ESS Spectroscopy division

Progress
Staffing
Rescoping
First science

PASCALE DEEN

Spectroscopy division

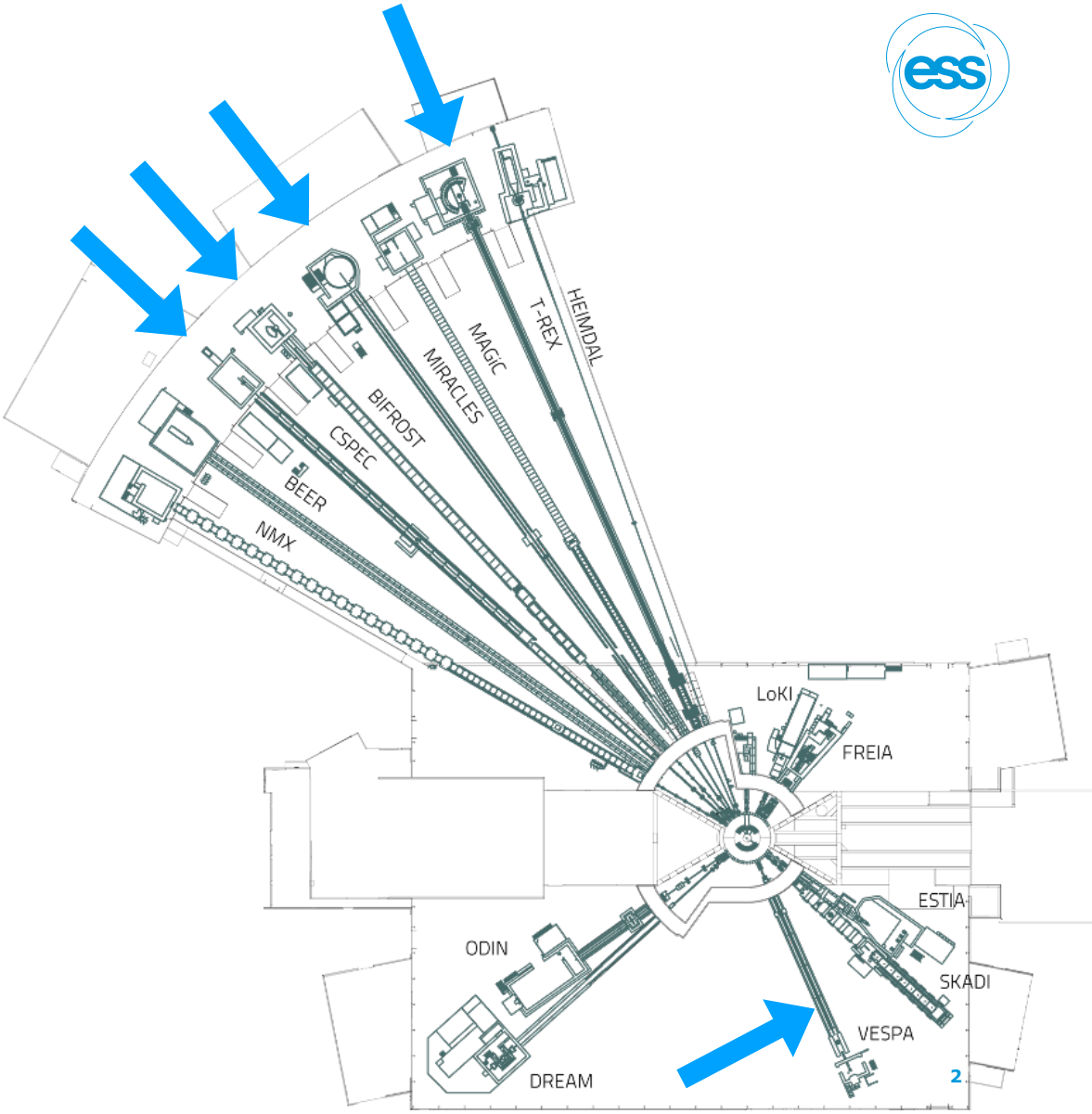
CSPEC Cold Chopper Spectrometer

T-REX Thermal Chopper Spectrometer

BIFROST Crystal Analyser Spectrometer

VESPA Vibrational Spectroscopy

MIRACLES Backscattering Spectrometer



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ESS Spectroscopy division

Progress
Rescoping
First science
Staffing

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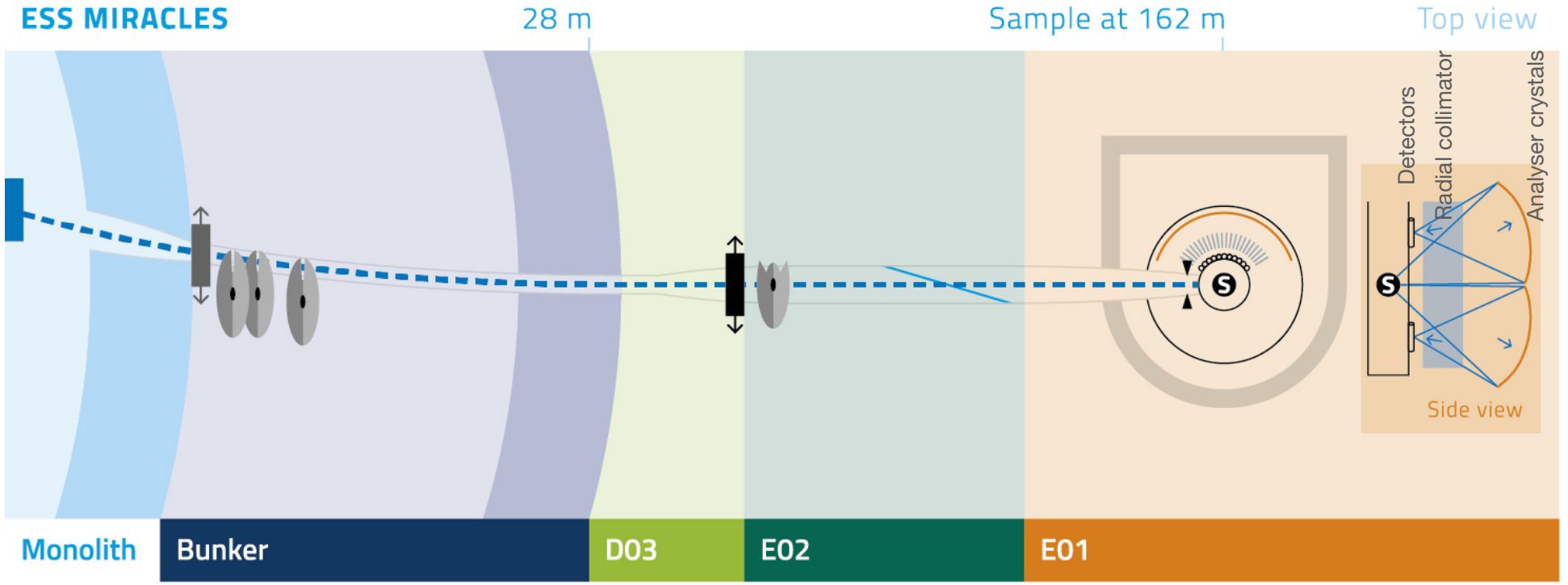
MIRACLES: High resolution backscattering spectrometer
Ready for hot commisioning TG5: June 2027

Lead scientist: Felix Villacorta (Bilbao), Jose Pereira (Bilbao)
Lead instrument engineer: Alex Conde Estebanez (Bilbao)



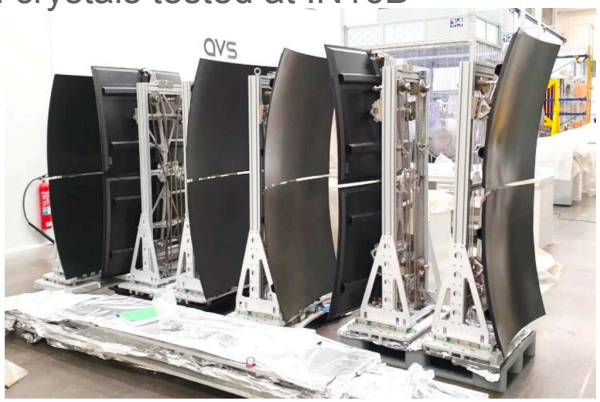
GOBIERNO DE ESPAÑA
MINISTERIO DE CIENCIA E INNOVACIÓN
Financiado por la Unión Europea NextGenerationEU
EUSKO JAURLARITZA GOBIERNO VASCO

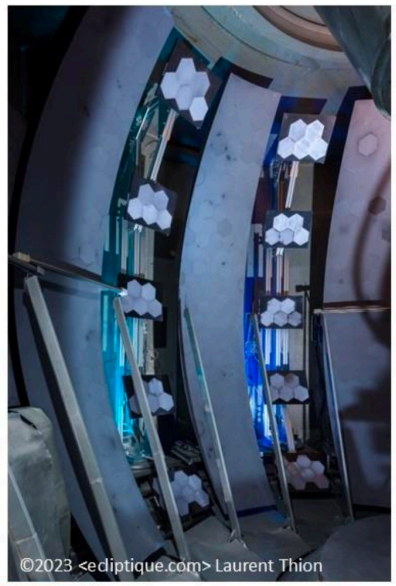
MIRACLES: High resolution backscattering spectrometer Progress

Panels and alignment for analyser system

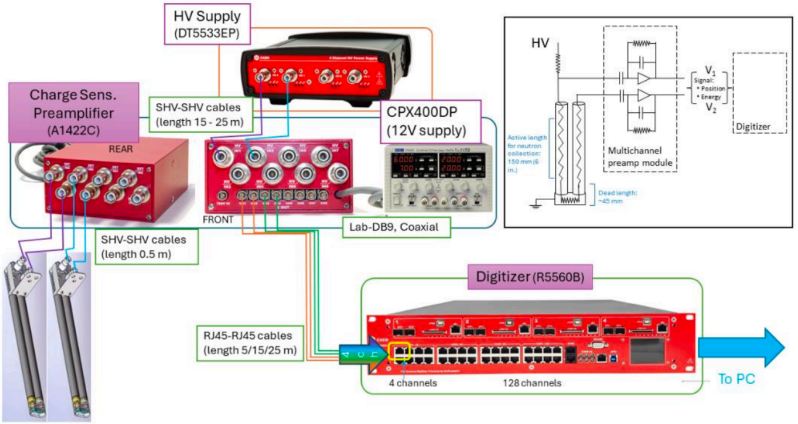
Si crystals tested at IN16B

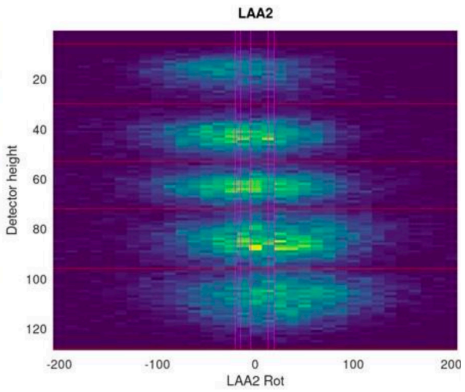
Detector tank





Detector developments





MIRACLES: High resolution backscattering spectrometer
Concerns & actions:

Choppers: Delayed delivery and technical challenges of fast speed choppers.

Common projects not prioritised for Tranche 2/3 instruments: electrical and conventional utilities, monitors, detector scope.

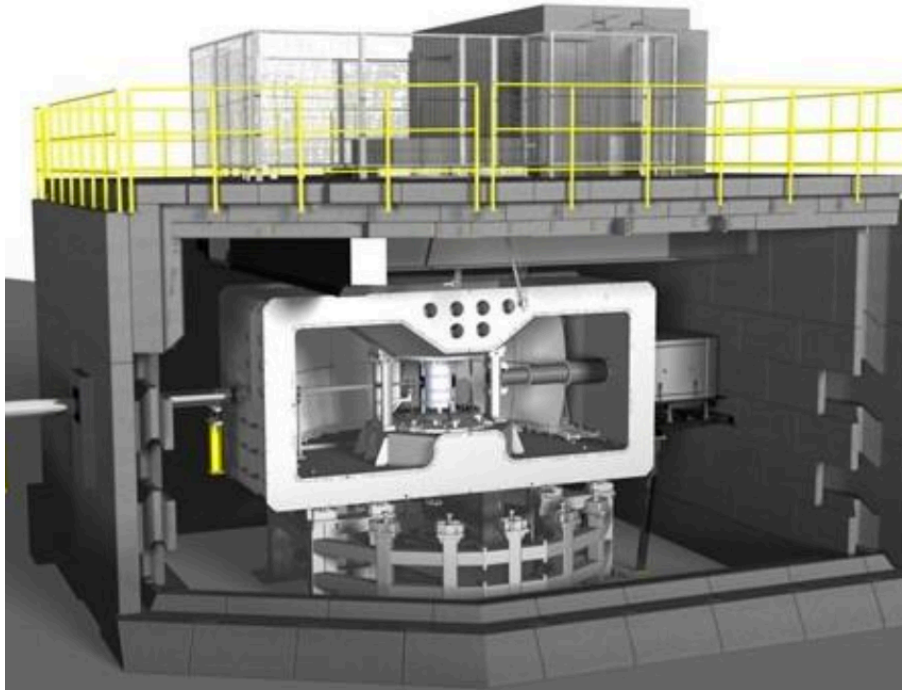
Lack of onsite staff
Position offered for instrument scientist based at ESS (October 2024), will need local engineering resources: position open for on-site engineer.

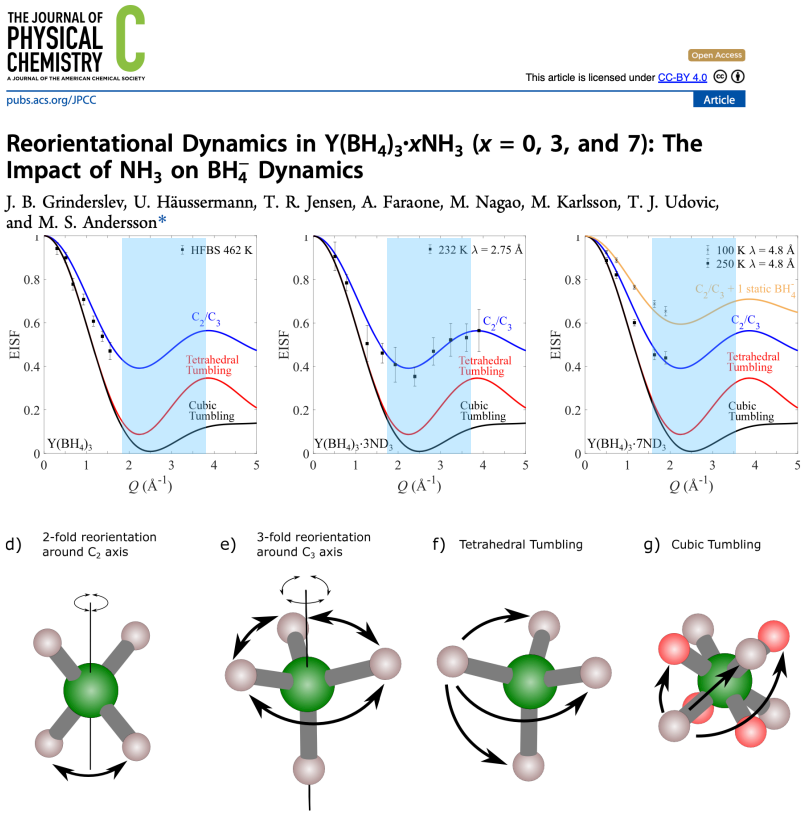
Data chain & workflow: Data scientist recruitment approved.

MIRACLES: Rescoping

The completion of the instrument will include the full coverage of the scattering system: a second analyser, radial collimator and ^{3}He detectors on the right side.

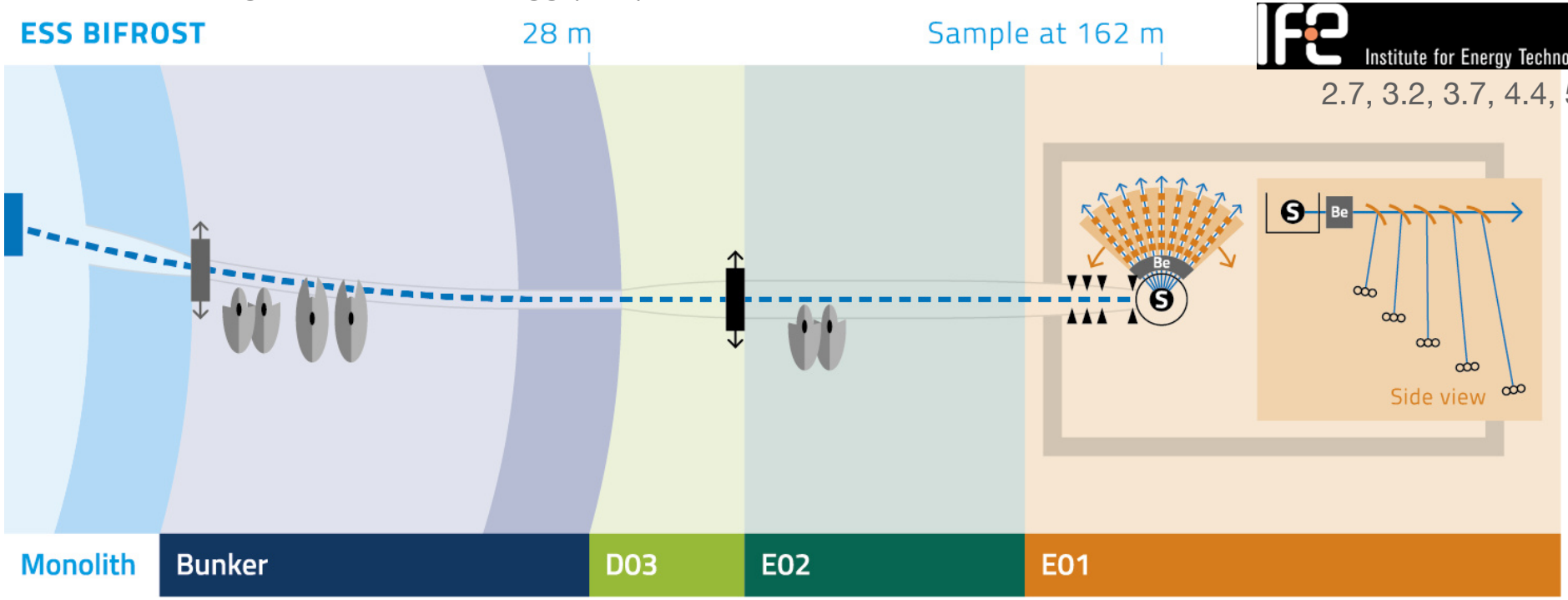
50% of right-side analyzer with Si(111) crystals (50%+),
50 % utilize Si(311) peaks, similar to other backscattering instruments (BASIS, DNA) and extend the Q-range to 3.8 Å.
Si(333) reflections from Si(111) crystals.





BIFROST: Extreme environment spectrometer
TG5: June 2025

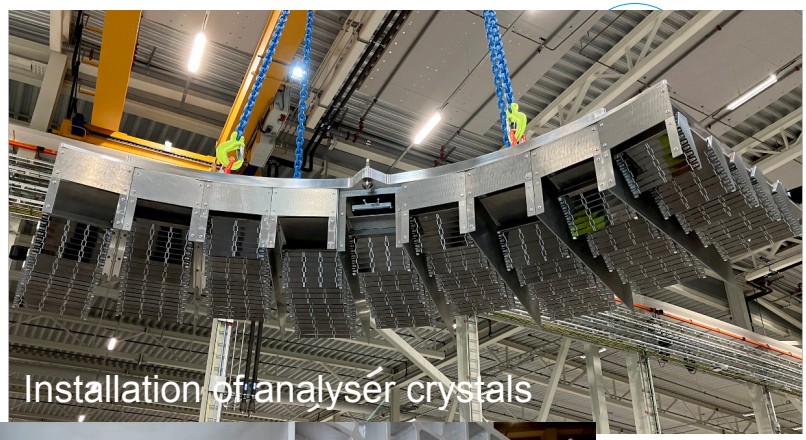
Lead scientist: Rasmus Toft-Peterson (ESS/DTU)
Lead instrument engineer: Liam Whitelegg (ESS)



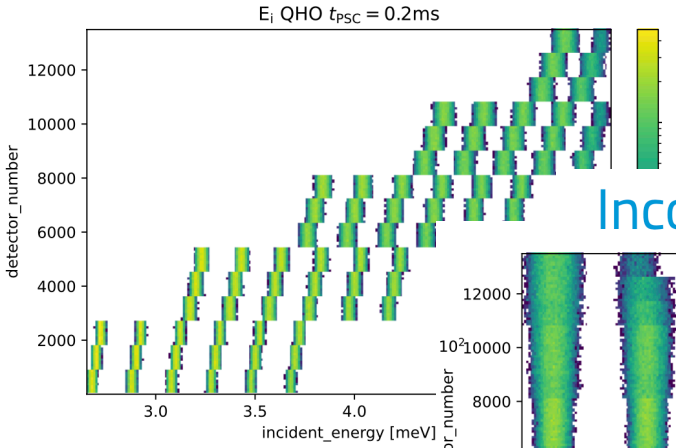
2.7, 3.2, 3.7, 4.4, 5 meV

λi = 1.5-6 Å
Radius of curvature = 1500 m: 1 x out of line of sight (Prior to bunker wall)
Bandwidth = 1.7 Å
Sample = 1 x 1 cm² - 0.1 x 0.1 cm²
Horizontal 7 - 135°, Vertical angular coverage = ±1.4°

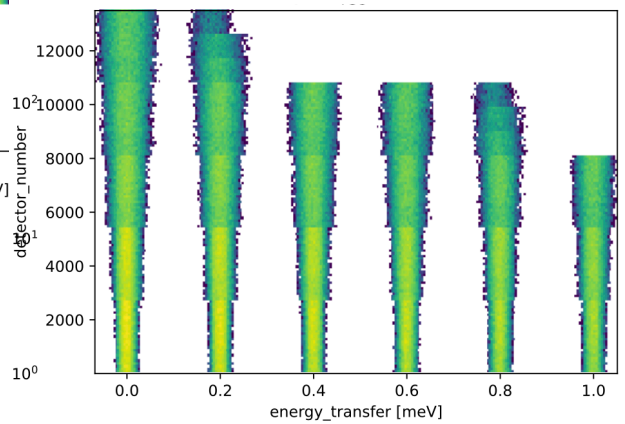
BIFROST: Extreme environment spectrometer
Progress:



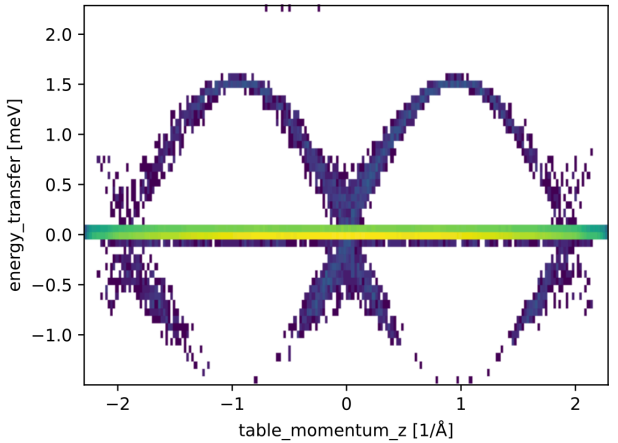
Bifrost: Extreme environment spectrometer
Data pipeline (IDS: Greg Tucker)
(current input : McStas data)



Incoherent inelastic



Coherent inelastic



Workflow requirements

Status	Description
✓	propagate `frame_time` to sample position
✓	calculate final (energy, wavelength, wavenumber, wavevector, velocity) from secondary geometry
✓	unwrap `frame_time` at sample to find `wall_time` at sample
✓	calculate incident (energy, wavelength, wavenumber, wavevector, velocity) from chopper cascade
✓	calculate energy transfer and lab-frame momentum transfer
✓	convert lab-frame momentum transfer to sample-table momentum-transfer
ongoing	normalize by incident wavelength-dependent flux
ongoing	normalize by detector efficiency, analyzer reflectivity, etc.
to-do	scale normalized intensity to absolute intensity units

Analysis requirements

Status	Software	Advantages	Disadvantages
✓	`scipp` +	event-based data, simple fitting, plotting	no high-level spectroscopy utilities
ongoing	`Horace`	extensive tof suite, resolution	detector-trajectory histograms
to-do	`MJOLNIR`	Bragg scattering spurions, visualization	flattened (Q_x, Q_y, E) histogram
	`Mantid`	event-based data	

BIFROST: Extreme environment spectrometer
Concerns & actions

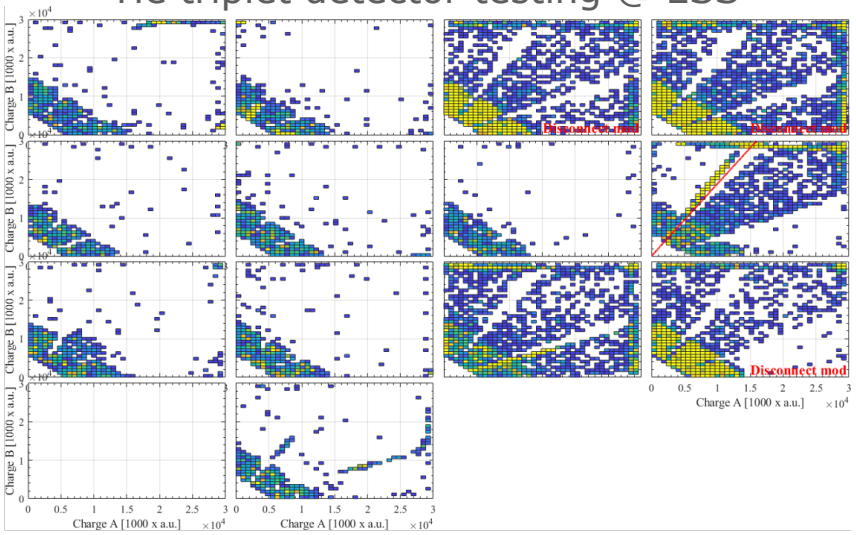
Cold commissioning - network to 1 instrument (Bifrost)
Energised only in D01 - not D03/E02/E01.

Without this holistic overview testing of instrument is not possible

Focus on PA is currently a distraction.

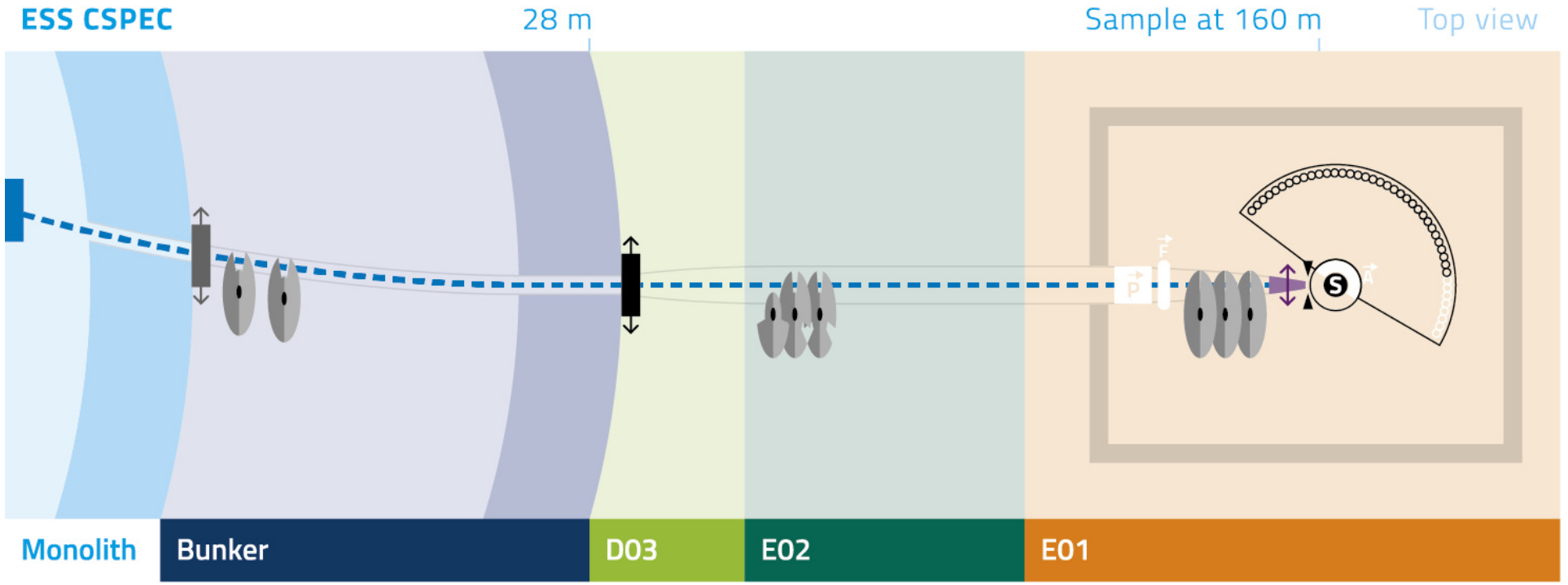
First science workshop: 4/5th February 2025. Engagement from community

^{3}He triplet detector testing @ ESS



The cold chopper spectrometer of the ESS
TG5: August 2027

Lead scientist: Daria Noferini (ESS)
Lead instrument engineer: Fernando Moreira (ESS)



- Cold neutrons (2-20 Å), ΔE/E = 1.5 % @ 4 Å.
- Focus flux on range of sample areas 4 x 2 cm^2 → 1 x 1 cm^2.
- Signal to noise = 10^5 (@5 Å, Vanadium).

The cold chopper spectrometer of the ESS
Progress:

The cold chopper spectrometer of the ESS
Progress:

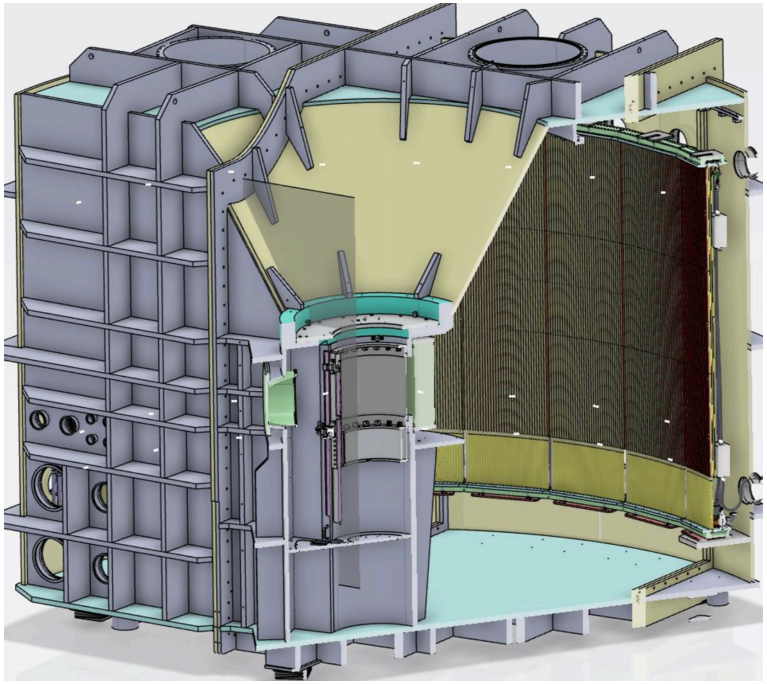

Collimator delivered, Kapton & Gd coating tested (ESS)

Installation of cave structure & hutch etc.. (as we speak)


In bunker guides & housing


Installation of out of bunker guides

CSPEC Detector kick-off meeting (contract signed): 16th/17th October 2024
ILL-ESS partnership for multitube ^{3}He detectors.



Engineering work commenced prior to kick off.
Engineering implementation of detector modules nearly complete.
Vanes not shown.

CSPEC: The cold chopper spectrometer of ESS
Concerns & actions

Working in a linear manner: Could really do with further engineering resources & technical writer to ensure timeline (beyond the IPL provided).

Common projects not prioritised for Tranche 2/3 instruments: electrical and conventional utilities, monitors, detector scope BUT team also do not have resources to focus on these.

ESS documentation criteria and requirements are difficult for many of our partner companies and laboratories to fulfil - leads to delays. Working actively to readjust.

Critical path is detector delivery for 4 modules at TG5, start with 1.

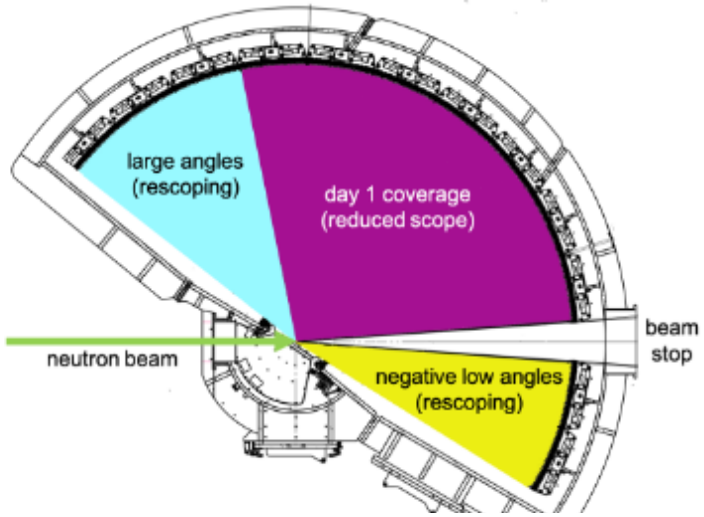
Rescoping

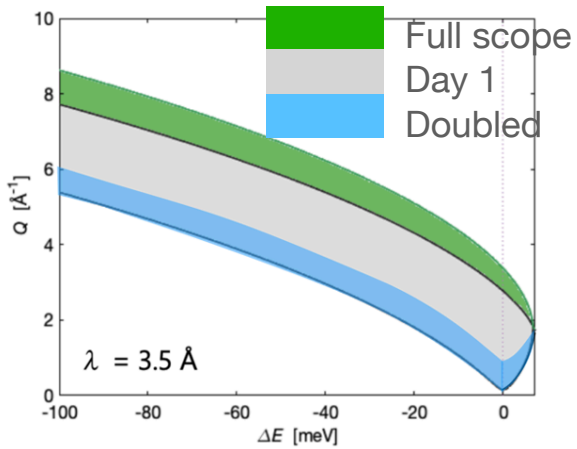
CSPEC: detector coverage from 58% to 100 %

(1) **^{3}He gas filling for complete detector (2.5 bar ^{3}He pressure)**

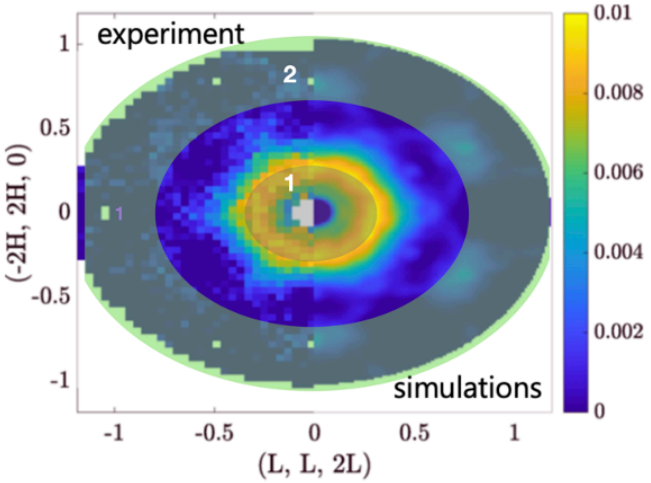
(2) Extend to 5 bar ^{3}He pressure

(3) PA

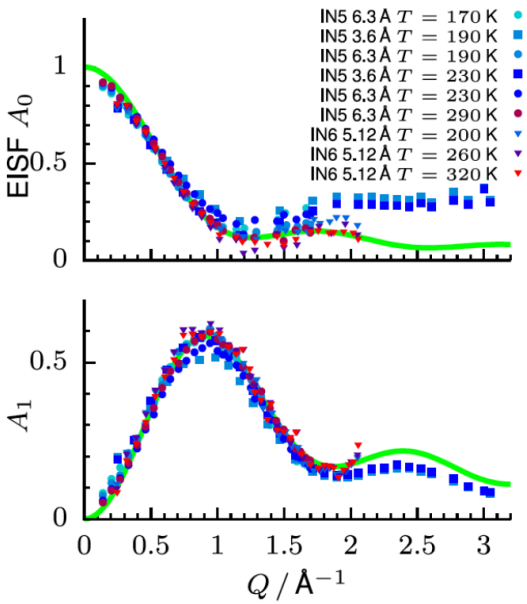




Single crystal frustrated magnetism



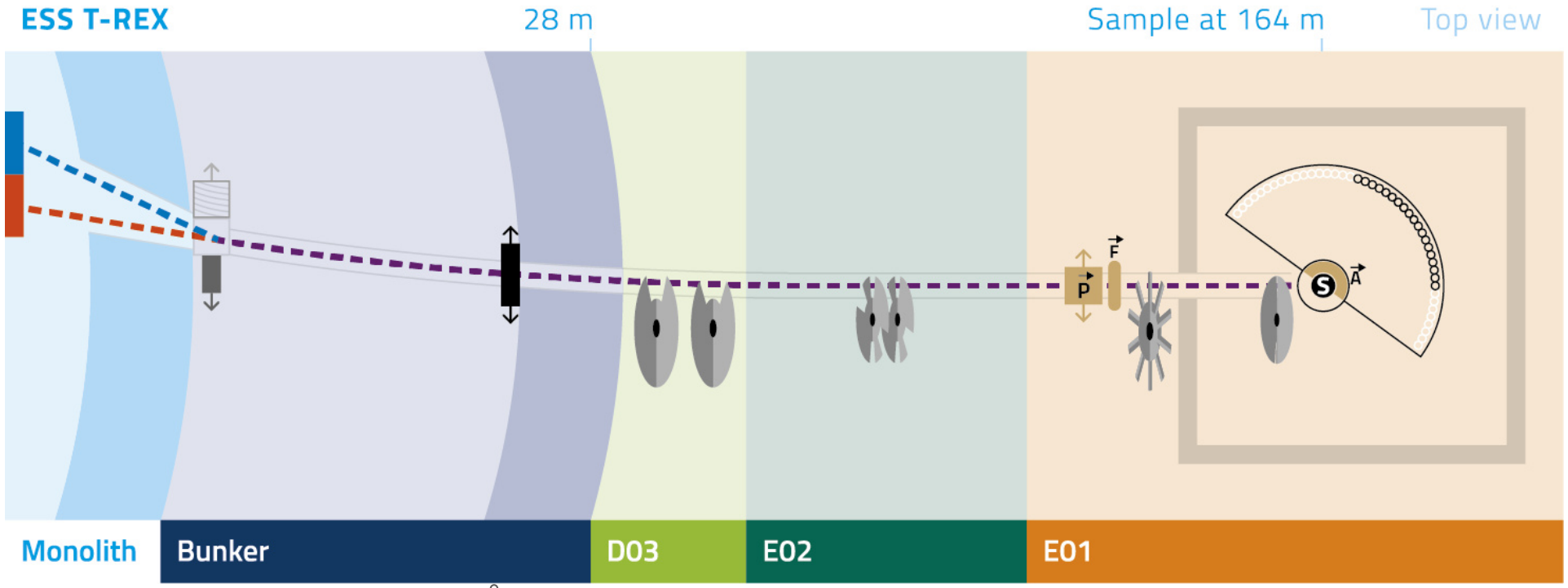
Ferrocene



Limited experimental signatures & Q range
Limits scientific capability
Day 1 scope FOM is not world leading.

T-REX: Bispectral chopper spectrometer with PA
TG5: August 2027

Lead scientist: Christian Franz (Julich)
Lead instrument engineer: Marcel Serwe (Julich)



- Bispectral extraction (0.7-6.5 Å, 2 - 160 meV), 1%–7% energy resolution.
- Focus flux on sample area 3 x 1 cm^2 (Div: ±0.25^o in the thermal band to ±1^o in the cold regime).
- Polarisation using PASTIS XYZ set-up.
- Novel B10 detector technology

TREX: The bispectral chopper spectrometer with PA.
Progress:


In-bunker guide installation


Heavy shutter installation


Detector tank ready for testing in Julich

TREX: The bispectral chopper spectrometer with PA. Progress:

Extensive activity on Multigrid detector

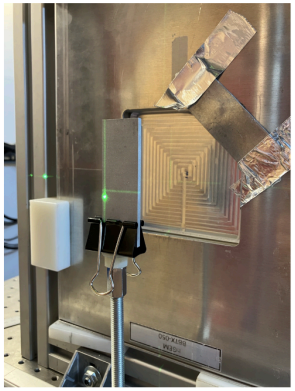
University of Glasgow

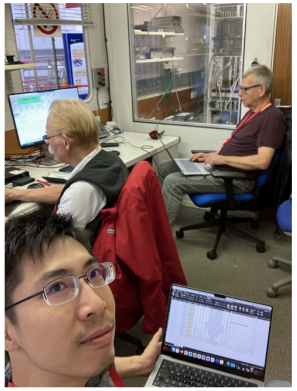
ess

UKRI Science and Technology Facilities Council

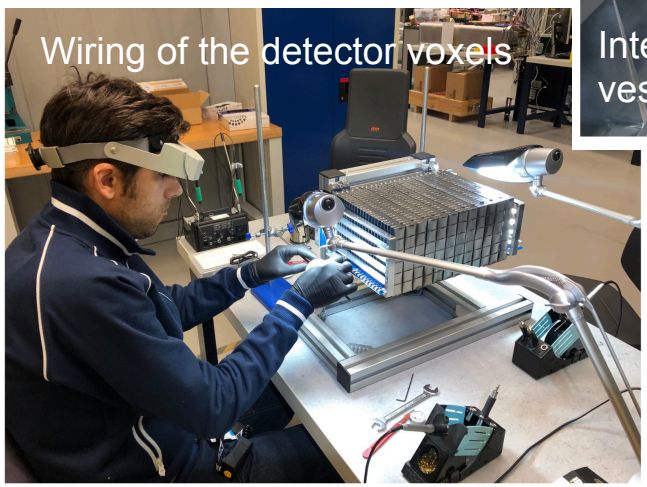
ISIS Neutron and Muon Source

Neutron transmission measurements, EMMA (ISIS)

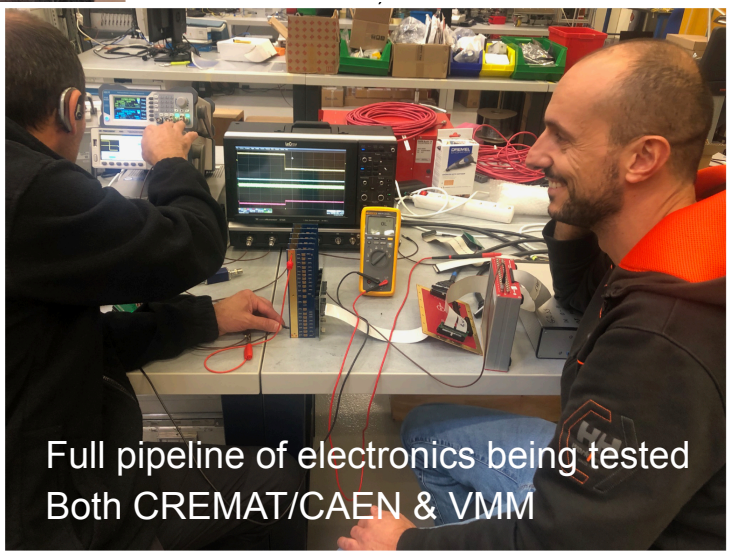




Integration test of detector into vessel (@ Julich)



Wiring of the detector voxels



Full pipeline of electronics being tested
Both CREMAT/CAEN & VMM

TREX: The bispectral chopper spectrometer with PA.
Concerns & actions

Common projects not prioritised for Tranche 2/3 instruments: electrical and conventional utilities, monitors, detector scope.

ESS documentation criteria and requirements are difficult for many of our partner companies and laboratories to fulfil - leads to delays. Working actively to readjust.

No staff member on site:
Recruitment completed for instrument scientist & will start 7th January 2025.
Concomitant recruitment of engineering resources.

Critical path is detector delivery.

Data chain & workflow: no current focus.

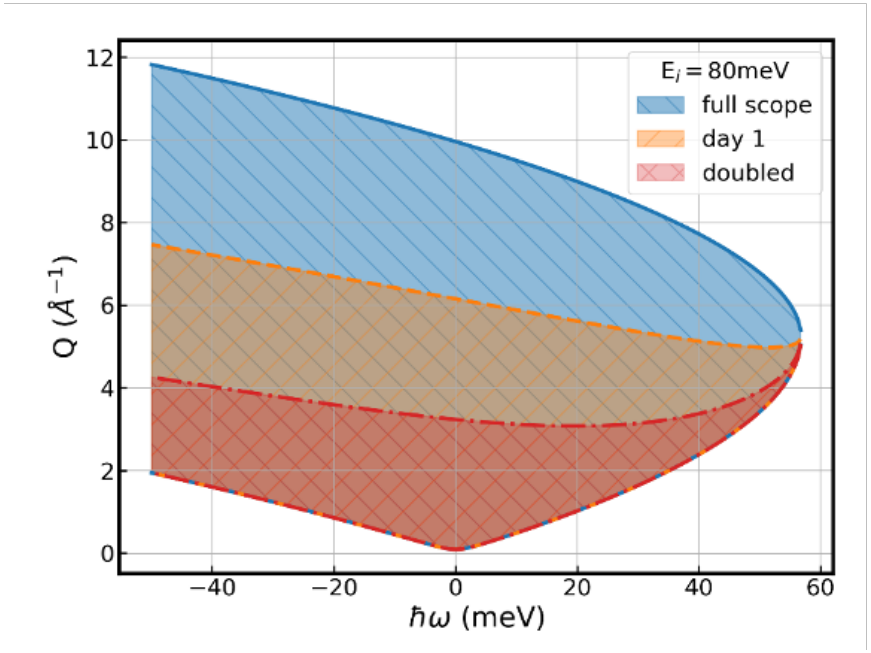
Rescoping

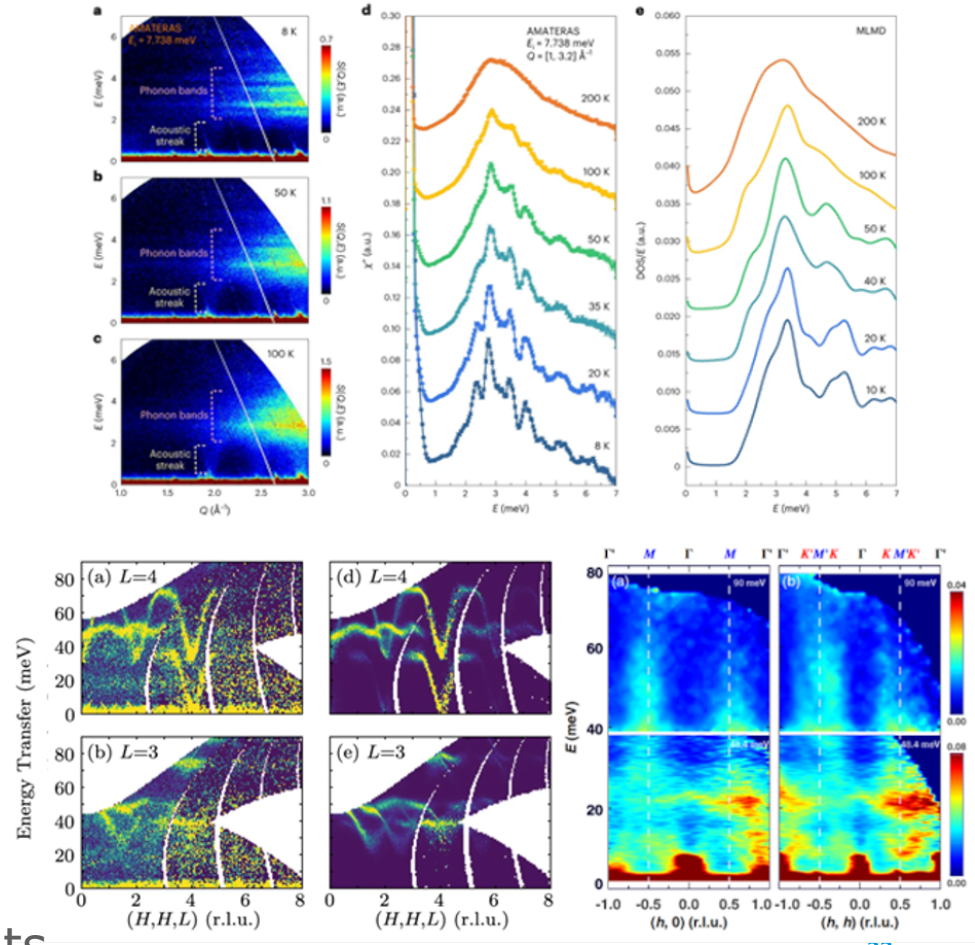
TREX:

(1) Detector coverage from 40% to 100%

(2) Advanced pulse shaping option with 4 blade pulse shaping chopper

(3) T0 chopper





Limited experimental signatures & Q range

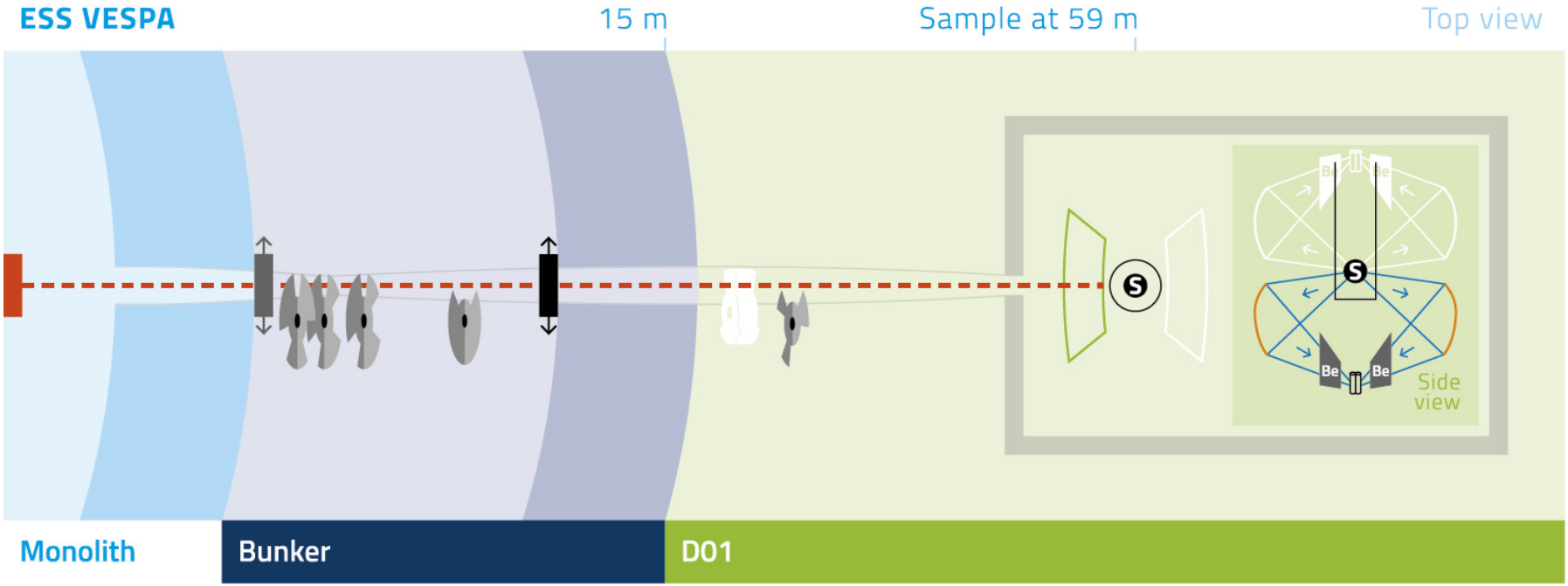
Limits scientific capability

Day 1 scope FOM is not world leading.

Note possible DG loss of competence if one waits.

VESPA: The vibrational spectrometer of the ESS
TG5: Replanning ongoing

Lead scientist: Adrien Perrichon (ESS)
Lead instrument engineer: Liam Whitelegg (ESS)



Direct view of the thermal moderator (Ei = 3 - 1000 meV)
Complex chopper cascade to achieve 3 subframes and variable resolution
Indirect-geometry crystal-analyser
Complex and compact secondary spectrometer:
280 ^{3}He tubes, 8500 HOPG crystals, 200 kg of cryo-cooled Be, in <2 m^{3} vacuum vessel

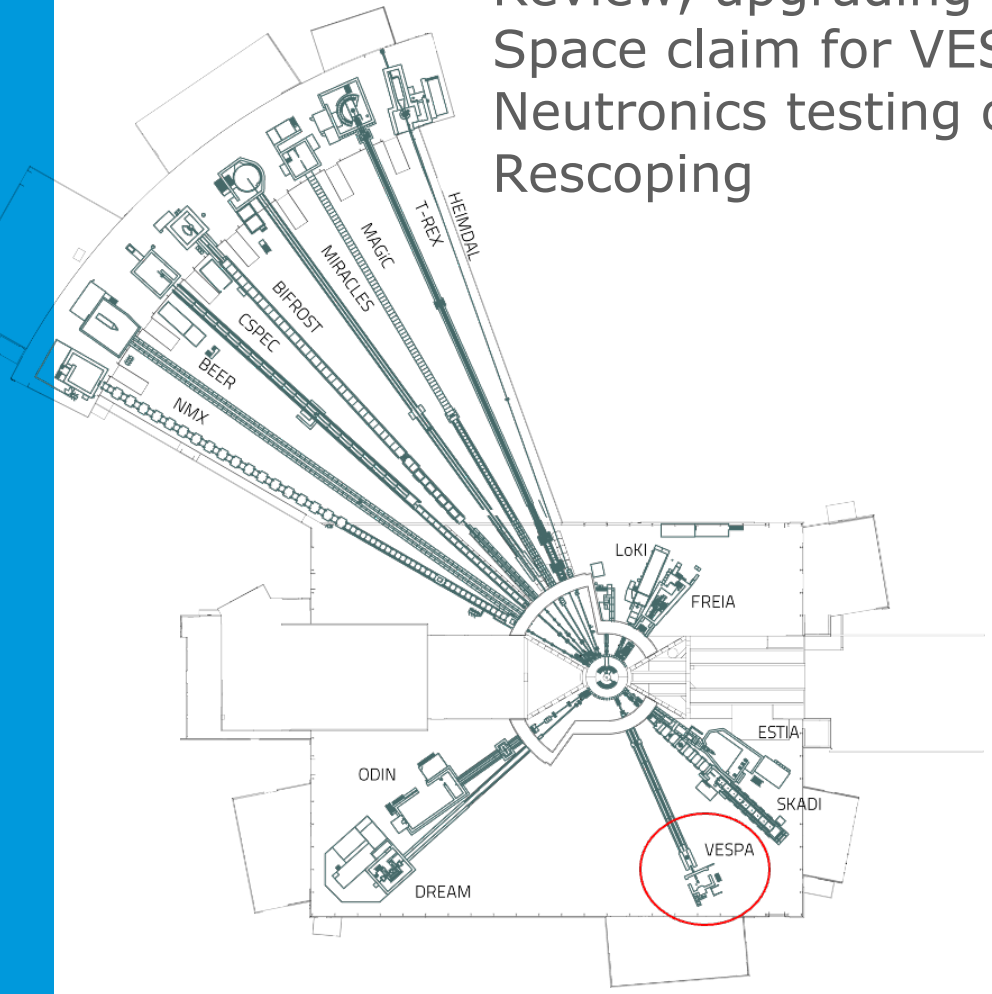
VESPA: The vibrational spectrometer of the ESS
TG5: Replanning ongoing

Staff recruitment in 2024

(January) Liam Whitelegg: Lead engineer (50%)
(March) Adrien Perrichon: Lead Scientist
(September) Rosa Camilleri Lledó: Lead Engineer
(October) Gianfranco Belcastro (ISIS/CNR): Engineer
[open] Mechanical engineer at ESS

STFC ISIS Facility collaborators
S. Parker, R. Bewley, J. Nightingale, D. Raspino

VESPA: The vibrational spectrometer of the ESS
TG5: Replanning ongoing



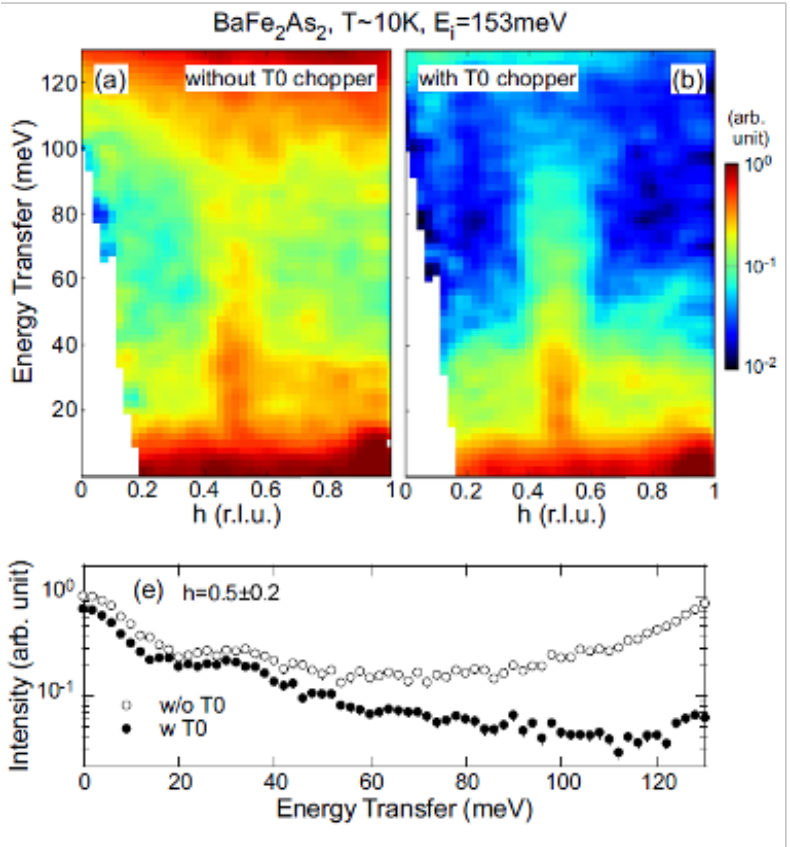
Review, upgrading and finalisation of VESPA design
Space claim for VESPA end-station
Neutronics testing of HOPG tiles
Rescoping

Primary
Chopper cascade
Slit system
Guide gaps and substrates

Secondary spectrometer
Update to TOSCA+ type geometry

Cave & sample preparation area
Evaluation of alternative designs

Rescoping
VESPA:
(1) T0 chopper
(2) Rescoping secondary spectrometer

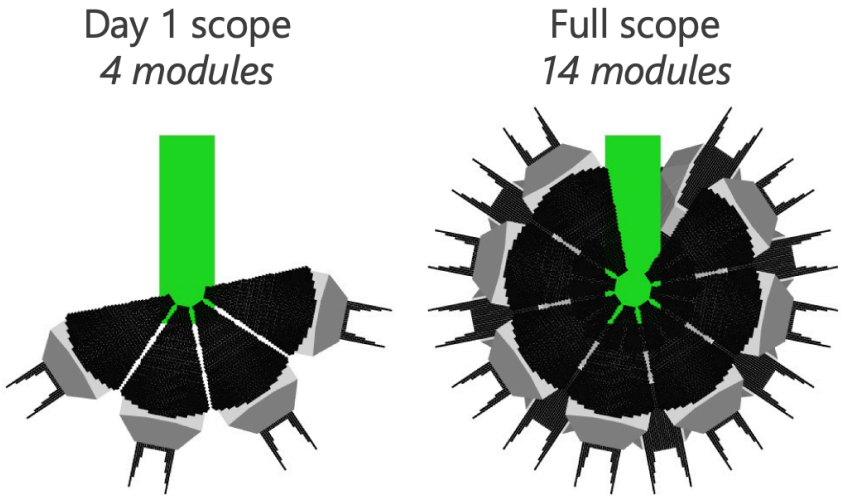


- Direct line-of-sight from moderator to sample
- Flood of epithermal and high-energy neutrons
- Secondary scattering events at unpredictable times
- The lack of T0 chopper would ruin the SNR of VESPA

4SEASONS at J-PARC

- Kajimoto et al., J. Phys. Soc. Jpn. **80** (2011) SB025

Rescoping
VESPA:
(1) T0 chopper
(2) Rescoping secondary spectrometer



Scope = 11% of nominal performance (Sr × reduced source power)

High-Resolution setting of VESPA only competitive if the instrument is fully rescoped
High-Flux setting of VESPA only state-of-the-art if the instrument is fully rescoped

ESS Spectroscopy division

Progress
Rescoping
First science
Staffing

PASCALE DEEN

Spectroscopy division: Rescoping priorities
PA not considered
Sample environment considered in the Scientific support division.

Instrument	Rescoping option	A: Scientific Impact (5: high, 1: low)	B: Manpower (1: high, 5: low)	C: Technical Risk (1: high, 5: low)	B: Cost	FOM: A*B*C
MIRACLES	Complete Analyser/collimator/detector coverage Si (1 1 1) & (3 1 1)	2	Can be included and delivered within current instrument construction: 2	5	**1.67 M€**	20
CSPEC	^{3}He full detector coverage (2.5 bar)	5	Minimal: 5	5	**2.025 M€**	125
CSPEC	^{3}He full detector coverage (5 bar)	2	Minimal: 5	5	**+4.375 M€**	50
T-REX	Full detector coverage	5	Significant (Detector group) 2	4	**>5 M€**	40
T-REX	Extra blades for P chopper	2	Julich chopper group: 3	2	**0.5 M€**	12
T-REX	T0 chopper	x	x	x	**0.85 M€**	?
VESPA	T0 chopper	5	Some (Chopper group) 4	4	**0.85 M€**	80
VESPA	Increase analyser modules	4	Can be included and delivered within current instrument construction: 4	4	**3.6 M€ for 10 (0.36 each)**	64

ESS Spectroscopy division

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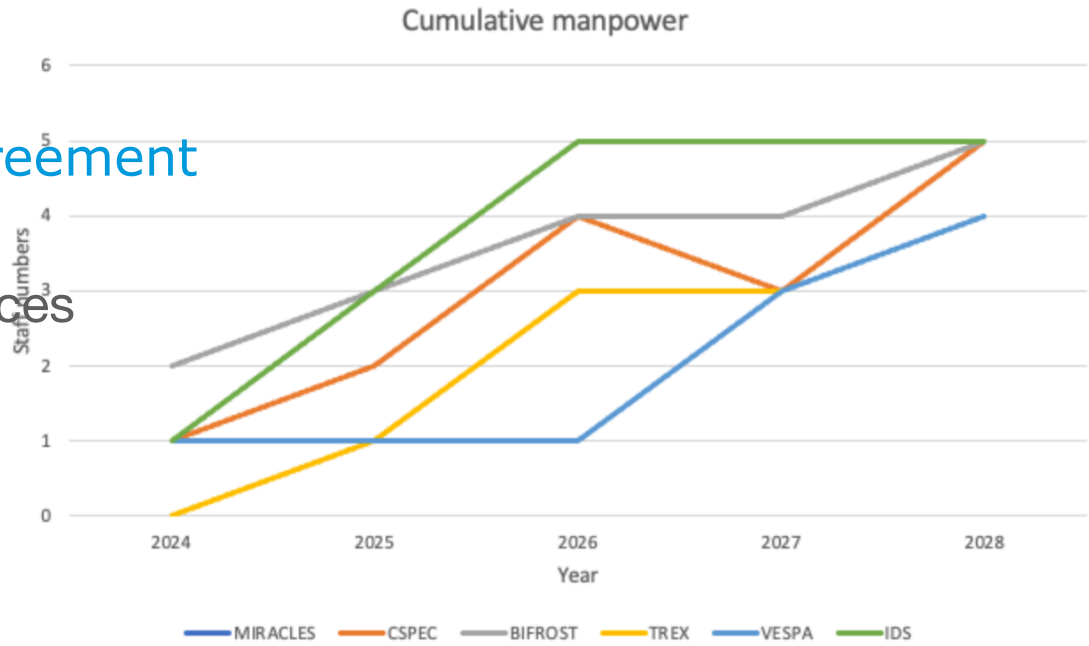
Spectroscopy division
Staffing expectation (on-site):
Contingent on SSO Review & Council agreement

Ensure concomitant onsite engineering resources



		2024						2028					
Instrument	TG5 Date	Scientist 1	Scientist 2	Scientist 3	IOE	Post-Doc	Data scientist	Scientist 1	Scientist 2	Scientist 3	IOE	Post-Doc	Data Scientist
MIRACLES	Q2 2027	0	0	0	0	0	0	1	1	1	1	0	1
CSPEC	Q1 2027	1	0	0	0	0	0	1	1	1	1	1	1
BIFROST	Q3 2025	1	0	0	1	0	1	1	1	1	1	1	1
TREX	Q2 2027	0	0	0	0	0	0	1	1	1	1	0	1
VESPA	Q1 2028	1	0	0	0	0	0	1	1	1	1	0	1
Spin echo	??												
Bold means Q3/4		Red is inkind											
Data Scientist													
Total for year						Spec Division	4					Spec Division	22
Note: VESPA Scientist 2 can be a computational material scientist.						IDS	1					IDS	5
Note: Bifrost scientist 2 is in-kind from KU													

ESS Spectroscopy division

PASCALE DEEN