Towards rescoping of ESS instruments

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The European Spallation Source (ESS) neutron instruments were initially approved for construction in 2013-2016 with performance estimates that, at that time, would significantly outperform equivalent world leading instruments. The ESS instruments were descoped, to meet financial limitations, first in 2014, for the first instruments chosen, with further descoping in 2016 for the rest of the instruments. A careful analysis of the effect of the descoping exercise was not, at the time, performed. In the 10 years since these decisions, there have been significant improvements at our partner facilities that have led to increased instrument performance.
In the last 18 months we have carried out a benchmarking analysis of ESS instruments' expected performances compared to performances of similar instruments in current world leading facilities. The document ESS-5290872, submitted to SAC32, provides an overview of the ESS instrument performance at the time of their proposal and today, after descoping at the ESS and upgrades at our partner laboratories.
The conclusion of the analysis is that in many instances a rescoping of the instruments is necessary to ensure the leadership of ESS worldwide. Furthermore:
(1) The rescoping of the instruments can be performed in a staged approach with current priority placed on the components outlined for each instrument to be completed for first science on each instrument.
(2) Reaching a stable 2 MW operational mode will be necessary to perform adequately.
(3) Further instrumental upgrades can be completed shortly after the instruments are in full operation ensuring a limited downtime.
It is noted that the support facilities are of paramount importance and these also need to be carefully considered and funded to optimise scientific output and the user experience.

Besides the financial burden, the rescoping of the instruments entails the use of resources that are now fully devoted to delivering the current scope in the construction project. In the current phase and because of the delays already experienced by the project, it is not possible to jeopardise the process and rescoping must be foreseen in the cases where outside resources can be exploited or if the impact on the in-house work is minimal. Nevertheless, it is important to start from now investigating the possibilities and anticipate procurement of elements or use of resources to be used later as well as make plans for steady state operation.

In the below sections overviews of the rescoping needs in the three instrument divisions is presented, including evaluations of the i) scientific impact, ii) manpower requirements, iii) technical risks, iv) and v) costs.

Based on the first four factors above, the following priority list was defined (for details see the descriptions from each division). Some of the cases have equivalent scientific priority, the numbering is indicative.

- FREIA shutters
- DREAM full coverage detectors
- VESPA T0 chopper
- CSPEC ^{3}He 2.5bar (full detector coverage)
- HEIMDAL detectors
- VESPA analyser modules
- ESTIA upgrades
- T-REX full coverage detector
- SKADI full coverage detector (pending validation of detector technology)
- NMX Gd coated detectors (to be started after instrument validation)
- MAGiC full coverage detector
- BEER texture detectors
- BEER multiplication choppers
- ODIN grating interferometry

SPECTROSCOPY Instrument rescoping

In this overview we present the most important needs for high performance of the spectroscopy instrument. Additional needs are presented in the individual instrument rescoping documents. Sample environment needs are not considered in this document.

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

VESPA

(1) T0 Chopper: **0.85 M€**

Resources needed: Requires significant resources from the chopper team.

The current SNR of TOSCA and VISION are estimated to 3×10^{-3}, and the Signal to Noise Ratio (SNR) target for next generation NVS instruments, TOSCA+ and VESPA, should be 10^{-4} or better. A T0 chopper will be essential to optimise the SNR on VESPA. VESPA is a straight guide instrument that views the thermal moderator. Previous instruments with such a guide configuration have observed a significant improvement in SNR with the introduction of a T0 chopper to remove the fast neutron prompt pulse. A particular, and published, example is that of 4SEASON, see Figure 1, showing that a T0 chopper can improve the SNR by an up to order of magnitude.

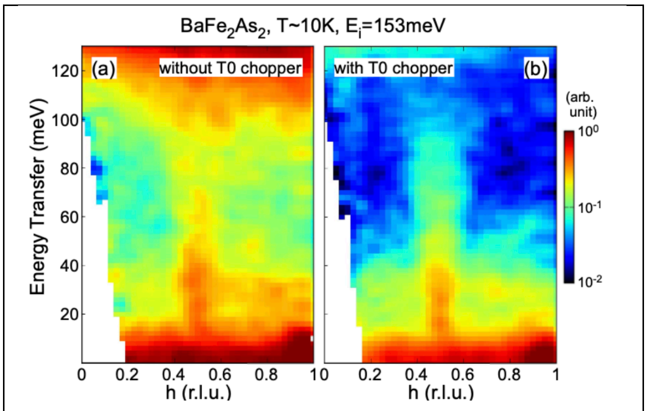

Figure 1: The effect of a T0 chopper on straight guide instrument 4SEASONS [1].

VISION, the vibrational spectrometer of SNS, studied the effect of a T0 chopper with test measurements of the empty cryostat while progressively dephasing their T0 chopper up to 30 μs from its nominal phase, private communications. Their results indicate that, in the TOF range where the pulse is generated, and where γ and epithermal neutrons can be directly detected by the detectors, the background increases by a factor 17. Note that these catastrophic degradations of the background occur when the T0 chopper is dephased by only 30 μs: the background increase would be worse if the T0 chopper was to be parked open. The ESS will have a long pulse and significantly larger source power than existing MW spallation facilities, and as such the background issues due to high energy neutrons can be expected to be significantly worse. In the absence of T0 chopper, the elastic line and the high energy region of the spectra, corresponding to the TOF range 0-10 ms, are expected to be unusable.

(2) Increase analyser modules: 10 x 0.36 = **3.6 M€**

Resources needed: The instrument team can implement these upgrades as part of the current instrument build.

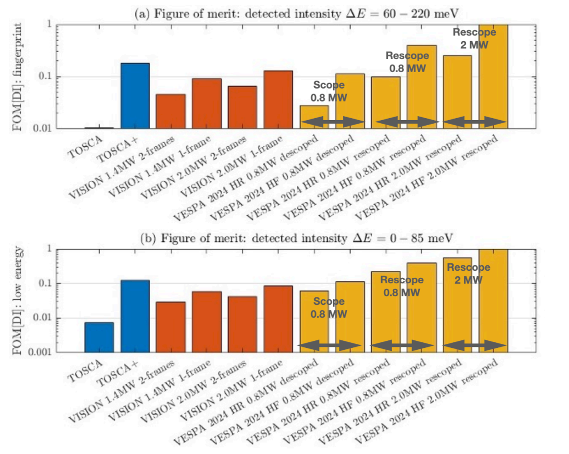

Figure 2: Normalised FOM of VESPA and other NVS instruments, for (a) the fingerprint region of the spectra and (b) at low-energy.

As most experiments are flux limited, a suitable figure of merit (FOM) is to consider a quantity proportional to the detected intensity:

$$\mathrm{FOM} = \Phi \cdot \frac{\Omega}{4\pi} \cdot T_{\mathrm{Be}} \cdot \eta \cdot \Delta\theta \cdot R$$

where Φ is the peak flux (brightness) on a 1×1 cm^2 area in n/s/cm^2, integrated in energy over the fingerprint or low-energy regions, Ω is the solid angle coverage of the analysers in sr, T_{Be} is the transmission of the beryllium filter in %, η is the detection efficiency of the detectors in %, $\Delta\theta$ is the mosaic spread of the analyser crystals in degrees, and R is the peak reflectivity of the analyser crystals in %.

The FOM metrics, normalised to the completed VESPA in high-flux (HF) setting and with 2.0 MW source power, are reported in Figure 2. The day 1 performance of a descoped VESPA with reduced source power are only 11% of that of the complete instrument at nominal power. In the fingerprint region, the high-flux setting of a descoped VESPA has comparable performance to those of VISION, while the high-resolution setting, which has an energy resolution comparable to that of VISION, has about 3 times less flux. Rescoping the instrument by fully completing the spectroscopy banks corresponds to a gain of 3.5 in detected intensity and makes the high-resolution setting on par with VISION. Note that both a fully rescoped instrument and the 2.0 MW source power are required to provide a significant improvement in flux compared to existing instrument.
In the low energy range, because of the large cold neutron brightness of ESS, even a descoped VESPA in high-resolution mode has comparable performance to those of the existing NVS instruments.
A fully rescoped instrument will make VESPA world leading, enabling significantly more sensitive measurements and, most importantly, in-situ studies that can access very weak hydrogenous content in the investigation of, for example, solids and liquids, soft matter, complex fluids, and biomaterials.

CSPEC

(1) ^{3}He completion (2.5 bar): **2.025 M€**

Resources needed: Only the procurement of ^{3}He is needed.

Cold chopper spectroscopy has seen enormous success in the last 20 years due the access of a broad 4 dimensional S(**Q**, ω) that can be mapped directly to theoretical developments. The broad overview, both for S(Q, ω) and S(**Q**, ω), significantly helps to restrict theoretical models and determine subtle variations in diffusive parameters and exchange interactions. The scope of the CSPEC detector, see Figure 3, provides 58% of the completed detector coverage with a ^{3}He pressure of 2.5 bar. This means that the broad **Q** coverage is compromised. In addition, the neutron detection efficiency is significantly reduced, with 2.5

bar, for λ< 6 Å, providing less than 2 x detection efficiency when compared to the world leading instruments, IN5 (5 bar), CNCS (6 bar), LET (10 bar) and AMATERAS (10 bar).
Figure 3 shows the day 1 scope coverage and the detector regions that need to be rescoped, these include a low negative 2θ region (in yellow) and the extended Q region (in turquoise).

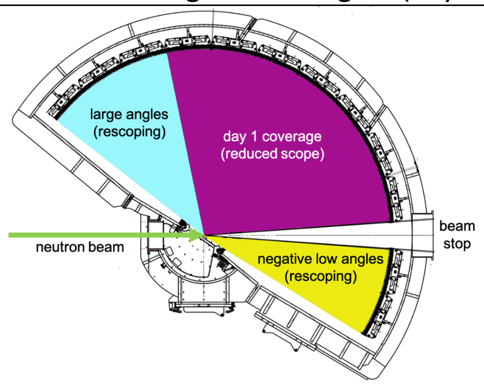

Figure 3: Detector coverage of the CSPEC instrument showing the scope of the instrument and the requested rescoping.

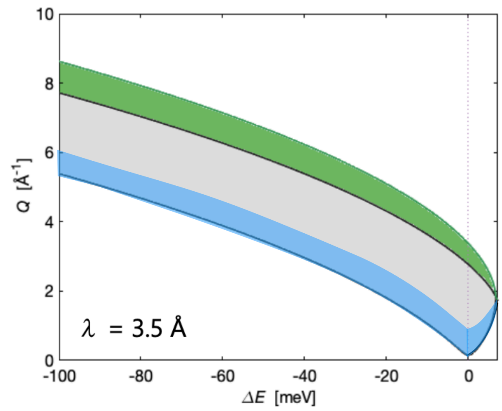

Figure 4: CSPEC S(Q, ω), for λ_i = 3.5 Å, showing full detector scope, with the scope reduction in blue (negative low angles) and green (large angles).

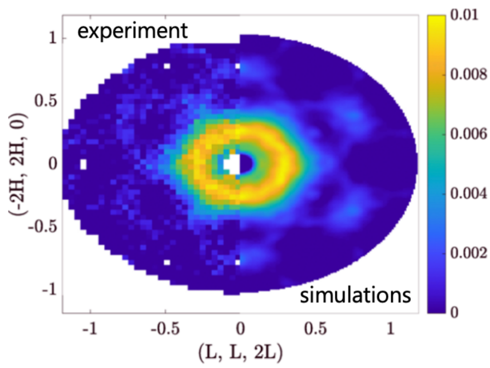

Figure 5: Single crystal magnetic S(Q, ω = ΔE) scattering of Yb3Ga5O12,) as measured on the old chopper spectrometer of the SNS, CNCS, with λi = 7.265 Å. Comparison of experimental data and RMC fit (left and right, respectively).

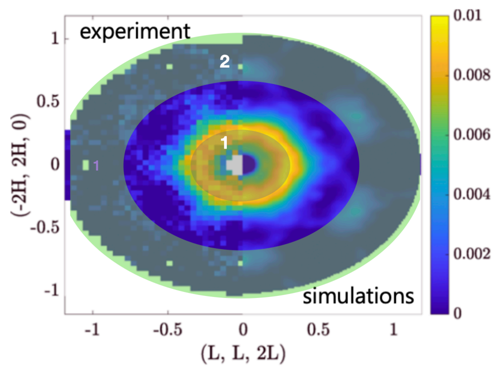

Figure 6: Data from Figure 5 with regions in green representing the regions where the CSPEC detector will be rescoped. Region 1 is the negative low angle region and region 2 is the large angle region.

Figure 4 shows the effect of this descoping on S(Q, ω) for λ=3.5 Å. Figure 5 shows a typical S(**Q**, ω) scattering profile measured to determine the low lying excitations in a hyperkagome frustrated magnet as measured on CNCS (SNS)[2]. Figure 6 marks the effect of the CSPEC detector descoping on such a data set. Region 1 will have limited detector coverage and thus detection efficiency is reduced by a factor of 2 and region 2 is not accessible with the current detector scope of CSPEC.

The FOM for time-of-flight spectroscopy is given by

$$\mathrm{FOM} = \Phi \cdot \Omega \cdot E$$

where Φ is the peak flux (brightness) in n/s/cm^2, Ω is the solid angle coverage of the detectors and E is the detector efficiency. Different scenarios are presented in Figure 7 comparing the world leading instruments, IN5, LET, CNCS and AMATERAS with CSPEC, current scope and full scope, 0.8 and 2 MW and 2.5 and 5 bar ^{3}He. In single pulse mode, the mode most commonly employed on current day spectrometers, it is clear that CSPEC will not be world leading until full detector coverage is provided with 2 MW ESS power. Increasing the detector efficiency further is not essential for early science. However, ensuring that the RRM mode is effectively employed will be essential since large gains in FOM can be made in this mode.

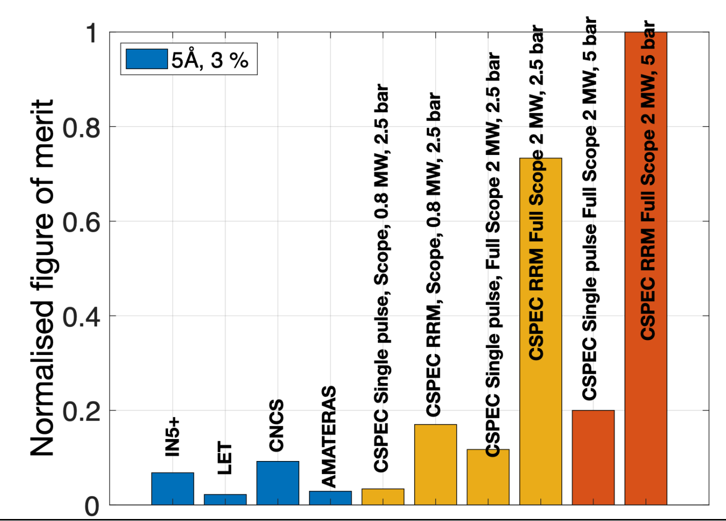

Figure 7: Comparison of the normalised FOM for tof spectrometers with the recently upgraded IN5, LET, CNCS (2 MW) and AMATERAS compared to CSPEC single pulse and RRM for 0.8 MW and 2 MW ESS power and 2.5 and 5 bar ^{3}He pressure.

The request is therefore that the CSPEC detector coverage shall be completed with 2.5 bar ^{3}He. Any further increase in gas pressure can be considered once the instrument is operational.

T-REX

(1) Complete detector coverage from 40 – 100 %. **2 M€ for detector boxes + detectors (cost to be provided by the detector group)**

Resources needed: Significant resources needed from the detector group – however these will be as a continuation of the current project and can possible be outsourced to a company.

Similar to the cold chopper spectroscopy, thermal chopper spectroscopy also benefits from scattering profiles across broad swathes of S(**Q**, ω).

The T-REX detector was descoped to 40% of its full coverage, see Figure 8, with like CSPEC, a descoping of a low Q negative detector region and a high Q region. We show a constant-energy slice of magnon scattering in a honeycomb ferromagnet at T = 1.7 K, measured with an incoming energy of 15 meV as measured on the recently commissioned instrument thermal chopper spectrometer of the ILL PANTHER, Figure 9. Superposed on Figure 9, Figure 10, are the regions that are affected by the descoping of detector on T-REX. In pink is the low Q region that will, in comparison to comparable instruments, have 50 % detection intensity. In green is the low Q region that will not be accessible with the current detector scope. Upgrading the detector can be done step by step whenever a new detector module, each covering 18° horizontal angle, is ready as integration time and cost allows.

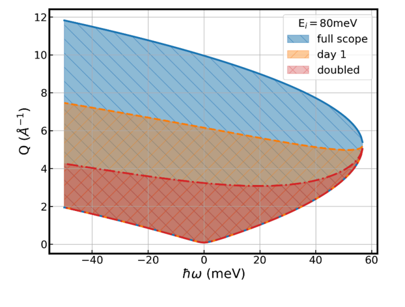

Figure 8: T-REX S(Q, ω), for λ_i = 1.01 Å, showing full detector scope, with the scope reduction in red (negative low angles) and blue (large angles).

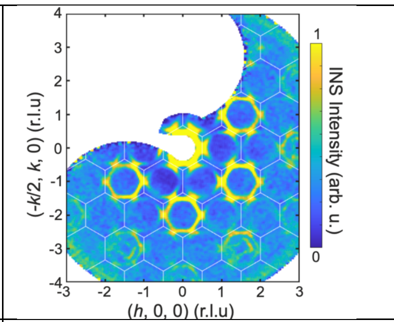

Figure 9: Constant-energy slice of magnon scattering in a hon-eycomb ferromagnet at T = 1.7 K, measured with an incoming energy of 15 meV. The data are integrated over energy transfers between 4 and 5 meV [3].

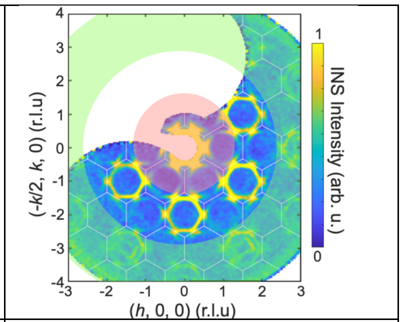

Figure 10: Data from Figure 9 with regions in pink and green representing the regions where the CSPEC detector will be rescoped. Pink region is the negative low angle region and the green region is the large angle region.

The normalised FOM for T-REX, presented in Figures 11 and 12, are given by

$$\text{FOM} = \Phi \cdot \Omega$$

where Φ is the peak flux (brightness) in n/s/cm^2, Ω is the solid angle coverage of the detectors. The full detector coverage is therefore needed to provide a significant improvement over existing instruments at 2MW ESS power.

Figure 11 shows the normalised FOM for thermal chopper spectrometers, Ei = 50 meV, ΔE/E = 5%, compared to T-REX with initial detector scope and 2 MW ESS power. Figure 12 shows the normalised FOM for thermal chopper spectrometers, Ei = 50 meV, ΔE/E = 5%, compared to T-REX with full detector coverage and 2 MW ESS power. It is again clear that it is essential for T-REX to have its full detector coverage and that full use of RRM modes must be available.

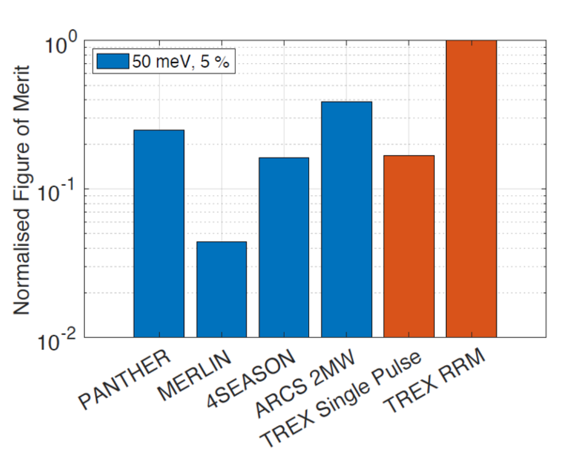

Figure 11: Normalised FOM for thermal chopper spectrometers compared to T-REX scope and 2 MW ESS Power.

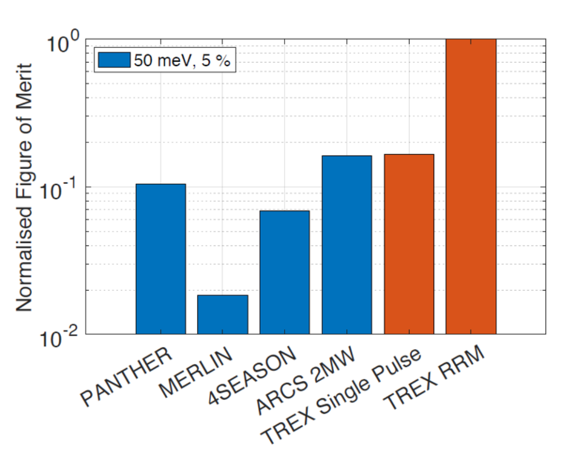

Figure 12: Normalised FOM for thermal chopper spectrometers compared to T-REX full scope and 2 MW ESS Power.

(2) Additional 2 discs for pulse shaping choppers. 0.5 M€ (current estimate)

Resources needed: Julich resources.

The P-chopper at 108m is cutting the long ESS pulse into sub-pulses up to 24 RRM (repetition rate multiplication) pulses and controls the incident wavelength resolution of these pulses. In day-1 scope, the chopper system is equipped with two chopper discs separated by 10cm along the neutron path. The chopper housing is already designed and built to host up to 4 discs in 2 pairs in over/under configuration, in day-1 scope only the two upper discs exist. All discs feature two openings of 35° and 20° for high-flux and high-resolution measurements, respectively. An upgrade to four discs would allow T-REX to decouple the energy resolution of the primary spectrometer from the repetition rate of the chopper by allowing advanced pulse shaping options. Essentially, the triangular transmission function of a two-disc assembly can be changed to a trapezoidal or rectangular shape, therefore cutting tails that worsen the resolution. This is especially useful in cases of deep inelastic scattering, where the resolution of the primary spectrometer can be matched to the already very good resolution of the secondary spectrometer providing a unique capability.

This is an upgrade that can be facilitated at a later stage.

(3) T0 chopper:
TREX has mitigated, in the first instance, the need for a T0 chopper by curving out of line of sight. Upon completion of hot commissioning the signal to noise levels will be determined and the possible need for a T0 chopper determined.

This is an upgrade that will be determined at a later stage.

MIRACLES
(1) Rescope: Complete the analyser bank with Si (1 1 1) and (3 1 1) analysers (plus detectors and radial collimator) to the right side. **1.67 M€**
Resources: The upgrade can be done without any disruption of the operation program, since all the integration, installation and adjustment features have already been manufactured, in anticipation to this completion effort.

MIRACLES will, within scope, provides analyser coverage with Si (1 1 1) crystals, on one side of the MIRACLES detector tank, that provides momentum transfer up to approximately 2 $Å^{-1}$. Rescoping the instrument will provide 50% more Si (1 1 1) on the other side fill the rest of the detector tank Si (3 1 1) analysers crystals to extend the Q-range up to 3.8 $Å^{-1}$, already a possibility on comparative backscattering instruments such as BASIS (SNS) and DNA (JParc). Extending the Q-range of the instrument will enable more detailed analysis over broader spatial scales often performed using several instruments. In-operando studies, as needed for example for rapidly screening battery materials, will particularly benefit from the extended Q-range. An example is shown in Figure 13 which shows a study on the reorientational dynamics of metal borohydrides using the high flux back scattering spectrometer (HFBS), the time-of-flight disc chopper (DCS) and the neutron spin echo (NSE) instruments at NIST. Rescoping MIRACLES with Si (3 1 1) would extend the Q range and will provide information up to 3.8 $Å^{-1}$, see blue region in Figure 13, in a single measurement thereby enabling the determination of different reorientational dynamics in complex materials. This rescoping is considered essential for MIRACLES to be competitive with current world leading instruments.

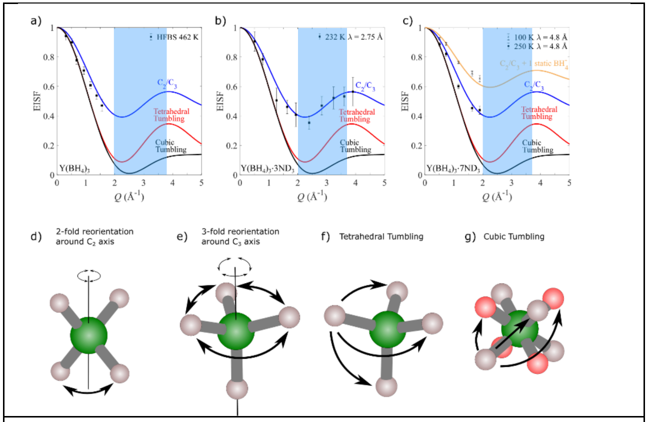

Figure 13: Figures from [4] EISFs determined from QENS spectra for (a) Y(BH4)3, (b) Y(BH4)3·3ND3, and (c) Y(BH4)3·7ND3 at different temperatures compared to EISF models for each respective system. (d-g) Representations of common reorientational motions for a tetrahedral anion.

Polarisation analysis on all instruments. Polarisation analysis (PA) provides tremendous opportunities for spectroscopy instruments. This has been exemplified by the successes on the chopper spectrometer LET of ISIS which has recently been equiped with neutron polarization analysis using a combination of a supermirror polarizer and ^{3}He wide-angle analyser system [5]. A particular example is that of a neutron spectroscopy PA study on water relaxation that shows significant coherent scattering of water from meso to intermolecular scales calling into doubt decades of work that considered most of the scattering profiles to be derived from incoherent contributions only. All spectroscopy instruments, except VESPA, have future proofed their instrument design to enable PA. T-REX will incorporate PA from day 1 but MIRACLES, CSPEC and BIFROST will require further technical developments that can be delivered once the instruments are operational. We therefore do not consider PA within this rescoping exercise.

[1] R. Kajimoto *et* al. *J. Phys. Soc. Jpn.* **80** (2011) SB025.
[2] L. Sandberg *et* al. *PHYSICAL REVIEW B* **104**, 064425 (2021)
[3] B. Fåk *et* al. *EPJ Web of Conferences* **272**, 02001 (2022)
[4] J. B. Grinderslev *et* al. *J. Phys. Chem. C*, **128**, 4431–4439 (2024)
[5] A. Arbe *et* al. *Phys. Rev. Research* **2** 2022015(R) (2020)

DIFF & IMAG Instrument Rescoping

by M.Feygenson

The item list below was prioritised purely on Scientific Impact, not figure of merit (FOM).

Instrument	Rescoping option	Procured by:	A: Scientific Impact (5: high, 1: low)	B: Manpower (1:high, 5:low)	C: Technical Risk (1:high, 5:low)	B: Cost (M€)	FOM A*B*C
DREAM	Full detector coverage (CDT)	Q1 2025	5	Significant (Detector group) 3	4	4.7	60
MAGiC	Full detector coverage (CDT)	Q3 2025	5	Significant (Detector group) 3	4	1.8 Including collimator & support	60
HEIMDAL	Full detector coverage (CDT)	Q3 2026	5	Significant (Detector group) 3	4	3.6	60
BEER	Texture detectors	Q1 2026	5	Significant (Detector group) 2	3	2.6	30
BEER	Multiplication Choppers	Q4 2025	4	Significant (Chopper group) 1	2	0.74	8
ODIN	Grating interferometer	Q1 2026	4	1, additional staff member to run the setup	1	>1.5 (TBC)	4
HEIMDAL	SANS option	Q2 2027	4	2	2	3.4	16
BEER	SANS option	Q3 2027	3	Significant (Detector group) 3	2	2.5	18
ODIN	SEMSANS	Q1 2026	3	Significant (Detector group) 3	2	0.8	18
MAGiC	Spectroscopy chopper	Q2 2026	3	Significant (Choppers group) 3	4, design was agreed with Choppers group	0.47	36
BEER	Additional sample stage	Q1 2027	3	4	4	0.8 (TBC)	48
ODIN	Diffraction detectors	Q2 2027	3	3	3	3.0	27

1. Completing the detector coverage

DREAM & HEIMDAL Detectors:

For the DREAM detector, we propose expanding its full coverage scope from the current 2.1 sr. to 5.1 sr. Similarly, for the HEIMDAL diffraction detector, the angular coverage should be increased from the existing 80 to 230°. This improvement would significantly increase the capability of both instruments. The revised scientific cases emphasize the ability to handle small sample studies and fast in-situ measurements, which are highly relevant to the energy storage, chemistry, and materials science research communities.

BEER Detector:
The BEER instrument would benefit from a doubling of its detector coverage, which includes the backscattering detector. This extension will not only enhance the rate of data collection—critical for in-situ measurements—but also extend the available d-range per pulse, which is currently limited to approximately 1.7 Å. Additionally, it will improve the resolution limits and make it possible to detect peaks that may have low intensity at the ±90^{o} detectors due to strong sample texture.

MAGiC Detector:
The MAGiC instrument is essential for neutron time-of-flight Laue single-crystal measurements. To fully realize its potential, additional development is necessary to extend both the detector support structure and the radial collimator coverage. These upgrades will ensure that MAGiC can continue to meet the demanding requirements of advanced crystallographic studies of single crystals.

2. **Recovering capabilities in engineering diffraction and imaging**

Additional Texture Detectors for BEER:
The inclusion of additional texture detectors in the BEER instrument is critical for understanding texture and its development during the thermomechanical loading of materials. This information is essential for the accurate interpretation of observed lattice strains. The off-plane detectors will enable monitoring of texture evolution even in-situ during mechanical testing, potentially reducing or eliminating the need for sample rotation. This capability is particularly important in complex sample environments, where sample rotation is often impractical or impossible.

Multiplication Choppers for BEER:
The installation of multiplication choppers will expand the resolution and intensity range of the BEER instrument. These choppers will support fast in-situ and in-operando measurements with relaxed resolution using pulse shaping modes, allowing access to 1-second time scales for dynamic processes, as initially envisioned in the original proposal. Additionally, an extra modulation chopper will introduce two more multiplication options: doubling the intensity at high resolution or achieving wider separation of modulation peaks, which is crucial for studying materials with complex compositions or low crystallographic symmetry.

Grating interferometer ODIN:
More info is needed, but the inclusion of dedicated staff to operate and optimize this setup for advanced imaging applications.

3. **Recovering SANS options for HEIMDAL, BEER and ODIN**

HEIMDAL is a unique hybrid instrument combining a thermal neutron diffractometer and a cold neutron small-angle neutron scattering (SANS) instrument. Recent optimizations to the cold guide design have significantly improved beam transport efficiency. These advancements also open the door for a potential upgrade to a full 10-meter SANS instrument, along with the option to integrate polarized neutrons using polarizing mirrors.

The integration of SANS capabilities with the diffraction detectors in the BEER instrument will greatly expand the accessible scale range. This improvement allows for the investigation of early-stage phase transformations—such as chemical partitioning and precipitate growth—before their signatures become detectable via diffraction. Simultaneously, it enables continuous monitoring of lattice strain evolution and phase composition changes, making it a powerful tool for materials research.

The SEMSANS (Spin-Echo Modulated Small Angle Neutron Scattering) option for the ODIN instrument is under consideration, although further details are required to finalize this upgrade.

4. Remaining Scope

MAGiC Spectroscopy Option:
Implementing a spectroscopy option for the MAGiC instrument requires the addition of choppers positioned close to the sample area. This enhancement offers strong synergy with the Spectroscopy Division. Moreover, combining polarization capabilities with the spectroscopy option provides an ideal setup for investigating dynamic responses in complex magnetic systems.

BEER Sample Handling:
Extended sample tower z-movement (up-down) to accommodate a wider range of sample sizes and types. The inclusion of an additional set of radial collimators to support a broader variety of gauge volumes. The development of a sample alignment system to improve the accuracy of sample positioning, which is critical for strain mapping, particularly for complex-shaped samples produced by additive manufacturing. This system will also expedite measurements by enabling automatic sample positioning and the ability to plan experiments in advance.

ODIN Diffraction Detectors:
Further details are required regarding the ODIN instrument’s diffraction detectors, with a comparison to the HEIMDAL science case needed to fully assess their potential.

HEIMDAL Imaging Option:
The HEIMDAL instrument's imaging capabilities can be enhanced by integrating TimePix3 detectors from the ODIN instrument. This will significantly improve the instrument's imaging performance and resolution.

TBL Upgrades :
Expansion of the experimental cave (requires an upgrade of the shielding) for a transmission measurement for fundamental scattering cross-section can be performed at TBL. A longer

distance between the sample and detector is needed to ensure that multiple scattering is minimized as much as possible. Also, a larger space for sample environment leads to more use case for testing/commissioning any equipment at TBL before installed at other instruments.

T0 chopper installation to minimize background from fast neutrons and gammas for cold-neutron experiments and ii) restrict pulse width for epithermal/fast neutrons for fundamental physics experiments and also time-of-flight (ToF) transmission/diffraction. This component has been proven successful at NOBORU (BL10), J-PARC, despite of short-pulse use case.

Gamma spectrometer can be installed inside the cave (together with some shielding) to carry out prompt-gamma neutron activation analysis (PGNAA). This experiment will not disturb the current scope of TBL, and improve a capability of the beamline for material characterization in terms of composition analysis.

LSS Instrument Rescoping

Andrew Jackson

Overview

The document covers assessment and ranking of the various known rescoping options for the Large Scale Structures instruments (LoKI, SKADI, Estia, FREIA, NMX). Not included here is the significant amount of scope for sample environment for the SANS and Reflectometry suites will need to support world leading research operations. This is assumed to be mostly covered by the capital purchases plans of the Science Support Division and the LSS Division (via instrument operations budgets). However, some items of sample environment will inevitably need significant development effort and a separate exercise of assessing and ranking SEE needs – with estimates of effort – will be needed.

Based on the figure-of-merit, combined with other constraints on when the work could be executed, the priority order for LSS is:

1) LoKI detector completion (FOM = 125)
   - Detectors already procured, installation pending
2) Various low-value addons for Estia (FOM = 80)
   - can be done whenever there is time/budget
3) FREIA fast shutter system (FOM = 75)
   - should be done now to have it installed before start of hot commissioning of FREIA
4=) NMX Isotopic Gd (FOM = 75)
   - supply chain issue
   - should wait for NMX to be commissioned -> procurement in 2027
4=) NMX extra detector (FOM = 75)
   - should wait for NMX to be commissioned -> procurement in 2027
6) SKADI completion of detector (FOM = 50)

- high manpower requirement
- should wait for detector to be fully validated -> procurement in 2027

7=) FREIA Polarised Beam (FOM = 20)
- can be procured whenever budget allows

7=) SKADI HR choppers (FOM = 20)
- disruptive, so plan for procurement in 2028/2029

9) FREIA resolution choppers (FOM = 16)
- very disruptive, so reassess and procure > 2029

10) Estia second beam path (FOM = 5)
- technically complex
- very disruptive and invasive to the instrument, so reassess and procure > 2030

11=) FREIA GISANS option (FOM = 1)
- this should be dropped as the science case is better covered by the combination of SKADI and Estia

11=) LoKI resolution choppers (FOM = 1)
- this should be dropped as higher resolution measurements are better done on SKADI and installing these choppers would reduce core science performance of LoKI

Assessment of Rescoping Options

The table below shows the scoring of the various options for the LSS instruments. Section 3 outlines the way I have used the scoring. The final column contains explanations/justifications for the scores. This approach does not cover **in what order** the rescoping should be done as some of the items should not be done until the base configuration of the instrument is proven – so some time after start of the user programme on the instrument. In the case of NMX there is also a supply issue for the components needed – giving an additional need to wait on execution.

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	Conclusion/Recommendation/Notes
LoKI	Complete detector coverage (add ~4 m^2)	5	Minimal : 5 (installation technician)	5	**1.04 M€$_{2013}$**	125	DONE : equipment has been procured. Installation pending.
	Resolution choppers	1	High : 1 (chopper group, new guide)	1	**2.16 M€ for 10 (0.36 each)**	1	I do not recommend pursuing this option as it will degrade core performance. The money is better spent towards another SANS instrument meeting the requirements natively that this would provide on LoKI. Also, if you need a higher resolution (lower dQ/Q) measurement then SKADI is available.
SKADI	Full detector	5	High: 2 (cabling, installation technician,	5	**2.5 to 4 M€**	50	Whilst this rescoping is key to unlocking the full potential of SKADI

	coverage (add 1m^2)		detector group scientist and technician, ECDC staff)				and providing world leading performance, there remain questions about the performance and integration of the SoNDE detector. Thus this rescoping should wait for demonstration of the SoNDE system fully working with our electronics and data readout chain using spallation neutrons and time-of-flight data processing on a standard sample. If SoNDE does not meet performance requirements a similar budget is needed to design and install ^{3}He alternative.
	High Resolution Choppers	2	High : 2 (chopper group, mechanical designer, installation technician)	5	**1 M€**	20	Concept needs development and evaluation, with re-assessment of science case.
Estia	Various options	5	Limited: 4	4	**1 M€**	80	Various different optics options that are all post-selene or in the cave. Could be executed as funds are available from normal ops budget if that is large enough.
	Second beam path with analysers	5	Very High: 1 (design, manufacturing oversight, disassembly/reassembly of Estia)	1	**5 M€**	5	This option would significantly enhance the performance for doing time-resolved polarised studies as it would enable measurement of all 4 spin channels simultaneously. However it is complex and labour and time intensive (requiring a complete replacement of the current Selene carriers and guides). Therefore this should not be performed until Estia has had a significant number of operating cycles and operation with the current guide system is fully understood.
Freia	Fast Shutter System	5	Moderate: 3 (MCA primarily)	5	**0.35 M€**	75	This option restores the core scope of FREIA to perform fast reflectivity measurements. It is thus vital to world leading performance. CR already prepared and discussed.
	Resolution enhancing choppers	2	High: 2	4		16	Replaces the final chopper single disc with a double disc arrangement that will improve bandwidth selection and flexibility – in particular for pulse-skipping mode. This should not be pursued until the instrument has had a significant number of operating days and the baseline configuration is well understood.
	Polarised beam	2	Minimal: 5 (installation technician, polarisation team support)	5	**0.5 M€**	20	This option will extend the capabilities of FREIA to support magnetic reference layer measurements for solid-liquid interfaces. This has proven to be an effective method to obtain contrast

							where it is difficult or expensive to use deuteration. These experiments will be possible on day 1 on Estia, so the overall science gain to the LSS suite is limited. Technical risk and installation effort is low as the instrument guide changer has been designed with a place for the polarizer, so only the polarizing guide needs to be procured and installed
	GISANS option	1	Very high : 1	1	**>5 M€**	1	Compared to the combination of SKADI and Estia, the scientific gains from GISANS on FREIA are low. To implement this would require a new detector vessel and likely extension of the cave.
NMX	Isotopic Gd converter for detectors	5	Limited : 4 (detector group)	5	**1 M€ - 4M€ (depending on source of 157Gd)**	75	The efficiency gain (from <5% with natural Gd to >20% with isotopically pure Gd) is significant and essential to obtain the full performance of the NMX instrument and make it world leading. The work is straightforward once the Gd sheet has been procured. Obtaining the isotopically pure 157Gd has become difficult and significantly more expensive as the primary supplier is in Russia. However, the detector system is not yet fully tested and integrated so this upgrade should wait until the instrument has been fully commissioned and some user experiments have been run.
	Additional detector module	5	Moderate : 3 (detector group)	5	**1 M€**	75	The addition of a static detector after the sample will increase the completeness of obtained diffraction patterns by approximately 33% - this translates to better quality structures being obtained for the same measuring time, or faster measuring for structures of the same quality as the day 1 scope. This will have a significant impact on the publishability of the data from NMX as completeness of structures is a major limiting factor in neutron protein crystallography. This scope can be achieved through either a new detector build or through rebuild/refurbishment of the prototype detector.

Ranking method:

Scientific Impact :
1 = very low; 2 = low; 3 = moderate; 4 = high; 5 = very high.

- Something with a score of 1 is either extremely niche science case, won't have noticeable impact on scientific output or quality, or is better covered on another instrument or instruments.

- Something with a score of 5 is either very high impact in terms of scientific output or quality, or is key to reaching world leading status.

Manpower Estimate :
1 = very high; 2 = high ; 3 = moderate; 4 = limited; 5 = minimal

- Something with a score of 1 has significant manpower resource requirements, such as needing most of the capacity of a technical group or dedicated support from multiple groups, for an extended period of time.

- Something with a score of 5 can be executed by LSS division staff with technician support and with limited support from a technical group.

Technical Risk:
1 = very high; 2 = high ; 3 = moderate; 4 = limited; 5 = minimal

- Something with a score of 1 has significant technical uncertainty, depends on significant development effort beyond adaptation to a given instrument.

- Something with a score of 5 is essentially "ready to procure" with minimal technical uncertainty and adaptation to a given instrument needed.