VESPA, the neutron vibrational spectrometer at the ESS

Spectroscopy STAP

PRESENTED BY ADRIEN PERRICHON

2025-10-21

Outline

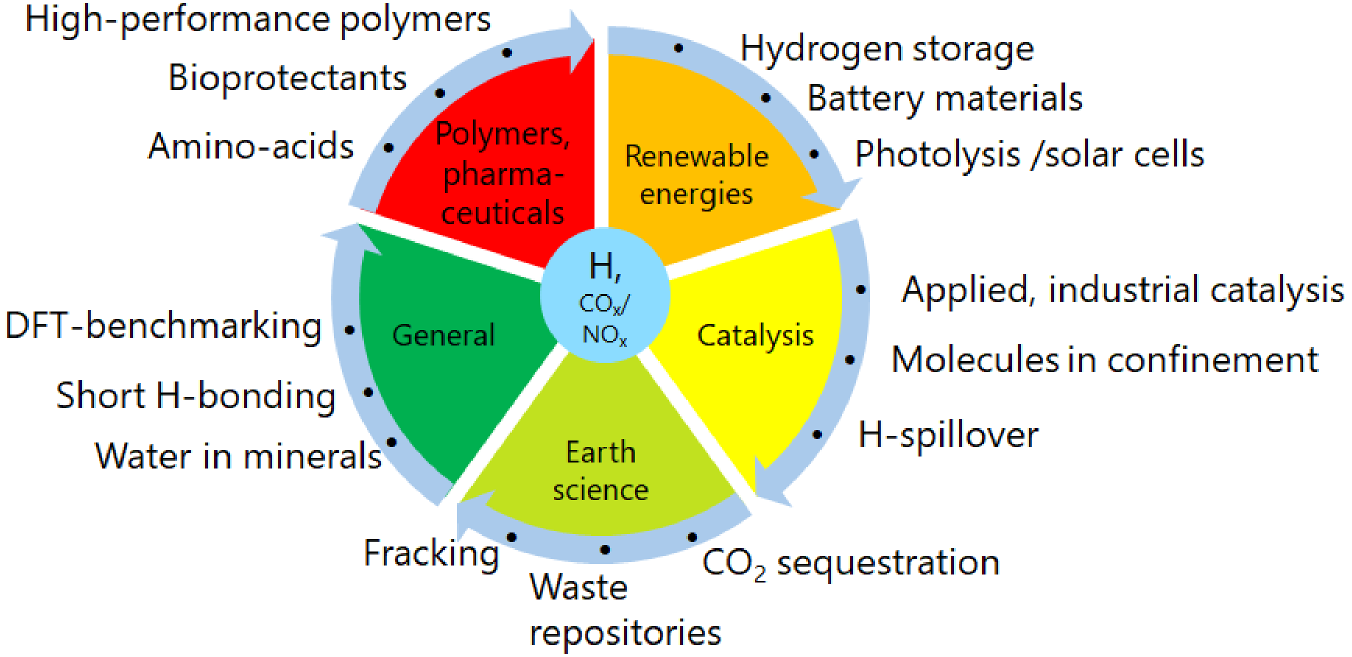
1. Introduction
2. Progress Report
3. Primary Spectrometer
4. Secondary Spectrometer – Scientific Concept
5. Secondary Spectrometer – Engineering & Prototyping
6. Cave & Hutch

Introduction

Introduction

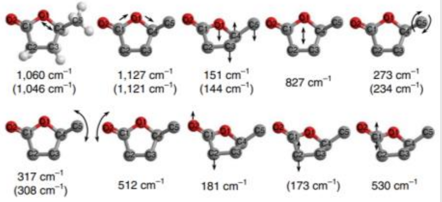
VESPA science

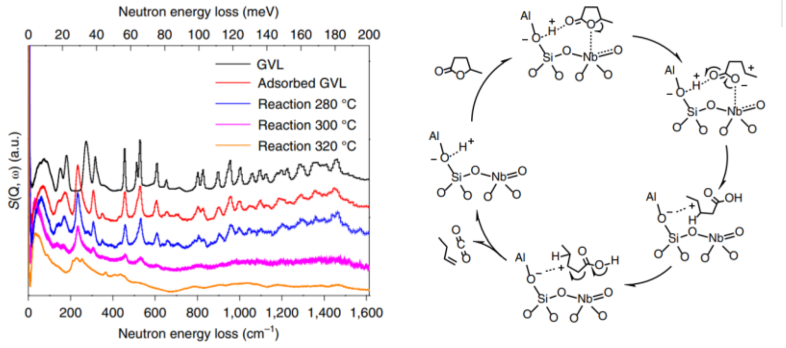
- Neutron Vibrational Spectroscopy (NVS) is the neutron analogue to infrared/Raman
- "Fingerprint" region: 480 – 1800 cm^{-1} (60 – 220 meV)
- Broad science case in chemistry, focus on catalysis & energy materials



Quantitative production of butenes from biomass-derived γ-valerolactone catalysed by hetero-atomic MFI zeolite

❖ Lin et al., Nature Materials 19 (2020) 86-93

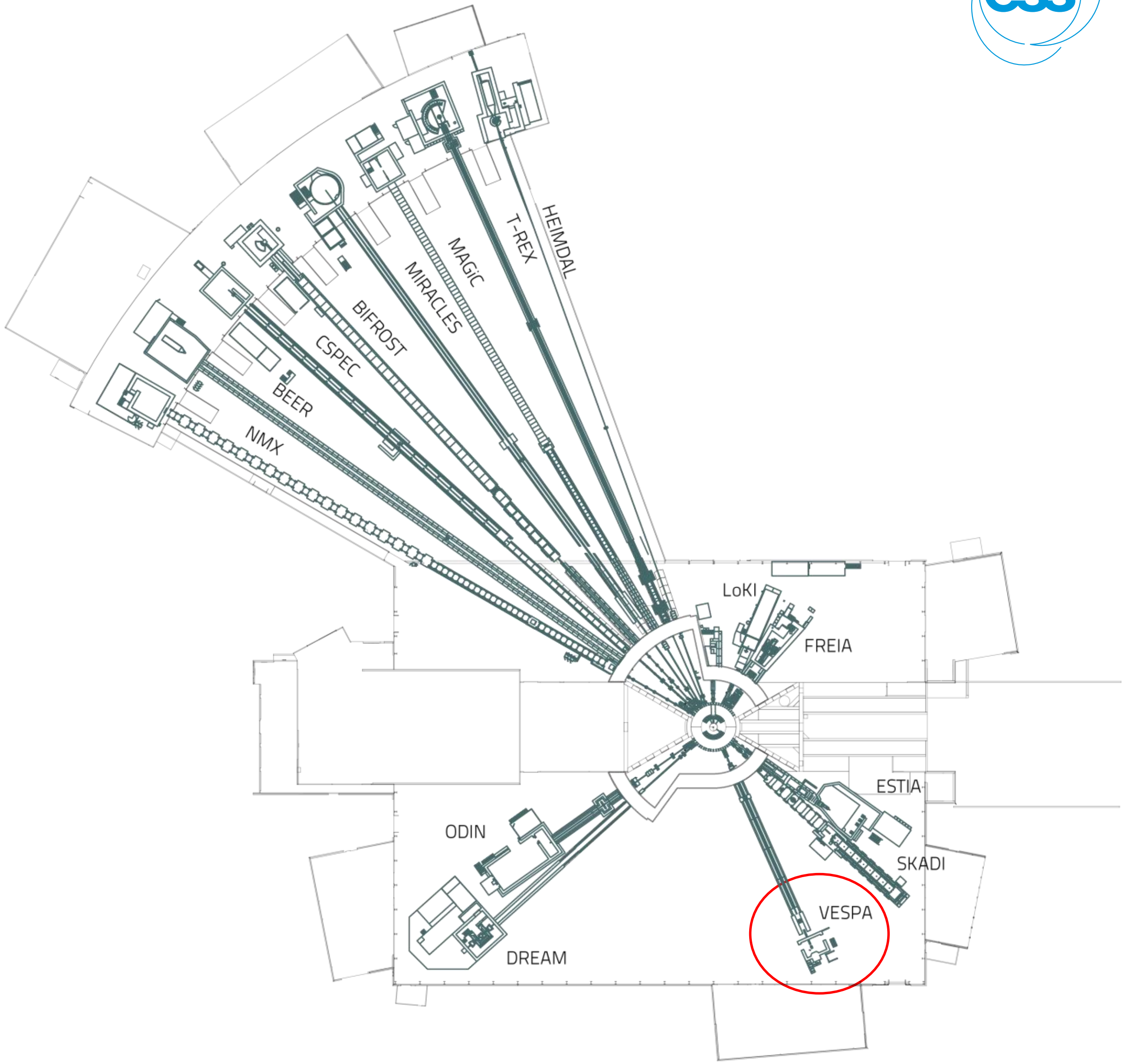




Introduction

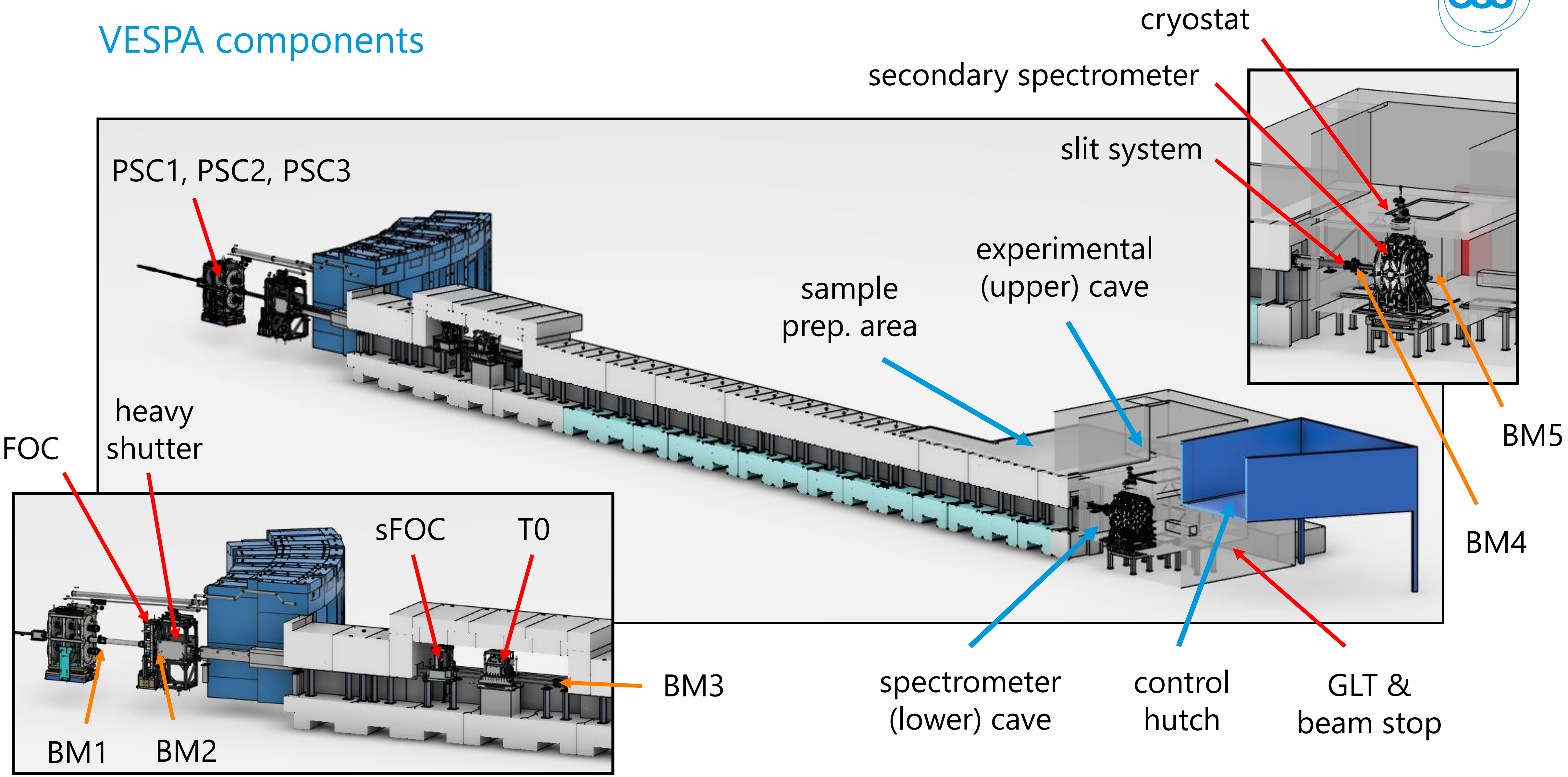
VESPA quick facts

- E7 beam port with direct view of the thermal moderator
- 59 m long instrument with a high-*m* elliptic supermirror guide
- Complex chopper cascade to achieve 3 subframes and variable resolution
- Broad band, Ei = 3–1200 meV
- Indirect-geometry crystal-analyser
- Complex and compact secondary spectrometer: >500 ^{3}He tubes, >12000 HOPG crystals, >250 kg of cryo-cooled Be, in <2 m^{3} volume



Introduction

VESPA components



Introduction

VESPA team

Team members	Affiliation, %FTE	Role
Adrien Perrichon	ESS, 100%	Lead Scientist
Monika Hartl	ESS, 100%	Instrument Scientist
Rosa Camilleri Lledó	ESS, 100%	Lead Engineer
Liam Whitelegg	ESS, 50%	Lead Engineer
Helen Popland	ESS, 100%	Mechanical Engineer
Alexander Johansson	ESS, 100%	Mechanical Engineer
Lorenzo Di Fresco	CNR, 50%	Project Engineer
Roberto Senesi	CNR, 20%	Project Sponsor

Consiglio Nazionale delle Ricerche

INFN Istituto Nazionale di Fisica Nucleare

UKRI Science and Technology Facilities Council

ISIS Neutron and Muon Source

Progress Report

Progress report

Update since April 2025

Project organisation and timeline

- VESPA has joined CEP, CUP, MCA in September
- New TG5 estimate in March 2029

Primary spectrometer

- Bridge beam guide (BBG) and light shutter – installation completed in September
- Supermirror guide – procurement ongoing with evaluation of the bid from Swiss Neutronics
- Choppers (PSC, FOC, sFOC) – preliminary design review completed in May
- T0 chopper – rescoping approved, to be delivered on time for day 1 operation
- Beam monitors – agreement that the front-end & integration will be transferred to ESS
- Slit system – not started

Progress report

Update since April 2025

Civil infrastructure (cave, beam stop, sample prep., hutch)

- All procurements transferred to ESS – procurement to be started in Feb 2026
- Concept design is ongoing (with support from Neutronics)
- Current plan: large cave expanding on E6 to allow installation/maintenance inside the cave

Sample exposure system

- Cryostat – specifications in preparation to start the procurement in Q1 2026
- Sample changer – not started

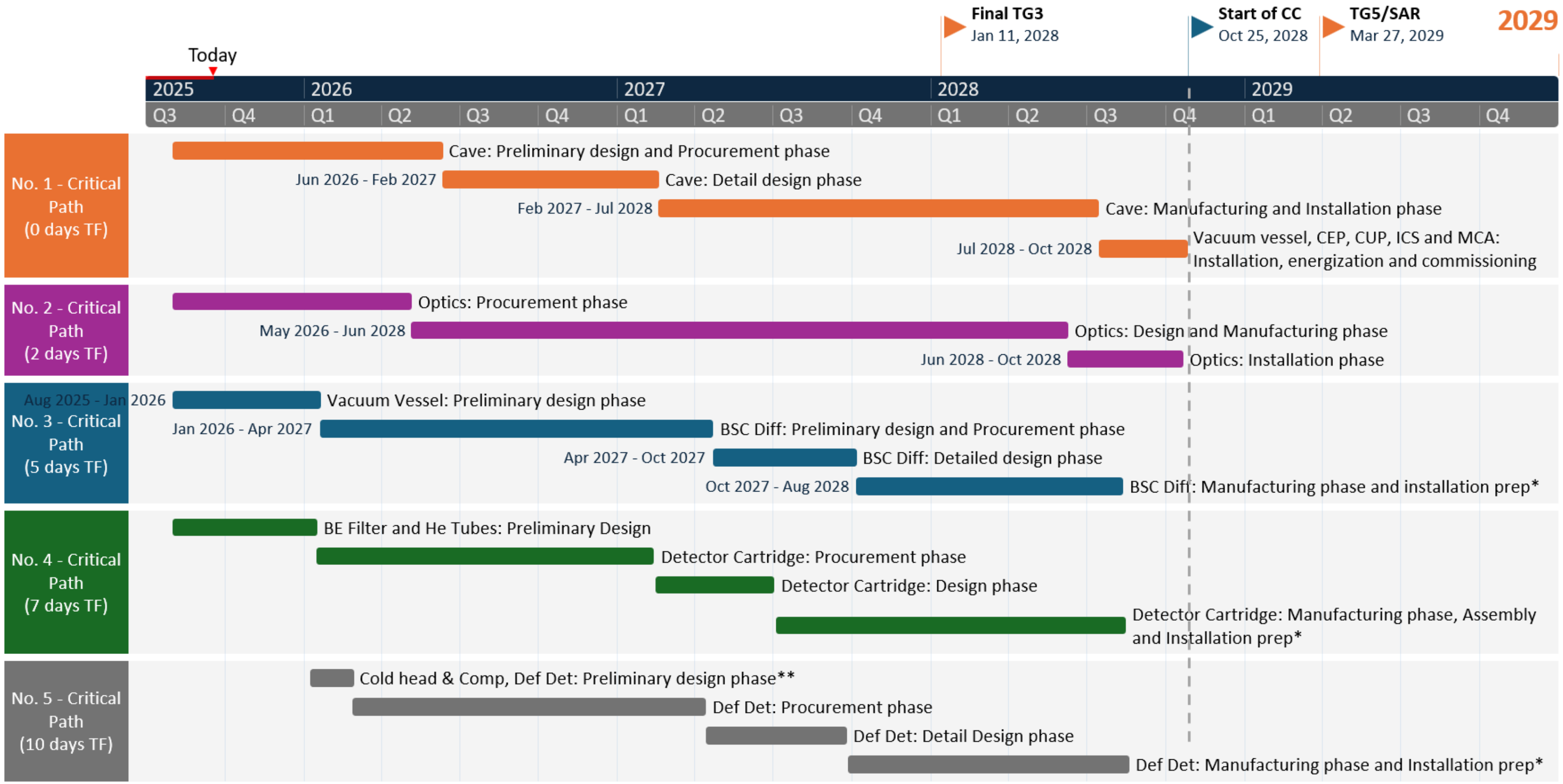
Secondary spectrometer

- Design – ongoing, with the aim to pass the preliminary design review in December
- Prototyping – analyser (backplate, coating, HOPG), gas box (windows)

Progress report

P6 as of August 2025

To be updated and re-baselined after PDR of secondary



Cave and guide have conservative durations for detail design and manufacturing

Guide procurement likely to be completed in Q1 2026

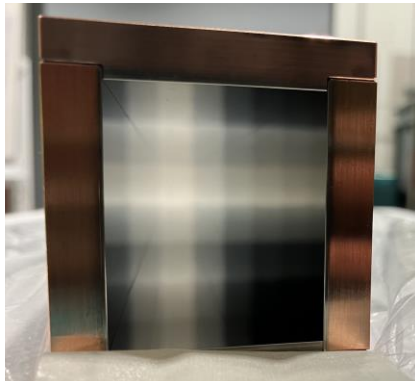
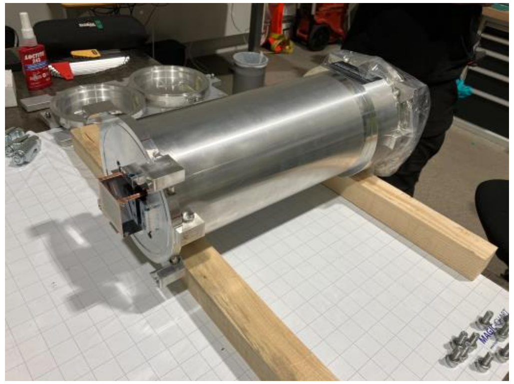
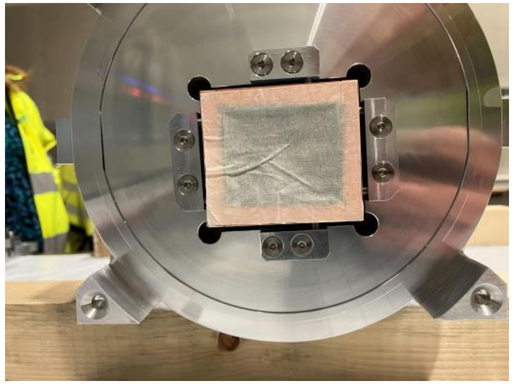
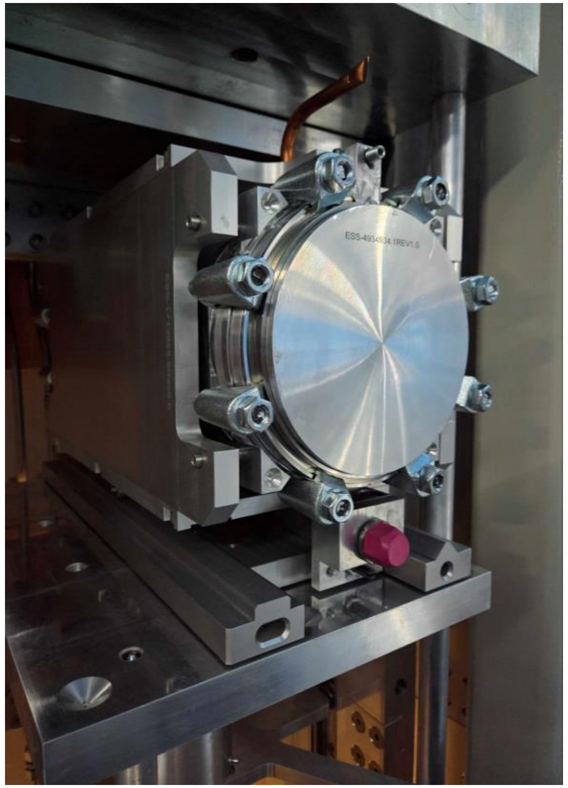
All paths of secondary spectrometer to be updated after PDR (December 2025)

Primary Spectrometer

Bridge beam guide (BBG)

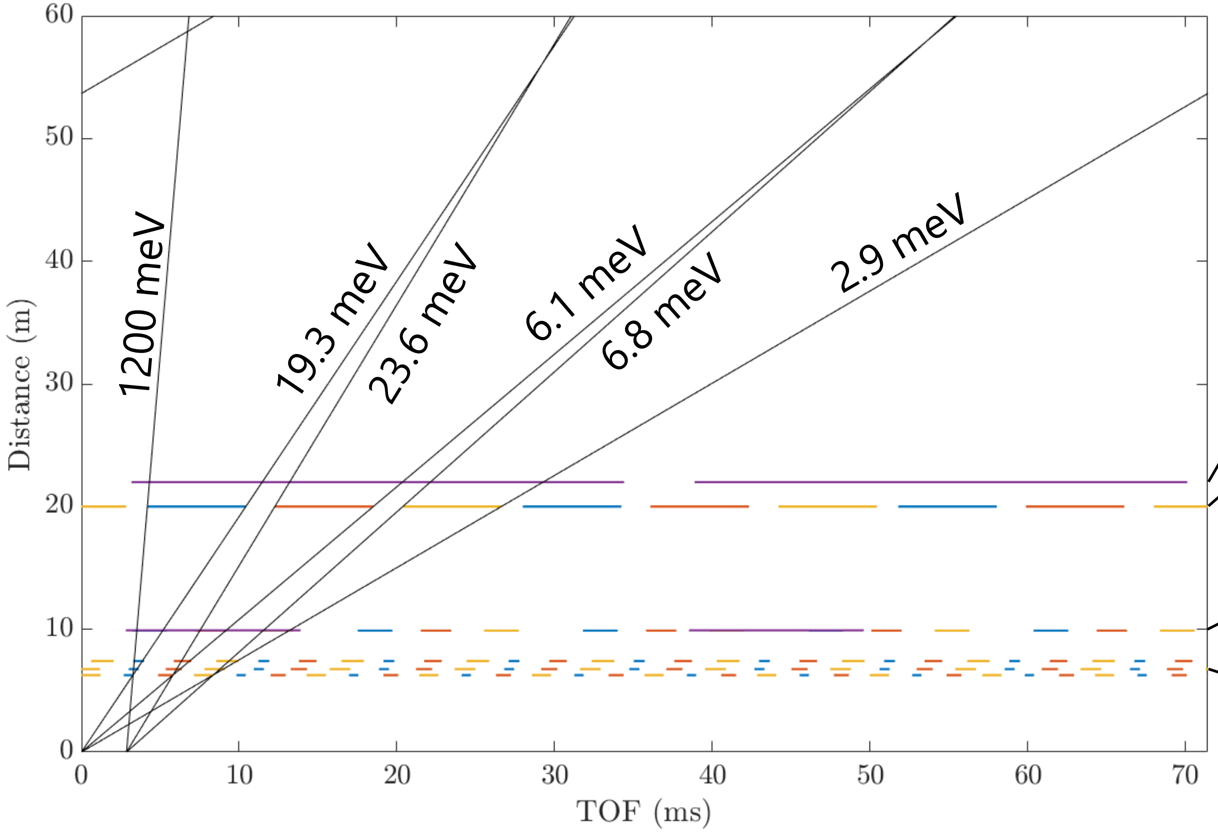
Guide section inside the light shutter (LSS)

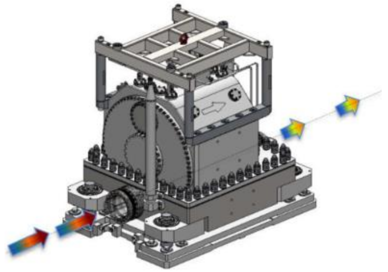
- Manufactured by Swiss Neutronics, tested and delivered to ESS end of May
- Installation in its casing, alignment and vacuum test in June
- Installation in the bunker in September

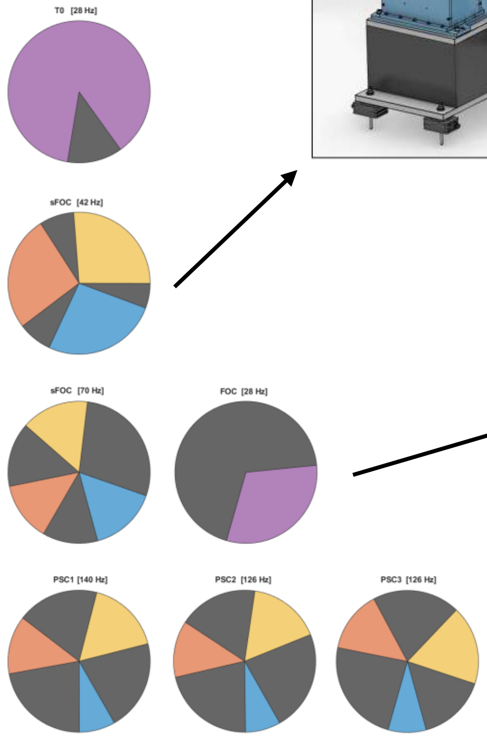





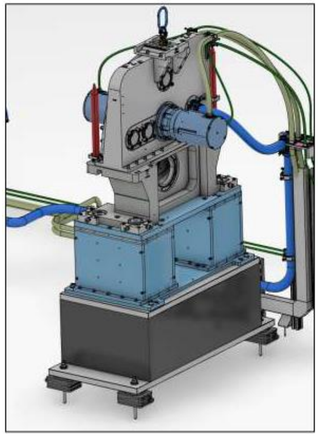

Primary spectrometer

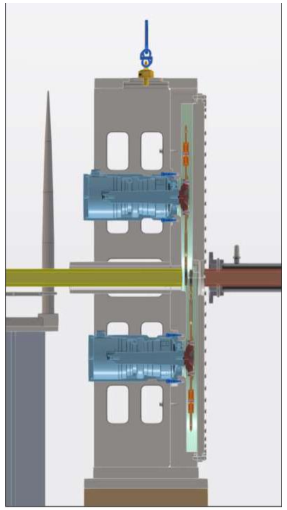
Time-distance diagram

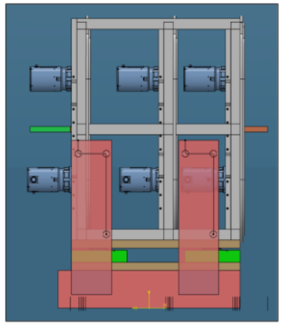










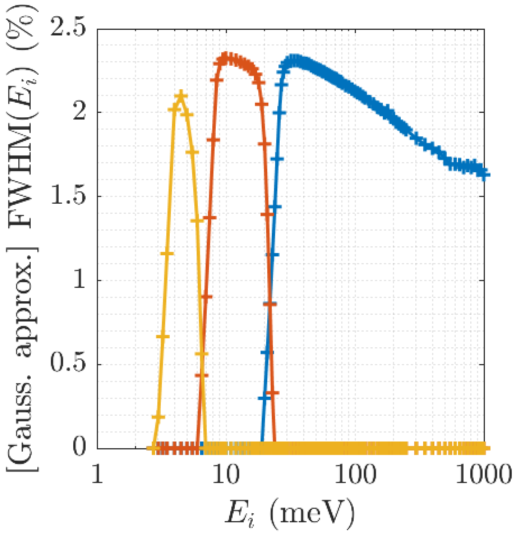


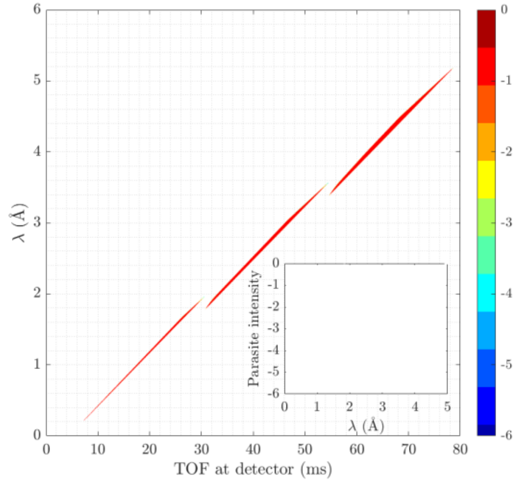
Primary spectrometer

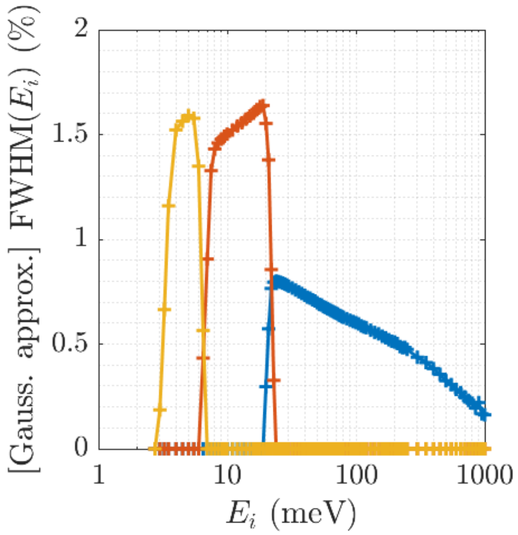
Resolution & Flux

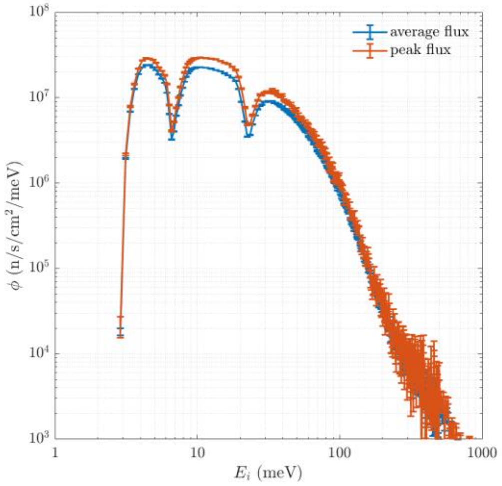
- Resolution of subframe 1 flexible from 0.8%Ei to 2.35%Ei, controlled through the PSC phases (<30s switch)
- Parasitic streams strictly suppressed
- High flux over the fingerprint (FP) region, 60-220 meV, and at low energy

Φ in n/s/cm²	FP	<85 meV
VESPA HF 2.0MW	19 e5	33 e8
VESPA HR 2.0MW	4.7 e5	18 e8
VISION 2.0 MW	9.1 e5	10 e8
VISION 1.4MW	6.4 e5	7.1 e8
TOSCA	3.7 e5	4.5 e8







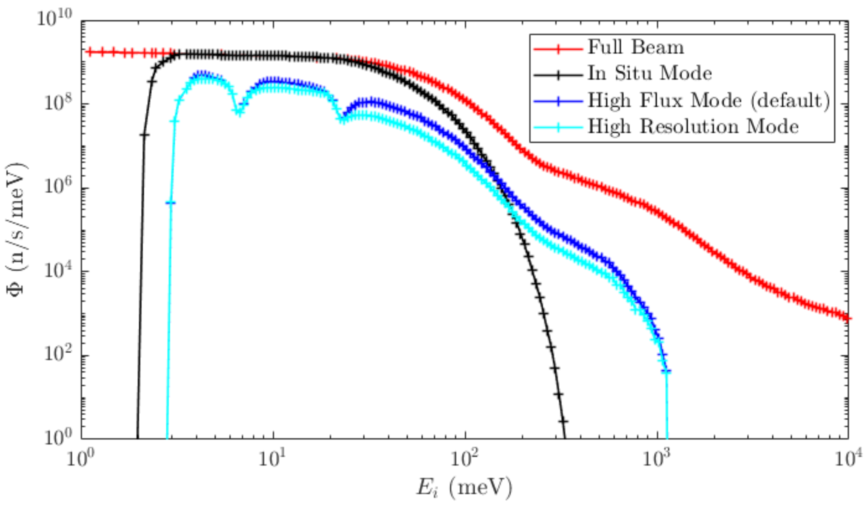


Primary spectrometer

Background management

Total flux (full beam at 5 MW) is very high! $\sim 10^{11}$ n/s

Operation Mode	Flux Φ (n/s)		
	Ei < 100 meV	Ei = 0.1 – 1 eV	Ei = 1 – 10 eV (*)
Full Beam / Transmission	6.93e10	4.87e9	1.28e8
In Situ	5.18e10	4.07e8	0
High Flux (default)	8.55e9	2.67e8	1.98e4
High Resolution	5.74e9	1.15e8	1.53e4



Strategies in place to minimise background

- T0 chopper for Ei > 1200 meV
- Beam stop moved outside the cave, starts 4.15 m after the sample
- Copper & steel collars around the guide in the bunker wall insert (BWI) and 5 m before the cave starts
- Absorber inside the secondary: Cd lining, B_4C cross-talk shielding, B_4C shroud

To be determined

- Cave wall lining vs secondary coffin
- Moderation vs absorption
- Beam stop design

Secondary Spectrometer Scientific Concept

Neutron Vibrational Spectrometers

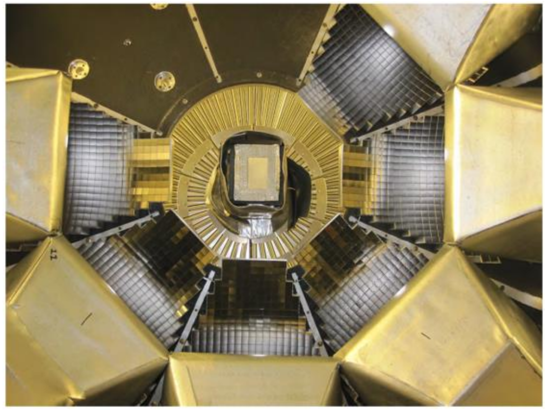
Indirect-geometry crystal-analyser spectrometers

Operational instruments

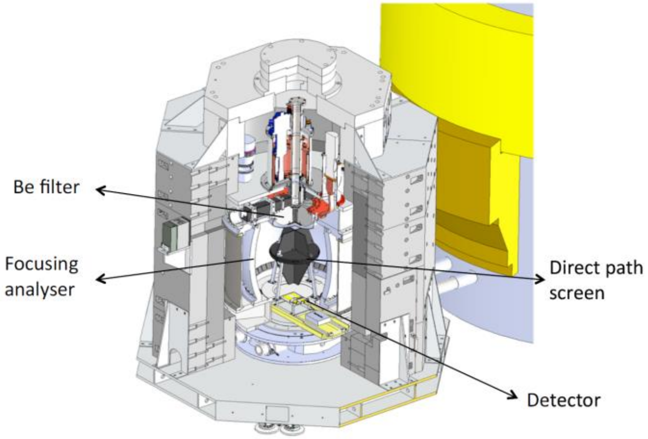
- TOSCA @ISIS, UK
- VISION @SNS, TN, USA
- Lagrange @ILL, France
- FANS @NIST, MD, USA
- NERA @FLNP, Russia

Upcoming instruments & upgrades

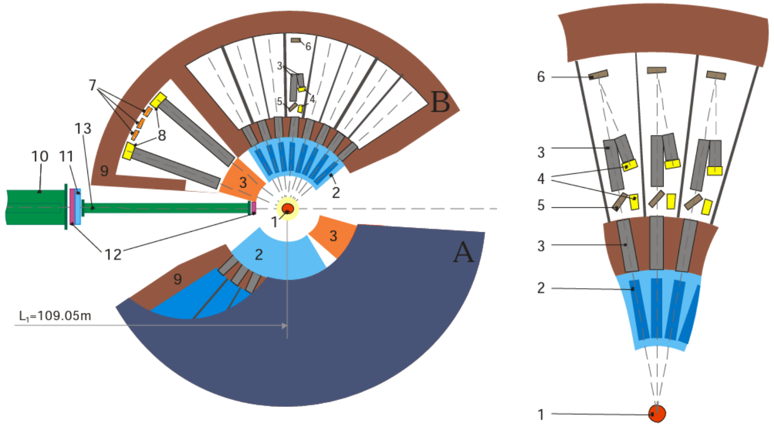
- VESPA @ESS, Sweden
- TOSCA+ @ISIS, UK
- iMovies @CSNS, China
- BJN @FLNP, Russia
- IN8(∗) @ILL, France
- B-WAVES(?) @SNS, TN, USA



- VISION, https://neutrons.ornl.gov/vision
- Seeger et al., Nucl. Instrum. Methods Phys. Res. A. **604** (2009) 719



- LAGRANGE, Jiménez-Ruiz et al., J. Phys. Conf. Ser. **549** (2014) 012004



- NERA, Natkaniec et al., J. Phys. Conf. Ser. **554** (2014) 012002

Neutron Vibrational Spectrometers

Indirect-geometry crystal-analyser spectrometers

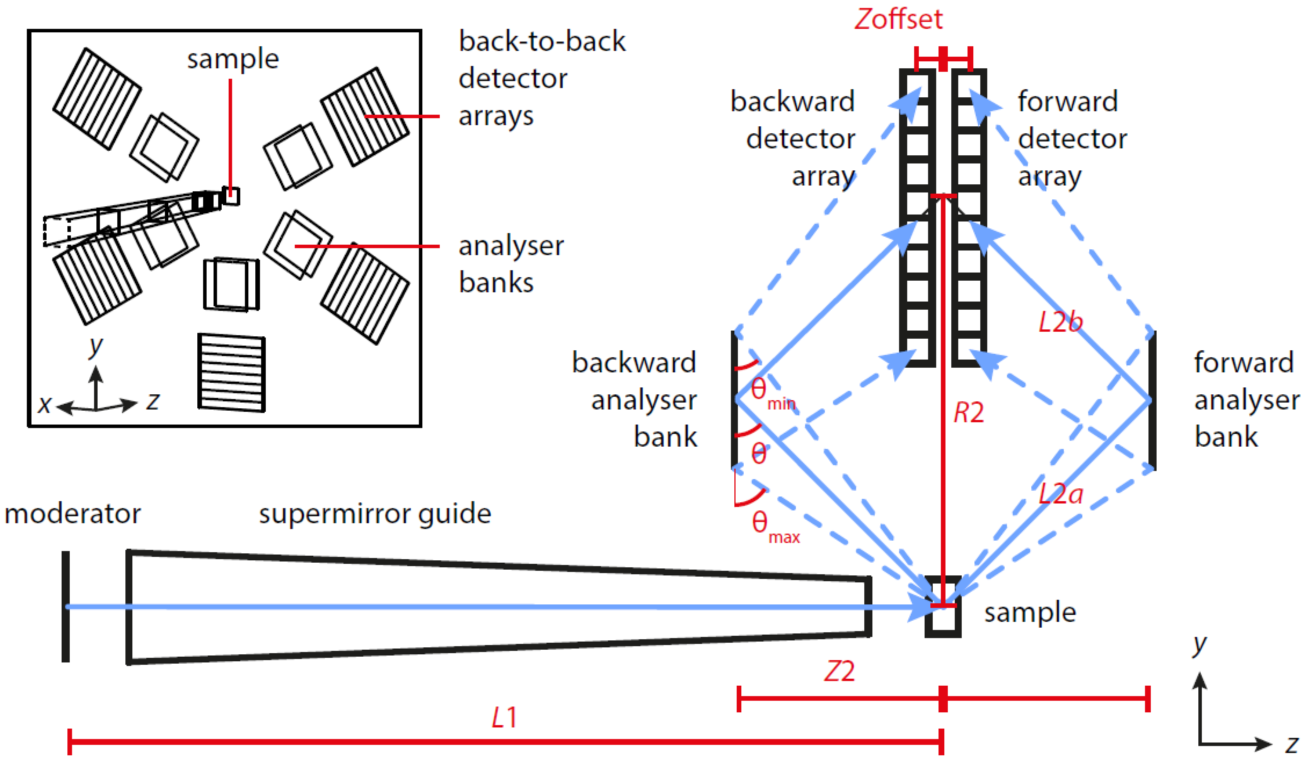
Instrument	Institut, Country	Status / Est. op.	Geometry	Ω (sr)	Resolution (% E_i) *
NERA	FLNP, Russia	Operational	2θ cylindrical	0.2	1.5-3, depends on scattering angle θ
TOSCA	ISIS, UK	Operational	wheel	1.0	1.5, depends on sample thickness
FANS	NIST, USA	Operational	2θ cylindrical	1.1	2-5 (Cu220), 2-7 (Cu311), depends on collimation
IN1 Lagrange	ILL, France	Operational	single barrel	2.5	2.6 (Cu220), 1.8 (Cu331), depends on sample volume/height and collimation
VISION	SNS, USA	Operational	wheel	3.5	1.5, depends on sample thickness
BWAVES	STS, USA	?	2θ cylindrical	1.3	3
BJN	FLNP, Russia	?	double barrel	5.8	4
iMovies	CSNS, China	2028	wheel	4.0	1-3 ?
TOSCA+	ISIS, UK	?	wheel	6.3	1.1 (0.8) depends on sample thickness
VESPA 2017	-	-	wheel	0.6	-
VESPA 2019	-	-	wheel	5.25	2.2 (HF), 1.0 (HR) depends on sample thickness
VESPA 2025	ESS, Sweden	2029	wheel	7.0	2.5 (HF), 0.8 (HR) depends on sample thickness

* Resolutions in the fingerprint region (50-150 meV), at the resolution plateau if applicable, else at 100 meV

Neutron Vibrational Spectrometers

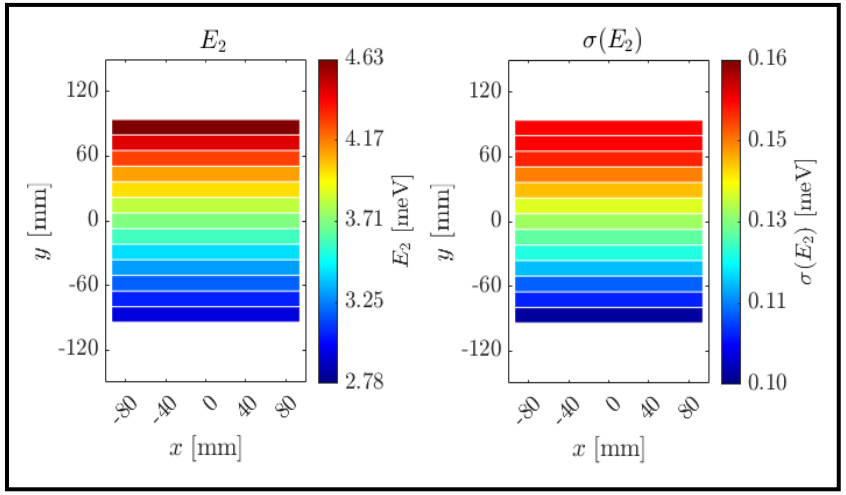
TOSCA's ideal wheel geometry

Time-focusing & energy-focusing geometry

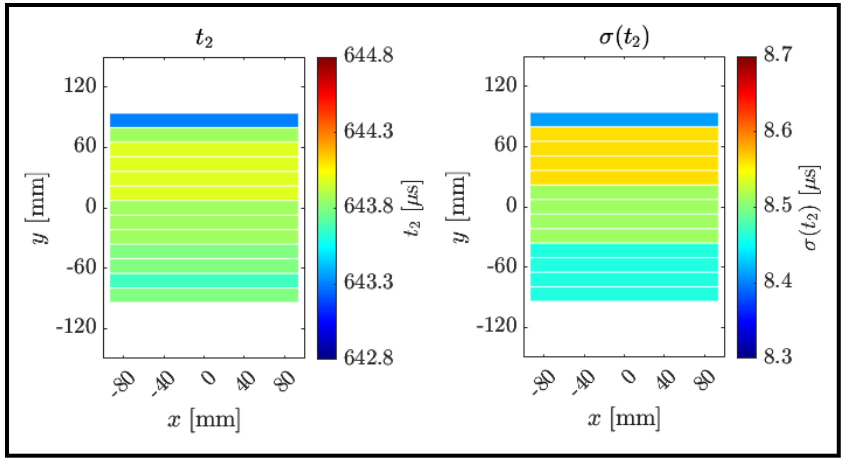


- Perrichon, Nucl. Instrum. Methods Phys. Res. A. **1041** (2022) 167401

Final energy (E_2) at detector



Secondary TOF (t_2) at detector



Secondary spectrometer

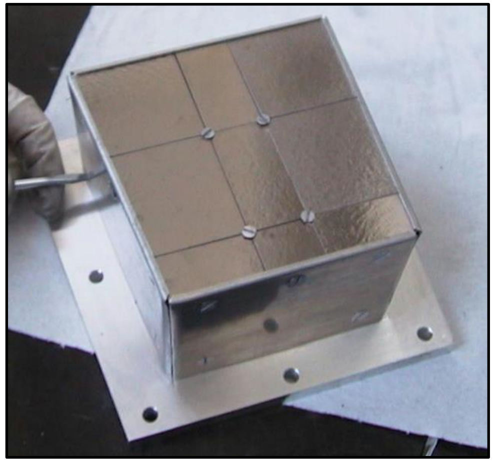
Several generations of wheel-geometry designs

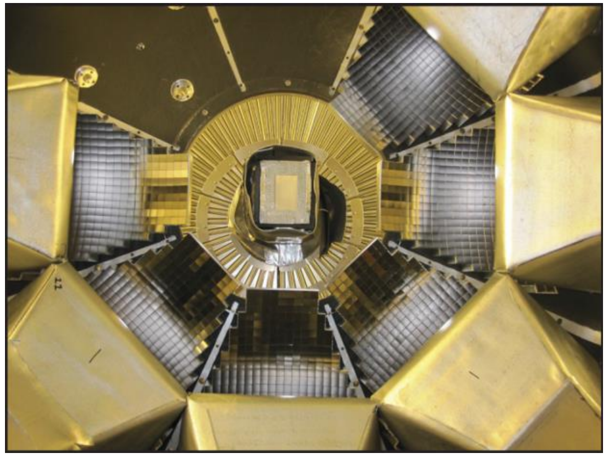
<u>TOSCA (VESPA 2016)</u>
Defocusing (flat)
Ω = 1.0 sr
$\Delta E_{th.}$ = 0.7% Ei

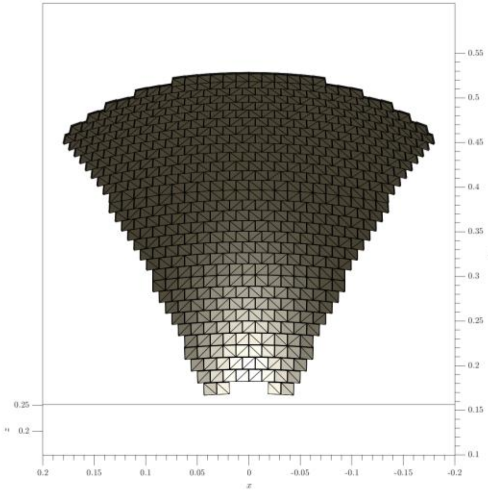
<u>VISION (VESPA 2019)</u>
Focusing (~elliptical)
Ω = 3.5 sr
ΔE = 1.5% Ei

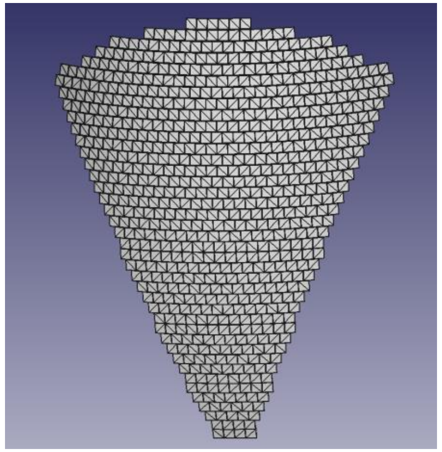
<u>TOSCA+ (VESPA 2024)</u>
Focusing (~parabolic)
Ω = 6.3 sr
$\Delta E_{th.}$ = 1.1% Ei

<u>VESPA 2025</u>
Focusing (~parabolic)
Ω = 7.0 sr
$\Delta E_{th.}$ = 1.1% Ei









Challenge of project timeline & opportunity of improved maintainability led to a simplification of the design (staggered vs back-to-back, vacuum vessel vs gas box), at equal performance and increased cost

Analyser design process

Rationale

1) The analyser must be focusing the scattered beam onto the detector array

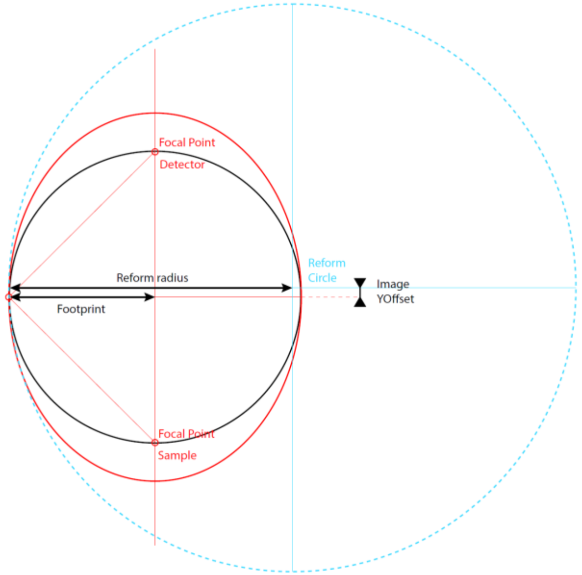
2) For a specific detector pixel, the (analyser contribution to the) resolution at the elastic line mostly depends on the secondary flight path uncertainty (σ_{L2}); the (analyser contribution to the) resolution at high energy mostly depends on the secondary flight path (σ_{t2}) < numerical optimisation

4) The spatial distribution of the mean values of E2, L2 and t2 is irrelevant given PSD; the geometry must minimise the uncertainties over the entire detector; many tiles illuminate the same detector pixel < holistic (entire analyser evaluated at once)

How?

Parametric model with enough flexibility to describe most backplate curvatures and historical "stepped" strategy, with limited number of parameters (10)

- Tile position defined by a 3D ellipsoid
- Tile angle defined by vertical/horizontal circles or focusing points



Analyser design process

Design guidelines

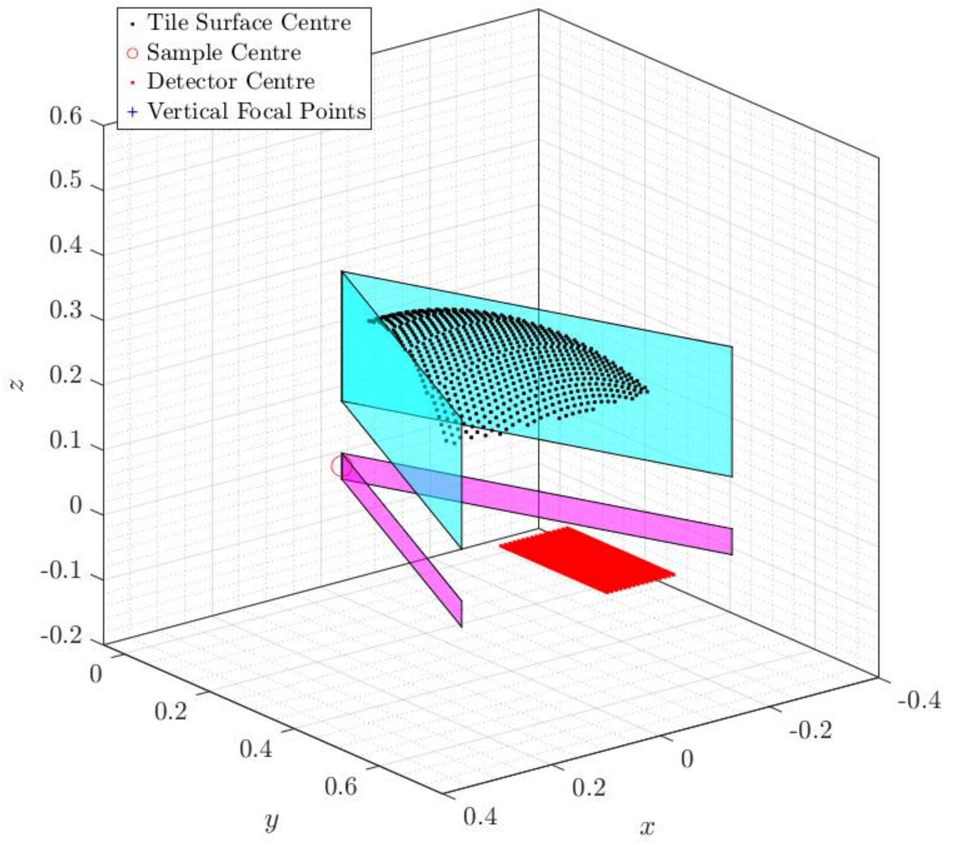
Best resolution is achieved by minimising the number of tiles contributing to the same detector pixel < maximise detector area & spread the image

Best resolution is achieved by limiting the width of a bank and increasing the number of banks – but negative to the intensity < sweet spot 40-50° polar

Best resolution and best filter are achieved the closer the detector is from the sample plane < minimise gap between forward/backward banks

Intensity is proportional to solid angle < maximise the polar and azimuthal coverage

Filter performances (filtering and transmission) improve the longer neutron path in Be is < minimise gaps Be/Detector and Be/Analyser(line-of-sight)



Analyser design process

Numerical optimisation 9 parameters (+3 fixed)

Focal circle radius = 320 mm (fixed)

Forced radial geometry defined by:

- φmin & φmax (fixed, solid angle of analyser)
- Detector position (fixed) and length

Vertical profile optimisation

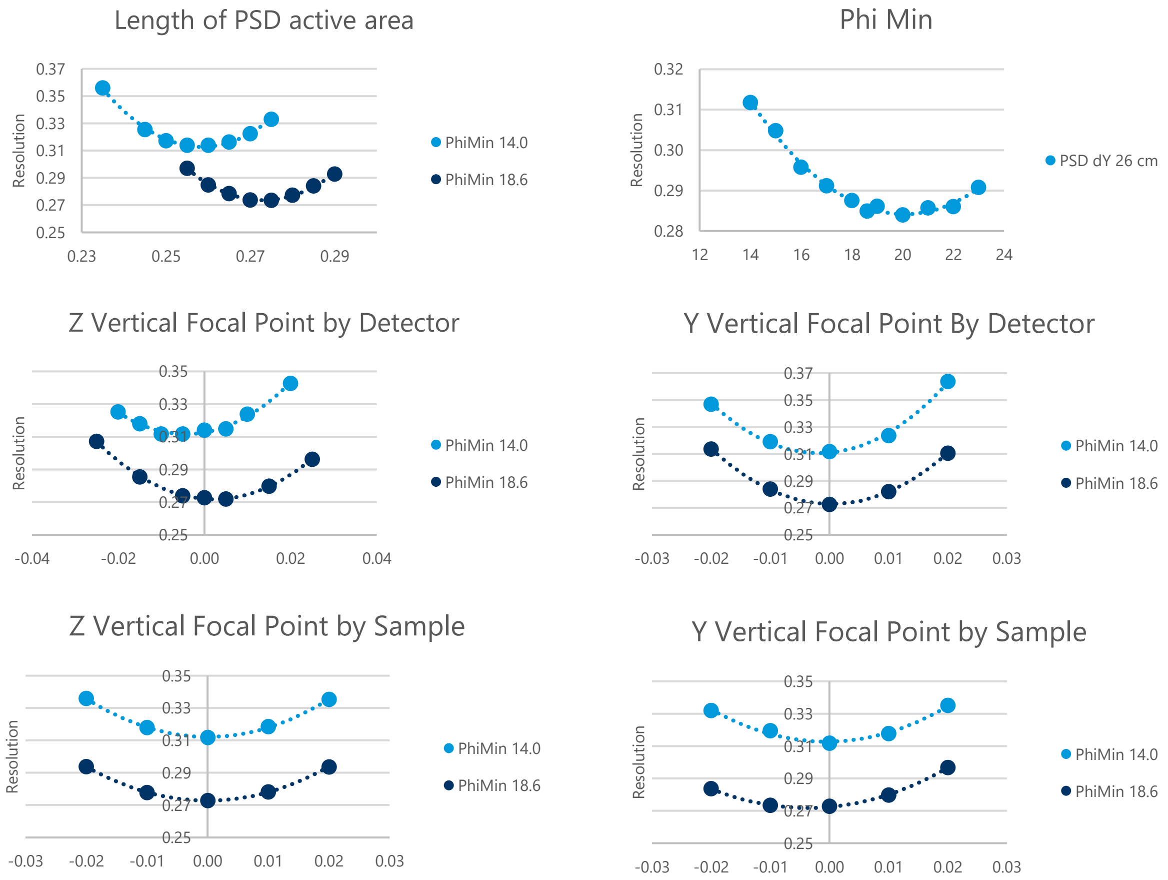
- Ellipse focal points by sample (y and z)
- Ellipse focal points by detector (y and z)

Horizontal profile optimisation

- Horizontal focusing radius
- Ellipse focal point by sample (z)
- Ellipse focal point by detector (z)

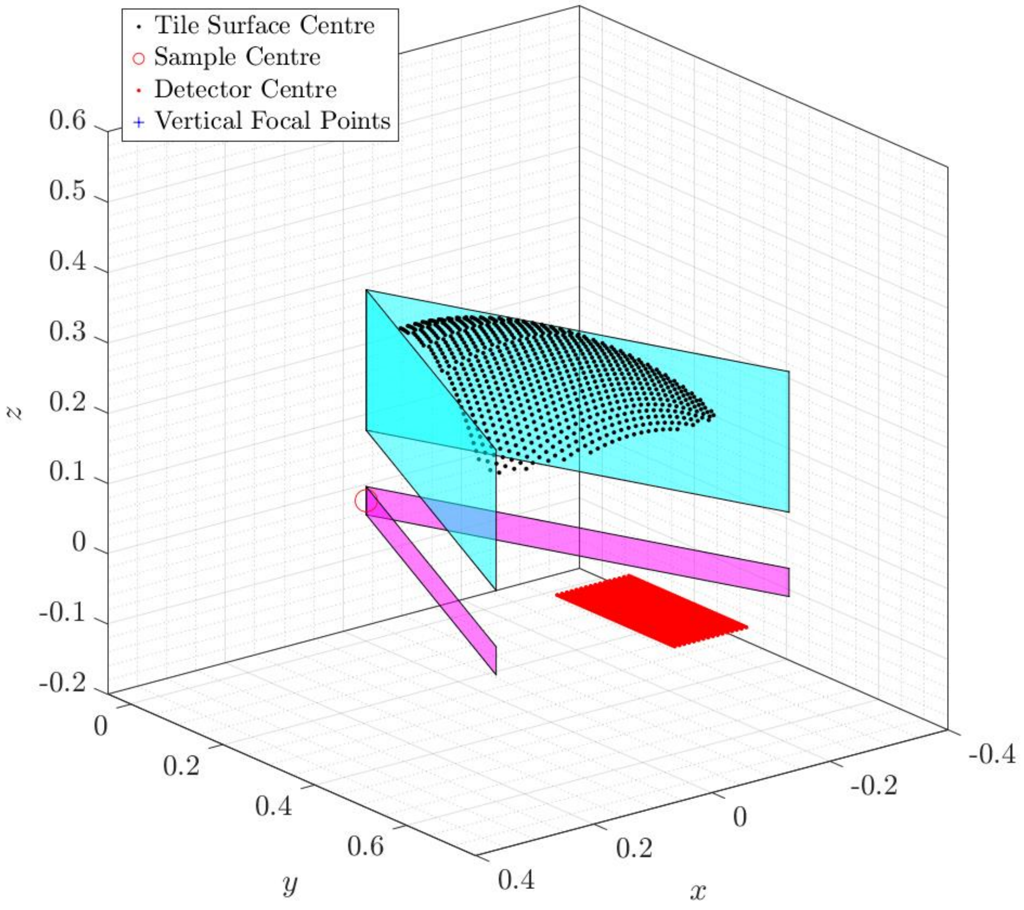
Collimator geometry is fixed to radial

Optimisation target: min(resolution)



Analyser design process

Iterative & joint optimisation of analyser, filter & detector



HOPG analyser

- 16 analyser modules
- 45° azimuthal, 18.6-67° polar
- Total coverage 7.0 sr
- 800 HOPG tiles per module, ~12800 HOPG tiles in total, ~1.84 m^2 of HOPG in total

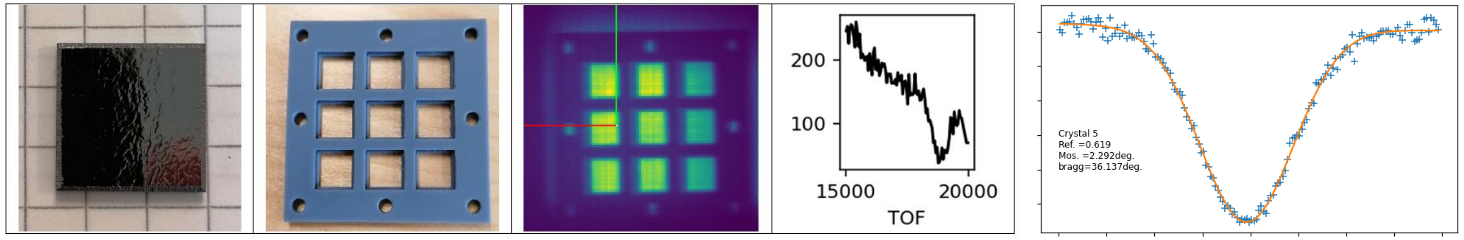
HOPG crystal

- 12×12×2 mm
- 3° mosaic spread
- Ongoing evaluation

HOPG crystal tests

Reflectivity & Mosaic spread – May 2025

- Optigraph crystals are highly variable, but their average performance is acceptable if outliers are removed
- Momentive have significantly improved their crystals: next batch of prototypes to be tested in Q4 on IMAT at ISIS



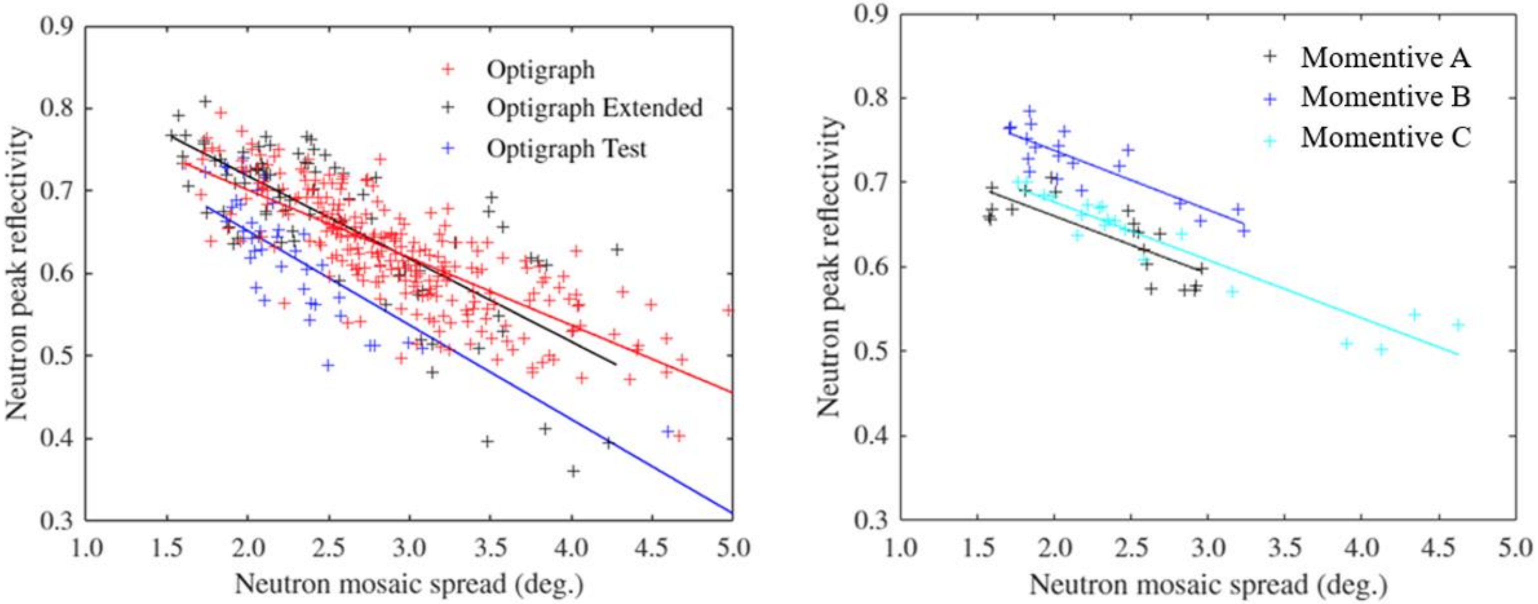


Figure 2 - Peak reflectivity as a function of mosaic spread measured on ALF at ISIS for HOPG crystals from (a) Optigraph abd (b) Momentive Technnologies.

Filter design process

Beryllium filter envelope and geometry

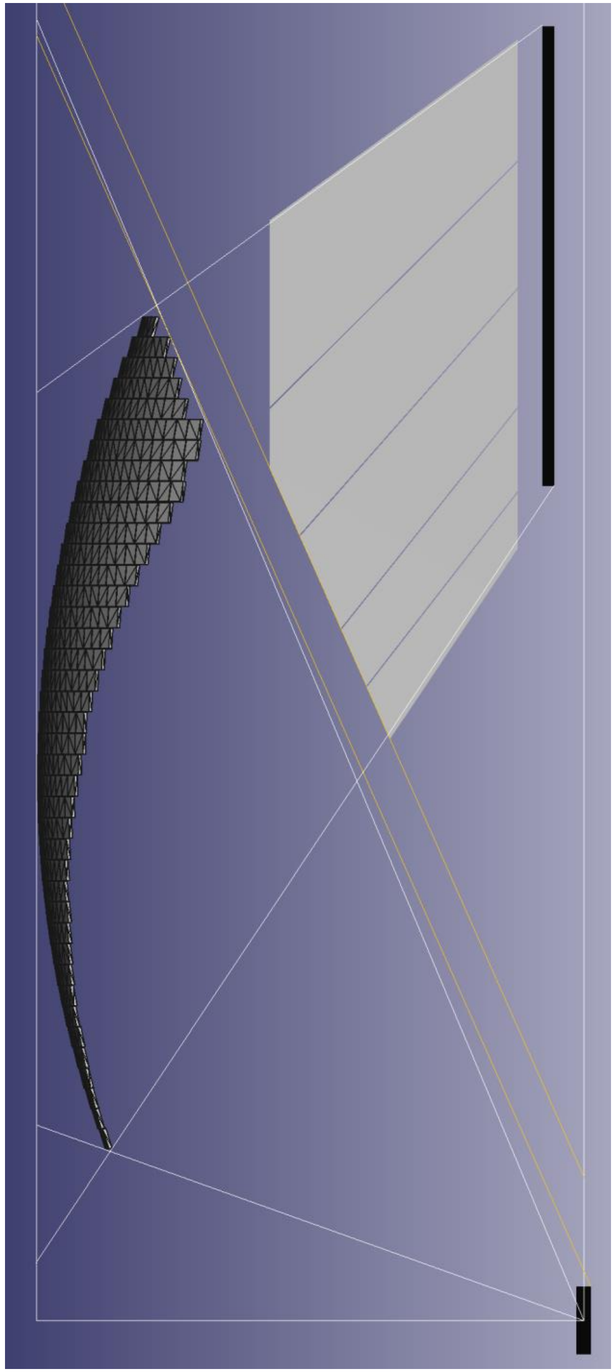
Fit into the wedge space between detector and analyser

Scientific requirements:

- Minimum path length 14 cm (VISION)
- Optimally 16 (CAMEA) to 20 cm (BIFROST)
- No line-of-sight from analysers to detectors without going through Be or significant shielding
- *No or minimal shadowing*

Engineering requests:

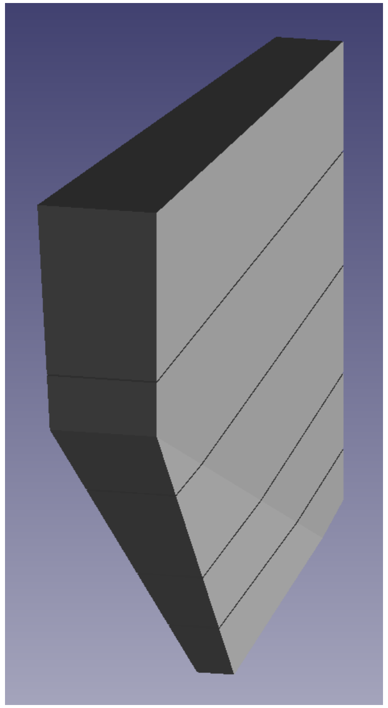
- Parallel illumination and filter planes
- Minimise the number of faces
- Increased gap between filter and detector
- Oversized Be (few mm) for tolerances

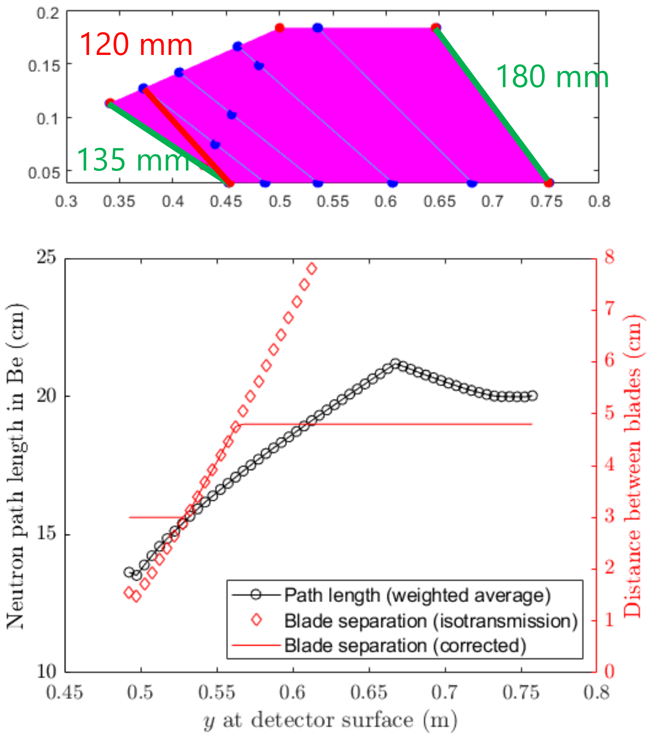


Filter design process

Beryllium filter envelope and geometry

VESPA 2025 (17.34 kg)





Beryllium filter

- 14–20 cm path length
- Transmission of high energy neutrons $\leq 10^{-4}$
- Transmission of analysed neutrons through the collimation $\geq$75%
- Simple, convex object with facets (machining)
- Beryllium mass ~17 kg per module, ~270 kg in total

Collimation materials

- Cadmium 750/800 μm sheets

Detector design process

Arrays of ^{3}He PSD tubes

TOSCA+ / VESPA 2019 design with ∅ 8 mm PSD tubes arranged vertically leads to severe saturation issues (ESS at 2 MW)

Estimate for the count rate φ

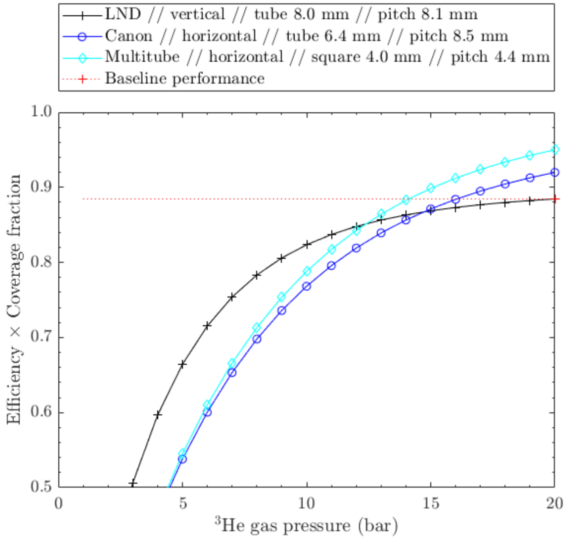
$$\varphi = \varnothing \times M \times R \times \frac{0.4}{4\pi} \times 0.8 \times 0.8 \times \sigma \times \frac{1}{N} \times \frac{V}{10}$$

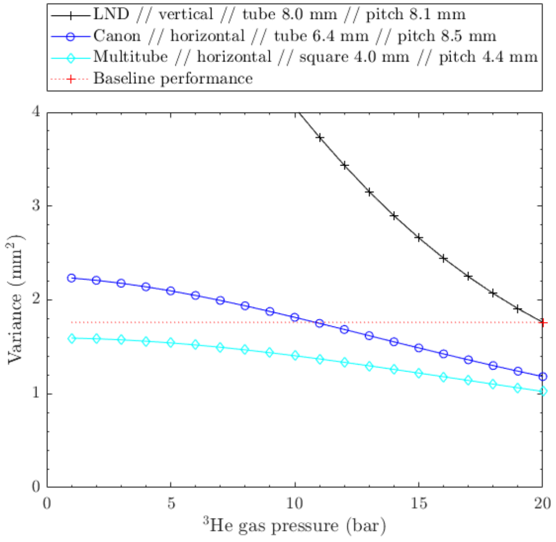
Table 1 – Count rates at 2 MW are reported for several scenarios of sample and beam spot

	N vertical/horizontal	Elastic φ in kHz per tube	Inelastic φ in kHz per tube
• 10% scatterer • 10 cm^2 beam	16 V	16,298	132
	27 H	15,452	126
	36 H	8,692	70.6
	54 H	3,864	31.4
• 10% scatterer • 3.2 cm^2 beam	16 V	5,216	42.4
	27 H	4,944	40.2
	36 H	2,782	22.6
	54 H	1,236	10.0
• 4% scatterer • 10 cm^2 beam	16 V	6,520	53.0
	27 H	6,182	50.2
	36 H	3,476	28.2
	54 H	1,546	12.6
• 4% scatterer • 3.2 cm^2 beam	16 V	2,086	17.0
	27 H	1,978	16.1
	36 H	1,112	9.04
	54 H	494	4.02

Solution: horizontal arrangement of tubes (TOSCA-style)

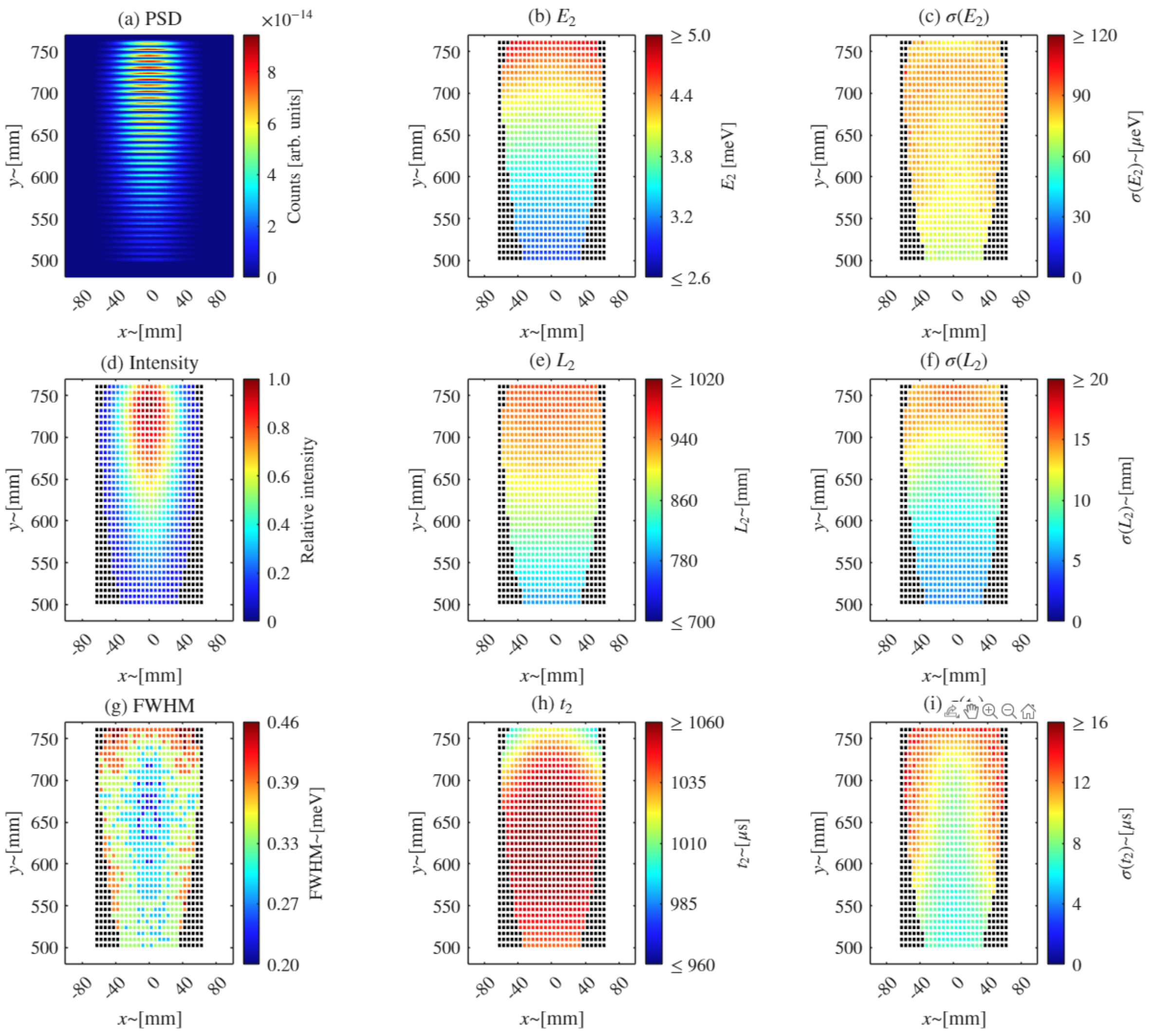
- Shorten the TOF range of saturation
- Good total efficiency because of 45° incidence
- Lower variance of tube compensates for larger pixel



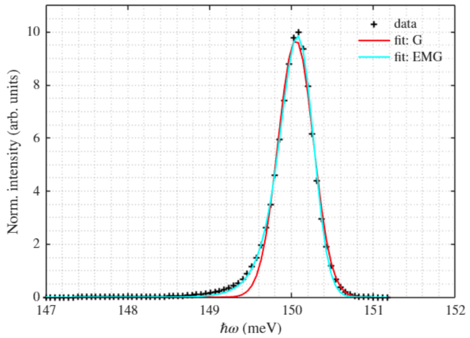


Predicted performance

“Per pixel” properties (16 PSD tubes)



Parameter	Value
Detector coverage	84.57%
Detector capture	95.30%
Filter transmission	79% - TBC
E2 (min – max)	2.96 – 4.86 meV
E2 (average)	3.94 meV
Resolution at 150 meV	0.33% (*)



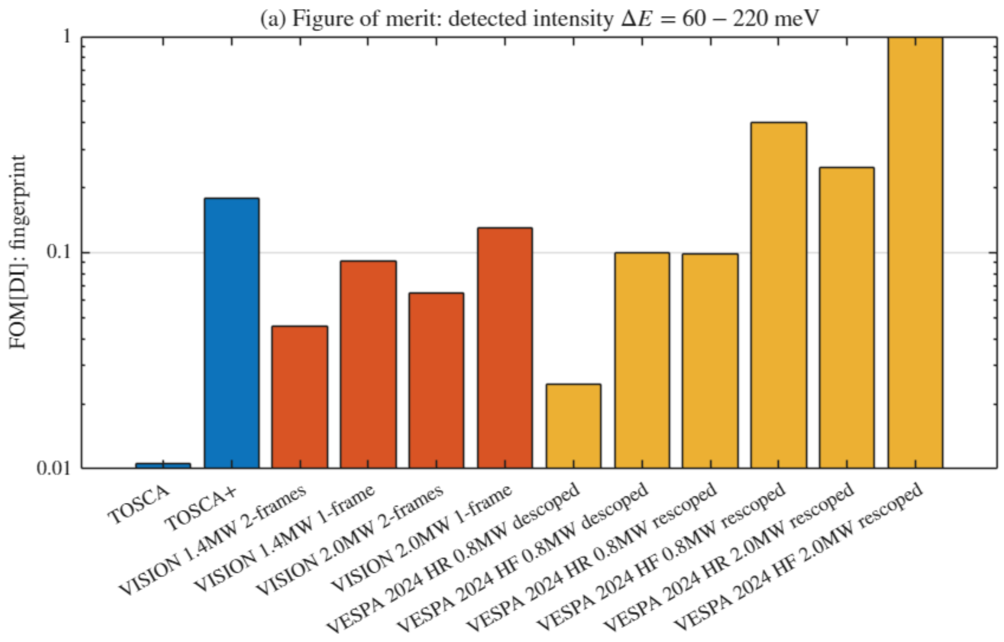
(*) Not including the contributions from tile thickness and detector electronics (1-2 μs std each), will be 0.5-0.6% Ei total

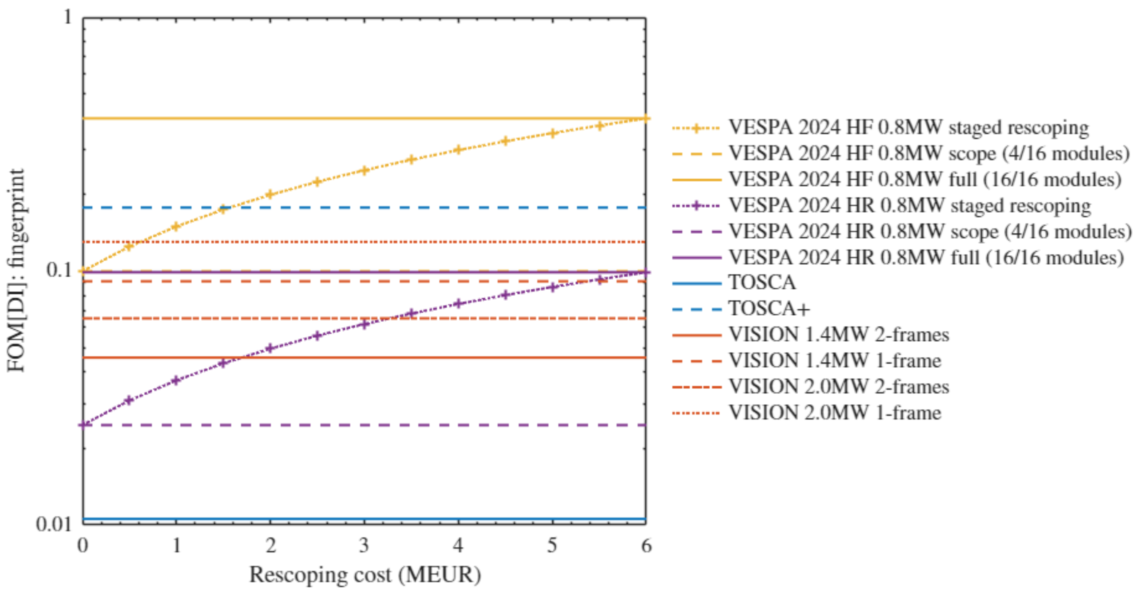
Rescoping of analyser modules

Figure-of-merit

Day 1 scope of VESPA is only 4 out of 16 modules

- Need 4 additional modules (50% coverage) to be equivalent to VISION
- Need full coverage to be world leading





Secondary Spectrometer Engineering & Prototyping

Secondary Spectrometer

One Module - Environments

Analyser – HOPG tiles

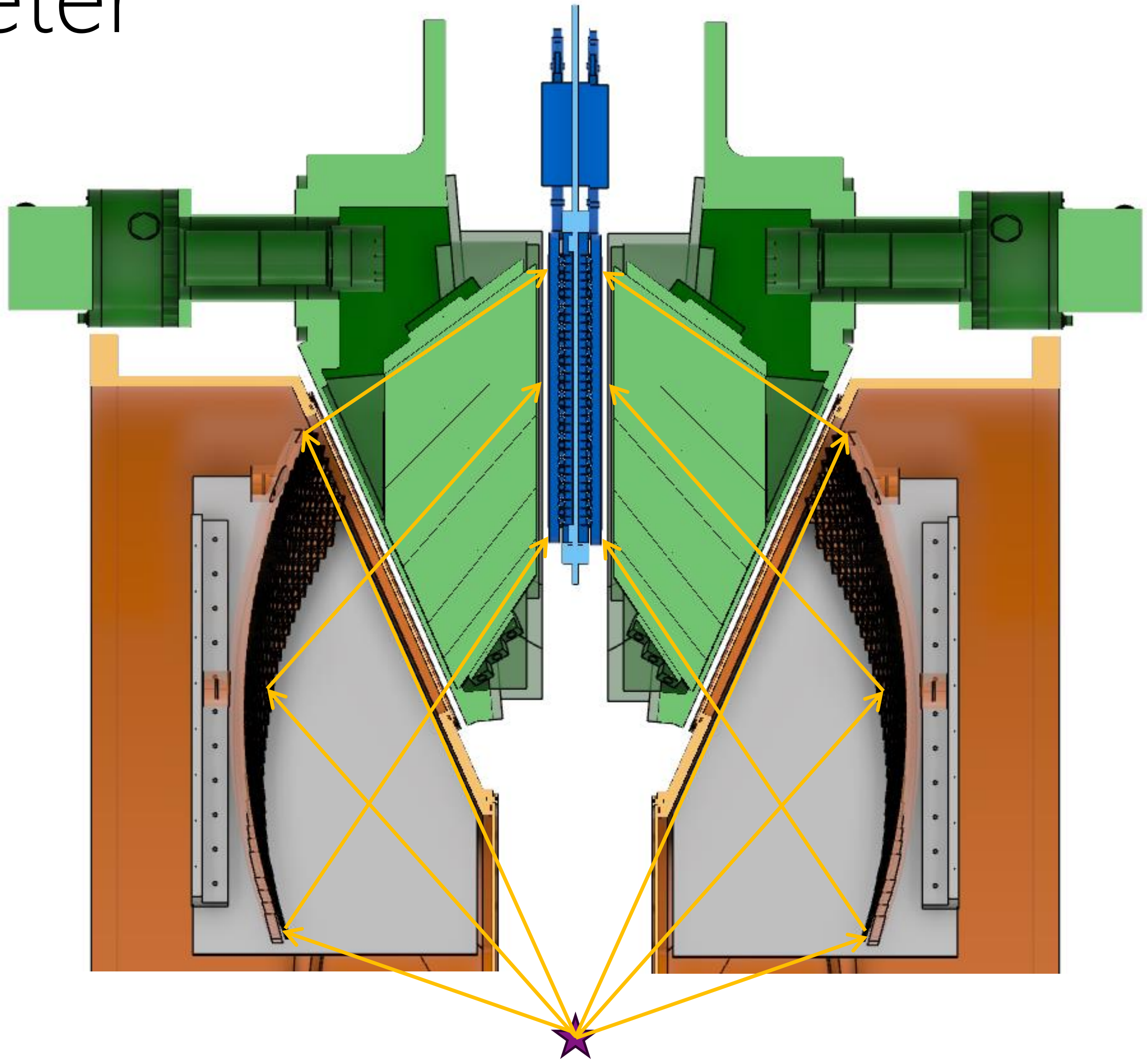
- Machined backplate coated with boron
- Shared helium environment at atm
- Cross talk shielding plate between modules

Filter – Beryllium

- Individual vacuum vessels
- Individual coldhead

Detector – He3

- Forwards-backwards detector pairs on one cartridge



Secondary Spectrometer

Complete System - Environments

Analyser – HOPG tiles

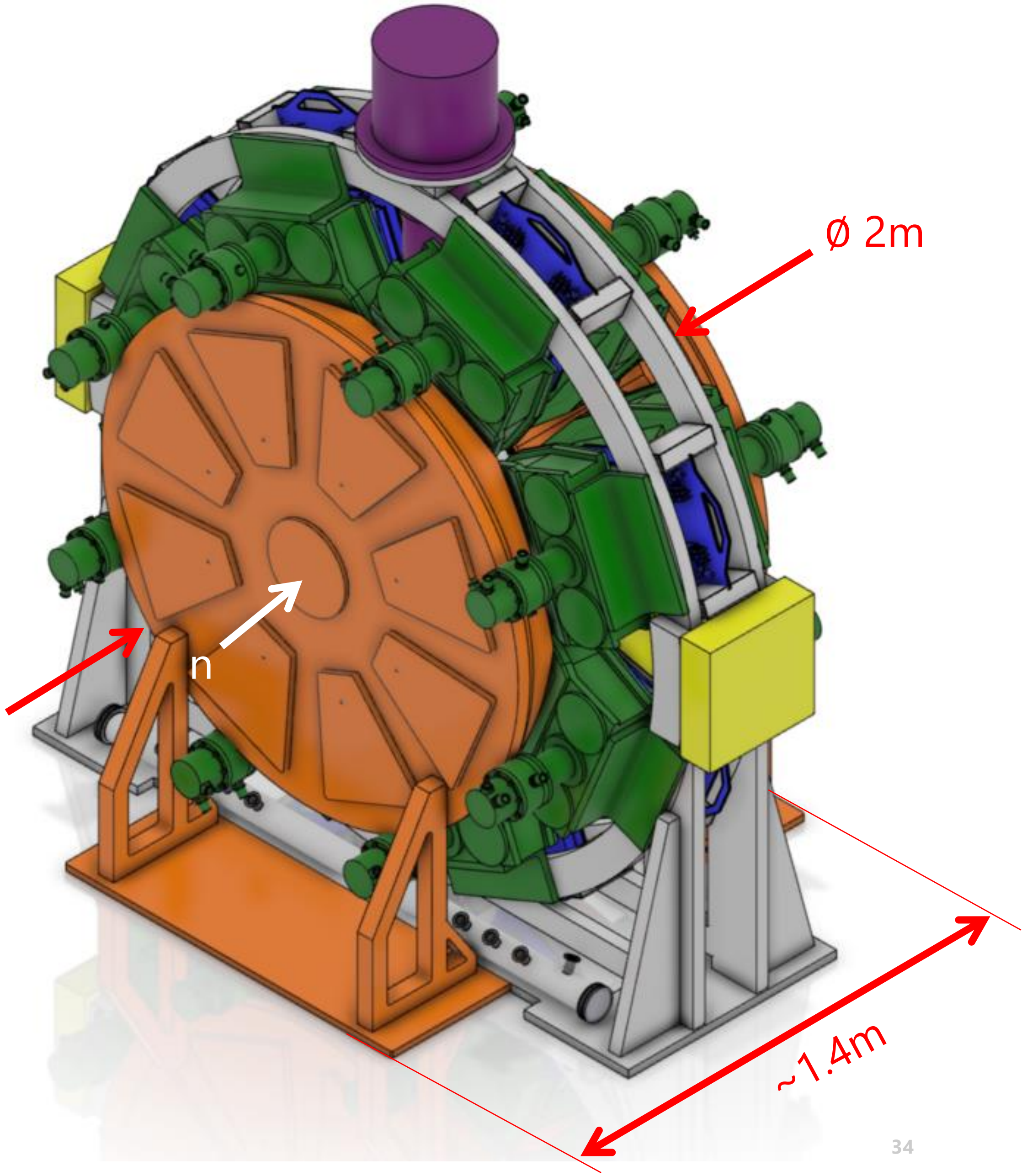
- Machined backplate coated with boron
- Shared helium environment at atm
- Cross talk shielding plate between modules

Filter – Beryllium

- Individual vacuum vessels
- Individual coldhead

Detector – He3

- Forwards-backwards detector pairs on one cartridge



Secondary Spectrometer

Complete System - Maintenance

Analyser – HOPG tiles

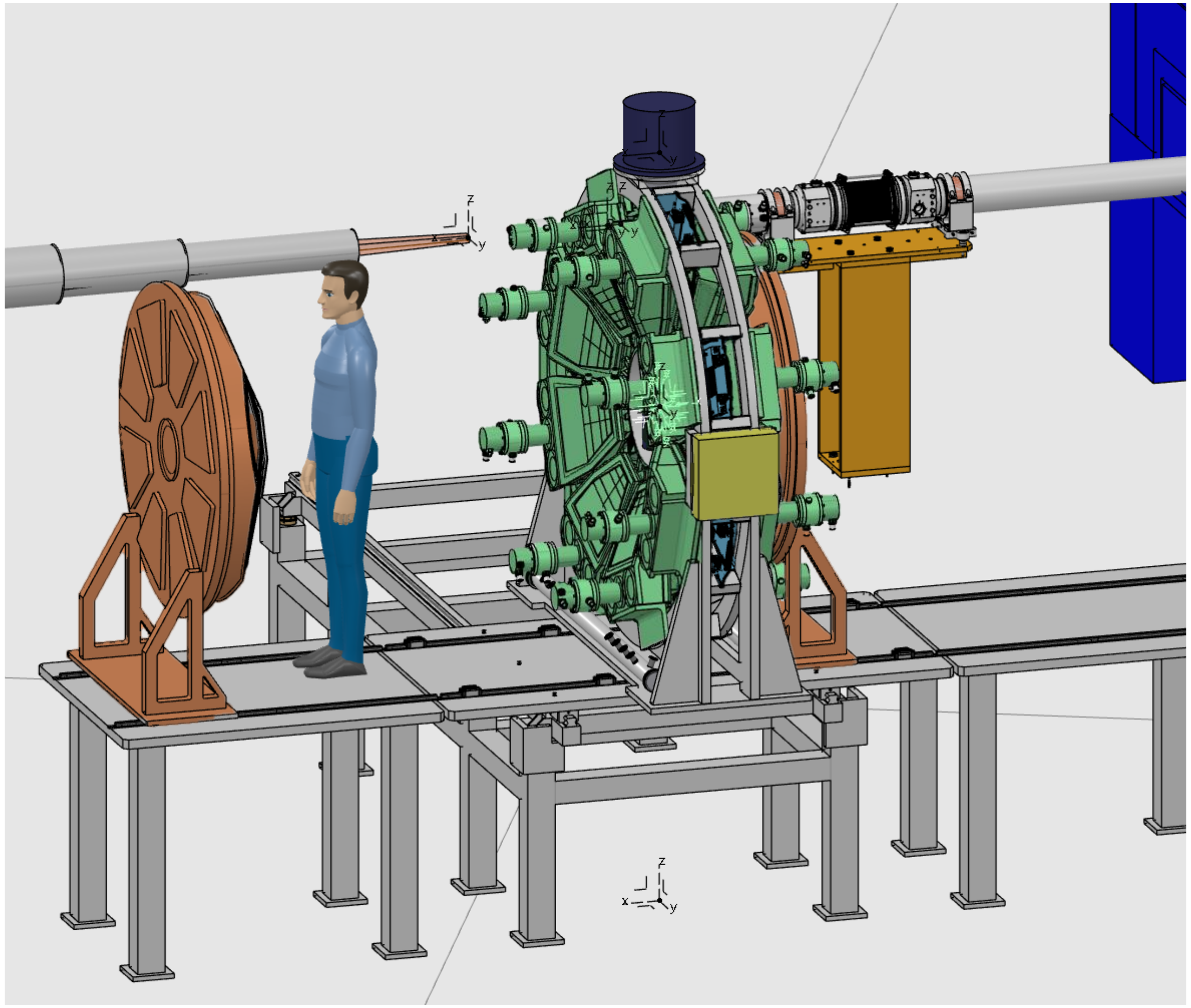
- Each gas box can slide out of the way for maintenance access
- Access for position adjustment of each analyser from backplate

Filter – Beryllium

- Independently remove cold heads
- Remove/add one filter as needed for upgrades/repairs

Detector – He3

- Pull cartridge out of secondary core structure

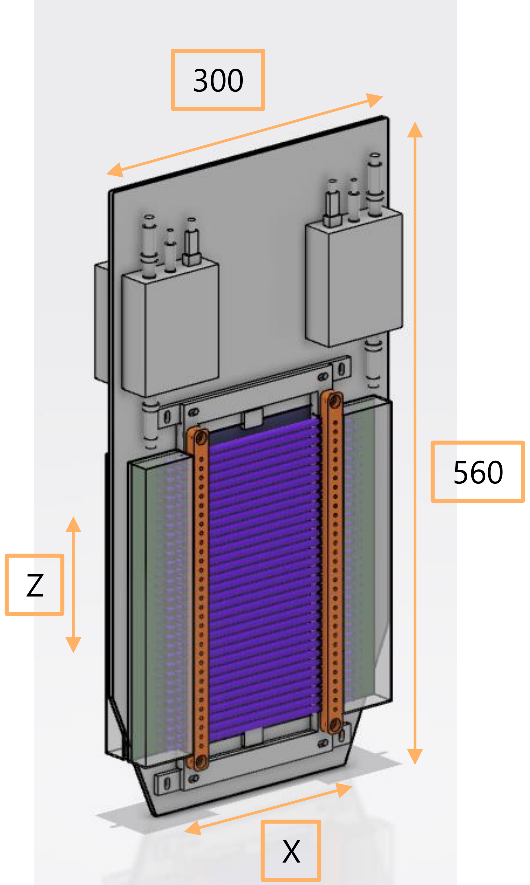


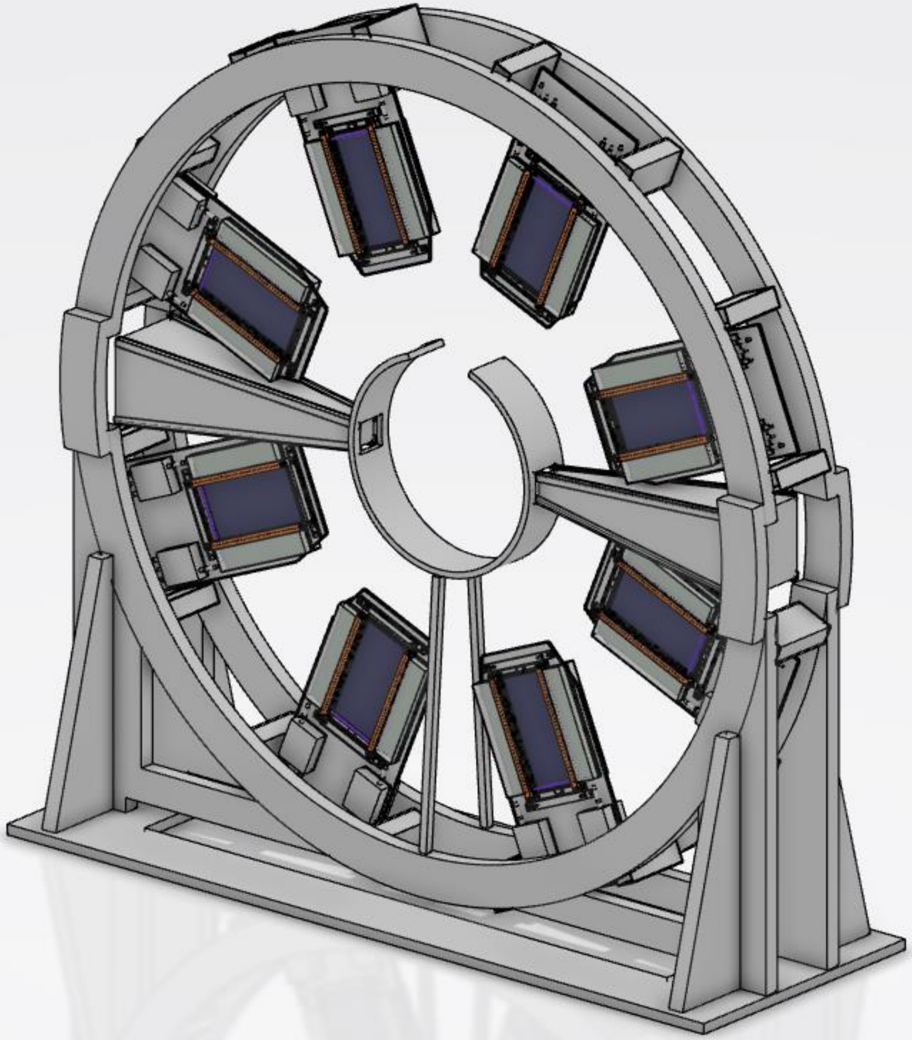
Secondary Spectrometer

Complete System - Maintenance

Detector cartridge

- 32-37 tubes ∅ 6 mm
- Horizontal arrangement
- PCB on each side, inside Faraday cage
- Grounding from the bulk metallic structure
- Preamps directly on the cartridge
- Cartridge in air
- Cartridge slides inside the structure on rails





The Beryllium Filter

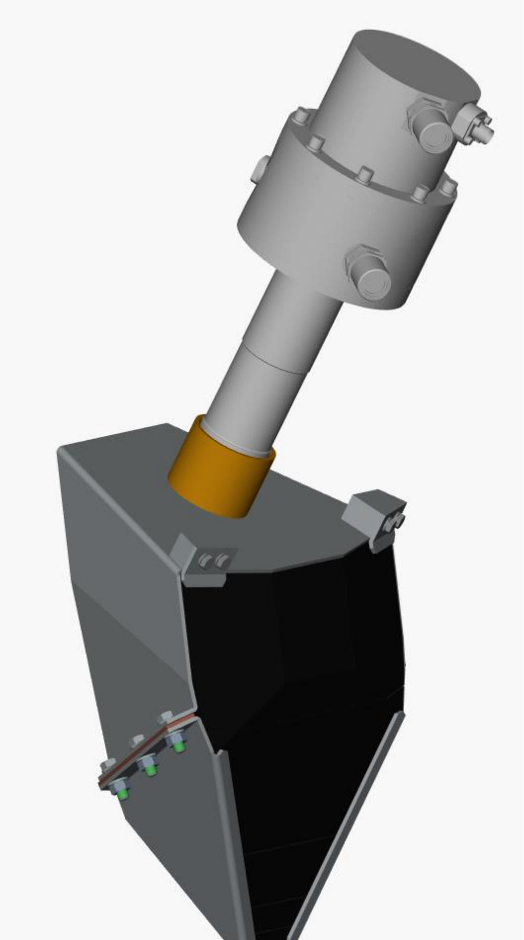
Thermal design challenges

Initial proposal to mount the filter directly to the cold head

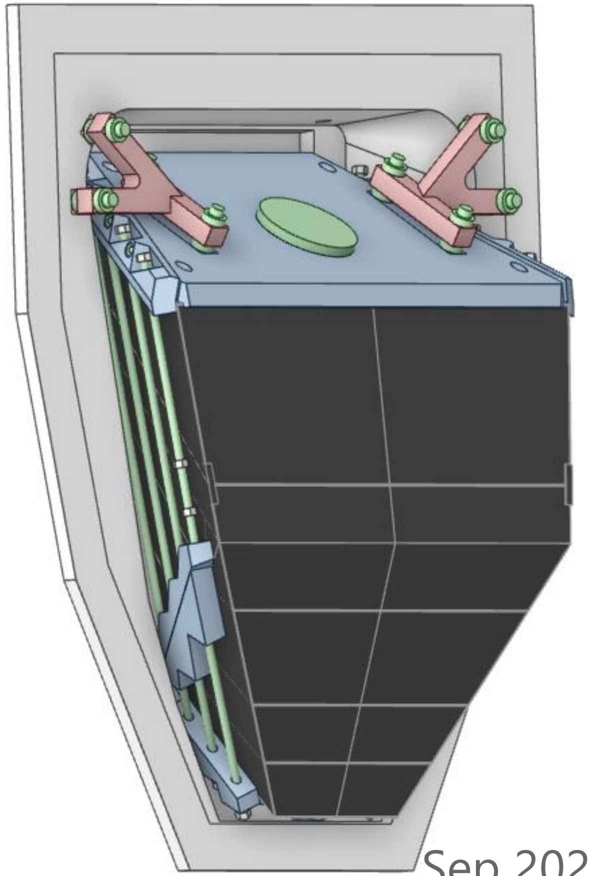
- Beryllium alone is currently estimated at 17kg
- cold heads considered had a load limit of 15kg perpendicular to their axis

Decoupling mass from the cold head creates conductive heat path from the vacuum vessel

- Optimise thermal isolation and stiffness
- Risk of condensation on outside of vacuum vessel
- New assembly challenges – how to access to access for connecting thermal link?



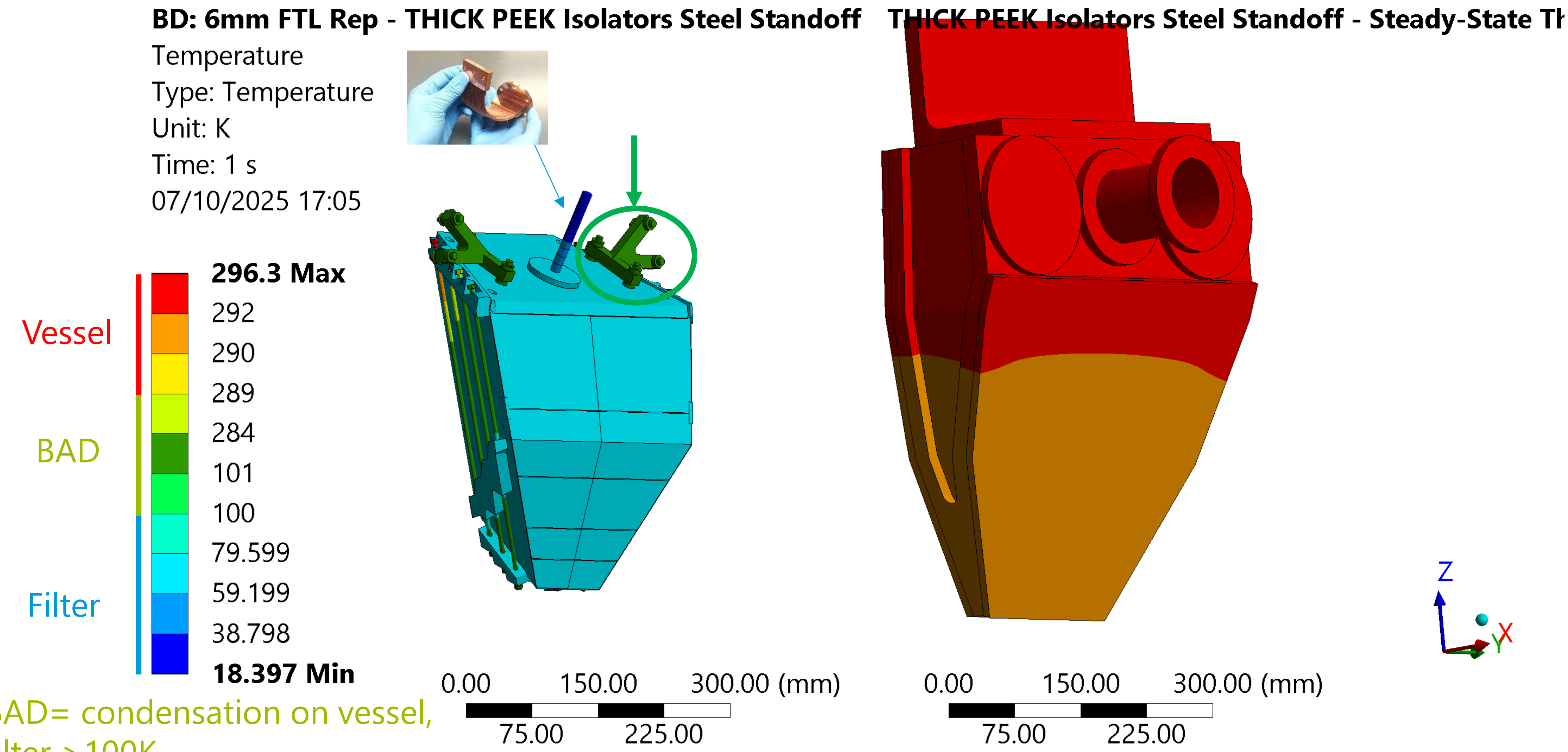
Jan 2025



Sep 2025

The Beryllium Filter - Thermal

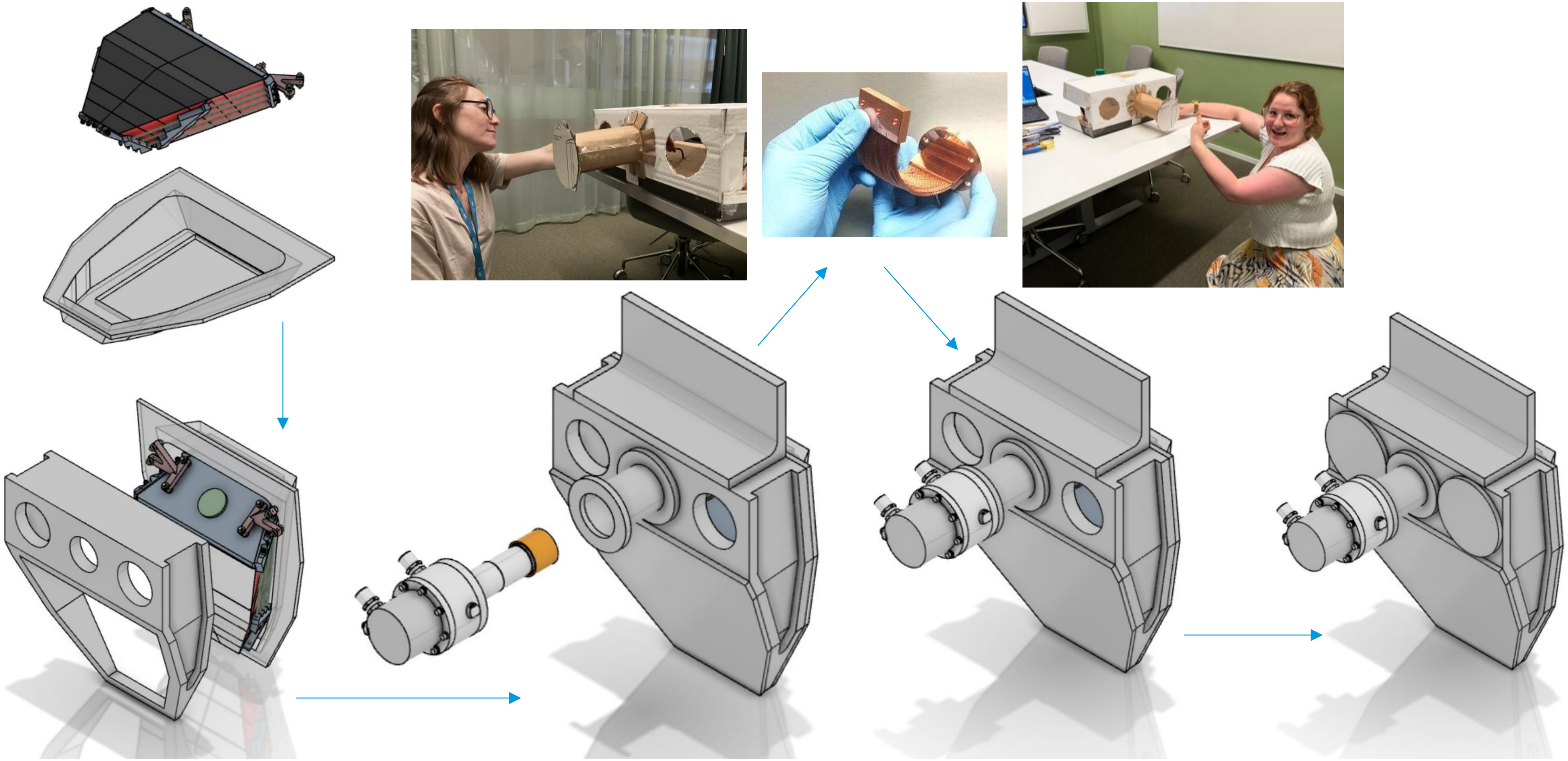
Thermal FEA outcomes



BAD= condensation on vessel, filter >100K

The Beryllium Filter – Vessel Assembly

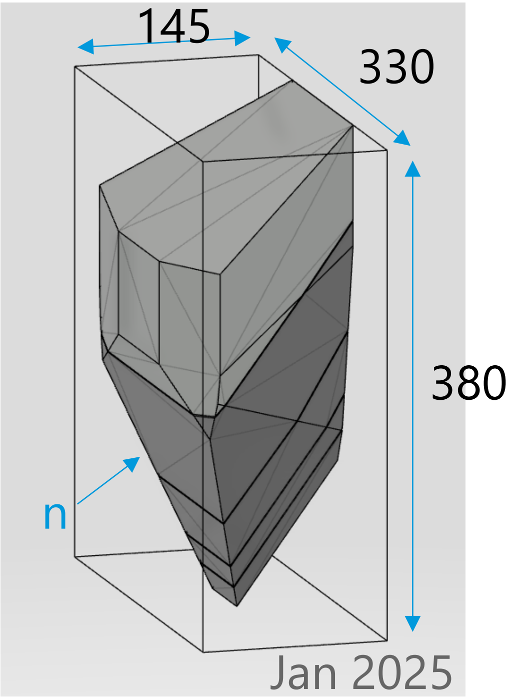
Assembly rapid prototyping

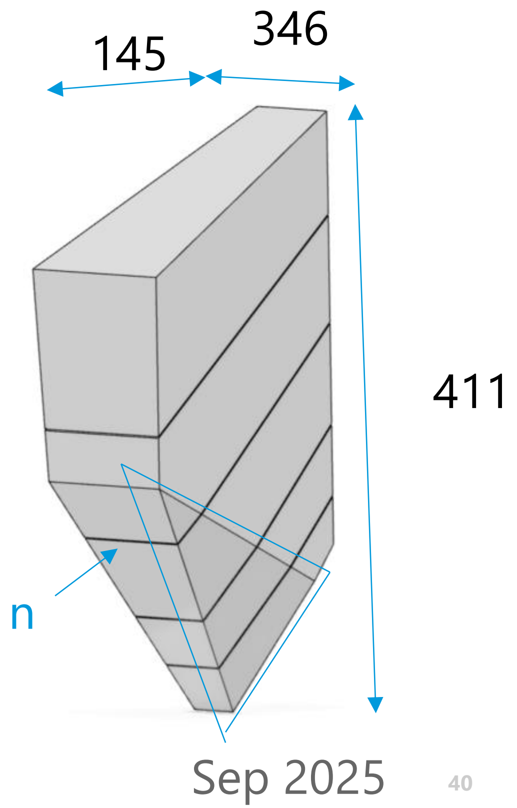


The Beryllium Filter

Mechanical Design Challenges

- Evolving science geometry based on analyser shape
- Negotiation with the scientist to make the shape easier to hold
- Thermal contraction between 300K to 80K – Beryllium contracts by ~1/3 the amount aluminium does
  - Any aluminium frame would shrink by ~1.2mm more than the beryllium ↕
- No useable parallel or perpendicular faces
  - Wedges acting in opposing directions



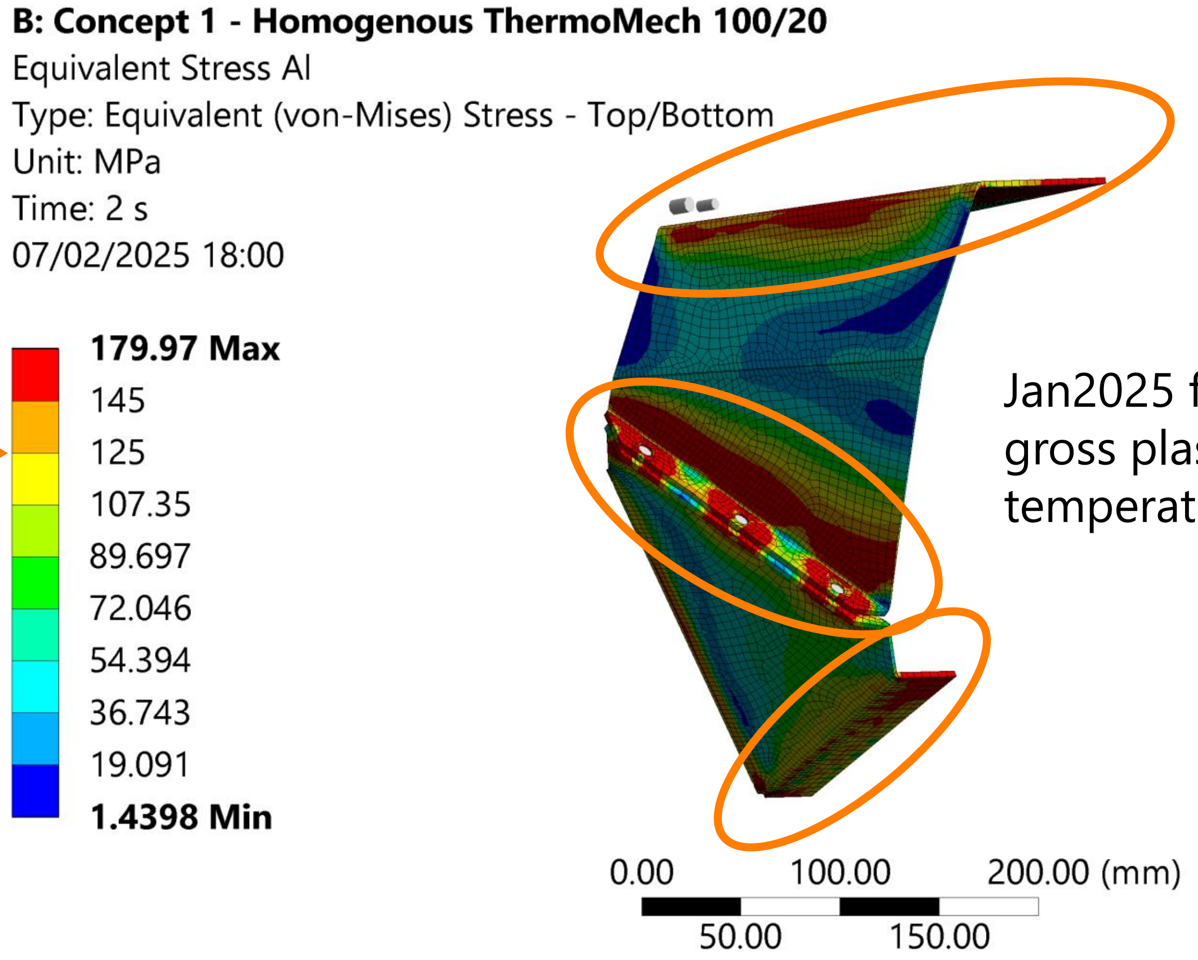


The Beryllium Filter - Mechanical

Proposed Mechanical Solutions (and the identified problems)

Stress due to thermal contraction at 20K

EN485-2 Yield Limit AW5083 3mm sheet



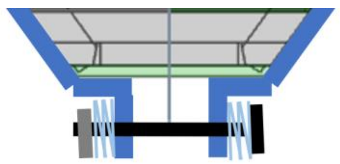
Jan2025 frame proposal : gross plastic yielding at low temperatures

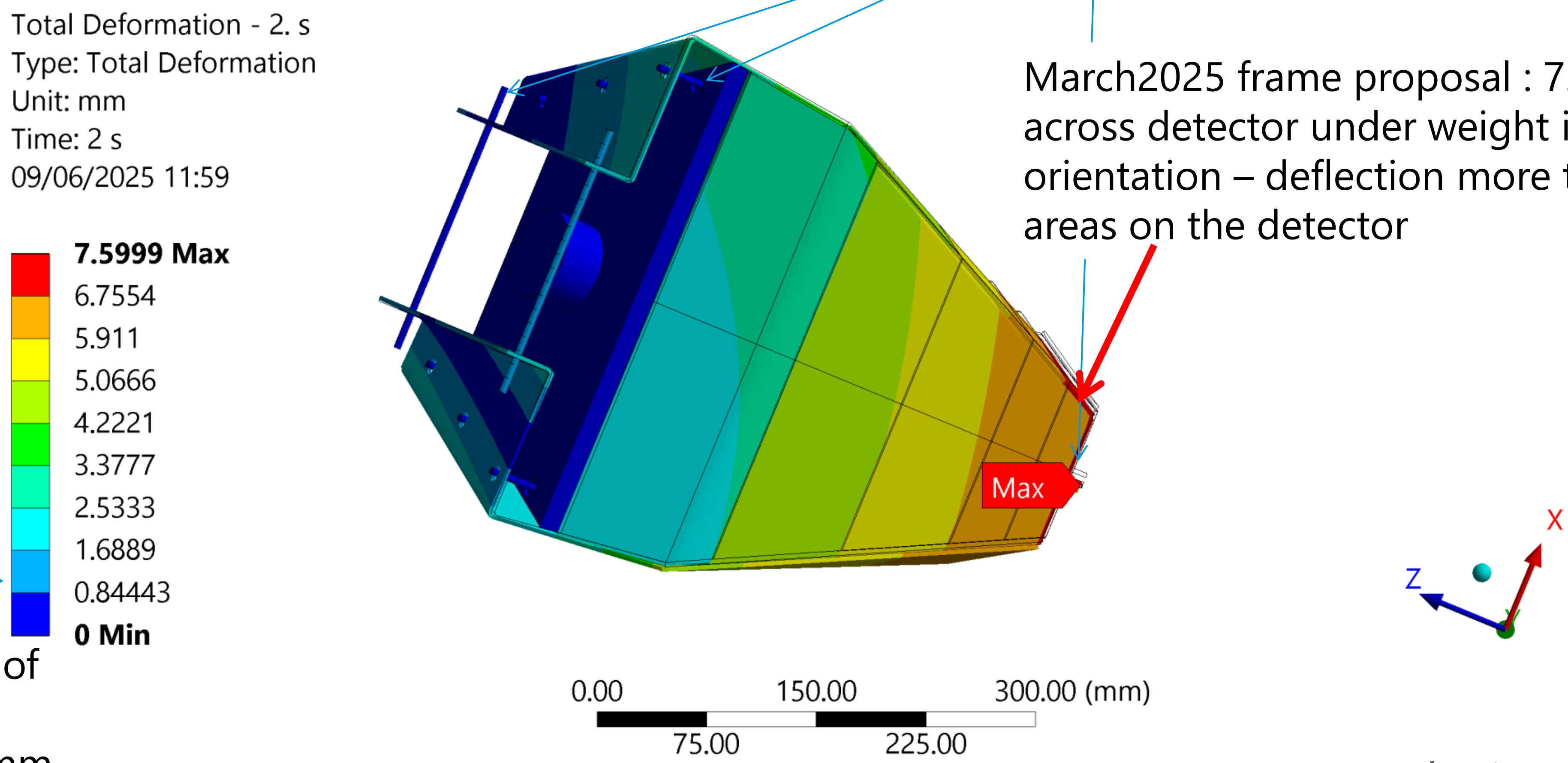
The Beryllium Filter - Mechanical

Proposed Mechanical Solutions (and their identified problems)

Deflection under gravity at 67.5° (295K)

Thermal float springs





March2025 frame proposal : 7.6mm deflection across detector under weight in the 67.5° orientation – deflection more than 2mm blocks areas on the detector

Acceptable movement of Be under gravity =1mm

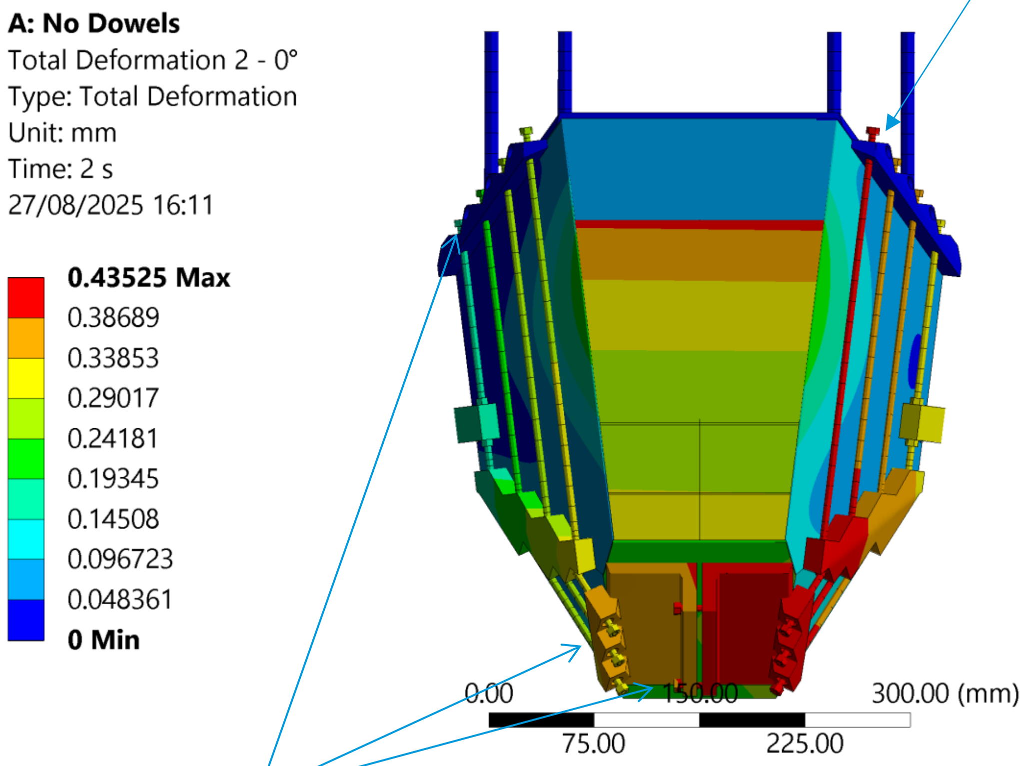
*True scale (1x) on deformation plot

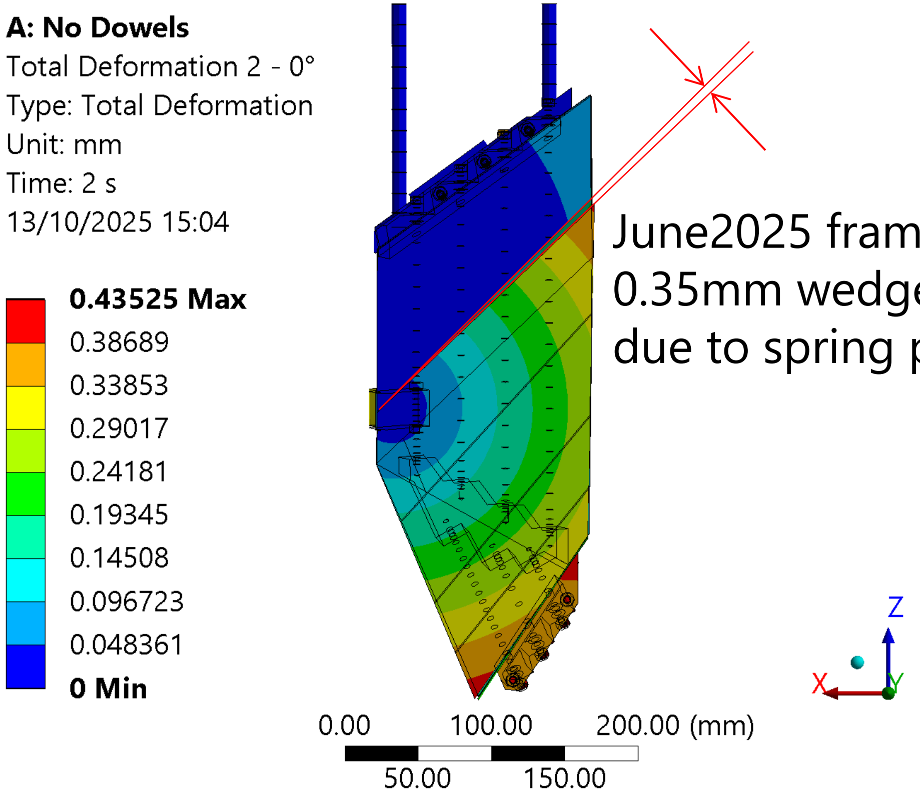
The Beryllium Filter - Mechanical

Proposed Mechanical Solutions (and the identified problems)

Deflection under gravity at 0° (295K)

Bent sheet changed for threaded rods and machined parts for better precision and stiffness





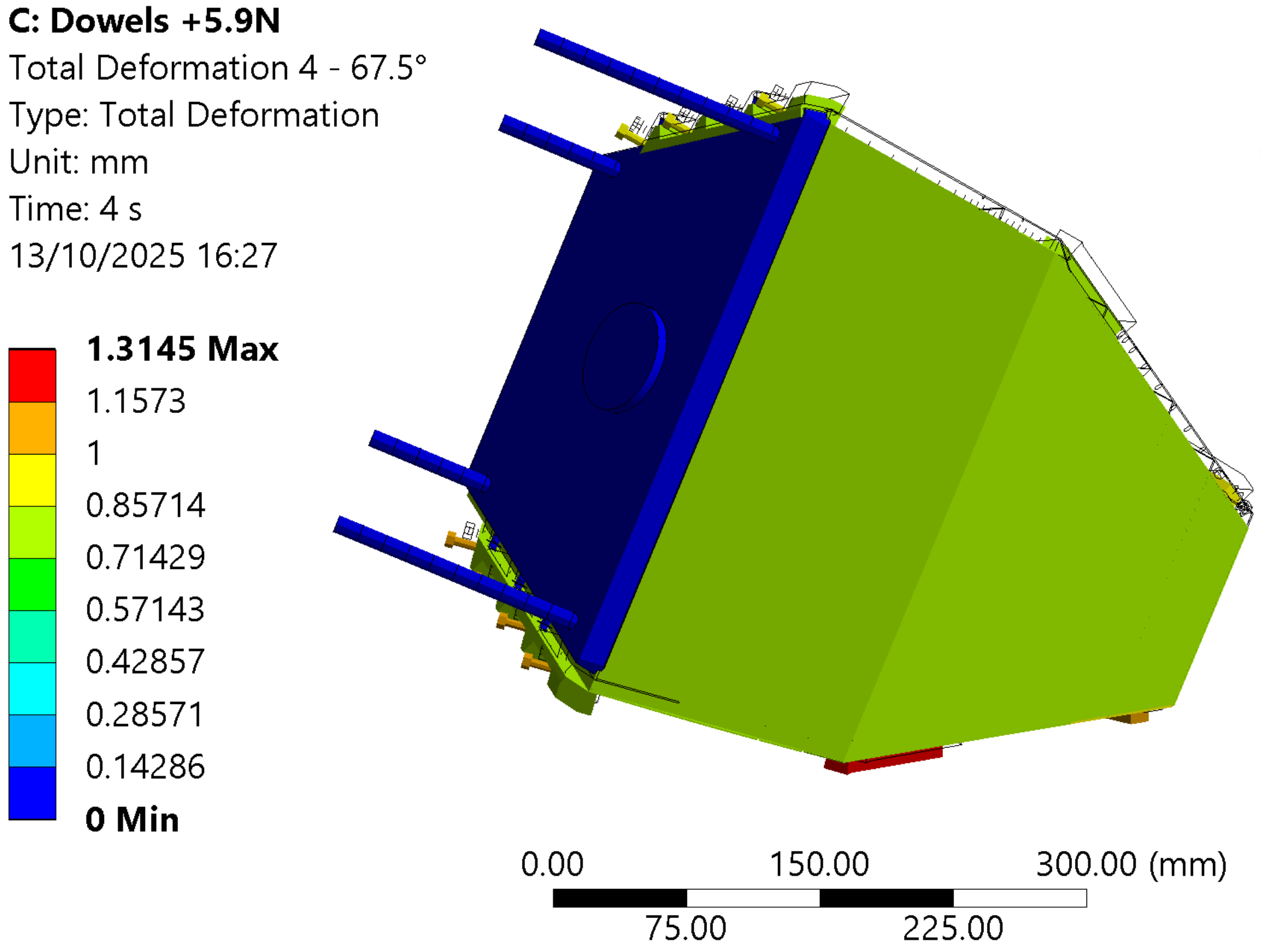
June2025 frame proposal : 0.35mm wedge separation due to spring preload

Pre-compressed Thermal Float Springs

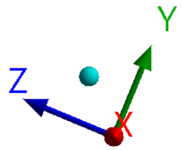
*10x scaling on deformation plot

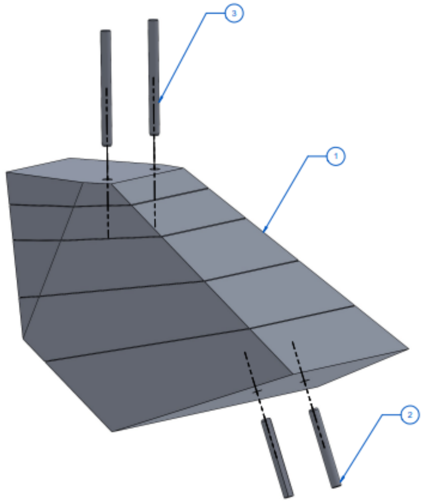
The Beryllium Filter - Mechanical

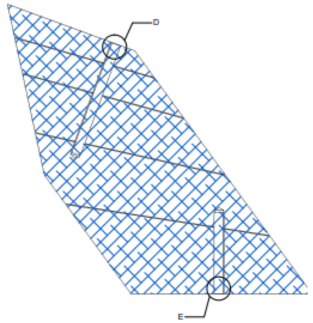
Proposed Mechanical Solutions



Acceptable position of Be under gravity







Jul2025: Exploring the option of including beryllium dowels with our Be machinist

*10x scaling on deformation plot

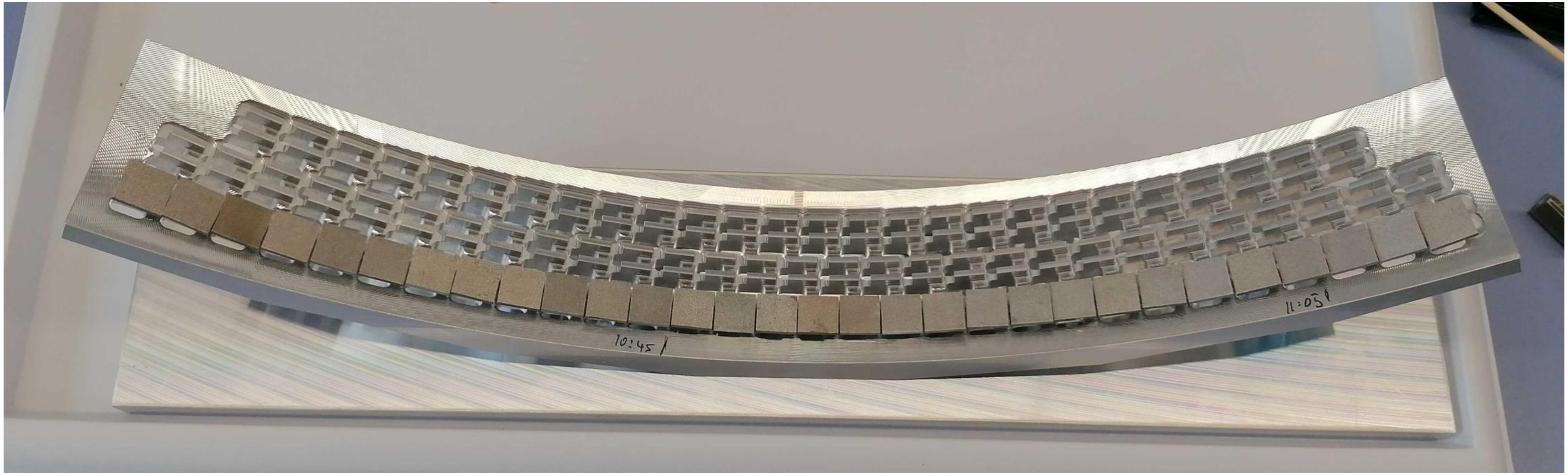
Analyser prototyping

Evaluation of compounded tolerances

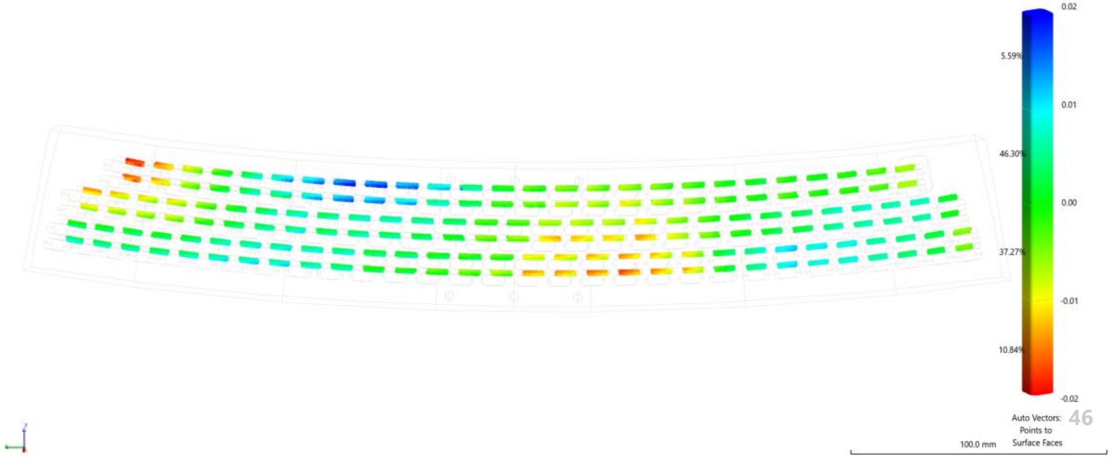
- Aluminum backplate – easy to machine compared to B-Al
- “Ridge & valley” design to minimise contact surface and gaps
- Thick B-epoxy absorber and glue
- What should be the dimensional tolerances (tile+epoxy+machining) to ensure feasibility and minimise gaps?

Analyser prototyping

Testing machining feasibility and tolerances



- Prototype with the full width of the analyser backplate to evaluate machining tolerances and gaps between tiles
- Excellent tolerances can be achieved with standard CNC +/- 20 microns
- Ongoing evaluation of assembly method



Analyser prototyping

Borated epoxy coating – first trials

Composition?
- 50% epoxy + 50% $^{10}B_4C$
- 50% epoxy + 50% ^{10}B

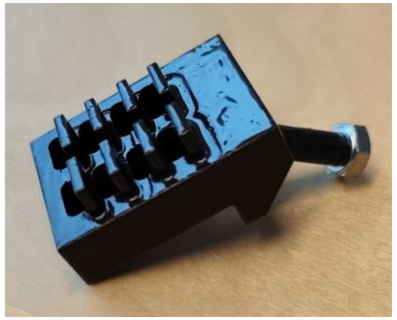
Application method?
- Dipping
- Vacuum coating
- Spray

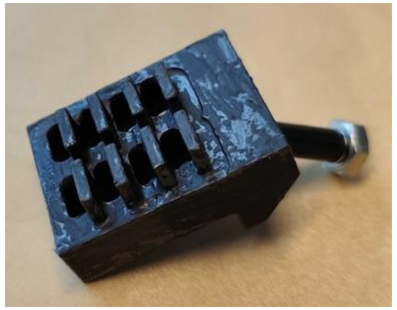
Curing conditions?
- Room temperature, 48h

Post-process?
- Machining to recover alignment surfaces

➢ Neutronics tests mid November on MARI

With ^{10}B





With $^{10}B_4C$

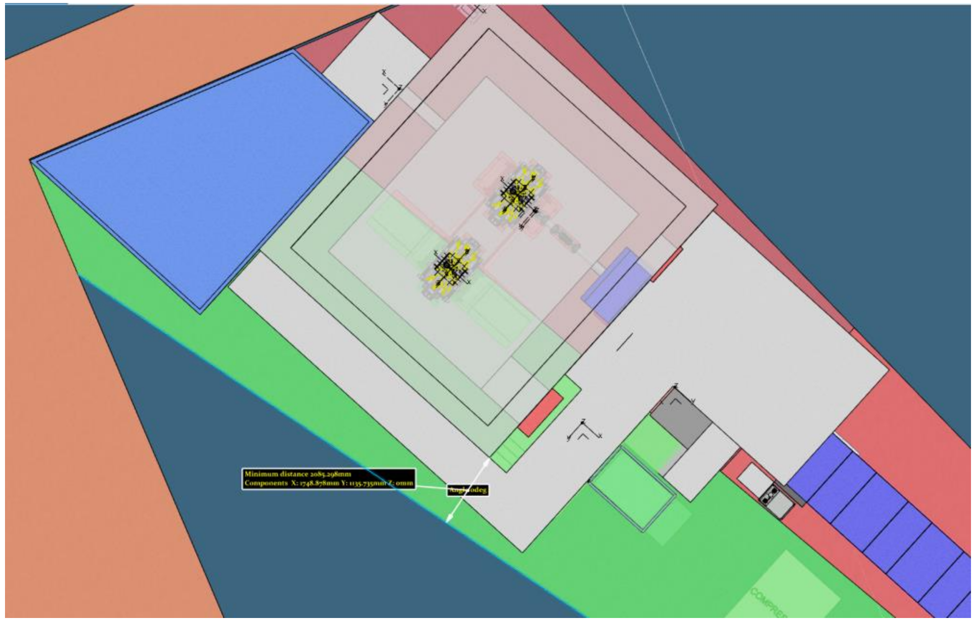
Cave & Hutch

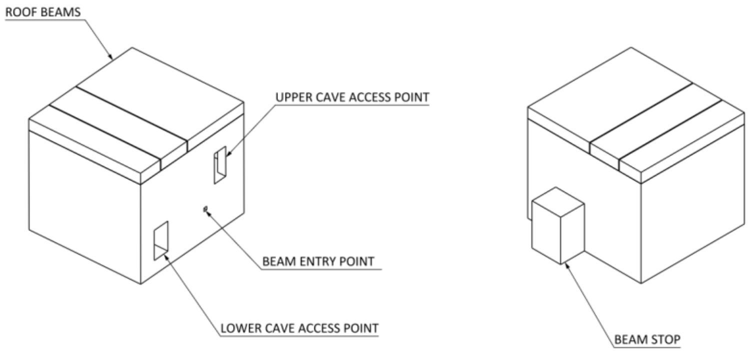
Cave & Hutch

Concept design & layout

VESPA was allocated the E6 wedge past 50 m to grow the cave to allow for:

- in situ installation in the lower cave
- in situ maintenance in the lower cave
- enough space to allow for concurrent experiment in the upper cave
- enough space for large sample environment kit (eg corrosive gas manifold)





Neutronics calculations ongoing to determine:

- Thickness of walls, ceilings, and doors
- Beam stop design/length/side shielding

Thank you for your attention!