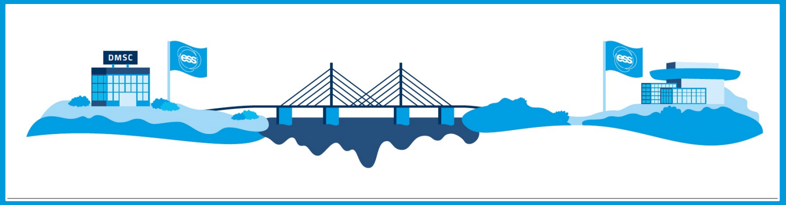
Welcome to Neuwave from the European Spallation Source

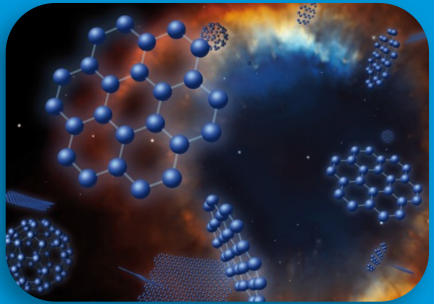
GIOVANNA FRAGNETO, SCIENCE DIRECTOR

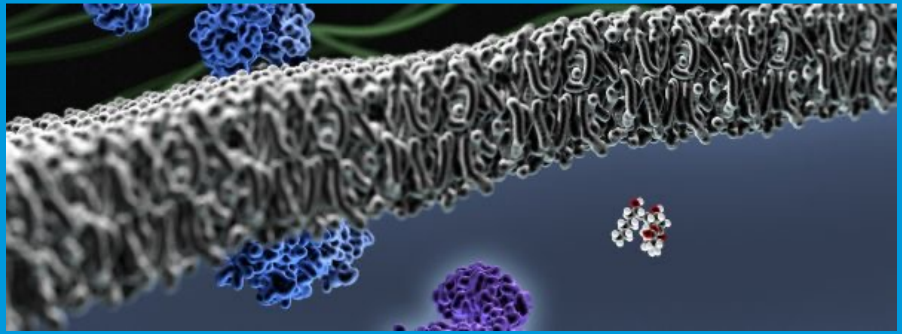
- **2003** European design of ESS completed
- **2009** Decision to site ESS in Lund
- **2012** ESS design update phase complete
- **2014** Construction starts on green field site
- **2019** Start of initial operations phase
- **2025** Beam on target
- **2026–2027** Early Science
- **2027–2028** User program

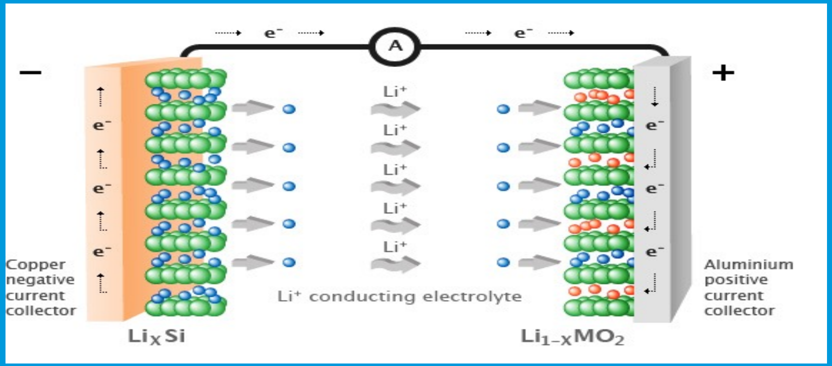


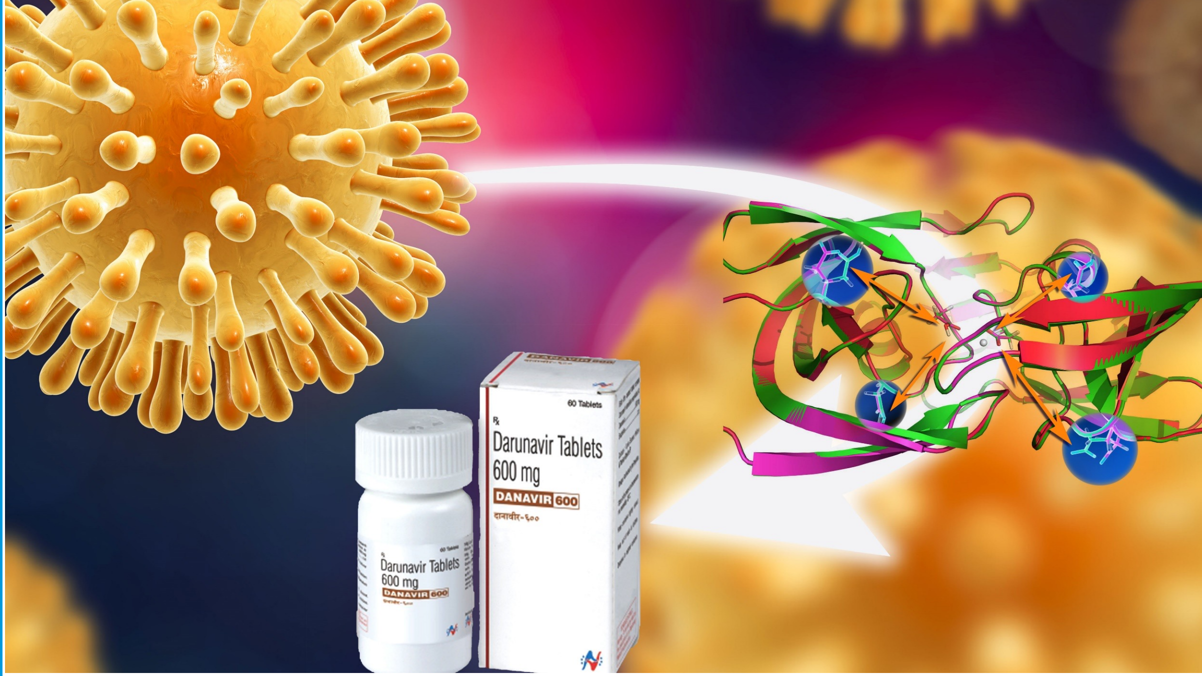
Science with neutrons

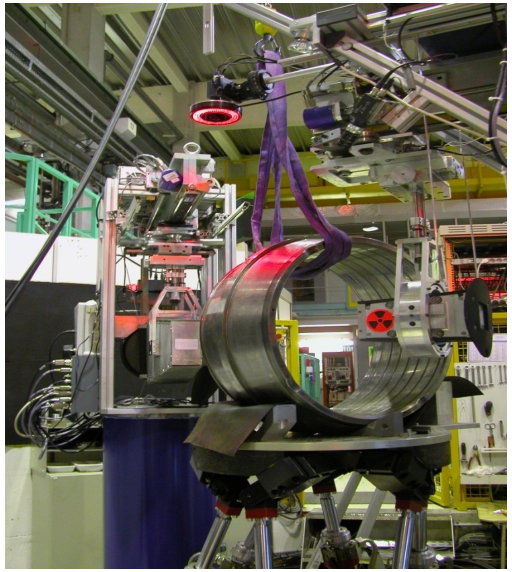
Understanding materials underlies all of modern technology.

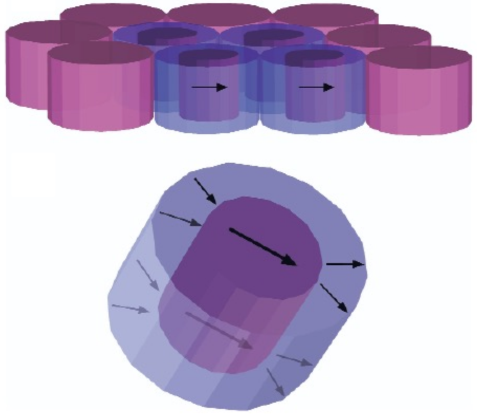


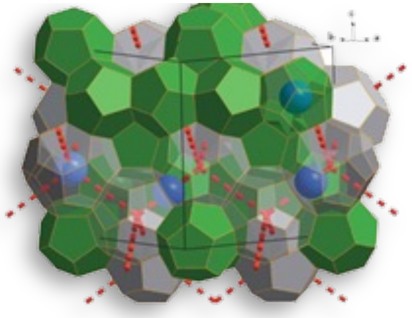






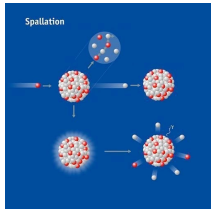




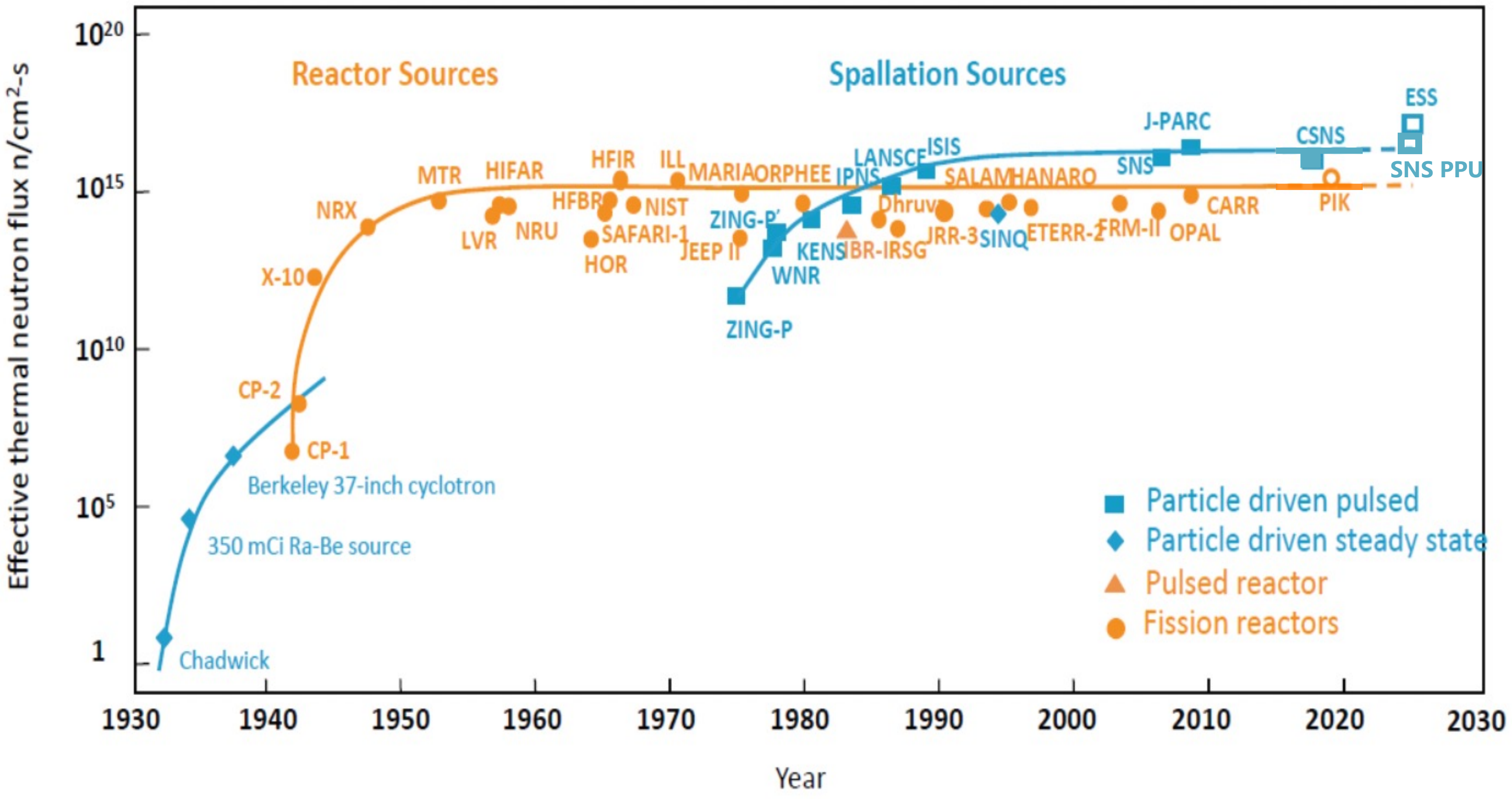


ESS peak flux 20 (2MW)-50 (5MW) brighter than the ILL

ESS mission



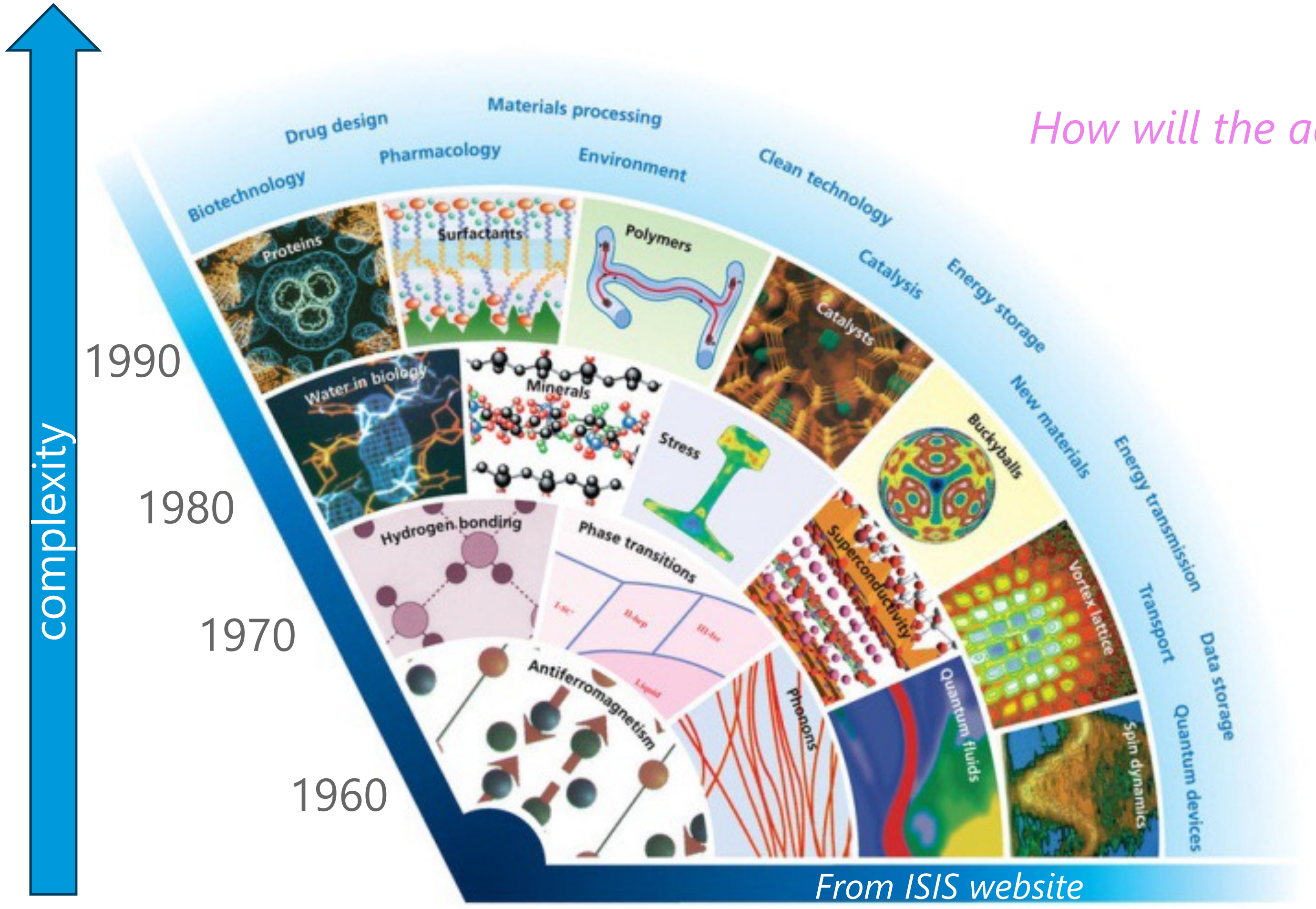
Long pulse (2.86ms) spallation neutron source fed by a linear proton accelerator (870MeV 2MW) and rotating Tungsten target



To build and operate the world most intense neutron source that will enable scientific breakthroughs in research relating to materials, energy, health and environment and address some of the most important challenges of our time

ESS will be an international user service facility

Naturally it will also host internal scientific activities in collaboration with users and user oriented



Future scientific challenges:

How will the advantages of ESS be used to meet societal challenges:

Improved understanding of materials and production processes

Elucidating disease processes and improving medical treatments

Helping the green energy transition

Developing the next generation of smart materials and IT

Furthering our understanding of the universe

ESS will be an international user service facility

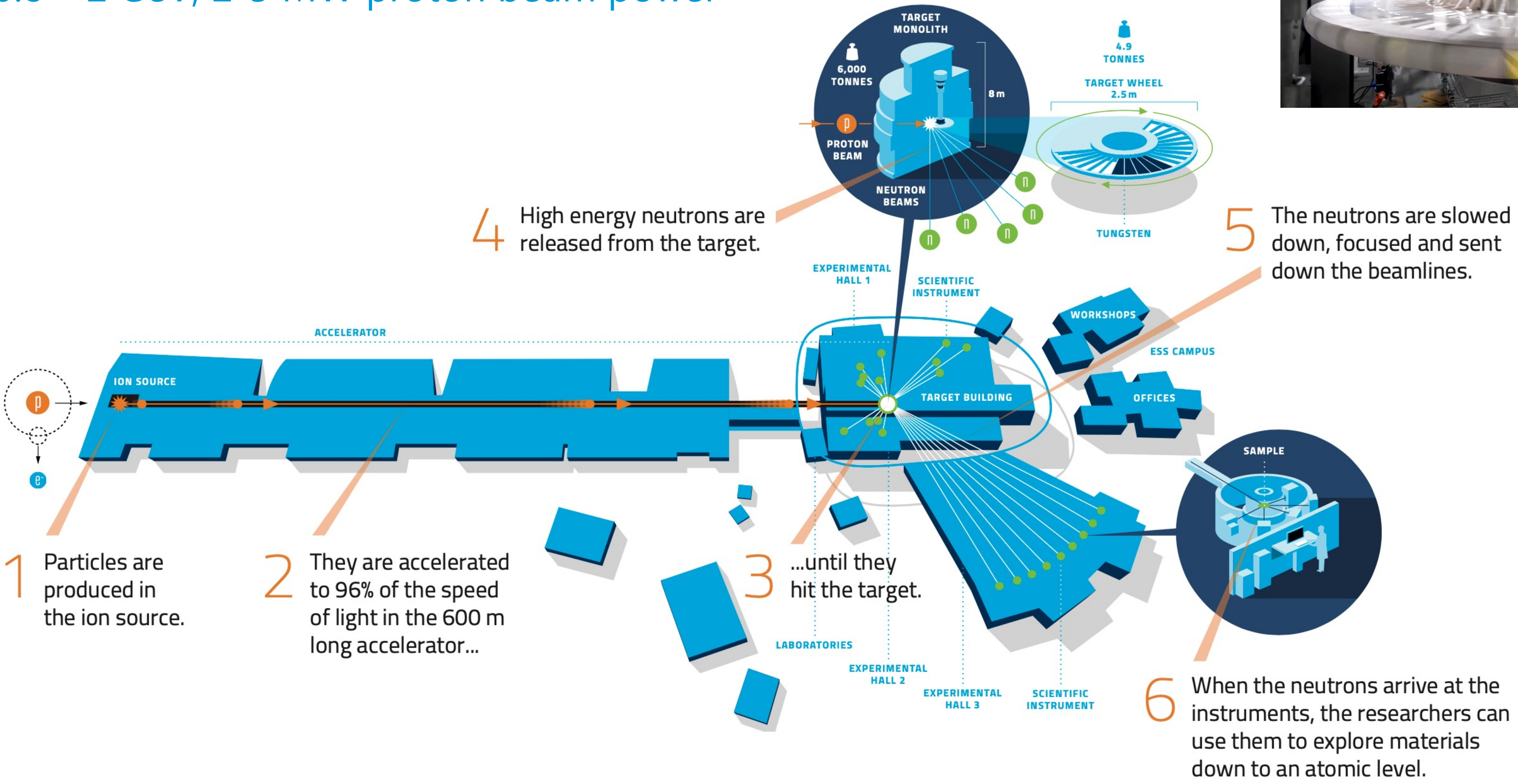
Naturally it will also host internal scientific activities in collaboration with users and user oriented

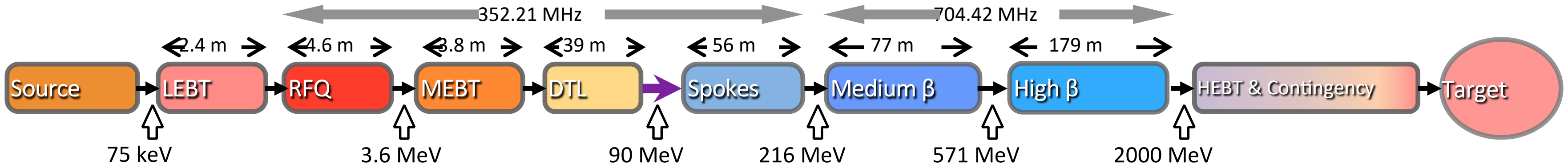
Advances expected in capabilities at ESS:

- Rapid data collection / short counting times to enable kinetics and high-throughput studies
- Probe broad size range to examine hierarchical structures
- Small samples for scanning, biological and complex samples
- Integrated flexible sample environment for non-equilibrium studies
- Integration of complementary techniques experimentally and in data analysis

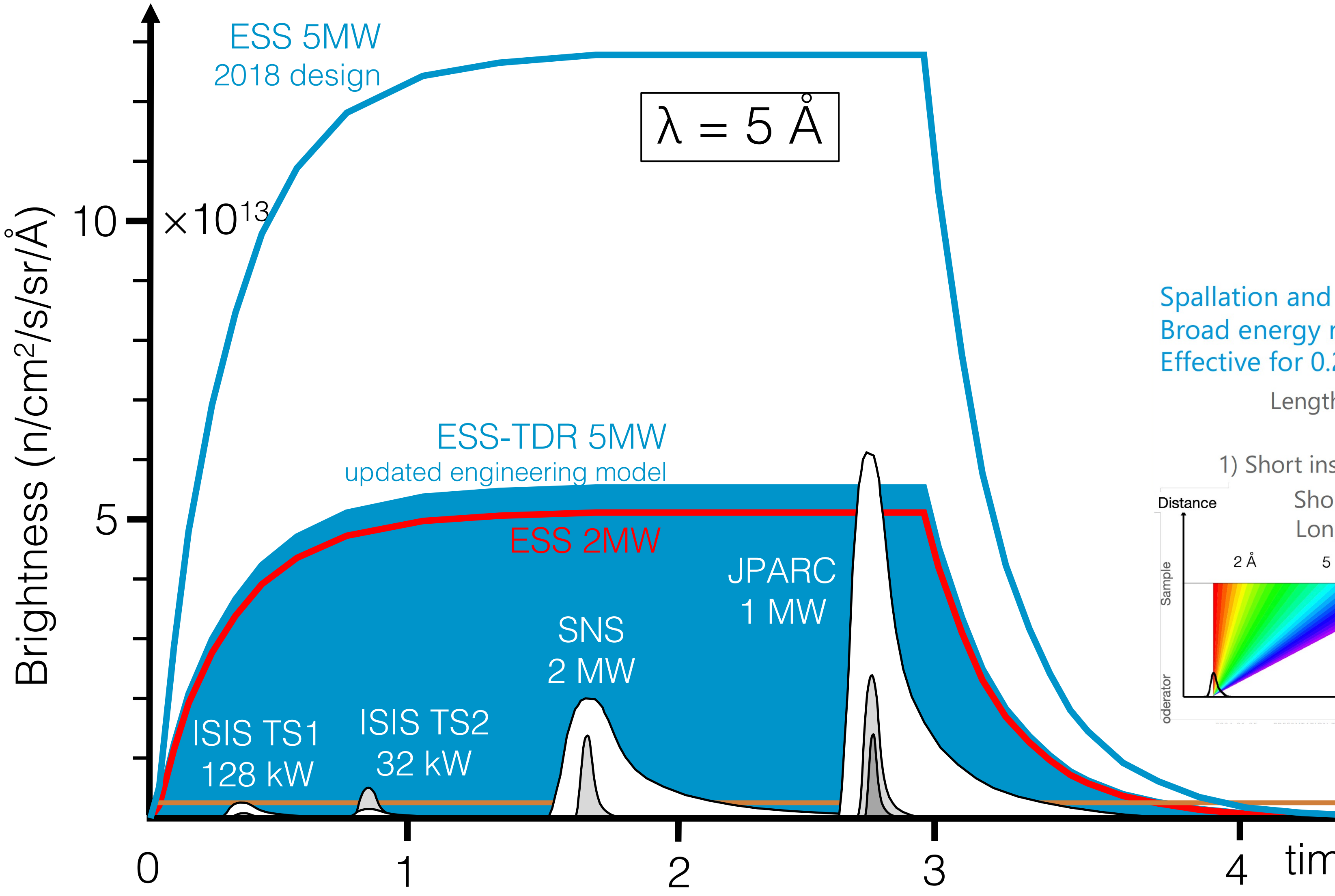
Long-pulse driven by linear accelerator pulse length 2.86 milliseconds

14 Hz, 0.8 – 2 GeV, 2-5 MW proton beam power

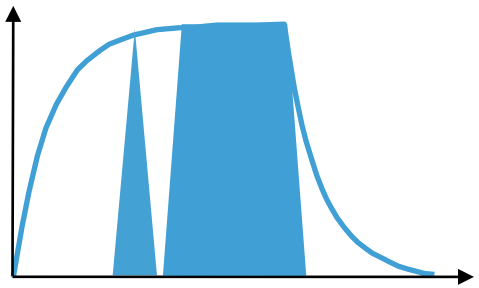




Long-pulse Performance and Flexibility



Possibilities of pulse shaping



$$\frac{\Delta\lambda}{\lambda} \propto \frac{\Delta T}{T}$$

Spallation and time of flight at ESS
Broad energy range from spallation & moderation process
Effective for 0.2-200 meV.

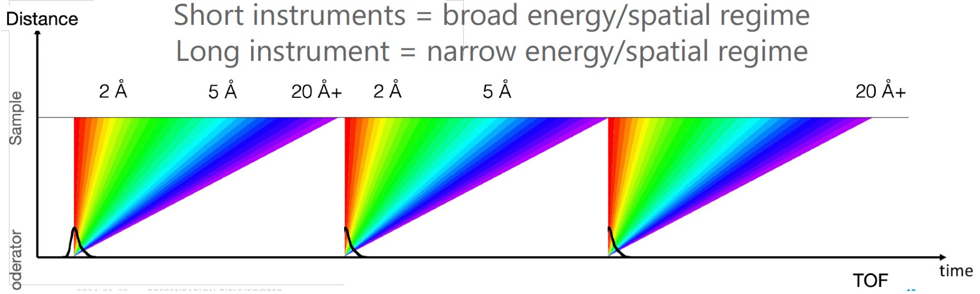
Length of instruments determined by science case.

14 Hz pulses. ΔT ≅ 71 ms

1) Short instruments = broad Δλ, long instrument = narrow Δλ

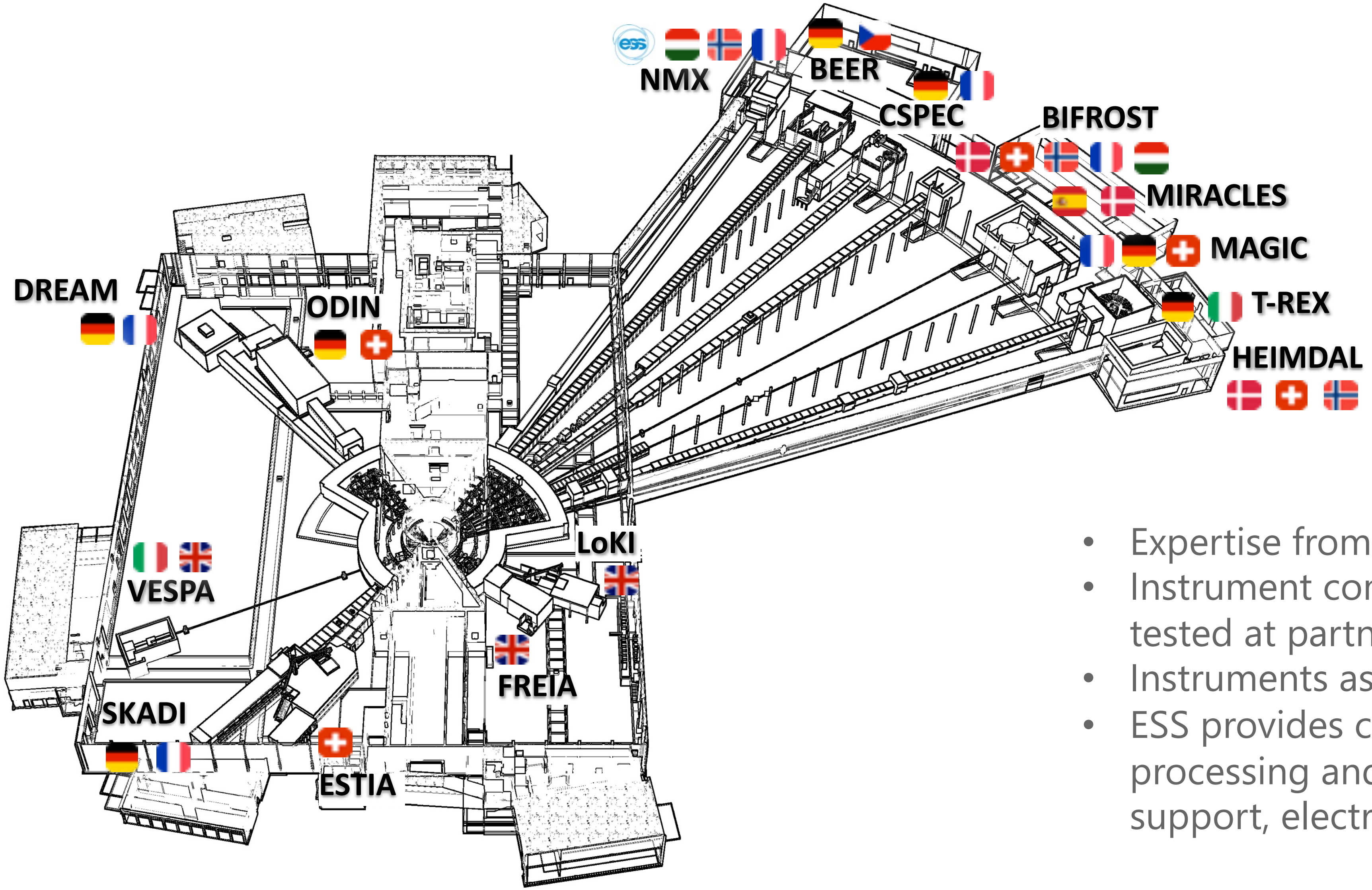
Short instruments = broad energy/spatial regime

Long instrument = narrow energy/spatial regime



Neutron Science Instruments at ESS

1 Imaging, 2 SANS, 2 Reflectometers, 5 Spectrometers, 5 Diffractometers, 1 Test Beamline



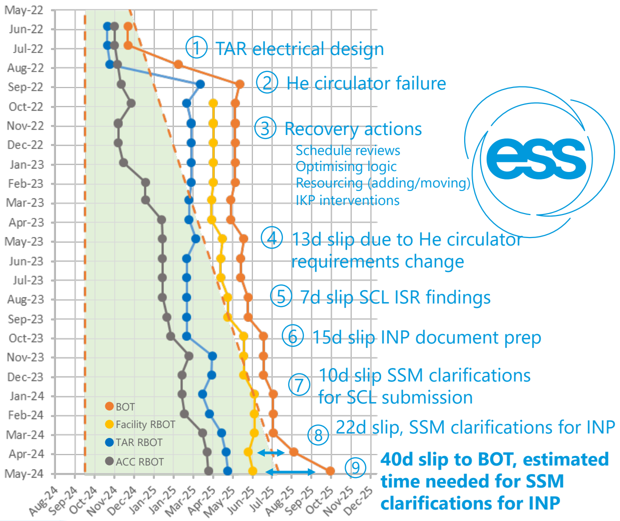
22 public instruments , 15 selected to date

- Life sciences
- Soft condensed matter
- Chemistry of materials
- Energy research
- Magnetism, superconductivity
- Engineering, geosciences
- Archaeology, heritage conservation

- Expertise from all around Europe
- Instrument components designed, built, and tested at partner institutes
- Instruments assembled and integrated at ESS
- ESS provides core - labs, data acquisition, processing and management, engineering support, electrical, utilities, safety systems,

2024

A crucial year for the project



Finish installation of CMs, RF, BI, Magnets
Conditioning of CMs and DTLs
Shielding and fire sealing
Backup compressor, H20 upgrade
MPS, PSS for BoD
Cryo cooldown with 27 CMs
SAR4/SRR4

Beam on Dump
~early 2025

A2T region

2024

2025

Last deliveries of Target components (e.g. He circ. A&B)
Target installation -> testing & commissioning

INP ref doc complete, receive SCL permit, submit INP permit

DMSC systems ready for Tranche 1
LOKI, ODIN, DREAM, BIFROST, TBL TG5/SAR

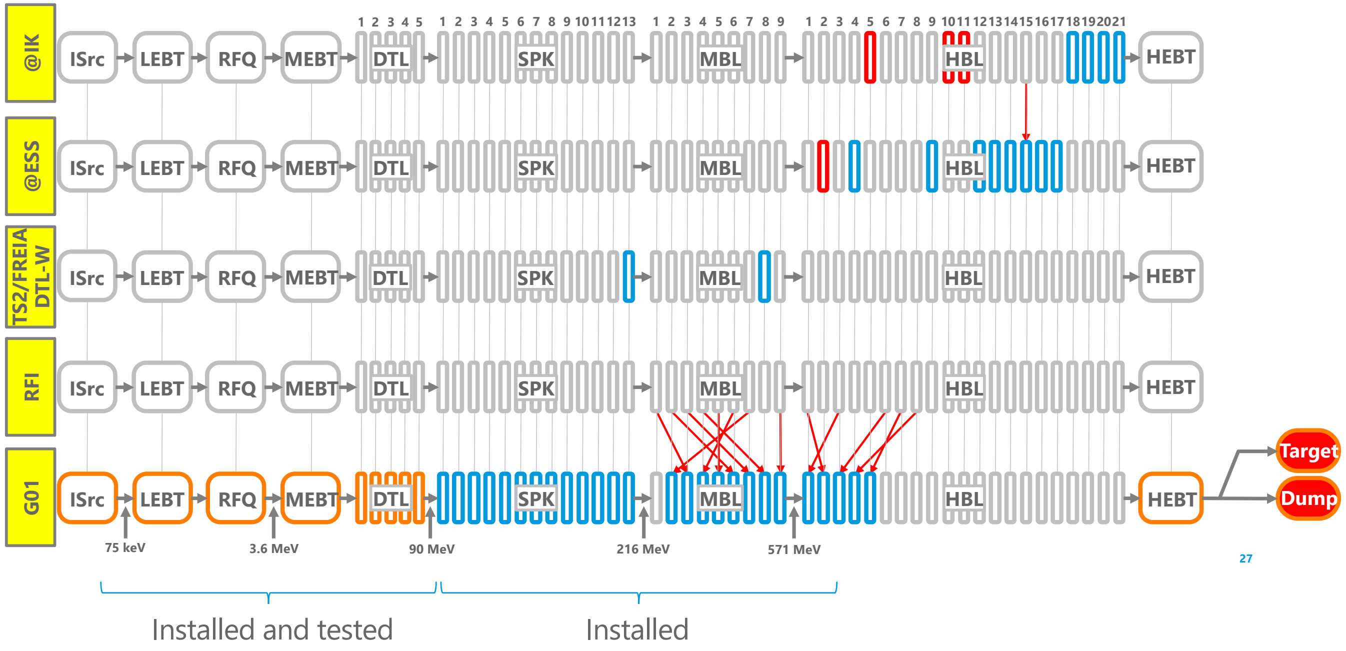
Integrated testing

Beam on Target
~autumn 2025

Post-BoT activities

Accelerator

- Normal Conducting Linac installation completed *(proton beam successfully transported to the DTL4 FC, achieving nominal current)*
- *Full* compliment of CMs ready for BOD/BOT (*2K operation achieved*)
- Gallery support systems are in good shape. All RF racks needed for BoT have been energized, now being soak tested.
- A2T region nearing completion



SCL license for trial operations was received late May

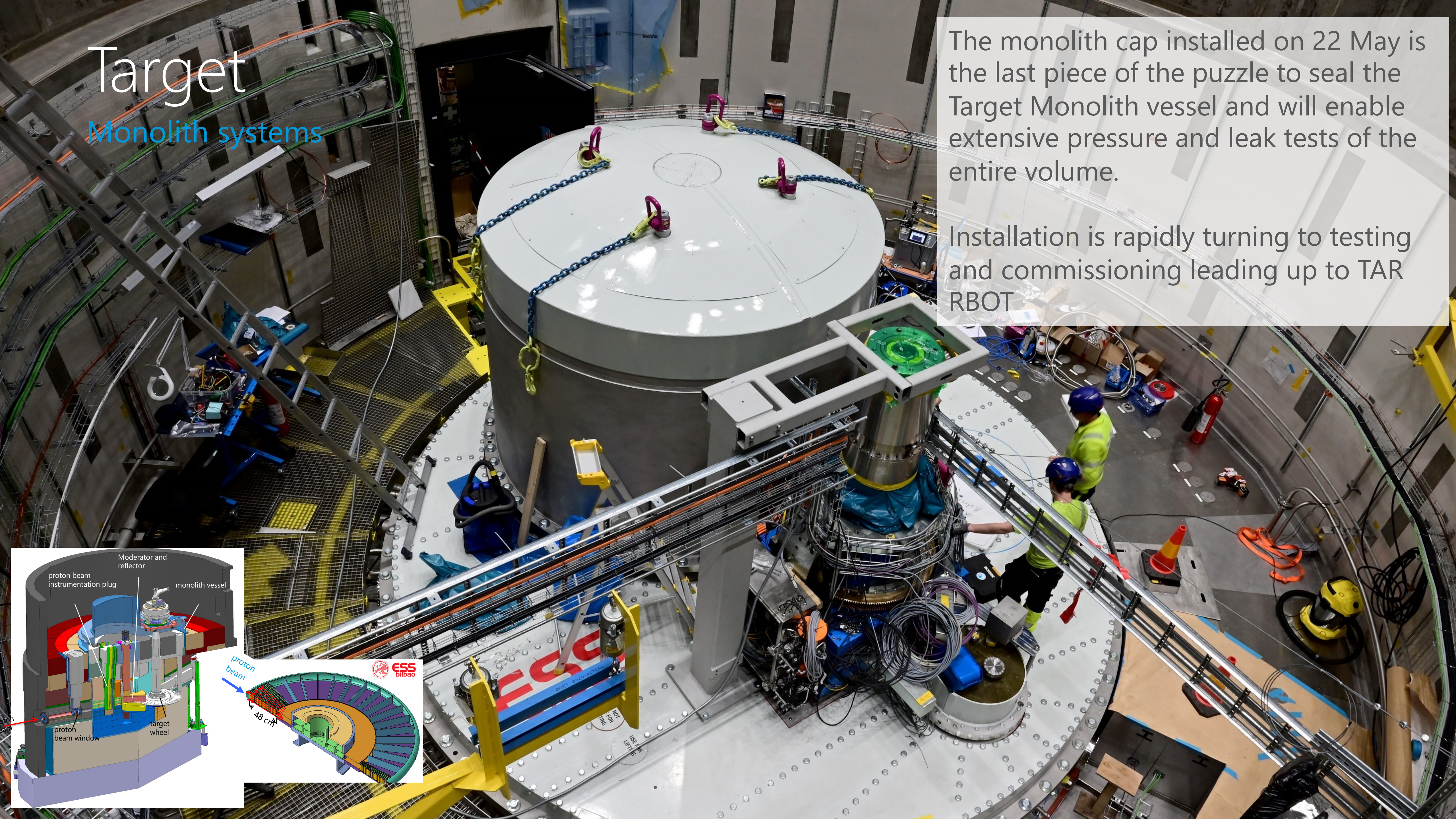
Week 5: The French state visit to the Accelerator tunnel celebrating the recent achievements leading up to beam operations at the end of 2024

Target

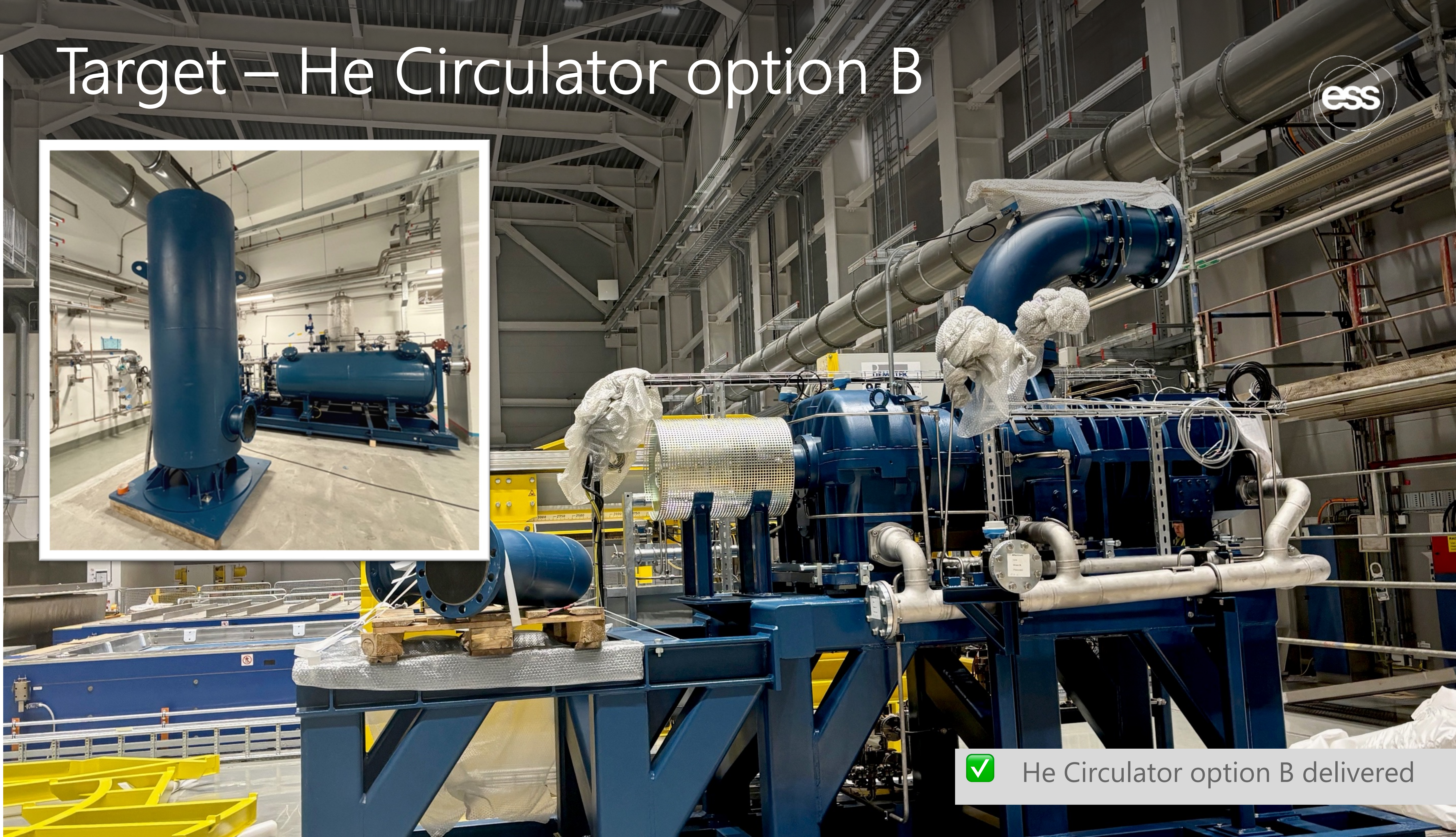
Monolith systems

The monolith cap installed on 22 May is the last piece of the puzzle to seal the Target Monolith vessel and will enable extensive pressure and leak tests of the entire volume.

Installation is rapidly turning to testing and commissioning leading up to TAR RBOT



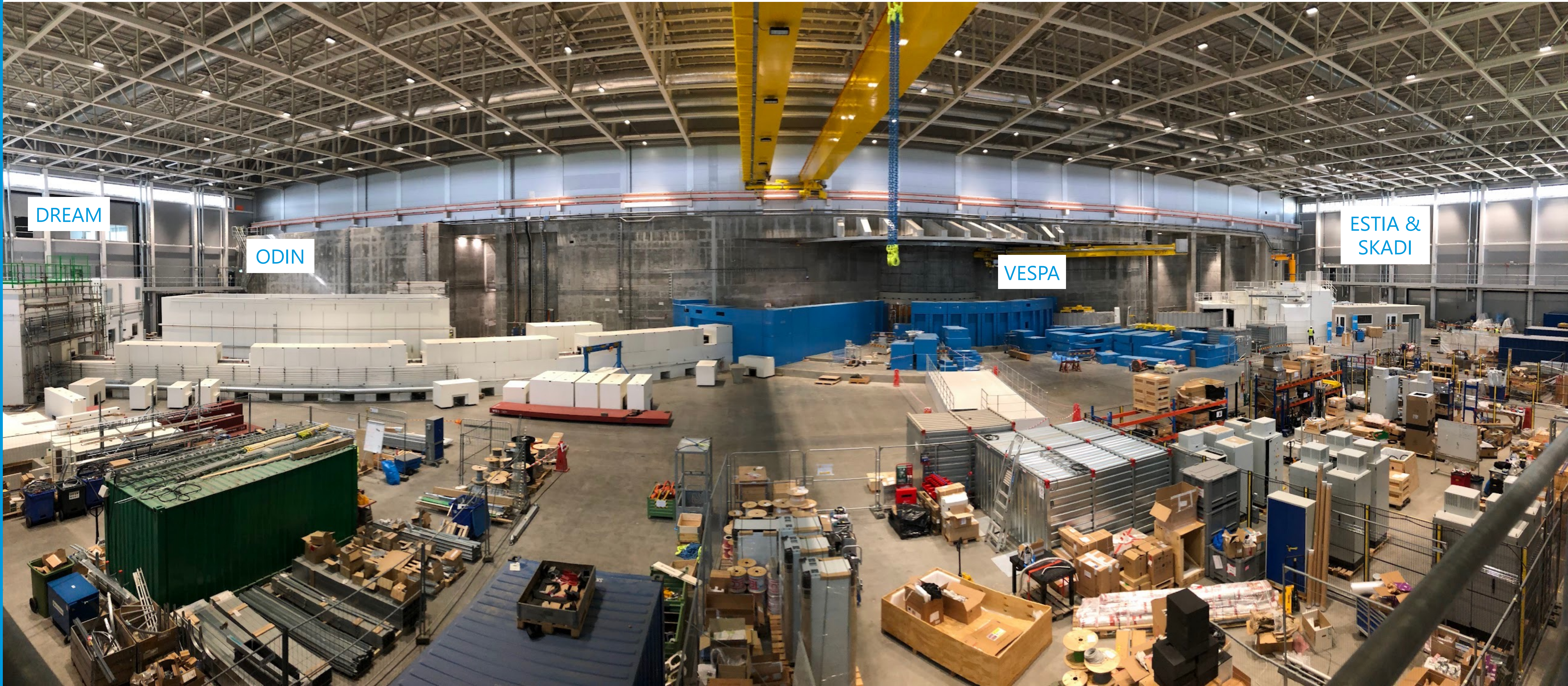
Target – He Circulator option B



✅ He Circulator option B delivered

Neutron Instruments

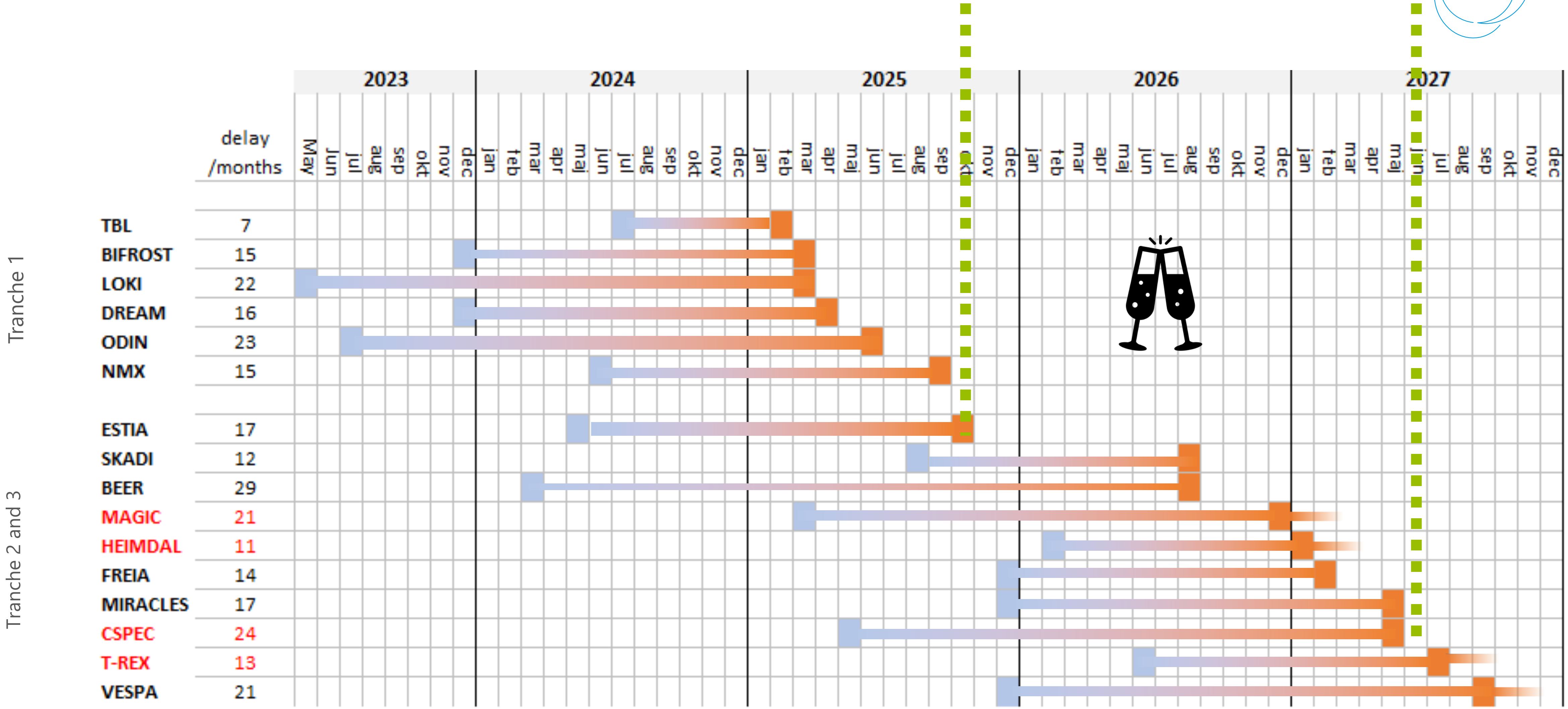
D01 side



Neutron Instruments

D03 side

Planning of neutron instruments

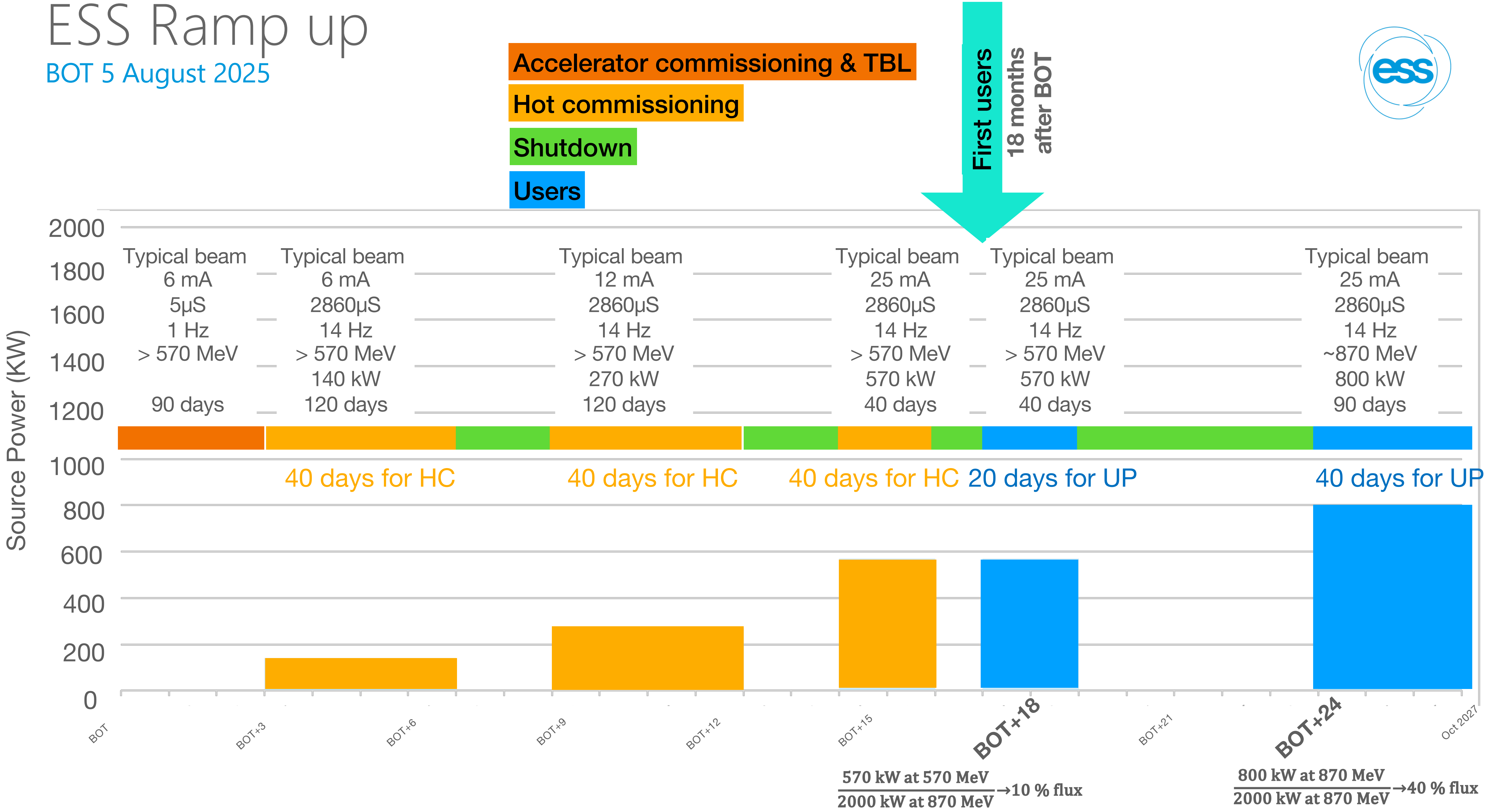


Updated with P6 21st of May live data (with the exception of T-rex and Magic where we've used the latest draft of the ongoing replanned plan)

replanning ongoing

ESS Ramp up

BOT 5 August 2025



The Science Directorate is in charge of completing and commissioning the instruments and delivering science and the user programme

Science Directorate

- Research Coordination Office

Diffraction and Imaging
- BEER
- DREAM
- HEIMDAL
- MAGIC
- ODIN
- TBL

Large Scale Structures
- ESTIA
- FREIA
- LOKI
- NMX
- SKADI

Spectroscopy
- BIFROST
- CSPEC
- MIRACLES
- T-REX
- VESPA

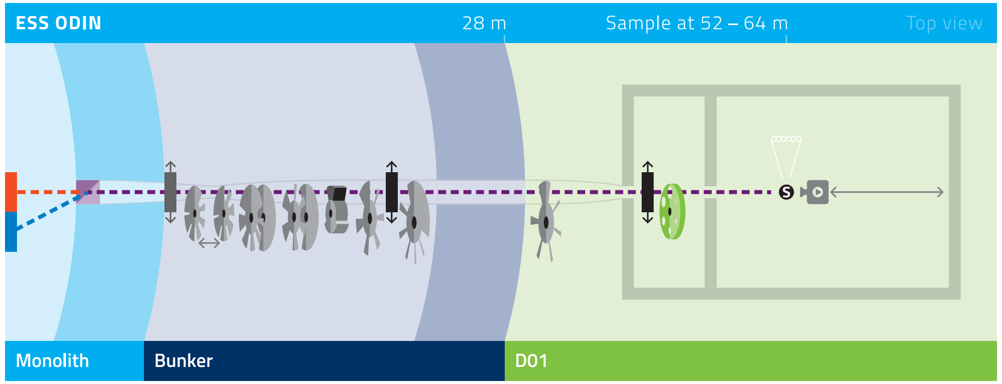
Data Management and Software Center
- Administration
- Data Analysis and Modelling
- Data Systems
- Scientific Information Management Systems
- INSTRUMENT DATA SCIENTISTS

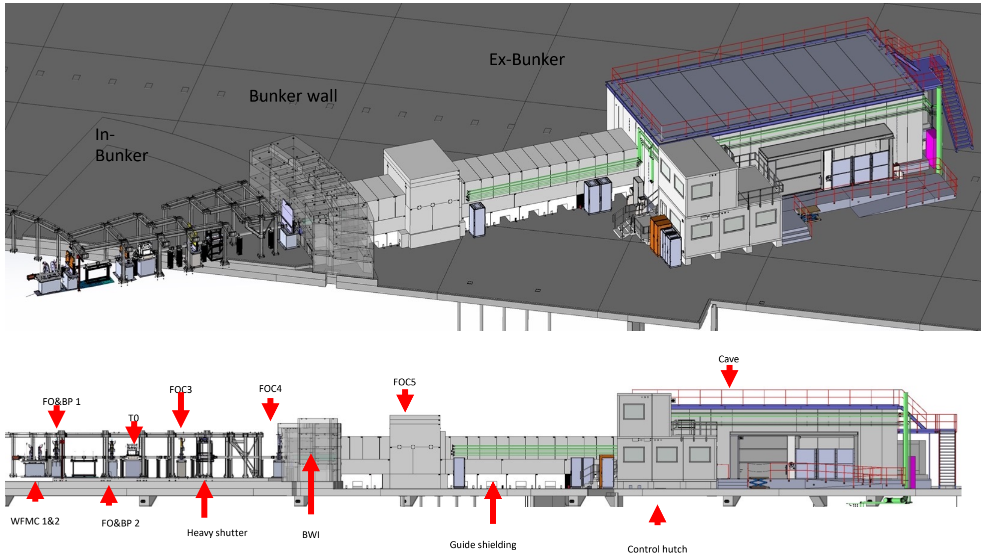
Scientific Support
- Chemistry and Life Science
- Materials Science and Physics

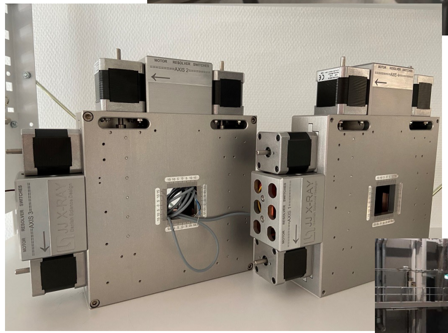
Neutron Scattering Systems
- Chopper
- Detector
- ECDC
- Motion Control and Automation
- NSS Planning and Coordination
- Technical Projects

ODIN

Optical and Diffraction Imaging with Neutrons







ODIN Quick Facts	
Instrument Class	Imaging
Moderator	Bispectral
Primary Flightpath	50 m (to pinhole)
Secondary Flightpath	2 – 14 m (pinhole to detector)
Wavelength Range	1 – 10 Å
Field of View	20 x 20 cm^2
L/D Ratio	Tunable 300 – 10000
Incident Beam Polarisation	Optional
Polarisation Analysis	Optional
Bandwidth at 14 Hz	4.5 Å
White Beam Mode	
Flux at Sample at 2 MW	1.2 x 10^9 n s^{-1} at 10 m, L/D = 300
Spatial Resolution	< 10 µm
TOF Mode without Pulse-Shaping	
Flux at Sample at 2 MW	9 x 10^8 n s^{-1} at 10 m, L/D = 300
Spatial Resolution	< 10 µm
Wavelength Resolution	Δλ/λ = 10% at λ = 2 Å
TOF Mode width Pulse-Shaping	
Flux at Sample at 2 MW	1 x 10^8 n s^{-1} at 10 m, L/D = 300
Spatial Resolution	< 10 µm
Wavelength Resolution	Adjustable <0.5% - 1% (constant for all λ)

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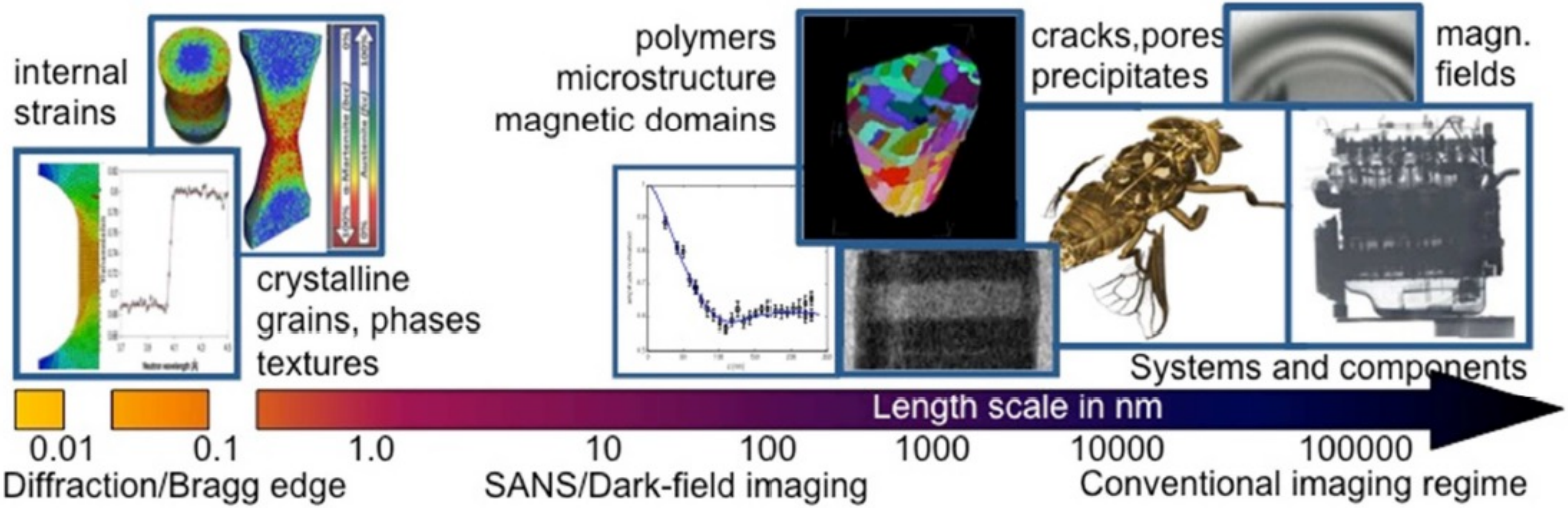
PAUL SCHERRER INSTITUT

ODIN

Science Case

M. Strobl, Physics Procedia, 69 (2015) 18-26



Descoping on ODIN included:

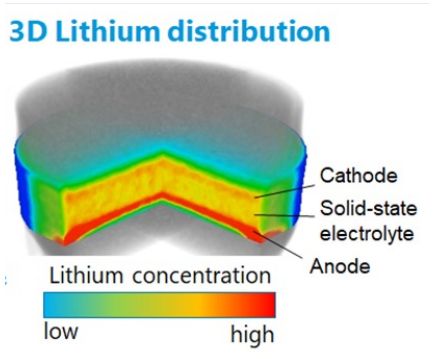
1. *High resolution imaging detectors*
2. *X-ray imaging capabilities*
3. *Diffraction detector(s)*
4. *Grating interferometry*
5. *Polarized capabilities*
6. *SEMSANS*

ODIN

Early Science Ideas

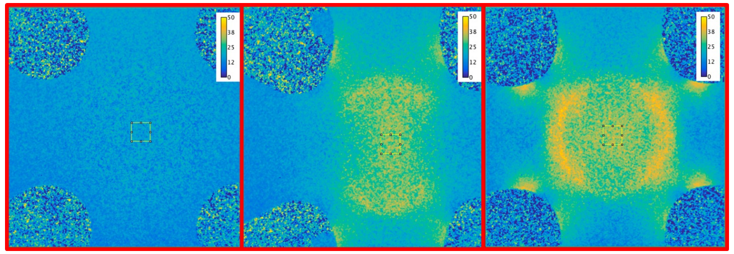
Attenuation tomography / time series (dual mode)

- Battery / battery material
- ANISSA project (ILL-HZB-LU-UM-WWU)
- exchange $^{7}Li/^{6}Li$
- cell development ongoing



Untextured phase mapping (diffraction contrast)

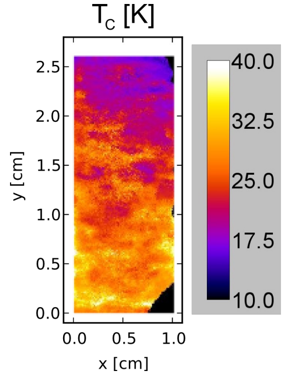
- Additive Manufacturing / engineering samples
- PSI
- no requirements from SE/Labs/external foreseen

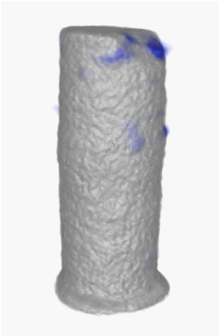


E. Polatidis, M. Morgano *et.al.*
Materials, **16** (2020) 1450

Polarized neutron imaging

- In-situ depolarization analysis of magnets under different conditions
- TUM
- Enabled by in-kind polarization project, SAM involvement

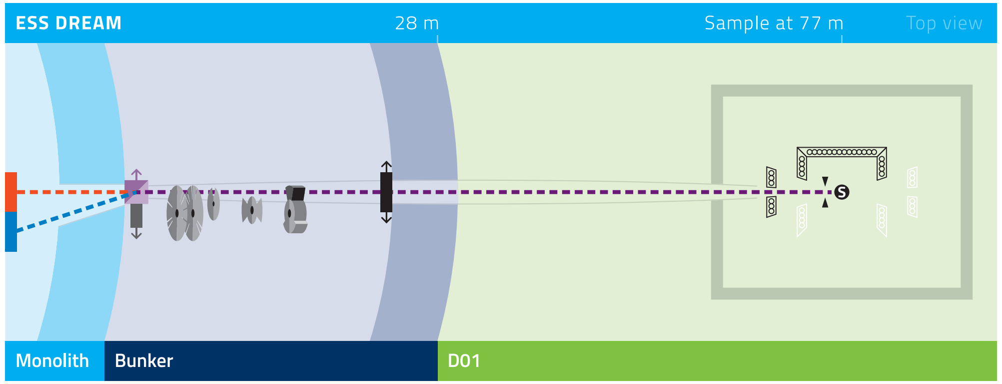




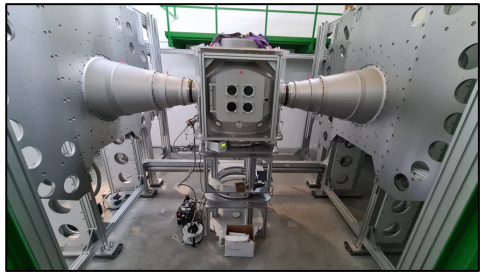
M. Schulz, *et.al.*
J.Phys. Conf., **211** (2010) 012025

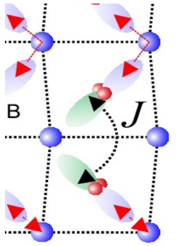
DREAM

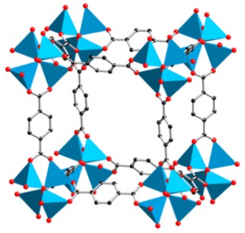
Diffraction Resolved by Energy and Angle Measurements



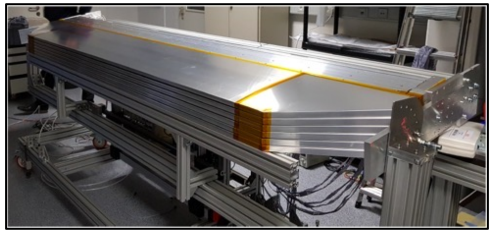
Sample vessel







Mantle & Endcap detectors



Experimental caves & Control hutches

Magnetism
superconductors
multiferroics
weak moments
orbital ordering
charge ordering

Energy Materials
Li, H -materials
in-situ measurements
multiphase
small coin cells

Nanostructures
magnetic nanoparticles
core-shell structures
real-time synthesis

Large Unit Cells
MOFs
catalysis
thermoelectrics
molecular sieves
H2- storage

Moderator	Bi-spectral
Primary Flightpath	76.5 m
Secondary Flightpath	1.1 m (end-cap and mantle detectors) 2.5 m (high-resolution and low-angle detectors)
Wavelength Range	0.5–4.1 Å
Flux at sample at 2MW	1.4×10^{7}ns^{-1}cm^{-2} (Δd = 3×10^{-4} Å) 1.0×10^{9}ns^{-1}cm^{-2}(Δd = 2.5×10^{-2} Å)
Q-Range	0.01 – 25 Å^{-1}
Detector Coverage	1.82 sr first day operations 5.12 sr full scope
d-spacing Resolution Δd	Adjustable 3×10^{-4} – 2.5×10^{-2} Å

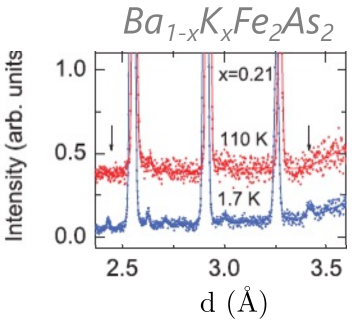
Orphée Laboratoire Léon Brillouin

JÜLICH FORSCHUNGSZENTRUM

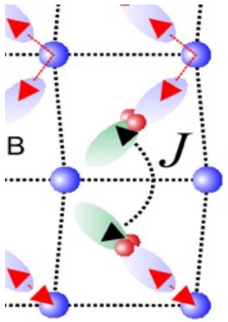
powders
single-crystals
nanoparticles
alloys
liquids

DREAM

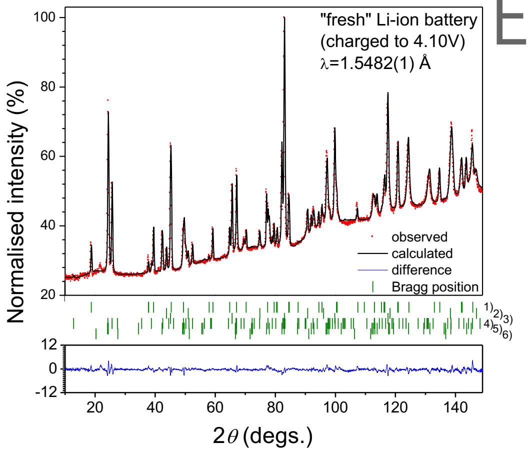
Magnetism



weak moments
phase diagrams of superconductors
multiferroics



orbital ordering
charge ordering
distortion
magnetic exchange

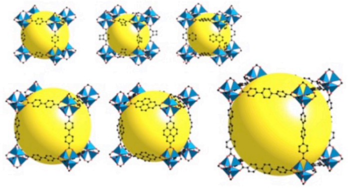


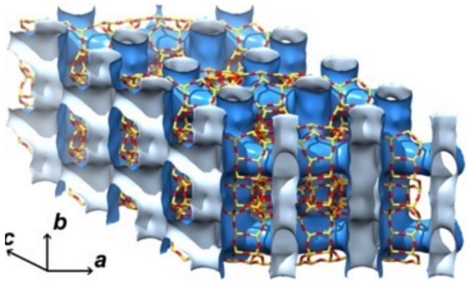
Energy Materials

multiphase
catalysts
in-operandi
batteries

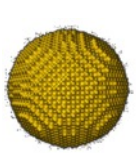
Large Unit Cells

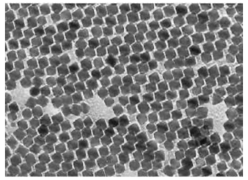
MOFs
thermoelectrics
molecular sieves
H_2 - storage





Nanostructures





many novel samples come in np
magnetic nanoparticles
core-shell structures
self-assembly
synthesis

Instrument Features

Bi-spectral (thermal + cold)
Pulse-shaping (high flux vs high resolution)
World-highest resolution in neutron powder diffraction
Low-angle scattering (nm-SANS) + polarized neutrons
New type of 3D detectors (^{10}B from CDT GmbH)

Courtesy M. Feygenson

DREAM

Early Science Ideas

Characterising DREAM main functionalities

- concept:

Neutron tests of novel components to provide a baseline for first user experiments

➔ *Bi-spectral moderator view*

➔ *Detectors performance*

➔ *Pulse shaping, world best resolution*

➔ *PDF data quality*

➔ *2D Rietveld*

- requirements:

Sample prep lab (OK)

Sample changer (ongoing)

Data reduction (DMSC, ongoing)

Magnetic nanoparticles

- concept:

Monitor magnet. profile of IONP to track and improve battery performance

➔ *Third party funding for novel instrument capabilities*

➔ *Cold neutron polarizer*

➔ *nm-SANS detector*

- current collaborators :

UU, MAX IV, Cologne, FZJ

- requirements:

Electrochemical cell (ongoing)

Benchtop testing of cell (ongoing)

DMSC & SAD interfaces (ongoing)

Hydrogenous materials

- Water confinement in porous materials:

  - concept:

  Unusual phase diagram of liquids confined in micro/meso-porous

  - requirements:

  Gas sorption from SAD (ongoing)
  High-Resolution diffraction (OK)
  nm-SANS detector (OK)

- Battery materials:

  - concept:

  Degradation of the electrolyte

  - requirements:

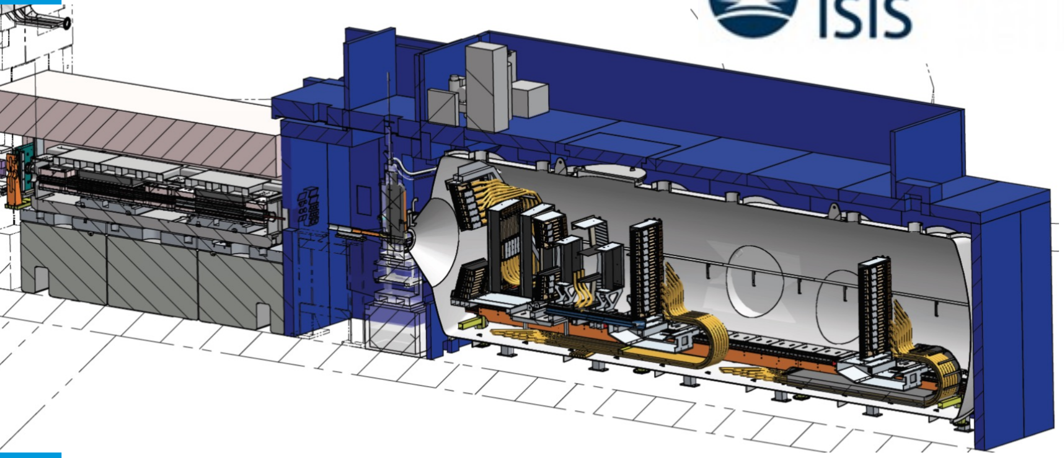
  Medium/High-Flux diffraction & PDF

current collaborators :

LLB, TUM, Collège de France

LoKI : Broad Band SANS

Science Case

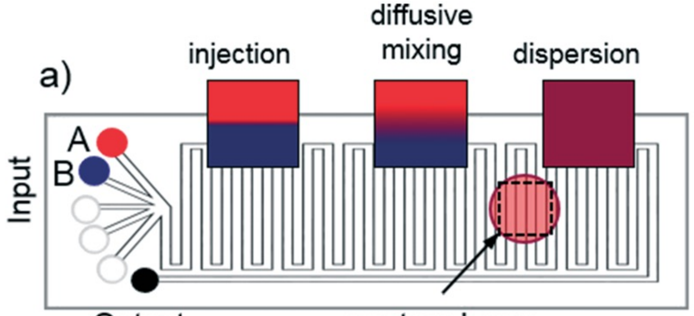


→ high flux, wide simultaneous size range, and a flexible sample area.

ABILITIES:

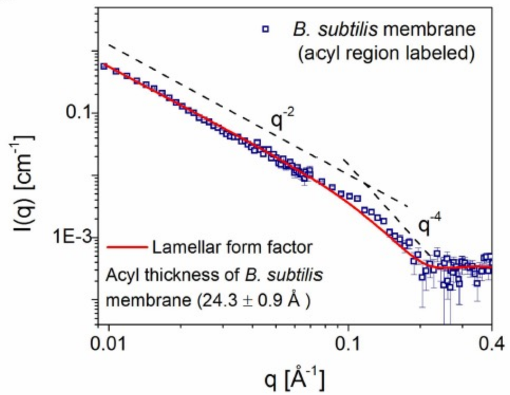
- Investigate **multiple length scale** systems (simultaneously 0.5-300 nm)
- Perform **“single-shot” kinetic measurements** on sub-second timescales.
- Perform experiments that use flow e.g. rheology & microfluidics **with small beam sizes**
- **High throughput** of regular SANS measurements

Microfluidic SANS:
High Throughput Mixing & Tailored Flow Geometry



Lab Chip, 2017, **17**, 1559

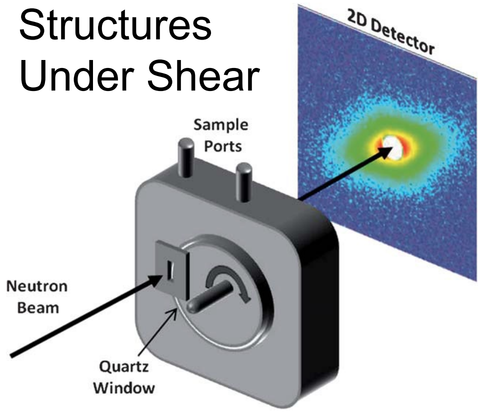
Biological Samples:
Weak Scatterers & Dilute Solutions



PLoS Bio, 2017, **15**, e2002214

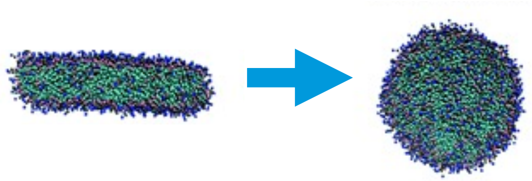
Rheo-SANS:

Structures Under Shear



Soft Matter, 2011, **7**, 9992

Non-Equilibrium Studies:
Self-Assembly & Kinetics



Colloid Polym Sci, 2010, **288**, 827

Courtesy J. Houston

LOKI Early Science (60% detector coverage & 0.5 MW)

Taking advantage of the wide simultaneous q-range & moderate flux

Performance @~0.5 MW:
- ➢ Comparable to SANS2D

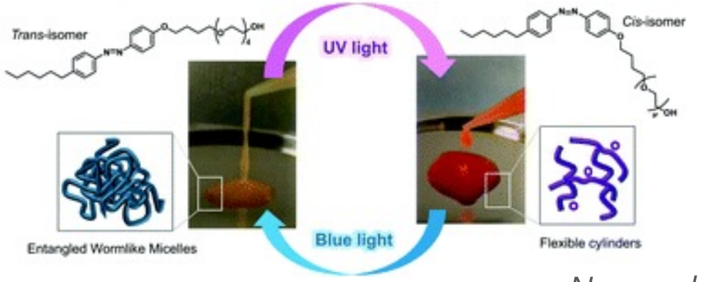
Performance @2 MW:
- ➢ ~5x compared to D22 (LoKI@14 Hz)
- ➢ ~20x SANS2D (LoKI@7 Hz)

Work with collaborators and expert users to:
- Investigate multiple length scale systems (simultaneously 0.5-300 nm)
- Perform experiments that use flow e.g. rheology & microfluidics
- Carry out work-horse SANS measurements with higher throughput
- Take advantage of pre-commissioned in situ sample environments

Some current ideas…

Photoswitchable worm-like micelles

R. Evans in Cambridge, UK

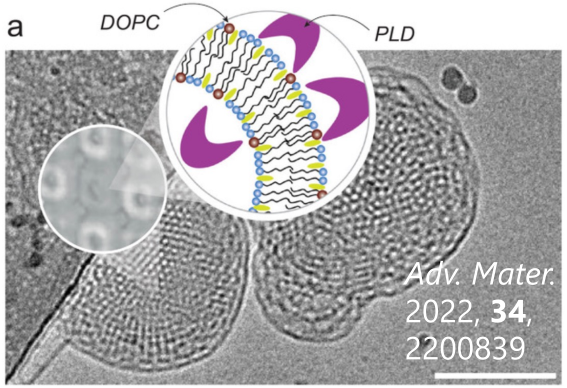


Nanoscale, 2020,**12**, 6300

System under flow ✓
Multiple length-scales ✓
In situ sample irradiation (adaptive sample environment) ✓

Lipid nanoparticles

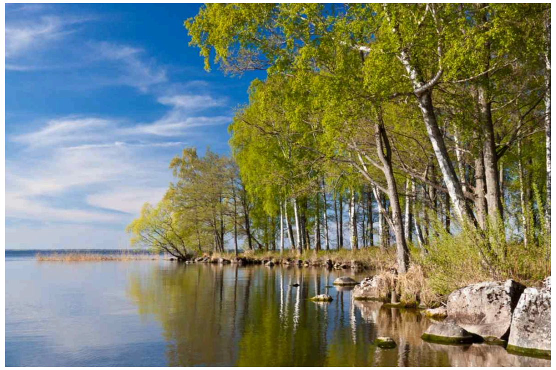
H. Barriga & M. Stevens at the Karolinska Institutet



Potential to involve ESS DEMAX ✓
Multiple length-scales ✓
Work-horse SANS experiments ✓

Dissolved Organic Matter

U. Olsson in Lund



JCIS Open, 2023, 11, 100091

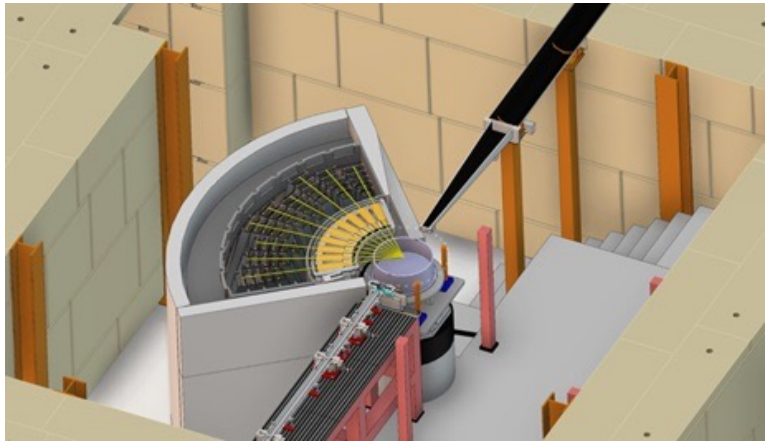
Multiple length-scales ✓
Workhorse SANS experiments ✓
Potential to involve ESS DEMAX ✓

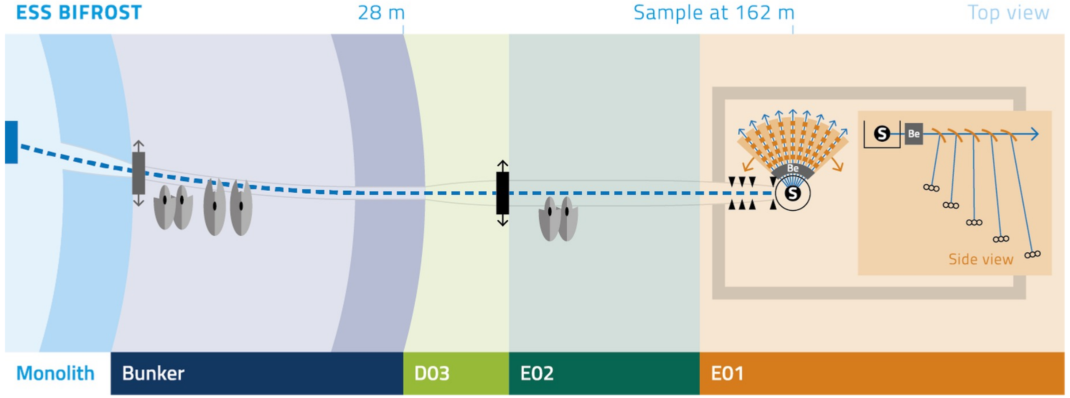
BIFROST

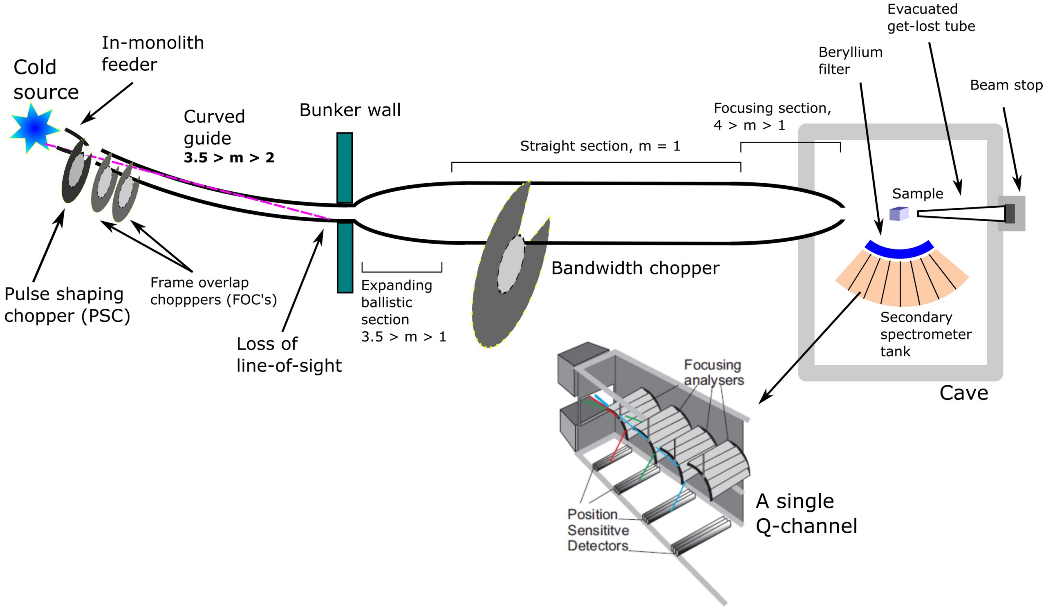
An innovative indirect time-of-flight spectrometer with multi-energy analysis

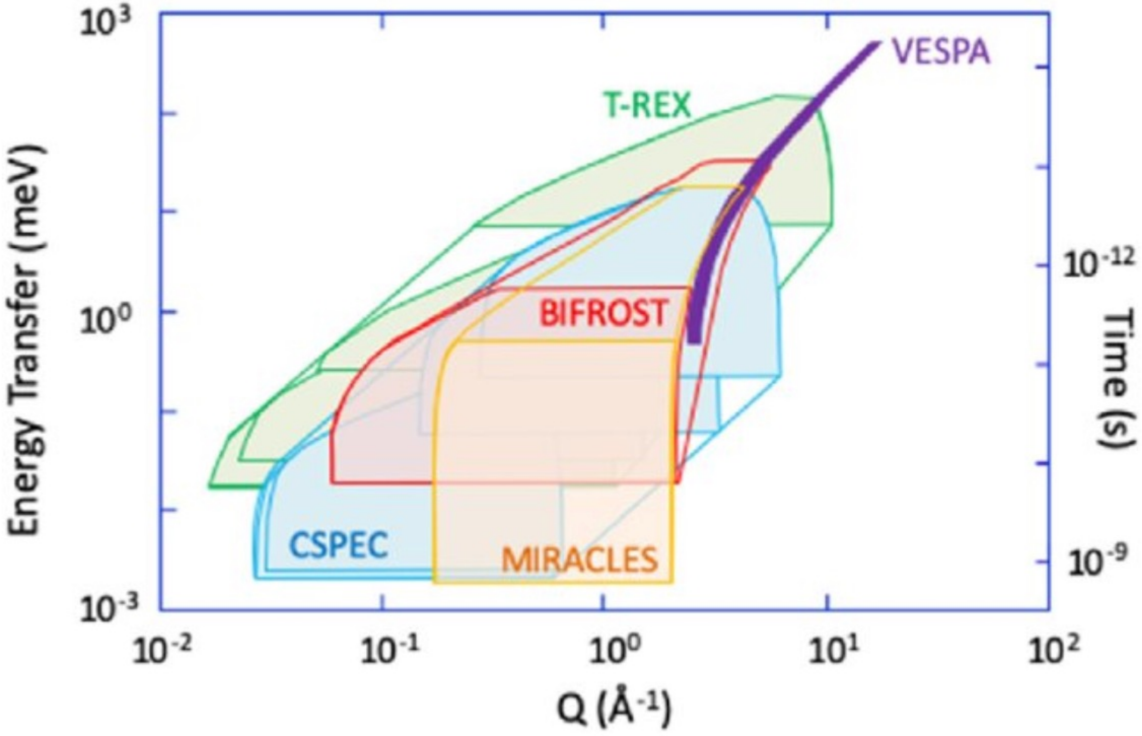
Resolving complexity of unconventional modes

Small samples – extreme environments



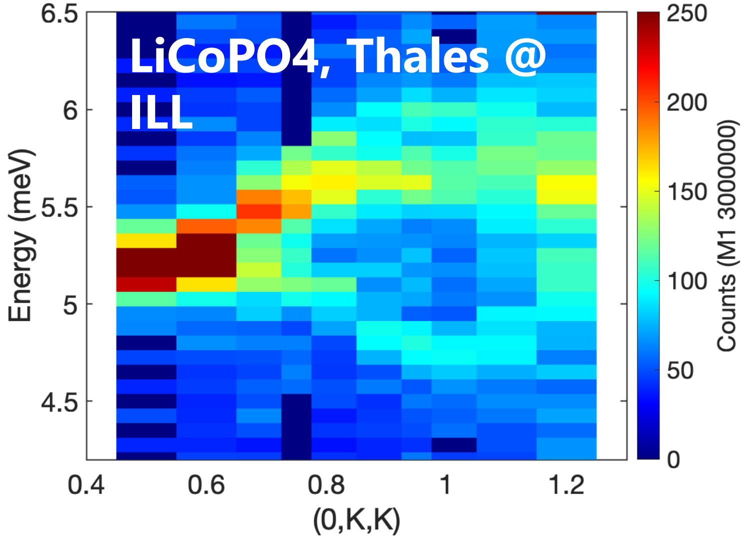






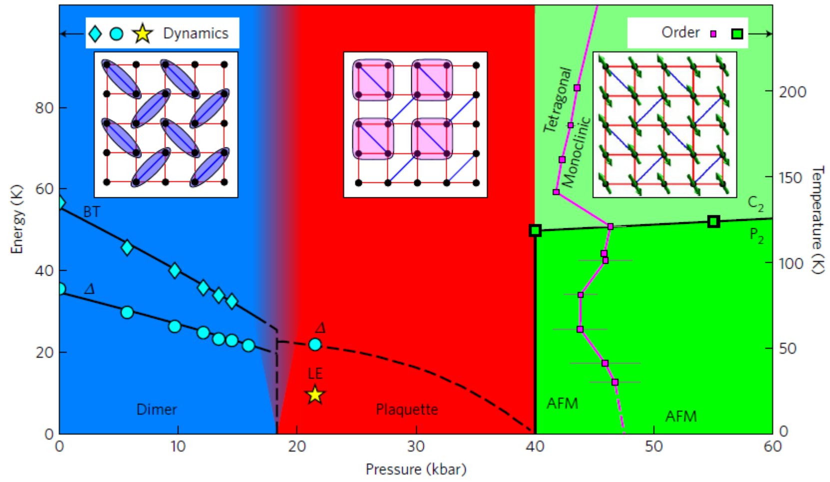
Early science on BIFROST

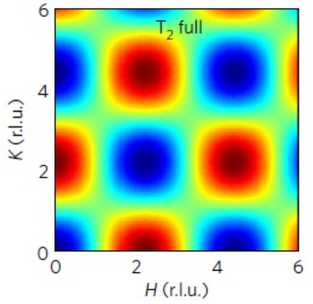
Early project @ 100 kW: Finally understanding LiCoPO4, a complex magnetoelectric with 4 spin wave branches and possible hybrid modes. Only small crystals available - on the feasibility limit today, we need more signal and better resolution -> BIFROST.

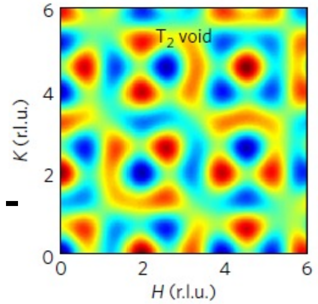


Early project @ 500 kW: Shastry Sutherland compound. Well known system, the 4 spin plaquette exists at high pressure

The nature of the plaquette is unresolved, needs a mapping experiment on small crystals under large pressure. Possible for the first time on BIFROST at 500 MW accelerator power.



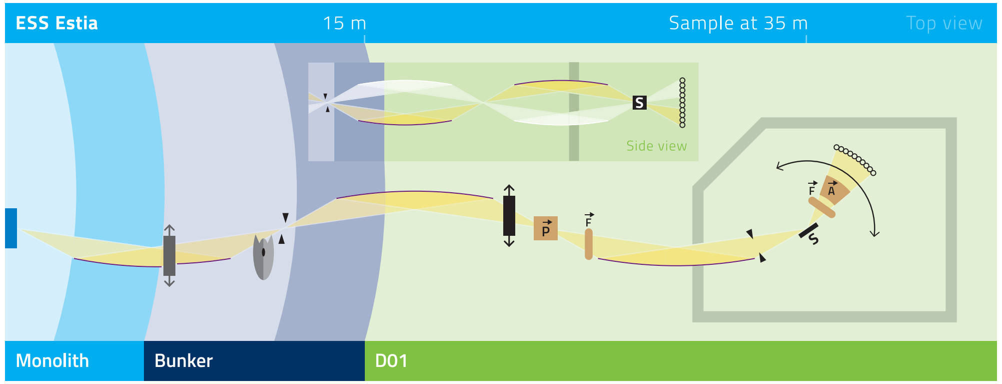


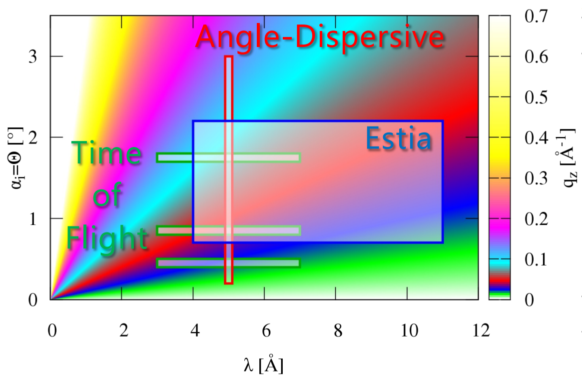


M. E. Zayed, et.al, Nature Physics, 13, 962, (2017) - **$SrCu_2(BO_3)_2$**

Estia

Focussing Polarised Reflectometer for Tiny Samples



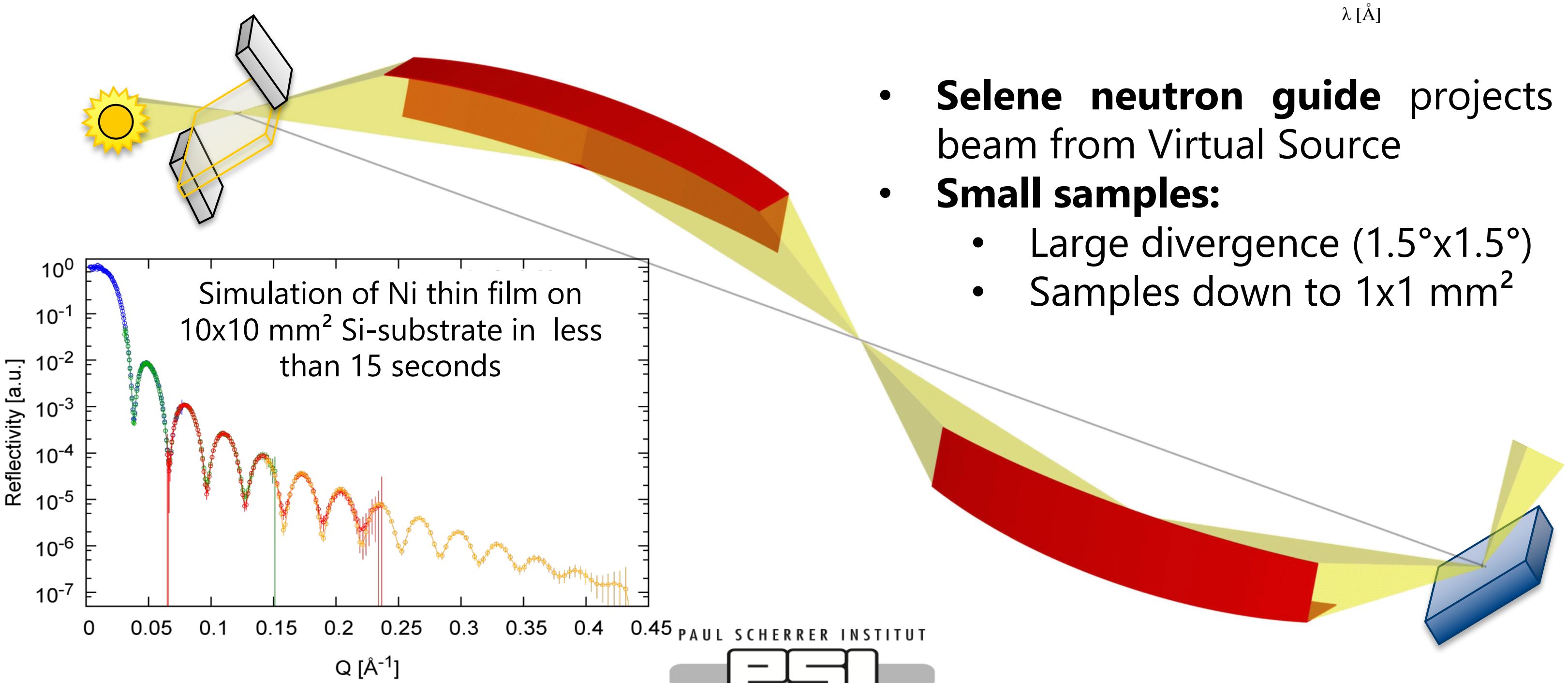


Estia Quick Facts.

Estia Quick Facts	
Instrument Class	Reflectometry
Moderator	Cold
Primary Flightpath	35 m
Secondary Flightpath	4 m
Wavelength Range	3.75–28 Å
Polarised Incident Beam	Optional
Polarisation Analysis	Optional
Sample Orientation	Vertical
Total Q-Range	0.001 to 3.15 Å^{-1}/−0.001 to −0.3 Å^{-1}
Standard Mode (14 Hz)	
Bandwidth	7 Å
Flux at Sample at 2 MW[a]	6×10^8 n s^{-1} cm^{-2}
Relative Q-Range	$Q_{max} = 2.85 \times Q_{min}$
Q-Resolution ΔQ/Q	7.8%–3.0% over Q-range
2-Pulse Skipping Mode (4.7 Hz)	
Bandwidth	21 Å
Flux at Sample at 2 MW[a]	2×10^8 n s^{-1} cm^{-2}
Relative Q-Range	$Q_{max} = 6.6 \times Q_{min}$
Q-Resolution ΔQ/Q	7.8%–1.3% over Q-range

[a] Full-divergence beam averaged over 5(H) × 10(V) mm².

- **Selene neutron guide** projects tiny beam from Virtual Source
- **Small samples:**
  - Large divergence (1.5°x1.5°)
  - Samples down to 1x1 mm²



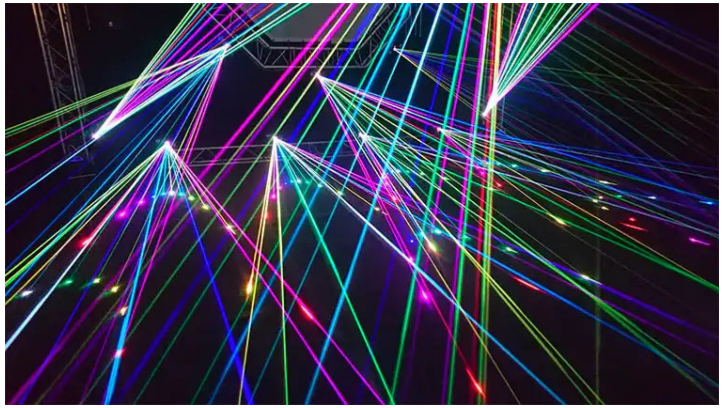
For the study of surfaces and interfaces including magnetic layers

PAUL SCHERRER INSTITUT

ESTIA Commissioning and Beyond

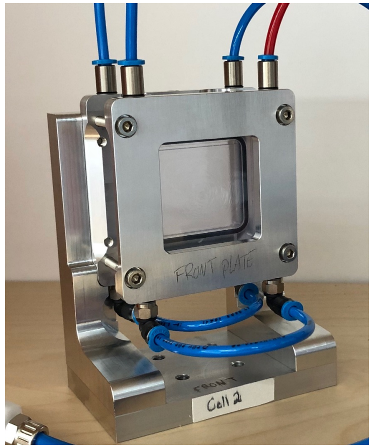
ESTIA is complicated!

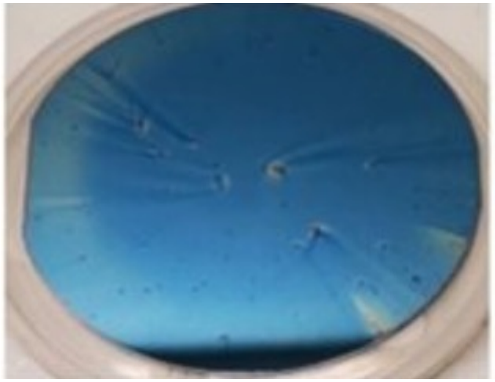
- Commissioning will be fun
- Made easier by PSI

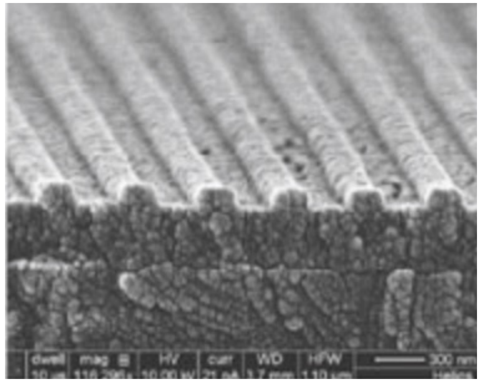


Early science will include

- Non-magnetic solid films
- Solid liquid experiments
- Simple magnetic systems
- Off-specular scattering tests

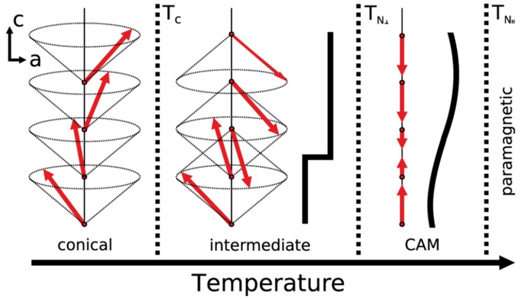


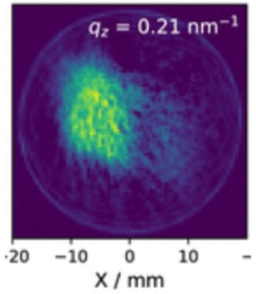




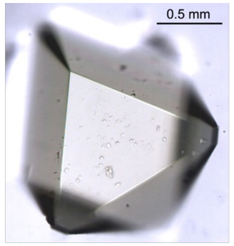
Full power (+FREIA)

- Complex magnetic systems
- Neutron reflectivity tomography...?

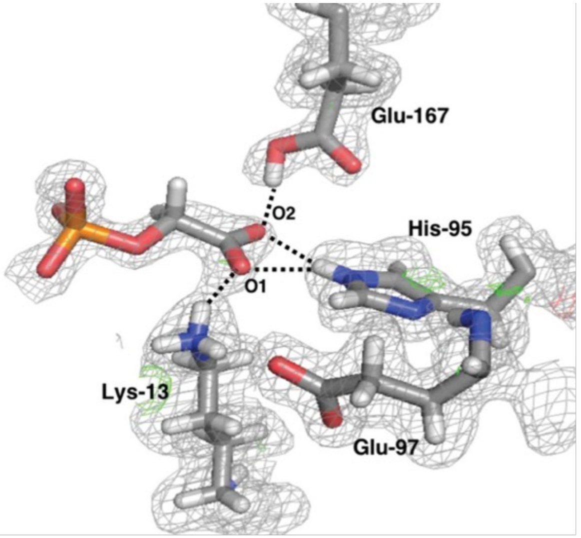




NMX Macromolecular Diffractometer



Oksanen, E *et al. J. R. Soc. Interface* 2009, ***6*** *Suppl 5*, S599-610.



Kelpsas, V., Caldararu, O. et al. (2021) *IUCrJ* **8** 633-643

Where are hydrogens important?

Enzyme mechanisms
Protein-ligand interactions
Proton transport across membranes

Neutron macromolecular crystallography

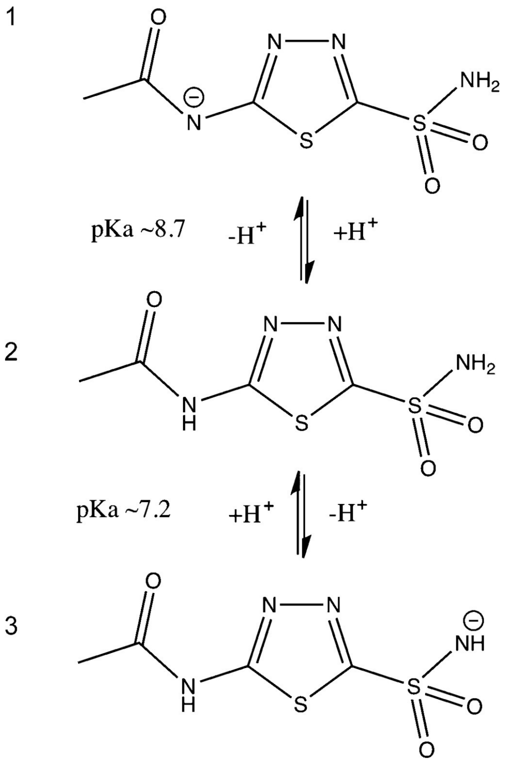
Hydrogens are visible
No radiation damage

Cold, TOF-Laue, Δλ<1.75 Å
158 m length
λ-range 1.8-10 Å
Robotic detector positioning
Gd-GEM detector

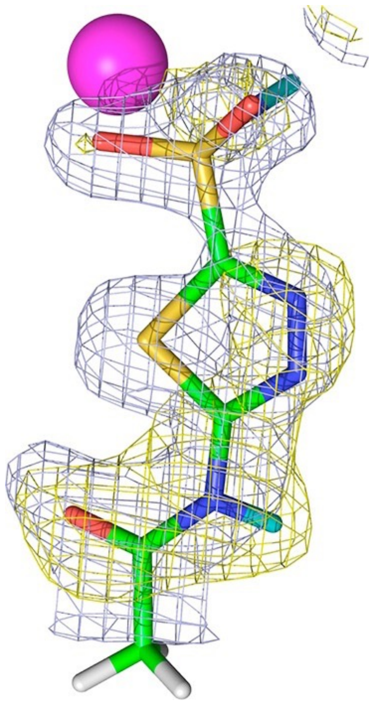
Why is hydrogen interesting?

Ligand binding and protonation states in Acetazolamide in Human Carbonic Anhydrase II

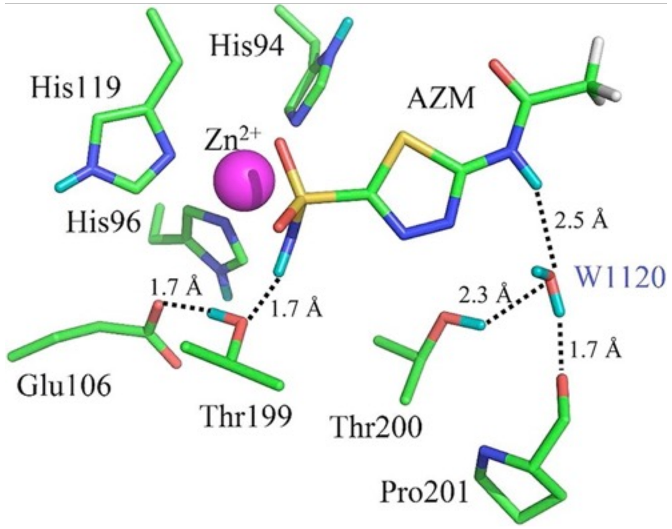
Three possible protonation states at physiological pH



Protonation state clearly determined by neutrons



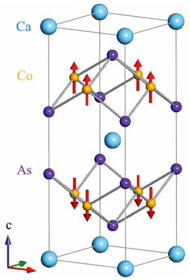
Provides fill picture of ligand binding

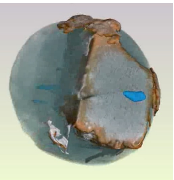


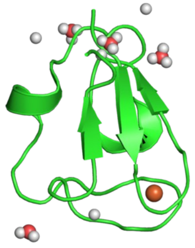
Fisher SZ *et al.* JACS (2012);**134**:14726-14729

Data Management and Software Center

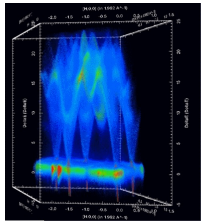
Support user from proposal to publication with scientific computing tools & services

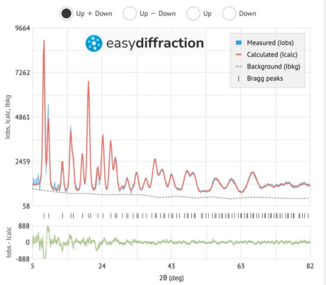


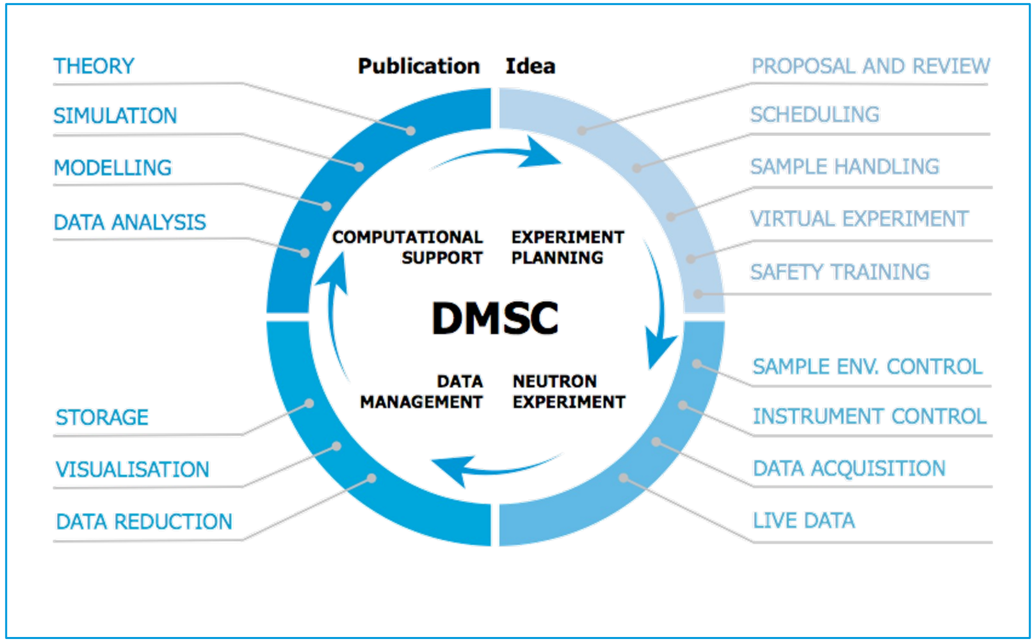


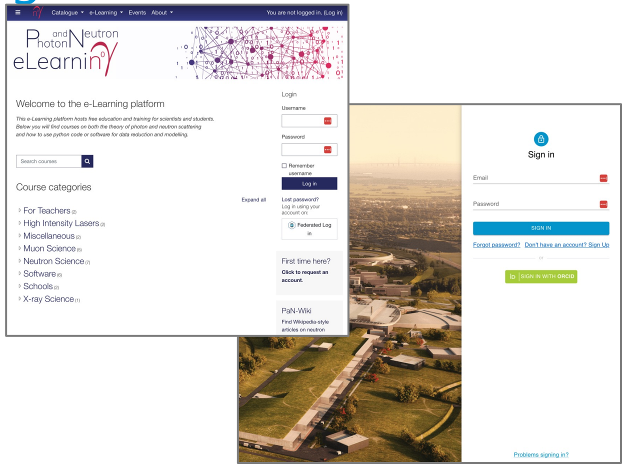


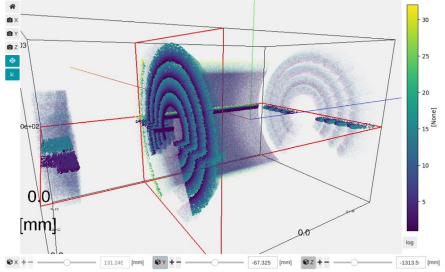
LOCATED IN DENMARK

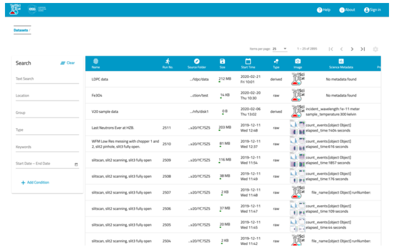


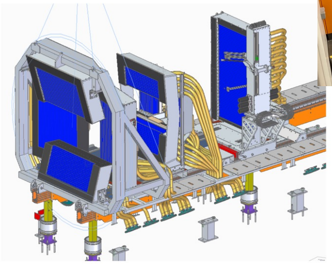


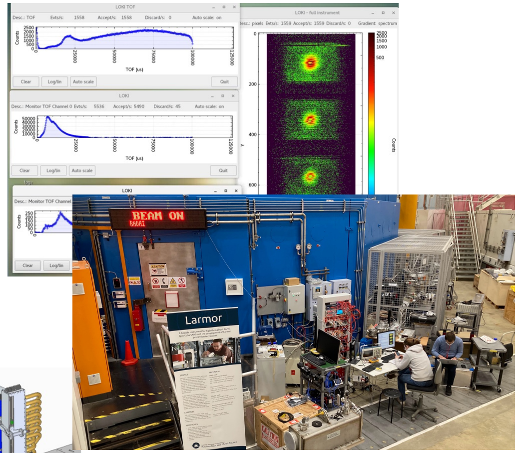


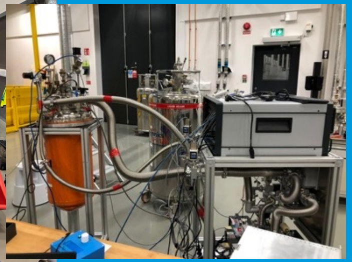




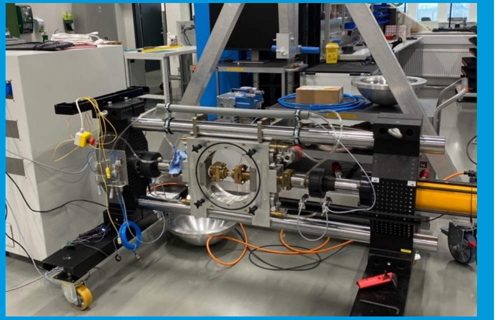








Sample environment & support laboratories



Materials and Physics Support

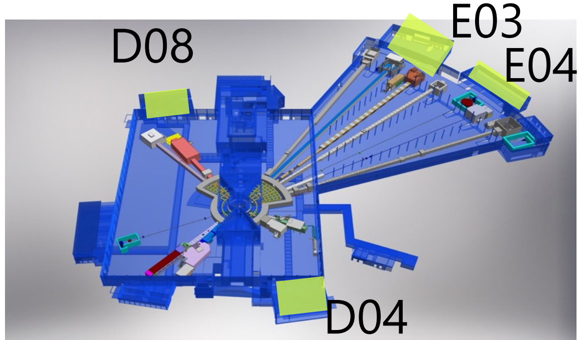
The MSPS scope:

- Provide sample environment systems and users support for low and high temperatures, magnetic and electrical fields, high-pressure and mechanical constraints.
- Provide SES control integration of complex systems and mechanical integration

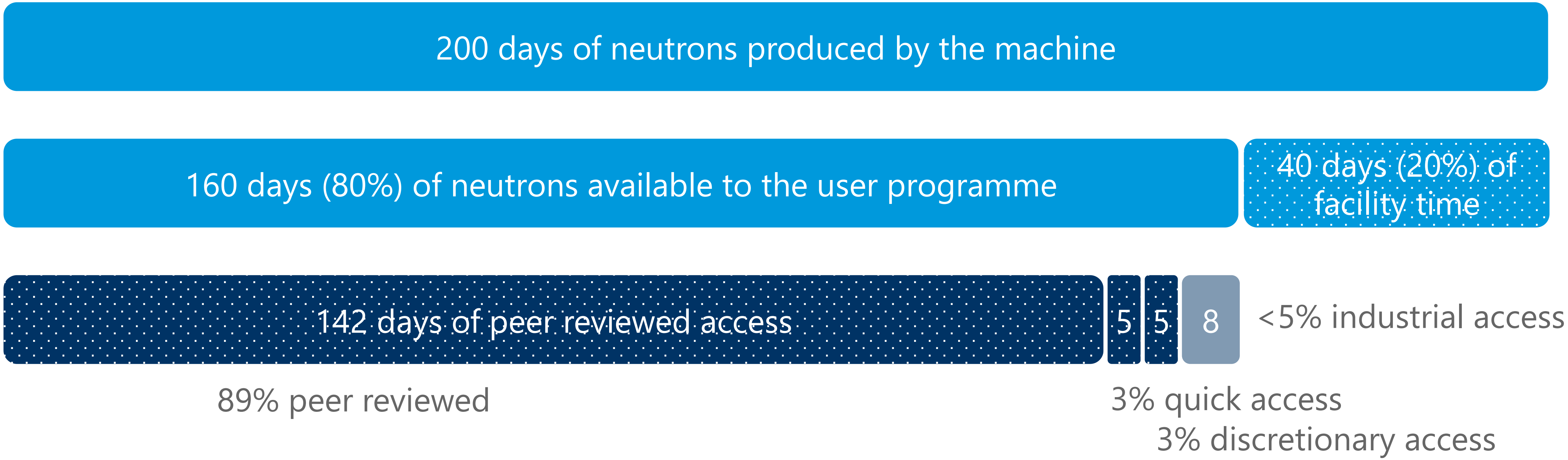
Chemistry and Life Science Support

The CLS scope:

- Support laboratories (Installation/Spallation Chemistry)
- Sample environment for chemistry, biology and soft matter
- Deuteration service
- Interaction Science



ESS proposal for Access to Neutron Instruments: work in progress



- **User programme to be offered to member countries proportionally to their financial contribution to the facility**
- Excellent science from non member countries will be possible via discretionary access
- ESS staff are invited to use the peer review process

ESS meetings organisation & first science brainstorm

REFLECTOMETRY – SXNS & ORSO (Grenoble - Jul)

NMX – ECM 34 – (Padova - Aug)

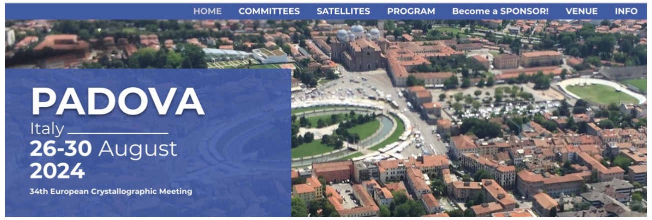
IMAGING – NEUWAVE 12 (Lund – Sep)

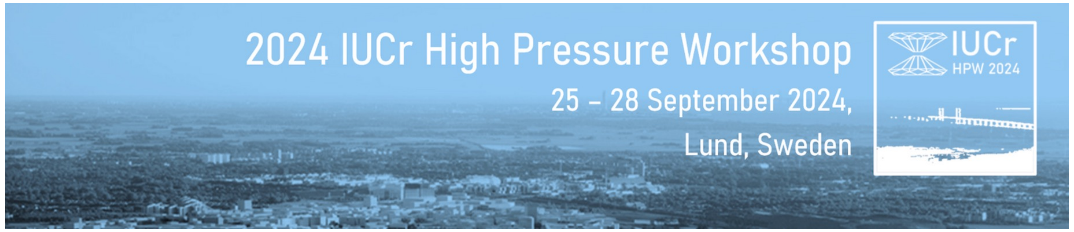
SANS - ECIS 2024 satellite – (Copenhagen - Sep)

DIFFRACTION - IUCr High Pressure (Lund - Sep)

ILL/ESS USER MEETING (Grenoble – Dec)

FUNDAMENTAL & PARTICLE PHYSICS (Lund – Jan)





Looking forward an exciting meeting and lots of ideas for great science at ESS!