CSPEC update

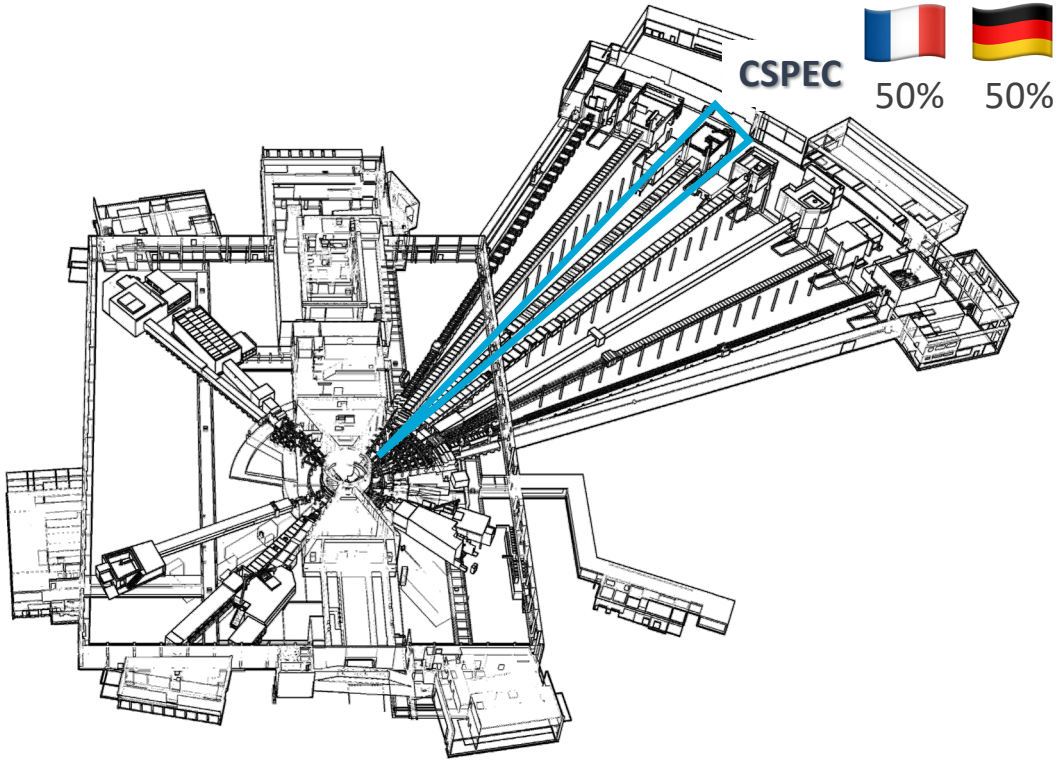
Daria Noferini (ESS) – daria.noferini@ess.eu

Spectroscopy STAP meeting 23.10.2024

CSPEC

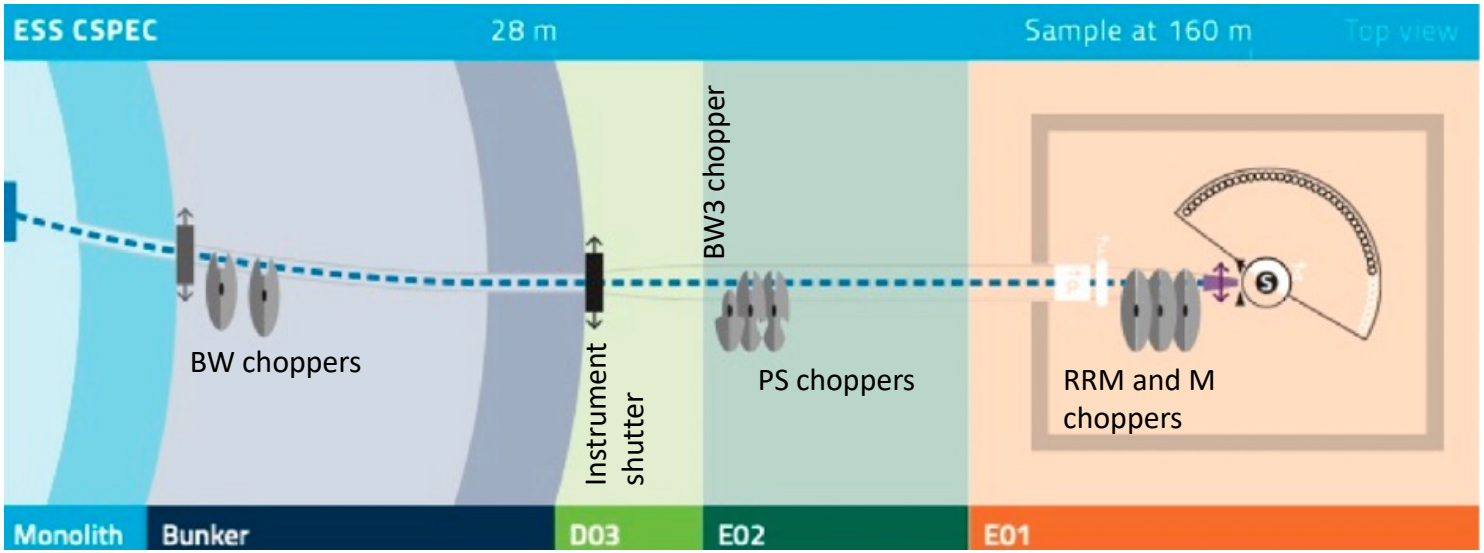
The Cold Chopper spectrometer of the ESS

Where to find us



CSPEC: The cold chopper spectrometer of the European Spallation Source, a detailed overview prior to commissioning – (https://doi.org/10.1063/5.0059907 or free version at https://arxiv.org/abs/2105.05552)

Overview



3.5 m sample to detector

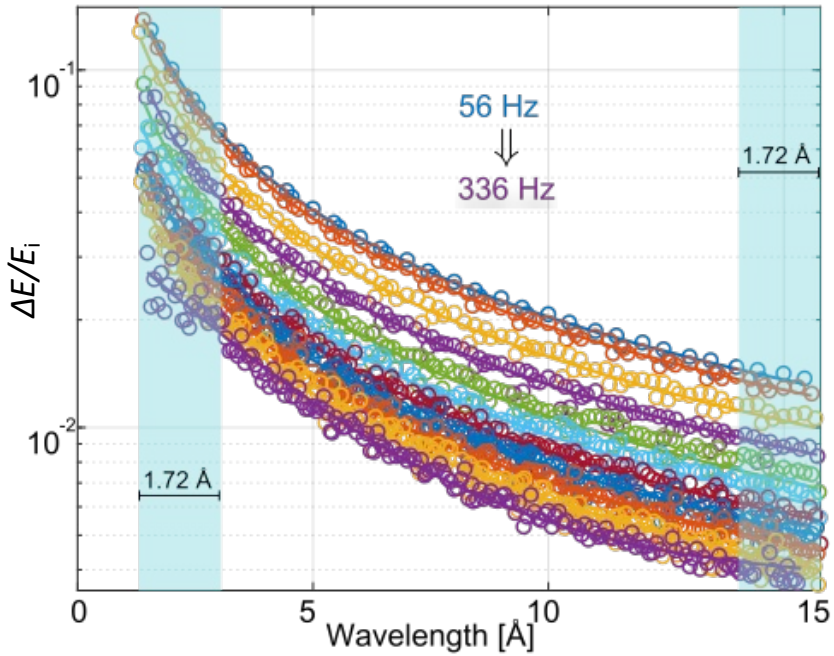
TG5: November 2025

CSPEC

The Cold Chopper spectrometer of the ESS

Specifications

λ range	2-20 Å
Energy resolution	1-5% of E_i
Detector coverage	-30°-140° [H] ± 26.5° [V] (full scope)
Beam dimension	4x2 cm^2 or 1x1 cm^2 (focussed)
Polarisation analysis	(foreseen)
Flux gain factor (@5MW, no RRM, 1 pulse)	2-6 with respect to current leading cold chopper spectrometers
Repetition Rate Multiplication	Wavelength band = 1.7 Å (approx. 6 pulses)
Signal-to-noise ratio	10^5 (@5 Å, vanadium standard sample)



Kinetic measurements, combined characterisations, small samples, *in situ*, *operando*…

K.H. Andersen, D.N. Argyriou, A. J. Jackson *et al.*, Nuclear Inst. and Methods in Physics Research, A 957 (2020) 163402
CSPEC: The cold chopper spectrometer of the European Spallation Source, a detailed overview prior to commissioning – (https://doi.org/10.1063/5.0059907 OR https://arxiv.org/abs/2105.05552)

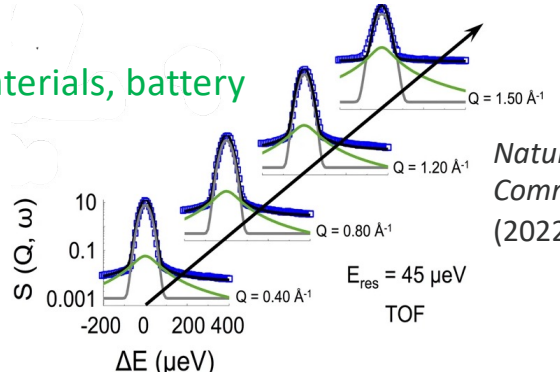
Science cases

INS and QENS (translations, rotations, quantum effects, spin dynamics, phase transitions, collective excitations, relaxation phenomena…)

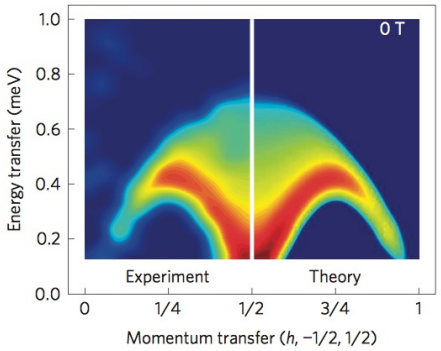
Energy materials: fuel cells membranes and electrolytes, thermoelectric materials, battery electrolytes, H-storage, organic photovoltaics…

Soft matter: polymers, nanocomposites, gels, surfactants…

Materials: clays, crystal growth, catalysis, quasi crystals…



Nature Communications, 13 (2022)



Nature Physics, 9, (2013)

Magnetism: spin glasses and fluids, quantum materials, frustrated compounds, magnetothermal, multiferroic materials, superconductors...

Liquids & glasses: monoatomic and molecular liquids, ionic liquids, glass forming liquids, liquid metals and alloys, glasses, confined fluids…

Biological systems: proteins, DNA, lipid membranes, pharmaceuticals & drug delivery…

Focus on small samples, in situ/operando, kinetics etc

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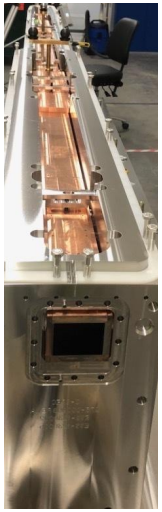
The Cold Chopper spectrometer of the ESS

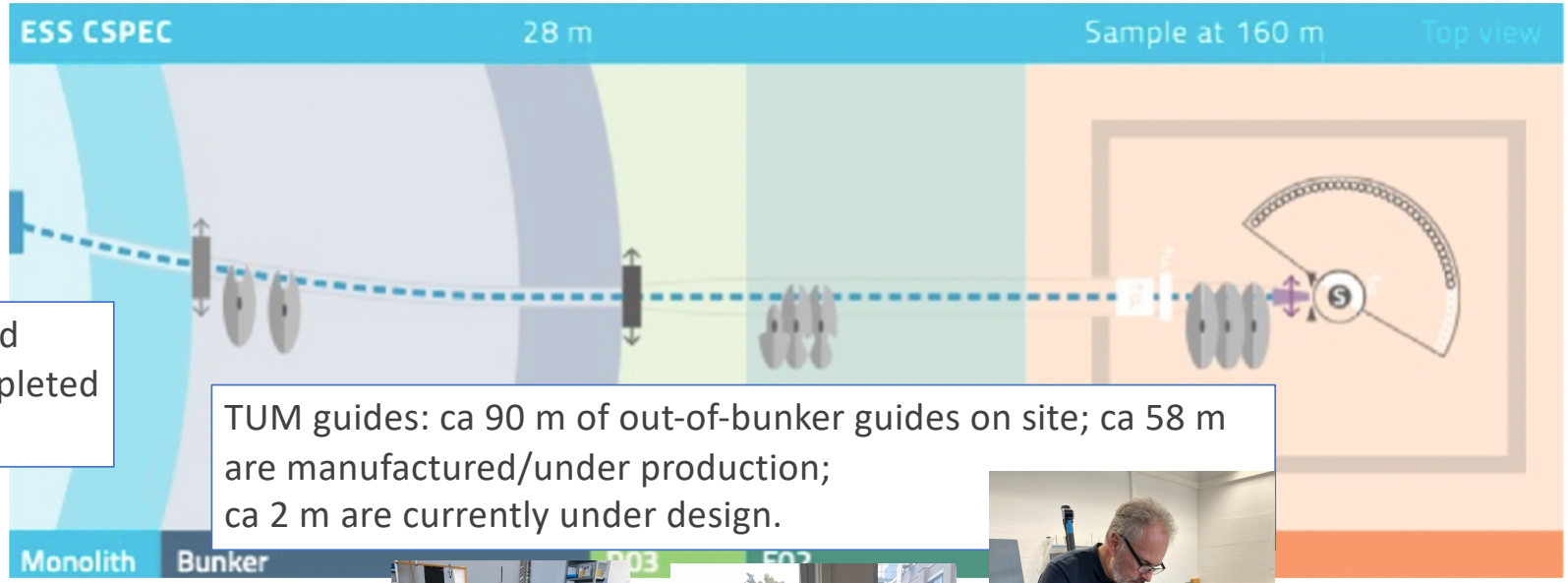
Guides

NBOA: installation completed
BBG: inspection on site completed
BWF: installation completed

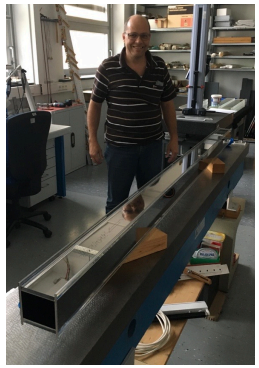


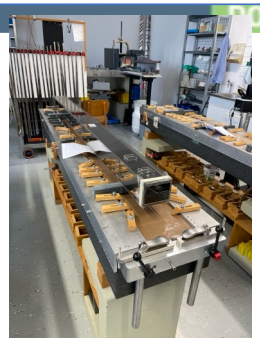
S-DH

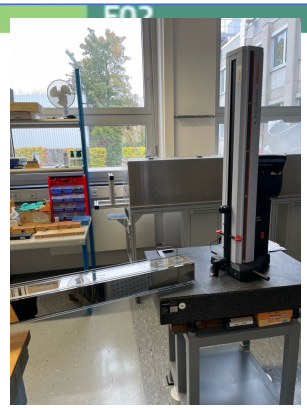
SwissNeutronics

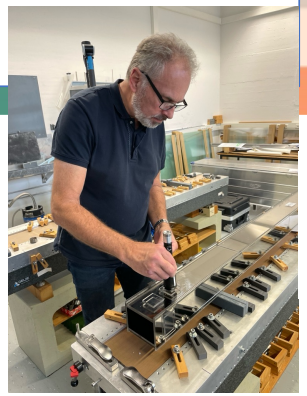


TUM guides: ca 90 m of out-of-bunker guides on site; ca 58 m are manufactured/under production;
ca 2 m are currently under design.









TECHNISCHE UNIVERSITÄT MÜNCHEN

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The Cold Chopper spectrometer of the ESS

Guide housings

In-bunker guide housings and support: FAT done, arriving on site

Out-of-bunker guide housings and supports produced, accepted and delivered

Moving towards installation of guides & guide housings:

Test early November
Installation campaigns in December 2024, spring and summer 2025

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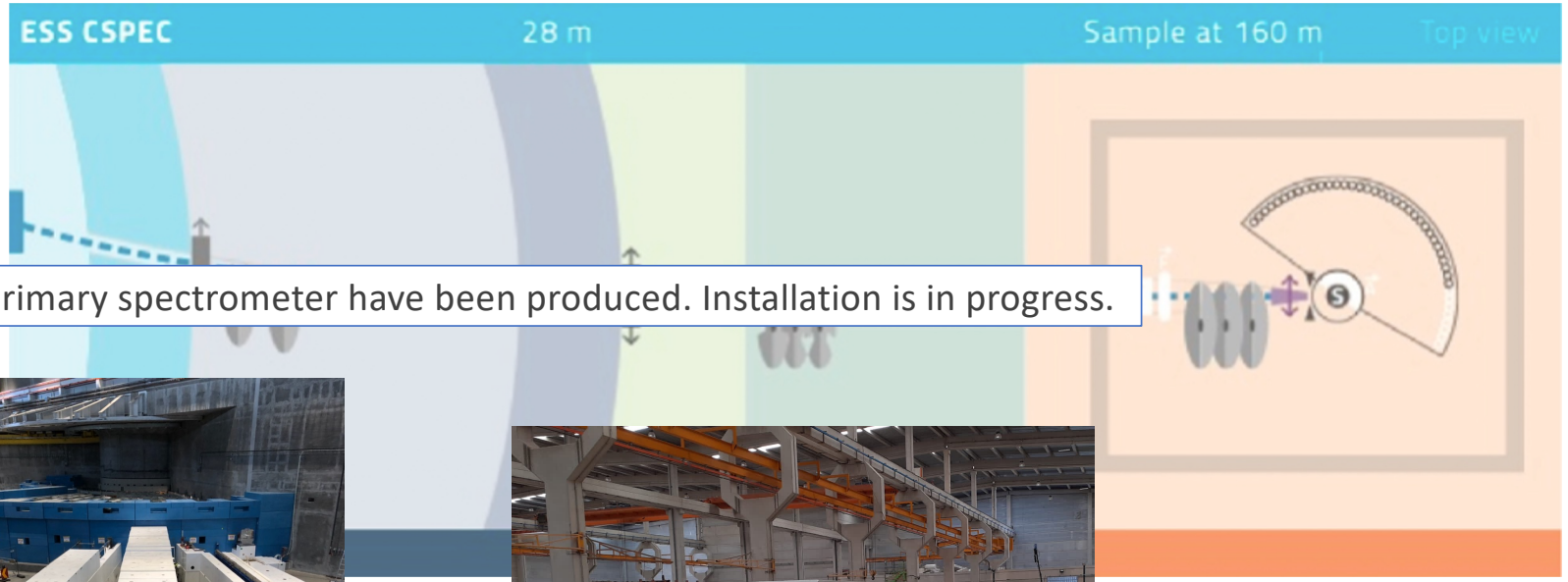
The Cold Chopper spectrometer of the ESS

Shielding

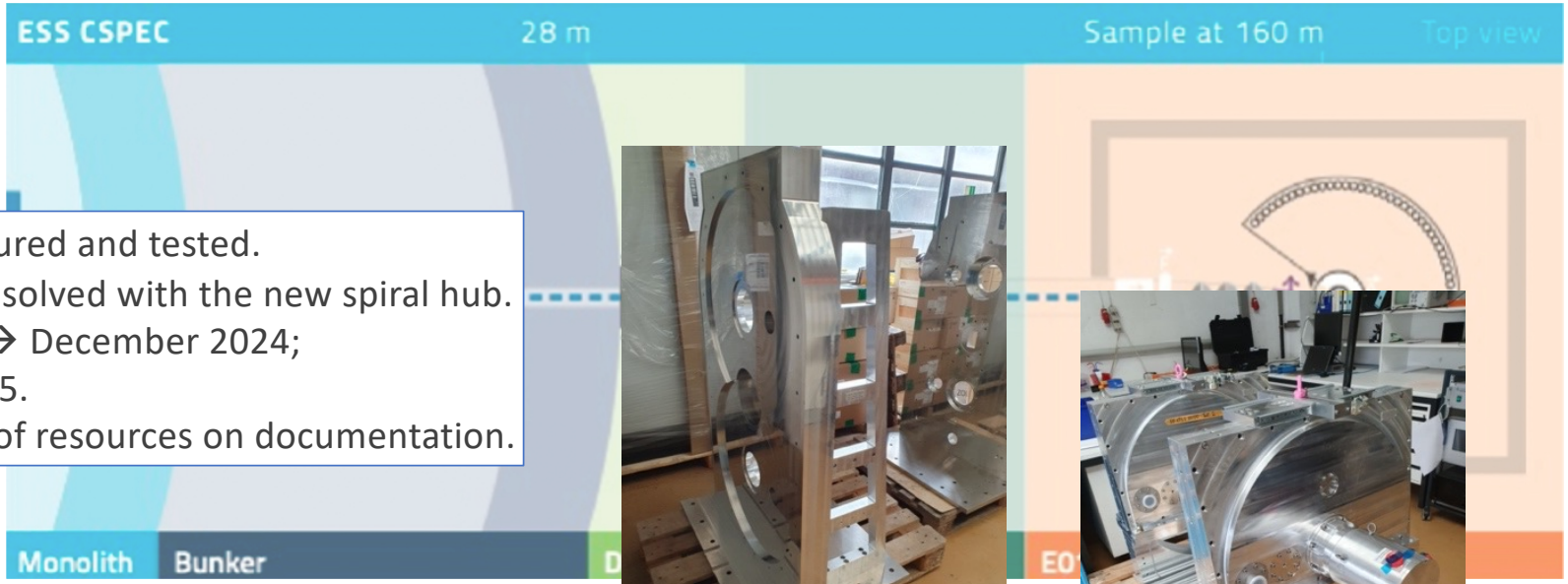
ESS common project

All the shielding blocks for the primary spectrometer have been produced. Installation is in progress.



Choppers

All the disks are manufactured and tested.
Some technical problems, solved with the new spiral hub.
Arrival on site: In bunker → December 2024;
Out of bunker → May 2025.
TG3 missing because lack of resources on documentation.



AIRBUS DEFENCE & SPACE

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The Cold Chopper spectrometer of the ESS

Detector tank

Detector tank installation: December 2024

sdms la chaudronnerie blanche

Cd sheets + borated PE blocks (bottom) → procurement

Borated PE blocks (side and top) → design

Detector tank

Assembly test at factory.
May 2024

sdms la chaudronnerie blanche ®

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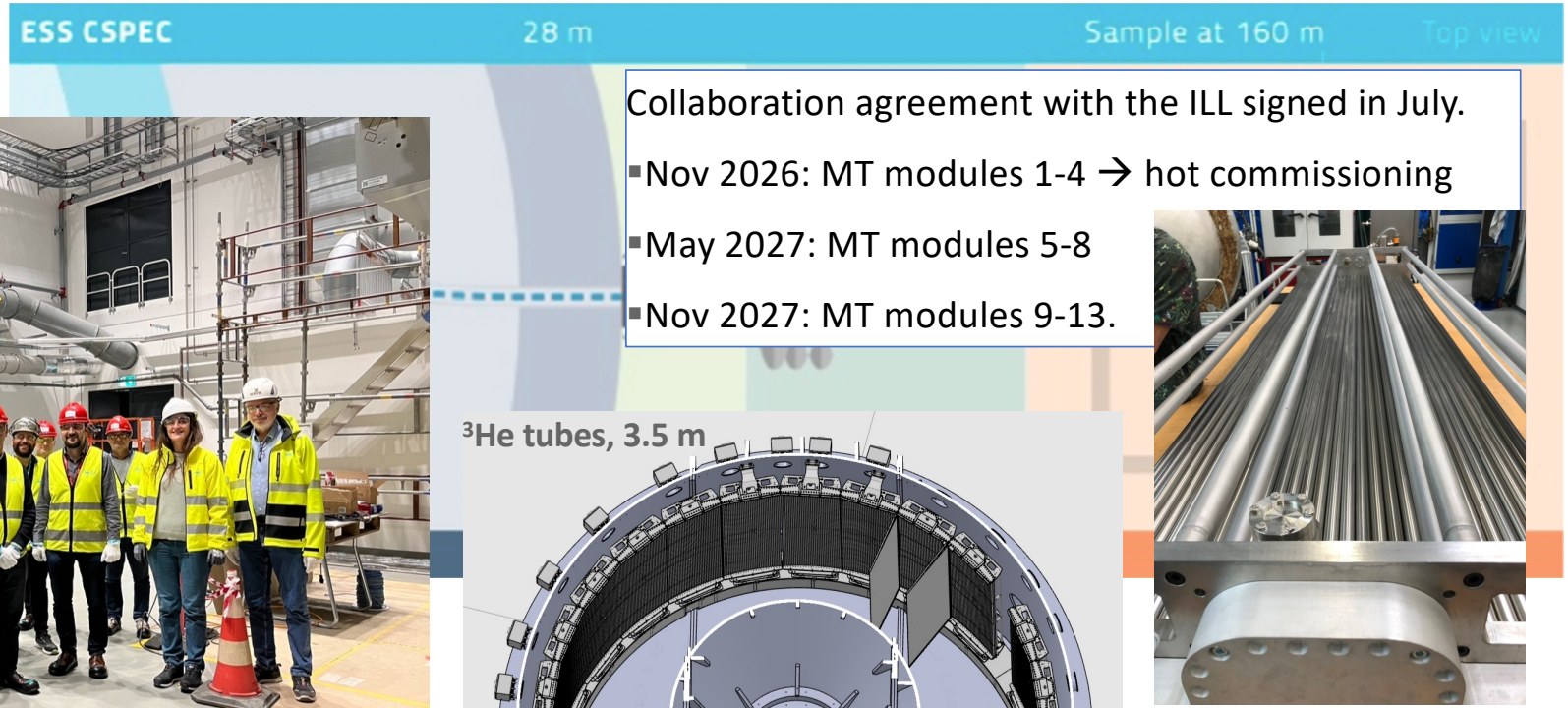
Detector

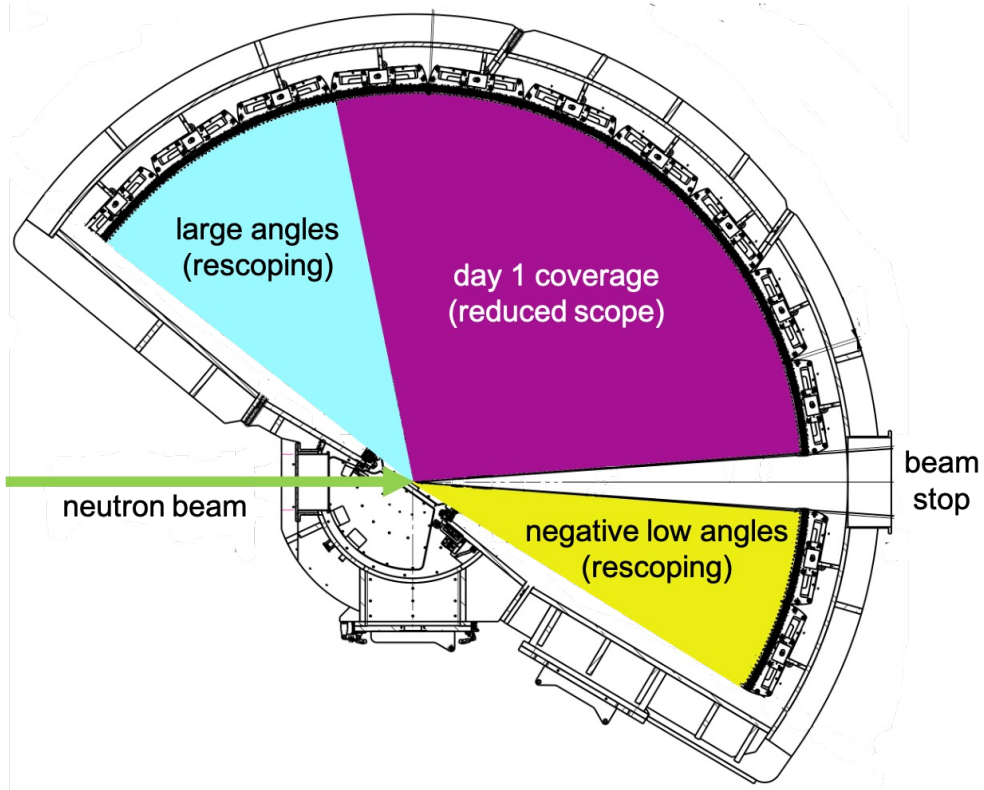
Kick off meeting@ESS, 16-17 October 2024

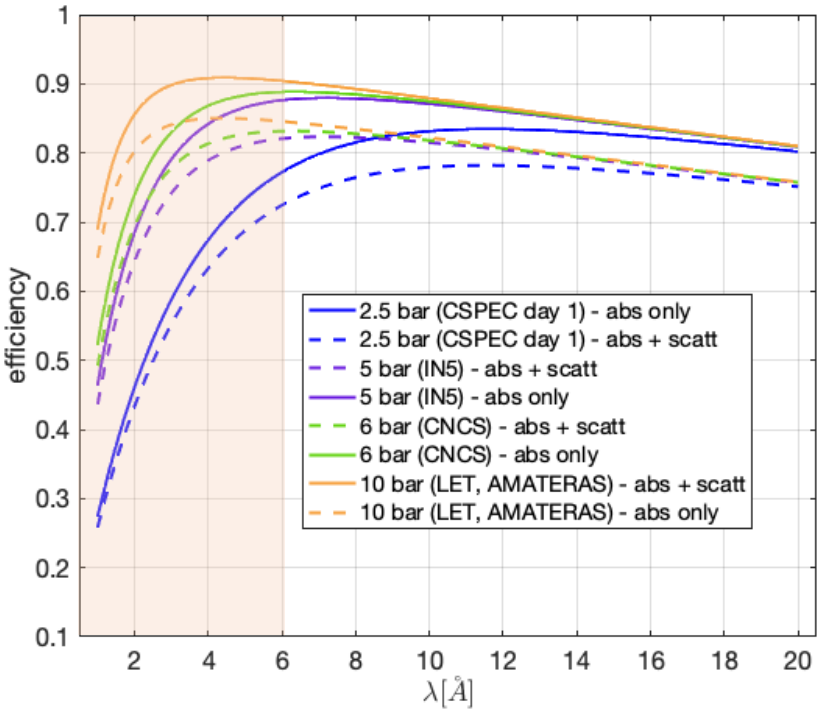


Collaboration agreement with the ILL signed in July.

- Nov 2026: MT modules 1-4 → hot commissioning
- May 2027: MT modules 5-8
- Nov 2027: MT modules 9-13.

Detector rescoping/upgrading

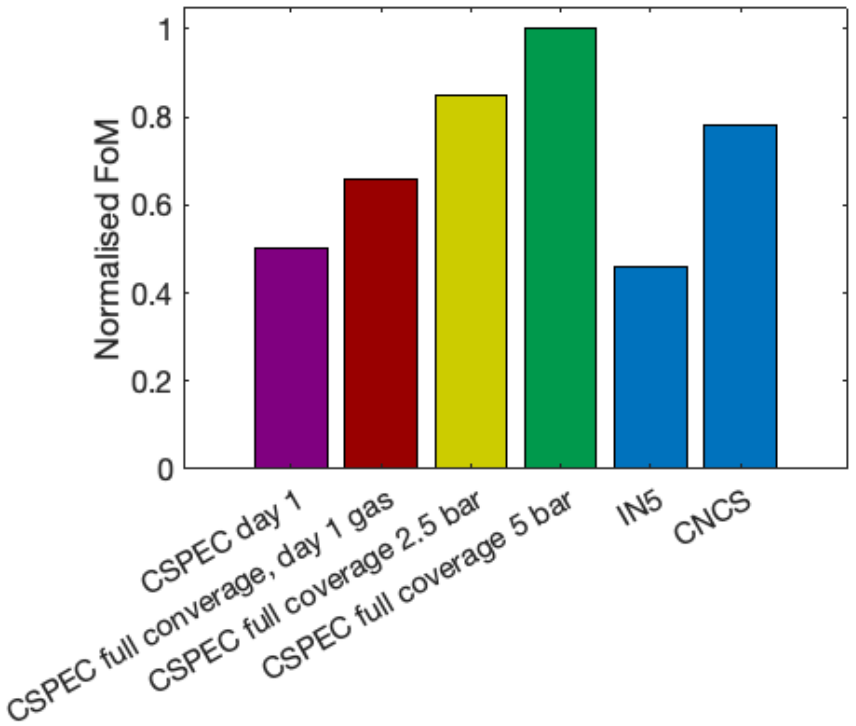




Reduced angular coverage, reduced efficiency

Detector rescoping/upgrading

FoM = Flux * Detector coverage * Efficiency



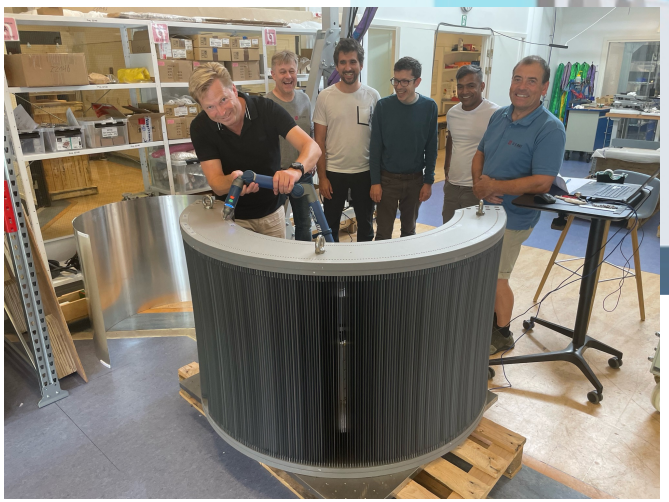
Upgrade	Estimate 1 (2700 EUR/l)	Estimate 2 (2000 EUR/l)
Full coverage 2.5 bar	2025 kEUR	1500 kEUR
Full coverage 5 bar	6399 kEUR	4740 kEUR

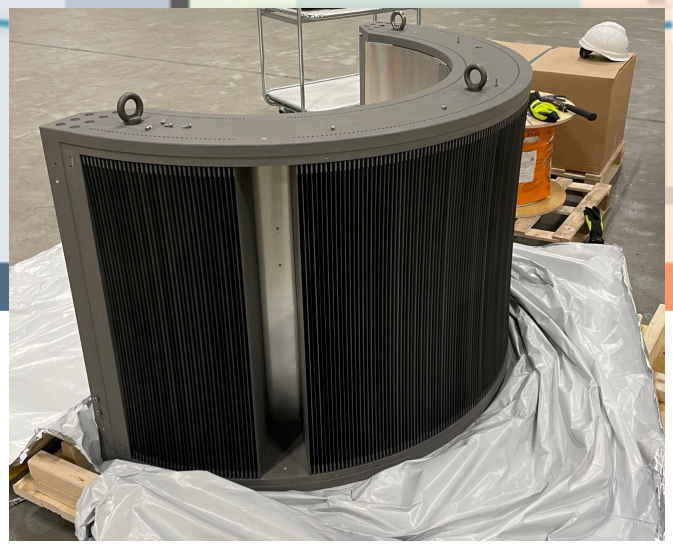
5 bar is the max pressure of the MT modules. For this estimate we consider 4.75 bar. The final details regarding the MT module design and the mixture of quenching gas and ^{3}He will determine the volume needed.

Beam stop region upgrade…

Collimator

The collimator is at the ESS.
Ongoing design work on the driving system (CSPEC team) → finalised in May 2025





JJ X-RAY
Danish Science Design

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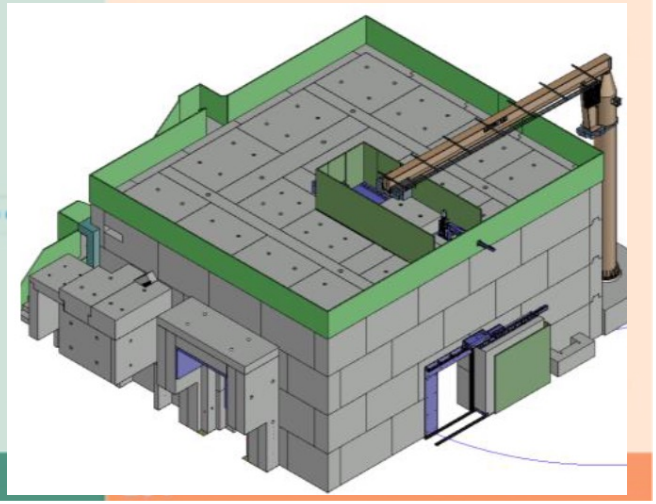
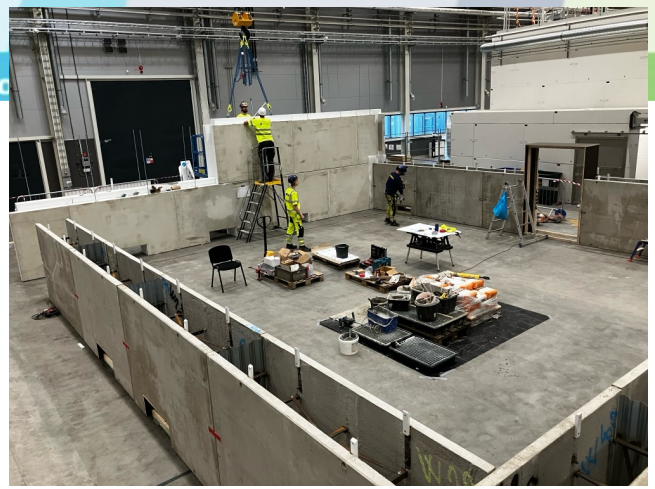
The Cold Chopper spectrometer of the ESS

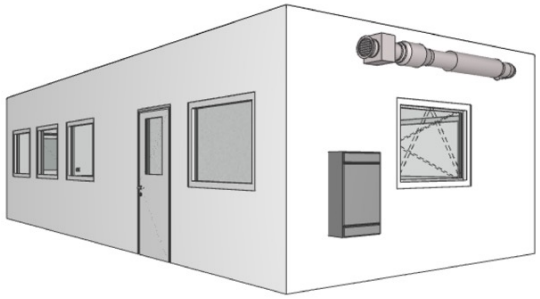
Cave & cabin





subTG3 passed in October

We're casting the blocks!



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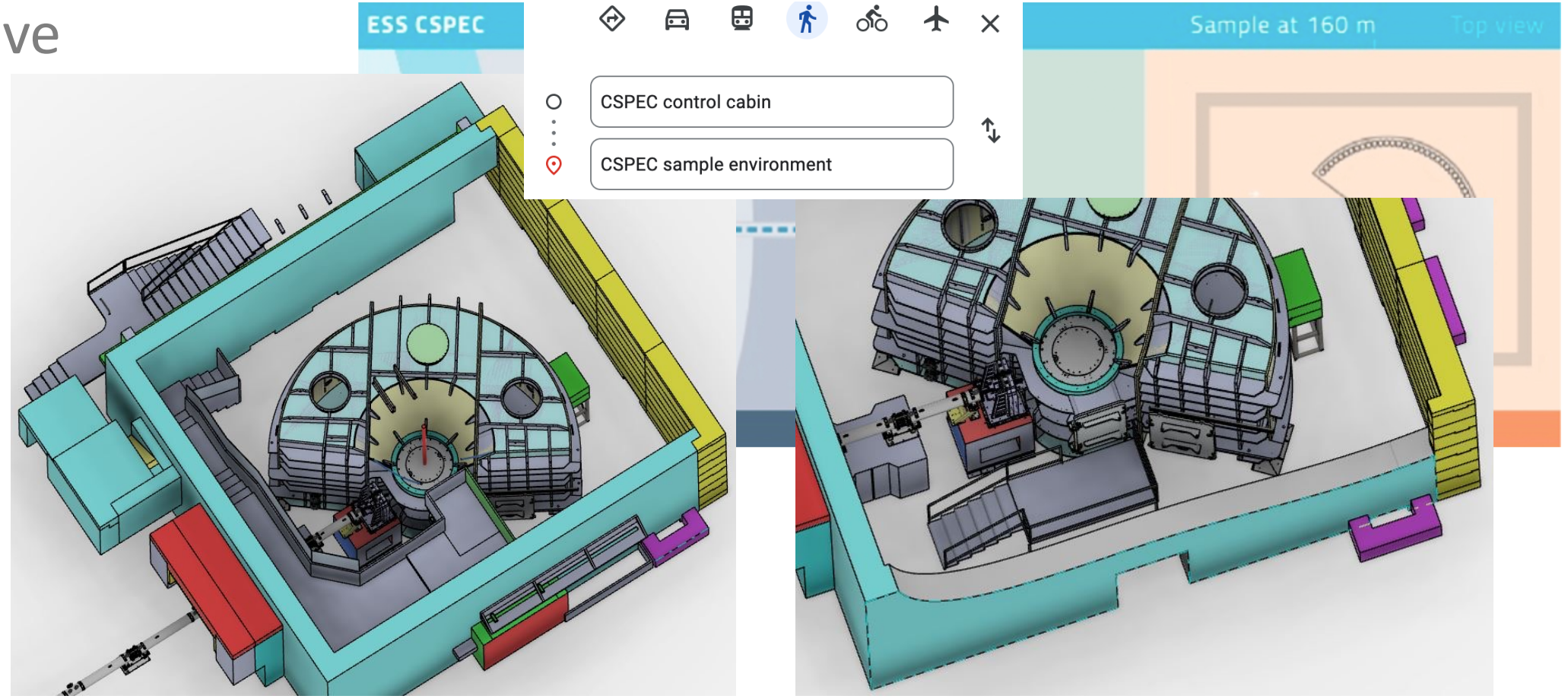
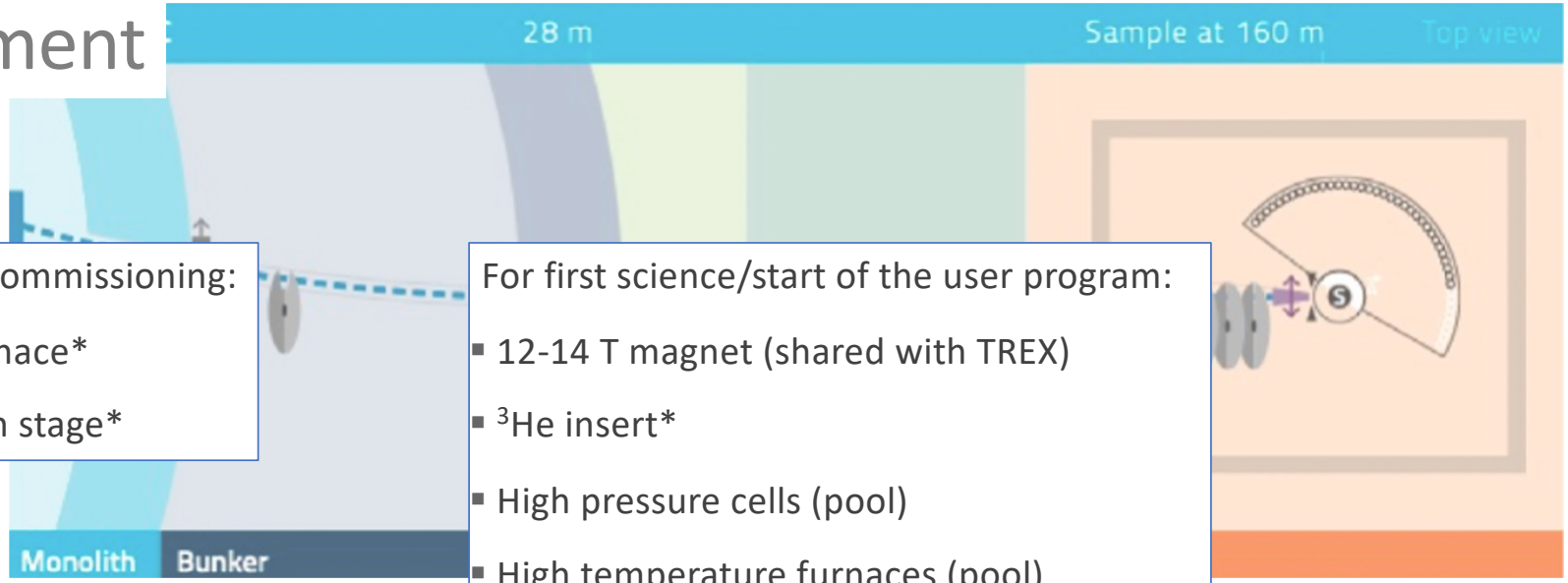
Cave



Sample environment



For hot commissioning:

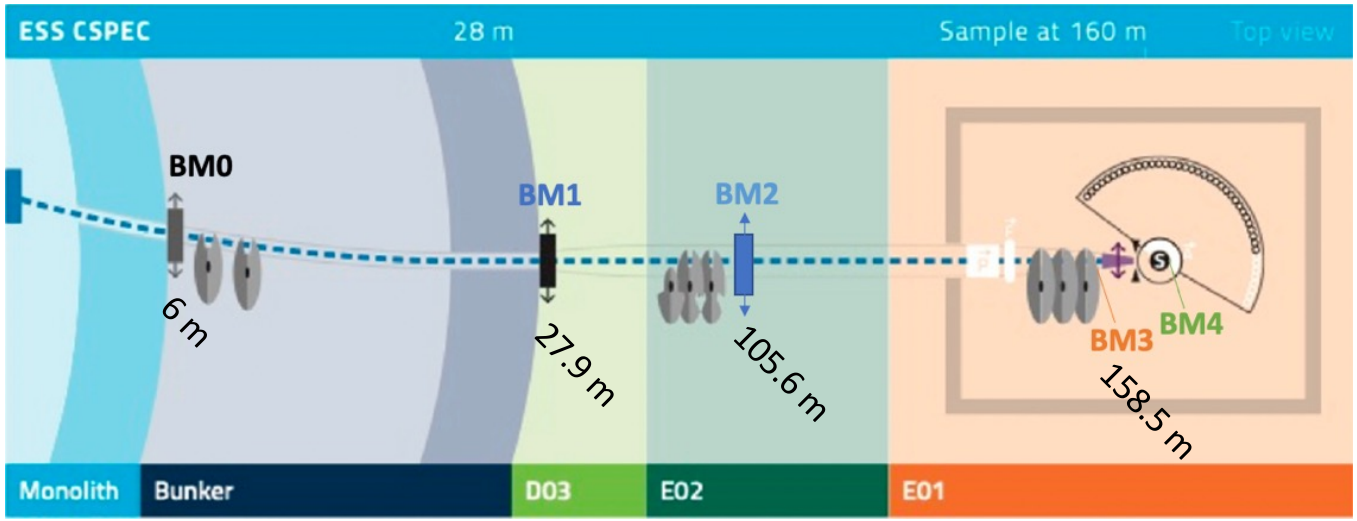
- Cryofurnace*
- Rotation stage*

For first science/start of the user program:

- 12-14 T magnet (shared with TREX)
- ^{3}He insert*
- High pressure cells (pool)
- High temperature furnaces (pool)
- Pump and probe setup (pool)
- Automatic sample changer* (likely later)

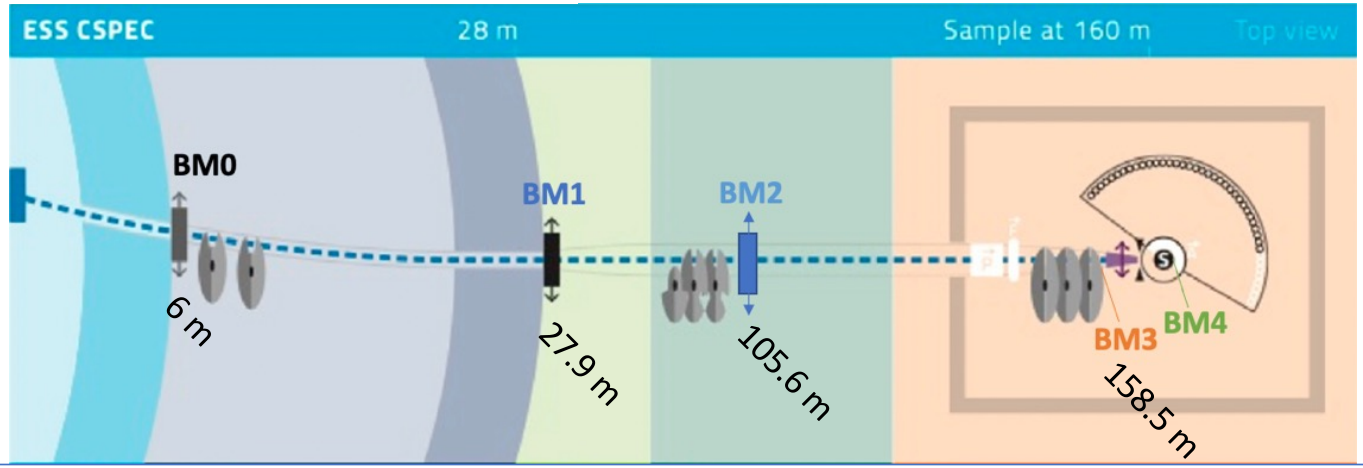
* CSPEC scope

Monitors (common project)



- BM0 (in-bunker, fixed): ionisation beam monitor (IBM), CDT Germany. Not CSPEC scope
- BM1 (removable): IBM or micromegas (MM), CEA, France
- BM2 (removable) and BM3 (fixed): MM
- BM4 (after sample): neutron camera (+ pool BM for commissioning and maintenance. Plans for a fixed transmission monitor for polarisation analysis (not day 1).

Monitors (common project)



BM0-BM4: tight space reservation (20 mm)!

BM0: “Harsh” environment. High flux at 2 MW. Flexible to follow the ramping up of the source.

BM1 and BM2: High flux at 2 MW. Opening time of the PS chopper: ca 55-670 µs. Large area for BM2 (115 x 74 mm x mm). Large dynamic range (3-4 orders of magnitude, 2 at fixed source power). BM1 close to the shutter → vibrations

BM3: Low attenuation needed. Opening time of the M chopper: 10-120 µs. Large dynamic range (3-4 orders of magnitude, 2 at fixed source power).

BM4: During operation: check the position of the sample & transmitted beam.

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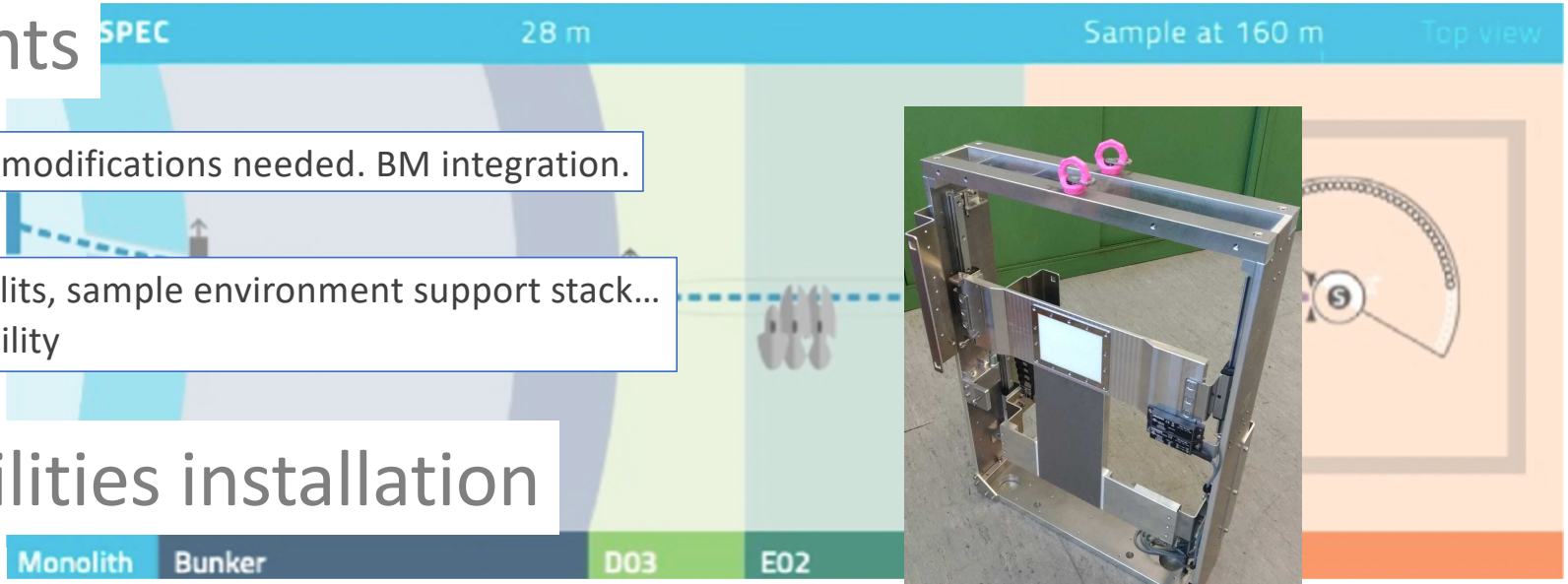
The Cold Chopper spectrometer of the ESS

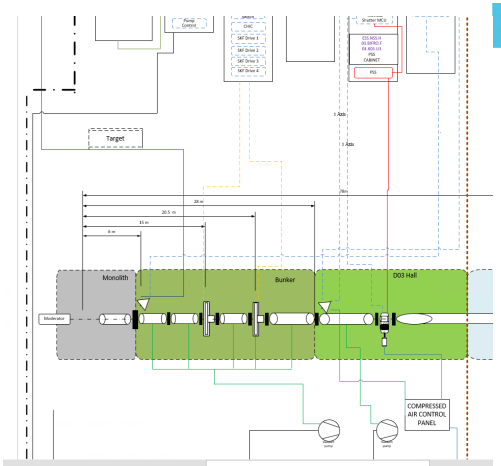
Other components

Shutter at the ESS. Some modifications needed. BM integration.

Guide exchanger, collimation slits, sample environment support stack…
→ waiting for designer availability



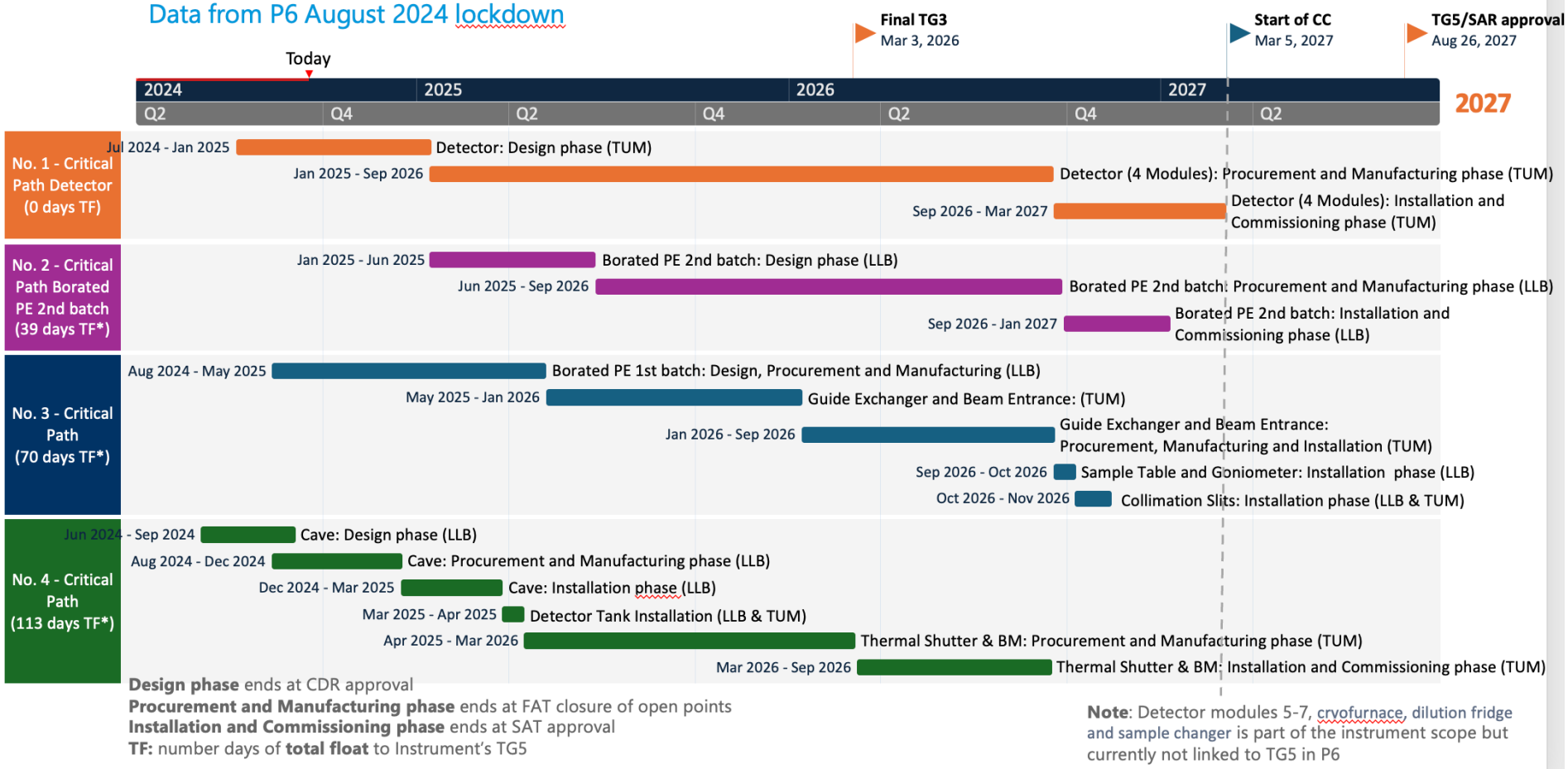
Electrical and utilities installation



CEP and CUP → priority in bunker; detailed plans for out of bunker after cave installation

CSPEC Critical Paths

Data from P6 August 2024 lockdown

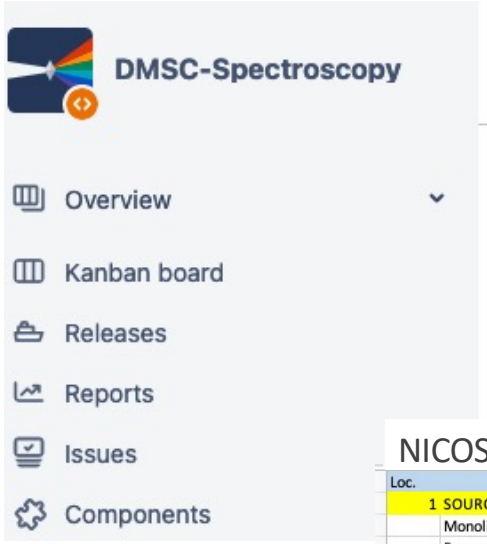


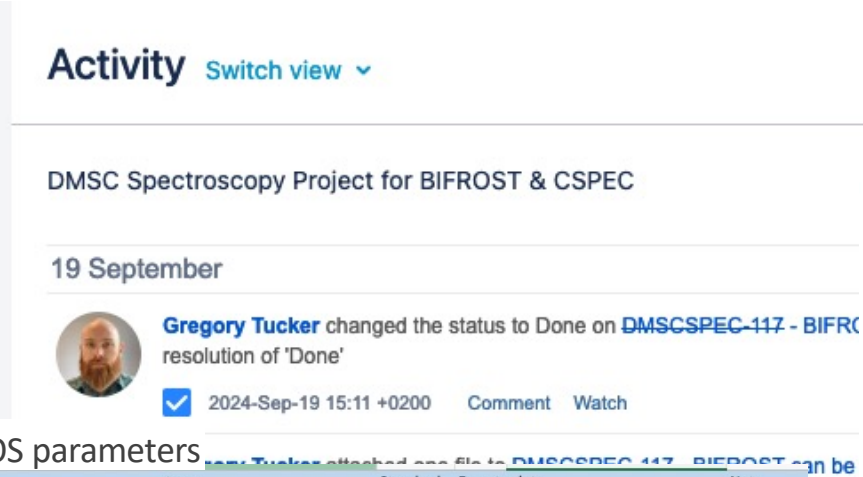
Design phase ends at CDR approval
Procurement and Manufacturing phase ends at FAT closure of open points
Installation and Commissioning phase ends at SAT approval
TF: number days of **total float** to Instrument's TG5

Note: Detector modules 5-7, cryofurnace, dilution fridge and sample changer is part of the instrument scope but currently not linked to TG5 in P6

Data acquisition and analysis

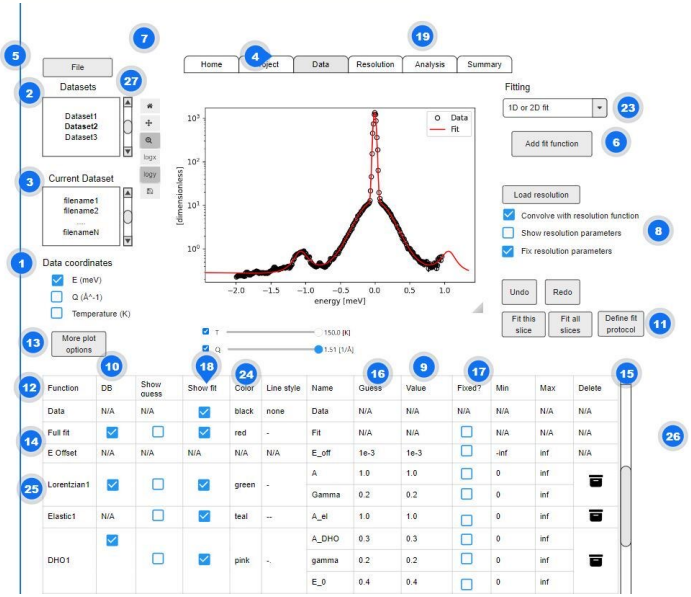
Working on different fronts, defining needs, wishes and priorities for instrument control, data acquisition, data reduction, data analysis…





NICOS parameters

Loc.		type	Standard	Expert	plot	Note
	1 SOURCE					
	Monolith shutter status	open/close	VO	VO	plot vs time?	still decidin
	Power	value (W)	VO	VO	plot vs time	
1--5	GUIDE					
	Guide vacuum pressure	value (unit?)	N	VO		~ 8 gauges,
	1 BM0					
	status	on/off	N	VC?	plot vs time?	we need to
	count rate	value (n/s)	VO	VO	plot vs time	
	2 BW1 CHOPPER					
	Status	on/off	VO	VC	plot vs time?	still decidin
	Speed	value Hz	VO	VC	plot vs time	



Hot commissioning

Standard samples

- vanadium
- $Na_2Ca_3Al_2F_{14}$, $Y_3Fe_5O_{12}$
- water

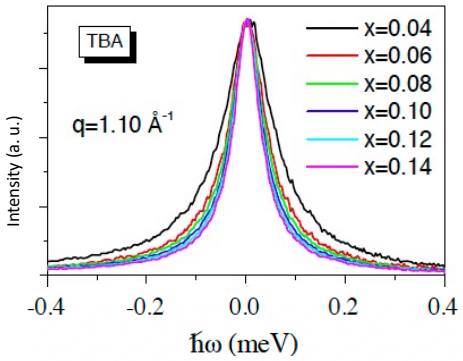
End-to-End Experimental Chain

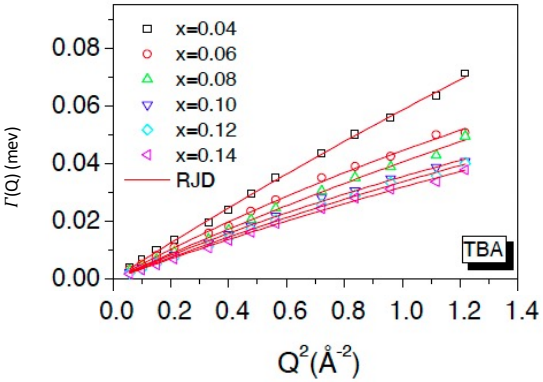
- already measured
- sample availability

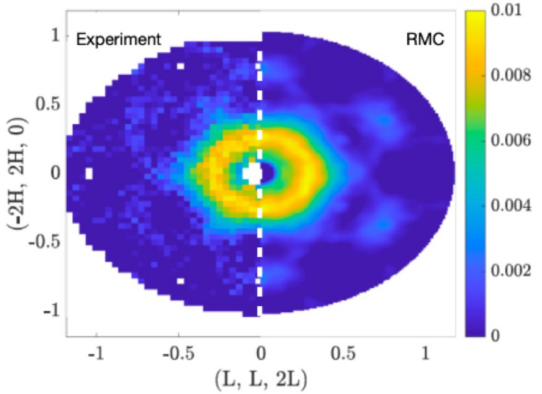
Examples:

- Aqueous solutions of tert-butyl alcohol-d
  measured at IN5, λ_0 = 10 Å, ΔE = 15 µeV FWHM. [ILL experimental report 30498]

- frustrated $Yb_3Ga_5O_{12}$ garnet
  measured at CNCS (E_i = 1.55 meV, ΔE = 37 µeV FWHM and E_i = 3.32 meV, ΔE = 109 µeV FWHM) (and IN5) [Phys. Rev. B 104, 064425, 2021]

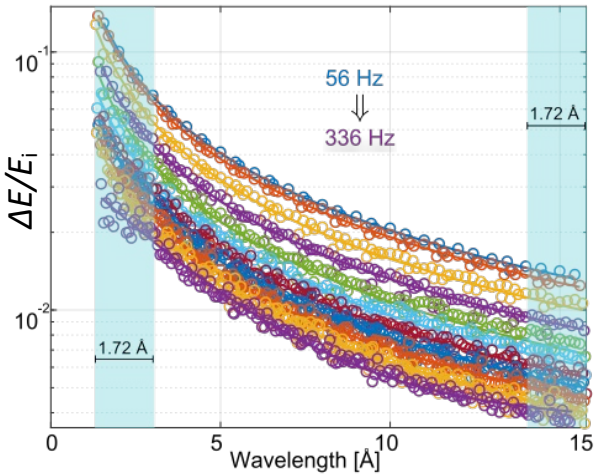






First science

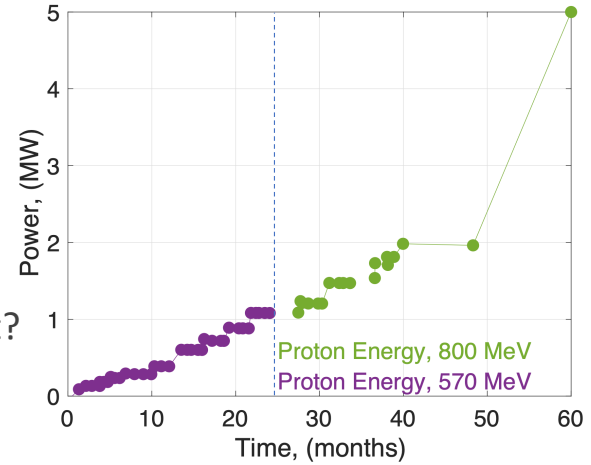
- Energy resolution (1.5% at 4 Å)
- *Q* resolution
- SNR 10^5 (at 5 Å)
- RRM (flux integration - long wavelengths)
- RRM (extended dynamic range – short wavelengths)
- Beam focussing
- Kinetics…



amorphous/powder and
single crystals/oriented samples

QENS and INS,
in different scientific fields

Flux? Days with neutrons? Detectors? Sample environment?



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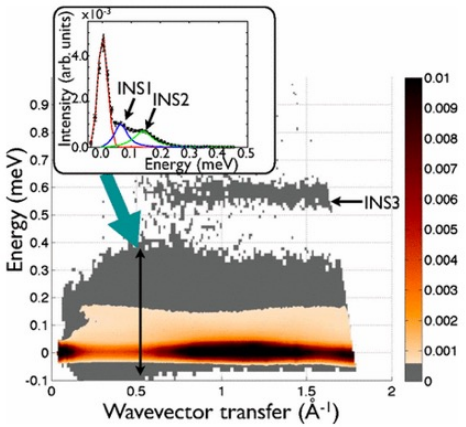
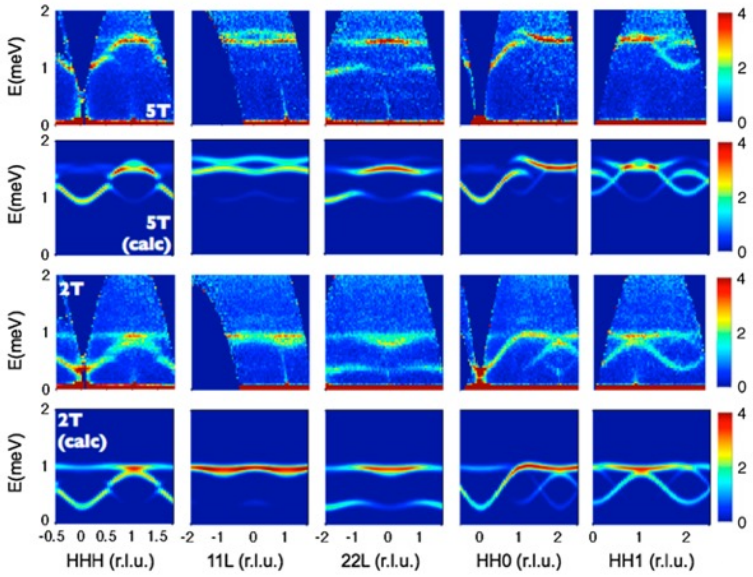
First science

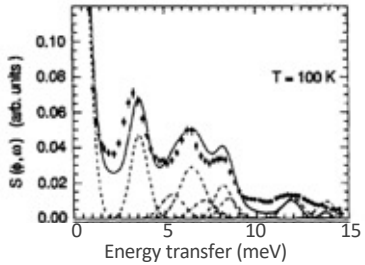
Something like…



Spin dynamics in the hyperkagome compound Gd_3Ga_5O.
Phys. Rev. B 82, (2010)

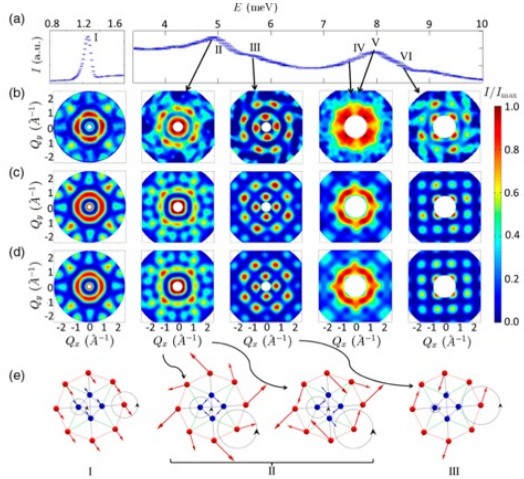


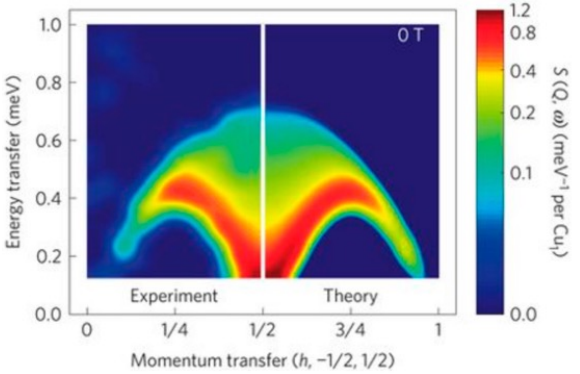
Quantum Excitations in Quantum Spin Ice.
Phys. Rev. X 1 (2011)



Neutron scattering determination of the crystal field parameters in $ErCu_4Al_8$ and $ErFe_4Al_8$ intermetallics.
Solid State Communications, 94, (1995)

Magnetic Exchange Interactions in the Molecular Nanomagnet Mn_{12}. Phys. Rev. Lett. 119, (2017)





Fractional spinon excitations in the quantum Heisenberg antiferromagnetic chain. Nature Physics 9, (2013)

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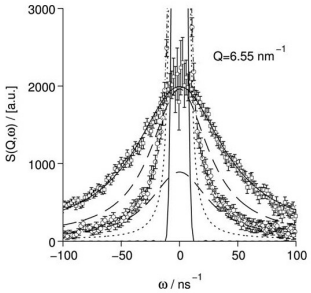
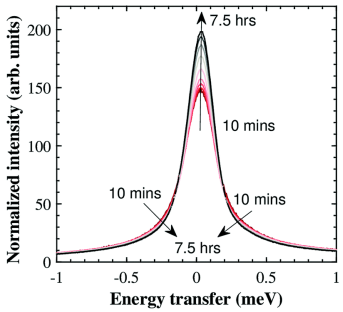
First science

Something like…

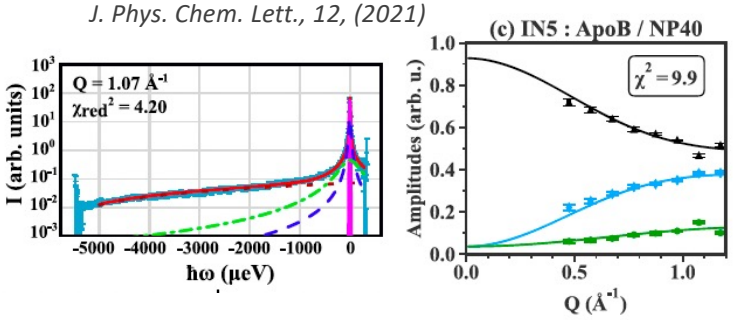


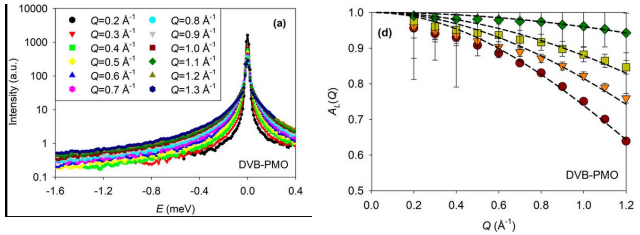
Fast internal dynamics in alcohol dehydrogenase J. Chem. Phys. 143, (2015)



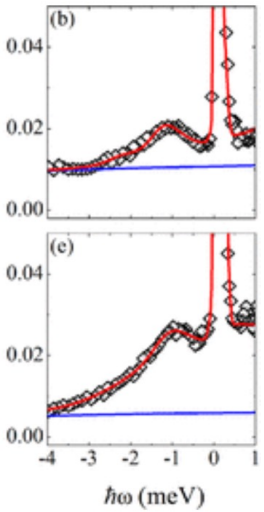
In situ quasi-elastic neutron scattering study on the water dynamics and reaction mechanisms in alkali-activated slags. Phys. Chem. Chem. Phys., 21, (2019)

Dynamics of Apolipoprotein B-100 in Interaction with Detergent Probed by Incoherent Neutron Scattering J. Phys. Chem. Lett., 12, (2021)

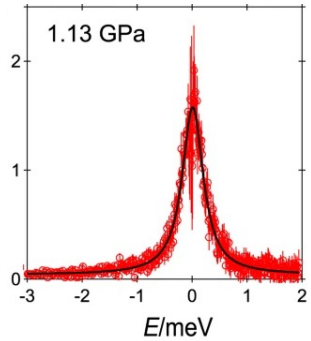




Dynamics of water confined in mesopores with variable surface interaction. J. Chem. Phys. 154, 094505 (2021)



Inelastic Neutron Scattering Investigation in Glassy SiSe2: Complex Dynamics at the Atomic Scale. J. Phys. Chem. Lett., 4 (2013)



Diffusion in dense supercritical methane from quasi-elastic neutron scattering measurements. Nature Communications, 12, (2021)

First science

CSPEC team

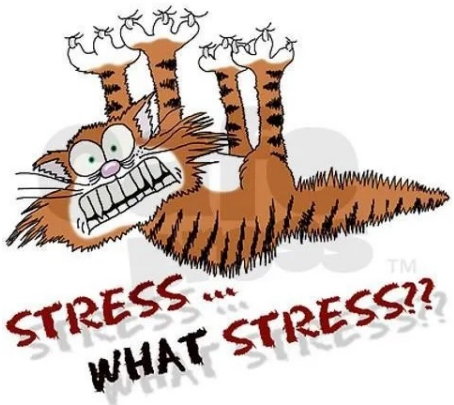




+ collaborators

Other friendly (and expert) users



Reliable instrument for the community, including new users!