CSPEC update

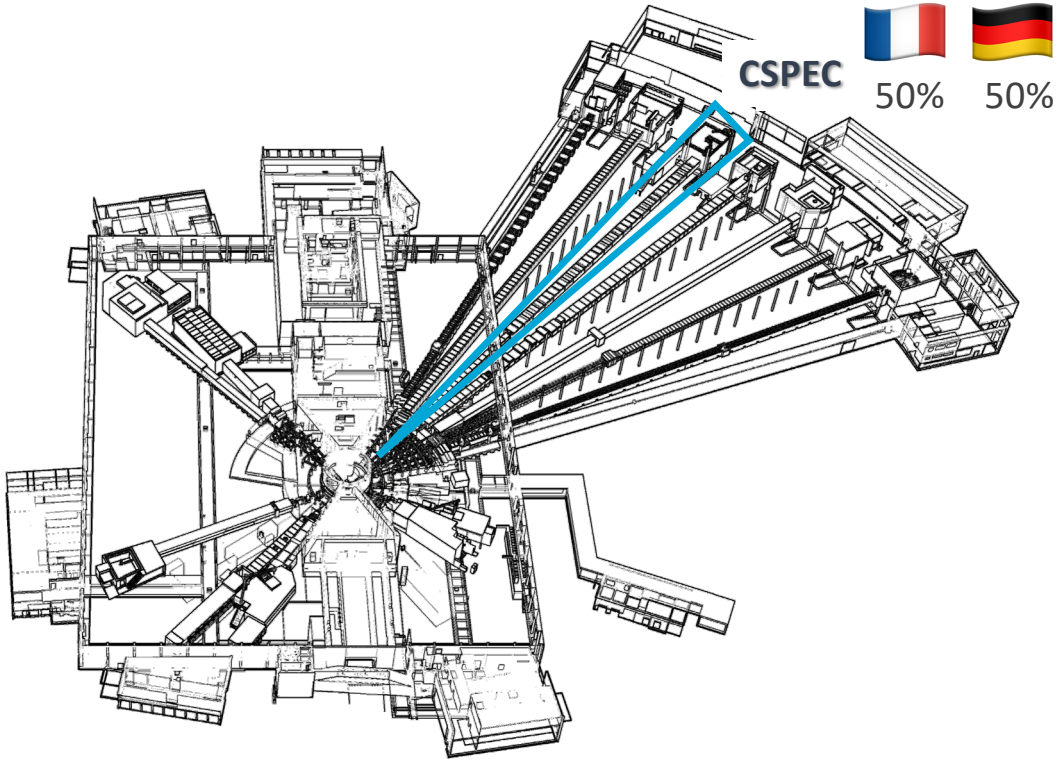
Daria Noferini (ESS) – daria.noferini@ess.eu

Spectroscopy STAP meeting 25.04.2023

CSPEC

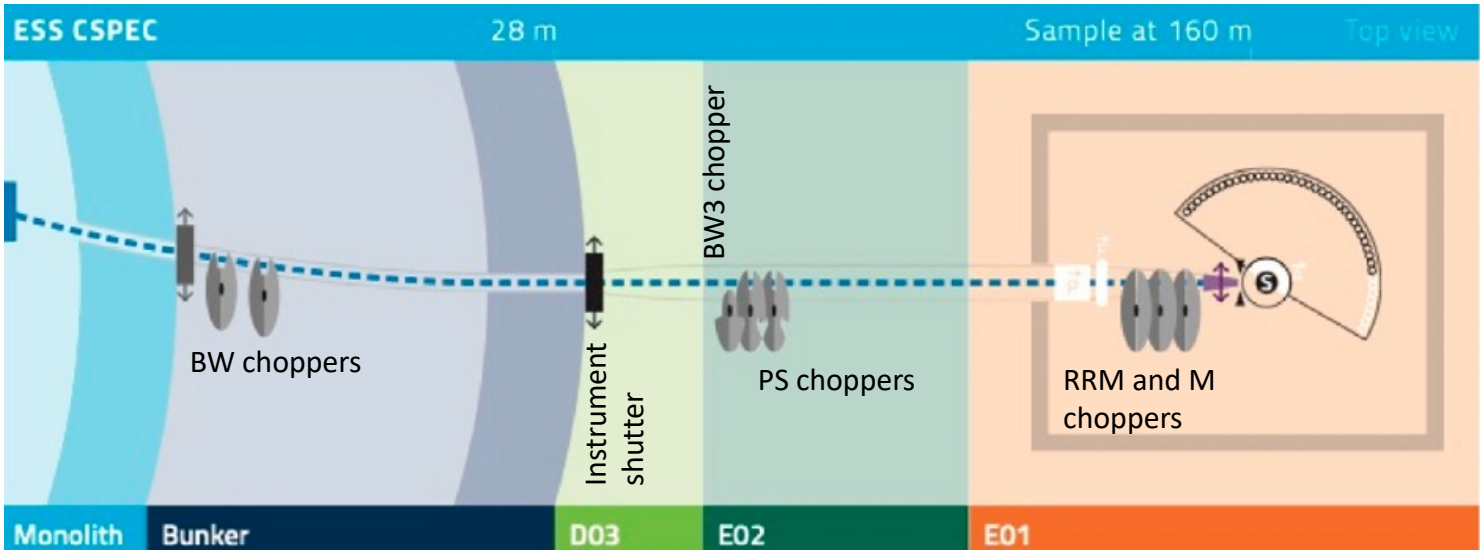
The Cold Chopper spectrometer of the ESS

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

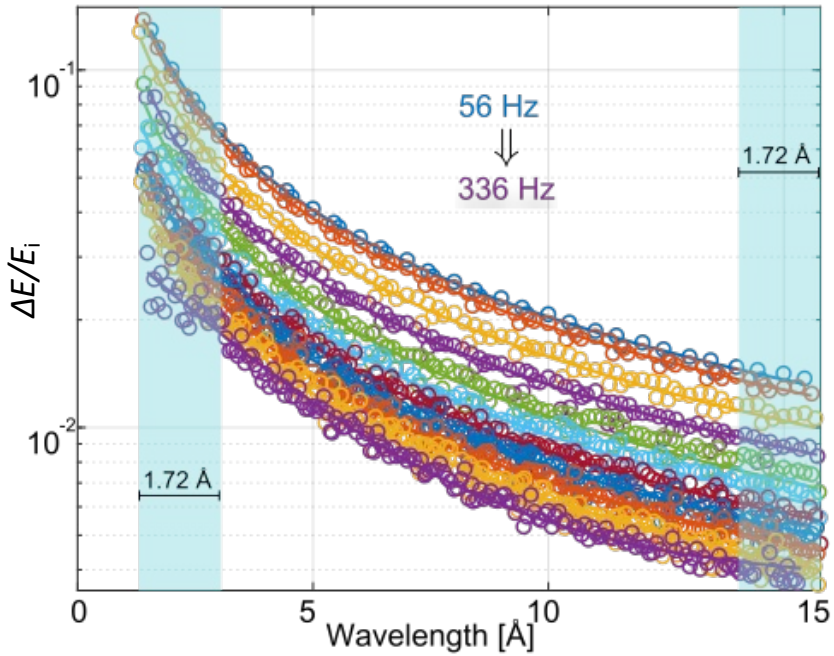
TG5: November 2025

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)

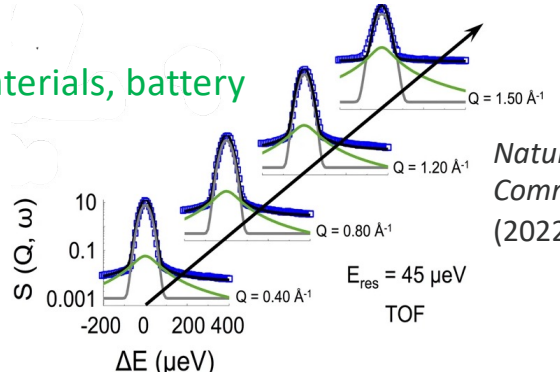
Science cases

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

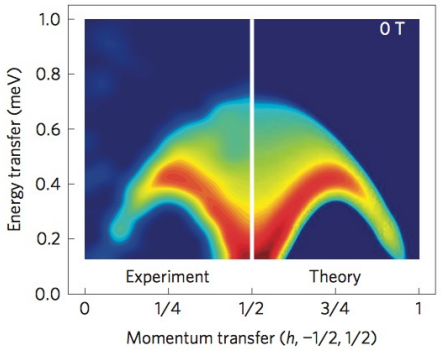
Energy materials: fuel cells membranes and electrolytes, thermoelectric materials, battery electrolytes, H-storage, organic photovoltaics…

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…

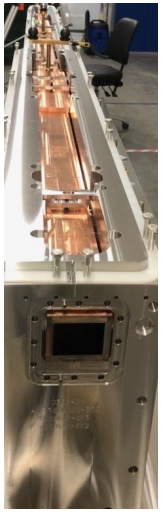
Focus on small samples, in situ/operando, kinetics etc

CSPEC

The Cold Chopper spectrometer of the ESS

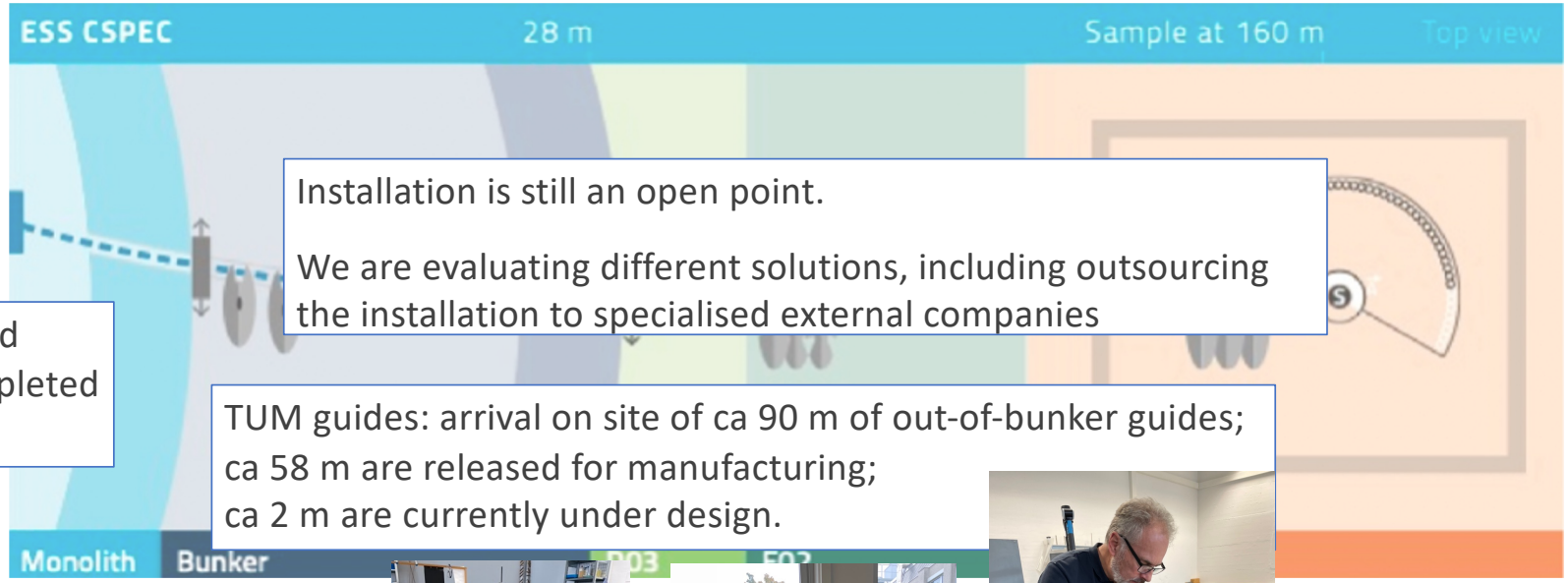
Guides

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



S-DH

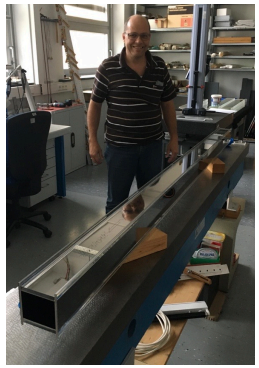
SwissNeutronics

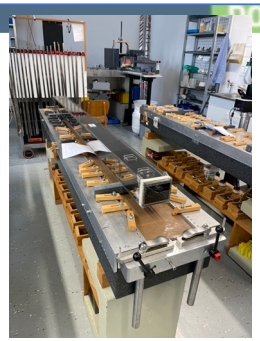


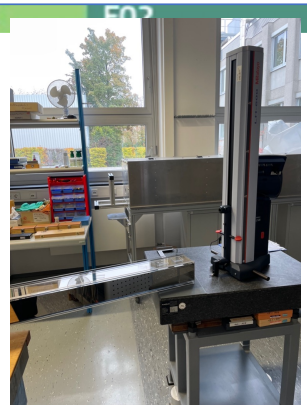
Installation is still an open point.

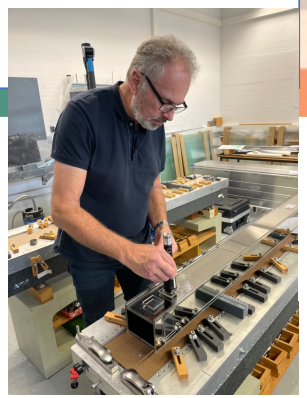
We are evaluating different solutions, including outsourcing the installation to specialised external companies

TUM guides: arrival on site of ca 90 m of out-of-bunker guides;
ca 58 m are released for manufacturing;
ca 2 m are currently under design.



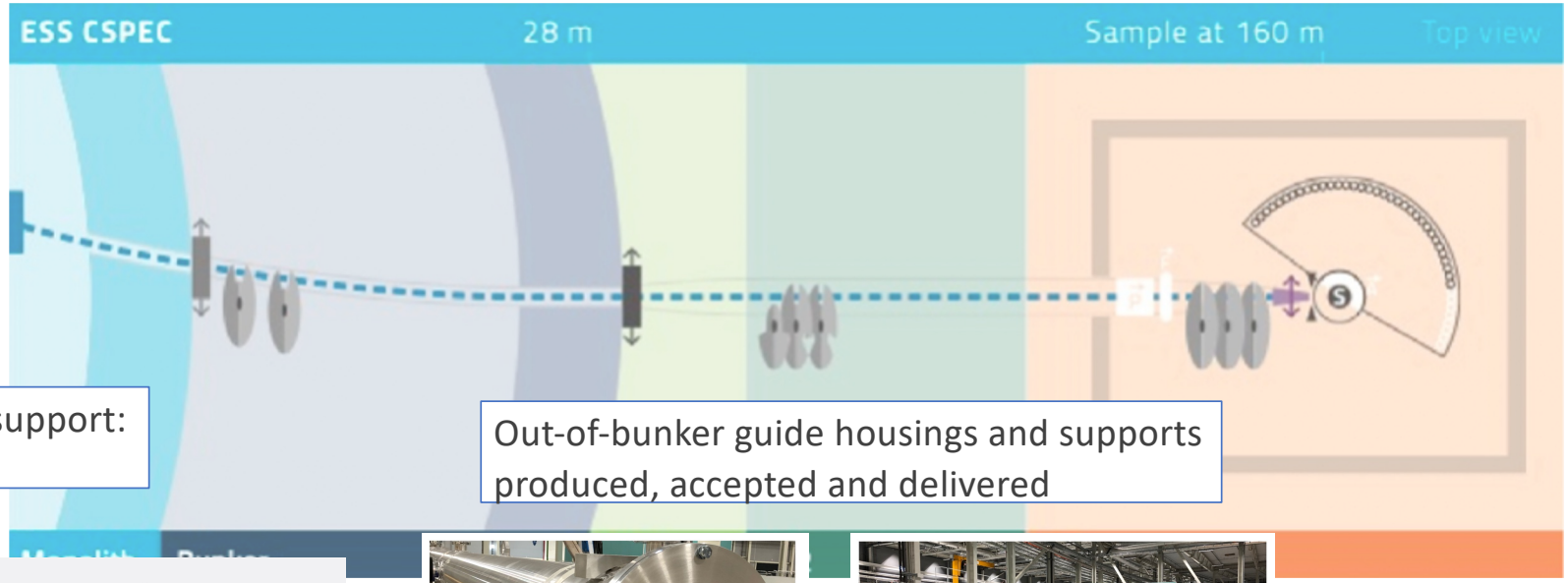




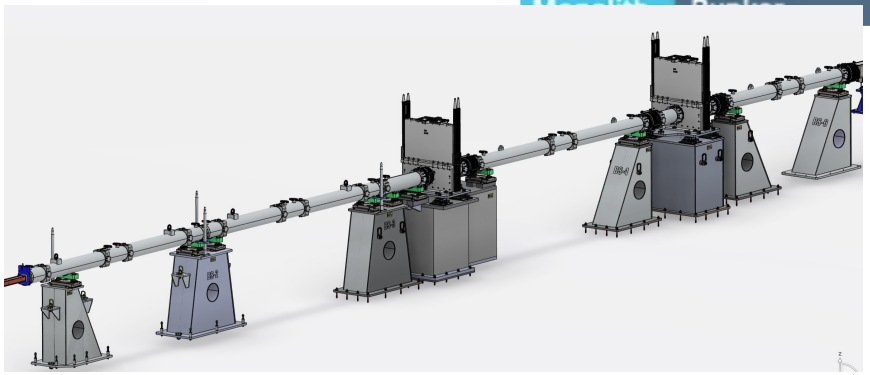


TECHNISCHE UNIVERSITÄT MÜNCHEN

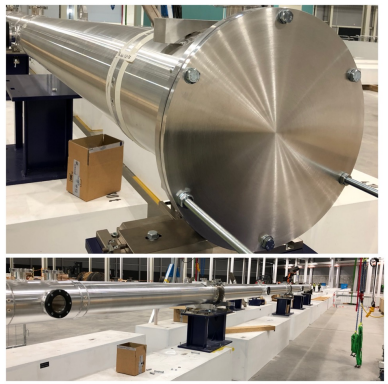
Guide housings



In-bunker guide housings and support: design in progress



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



CECOM HIGH PRECISION SOLUTIONS

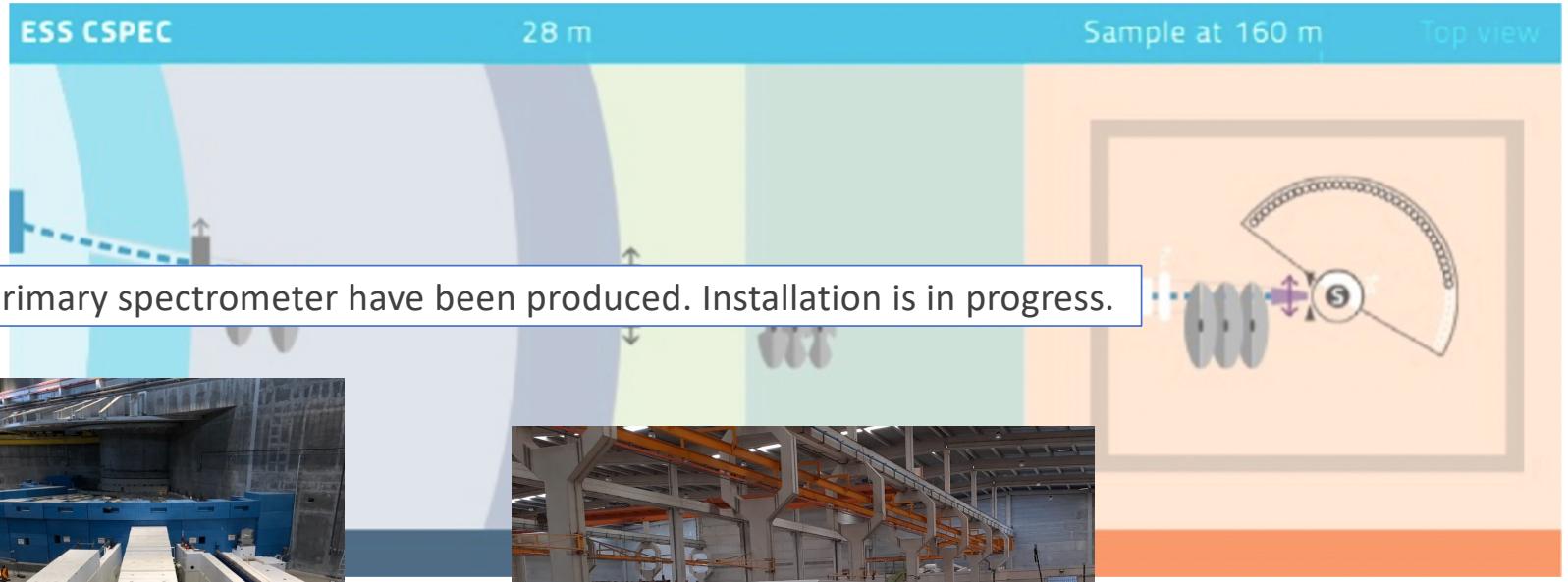
CSPEC

The Cold Chopper spectrometer of the ESS

Shielding

ESS common project

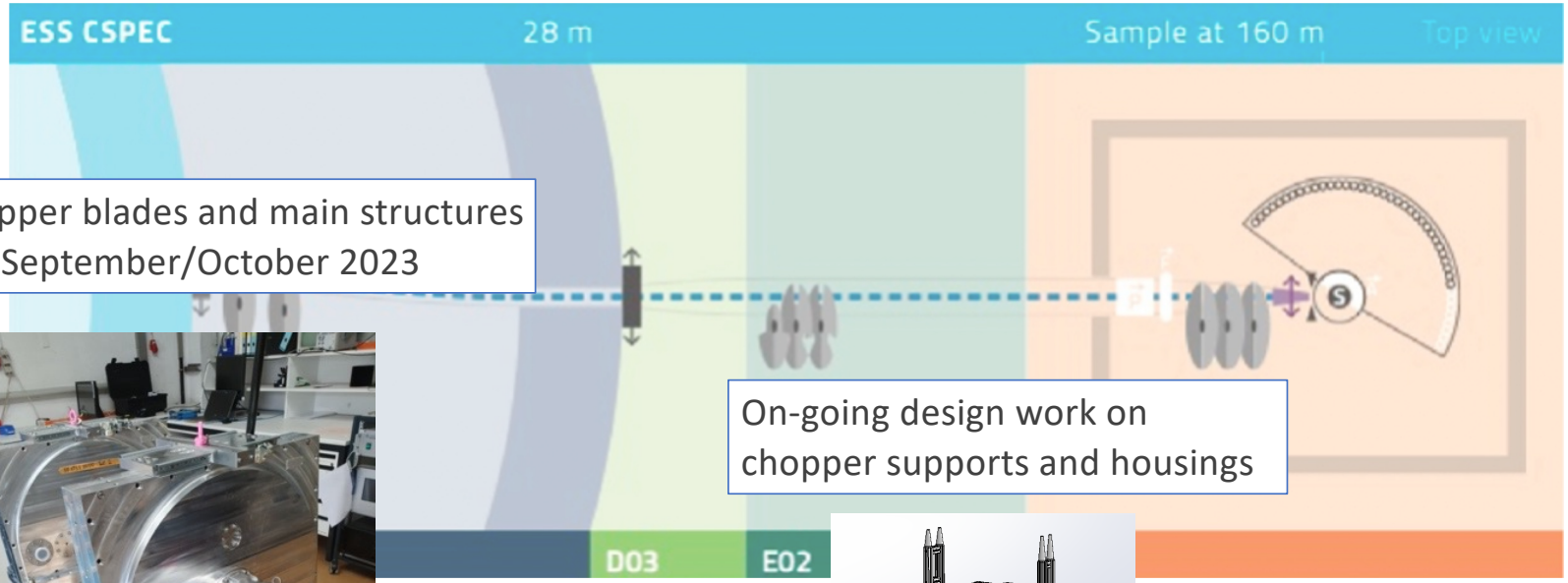
All the shielding blocks for the primary spectrometer have been produced. Installation is in progress.



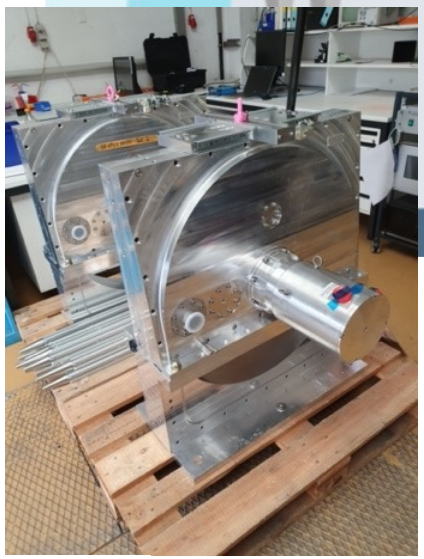
CSPEC

The Cold Chopper spectrometer of the ESS

Choppers

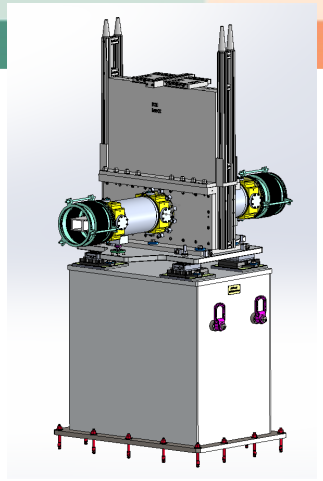


Manufacturing of the chopper blades and main structures is progressing well → FAT September/October 2023

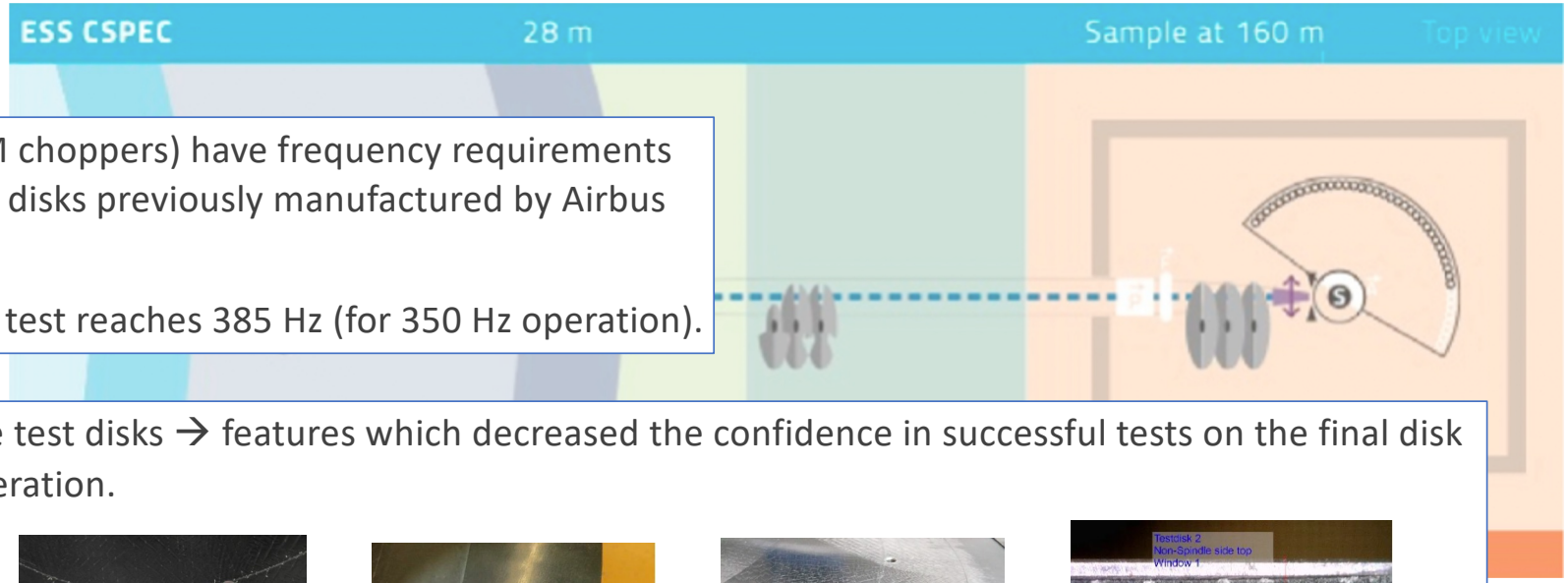


AIRBUS DEFENCE & SPACE

On-going design work on chopper supports and housings



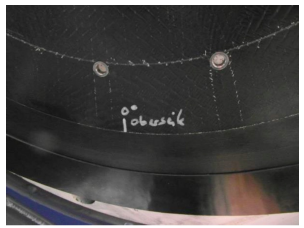
Choppers

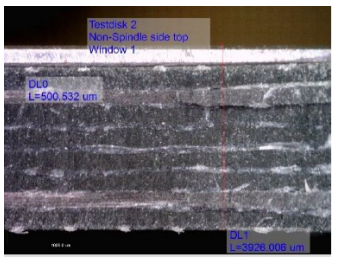


CSPEC fast disks (M and RRM choppers) have frequency requirements that were never matched by disks previously manufactured by Airbus (e.g. LET or DREAM).

First time that an overspeed test reaches 385 Hz (for 350 Hz operation).

During the tests on the test disks → features which decreased the confidence in successful tests on the final disk and safe long-term operation.





The team agreed to reduce the operational speed to 336 Hz (still within scientific specifications)

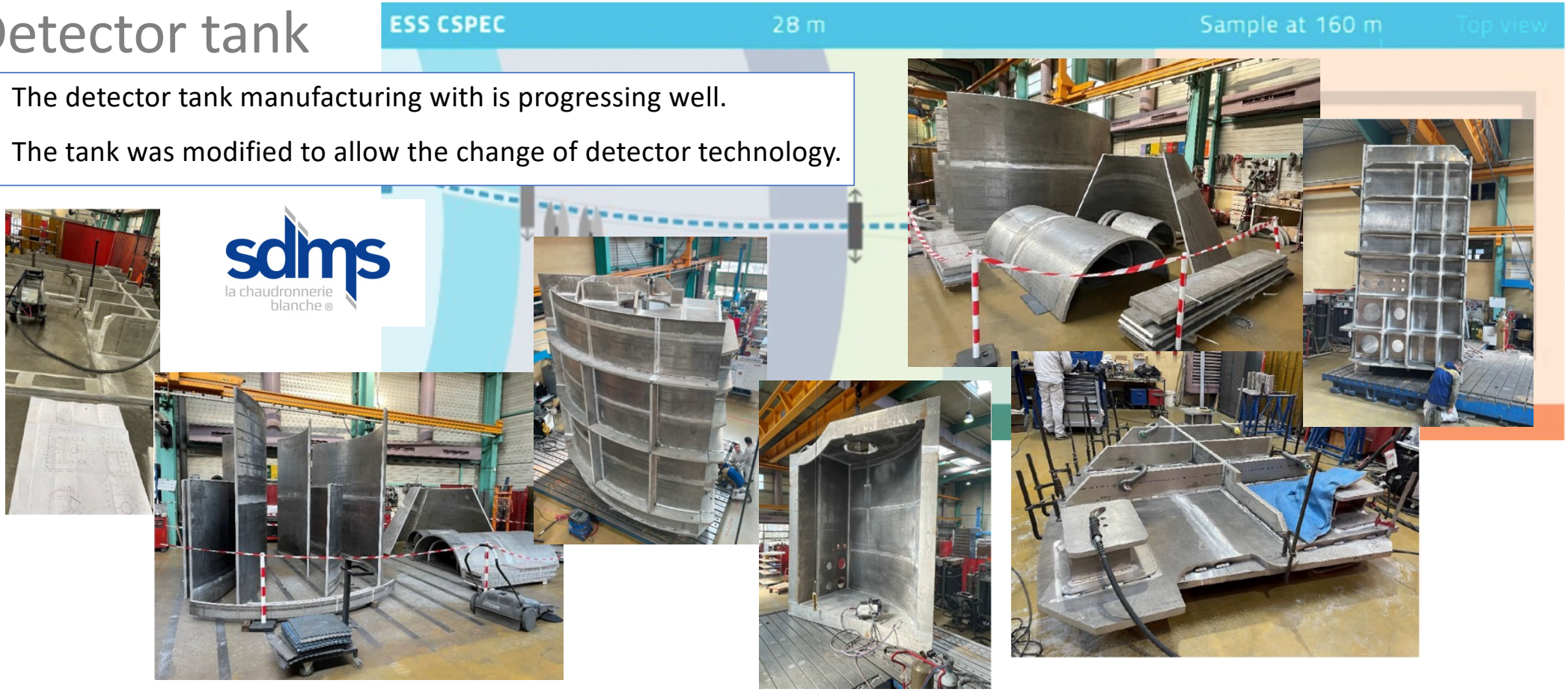
CSPEC

The Cold Chopper spectrometer of the ESS

Detector tank

The detector tank manufacturing with is progressing well.

The tank was modified to allow the change of detector technology.

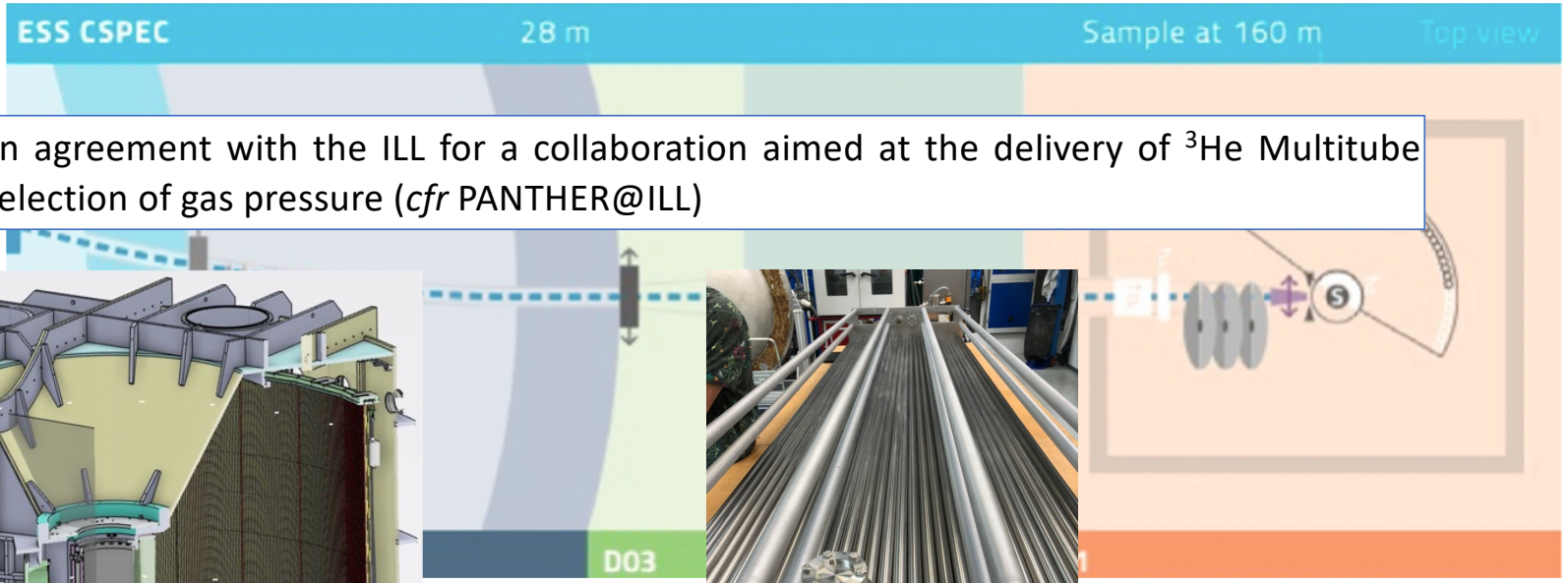


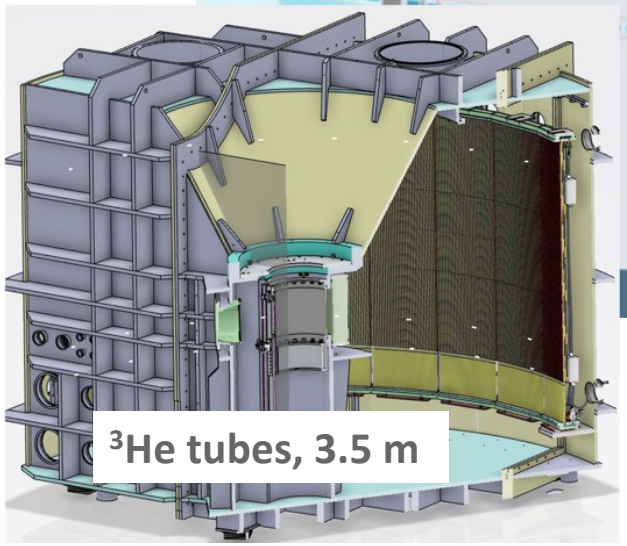
Installation → April 2024

Cd sheets + PE blocks → design and procurement coming soon

Detector

We are working to finalise an agreement with the ILL for a collaboration aimed at the delivery of ^{3}He Multitube detectors (MT) with flexible selection of gas pressure (*cfr* PANTHER@ILL)





See talk from Kevin Fissum after lunch!

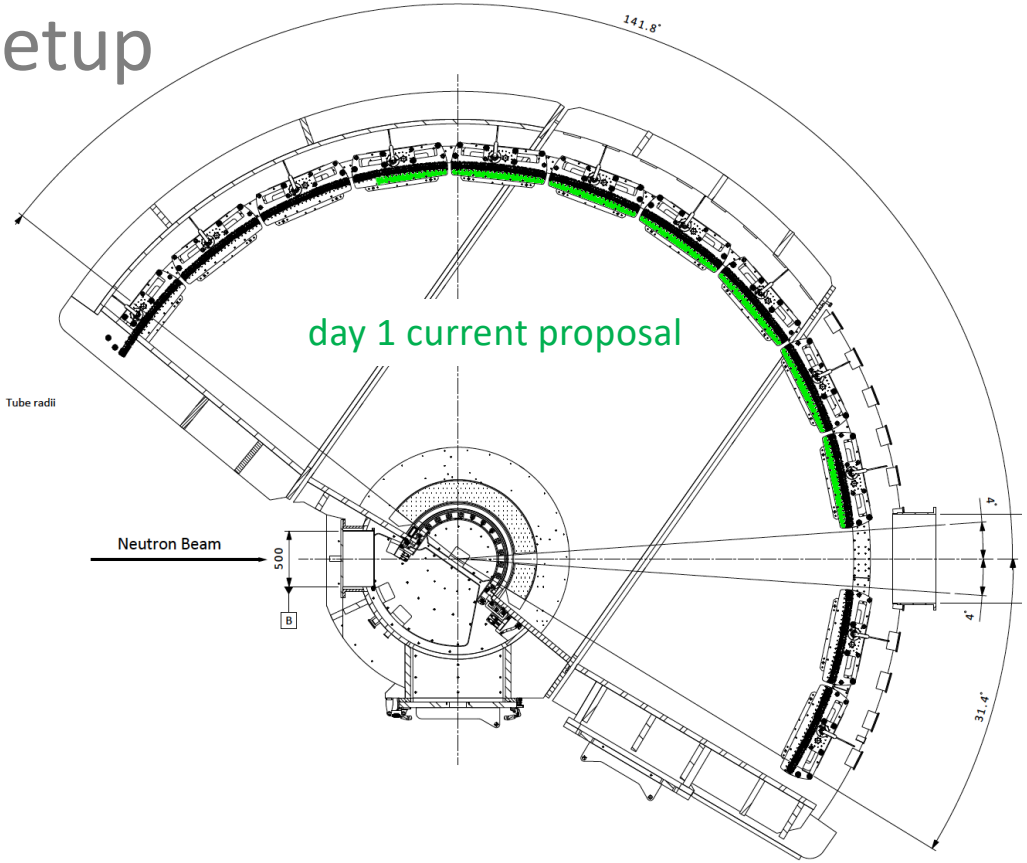
Detector: from design to day 1 setup

original design: ± 30° [vertical] (4 m height),
-30°-140° [horizontal]

scope-setting meeting : ± 26.5° [vertical] (3.5 m height),
-30°-140° [horizontal]

ConOps (2017) proposal for day 1: full horizontal coverage, 50% of the electronic channels covered (MG) – technically unfeasible

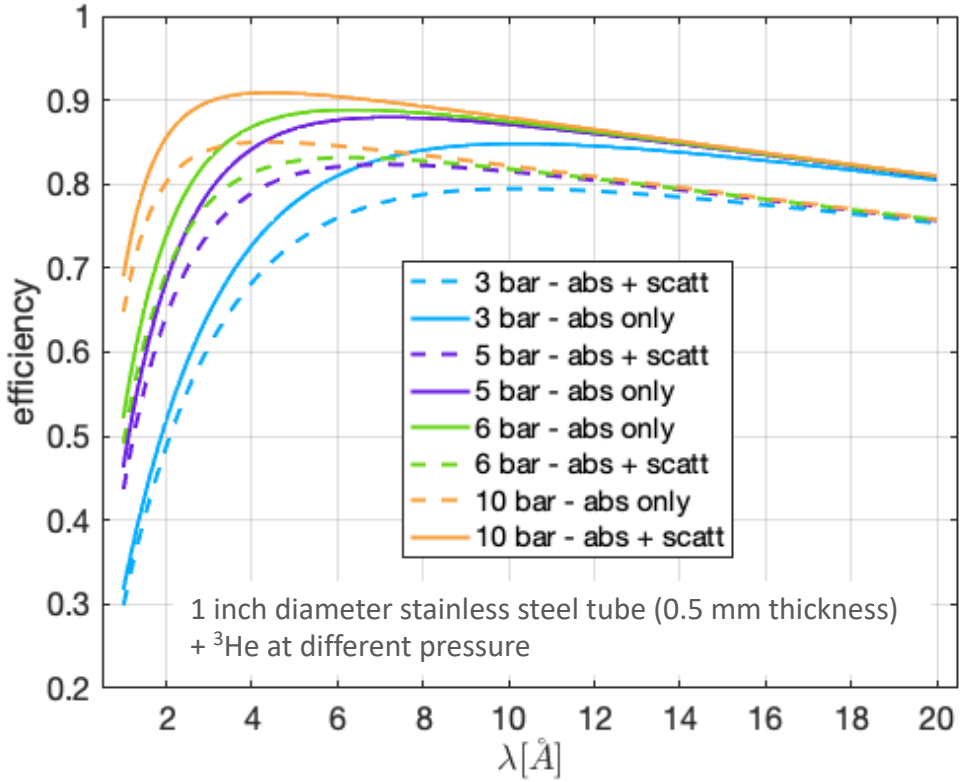
current day 1 proposal: full vertical coverage (3.5 m),
58% of the horizontal coverage



The reduced angular coverage is problematic for the many studies which need an extended *Q*-range to properly model and understand the dynamics (*e.g.* diffusion and local motions in energy materials, soft matter, biophysics etc)

Detector: from design to day 1 setup

Unlucky time for change of technology (relative peak of ^{3}He price)

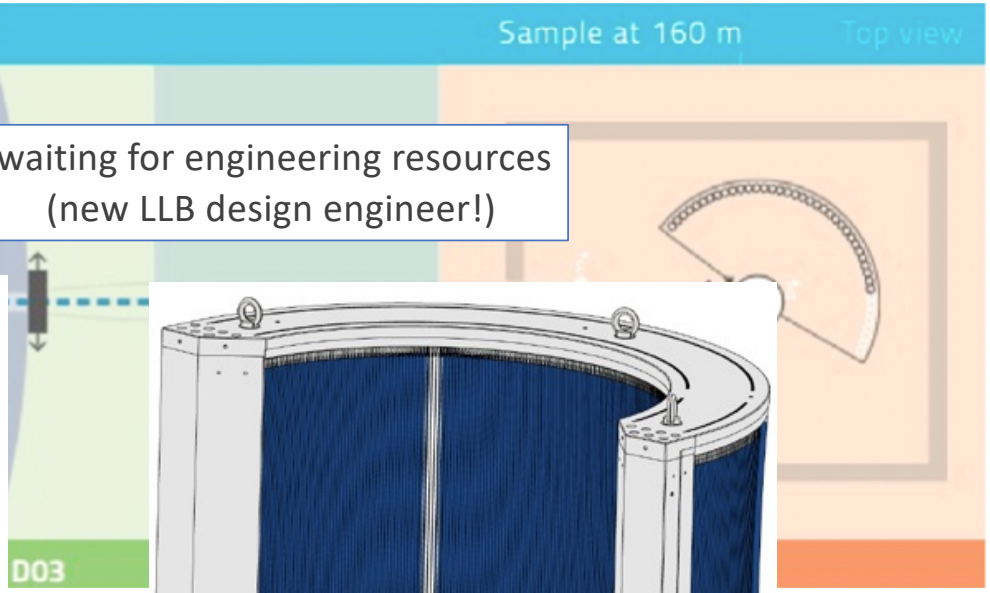


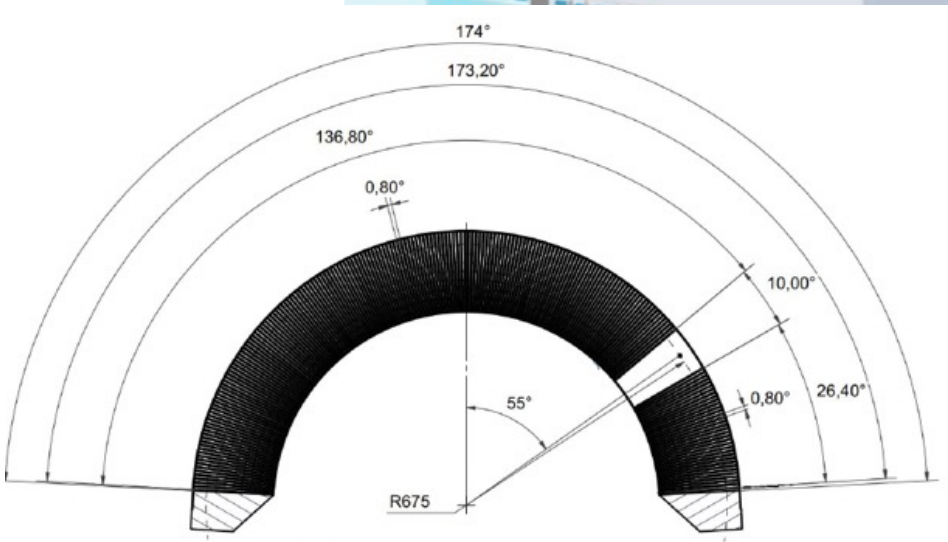
CSPEC day 1 proposal: 3 bar (budget limitations and technical feasibility of MG at scope setting meeting)
IN5: 5 bar
CNCS: 6 bar
AMATERAS, LET: 10 bar

The low efficiency limits early “days” science and challenging experiments (small samples, operando, in situ, kinetics…
i.e. the focus of CSPEC!)

Collimator

Manufacturing almost completed. The collimator drive design → waiting for engineering resources (new LLB design engineer!)



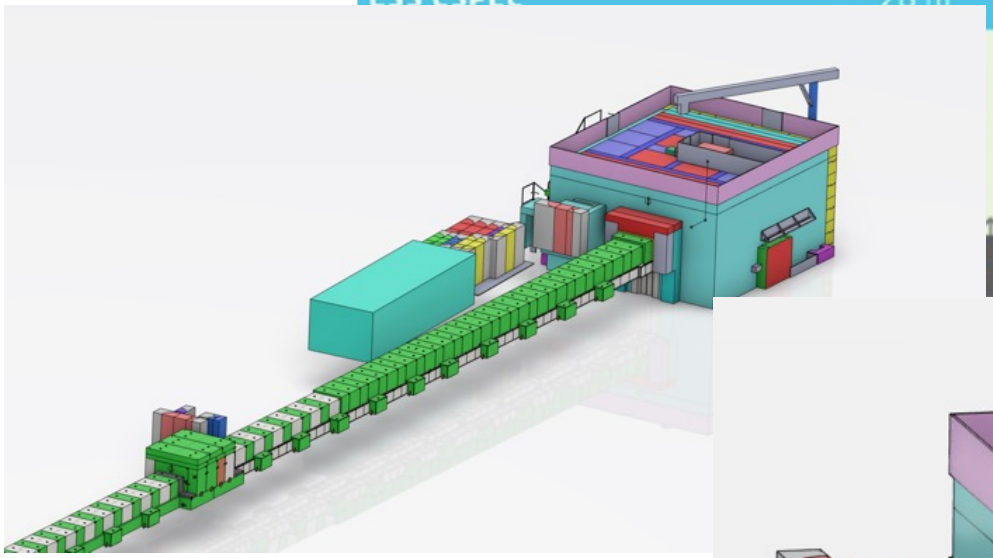


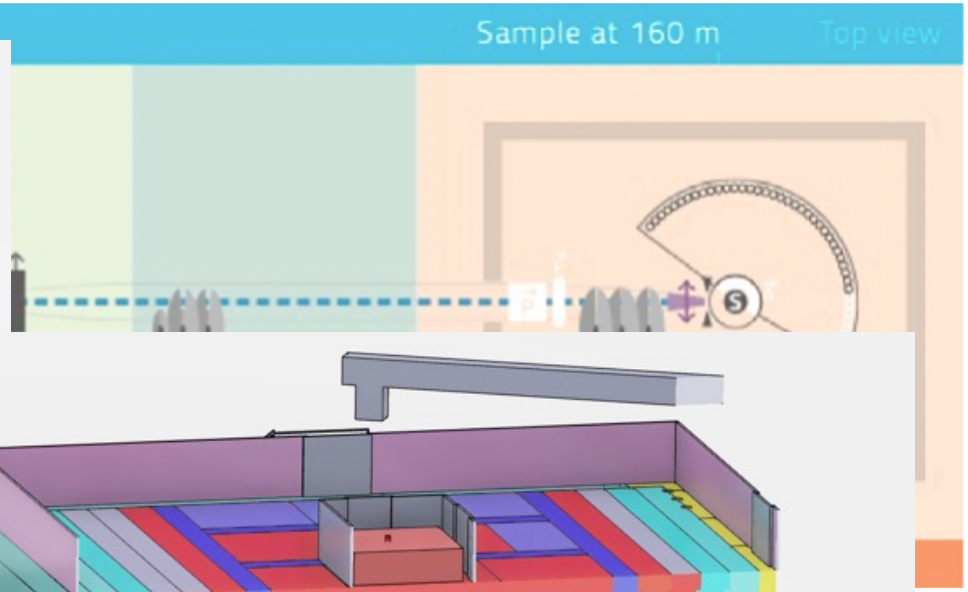
JJ X-RAY
Danish Science Design

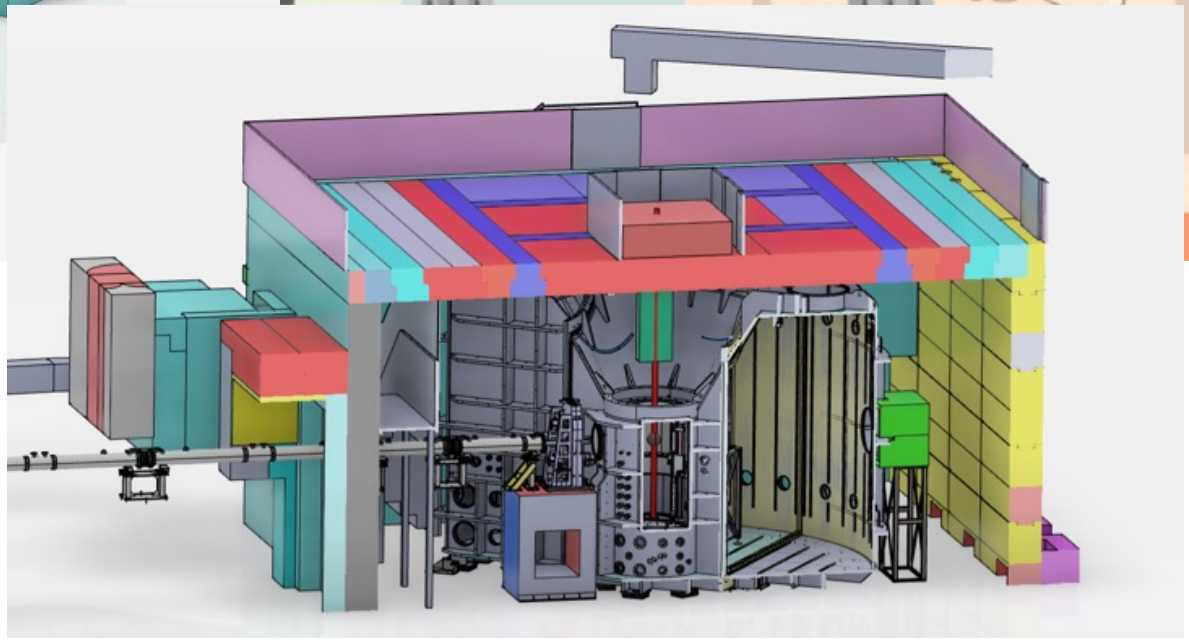
CSPEC

The Cold Chopper spectrometer of the ESS

Cave







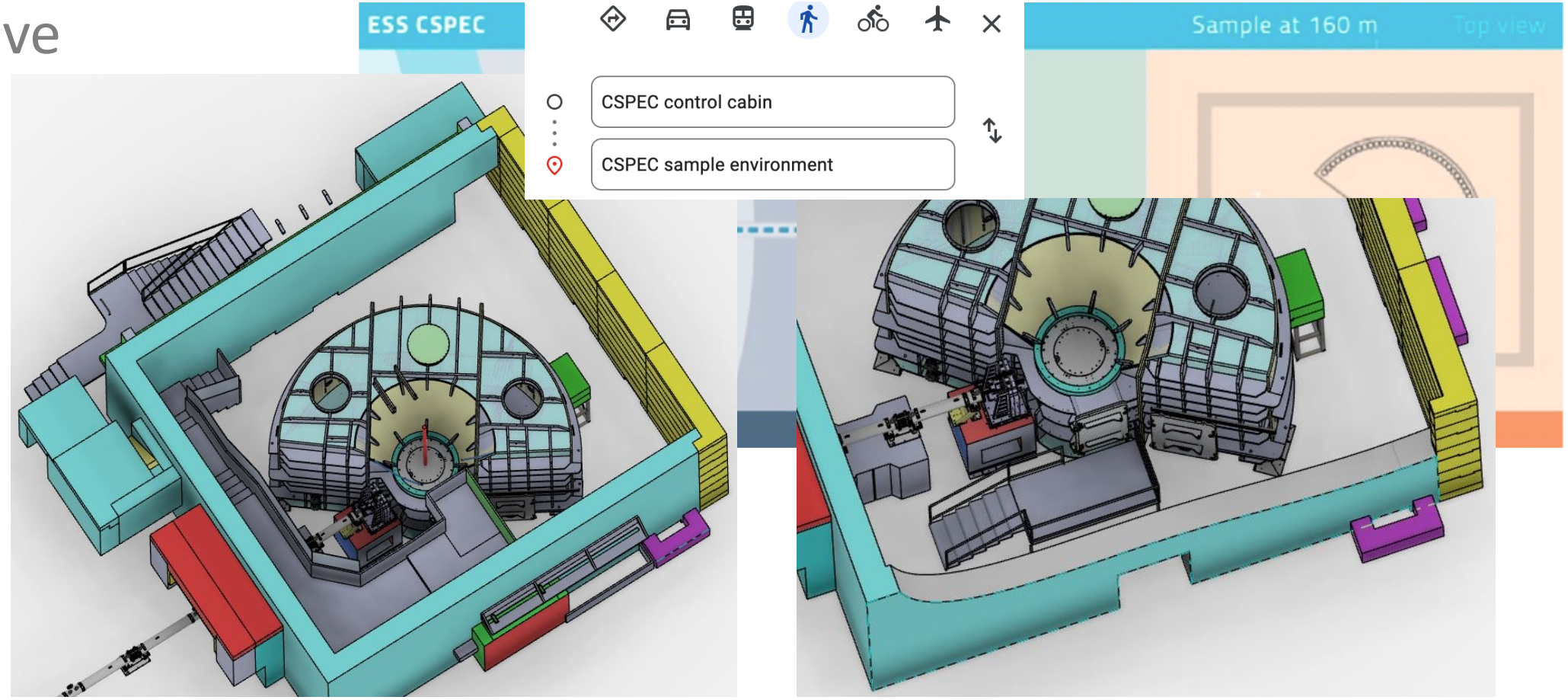
The tender closed at the end of March. We are currently evaluating the offers and starting the negotiations.

Control cabin, instrument crane, false floors for the racks → not part of the current tender (out for tender separately in the next future).

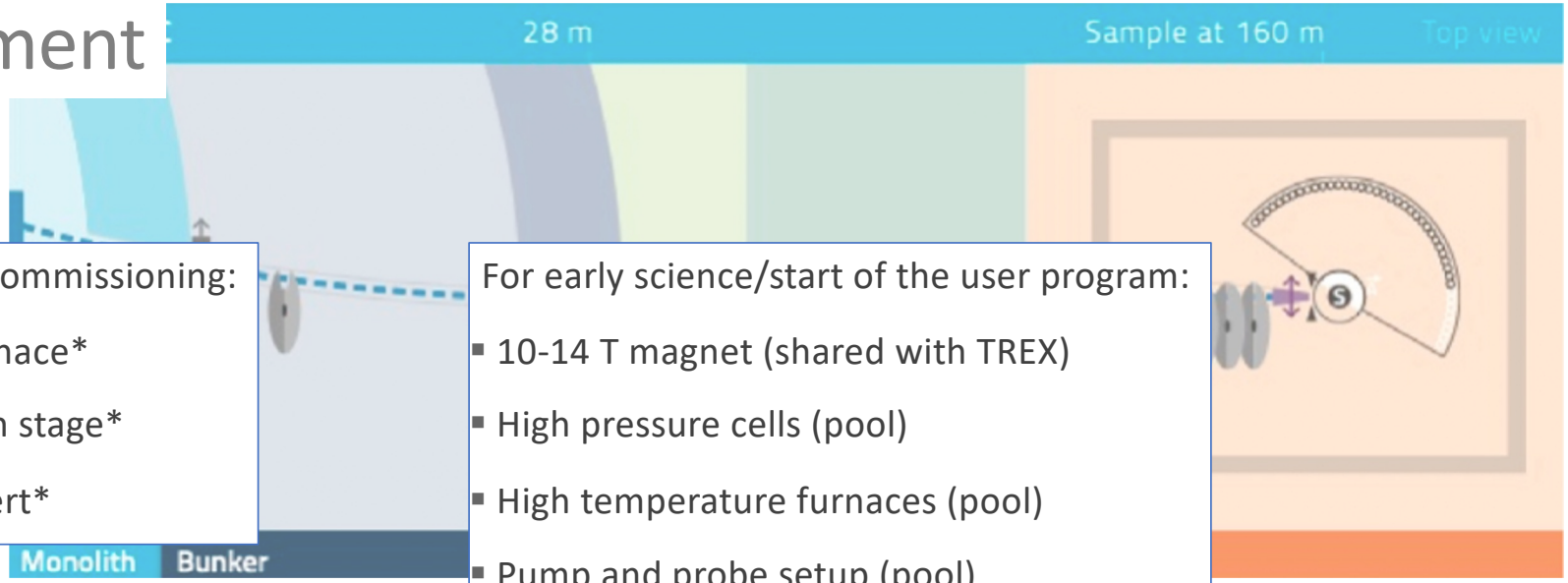
CSPEC

The Cold Chopper spectrometer of the ESS

Cave



Sample environment



For hot commissioning:

- Cryofurnace*
- Rotation stage*
- ^{3}He insert*

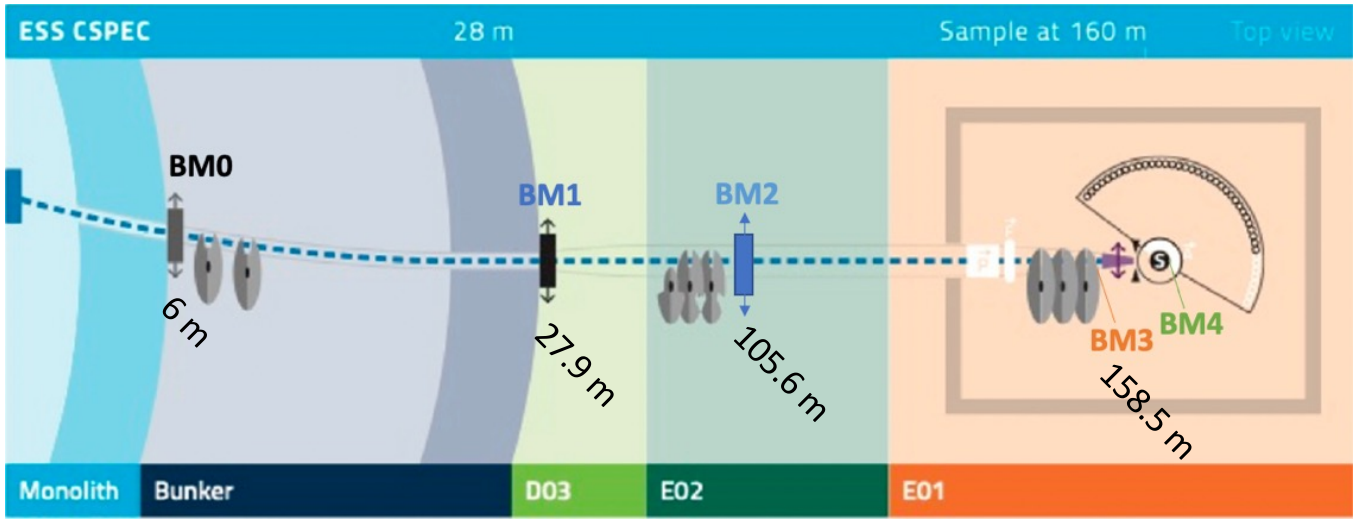
For early science/start of the user program:

- 10-14 T magnet (shared with TREX)
- High pressure cells (pool)
- High temperature furnaces (pool)
- Pump and probe setup (pool)
- Automatic sample changer*

See talk from Alex Holmes tomorrow!

* CSPEC scope

Monitors



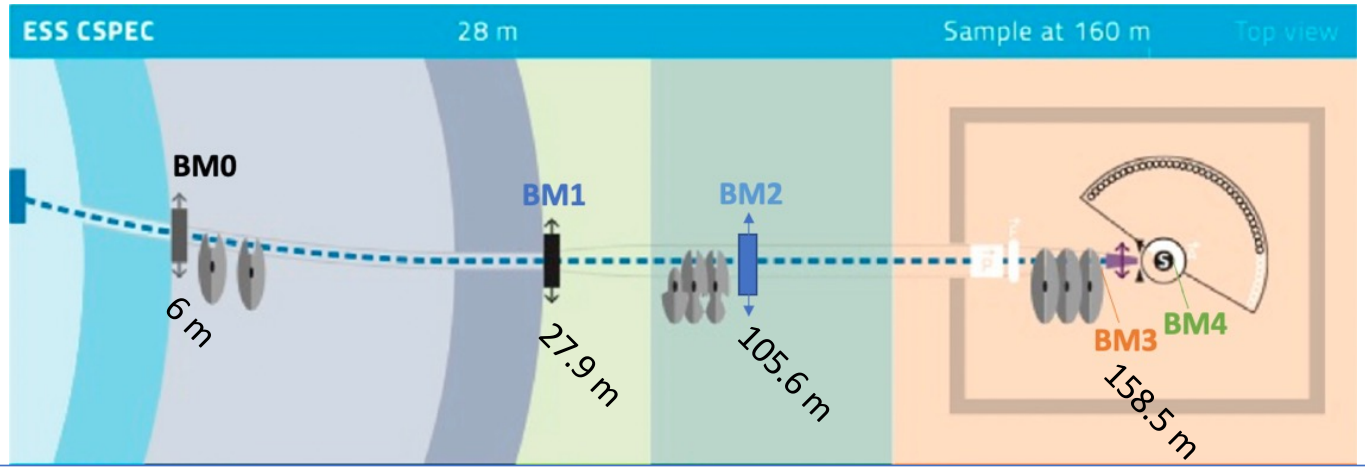
BM0: ESS requirement (not CSPEC scope). Fixed in position during experiments

BM1 and BM2: guide and chopper diagnostic. Removable (remotely).

BM3: guide and chopper diagnostic + normalisation. Fixed in position during experiments.

BM4: post-sample beam diagnostic + transmission. Removable (by hand).

Monitors



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

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

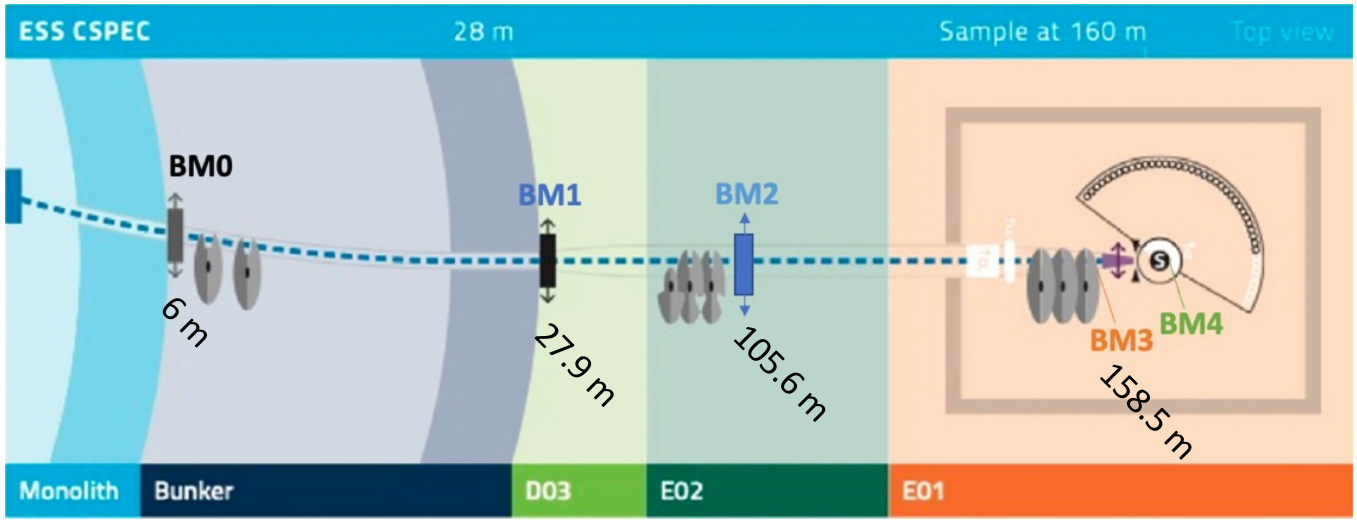
BM1 and BM2: High flux at 2 MW. Opening time of the PS chopper: ca 55-670 µs. Large area for BM2 (115 x 74 mm x mm). Large dynamic range (3-4 orders of magnitude, 2 at fixed source power).

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.

Monitors

See talk from Kevin Fissum after lunch!



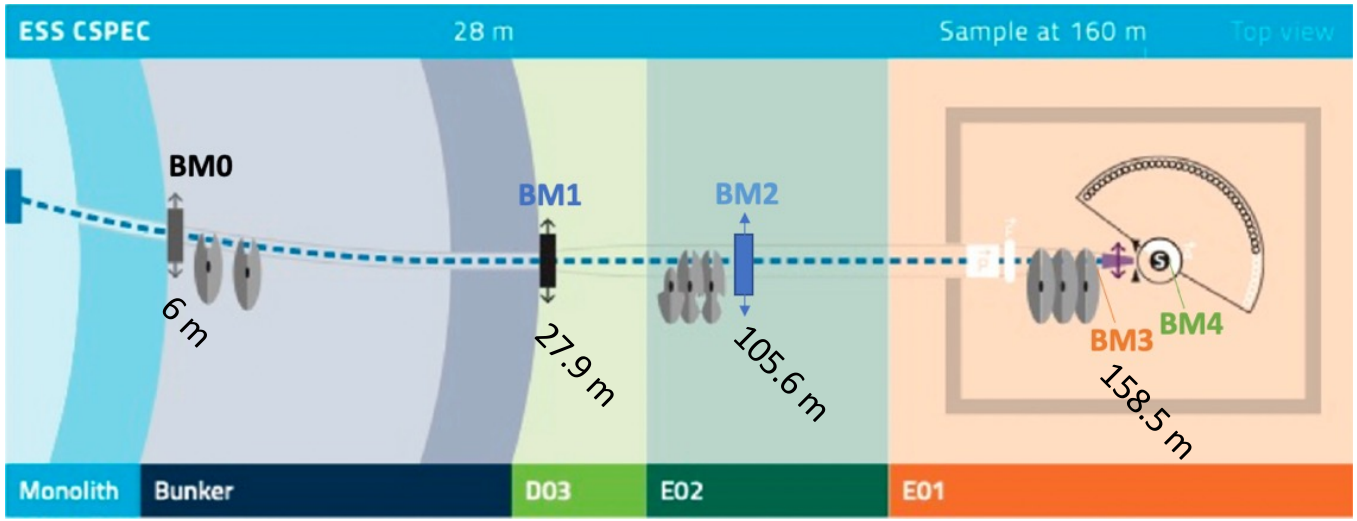
Pillars from the BM common project (reloaded):

- reduce the number of technologies per instrument and across instruments
- fundamental requirements + budget + timeline
- tests, tests, tests!

***I. Katsioulas**, F. Piscitelli, D. Noferini*

Monitors

See talk from Kevin Fissum after lunch!



BM0 → Ionisation Beam Monitor (IBM), CDT, Germany

BM1-BM3 → MicroMegas (MM), CEA, France

BM4 → Neutron camera

~~Tests planned at EMMA@ISIS (May 2023)~~
→ Tests at Morpheus@PSI and AMOR@PSI (June 2023)

Radiation hardness tests (end 2023)

Prototypes in October 2023 (including electronics)
→ tests

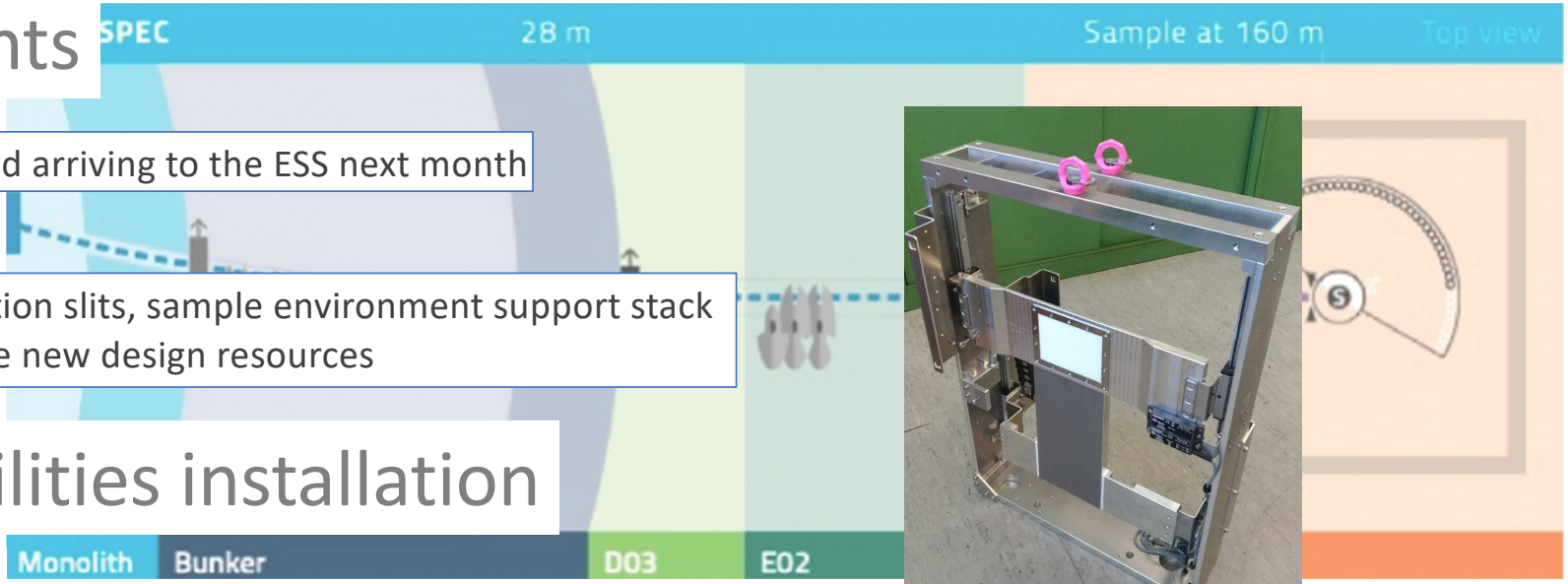
CSPEC

The Cold Chopper spectrometer of the ESS

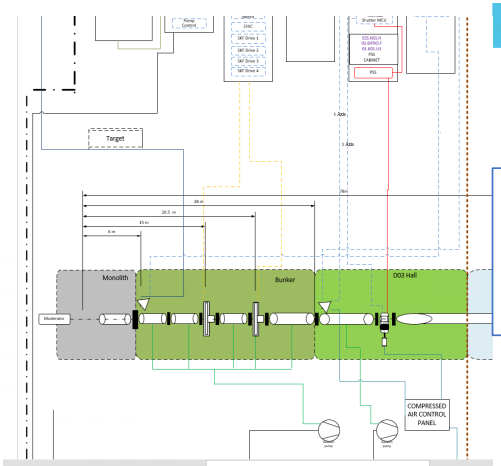
Other components

Shutter tested at TUM and arriving to the ESS next month

The guide exchanger, collimation slits, sample environment support stack
→ on hold and waiting for the new design resources



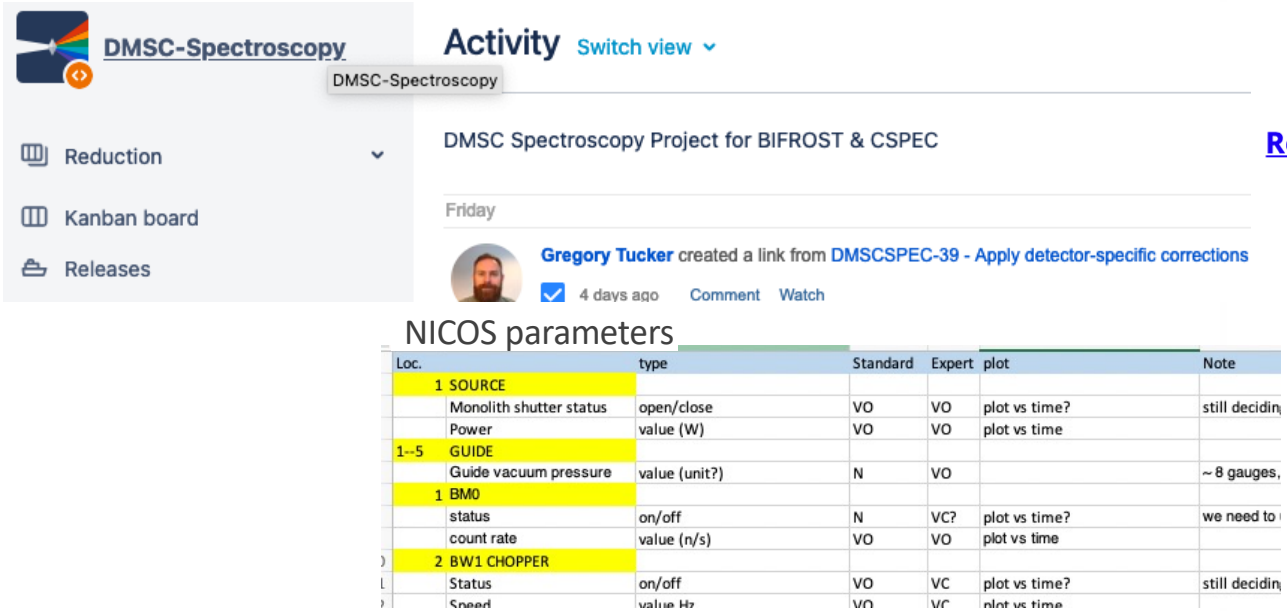
Electrical and utilities installation



Piping and Instrumentation Diagram (P&ID) work in progress → basis for a kick-off meeting with the ESS electrical team; the discussion with the ESS technical team for utilities will start after the first model of the cave is provided by the supplier

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	

Requirements for data analysis

- DMSCSPEC-57 Other analysis software
- DMSCSPEC-56 Mantid analysis software
- DMSCSPEC-55 MJOLNIR analysis software
- DMSCSPEC-54 PACE analysis software
- DMSCSPEC-53 QENS analysis software

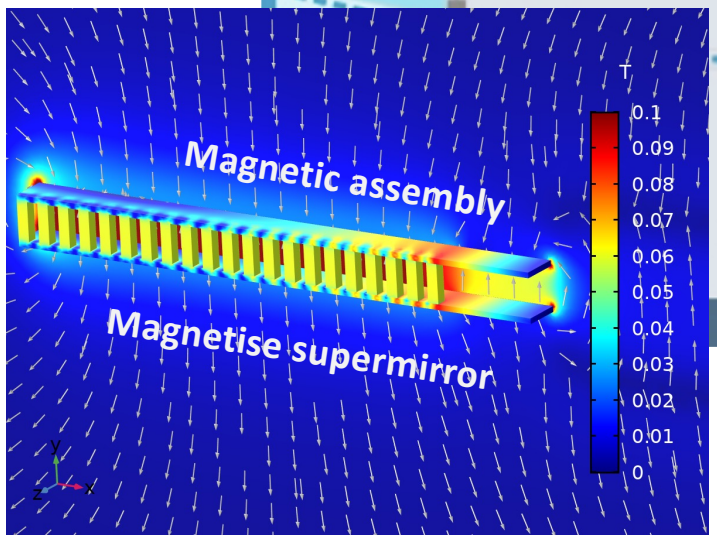
Requirements for data reduction

- DMSCSPEC-34 🔥Conversion of event parameters, density-of-states
- DMSCSPEC-32 🔥Conversion of event parameters, poly-crystal
- DMSCSPEC-31 🔥Conversion of event parameters, single-crystal
- DMSCSPEC-39 🔥Apply detector-specific corrections
- DMSCSPEC-46 Output histogrammed event data to externally defined formats
  - DMSCSPEC-50 🔥Output histogrammed event data to NXspe files
  - DMSCSPEC-52 🔥Output histogrammed event data to MJOLNIR files
  - DMSCSPEC-51 🔥Output histogrammed event data to SQW files
  - DMSCSPEC-49 🔥Output histogrammed event data to text files
- DMSCSPEC-45 Output event data to externally defined formats
  - DMSCSPEC-48 Output event data to whole-experiment archive
  - DMSCSPEC-47 👥Output to MDWorkspace

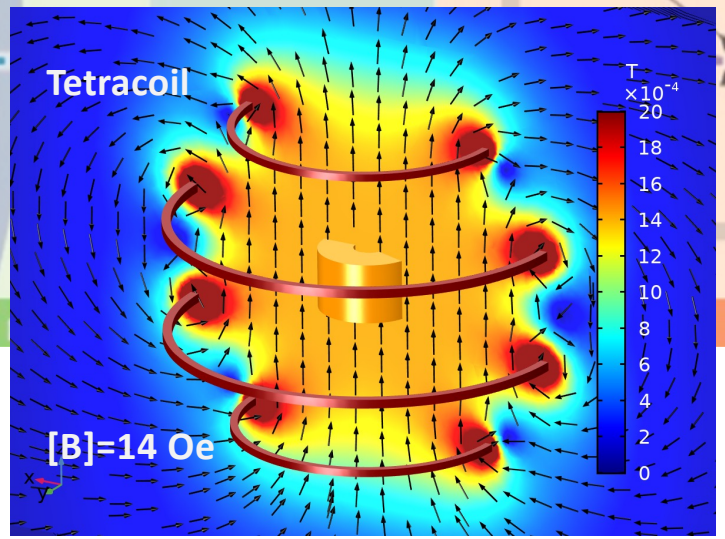
See talk from Greg Tucker in some minutes!

Forecasted upgrade: polarisation analysis

Polariser: Supermirror
Integrated polariser and spin-flipper



Analyser: Polarised ^{3}He
MEOP + "Local-filling" to fill the cell.



Expected timeline: June 2023 – October 2030

See talk from Hal (Wai Tung Lee) tomorrow for all the details!

Hot commissioning

Standard samples

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

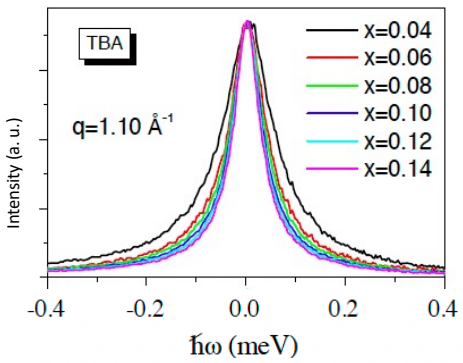
End-to-End Experimental Chain

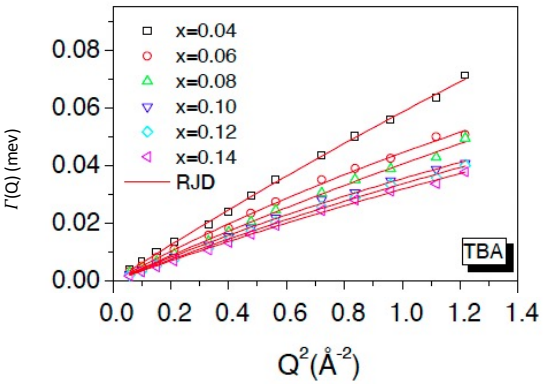
- already measured
- sample availability

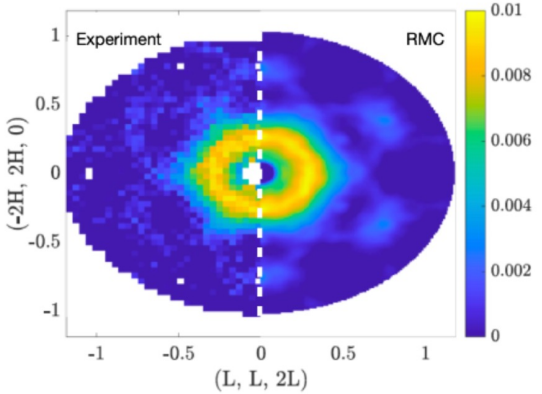
Examples:

- 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]

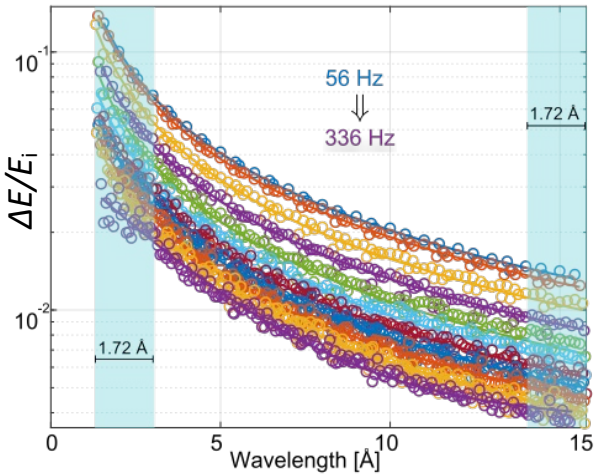






First science

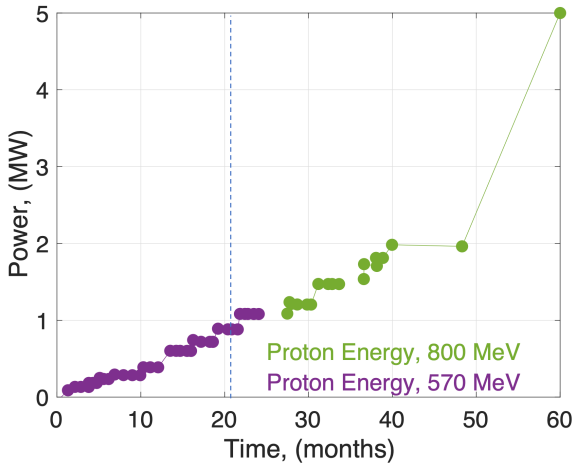
- Energy resolution (1.5% at 4 Å)
- *Q* resolution
- SNR 10^5 (at 5 Å)
- RRM (flux integration - long wavelengths)
- RRM (extended dynamic range – short wavelengths)
- Beam focussing
- Kinetics…



amorphous/powder and
single crystals/oriented samples

QENS and INS,
in different scientific fields

Flux? Days with neutrons?

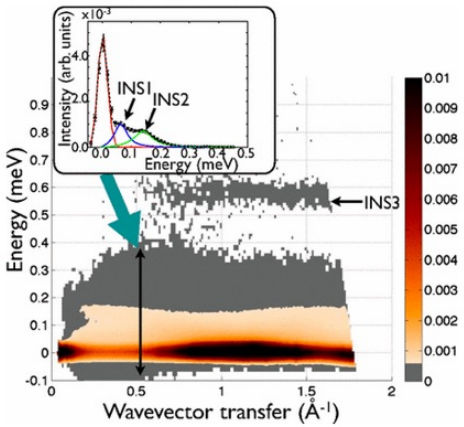


CSPEC

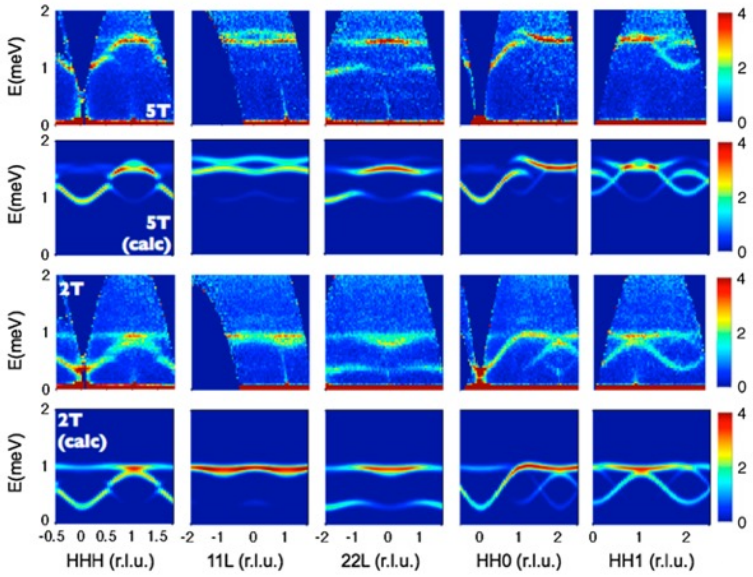
The Cold Chopper spectrometer of the ESS

First science

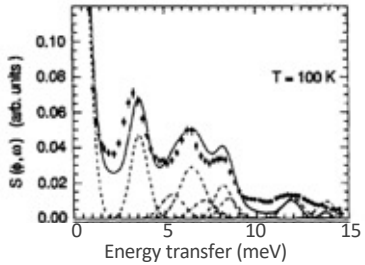
Something like…



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

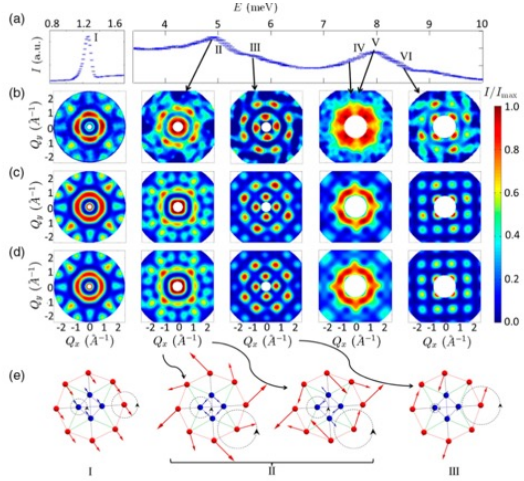


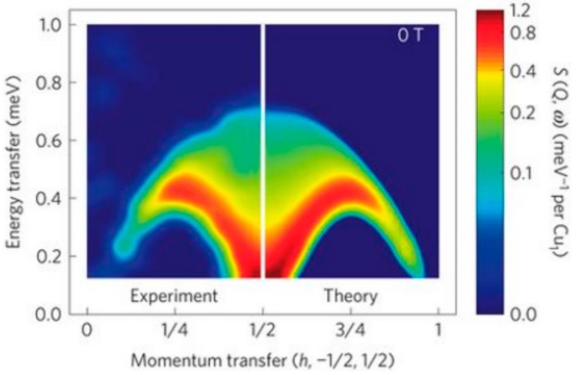
Quantum Excitations in Quantum Spin Ice.
Phys. Rev. X 1 (2011)



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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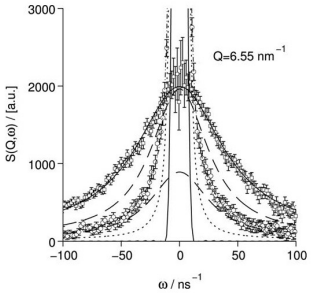
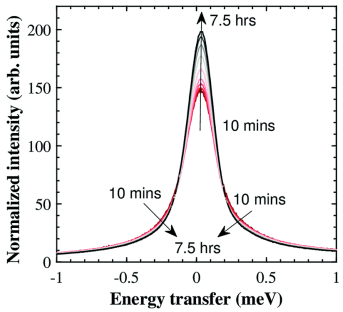
The Cold Chopper spectrometer of the ESS

First science

Something like…

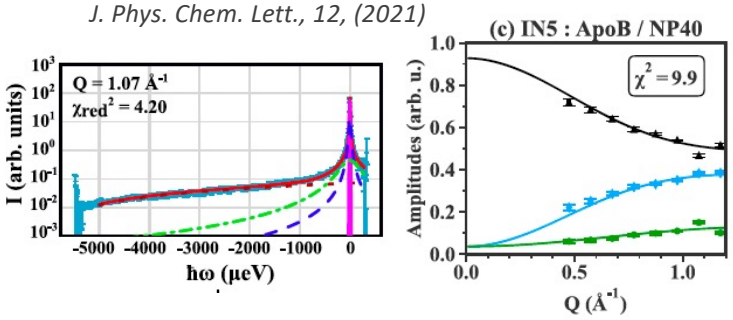


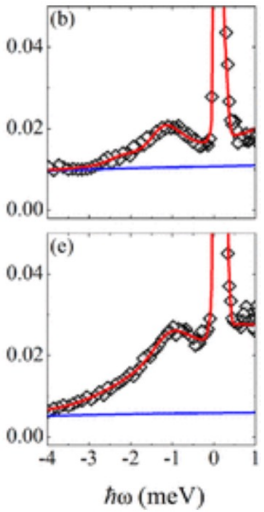
Fast internal dynamics in alcohol dehydrogenase J. Chem. Phys. 143, (2015)



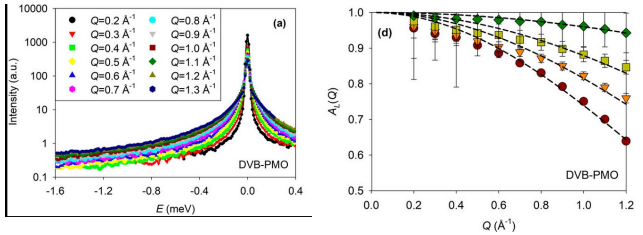
In situ quasi-elastic neutron scattering study on the water dynamics and reaction mechanisms in alkali-activated slags. Phys. Chem. Chem. Phys., 21, (2019)

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

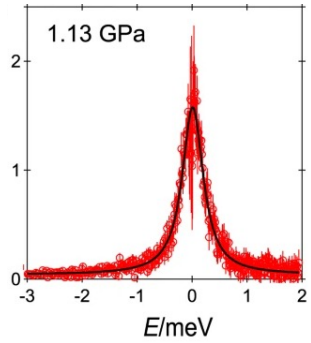




Inelastic Neutron Scattering Investigation in Glassy SiSe2: Complex Dynamics at the Atomic Scale. J. Phys. Chem. Lett., 4 (2013)



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



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