

ESS Bilbao

MIRACLES STAP Spectroscopy

José E.M. Pereira & Félix J Villacorta,
on behalf the MIRACLES Team

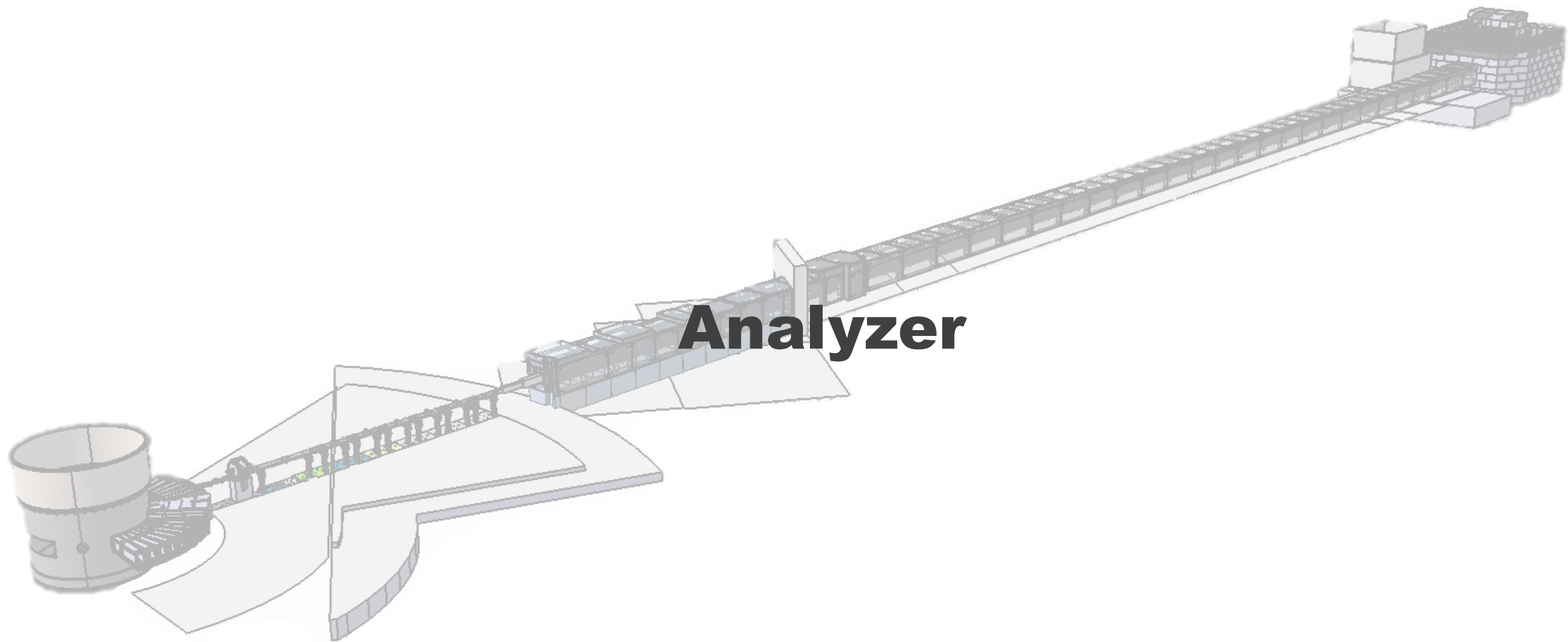
26/04/2022



Outline

STAP (charge to instrument teams):

- *Status project (scope)*
 - *Analyzer*
 - *Detectors*
 - *Scattering Vessel*
 - *Experimental Station*
 - *In-bunker Beamline*
 - *Out-of-bunker Beamline*
 - *Common Projects & Scope Setting*
- *First Science*
- *Upgrade to Completion.*
- *Project management (schedule, risks)*



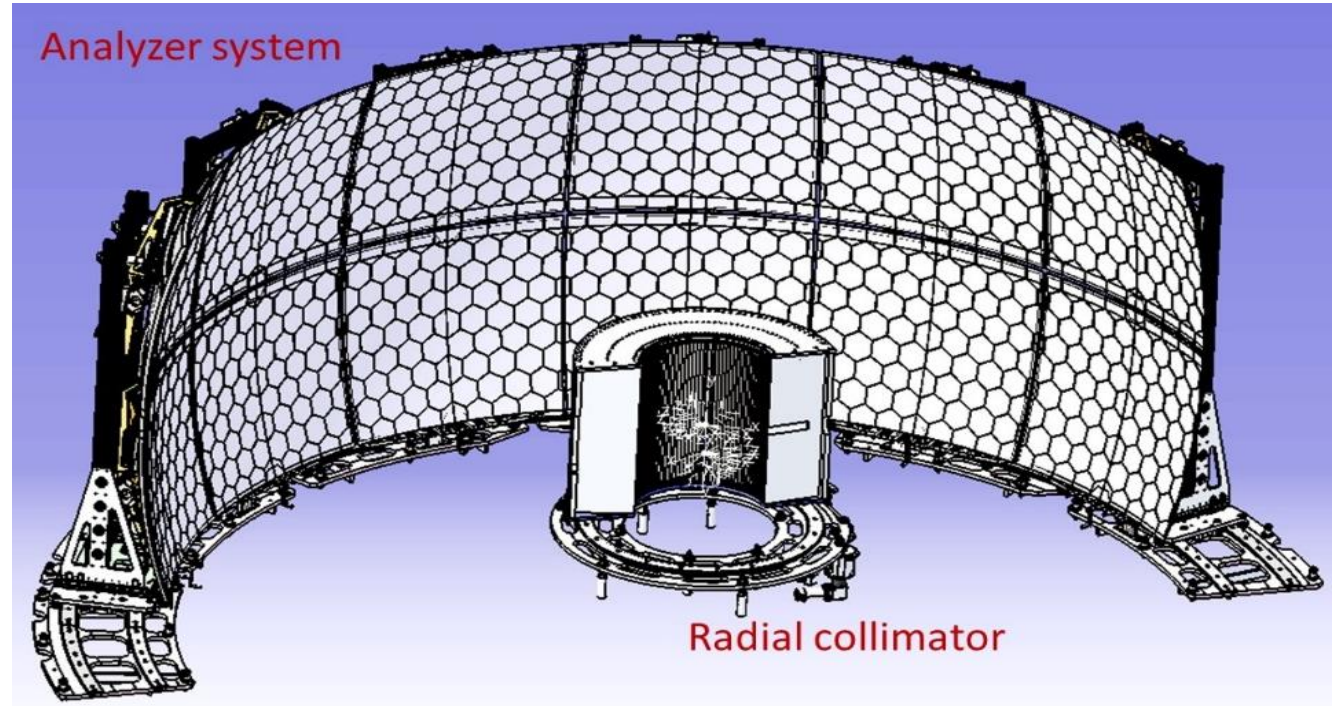
Analyzer



Analyzer system

MIRACLES analyzer consists of:

- 2-spherical monochromator of radius 2.5 m,
- 12 spherical plates (6 plates for the top set and 6 for the bottom set),
- 1032 Si(111) wafers, 6 in. diameter, cut into hexagons, with $\sim 700 \mu\text{m}$ (like DNA, IN16B, EMU, Spheres,...).
- The Si wafers are pressed and directly glued onto the curved backing plate.



The Si crystals forming the analyzer will be coated in the rear part with Gd_2O_3 paint, thus, suppressing possible background neutrons scattered by the glue or the analyzer panels/supports/structure.

Analyzer system

The mechanical assembly of the analyzer is in the manufacturing stage (an early manufacturing process of the panels was carried out).



(Left) mold (Right) one of the panels of the analyzer.

Prototype analyzer

- ❑ PDR MIRACLES Scattering System: a systematic study is desirable[...] *“If the team plans to test the neutron reflectivity for different wafer thickness this probably needs to be done under realistic conditions and might require a backscattering spectrometer.”*
- ❑ STAP 2021: *“More information would be desirable concerning the analyzer crystal assembly (a prototyping had been suggested a year ago)”*

- Systematic study is under way

- ❖ Prototypes

- ❖ Measurements scheduled by 2023

- Thickness: 575 - 1250 μm
- Surface: etched vs. as-cut
- Method: CZ vs. FZ

- A collaboration:



From BATS to MIRACLES: Paving the way for European high-resolution neutron spectroscopy

Prof. Dr. Frank Schreiber
Eberhard Karls Universität Tübingen

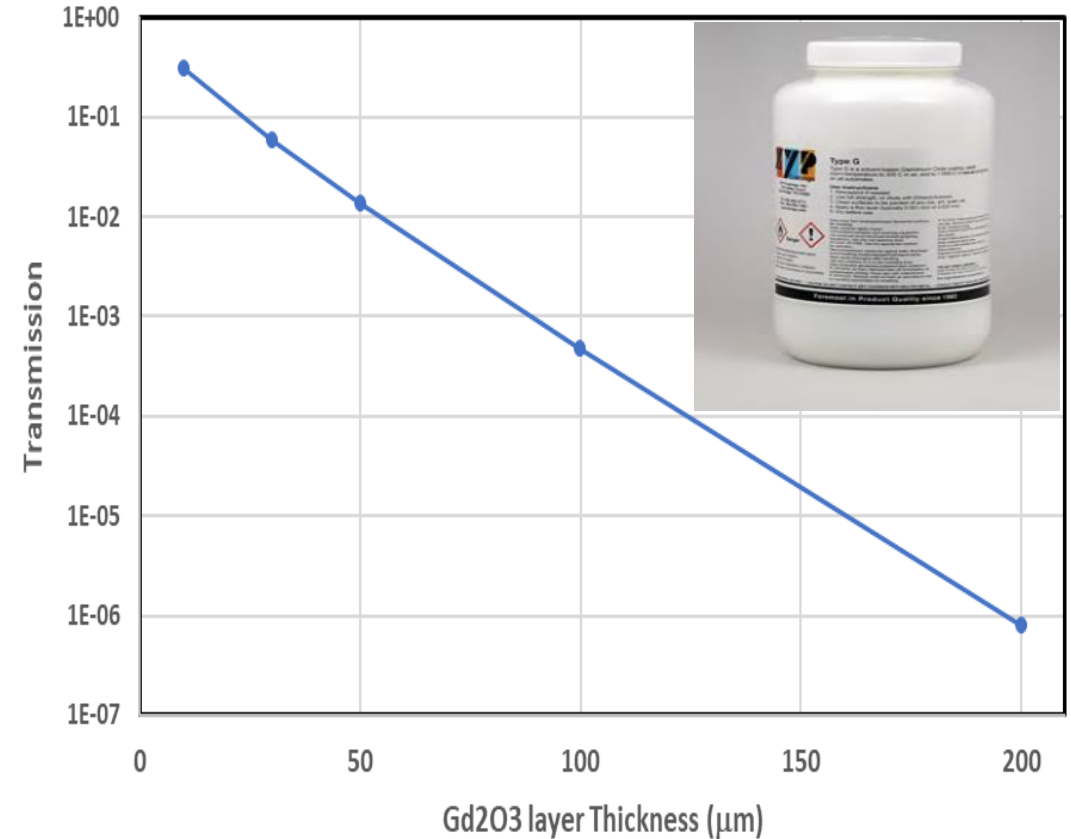
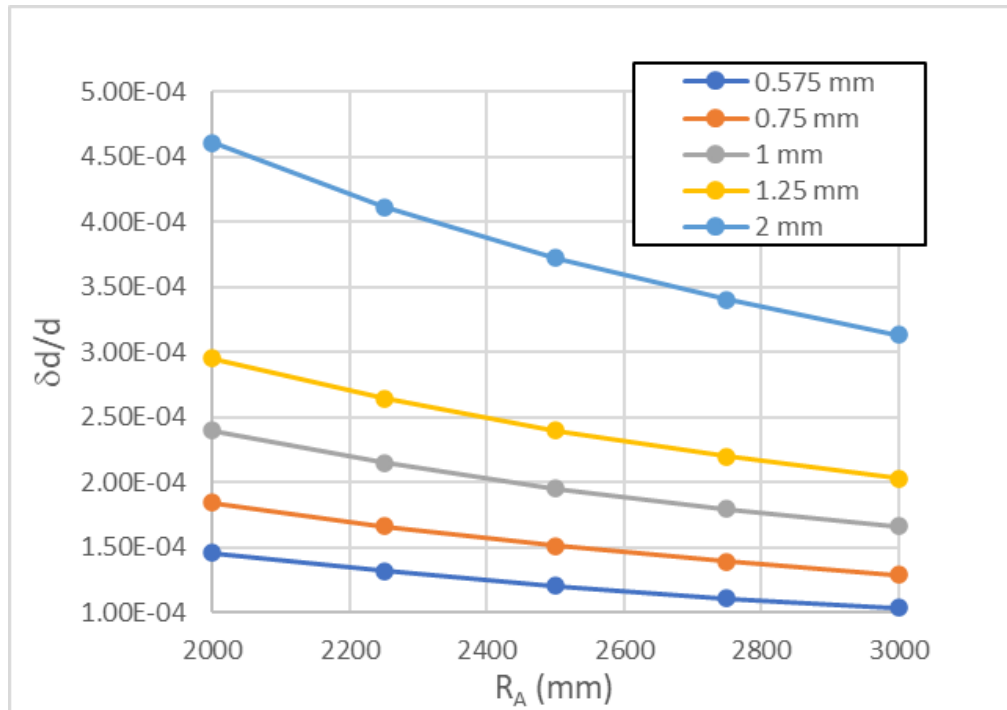
High-resolution neutron backscattering spectroscopy benefits from substantial technical progress in recent years enabling new types of experiments. These include for instance measurements accessing hierarchically superimposed diffusive motions on the nanosecond time and nanometer length scale in a wide range of complex materials and fluids. Accordingly, the demand for beam time is very high. This project aims to add new capabilities and strengthen the European landscape of neutron backscattering spectroscopy by (1) ensuring reliable chopper operation of the BATS option on IN16B at the ILL given the high radiation loads and (2) by extending backscattering analyzer techniques at low scattering angles. These new capabilities will be established with demonstration experiments on IN16B at the ILL and will enable backscattering spectroscopy in the most reliable user operation and in the widest possible range in energy and momentum transfer. Work package (2) will moreover enhance the synergy with the MIRACLES team at the ESS.

After purchasing the support structure and the silicon wafer material, the collaboration between IN16B and MIRACLES will continue with the process of crystal preparation, coating their back side with a neutron absorbing layer and gluing to the panels. Careful choice of the crystal parameters, coatings and assembly of the structure are vital parameters in achieving the desired energy resolution with optimum flux and minimal background. Realisation of this task will coincide with the preparation of prototype analyser panels for MIRACLES by ESS Bilbao. By participating in the subsequent commissioning phase, the MIRACLES team will get the opportunity to test their prototypes under real operating conditions in the IN16B spectrometer. This will help to prove the suitability of the chosen MIRACLES analyser design and contribute to the optimum performance of the future spectrometer at ESS.

Prototype analyzer

The performance of the spectrometer, in terms of energy resolution and flux, depends critically on the features and the assembly procedure of the Si(111) wafers.

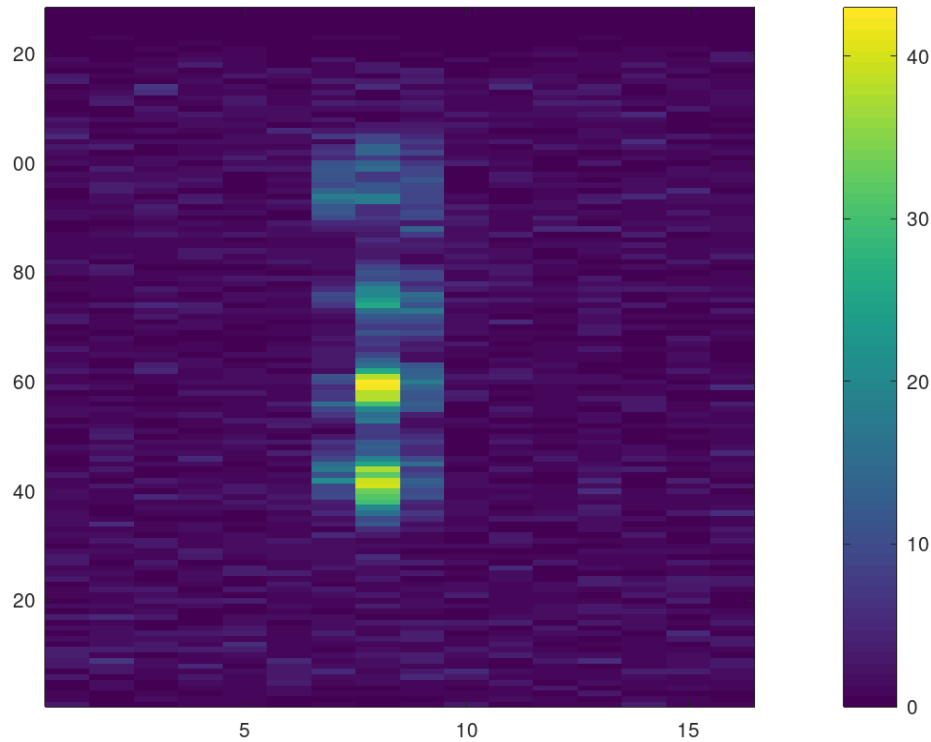
A systematic analysis, that includes prototyping and testing, prior to manufacturing is essential to validate the manufacturing and assembly process of the analyzer.



Neutron transmission of a Gd₂O₃ paint layer (with 50% Gd₂O₃ content) as a function of the layer optics (to confirm that 80 μm thickness is enough to achieve a transmission of 10^{-5}).

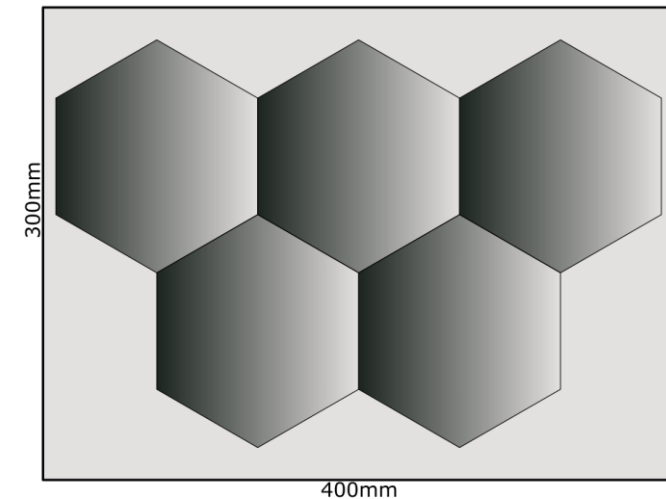
Prototype analyzer

For the experiment, 10 panels distributed in 2 prototypes will be mounted with different Si crystals samples each, distributed into distinguished areas, onto spherical surface with a radius of 2000 mm.



A vertical distance of about 45 cm between the plates, and we got the detector image nicely separate.

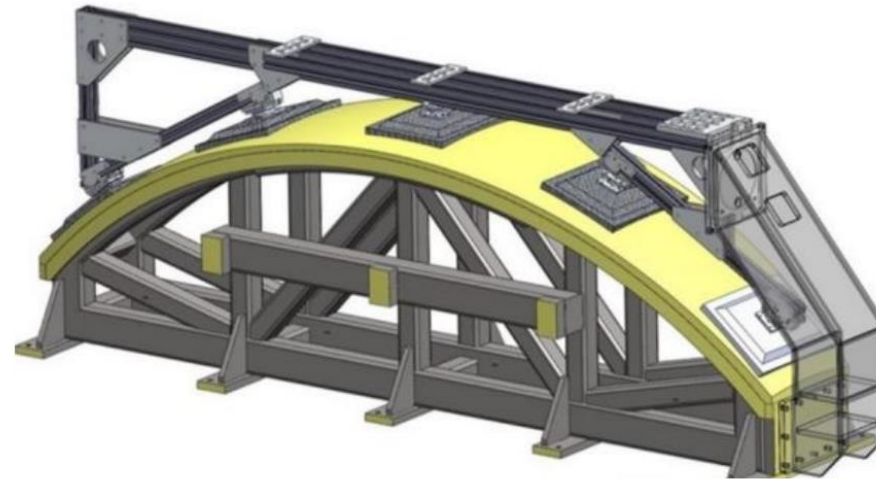
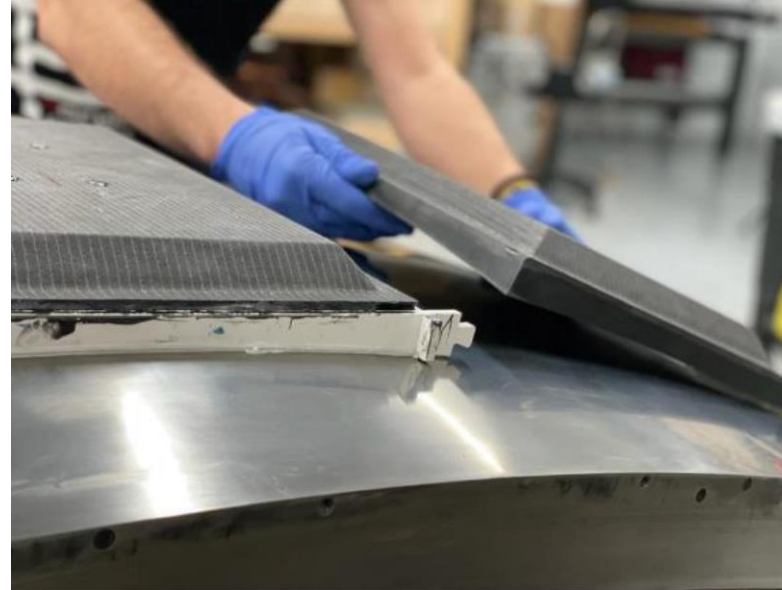
PANELS	
Growth method	Czochralski (CZ) or Float Zone (FZ) (FZ only for the 700 μm)
Orientation	$\langle 111 \rangle \pm 0.1^\circ$ ($\pm 0.05^\circ$ best effort)
Thickness	575, 700, 1000 and 1250 μm
Diameter	6 inches (≈ 150 mm) Hexagonal shape
Surface treatment	SSP / etched or as cut



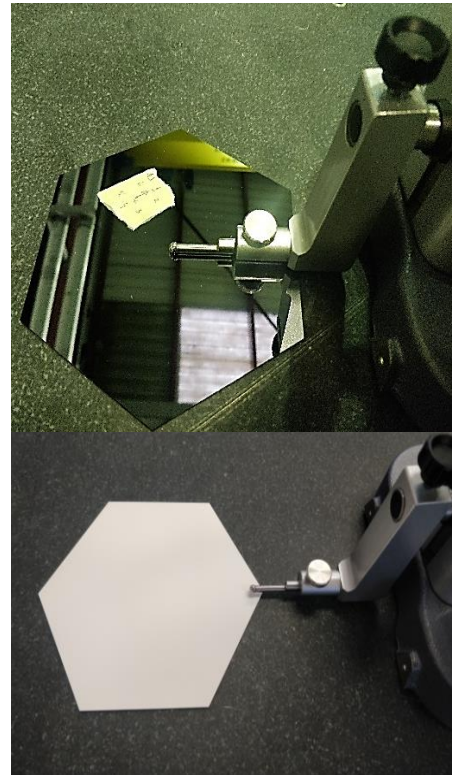
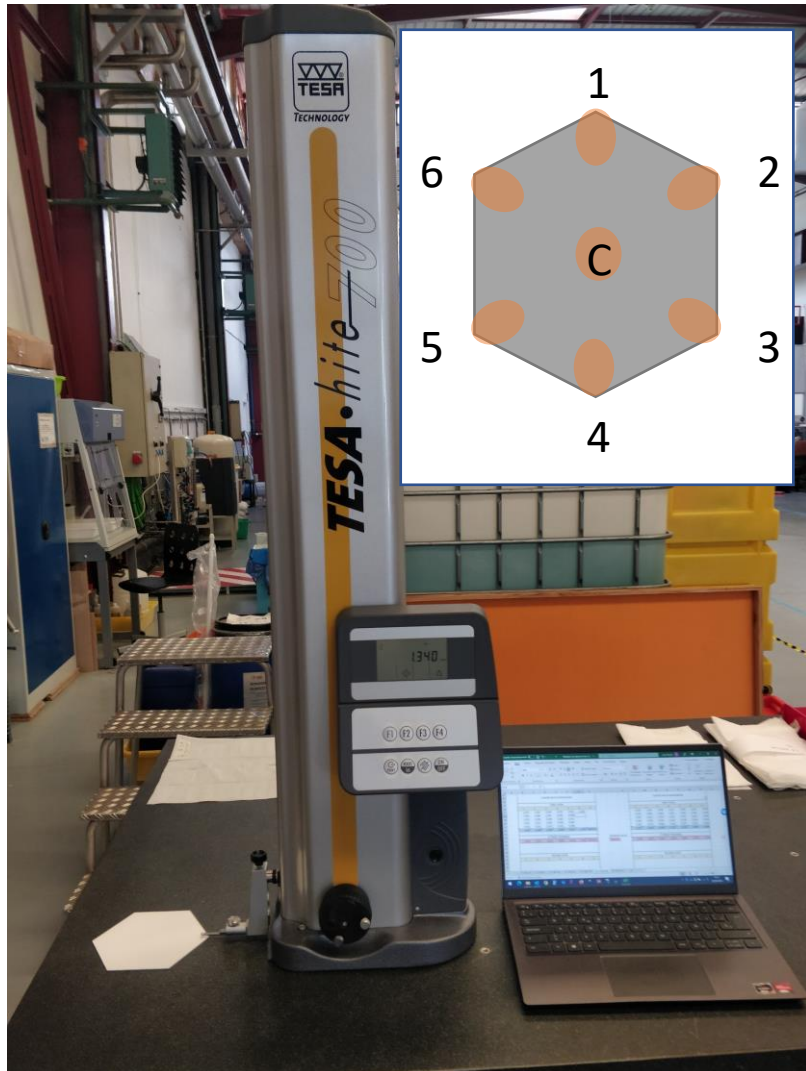
Prototype analyzer

Two prototypes are being manufactured to validate the Gd paint coating procedure and the gluing procedure as well as to evaluate the effect of different fabrication conditions of the Si crystals.

The absorbent coating paint that will be used is from ZYP: Type G. Type G is a Gadolinium Oxide coating which uses very high purity (99.99%) Gd_2O_3



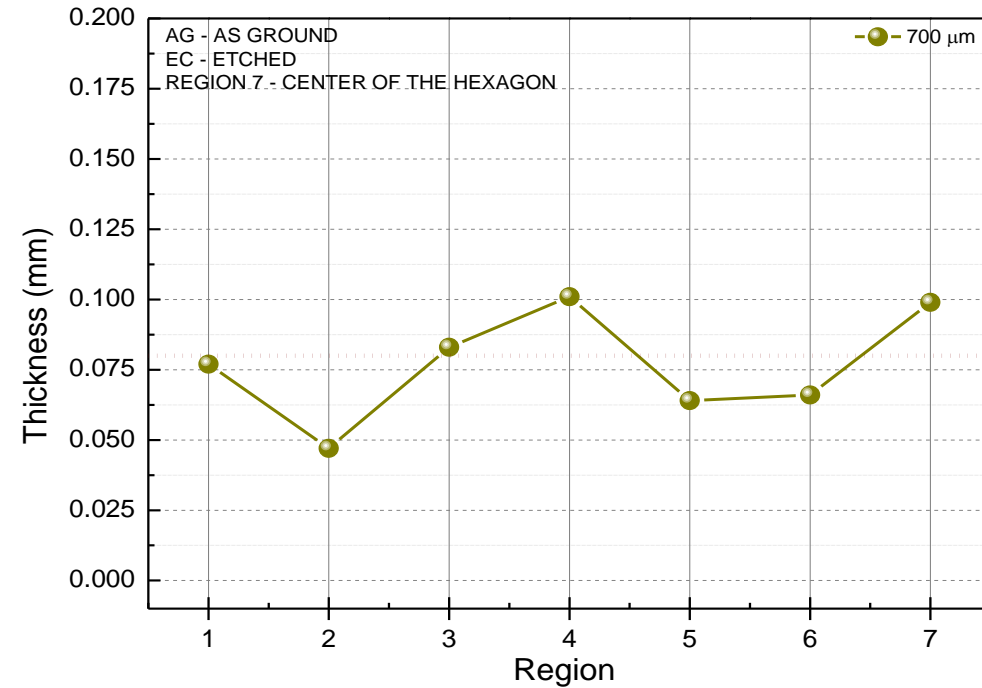
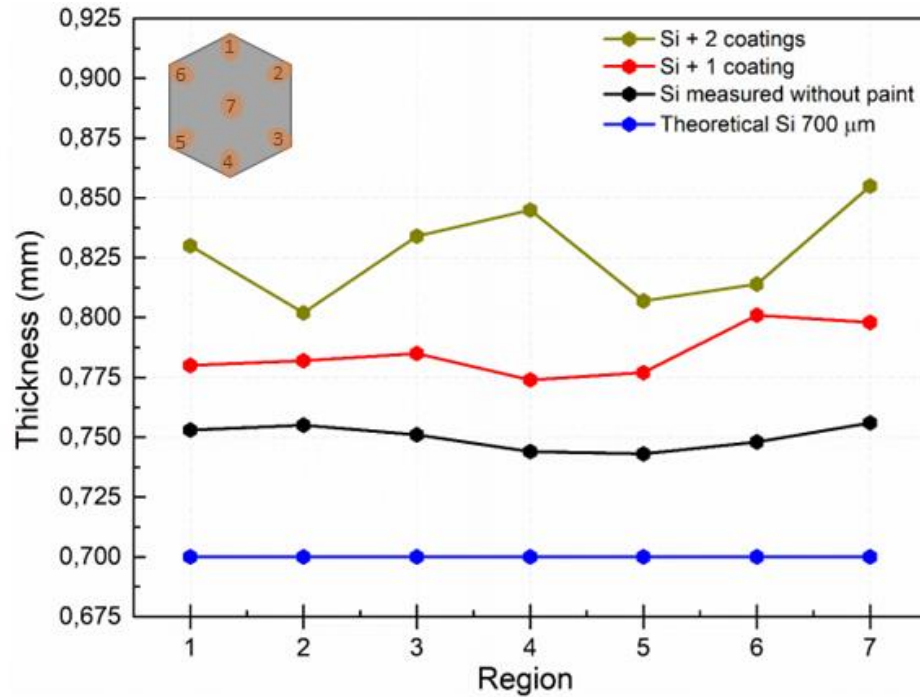
Prototype analyzer



- The thickness of the Si wafer is measured using a height gauge TESA-Hite Magna 700 at several points in each hexagon, mostly at the edges and corners.
- Thickness checked before and after painting.
- Deposition of the Gd_2O_3 paint in the Si wafer with the spray gun.

Prototype analyzer

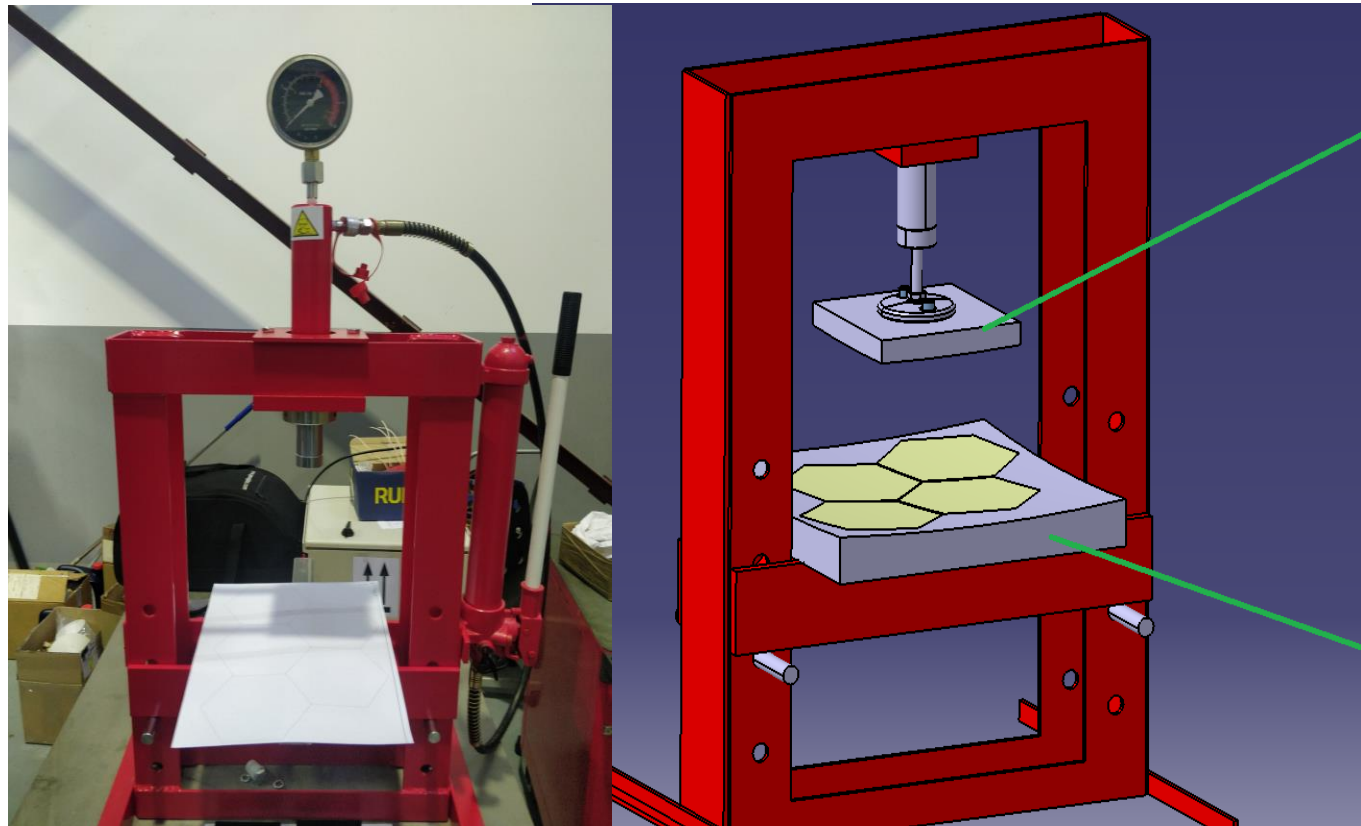
For every coat (every pass) an average coating of $\sim 40 \mu\text{m}$ is achieved. Hence, two passes are needed to achieve the $\sim 80 \mu\text{m}$ required.



Prototype analyzer

Gluing test

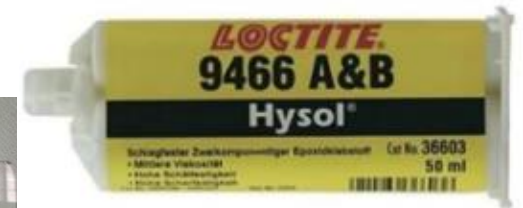
A curved surface (2000mm radius) with similar configuration of the IN16B panel will be used for to test the gluing process.



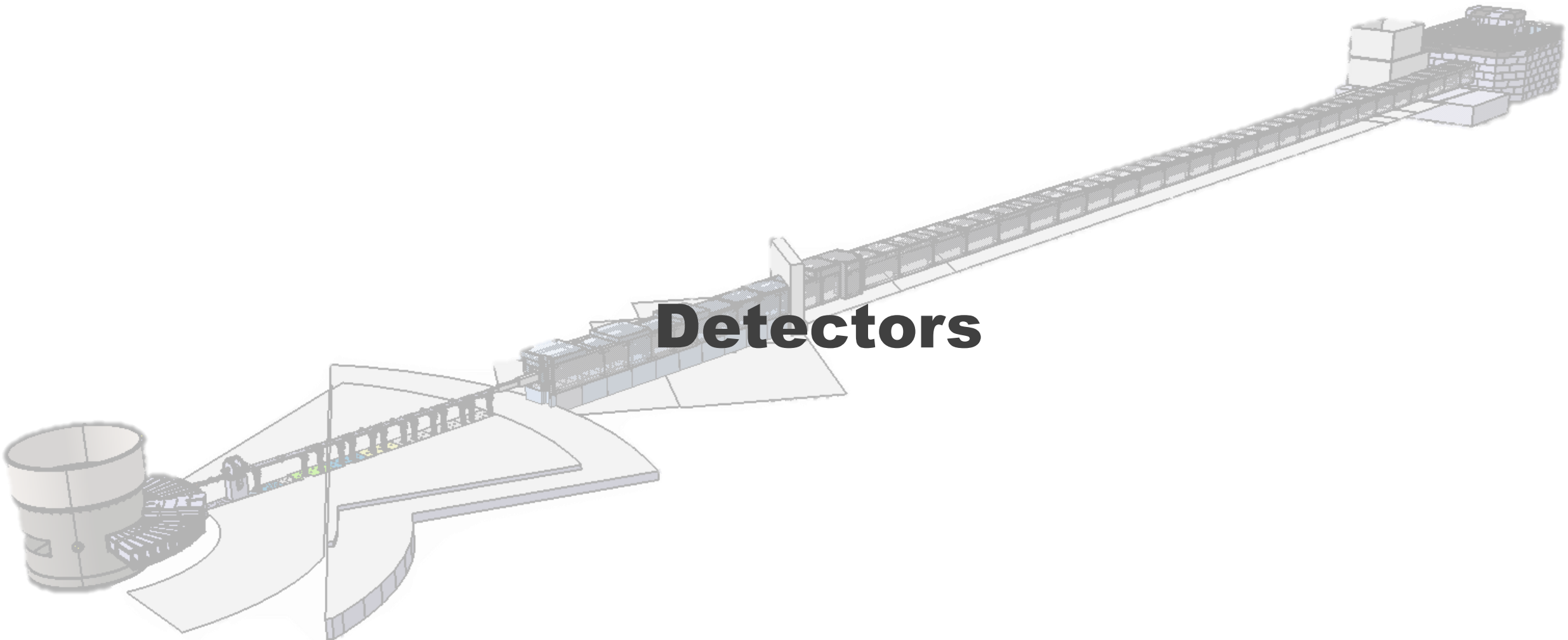
pisador convexo



pieza composite concava



Example of a possible distribution of the glue in the Si surface.

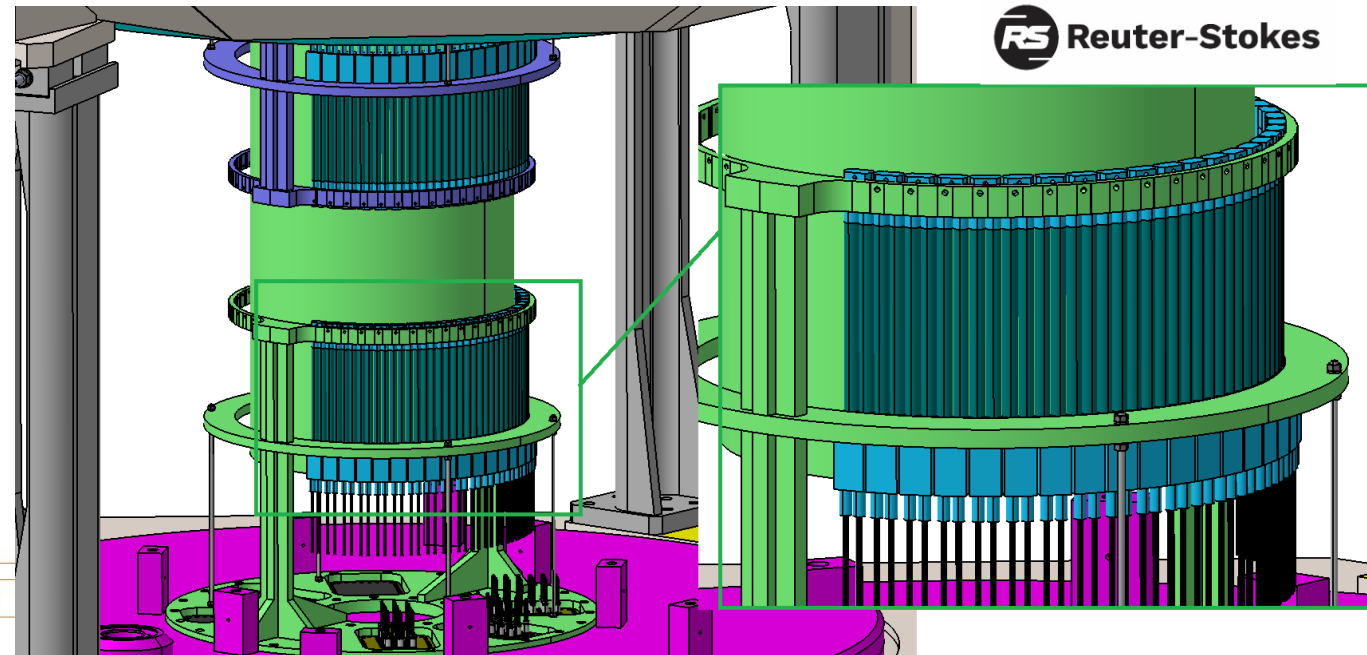


Detectors

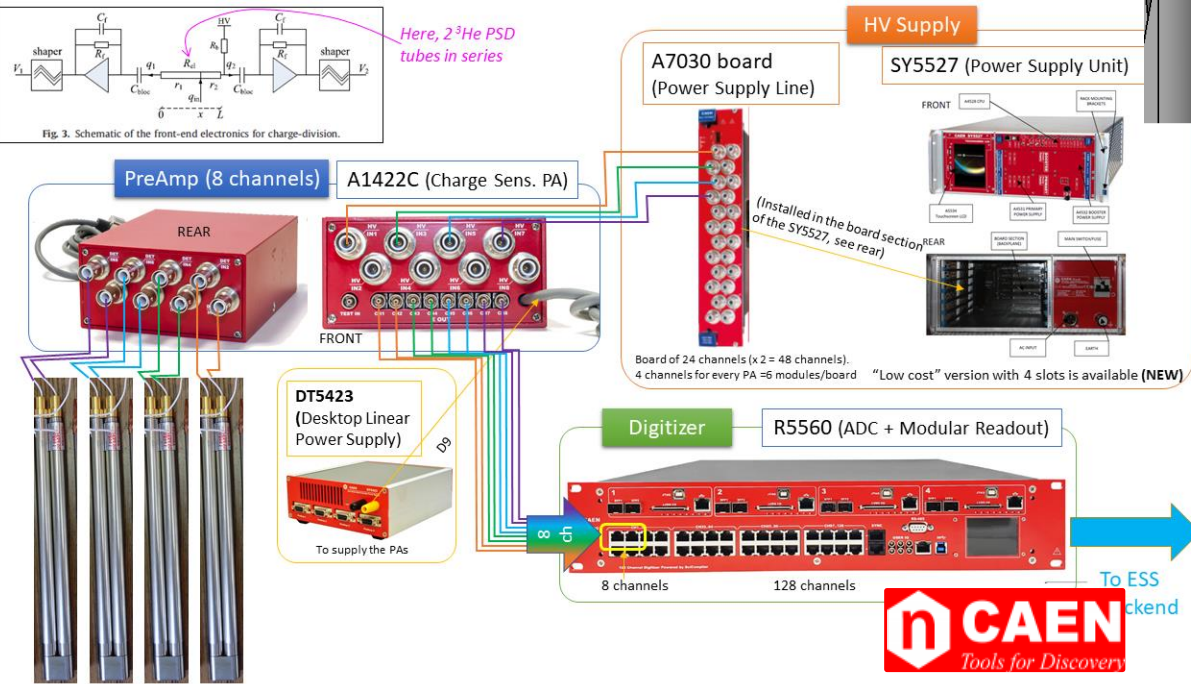


Detectors

- ❖ Horizontal coverage: $[9.48-165]^\circ$
- ❖ $R=230$ mm;
- ❖ 96 detector tubes
 - ❖ Active length $\Delta l=150$ mm
 - ❖ Diameter $\varnothing=12.7$ mm
 - ❖ $P_{3\text{He}}=8$ atm
- ❖ Minimizing gap between tubes: $\sim 0,5$ mm



RS Reuter-Stokes

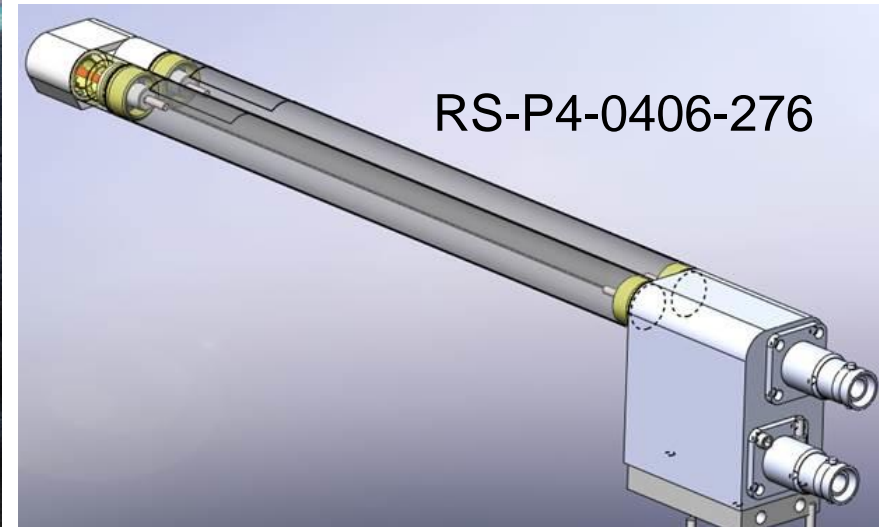
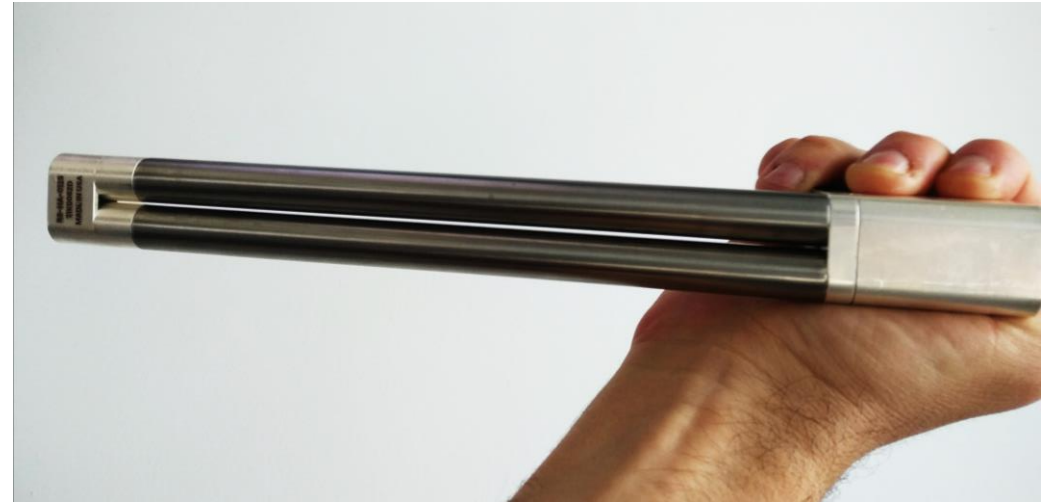


- ❖ PSD
- ❖ Digitizer CAEN R5560 (128 ch)
- ❖ Multichannel preamp
- ❖ CAEN HV supply



Detectors & Front end: experimental

- ^3He tube pairs U-shaped prototype
- Preamps CAEN
- Tests at UPM (Am-Be source 2 Ci)
 - Validating U-shaped detectors
 - Choosing the right preamp
 - Checking frontend

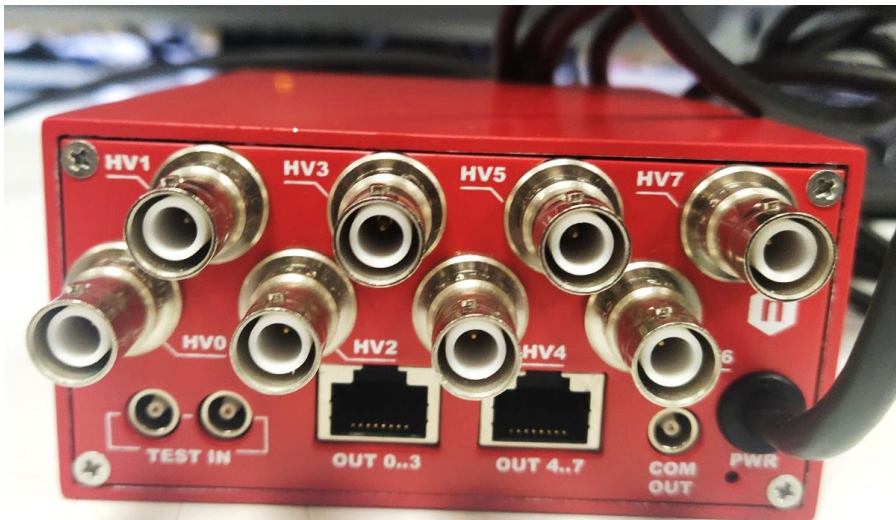


Multichannel Preamplifiers



A1422C

- 8-channel PA
- Customized signal output (RJ45)
- Compact design (ideal for MIRACLES)
- Total gain: ~ 2 V/pC
- Already available since 2010's



R1443

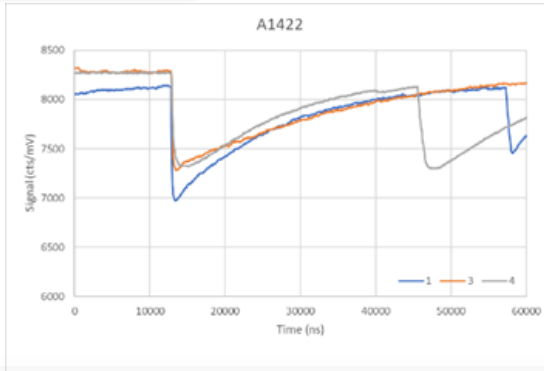
- 32-channel PA (1 same HV supply)
- Signal output RJ45
- 19" rack unit (2U height)
- Total gain: 2.25 V/pC
- In the market since September 2022



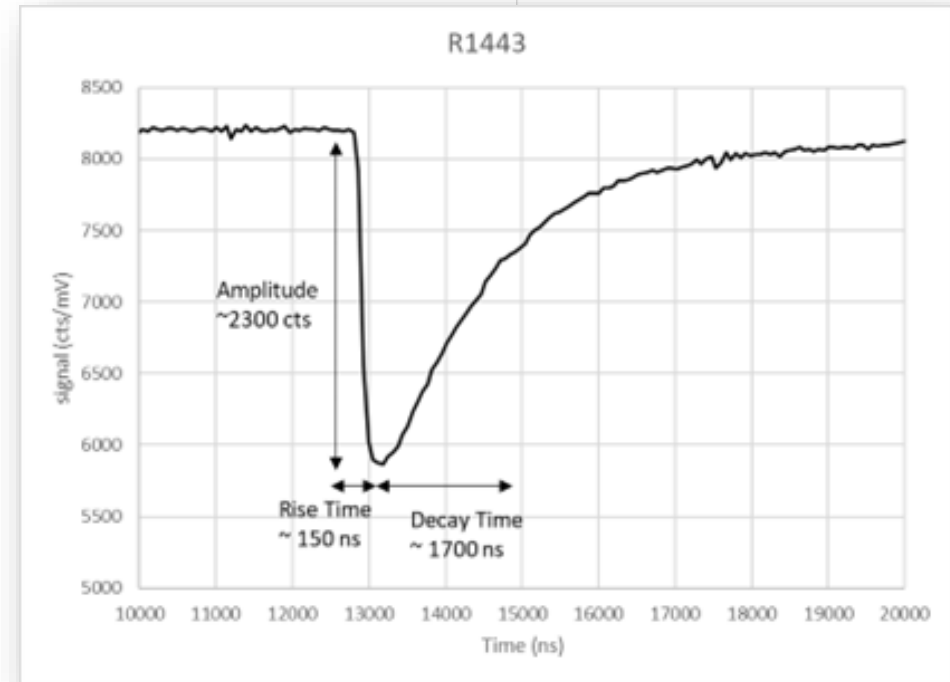
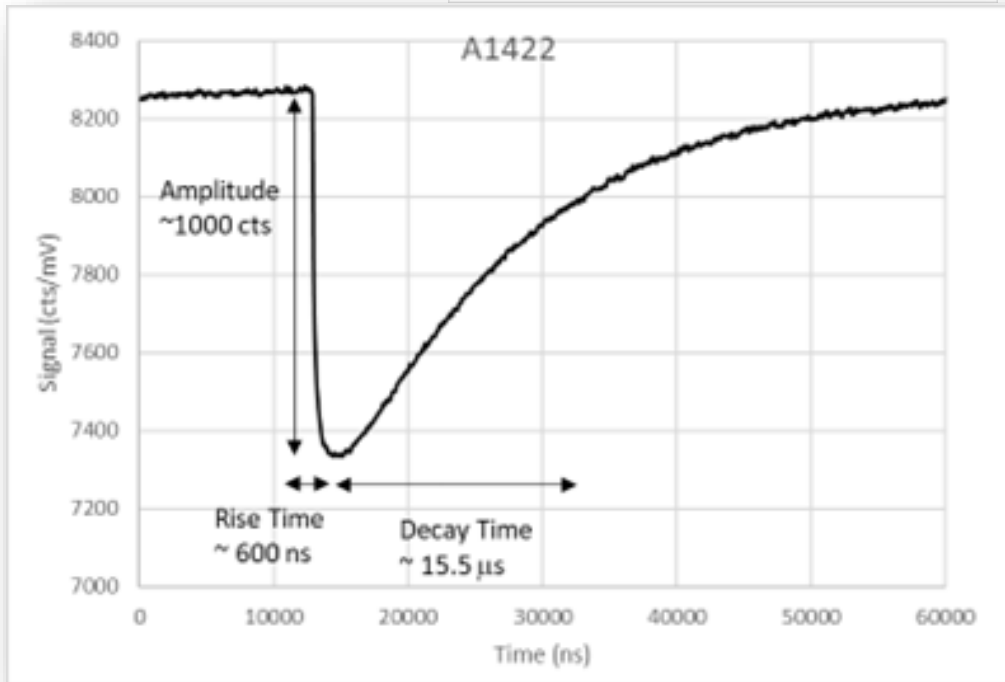
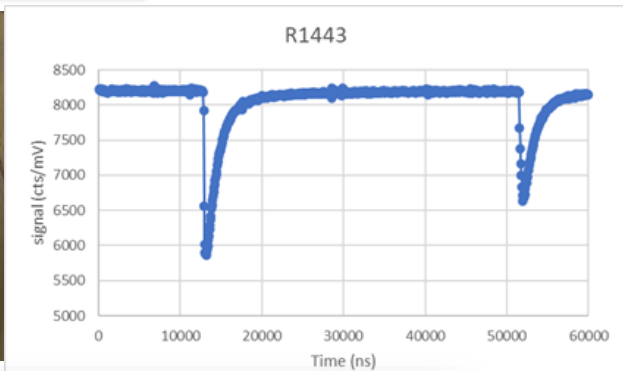
Multichannel Preamplifiers



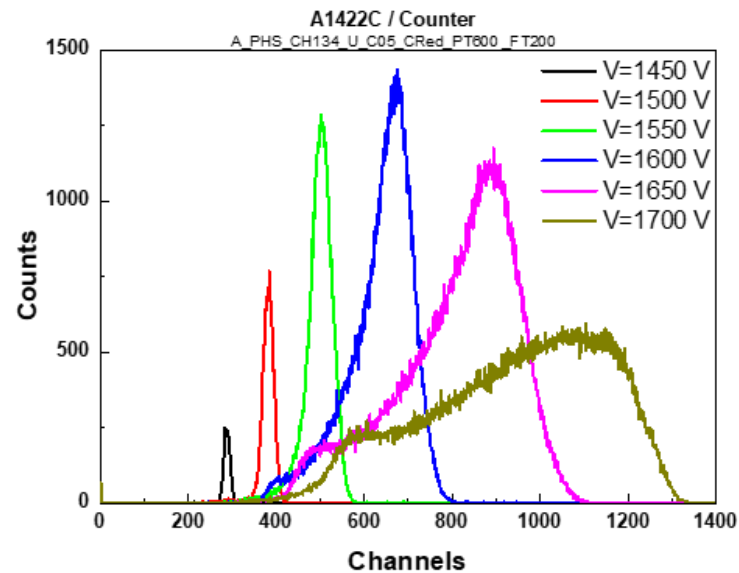
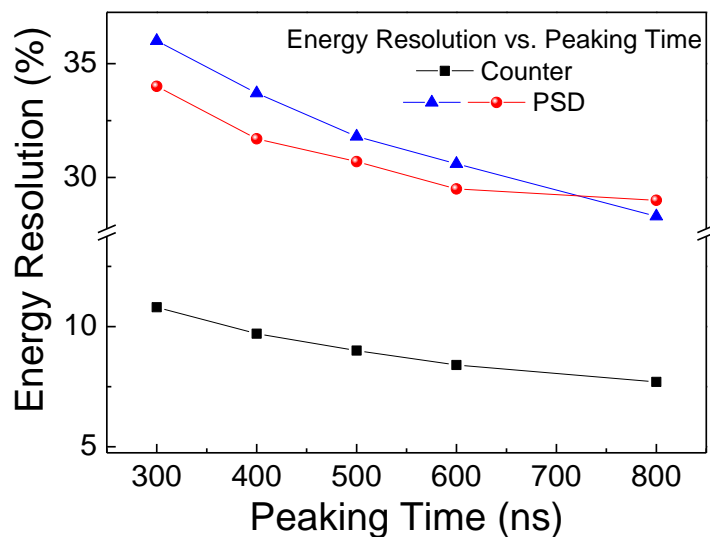
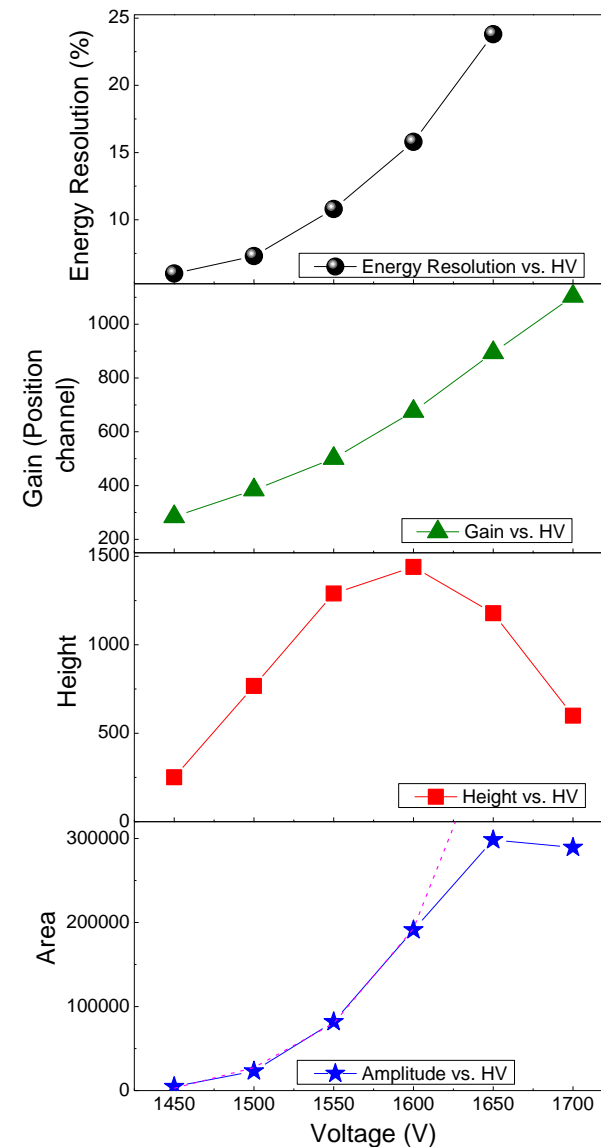
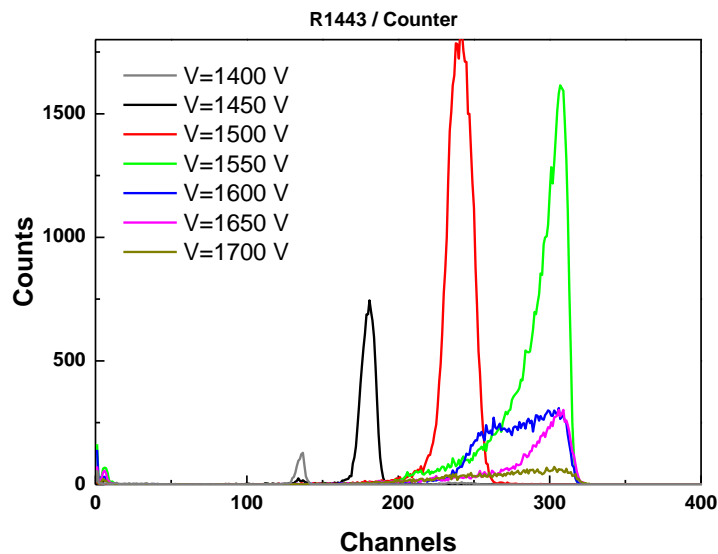
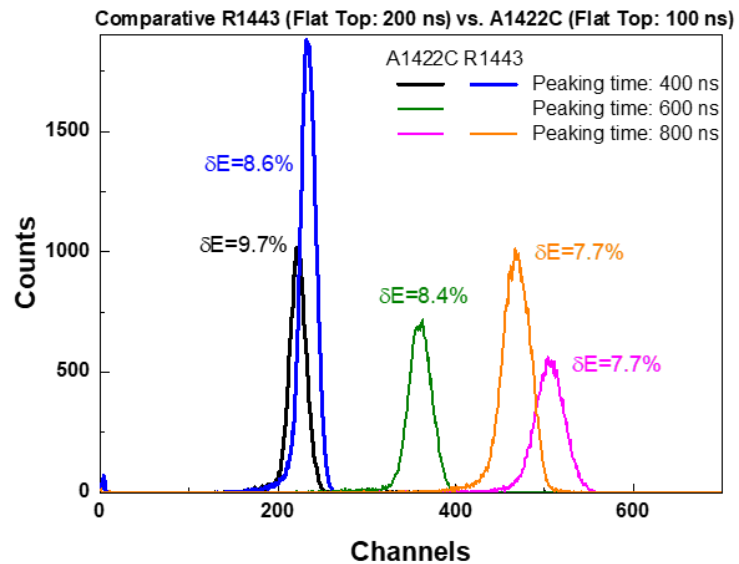
A1422C



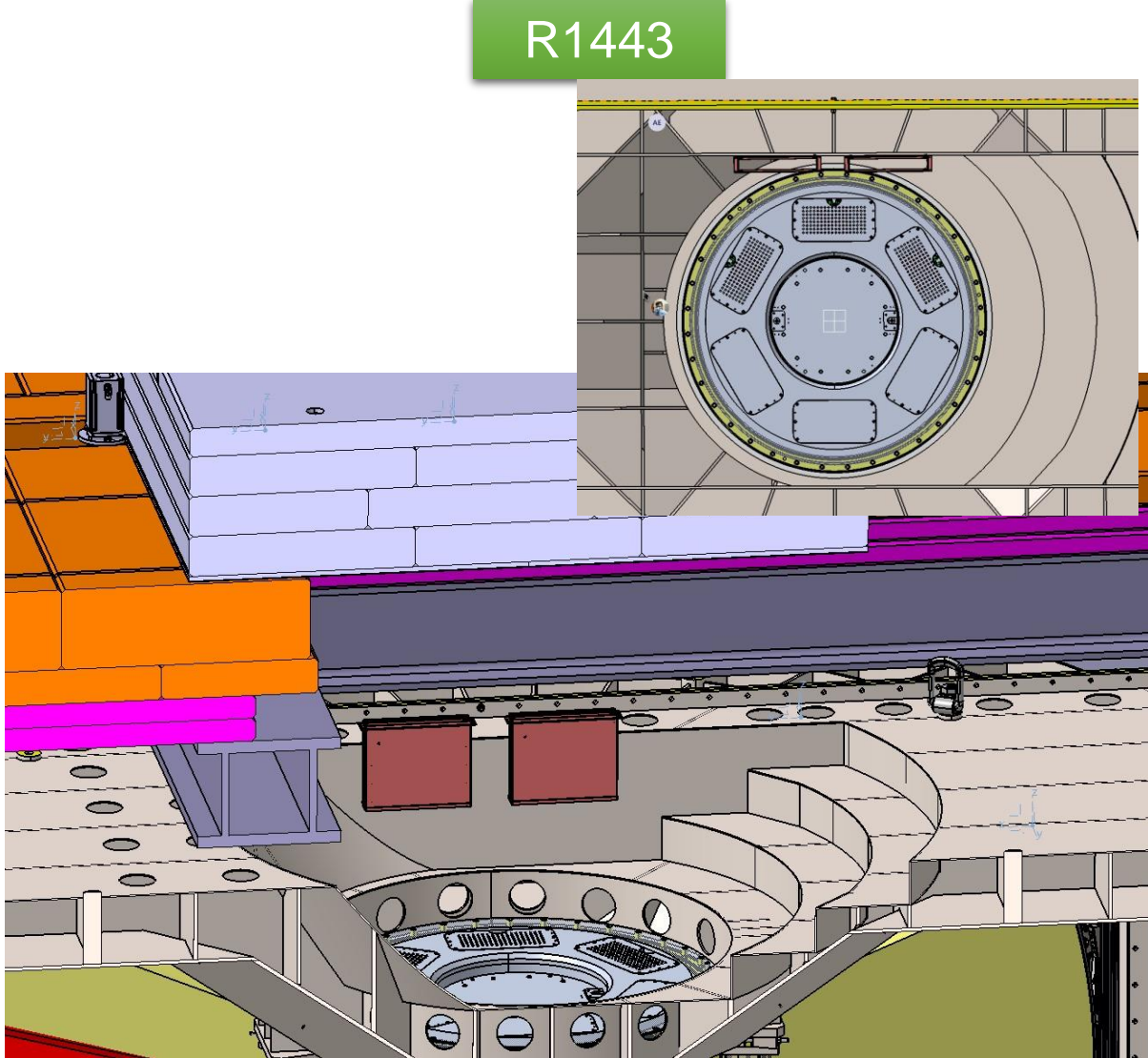
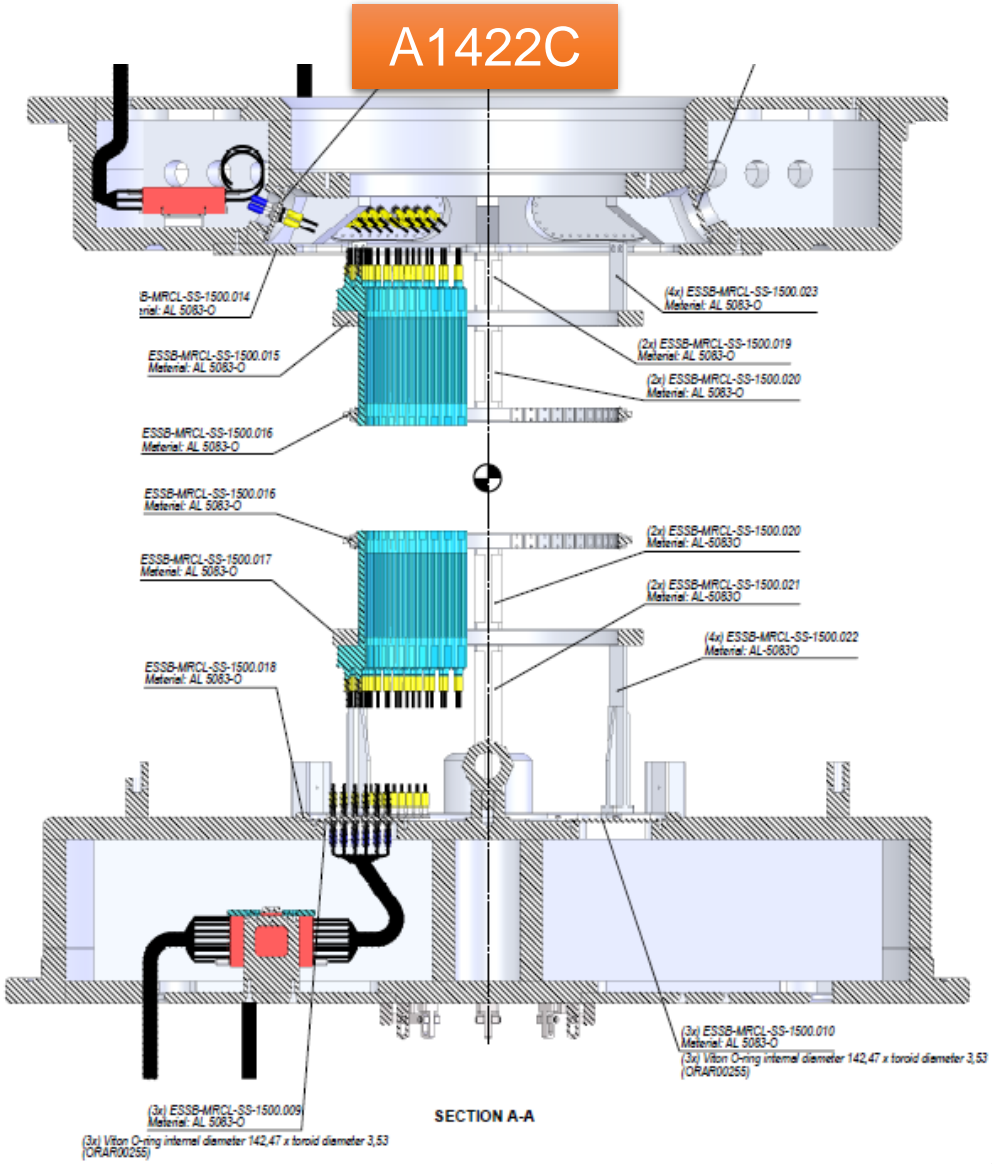
R1443



Preamplifiers: results



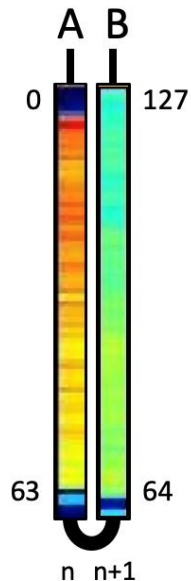
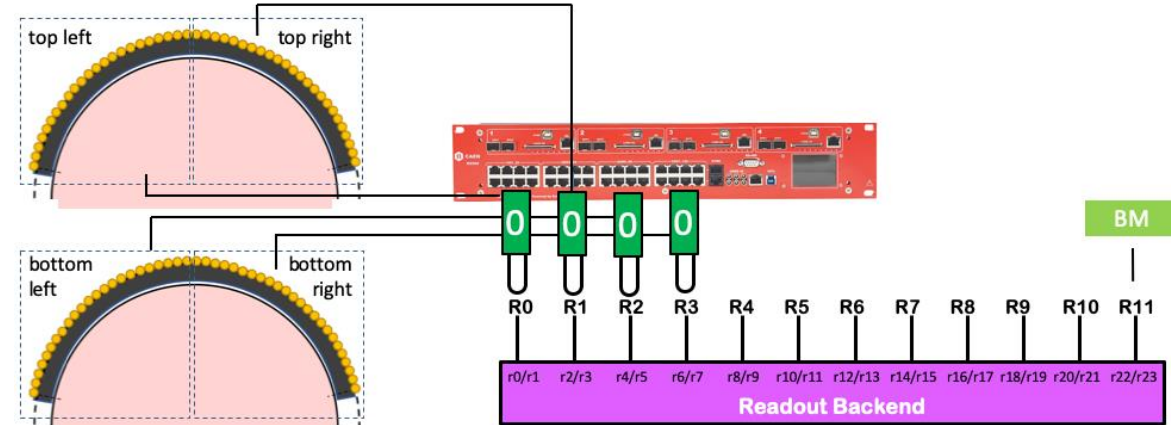
Preamplifiers integrated in MIRACLES



Integration DMSC-MIRACLES

- w/ Morten Jagd Christensen (ESS)
- DAQ chain, from detectors to data management:
- Starting with ring allocation & digital mapping
- Geometrical resolution 64 discrete units

$$pos(A, B) = \frac{A}{A + B}$$



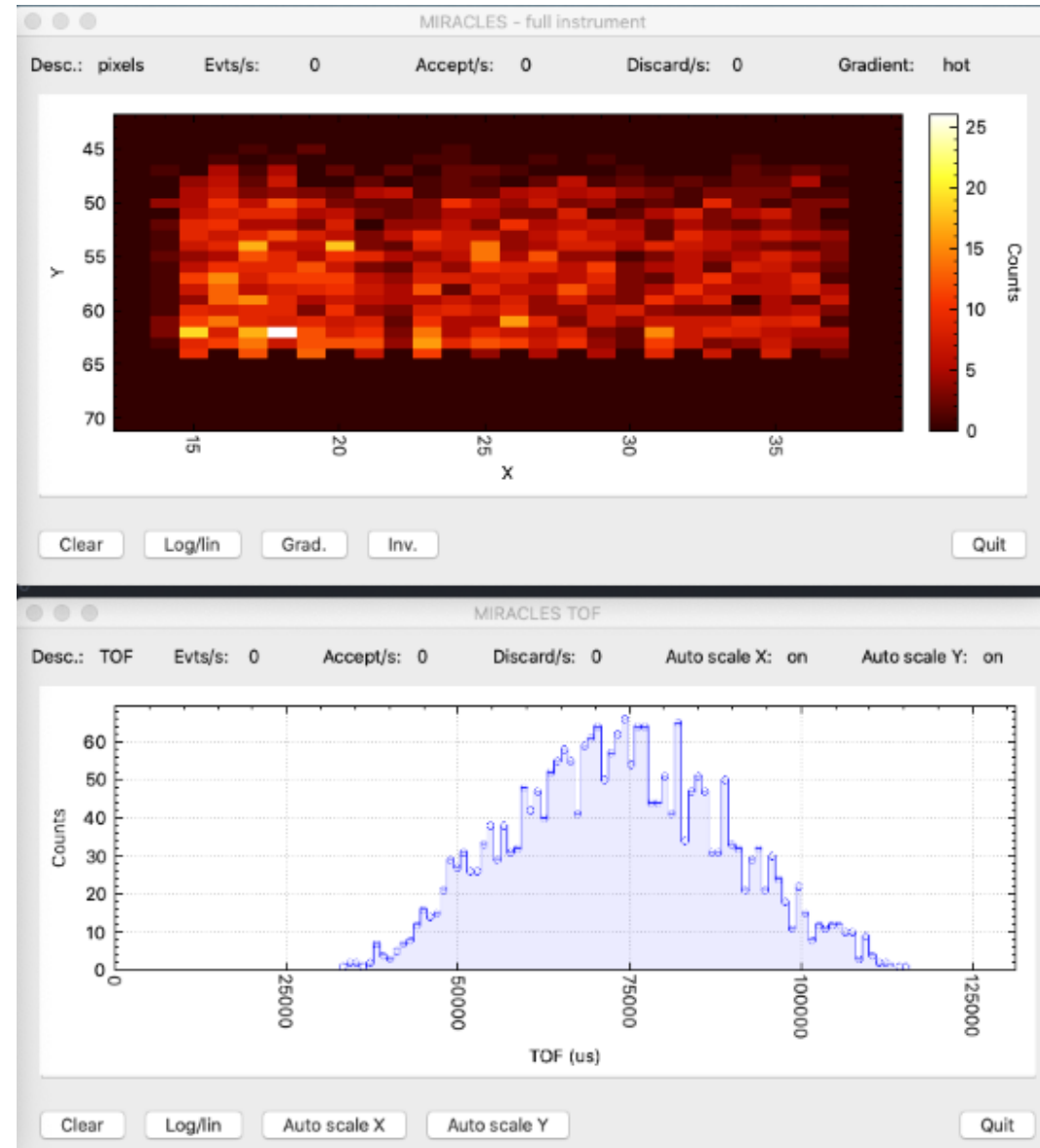
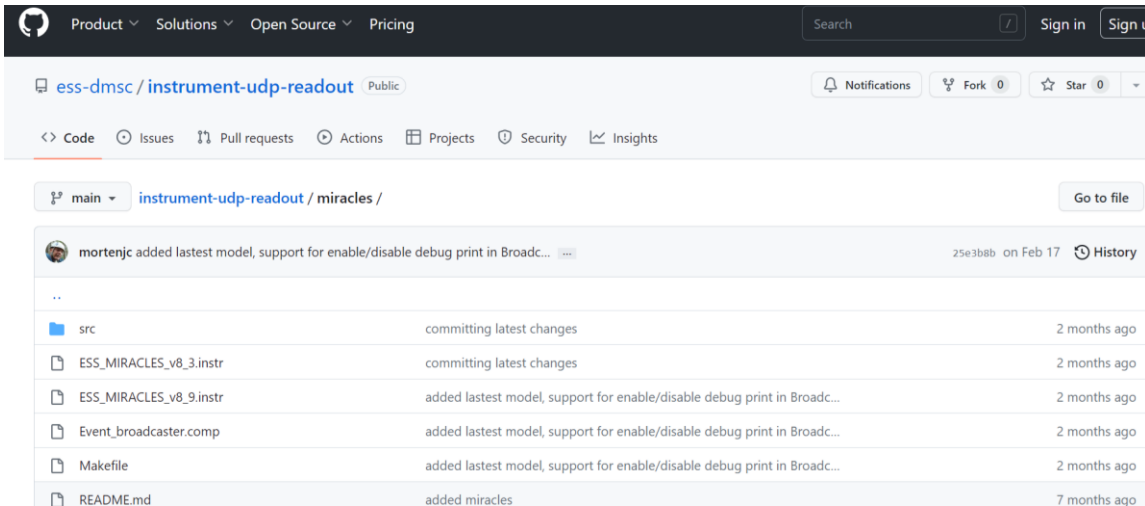
tp 0	tp 23
1 (0, 0)	(47, 0) 48
tube 1	tube 47
upper bank	
3025 (0, 63)	(47, 63) 3072
3073 (0, 64)	(47, 64) 3120
tube 49	tube 95
lower bank	
6097 (0, 127)	(47, 127) 6144



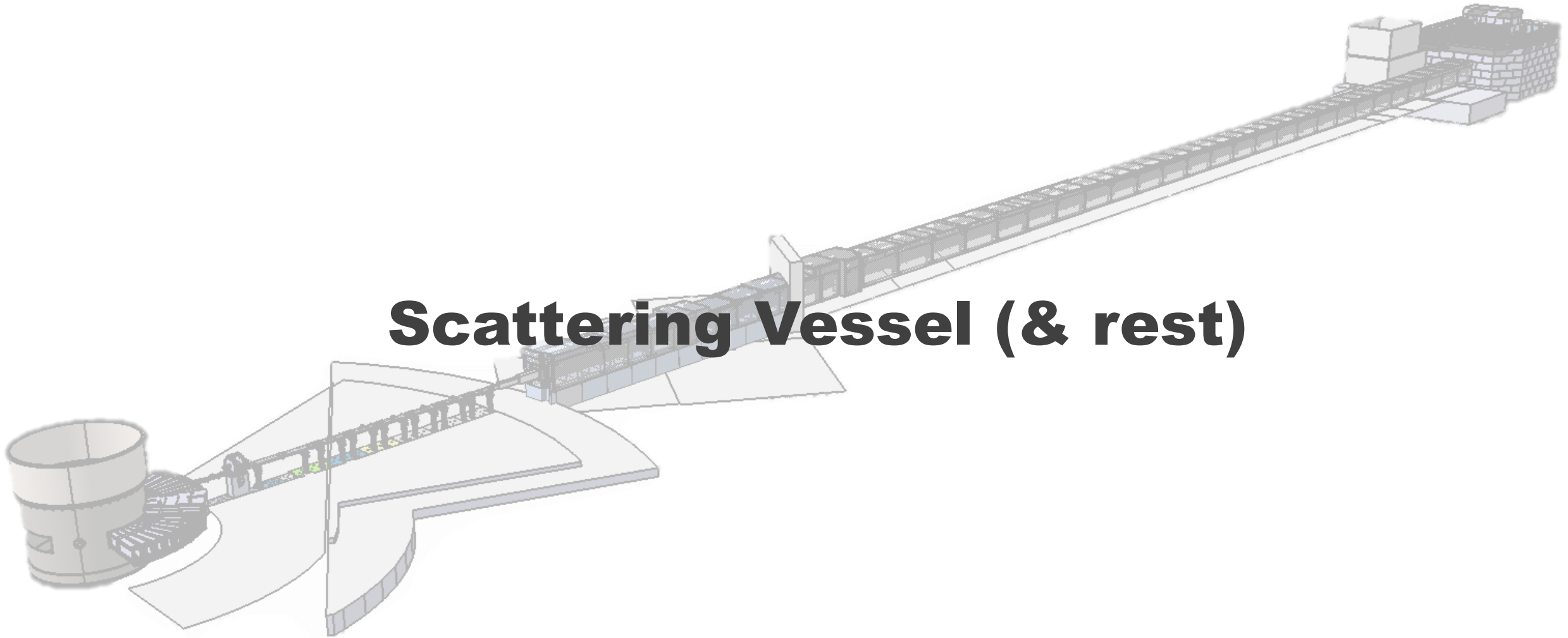
Integration DMSC-MIRACLES



- Digital Twin: connecting the MIRACLES McStas simulation to the EFU, through Kafka and into a consumer that provides live visualisation of the detector image and 'TOF'
- Early integration: Eventhough neither the instrument model, the detector tubes or the EFU are complete this allows us to validate the full acquisition chain.
- It is only a small step to also provide a Nexus file so that we can extend the integration to include data analysis.

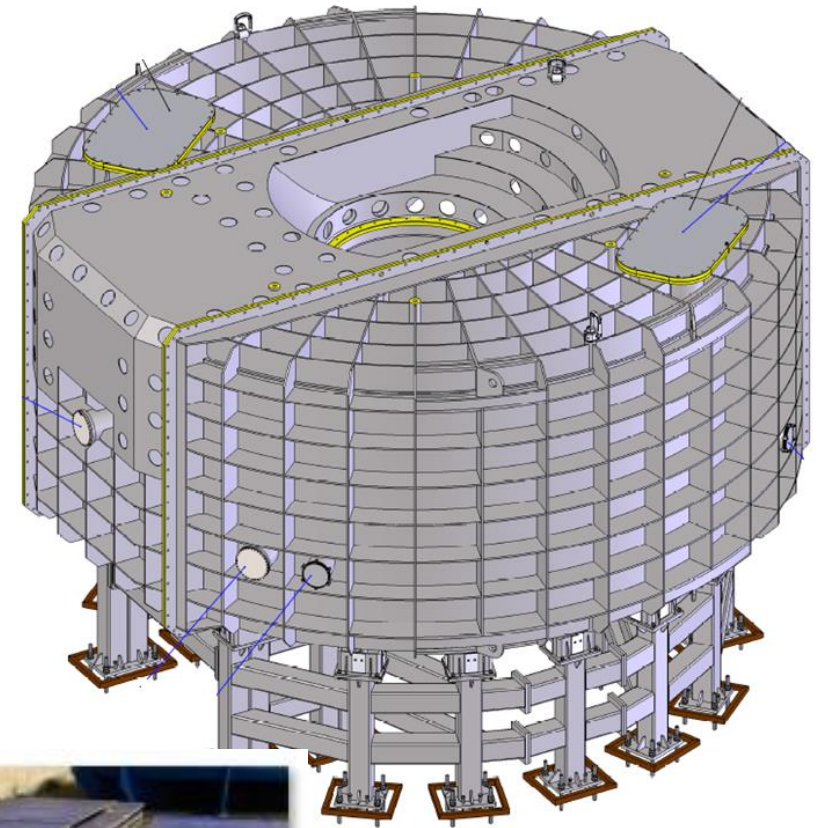


Scattering Vessel (& rest)



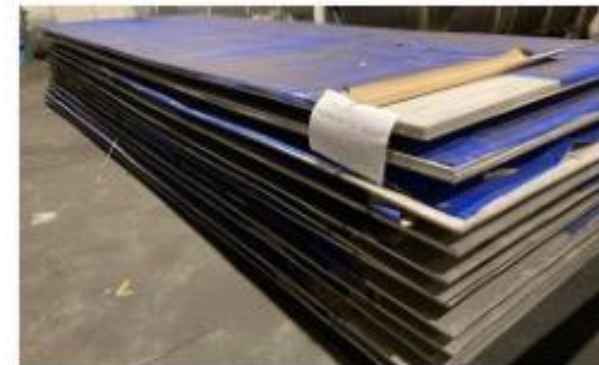
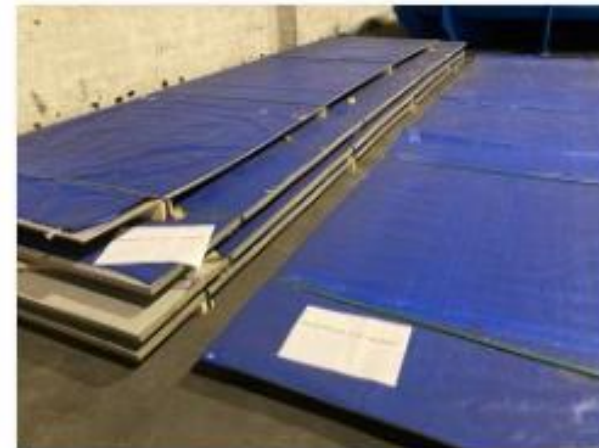
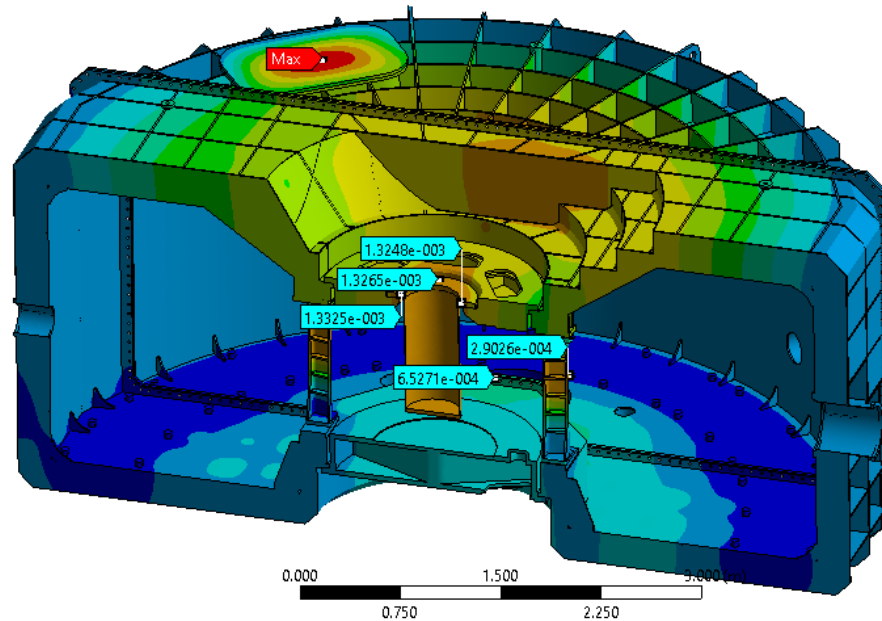
Scattering Vessel

- ✓ Design complete and approved: in production
- ✓ Access to sample area incorporated
- ✓ Deflection at sample position: ≤ 1.5 mm (vertical)
- ✓ Steel 316L (in agreement with Polarization Analysis)
- ✓ Vacuum $< 1 \times 10^{-3}$ mbar
- FAT: Q1-2024



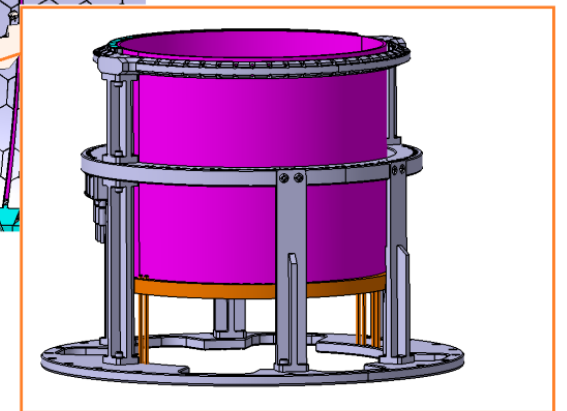
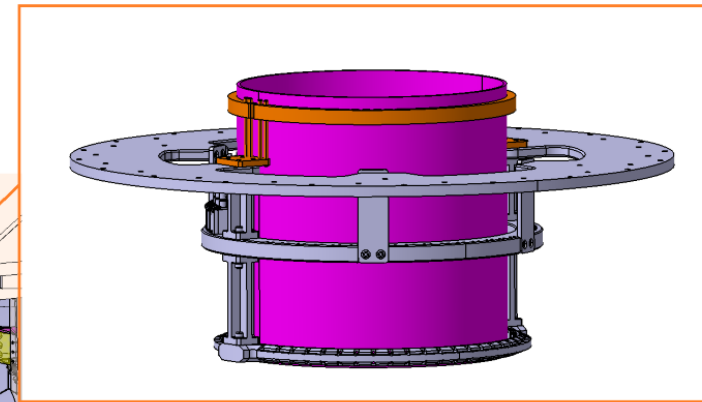
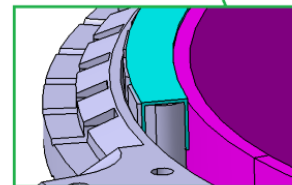
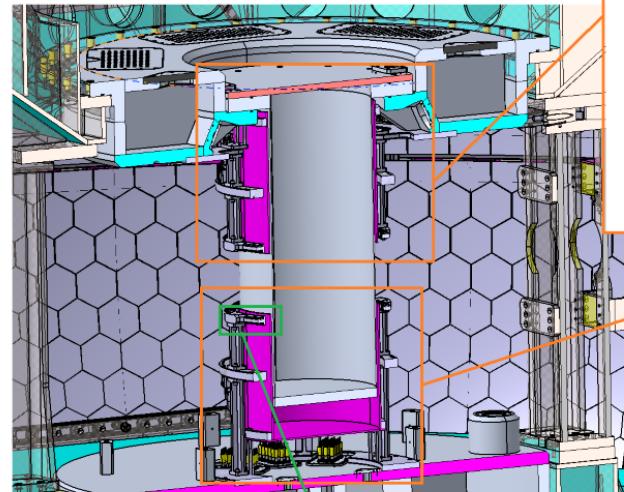
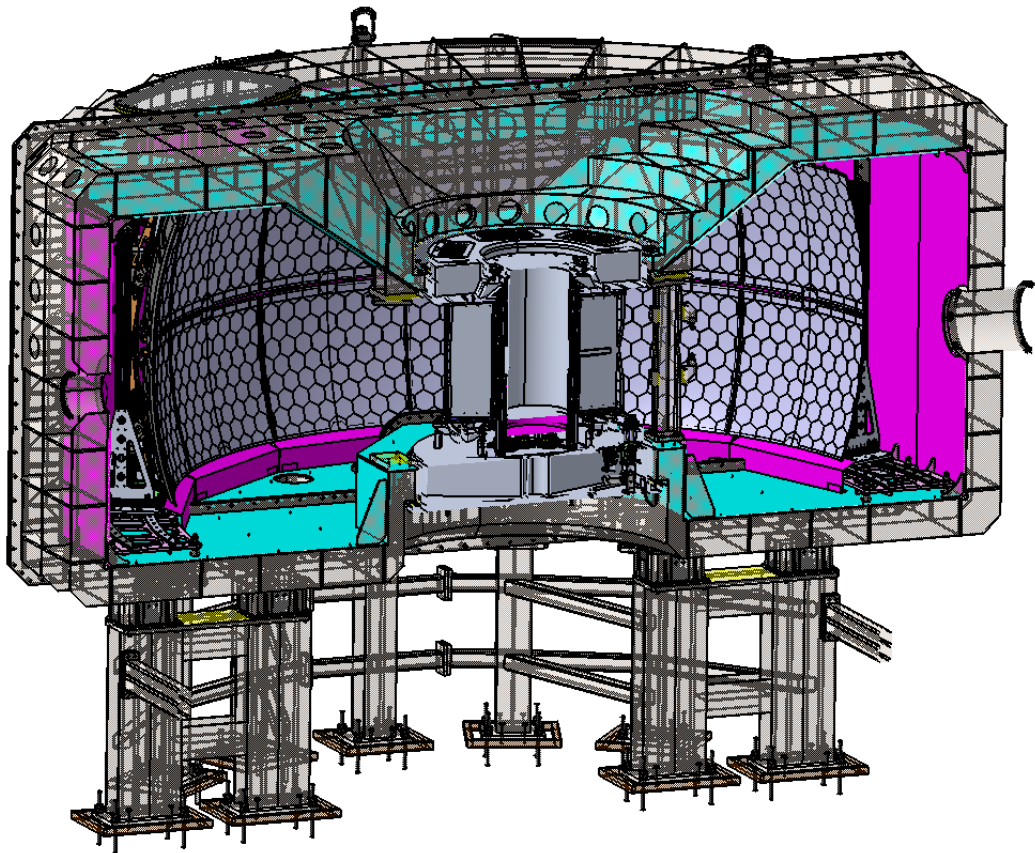
Total Deformation 2
Type: Total Deformation
Unit: m
Time: 2

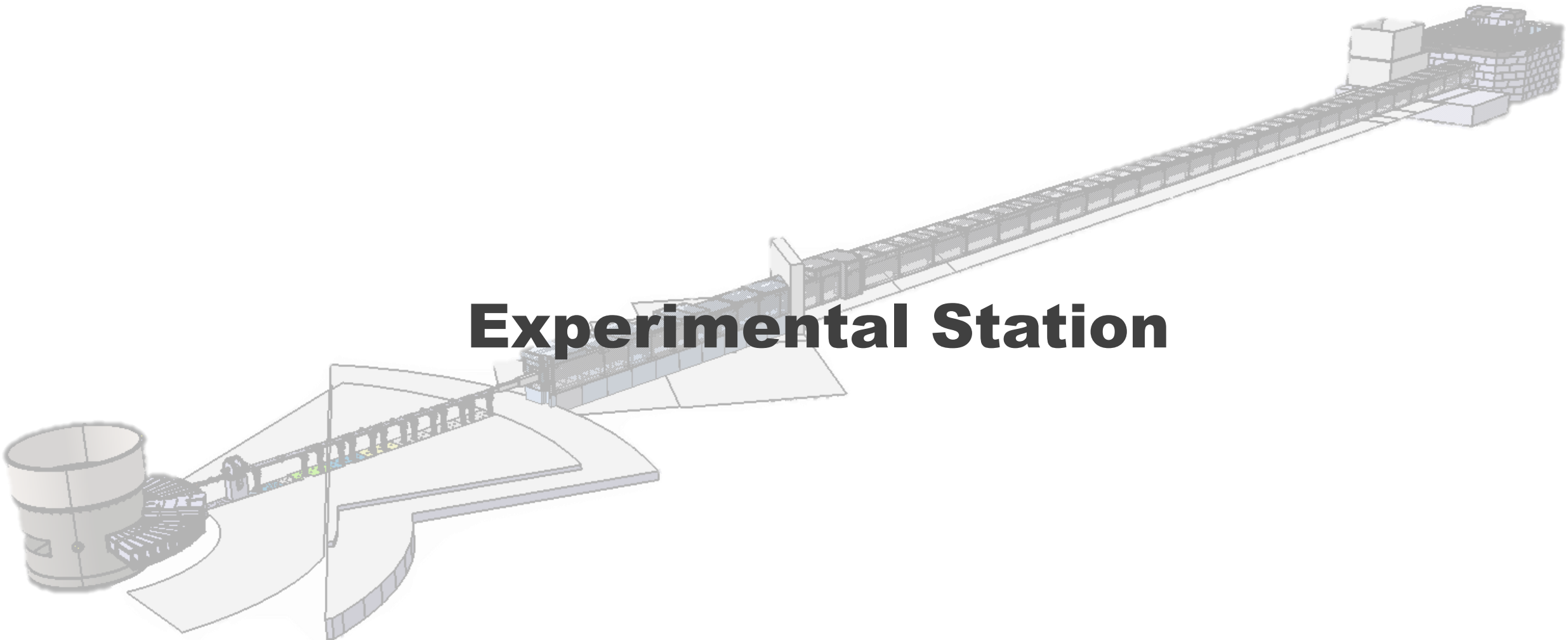
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0.0014544
0.0012895
0.0011246
0.00095967
0.00079475
0.00062984
0.00046492
0.0003
5.7958e-7 Min



Vessel shielding

- ❑ Shielding: Cd plates and flexible B4C
- ❑ Detector shielding: 5 mm B4C / 1 mm Cd (on the detector side) *[Thanks Rasmus!]*
- ❑ Tender: Q3-2023



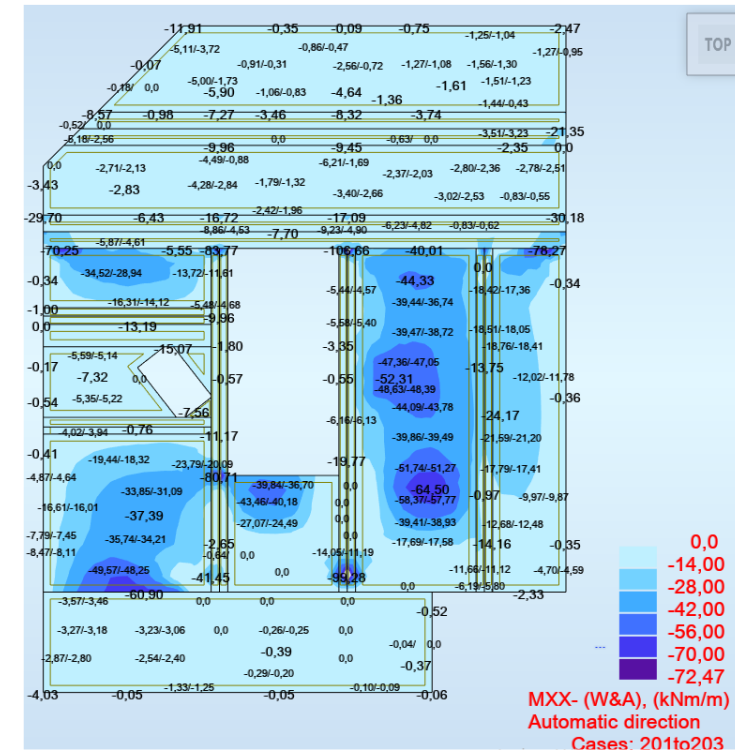
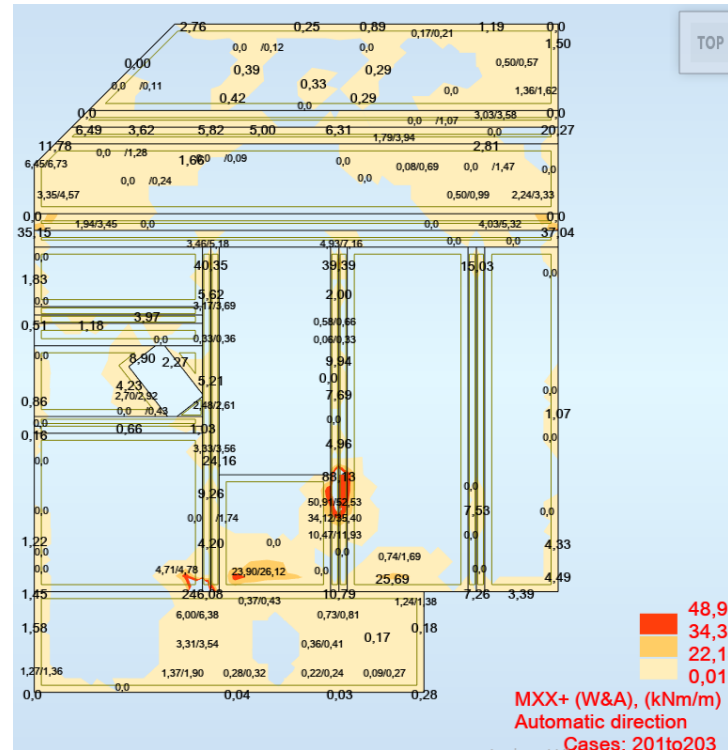
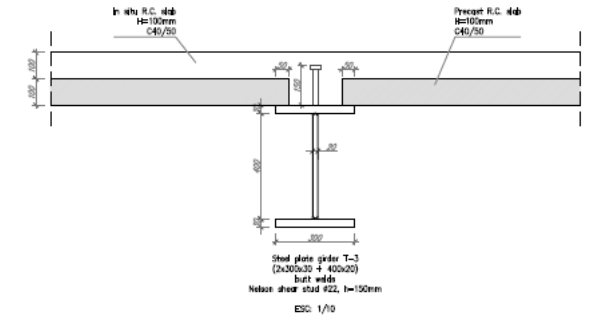
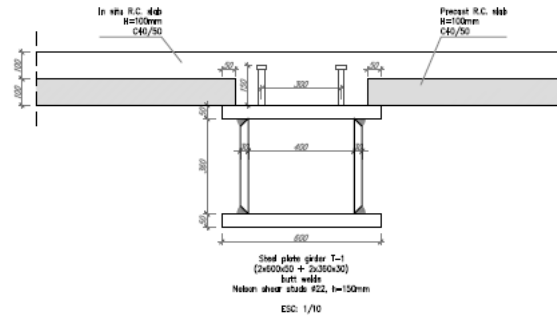
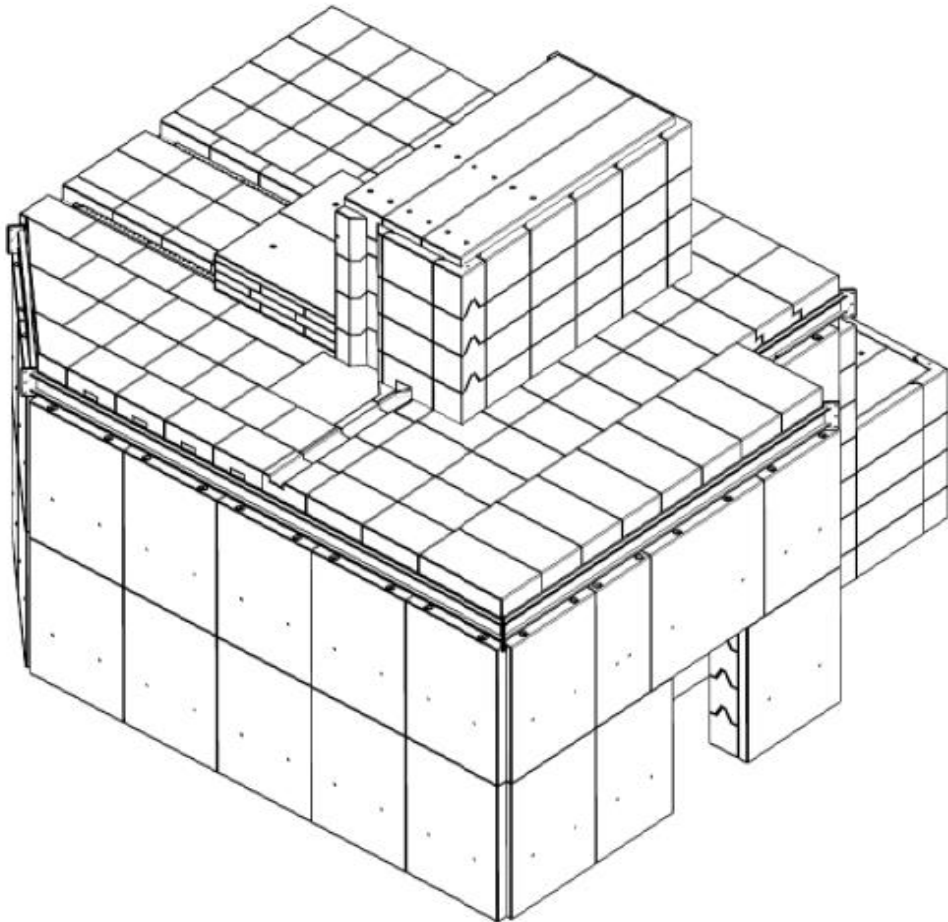


Experimental Station

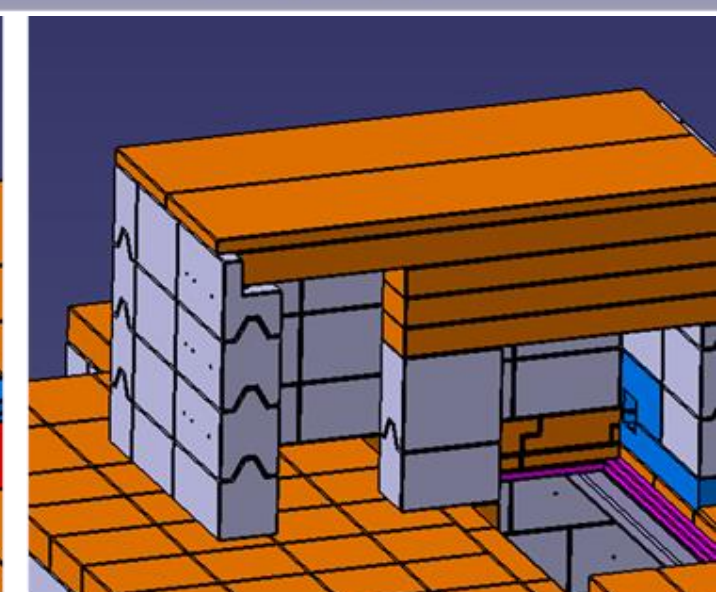
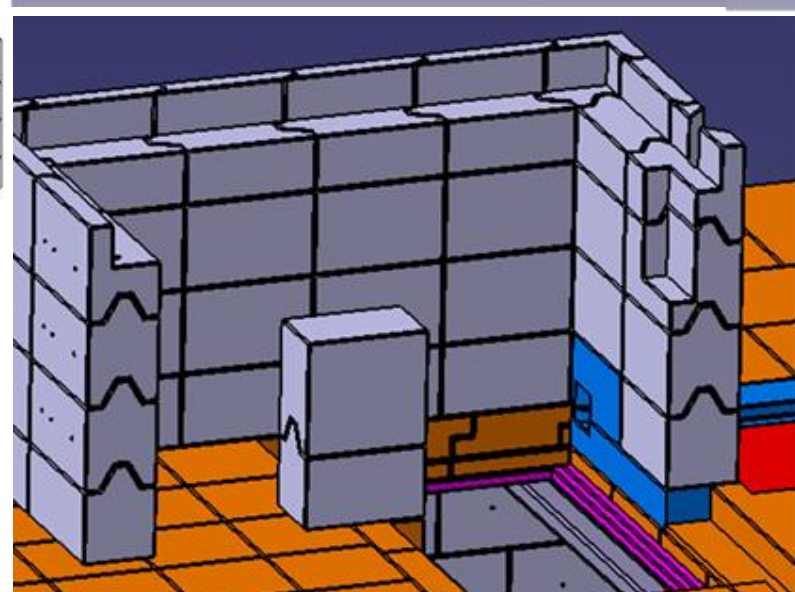
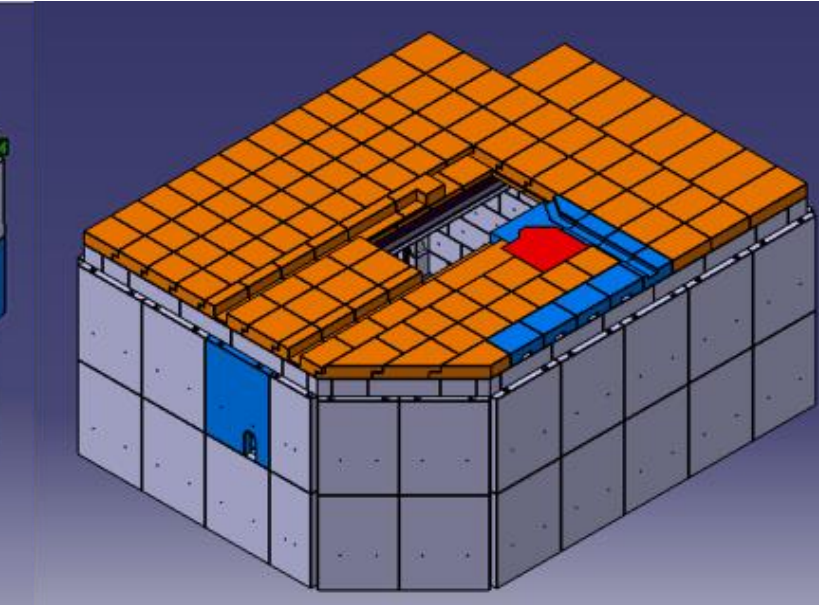
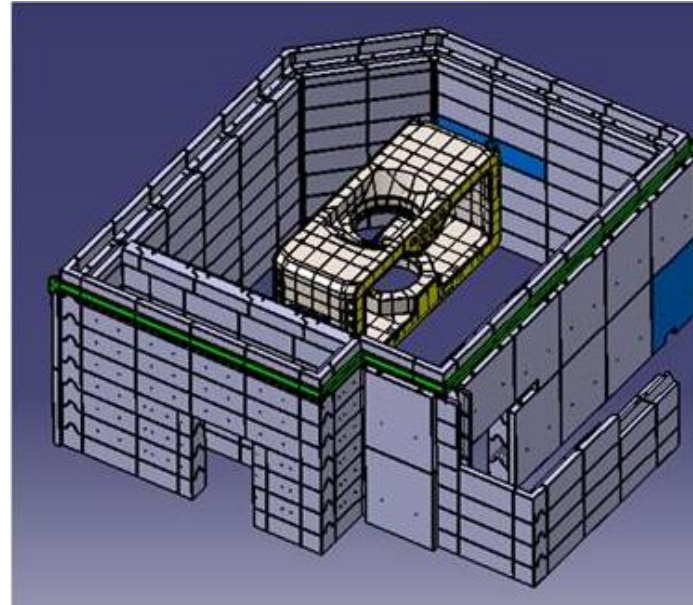
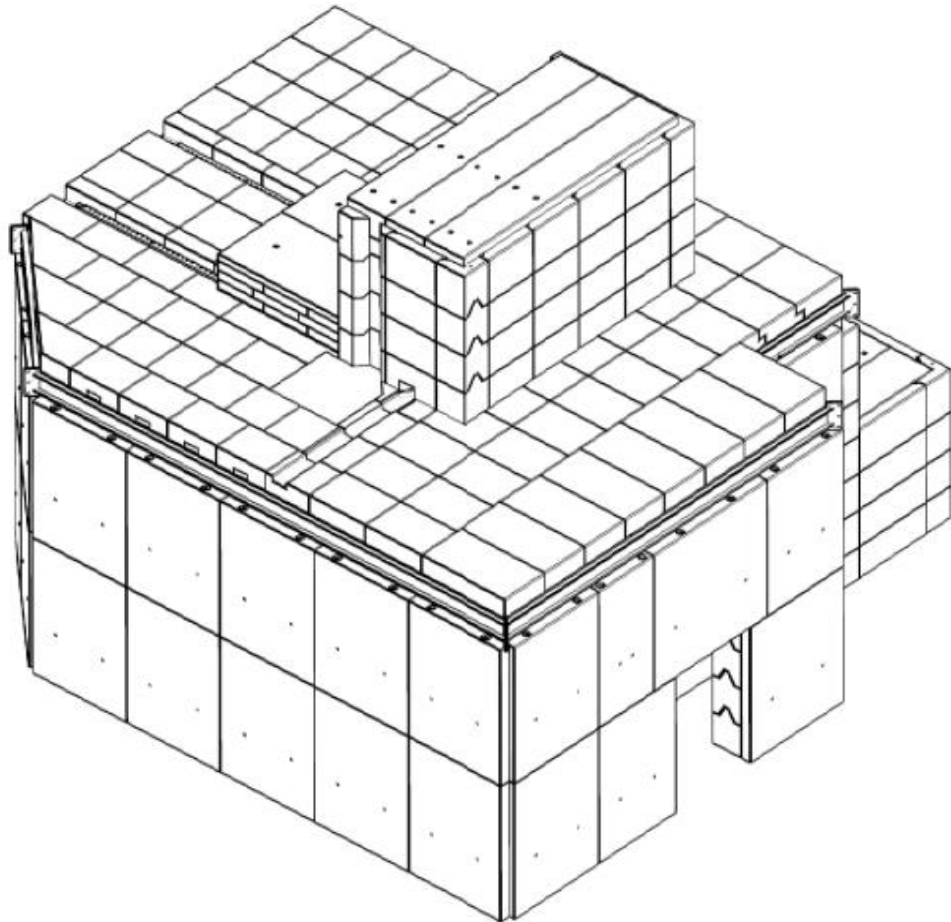


Cave design

- Preliminary design & structural calculations
- Too large and too heavy: need a second round
- Reviews (IDR & CDR) after summer

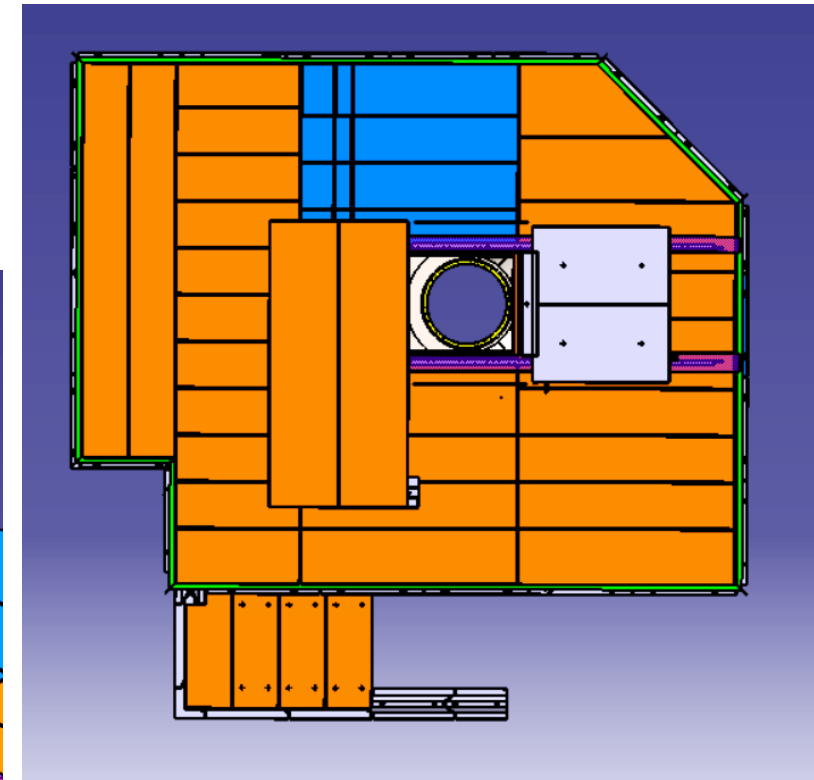
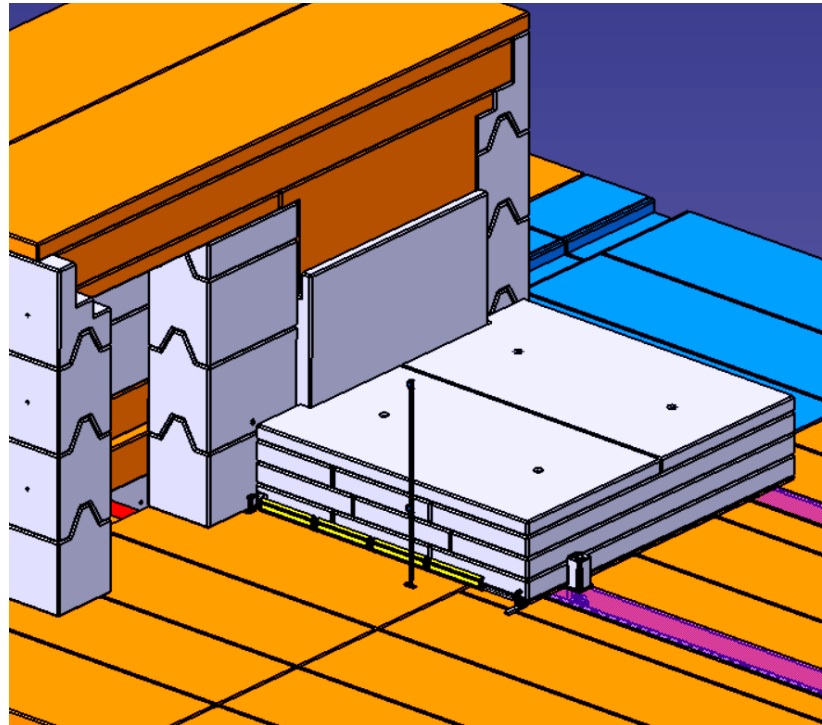
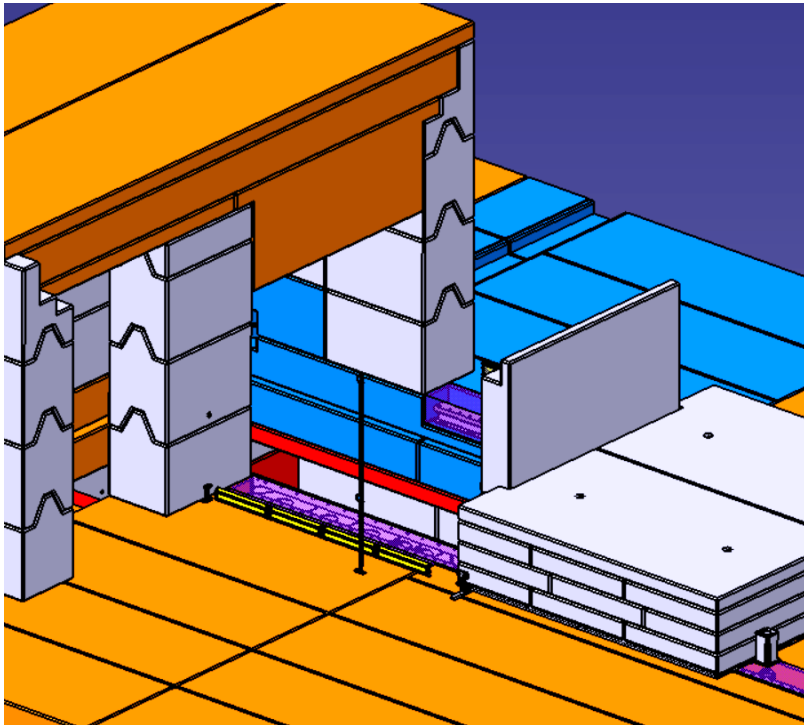


Cave design



Sliding slab

- Concrete multiblock slab (15-20 Tons)
- Guided by railed guides.
- Gearmotor which will move the load along the HEPCOMOTION MHD rack and pinion element.
- Connected to PSS & Shutter

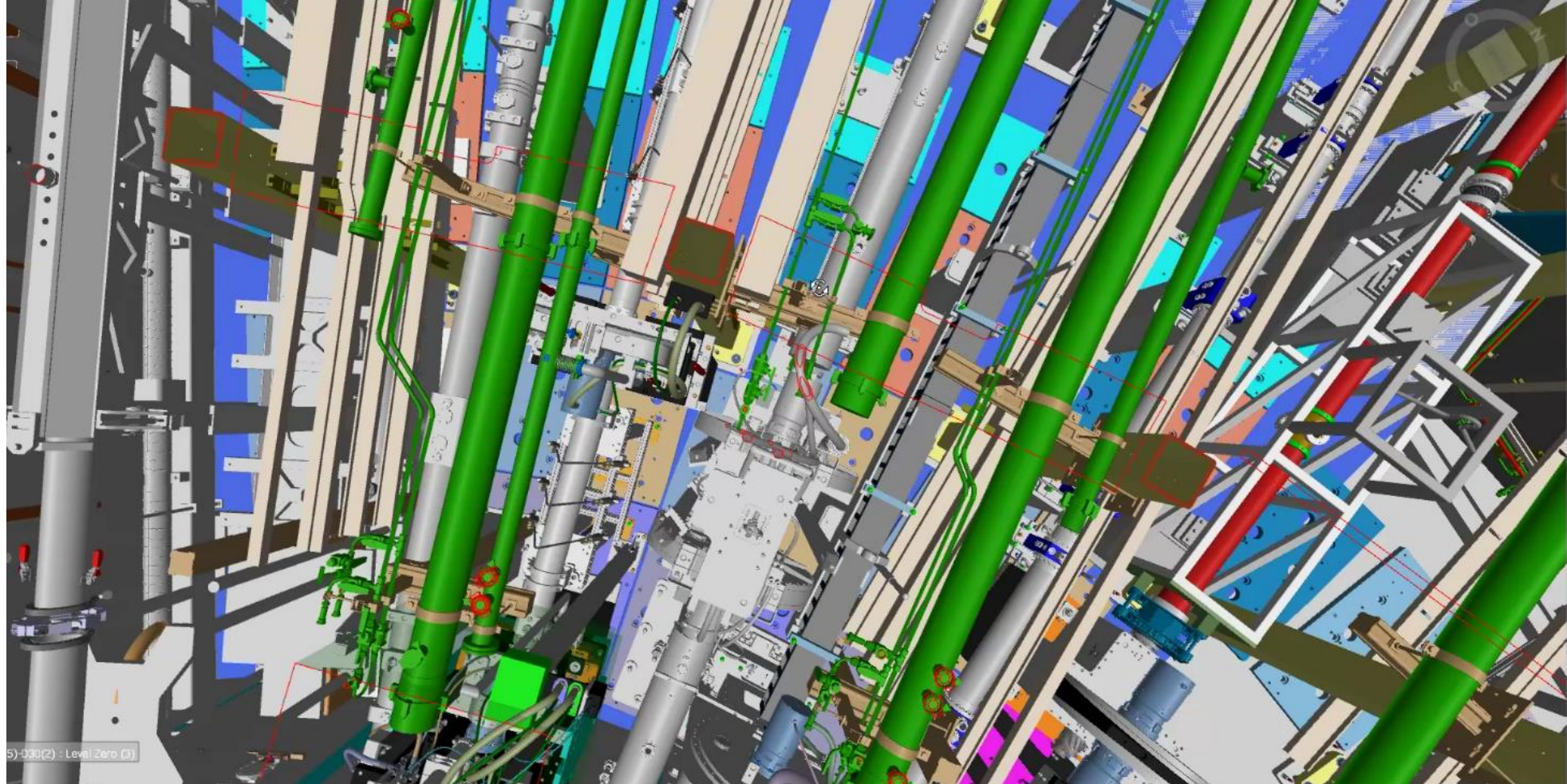




In-bunker Beamline

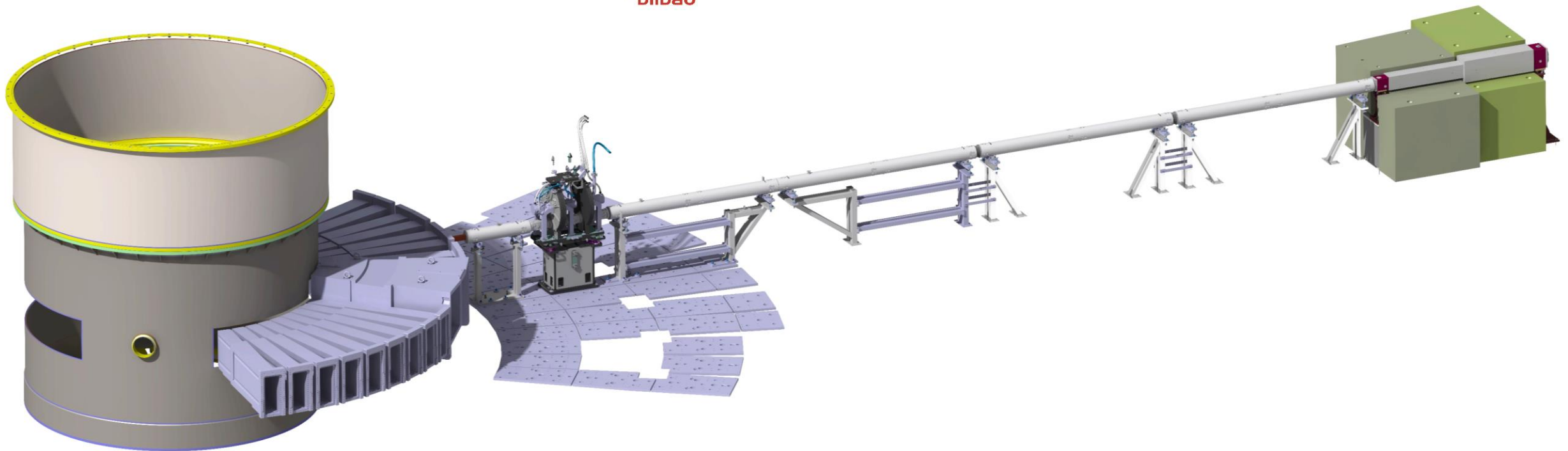


In-bunker integration



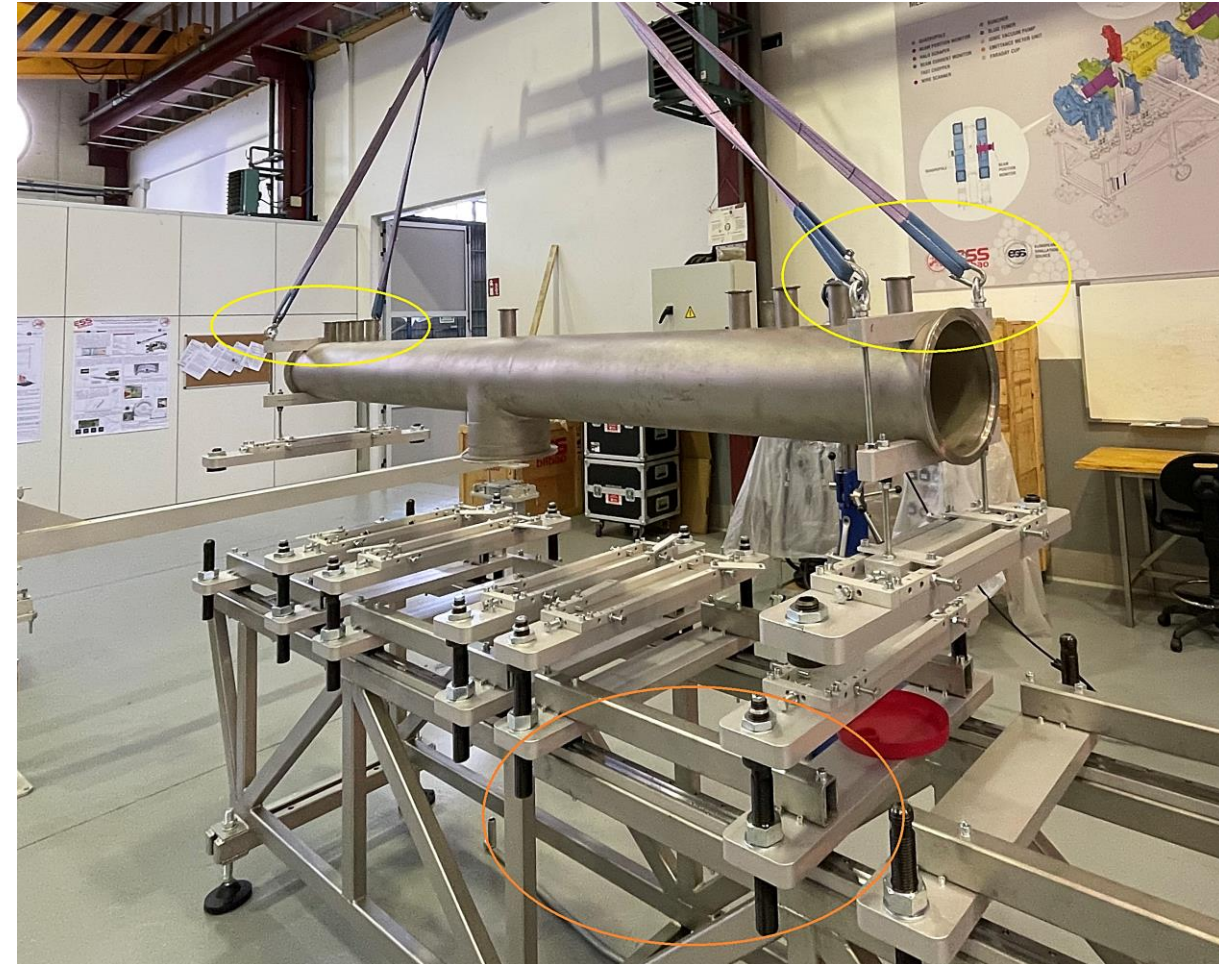
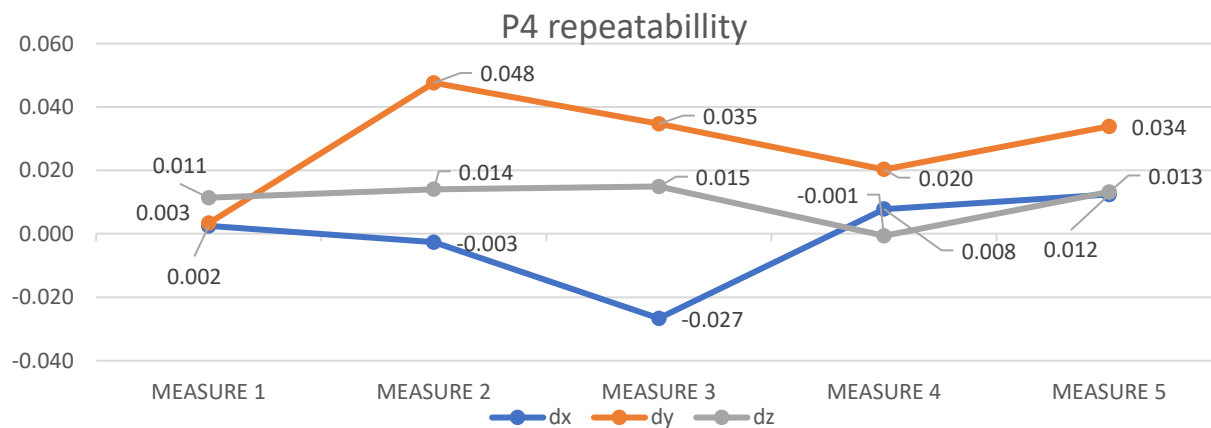
In-bunker integration

- Choppers
- In-bunker guide
- BWI
- Infrastructure
- Guide housing alignment & supports
- Coordination

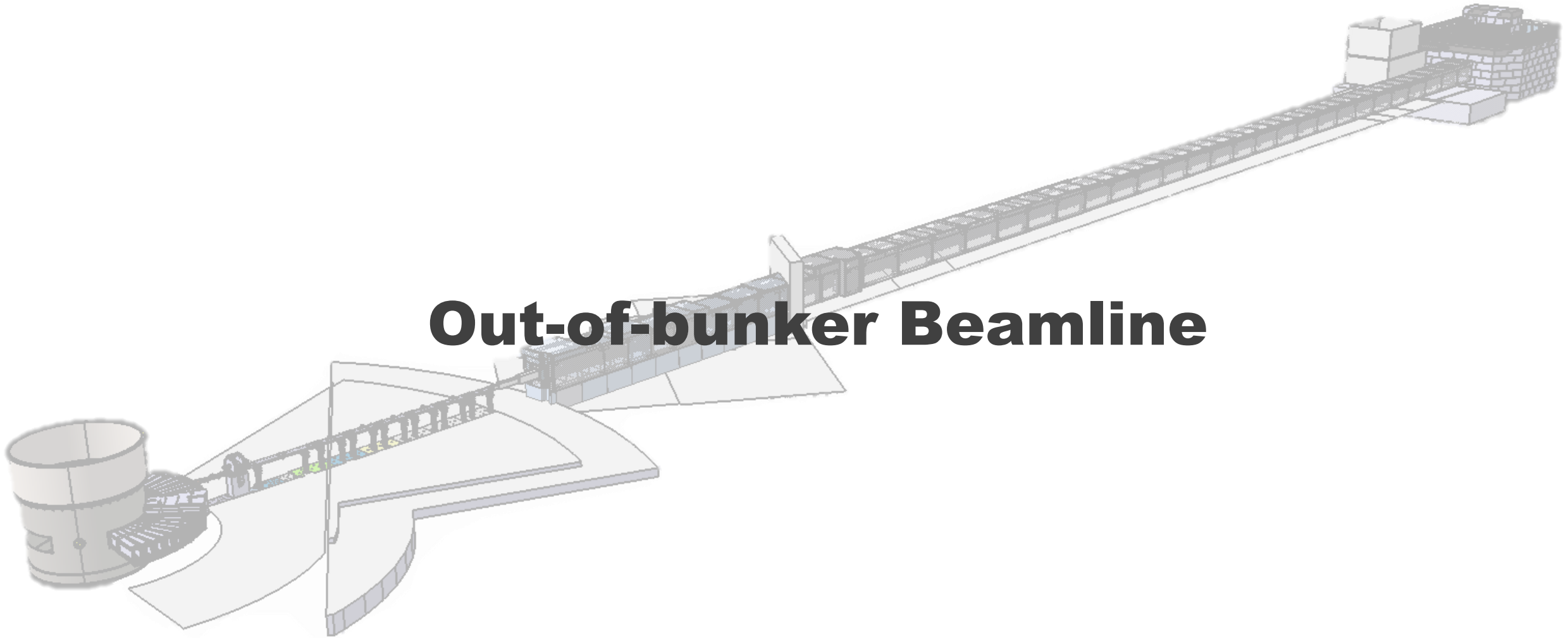


In-bunker housing alignment system: repeatability

- ✓ Remote handling
- ✓ A mock-up guide of a guide housing on a support that already exist was assembled and tested
- ✓ Kinematic reassembly of the system is achievable on an approx. average of 0.030 mm with a maximum deviation observed of 0.058 mm.



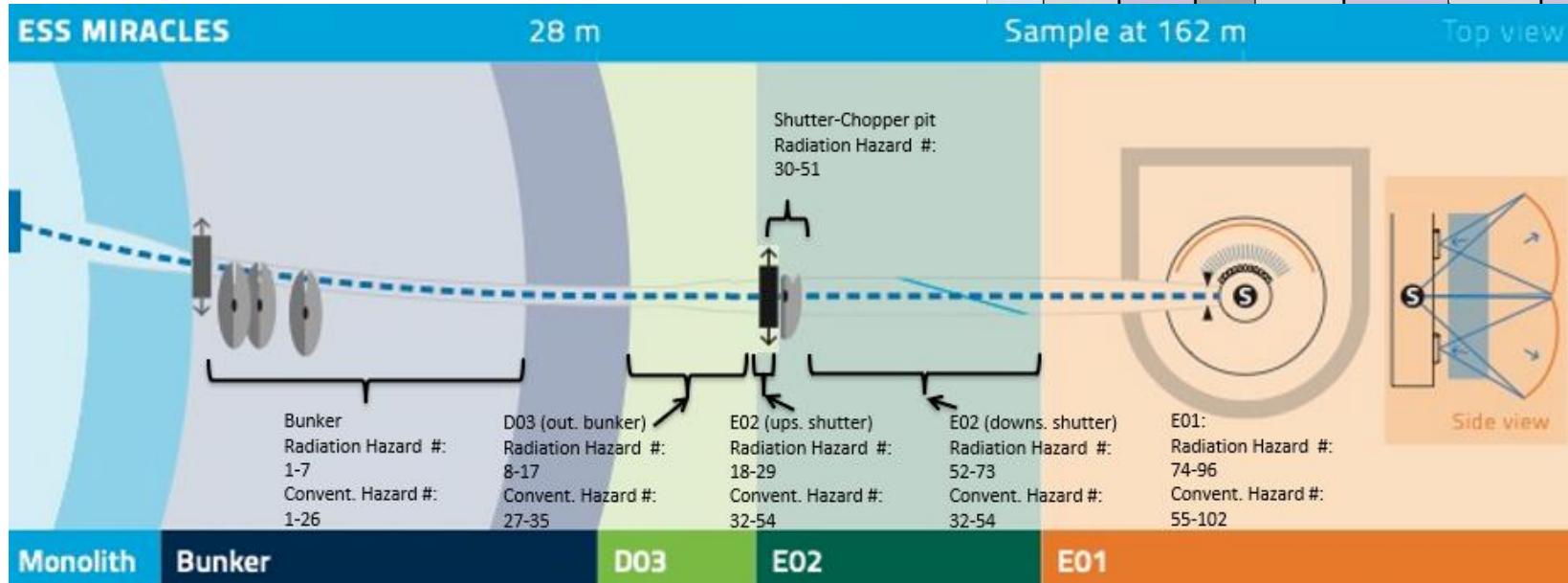
Out-of-bunker Beamline

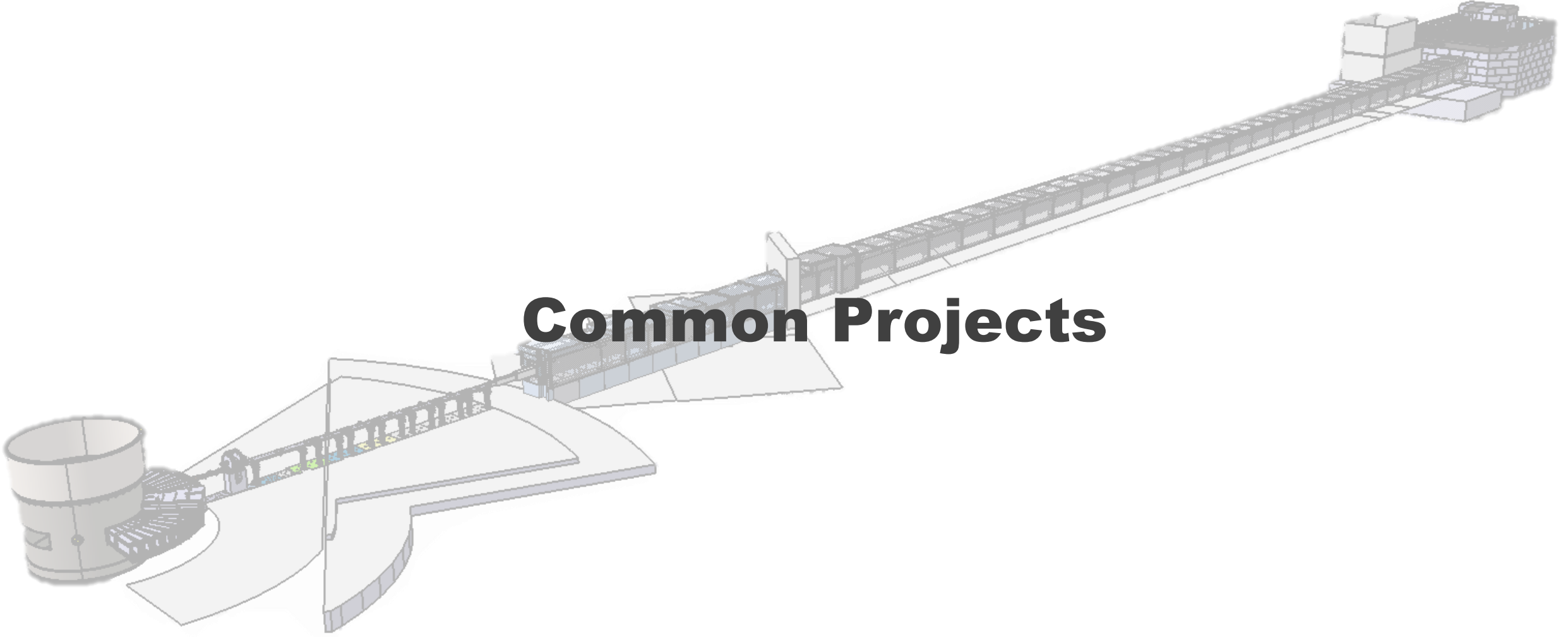


Instrument Hazard Analysis

- Listing Radiation & Conventional Hazards
- Towards 2nd draft [Thanks Pascale]
- Input for Hazard Identification Workshop & PSS

Building	Radiation Hazard Identification				Cause / Initiating Event	Person Affected	Source of Hazard	Sub Mode / Task	Likelihood per year (From H Category) ESS-0000004	Risk Estimation and Reduction		
	1 Instrument Area	2 Instrument Sub-area	3 Radiation Hazard Number	4 Mode						11 Severity	12 Likelihood*Severity	13 Actions to Mitigate Risk (Risk Controls)
D03	Primary Spectrometer	Bunker	1	Proton beam Off	Access to the bunker during maintenance	Exposed worker without radiation safety task	Activated instrument components. Choppers/Guides/Monitors	N/A	H1 1	dose < 2 mSv/event		a) Shielding and barriers to prevent access to the bunker area beyond where the work takes place b) Signage.
D03	Primary Spectrometer	Bunker	2	Proton beam Off	Access to the bunker - Barriers and signage disregarded -	Exposed worker without radiation safety task	Activated instrument components. Choppers/Guides/Monitors	N/A	H3 1X 10 ⁻³	2 < dose < 10 mSv/event		Radiation safety training required by all workers prior to accessing site. Badge access only. MIRACLES staff and users do not have access. Managed by bunker risk assessment.
								N/A	H3 1X 10 ⁻³	2 < dose < 10 mSv/event		Radiation safety training required by all workers prior to accessing site. Badge access only. MIRACLES staff and users do not have access. Managed by bunker risk assessment.
								ionising	N/A	H3 1X 10 ⁻³	dose > 20 mSv/event	Check of bunker prior to closing. Audio and visual alarm prior to proton beam opening. Emergency stop of proton beam.
								ionising	N/A	H4 1X 10 ⁻⁶	dose > 20 mSv/event	Check of bunker prior to closing. Audio and visual alarm prior to proton beam opening. Emergency stop of proton beam.
								ionising	N/A	H4 1X 10 ⁻⁵	dose > 20 mSv/event	Radiation safety training required by all workers prior to accessing site. PSS lock of bunker.
								ionising	N/A	H3 1X 10 ⁻³	dose > 20 mSv/event	Radiation safety training required by all workers prior to accessing site. PSS lock of bunker.
								on from	N/A	H1 1	dose < 2 mSv/event	Guide shielding to achieve radiation levels equal or less than 3 microSv/year on touch. Pit prevents radiation with beam on but this is with beam off.





Common Projects

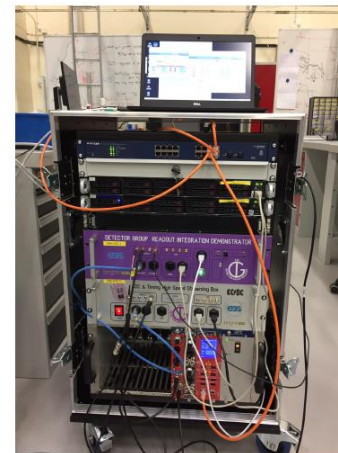


MIRACLES: NSS Common Projects

ESS Common Project	MIRACLES Involvement	Status
Beamline Shielding	In	Preliminary design ongoing
Beam Monitors	In	Project Frozen
Choppers	In (racks only)	Racks at ESS
Electrical	Under discussion	Requirements document ongoing
Utilities	Under discussion	Requirements document agreed, waiting for offer



MIRACLES Distribution Board

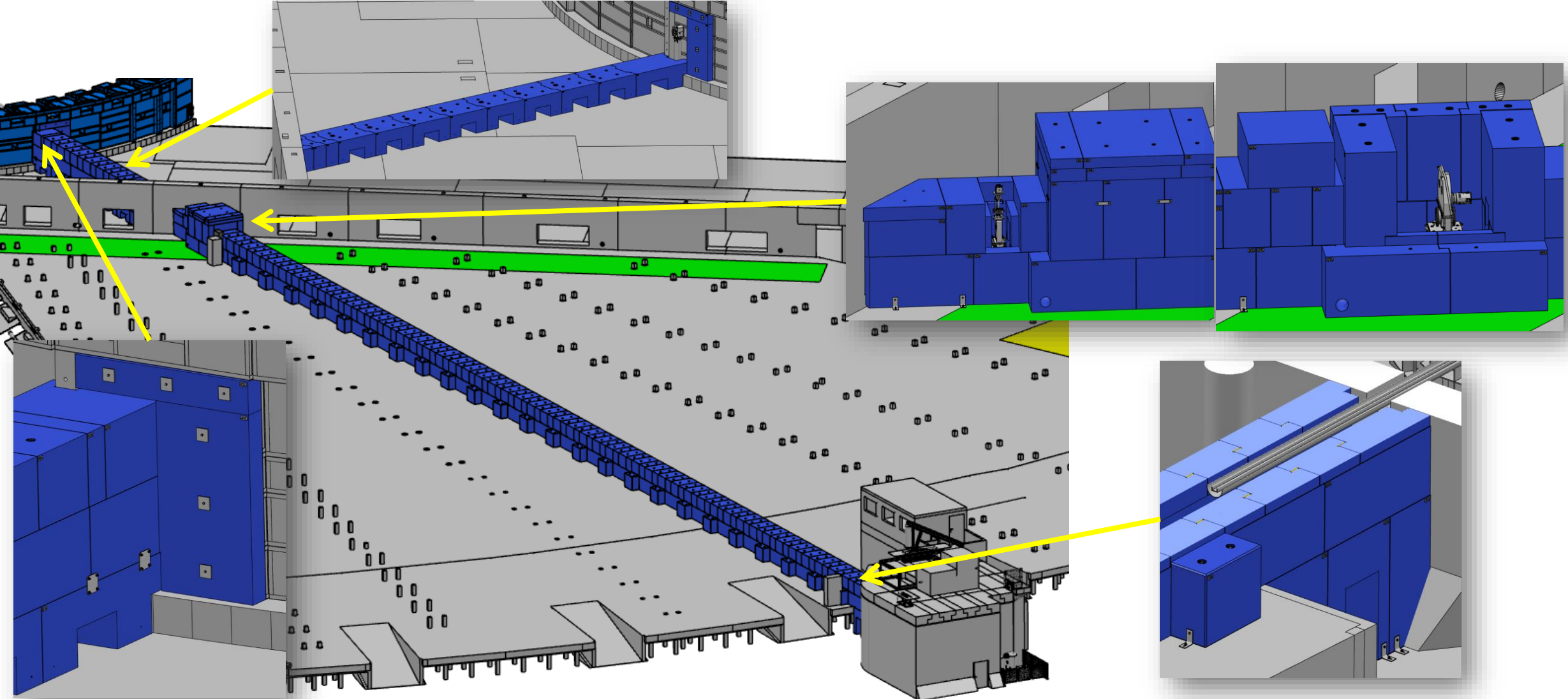


Baseline DAQ for BMs in the Utgård



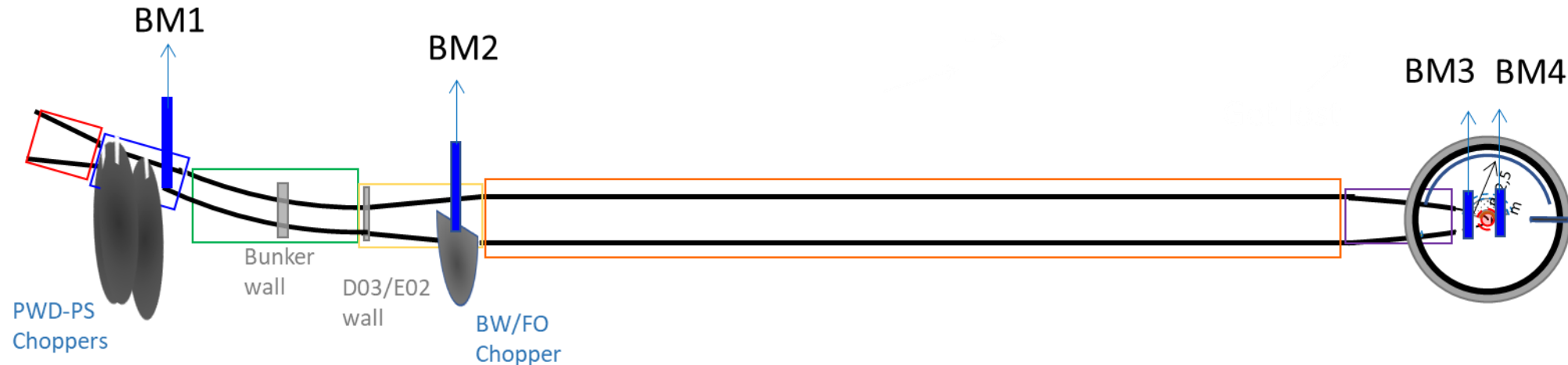
The two MIRACLES Chopper racks

NSS Common Shielding Project (MIRACLES Beamline)



NSS Beam Monitors Common Project

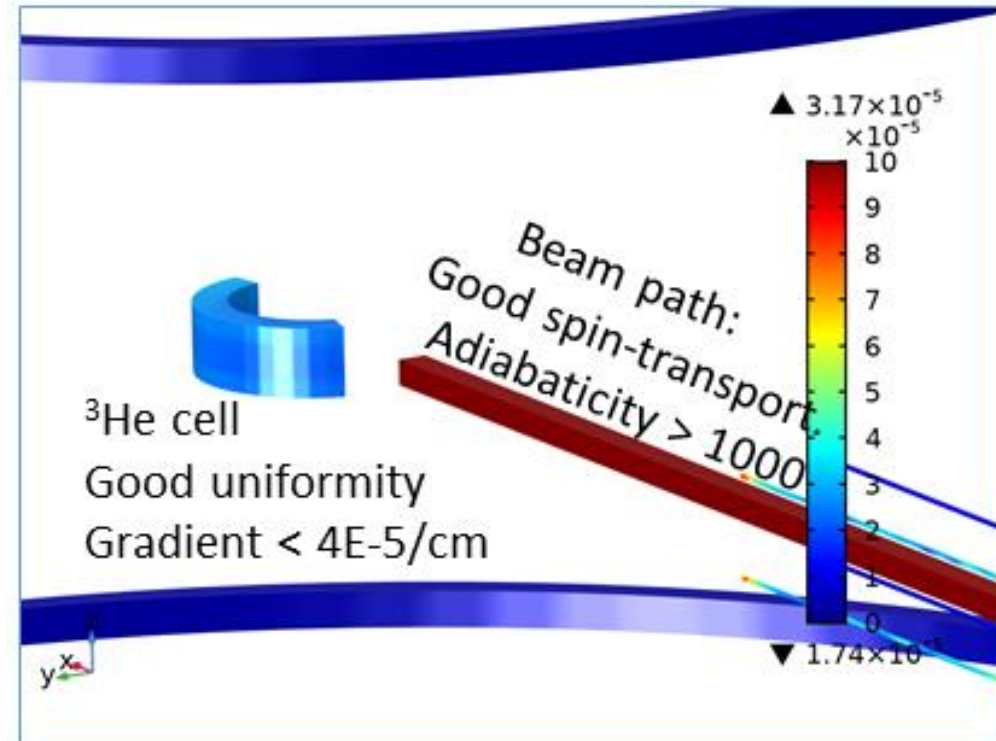
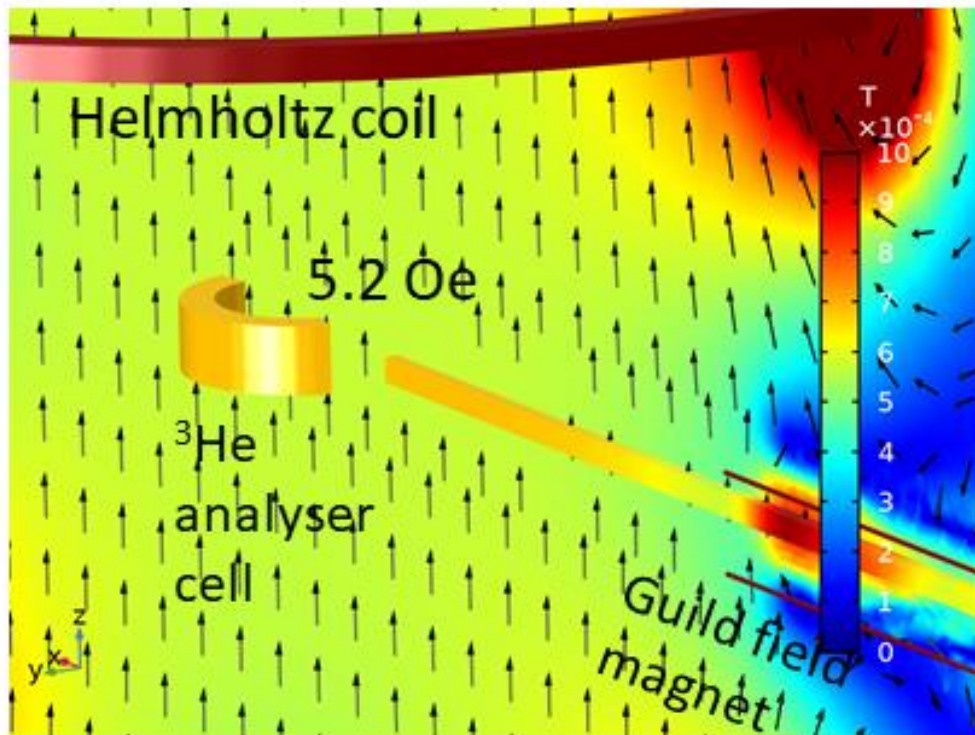
- Project frozen, but will progress with new PL [*and Daria*]
- At the moment, the idea is only to get focused on the in-bunker beam monitor (BM1)



#BM	Grounding zone	Purpose	Beam profile (y×z, vertical×horizontal mm ²)	Placement	Moveable	Remote handling (RH)	Technology	Efficiency	Converter specs (gas, solid)	FEE/ADC	Assister	Gas/Flow
1	bunker	PWD, PSC diagnostics	80 x 60	air	N	TBD	pulse mode ionisation chamber I-BM	<1e-6	100 nm 10B4C or 0.13 mg 235UO ₂	ESS/ADC 100	KC705	none, sealed
2	intermediate	BW, FO chopper diagnostics	110 x 130	air	N	N/A	GEM	<1e-5		GEMINI	NI	N ₂ +Ar/CO ₂
3	cave	pre-sample/normalisation	30 x 30	vacuum (1e-3 mbar)	N	N/A	MWPC	<1e-3		ILL/ADC100	KC705	none, sealed
4	cave	post-sample	100 x 100	vacuum (1e-3 mbar)	Y	N/A	MWPC	<1e-3		ILL/ADC100	KC705	none, sealed

Polarization Analysis Capability

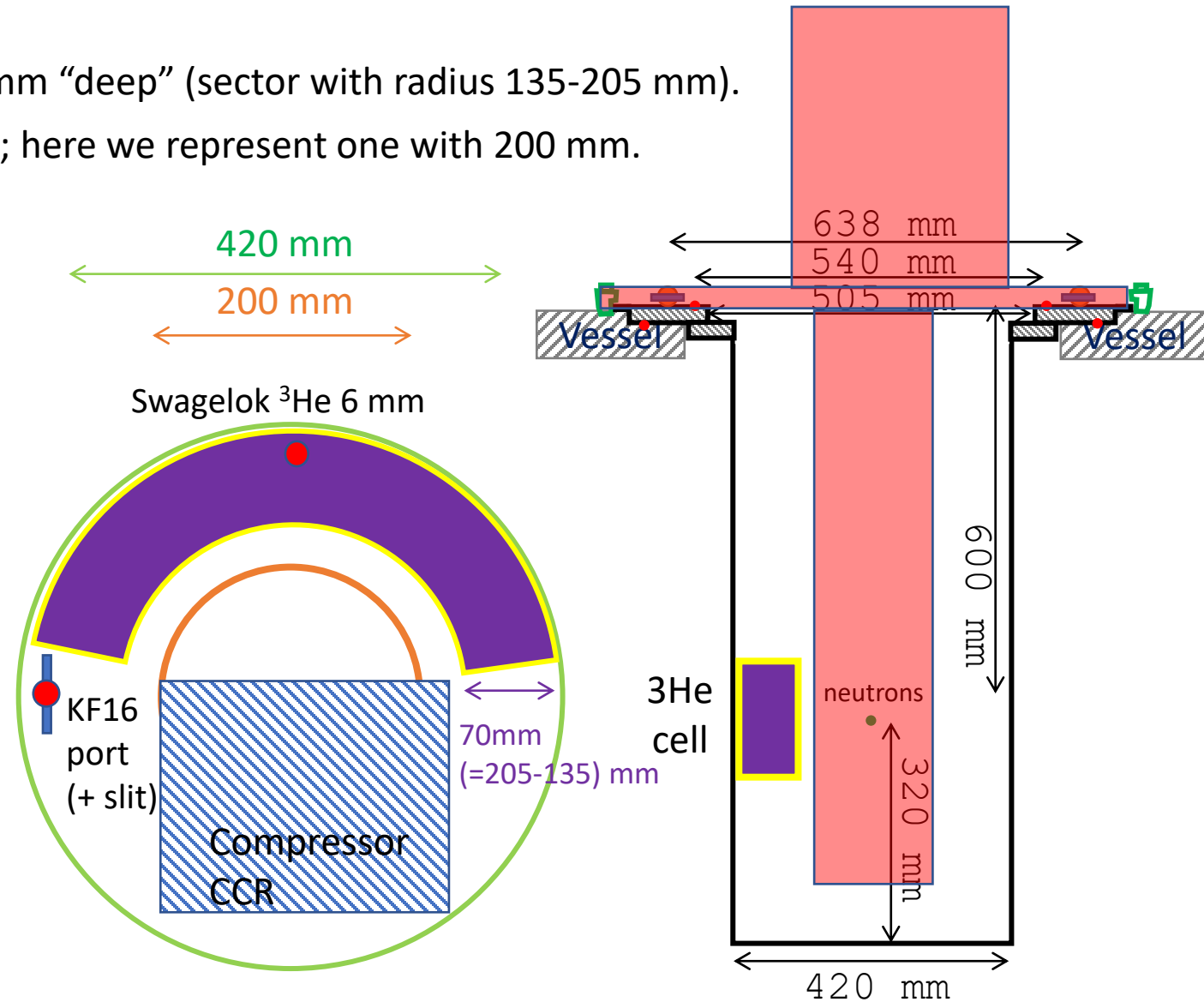
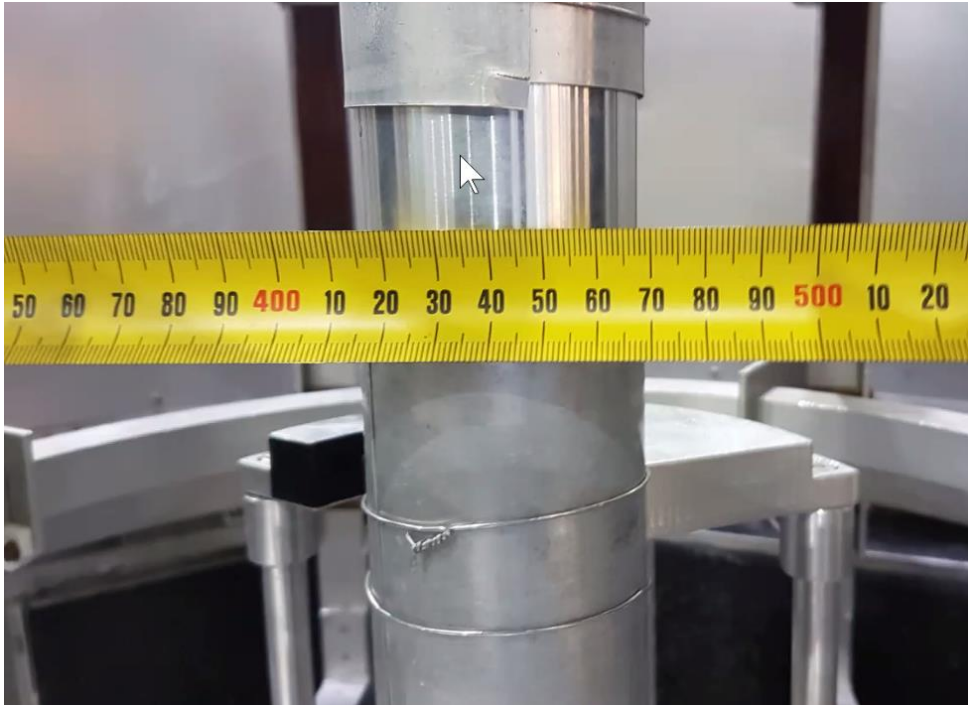
- ✓ Good timing between both projects
- ✓ Integration of PA components done
- ✓ Conceptual → Preliminary design
- ✓ Swedish IK contribution



CCR & ^3He cell

Agreed with Hal:

- For cold neutrons, the ^3He cell is about 60-70 mm “deep” (sector with radius 135-205 mm).
- A thin-tailed CCR (diameter <100 mm) can help; here we represent one with 200 mm.
- Swagelok ports 6 mm are needed in the flange.



Scope Setting: Sample environment equipment list

Essential on Day 1:

- CCR
- Humidity chamber
- Automatic sample changer (6-8 samples)

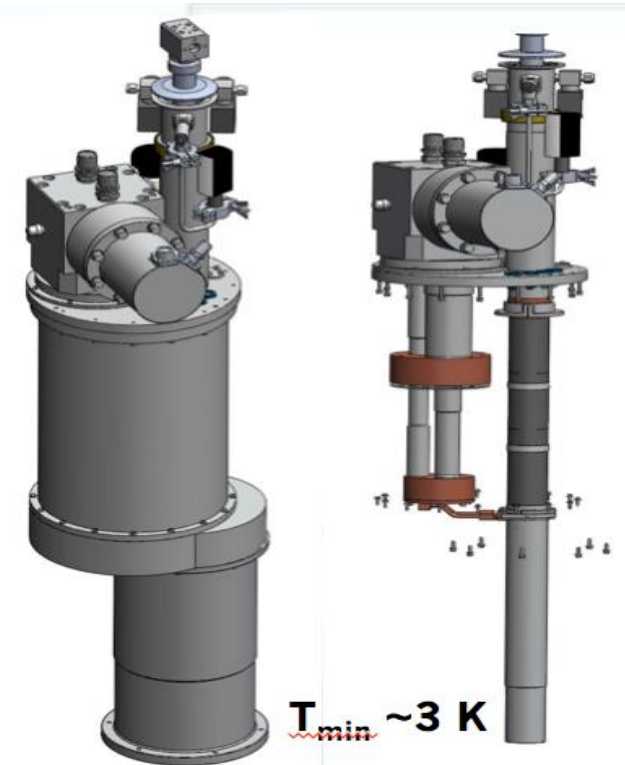
- MIRACLES will have a dedicated CCR.
- The CCR will be the workhorse SEE for MIRACLES (3-300 K). Option to 600 K.

Essential:

- OC / cryofurnace (with dilution insert option)
- Furnace
- Cryomagnet
- Electric field polarization
- Pump probe laser
- Electrochemical cell
- Gas process handling
- High pressure cell

Good to have:

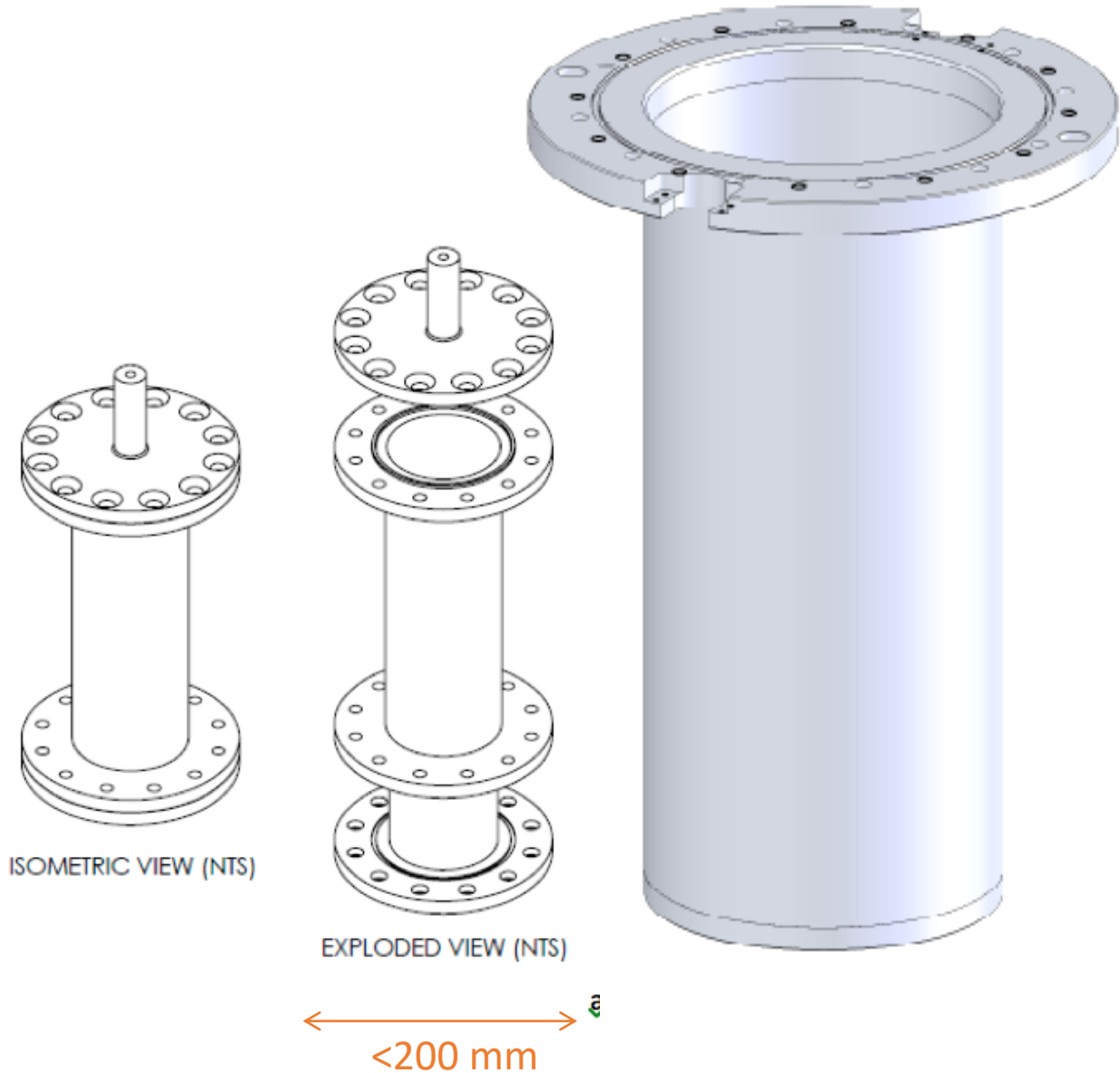
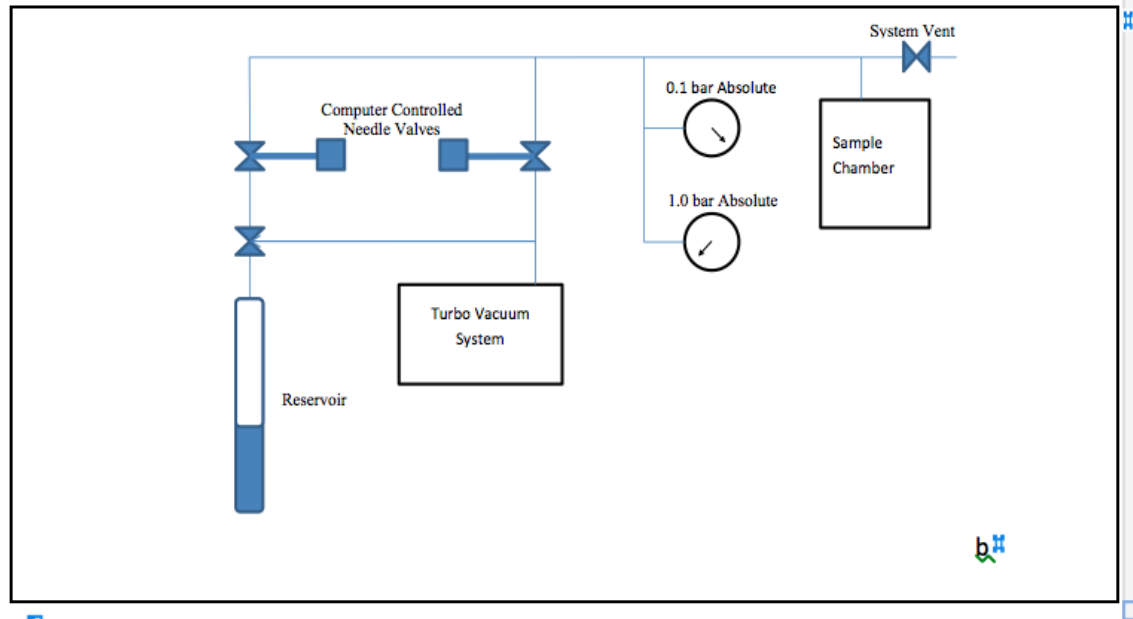
- In-situ Raman-QENS
- DSC
- Biofurnace



Humidity Chamber

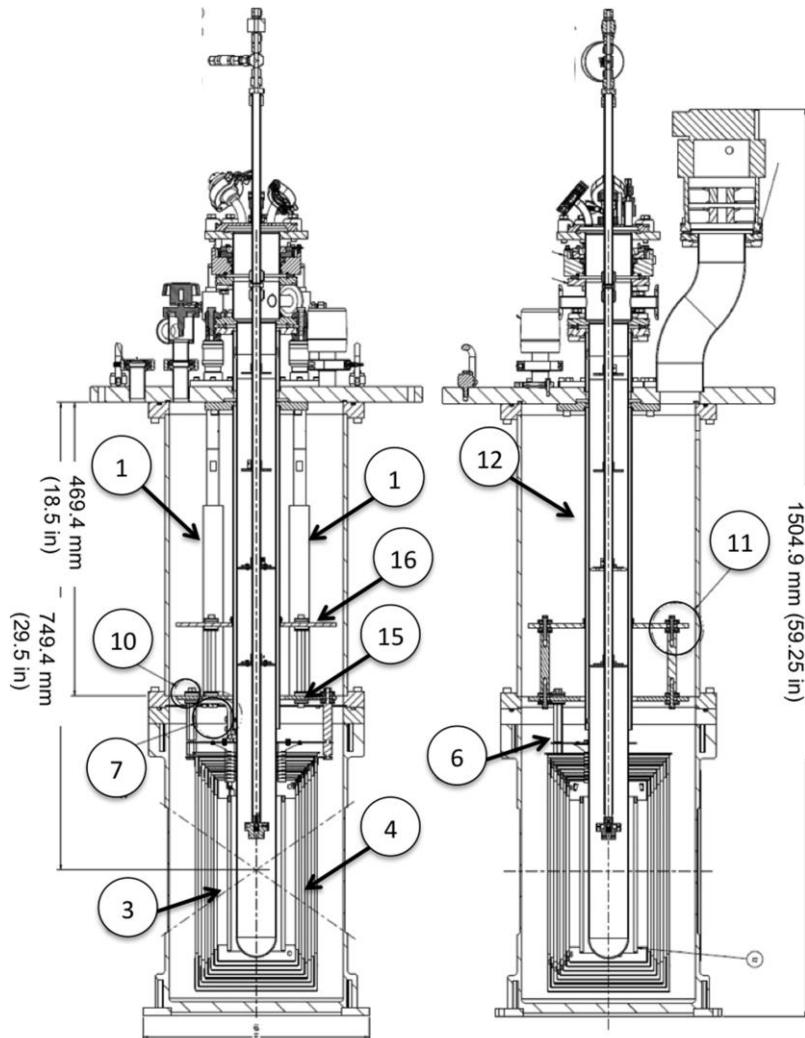
- Temperature $T = 10^{\circ} \text{C} - 80^{\circ} \text{C}$
(Commercial: $10^{\circ}\text{C} - 60^{\circ}\text{C}$)
with stability $dT = \pm 0.01^{\circ} \text{C}$,
- Humidity r.H. = $0\% - 100\%$
(Commercial: $5\% - 95\%$)
with stability $d(\text{r.H.}) = \pm 0.1\%$

Commercial manufactures (Anton Paar, Hiden, ...).
The port and slit can fit perfectly in the adaptive flange

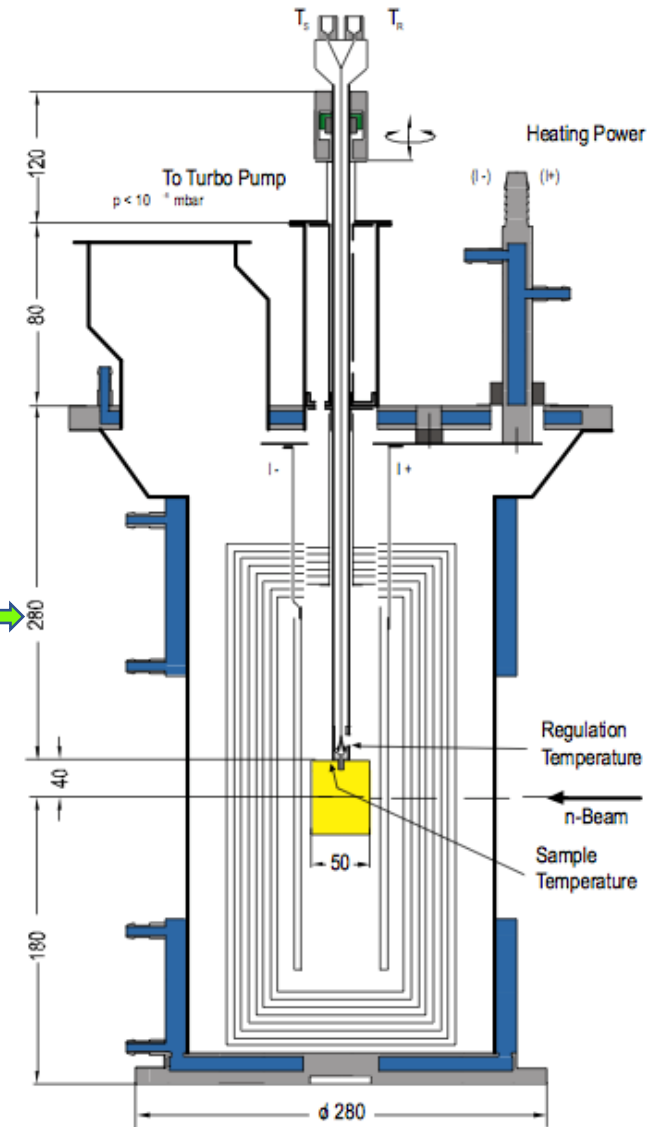


Furnace

- Top loading Al-Nb
- Minimum Temperature range: 300° C – 1500° C
- Photos (Left: ARCS) and (Right: ESS UK IK ISIS-SE and company AS SCIENTIFIC)



Make this
600 mm?! →



Pump-probe laser & Electric Field Polarization

External (dimensions are adaptable for MIRACLES):

- Electric field polarization (IK – Italy – F. Natali)
- Pump-probe laser (IK – Estonia – J. Pieper)

PRL 100, 228103 (2008)

PHYSICAL REVIEW LETTERS

week ending
6 JUNE 2008

Transient Protein Softening during the Working Cycle of a Molecular Machine

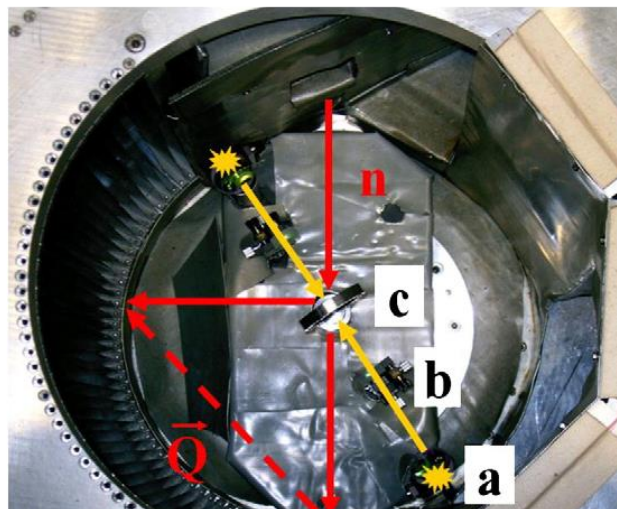
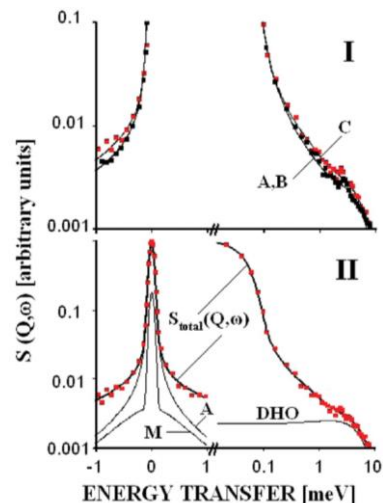
Jörg Pieper,^{1,*} Alexandra Buchsteiner,² Norbert A. Dencher,³ Rued E. Lechner,^{2,3} and Thomas Hauß^{2,3}

¹Max-Volmer-Laboratories for Biophysical Chemistry, Technische Universität Berlin, Strasse des 17. Juni 135, 10623 Berlin, Germany

²Hahn-Meitner-Institut Berlin, Glienicker Str. 100, 14109 Berlin, Germany

³Physical Biochemistry, Department of Chemistry, Technische Universität Darmstadt, Petersenstrasse 22, D-64287 Darmstadt, Germany

(Received 13 December 2007; published 3 June 2008)



1 Electric Field Induced Polarization Effects Measured by in Situ 2 Neutron Spectroscopy

³Rosanna Ignazzi,[†] Will P. Gates,[‡] Souleymane O. Diallo,[§] Dehong Yu,^{||} Fanni Juranyi,[‡]
⁴Francesca Natali,^{¶,v} and Heloisa N. Bordallo^{*,†,‡,||,⊙}

⁵Niels Bohr Institute, University of Copenhagen, Universitetsparken 5, 2100 Copenhagen Ø, Denmark

⁶Institute for Frontier Materials, Deakin University, Burwood, VIC 3125 Australia

⁷Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, United States

⁸Australian Centre for Neutron Scattering, Australian Nuclear Science and Technology Organisation, Lucas Heights, NSW 2234, Australia

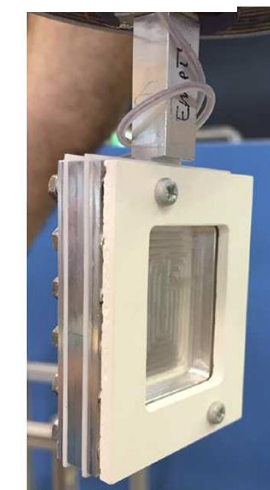
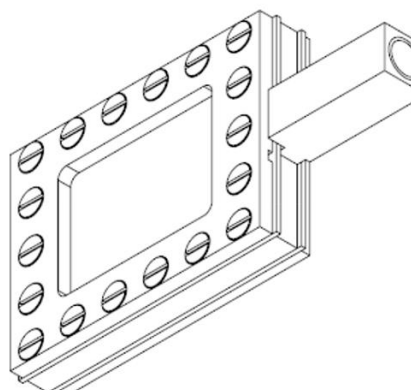
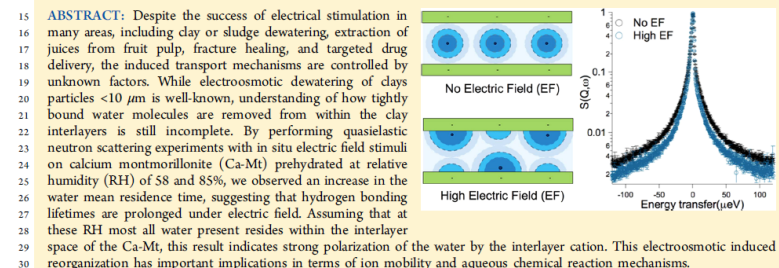
¹⁰Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institute, CH-5232 Villigen, Switzerland

¹¹Institute of Materials, Research National Council (CNR-IOM), 34149 Trieste, Italy

¹²VInstitut Laue-Langevin, BP 156, F-38042 Cedex 9, Grenoble, France

¹³European Spallation Source ESS AB, P.O. Box 176, SE-221 00 Lund, Sweden

¹⁴Supporting Information



15 **ABSTRACT:** Despite the success of electrical stimulation in
16 many areas, including clay or sludge dewatering, extraction of
17 juices from fruit pulp, fracture healing, and targeted drug
18 delivery, the induced transport mechanisms are controlled by
19 unknown factors. While electroosmotic dewatering of clays
20 particles <10 μm is well-known, understanding of how tightly
21 bound water molecules are removed from within the clay
22 interlayers is still incomplete. By performing quasielastic
23 neutron scattering experiments with in situ electric field stimuli
24 on calcium montmorillonite (Ca-Mt) prehydrated at relative
25 humidity (RH) of 58 and 85%, we observed an increase in the
26 water mean residence time, suggesting that hydrogen bonding
27 lifetimes are prolonged under electric field. Assuming that at
28 these RH most all water present resides within the interlayer
29 space of the Ca-Mt, this result indicates strong polarization of the water by the interlayer cation. This electroosmotic induced
30 reorganization has important implications in terms of ion mobility and aqueous chemical reaction mechanisms.

Cryomagnet (5 T) : like VM-3 (Berlin)



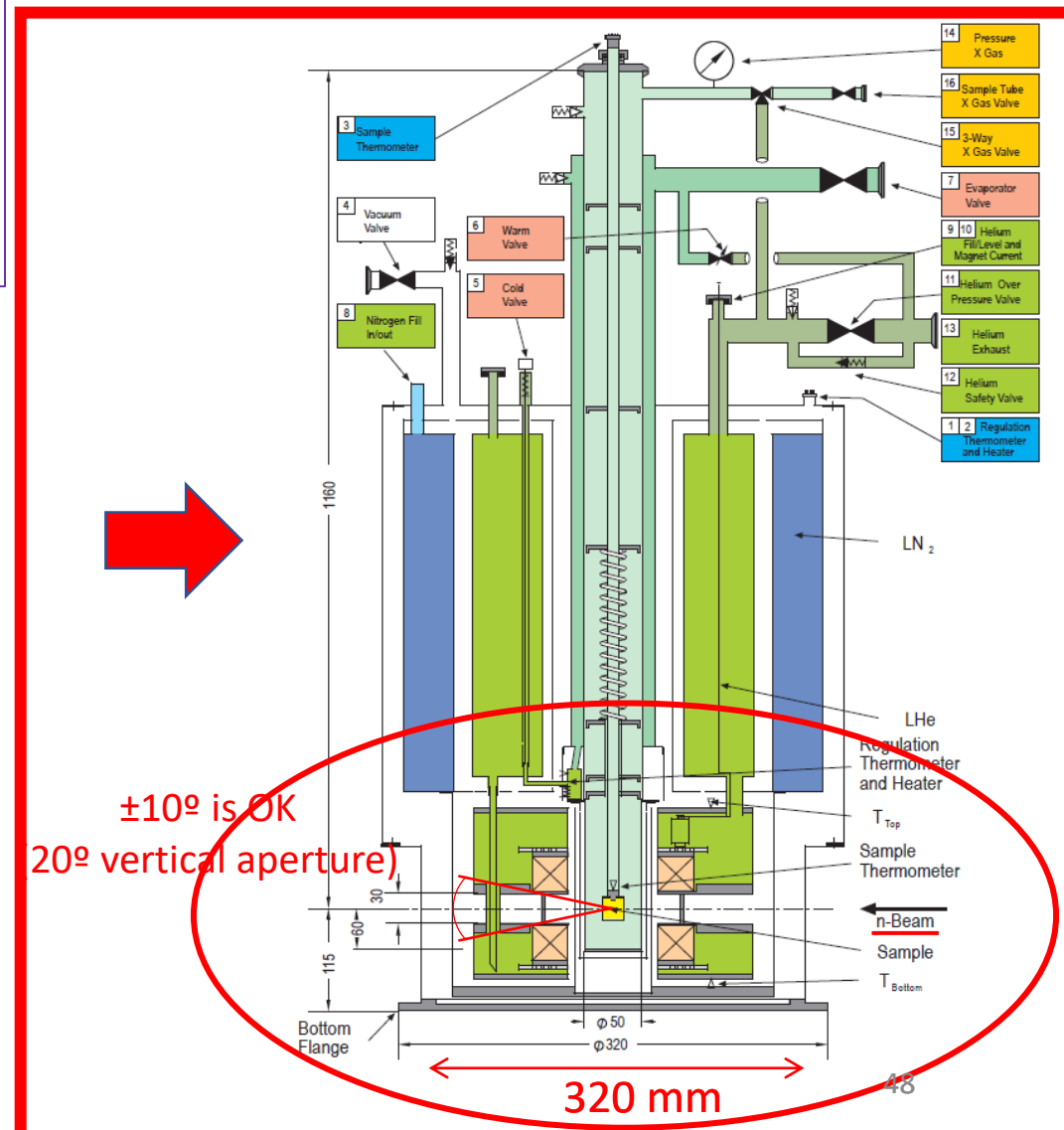
- Modified orange cryostat (L-He also for magnets; field up to **5 T**)
- Vertical aperture (through slight modification without affecting the magnets' distance: **$\pm 10^\circ$**)
- Diameter: **320 mm**

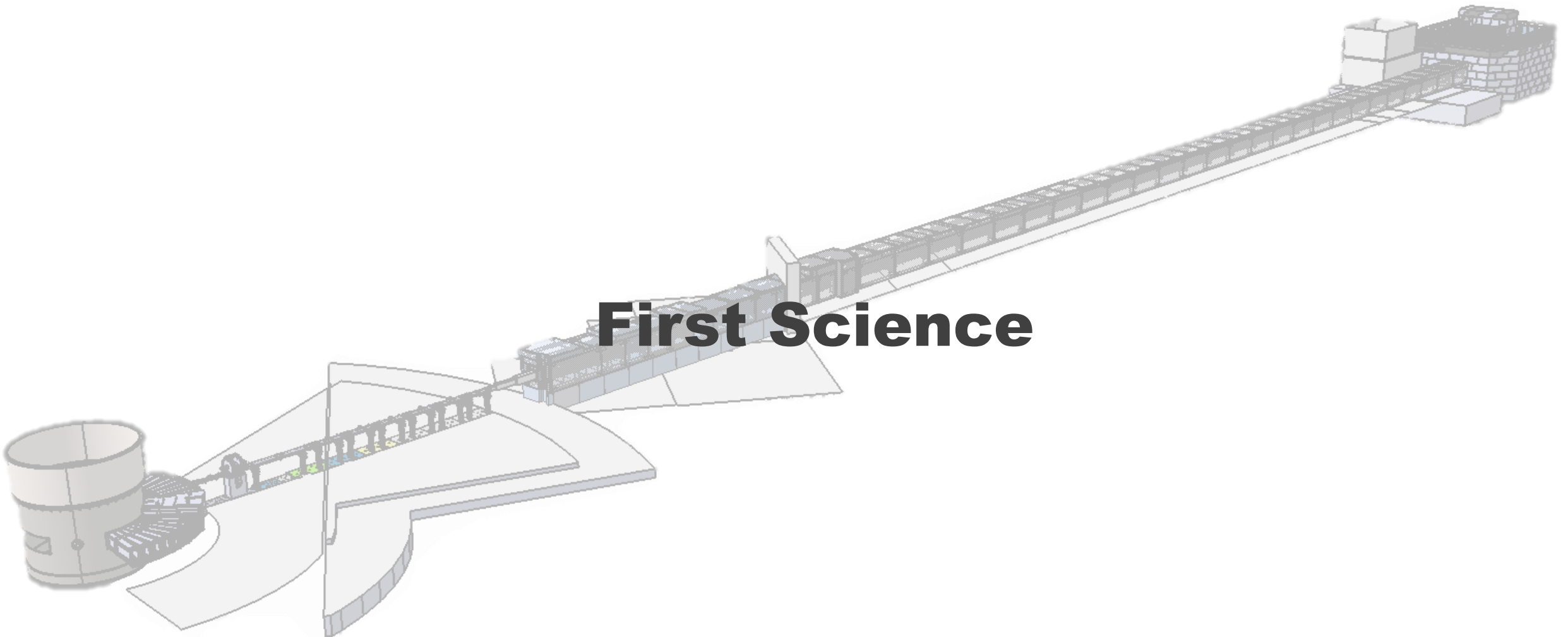
5.3 Vertical Magnet VM - 3

Specifications:

Manufacturer:	AS Scientific Products Ltd., Abingdon, GB
Temperature Range:	1.5 K - 300 K
with Dilution Insert:	50 mK - 1.2 K
Sample Diameter:	< 50 mm
with Dilution Insert:	< 40 mm
Split:	30 mm
Angle:	0°
LN ₂ -Hold Time:	24 h
LHe-Hold Time:	24 h
Magnetic Field (max):	5 T (symmetric)
horizontal Access:	Total view 345° (15° dead angle)
Total Thickness of Al-Screens:	2 x ca. 8 mm (no beam-in windows)
Thermometry Sensors:	Cernox®
Scheduled Position:	E1, E2, E3, E4, E6, V1, V2, V3, V4

This vertical magnet is a modified version of an Orange Standard cryostat



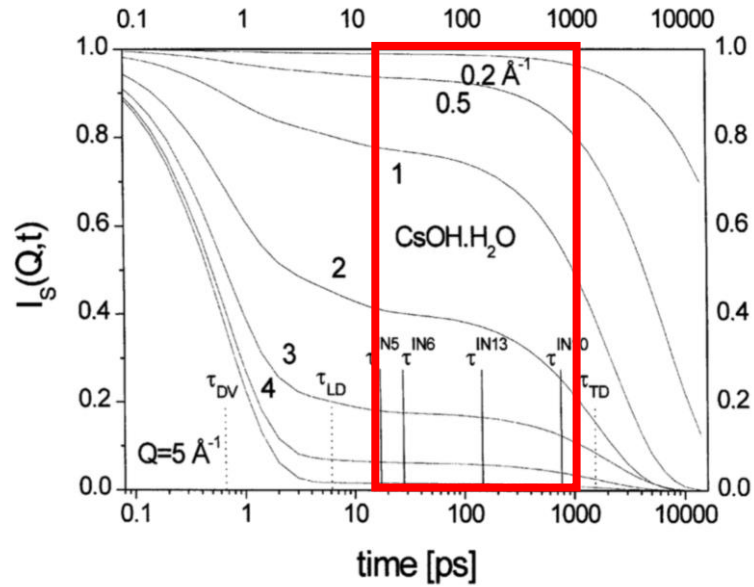


First Science

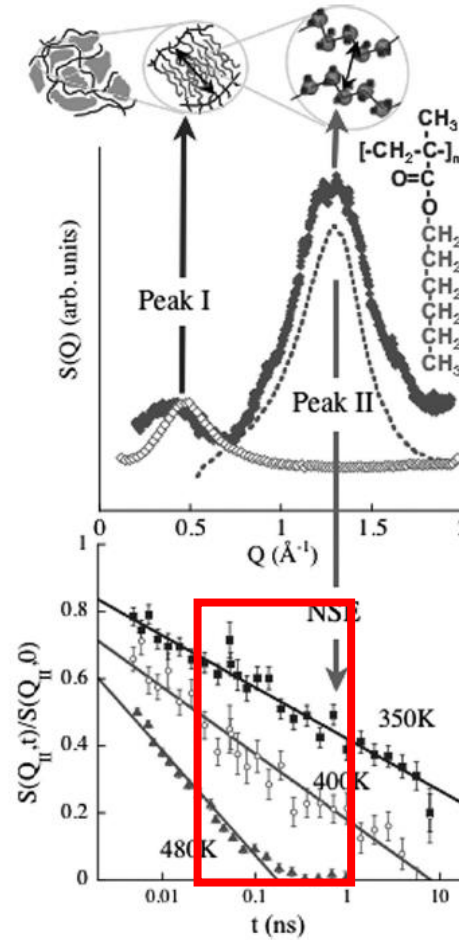


MIRACLES First Science

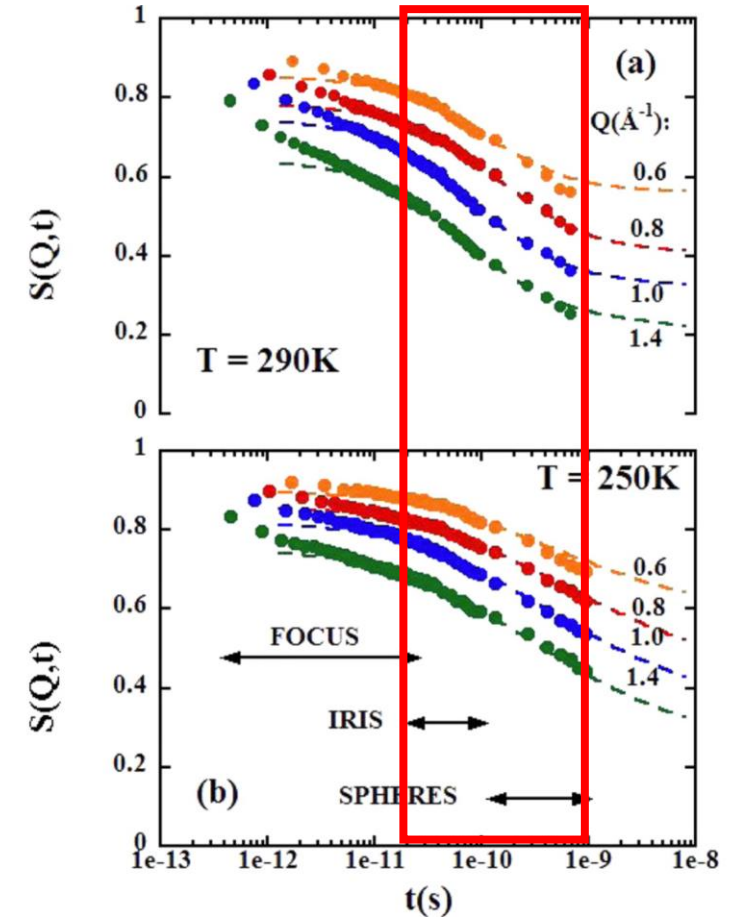
Carrying out one experiment at different timescales



R. E. Lechner, Physica B 301 (2001) 83–93



Arantxa Arbe & Juan Colmenero (2010), Neutron News, 21:3, 11-14



G. Goracci et al. Macromolecules. 48 (2015) 6724-6735

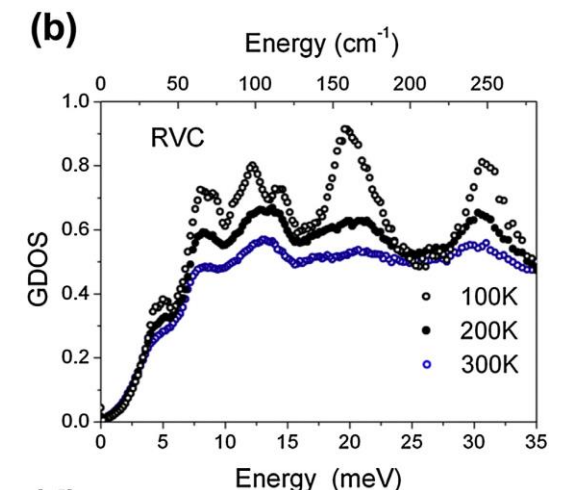
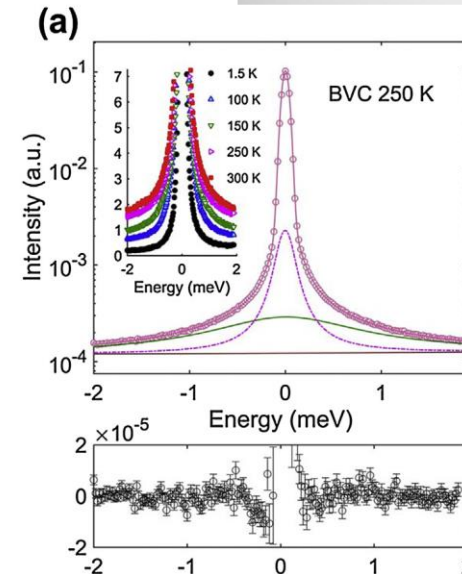
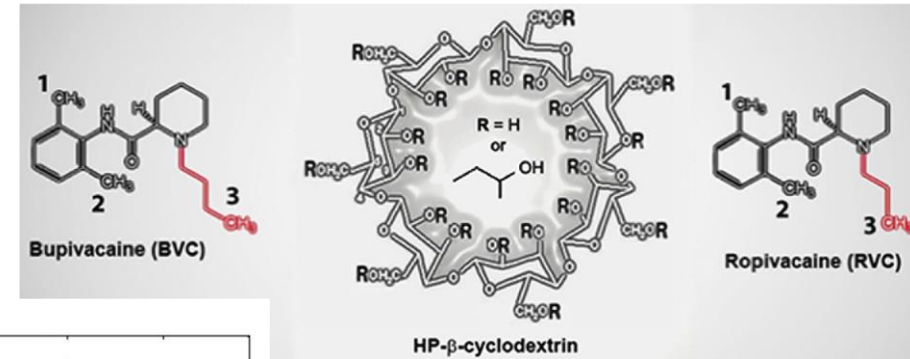
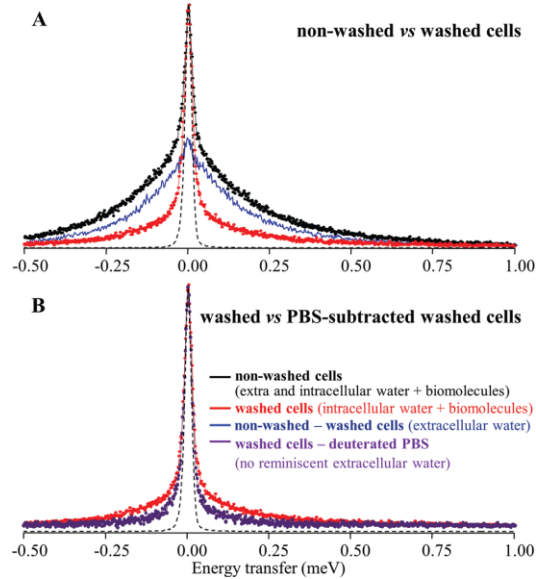
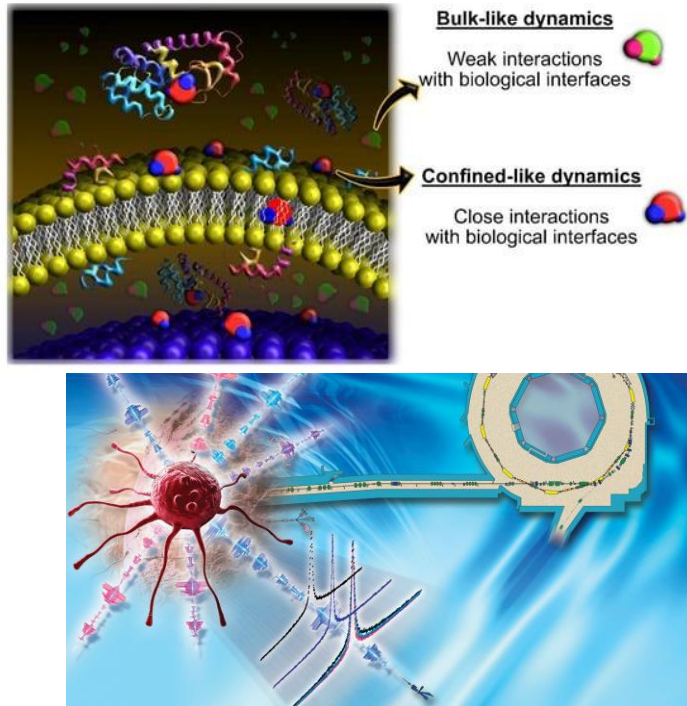
MIRACLES First Science

Mobile vs. Immobile fraction & Complex diffusive behavior (molecular crowding):

- Dynamics of water IN and AROUND cells
- Improving drug delivery systems relying on slow dynamics or control of docking

☐ Test capability of high and variable resolution

☐ Test INS

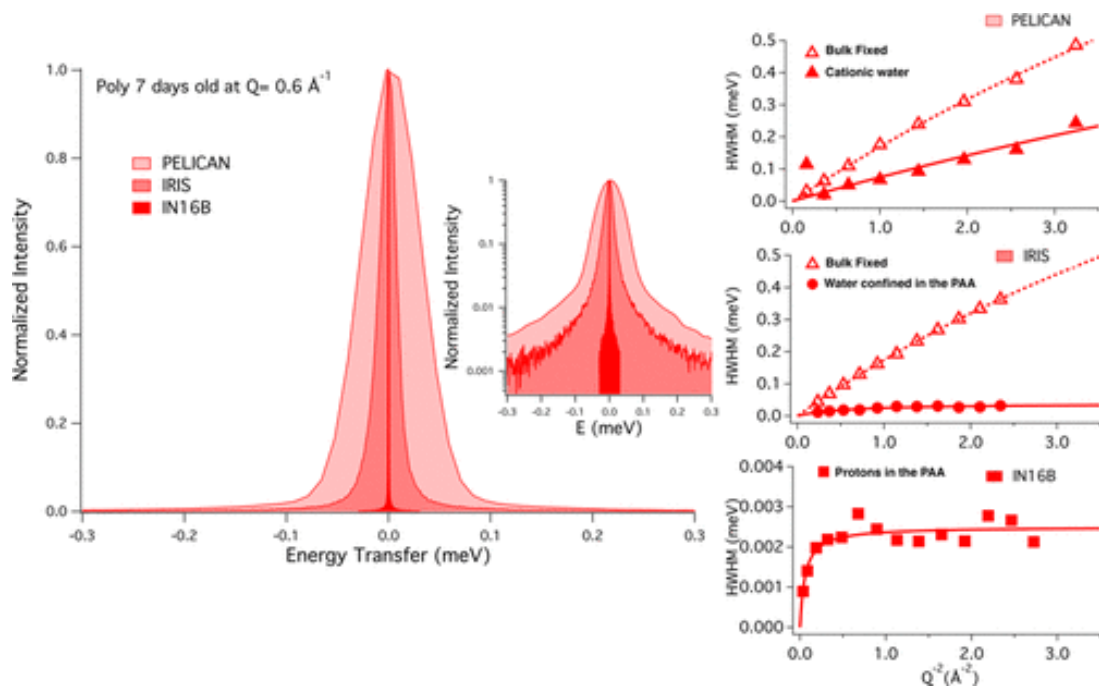


MIRACLES First Science

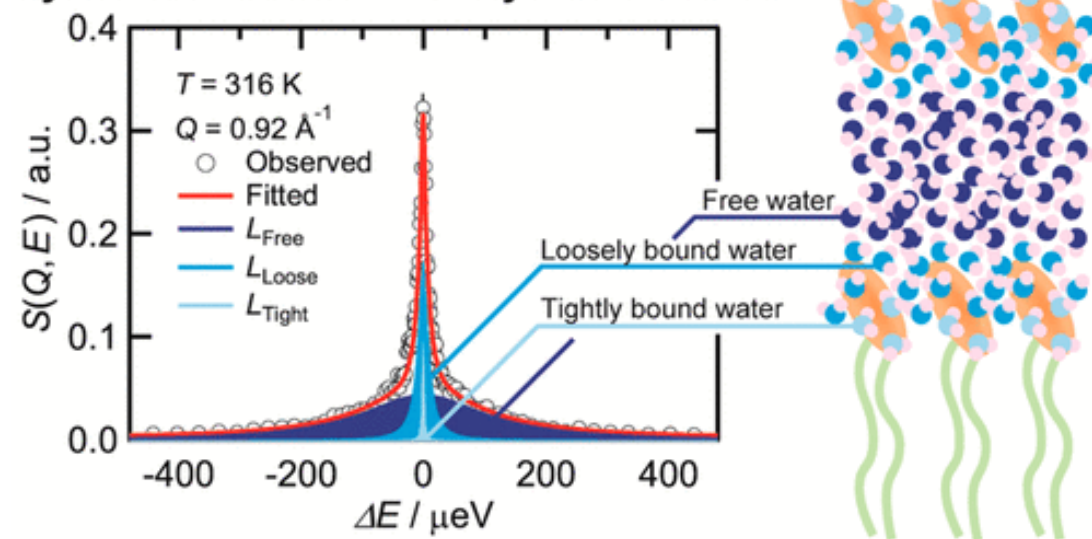
Fast protein dynamics and stability.

(Many times, this type of study is restricted to elastic window scan quasielastic signal is very often neglected because of poor statistics)

- ❑ Test MIRACLES high flux
- ❑ Variable energy resolution QENS
- ❑ Q-dependent measurements

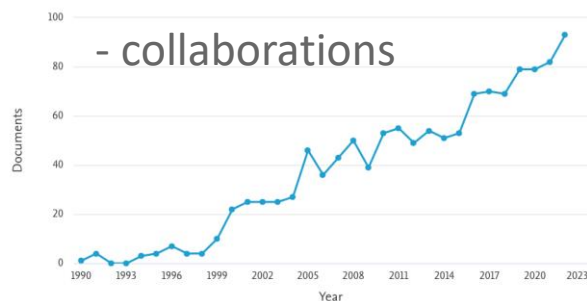
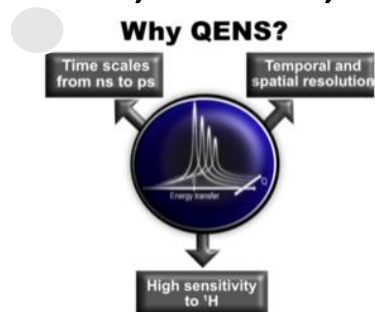


Dynamical Behavior of Hydration Water



MIRACLES First Science: Ideas

- Idea 1
- Water, water, water



- - requirements from SE/DMSC/Labs/external developmental

- Idea 2
- Understanding and predicting how amino acid substitutions affect proteins



Integrative Structural Biology at the University of Copenhagen

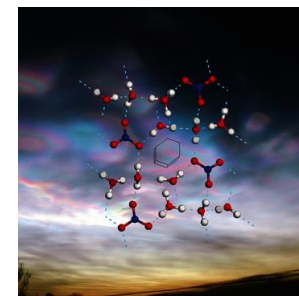


Rasmus Hartmann-Petersen & Kresten Lindorff-Larsen

*Molecular Biology and Evolution, 38, 2021, 3235–3246

- - SE: sample changer
- - DMSC: complex data analysis

- Idea 3
- Climate change and cloud formation



- - Grothe – TU Wien
- <https://www.tuwien.at/tch/pc/physikalische-chemie-der-atmosphaere>
- - Gates and Iles groups – AUS*
- * *J. Phys. Chem. C* 2022, 126, 21061–21070
- - SE: T & P (& Raman)
- - DMSC: complex data analysis



Upgrade to Completion

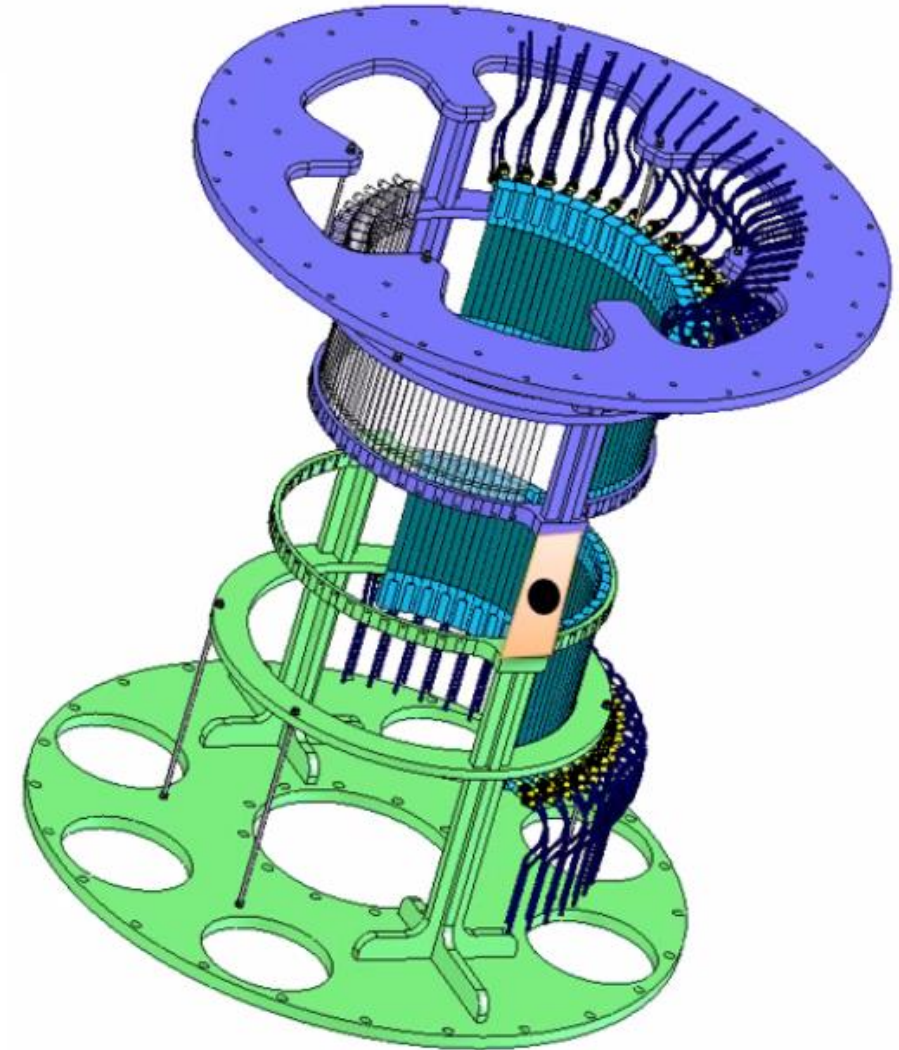
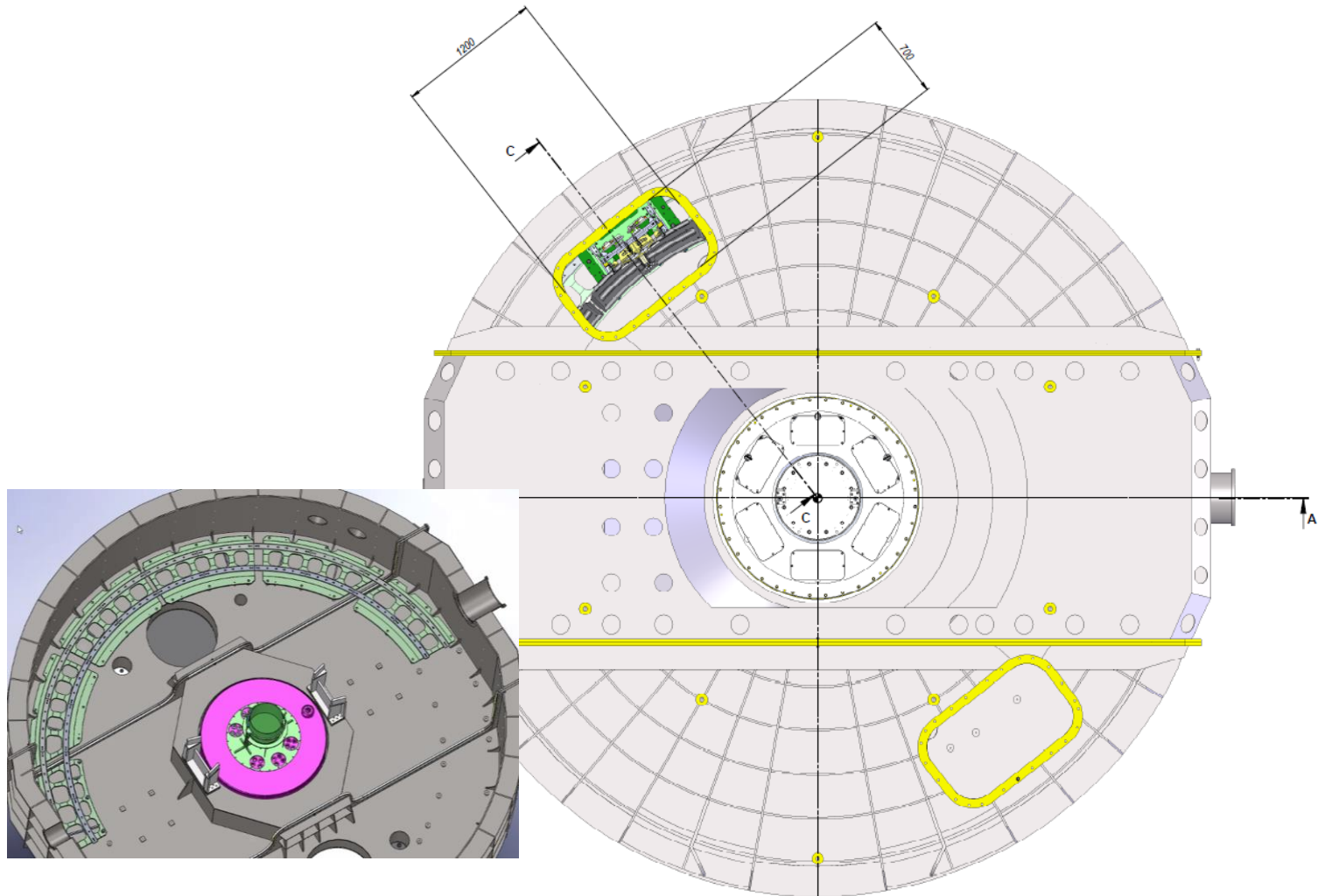


ESS
bilbao



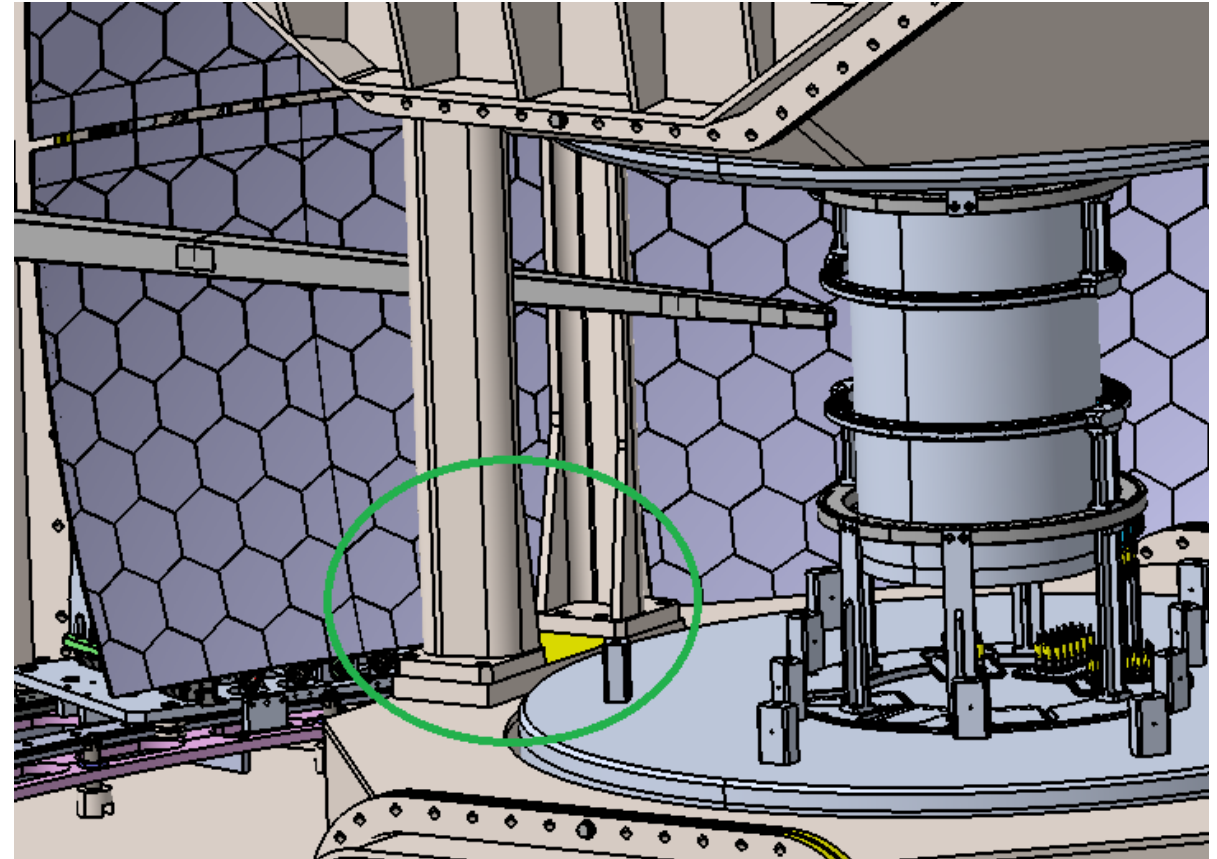
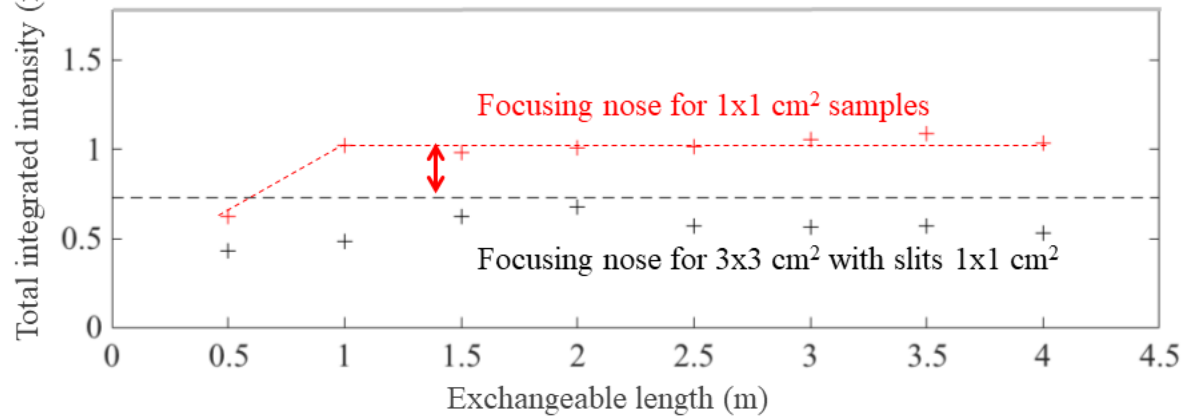
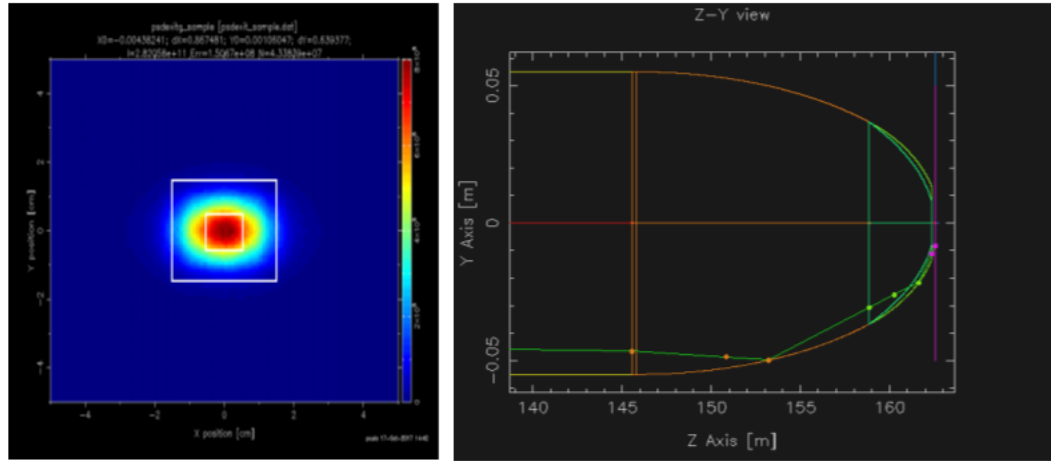
Full angular coverage

Design of scattering system allows completion of the instrument



Guide exchanger

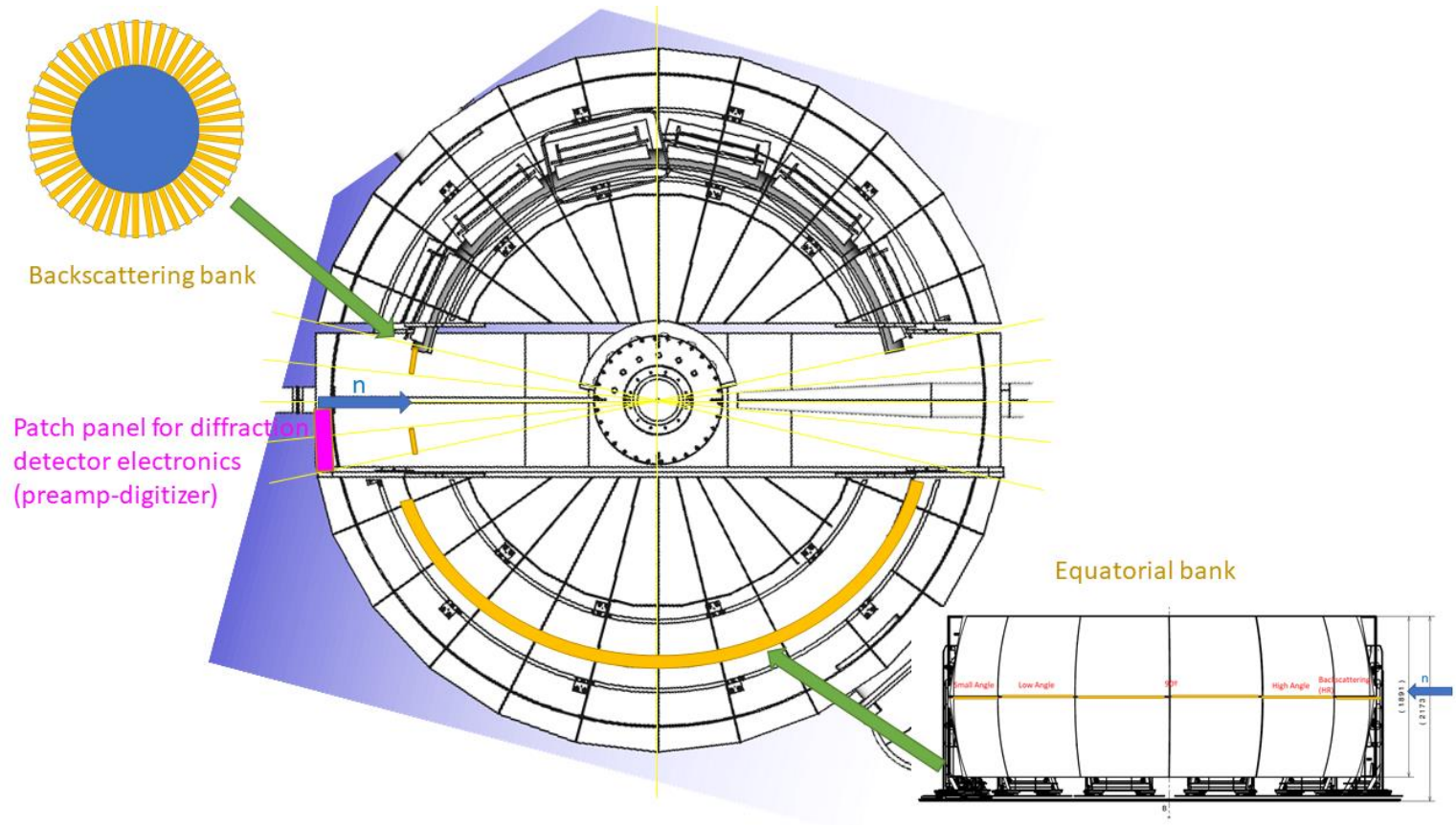
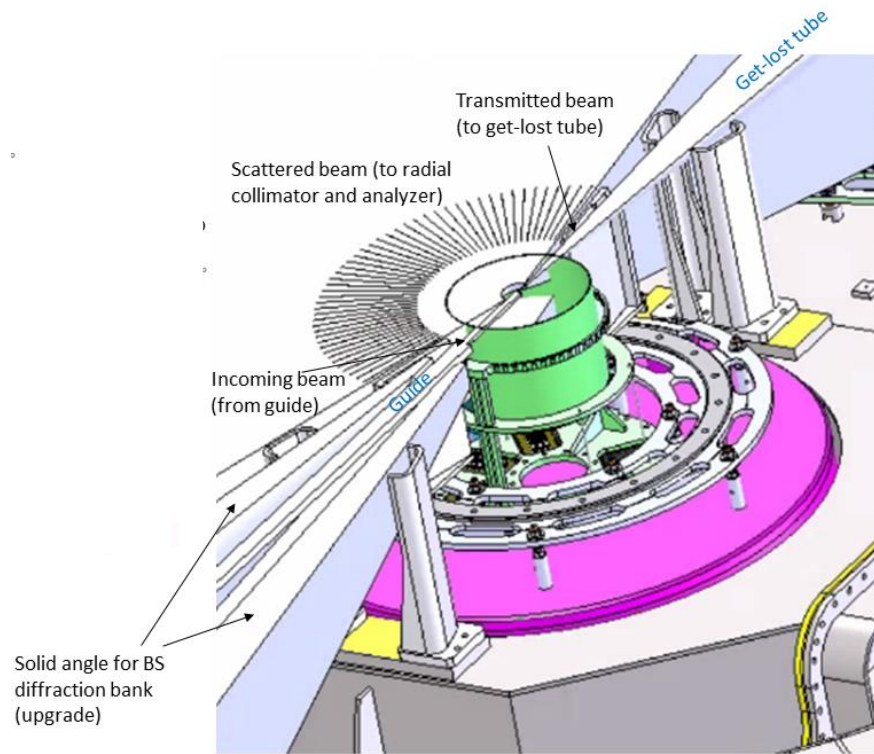
Gaining up to 70% for small samples (1x1 cm²)

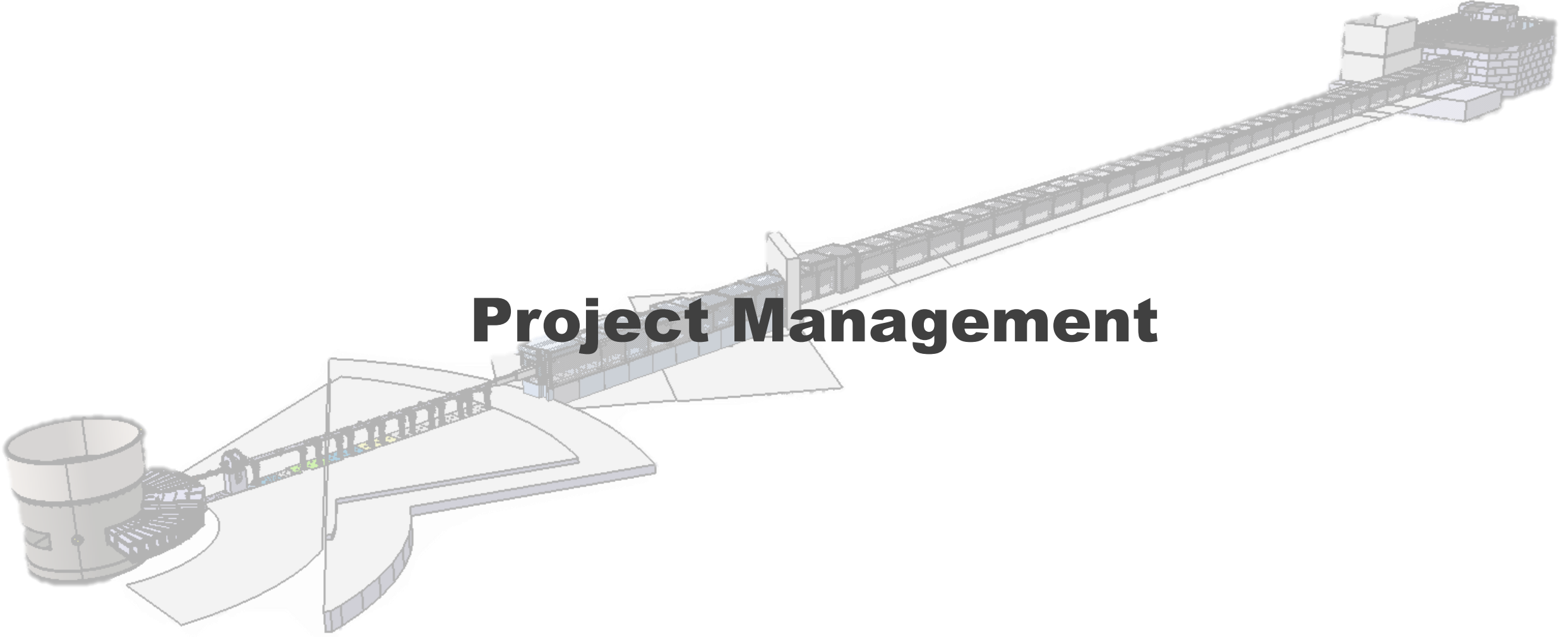


Diffraction

Detectors for diffraction in:

- Equatorial position
- Backscattering





Project Management



Risks & challenges

- Main risks: Cost & Schedule
- Quality risks anticipated

Top 5 Risks				
Title	Rating	Category	Partner	Treatment
Cave design	12	Schedule	ESS-Bilbao	Reduce
Delayed delivery and technical challenges of fast choppers	10	Quality	ESS-Bilbao	Avoid
Problems with the supply of detectors	9	Schedule	ESS-Bilbao	Observe
Increasing cost associated to scope creep	8	Cost	ESS	Reduce
Deterioration of analyzer components	5	Quality	ESS-Bilbao	Avoid

Top 5 Issues						
Title	Rating	Category	Partner	Cost	Delay	Quality
Unsuitable beam monitors	16	Schedule	ESS	<25k€	7-12 months	It is certain that high level goal can't be reached with minor impact on science case
Delayed delivery of in-bunker guide components	9	Schedule	ESS-Bilbao	N/A	4-6 months	N/A
Delayed delivery of key guide components: BWI	9	Schedule	ESS-Bilbao	N/A	4-6 months	A technical requirement can't be met, but high level goal reached
Choppers cost increase	9	Cost	ESS-Bilbao	100-300k€	<1 month	Margin between delivered results and technical requirements reduced
Electrical infrastructure lack of installation resources	9	Cost	ESS-Bilbao	100-300k€	N/A	A technical requirement can't be met, but high level goal reached

Status of MIRACLES instrument (Mar'23)



SubTG3s: Along 2022-2023
Installation (bunker): Q4-2023 / Q1-2024
Installation (E01): 2024-2025
Installation (E02): 2025
Completion: 2025

Choppers (all) (ESS-B)
 Des. & Mfg. **AERInova**
 SubTG3 approved: Nov-22 & Mar'23
 Delivery: Oct '23 (in-bunker)
 Jan'25 (out-of-bunker)

Chopper racks (ESS)
 NSS Common Project

BWI (ESS-B)
 Des. & Mfg. **S-DH**
 SubTG3 approved: Mar'23
 Delivery: Sep'23 (tentative)

NBOA (ESS-B)
 FAT Sep '21 **SwissNeutronics**
 Delivery: Oct '21

In-bunker Guide (ESS-B)
 Des. & Mfg. **SwissNeutronics**
 SubTG3 approved: Nov-22
 Delivery: Jan'24

In-bunker Guide supports (ESS-B)
 SubTG3 (in-bunker) approved: Nov-22
 Tender (Mfg.): Apr '23
 Delivery: Nov '23 (in-bunker)

Out-of-bunker Guide supports (ESS-B)
 SubTG3: May'23
 Tender (Mfg.) Sep '23
 Delivery: '24-'25

Thermal shutter (ESS-B)
 SubTG3 approved: Mar'23
 Tender (Mfg.): Jun '23
 Delivery: Jan'25

Beam Monitors (ESS)
 NSS Common Project

Control Room (ESS-B)
 FM Control Hutch?
 Delivery: Dec '24

Vessel (ESS-B)
 Des. & Mfg. **QVS**
 SubTG3 approved: Mar'23
 Delivery: Sep '24

In-vessel (ESS-B)
 Des. & Mfg. **QVS**
 SubTG3 : Feb'23
 Delivery: Sep '24

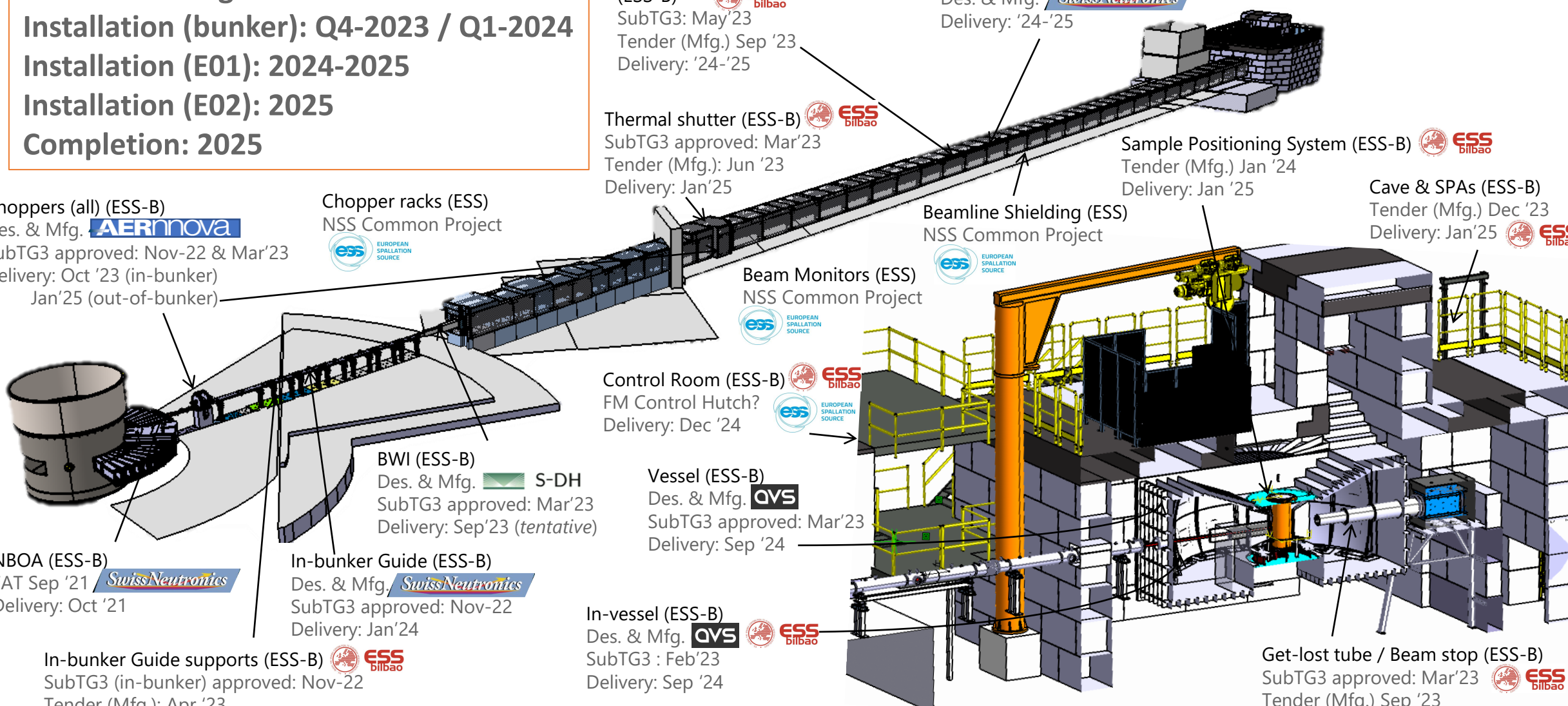
Out-of-bunker Guide (ESS-B)
 Des. & Mfg. **SwissNeutronics**
 Delivery: '24-'25

Beamline Shielding (ESS)
 NSS Common Project

Sample Positioning System (ESS-B)
 Tender (Mfg.) Jan '24
 Delivery: Jan '25

Cave & SPAs (ESS-B)
 Tender (Mfg.) Dec '23
 Delivery: Jan'25

Get-lost tube / Beam stop (ESS-B)
 SubTG3 approved: Mar'23
 Tender (Mfg.) Sep '23
 Delivery: Sep '24



TG3 dates

Sub-TG3.1 – In-bunker BTCS: August-2022

**Sub-TG3.2a – Out-of-bunker BTCS Part I (BWI, FO chopper, Shutter):
November-2022**

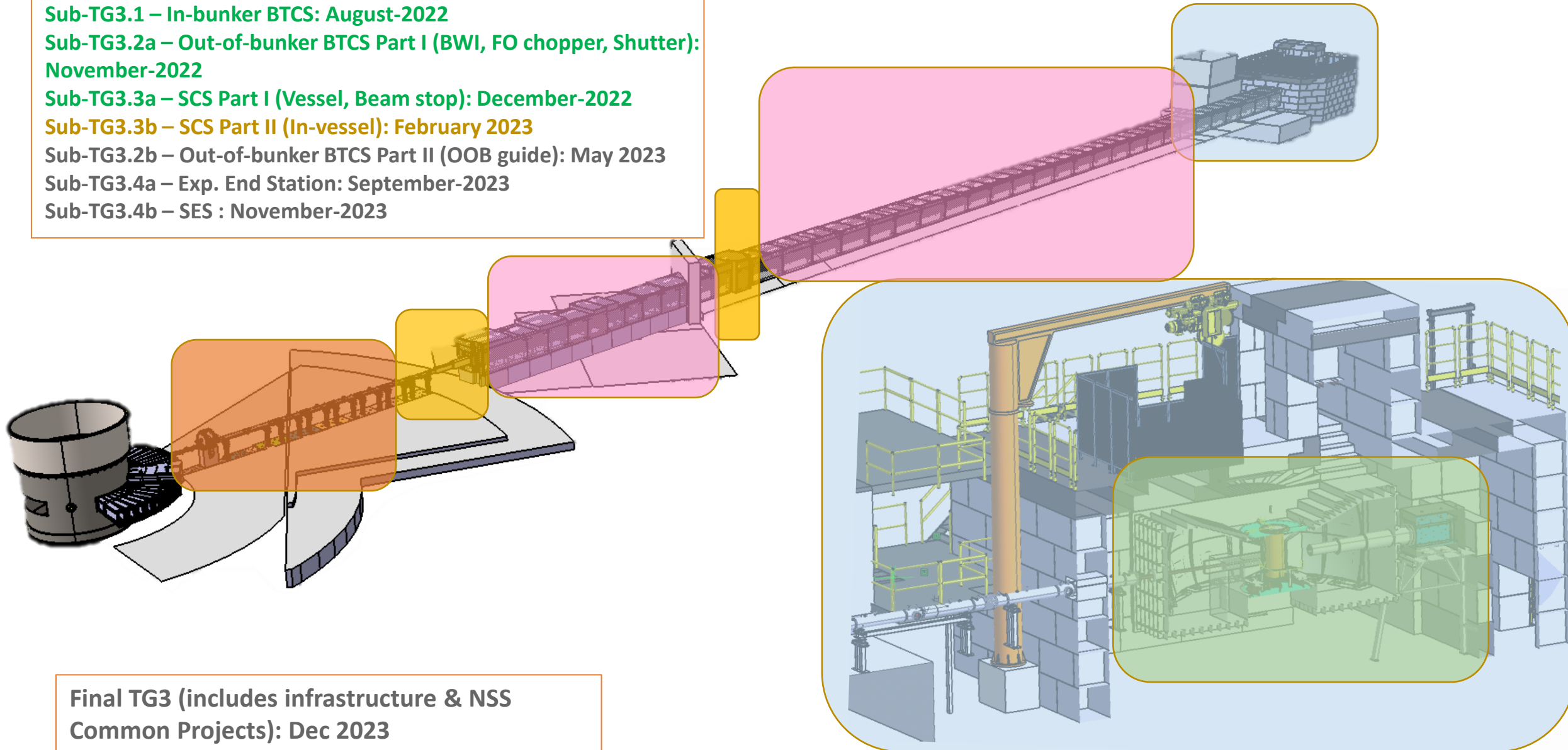
Sub-TG3.3a – SCS Part I (Vessel, Beam stop): December-2022

Sub-TG3.3b – SCS Part II (In-vessel): February 2023

Sub-TG3.2b – Out-of-bunker BTCS Part II (OOB guide): May 2023





Sub-TG3.4a – Exp. End Station: September-2023

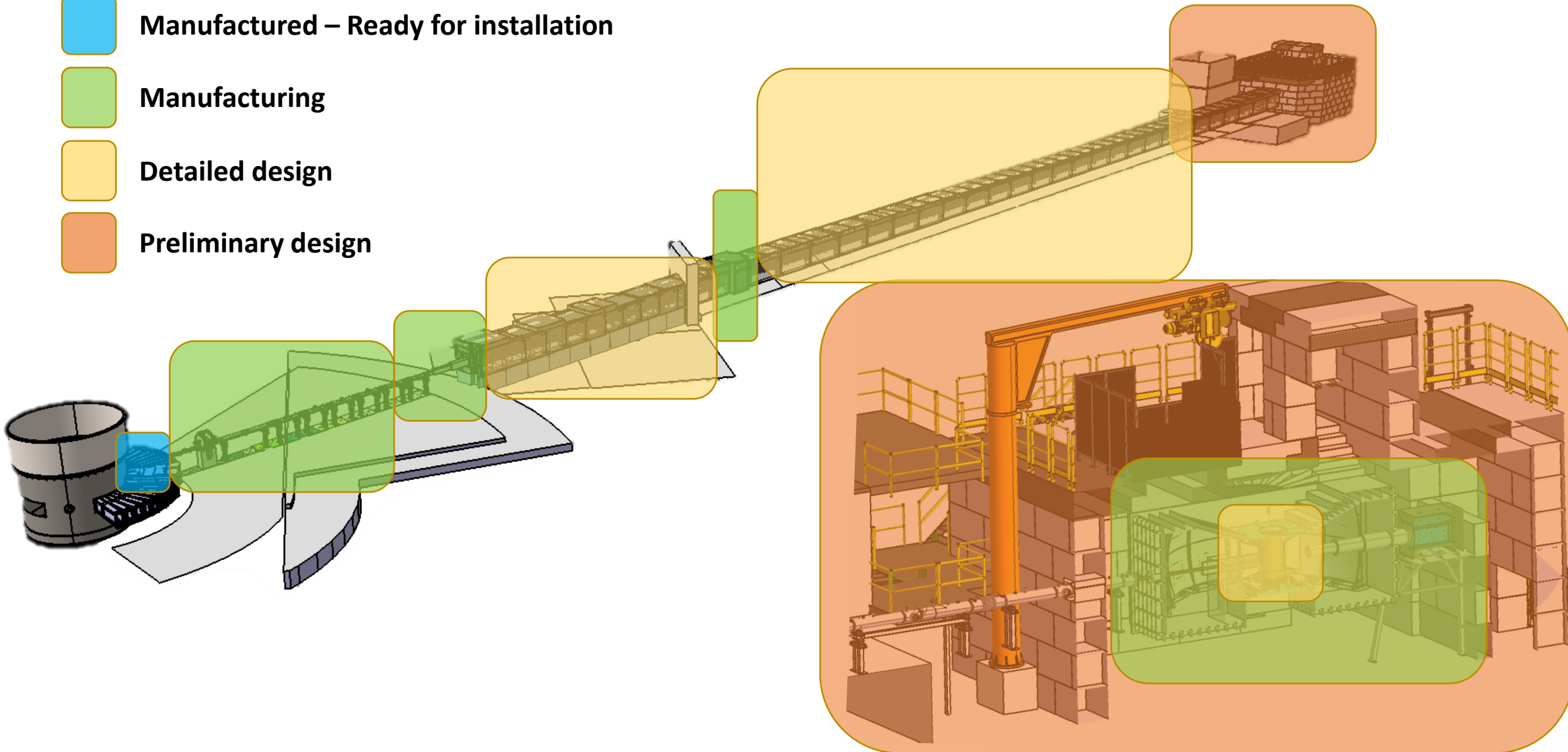
Sub-TG3.4b – SES : November-2023



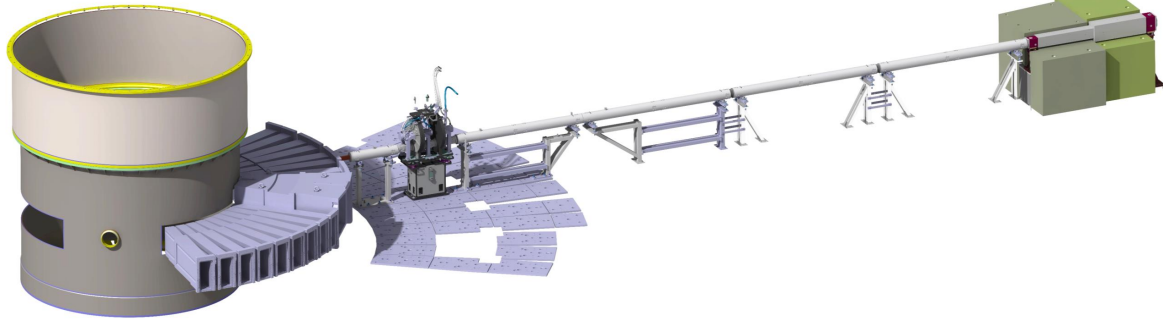
**Final TG3 (includes infrastructure & NSS
Common Projects): Dec 2023**

Maturity level

-  **Manufactured – Ready for installation**
-  **Manufacturing**
-  **Detailed design**
-  **Preliminary design**

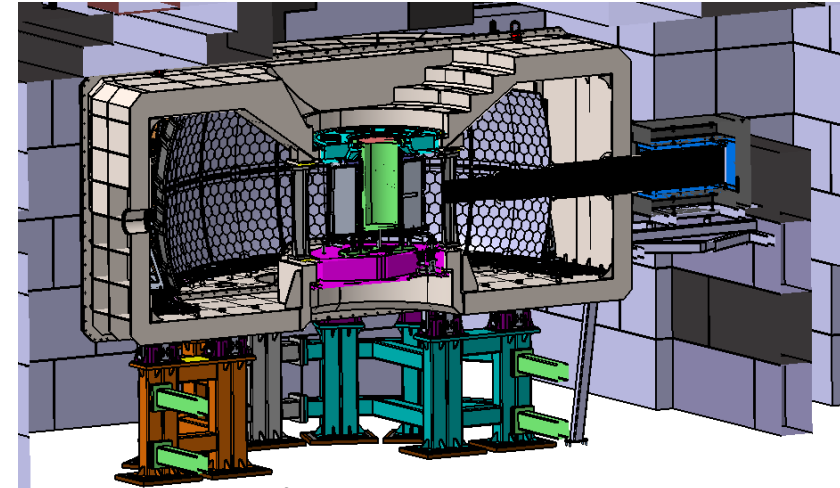


Installation schedule MIRACLES (proposal)



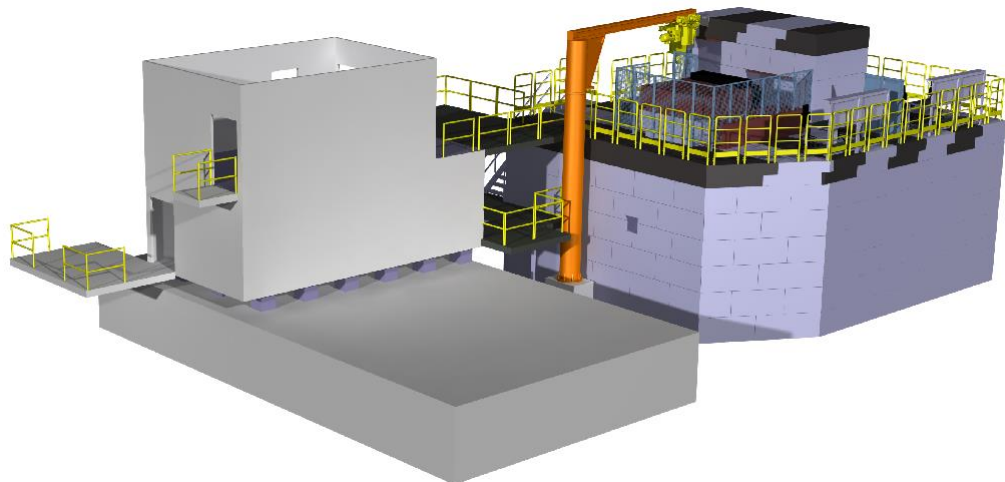
In-Bunker Beamline

- October 2023 – February 2024



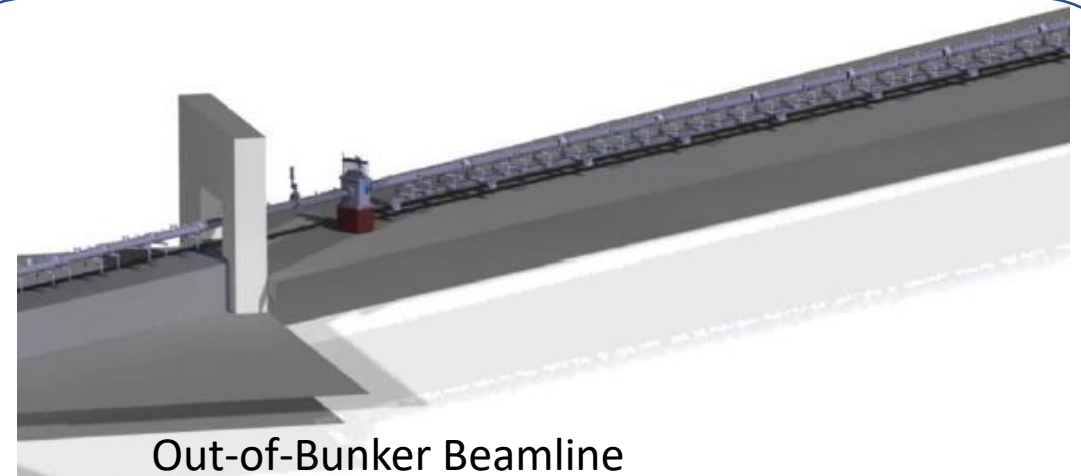
Scattering Characterization System

- September 2024 – December 2024



Experimental End Station

- January-March 2025



Out-of-Bunker Beamline

- D03 & E01: March – July 2024
- E02: March – July 2025

MIRACLES core team



Alex Conde



Aitor Zugazaga



Idoia Mazkieran



Iván Aranda



Giles Harper



Octavio G del Moral



Roberto Martínez



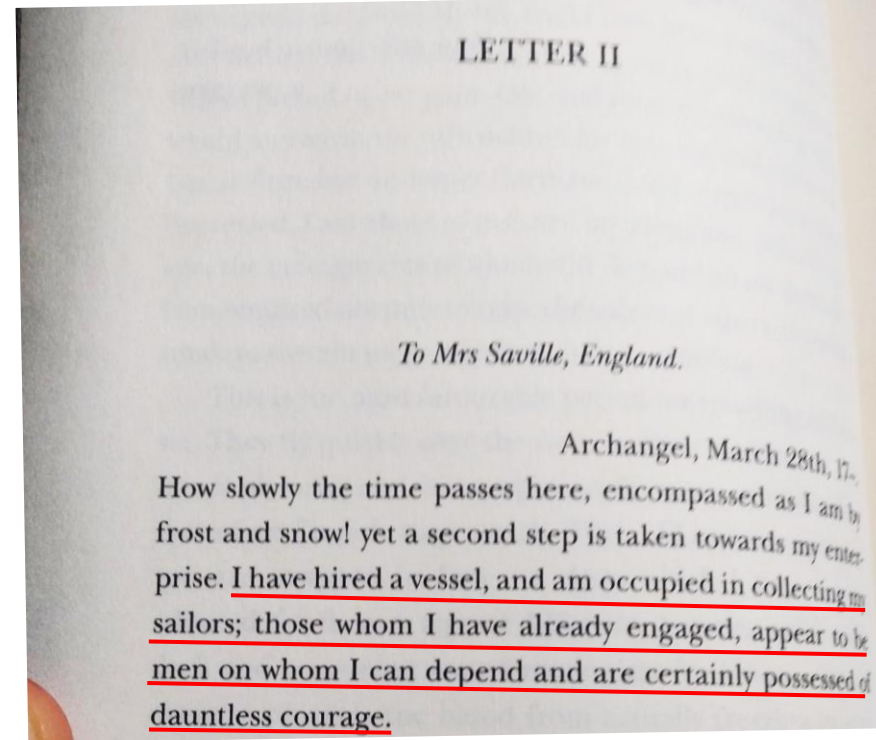
Jose Pereira



Heloisa N. Bordallo



Félix J. Villacorta





ESS Bilbao

