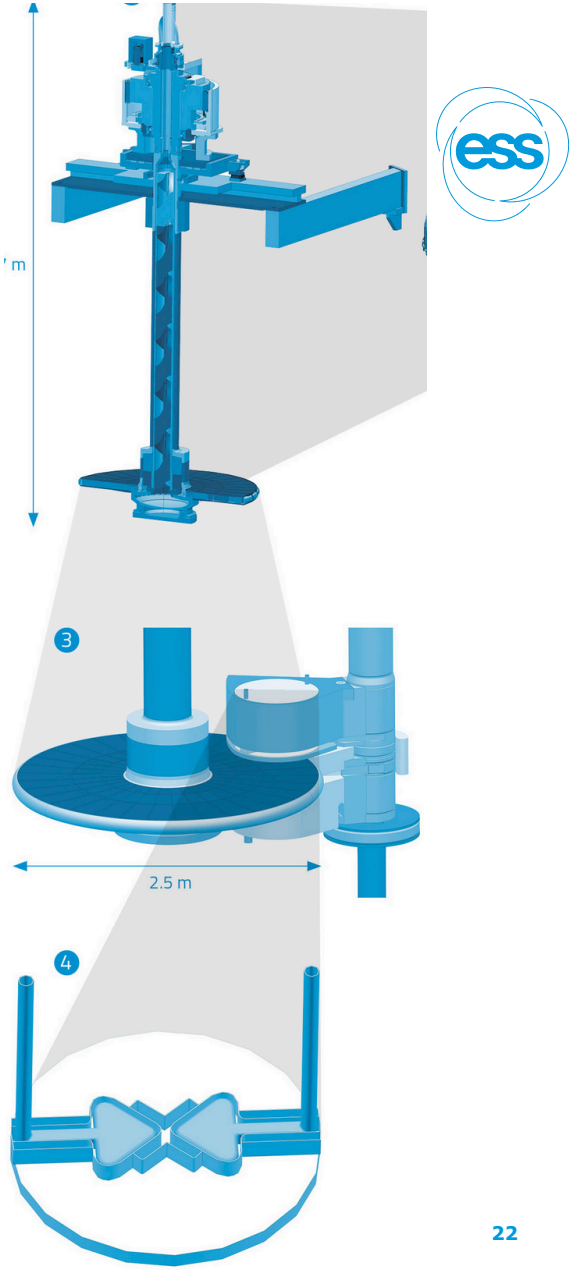
Damaged lower part of the journal bearing of the rotor in the circulator #1



Damaged upper part of the motor for the circulator #2

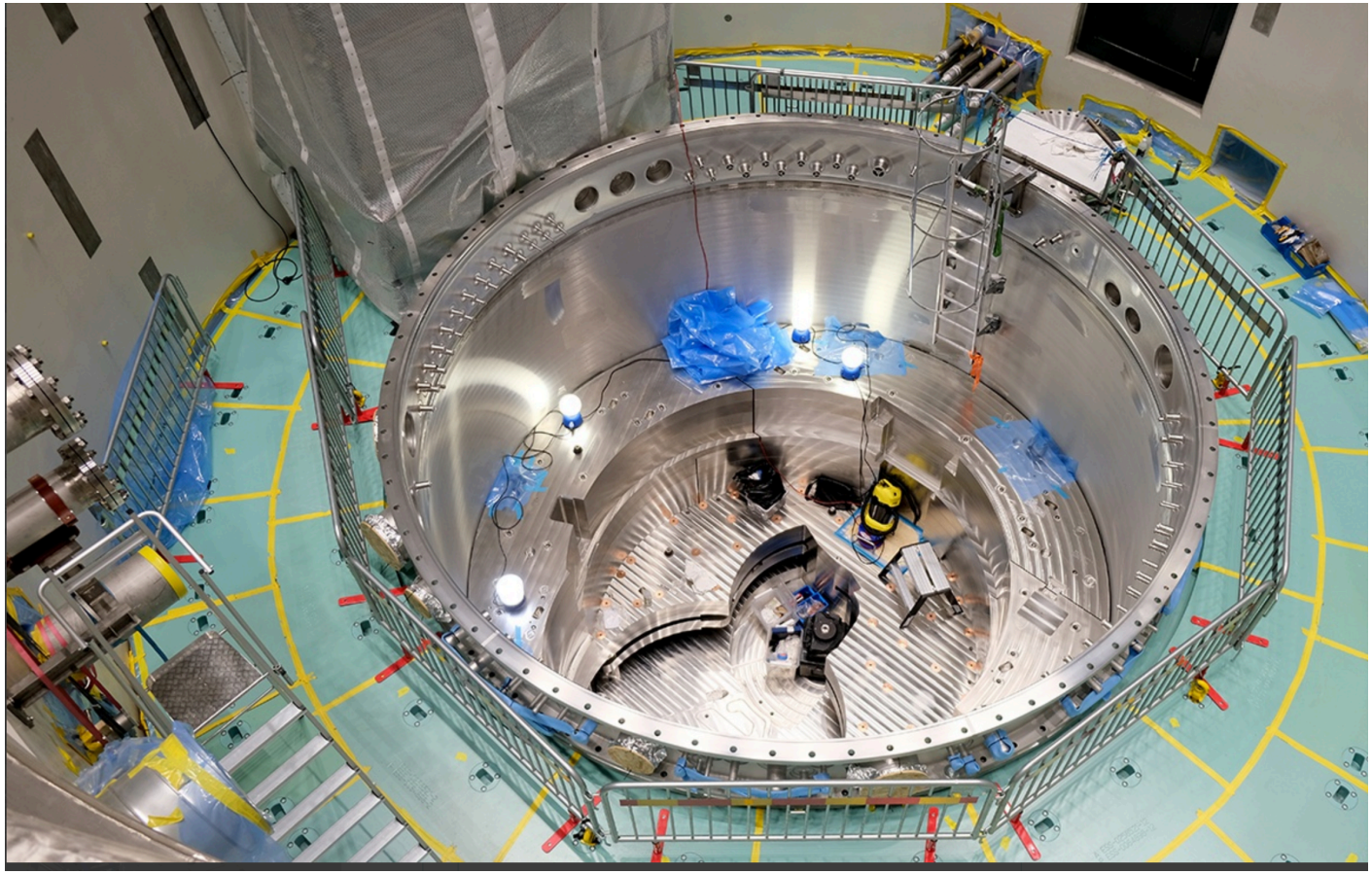
Target monolith



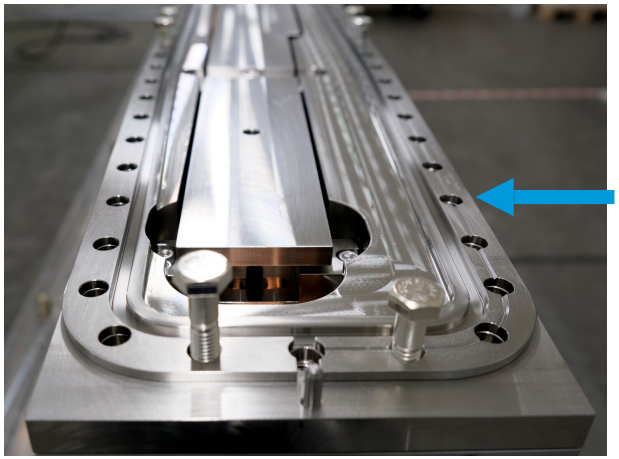


Target monolith and vacuum vessel before installation of shielding

Target monolith shielding



Beamports



In-monolith optics for an instrument …

… get put into a beamport

Surveying the beamport inserts containing in-monolith optics from inside the target vessel

Helium cooling system for the neutron optics

Beam plugs

D01 (South and East Sectors)

D01 (West sector)

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