INSTRUMENT PROPOSAL FOR SINGLE CRYSTAL DIFFRACTION - HUGIN AND MUNIN

	Name	Affiliation
Main Proposer	Alexandra Gibbs	Centre for Designer Quantum Materials and School of Chemistry, University of St Andrews (UK)
	Werner Schweika	European Spallation Source (Sweden)
Contributors	Jonathan White	Paul Scherrer Institut (Switzerland)
	Malcolm Guthrie	Oak Ridge National Labs (USA)
	Craig Bull	ISIS Neutron and Muon Source (UK)
	Bianca Haberl	Australian National University (Australia)
	Andrzej Grzechnik	Aachen University (Germany)
	Nick Funnell	ISIS Neutron and Muon Source (UK)
	Chris Ridley	Oak Ridge National Labs (USA)
	Mads Hansen	University of Cambridge (UK)
	Dominique Laniel	University of Edinburgh (UK)
	Klaus Lieutenant	Forschungszentrum Jülich (Germany)
	Francesca Miozzi	ETH Zurich (Switzerland)
	Esko Oksanen	European Spallation Source (Sweden)
	John Loveday	University of Edinburgh (UK)
	Felix Villacorta	ESS-Bilbao (Spain)
ESS Contact	Mikhail Feygenson	European Spallation Source (Sweden)

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1. EXECUTIVE SUMMARY

The instrument **Hugin-Munin** on beam port S4 will be a platform for small single crystal studies: a new state-of-the-art explorative single crystal materials observatory. **Hugin** offers a bi-spectral view to thermal and cold sources, while **Munin** delivers the wavelength spectrum >1.8 Å with optimal flux. Together they provide the most competitive parameters and scope for crystal and magnetic structure determination using the full long pulse in TOF Laue diffraction, with at least one order of magnitude higher flux than at any other neutron source. Beyond its use for routine cases, the pairing is designed to deliver definitive structural and magnetic information on samples too small, complex or constrained by sample environment for current workhorse instruments. A Web of Science search with key words "neutron diffraction" and "single crystal" shows a current output of around 300 publications per year. Crystallography and magnetic structure determination from small crystals will therefore be an immediate user community for Hugin and Munin. Next, searches combined with "quantum materials" or "high pressure" identify in each case 40 pubs/y. These topical research areas represent some of the most challenging cases of extremely small-crystal studies that often rely on tiny high-quality crystals in possibly multi-grain samples. An optional feature will be tuning resolution with pulse shaping choppers, when needed, e.g. for measurements of small powder samples. Hugin and Munin are not redundant variants of the same concept, but occupy genuinely distinct optimisation spaces in wavelength band, operating mode, science reach, and user capacity, such that the combined concept is materially stronger than a single compromise beamline. At the same time, the overall setup is cost-efficient due to the inherent optimisation for small samples and well suited to staged construction.

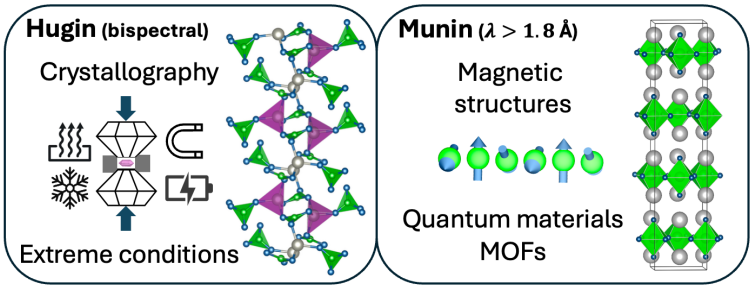

Figure 1: Dual instrument concept and preferences.

Small single crystals are crucial in driving progress in quantum and functional materials, particularly in quantum magnetism and multiferroics, where strong structure–property relationships and sensitivity to disorder demand high-quality, single-domain samples [1,2]. As the scope and scale of functional and quantum materials research continues to expand, experimental capacity for small single crystals will be a critical bottleneck; research on promising new materials cannot simply wait for large crystals to be grown. Here, synchrotrons have taken the lead through highly standardised high-throughput schemes (e.g. block-allocation grants) and remote single crystal measurements that streamline discovery workflows across organic, hybrid and inorganic materials. The exceptional flux of Hugin and Munin will support a comparable high-throughput approach using neutrons, for both nuclear and magnetic structures—a unique offering. The world-leading high flux spallation source characteristics of the ESS enable efficient time-of-flight Laue diffraction, facilitating rapid determination of superstructures in complex layered and large-unit-cell materials, as well as magnetic propagation vectors, that would otherwise often require preliminary synchrotron experiments. The instrument platform is ideally suited to current developments in large-unit-cell materials such as layered oxides and oxychalcogenides, and to the increasingly important family of coordination polymer materials (e.g. MOFs, COFs).

Together, the twin instruments transform the usual disadvantage of small single crystals into a strength, by exploiting their single-domain, high-quality nature on timescales compatible with modern materials discovery. This joint capability between the instruments directly supports research addressing current and future societal challenges in areas such as energy, quantum technologies and sustainable chemistry.

Within this broader programme, high pressure represents a flagship extreme-conditions capability, rather than a separate scientific identity. Extremes of environment are becoming ever more accessible in the physical sciences, giving us access to unprecedented states of matter and geologically and industrially relevant conditions. As an exemplary extreme, high-pressure science has underpinned some of the most significant discoveries of the 21st century, from elucidating fundamental properties of the Earth's core to finding new phases of ice, synthesising ultra-hard materials such as diamond, and achieving record-breaking high-T_C superconductivity in hydrides. Neutron diffraction at high pressure has been central to many such advances, for example in discovering and characterising many of these new forms of ice. In recent decades, synchrotrons have pioneered high-throughput experiments using tightly focused, high-flux beams in combination with compact diamond anvil cells (DACs). The combination of standardised DAC physical property measurements with routine laboratory diffraction has transformed DAC-based high-pressure research from a niche specialism into a more widely accessible technique. **Hugin**-**Munin** will enable neutron science to extend this capability in a uniquely complementary - not exclusive - way by allowing measurements on the very same DAC at both synchrotron and neutron sources, and for extreme environments: in-situ gas loading of single crystal MOFs, thus far a synchrotron speciality [3], is a key exemplar of game-changing complementary capability brought about by the combination of ESS brightness and cold neutrons.

This instrument pair will together allow the ESS both to set the scientific agenda for coming decades and to remain agile in responding to emerging priorities across the physical sciences spectrum.

2. SCIENTIFIC CASE

Small single crystals provide particular opportunities to answer questions which are not possible to address with larger single crystals in realistic timescales, for example due to the difficulties in preparing larger crystals, requiring months or years of effort, or the formation of twins and other domain structures. Being able to probe materials as soon as they are discovered makes a dramatic difference to the materials pipeline, essential if we are to meet the challenges of the modern research environment. Materials discovery is accelerating but neutron science struggles with the need for high-throughput characterisation and the small size of crystals of many new materials. Synchrotron facilities have pioneered the high-throughput model and being able to complement this with neutron data would be indispensable, particularly for the cases of materials containing both light and heavy elements, extremely common in functional and quantum materials, where absorption limits data quality from synchrotrons. In addition, the opportunity to study the magnetism of these materials in a high-throughput way is game-changing – going from 4-day experiments to half a day changes the research landscape dramatically. This also improves accessibility via both capability and capacity increase. Within the broader theme of high-throughput neutron diffraction for modern materials discovery, quantum materials emerge as one of the clearest and most impactful science drivers.

These advantages are not limited to high-throughput characterisation: access to extreme conditions on similarly small scales is equally powerful. Again, using high-pressure science as our example, this underpins a wide range of research fields spanning Earth and planetary sciences, chemistry, physics and engineering. Pressure is a clean, continuously tuneable and uniquely powerful thermodynamic variable that can be applied to essentially any material to modify its atomic structure, giving it a uniquely broad scope. It can drive the formation of entirely new materials, transform the phases and structures of known compounds, and stabilise novel ground states and structures that are inaccessible at ambient conditions. The flexibility and wide applicability of high-pressure and single-crystal techniques not only argue strongly for expanded capabilities and capacity but also highlight the imperative to be ready for unforeseen scientific challenges in the coming decades.

The scientific case presented here focuses on current priority areas in which **Hugin–Munin** can play a decisive role, as well as on directions that we anticipate will become major future challenges.

2.1. Key scientific drivers

Quantum materials, as a particularly powerful driver within the broader modern materials-discovery landscape: Towards the middle of the 21st century, quantum materials will shift from laboratory curiosities into the technologies underpinning key societal functions [4]. Consequently, the central research frontier will shift from identifying exotic phases to establishing quantitative microscopic mechanisms by which small structural changes govern emergent behaviour. Prominent examples we can currently anticipate include pressure-tuned bandwidth control in Mott and metal-insulator transitions, field-driven topological textures and chiral magnetic order, coupled spin-lattice-charge instabilities, altermagnetism and symmetry-breaking phenomena underlying multiferroicity and non-reciprocal transport [5–7]. Beyond these currently identifiable cases, the first century of quantum materials research shows that new classes of emergent phenomena are certain to arise in the future, particularly as materials complexity and available control parameters continue to expand. A persistent bottleneck in this research is that many of the most relevant compounds are available only as microcrystals with characteristic dimensions of 10–300 micron. Their most informative states must be accessed under extreme conditions of pressure, magnetic field and low temperature [4]. An example of particular current interest is looking for correlated states at the edges of the altermagnetic state [8]. Under such constraints, the unique capabilities of neutrons, namely the sensitivity to light elements, subtle symmetry lowering, magnetic order, domain populations and weak magnetic moments, are intrinsically challenging to exploit. Without this microscopic foundation provided by neutrons however, phase diagrams remain phenomenological and the transition from correlation-driven discovery to predictive materials design remains elusive.

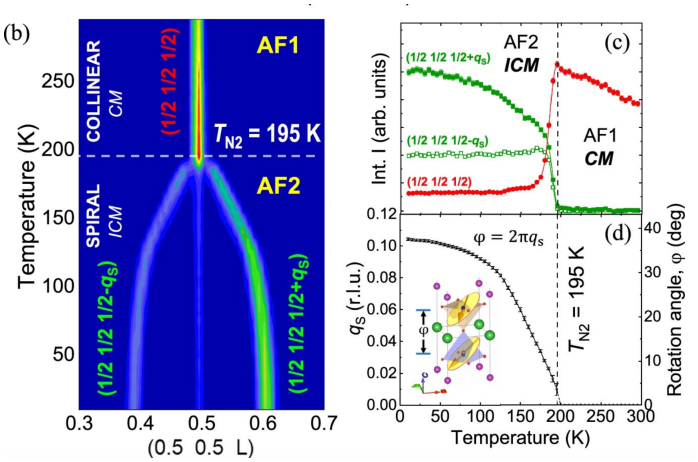

Figure 2: Single crystal neutron diffraction has proven essential to understanding and tracking the complex magnetism in high temperature multiferroic $YBaCuFeO_5$, data shown here are from D9 at the ILL **[2]**

Functional materials: High-throughput materials discovery has a special place in the functional materials community, and AI methods are contributing to this, combined with the ability to set up automated synthetic explorations [9–11]. Materials such as oxide ion conductors and lithium-based battery materials typically contain light elements as a key component, often in combination with much heavier elements [12,13]. The special capability of neutrons to interrogate such materials, and in a high-throughput manner, makes the instrument concept groundbreaking [14]. It builds upon recent successes in the field of electron diffraction in allowing study of a single powder grain, but with the enhanced insight that neutrons can provide as a true bulk probe into subtle structural distortions, domains and magnetism. Framework materials such as metal-organic frameworks (MOFs), covalent organic frameworks (COFs) and zeolites are a quintessential class of functional materials where the large pores allow a range of functionalities such as gas storage, catalysis and carbon capture. Rather than targeting large single crystals, these are typically synthesised as microcrystalline powders both in the laboratory, for fundamental research, and industrially for applications. The opportunity to do routine structural studies on such materials directly after discovery and/or in the exact form in which it will be used will be a step-change in neutron capability. High pressure is a key tuning parameter for materials with useful functional properties, enabling both the creation of new compounds and the study of polymorphism and fundamental structure–property relationships [15–

18]. As a continuously variable parameter, pressure allows smooth exploration of phase space, making it possible to track the evolution of physical properties with controlled distortions of the crystal structure and thereby elucidate structure–property correlations [19].

Pharmaceuticals: Neutron diffraction is especially valuable for drugs and biomolecular systems, where hydrogen positions and interactions govern function; in single crystals, hydrogen scattering can often be managed without perdeuteration. This is particularly important for high-pressure studies of polymorphism, which affects safety, efficacy, processing, and patentability [20]. Access to very small crystals also enables studies of metastable and difficult-to-crystallise forms, while current reliance on X-ray diffraction for tiny pressure-grown crystals has limited broader progress [21].

Energetic materials: High-pressure neutron diffraction reveals the structures and pressure response of energetic materials, informing detonation mechanisms and theory [20]. Its sensitivity to light elements and lack of radiation damage are major advantages over synchrotron methods [22].

Hydrides: Hydrides are central to hydrogen storage and high-temperature superconductivity, and neutrons are essential for locating hydrogen. Super-hydride research has pushed the limits of superconducting transition temperatures, T_c, to near room temperature, however, these materials need mega-bar pressures to be stabilized [23–26]. This has barred structure determination of the hydrogen sub-lattice, making the field reliant on ab-initio calculations. In recent years, however, hydride superconductor research has shifted towards ternary hydrides to enable lower synthesis pressures. Rapid computational discovery, powered by machine learning, has produced many predicted materials [27–31], including new families of hydride superconductors, some with transition temperatures approaching 160 K. Several of these predicted compounds require synthesis in the range 0-30 GPa, making them prime targets for Hugin-Munin. Ongoing synthesis attempts of predicted ternary hydrides highlight the need for neutrons to unambiguously determine the structure of these materials [32–34]. A stretch goal of neutron diffraction up to 1 Mbar would make a decisive contribution here.

Earth & planetary sciences: Understanding Earth's deep interior requires studying phases stable only at high pressure and temperature. Neutron diffraction is crucial for locating hydrogen in candidate water-bearing and other light-element-rich phases, and for determining how they influence deep-Earth properties. Neutrons are equally important for hydrates and high-pressure ices. Hugin-Munin offers the exciting prospect of the first full structures of the superionic phases of ice and ammonia [35]. These phases, thought to play a role in the unusual magnetic fields of Neptune and Uranus [36], have recently been identified by X-ray diffraction [37,38] but nothing is known experimentally about their H-sublattices.

Fundamental physics and chemistry: Simple elements, molecules, and compounds remain a rich area of high-pressure research [39]. Opportunities include structures of the broken-symmetry phases of hydrogen and deuterium, a long-standing problem involving quantum rotational states, H-bond centring in systems like ice and squaric acid ($H_2C_4O_4$), which test models of the proton as quantum object [40–42] and pressure ionisation in systems like ammonia hemihydrate, here the effect has been predicted but structural information is sparse [43,44].

Materials complexity: In parallel with the scientific themes outlined above, there is a clear trend toward increasing materials complexity—in elemental composition, structural motifs and mesoscopic organisation (e.g. correlated disorder) [45]. This is mirrored by growing complexity in the samples themselves, which are often available only as small single crystals or limited powder quantities. In quantum and functional materials research, in particular, large high-quality single crystals frequently cannot be grown on the timescales required [46–48], have properties dominated by domain walls [49], do not attain the quality needed to exhibit the targeted phenomena [50] or must be small to allow specific physical property studies [51]. Consequently, there is a strong drive to advance analytical capabilities so that the pace of materials discovery and optimisation remains sufficient to meet technological and societal demands.

Protein structures (optional future capability, complementary to NMX): Hydrogen atoms play a key role in most biochemical processes, but they cannot in general be visualised using the standard techniques of X-ray crystallography or cryo-electron microscopy. Neutrons can be used to determine hydrogen positions in macromolecular structures, but crystal size is limiting. The use of polarised neutrons combined with dynamic nuclear polarisation DNP [52] promises to enable significantly smaller crystal sizes as well as enhanced signal on the hydrogens. This could revolutionise neutron macromolecular crystallography and open the field to a large number of new users. It is straightforward to include neutron polarisation for the instrument Munin offering an immediate step into this alternative field, when a success of DNP can be proven.

2.2. Potential societal relevance of the science case

The scientific scope of Hugin and Munin encompasses a broad range of applications with significant societal relevance. The quantitative microscopic understanding of quantum materials is a prerequisite for transitioning emergent quantum phases into robust and scalable technologies. Progress in this area underpins European strategic priorities in quantum technologies, including sensing, information processing and secure communications. It also supports advances in energy and digital efficiency, through materials enabling lower-loss electronics, novel switching mechanisms and adaptive functionality. Furthermore, quantum materials are increasingly central to advanced functional materials for electrification, including magnetoelectrics and multiferroics.

By reducing uncertainty early in the materials discovery pipeline, neutron-enabled insight fosters innovation while lowering risk, cost and time associated with materials development and exploitation. The ability to generate and probe extreme conditions enables the creation and characterisation of deep-Earth minerals and improved insight into the composition and evolution of planetary bodies.

These instruments will enable the synthesis and detailed characterisation of novel hydrides for hydrogen storage, as well as systematic studies of how energy materials respond to compression—knowledge that is crucial for guiding the rational design of next-generation technologies. Beyond the energy sector, high-pressure studies remain vital across multiple industries. Pharmaceutical materials, particularly with respect to polymorphism and the development of deuterated drug compounds, continue to require precise structural insight under varying thermodynamic conditions. Similarly, the characterisation of energetic materials is central to applications in mining, propulsion, and the development of new fuel systems for emerging technologies.

The unique strengths of neutron diffraction—sensitivity to hydrogen, the ability to discriminate neighbouring elements, and the capacity to exploit isotope substitution—provide decisive advantages for these investigations, especially when working with rare or precious samples. By enabling scientists to observe how materials form, transform, and respond under pressure, Hugin and Munin support a virtuous cycle in which fundamental discoveries drive applied innovation, and societal challenges, in turn, motivate deeper scientific exploration.

2.3. Potential new science

For functional and quantum materials **Hugin–Munin** offers a unique opportunity to probe the structure and magnetism of small single crystals produced in the limited volumes of multi-anvil presses (e.g. the orbital-molecule compound $In_2Ru_2O_7$ [53], and TiOF [54]), or via routes such as hydrothermal synthesis that typically yield only small crystals under research-laboratory, rather than optimised industrial, conditions. This capability substantially strengthens the virtuous cycle between theory and experiment by accelerating the feedback between prediction, synthesis and characterisation in such complex materials. Chiral materials are a particularly active frontier in both functional and quantum materials research [55,56]. Their study requires single-enantiomer crystals - extremely challenging to

grow reproducibly. The ability to measure manually separated enantiomers, or small single-enantiomer crystals, by neutron diffraction would represent a step change in this important area.

Hugin-Munin will provide access to definitive neutron information on quantum and functional materials microcrystals under extreme conditions, providing access to currently inaccessible scientific regimes. The instrument will enable direct determination of how pressure- and field-induced structural distortions modify magnetic exchange, anisotropy and topology at the microscopic level in frontier materials. This capability will allow quantitative testing and refinement of theoretical models describing emergent behaviour in strongly correlated and topological systems much earlier in a materials discovery context than possible now. It further enables the study of weak, complex or multi-component order parameters that are invisible or ambiguous using alternative probes.

In Earth and planetary sciences, access to hydrogen positions in high pressure environment would constitute a breakthrough. It allows for a precise determination of mineralogical structures for hydrogen and water bearing phases, significantly improving our capabilities to model processes taking place in the deep Earth as well as planets and icy satellites inside and outside the solar system. Furthermore, the ability of Hugin-Munin to use standard X-ray DACs for experimentation also offers to scope to finally include associated techniques for multi-extremes that are routinely possible at synchrotrons. The prime example is the laser-heated DAC that offers simultaneous temperatures up to ~5000 K at megabar pressures and is critical in earth & planetary sciences and also materials synthesis. No equivalent has yet been set up for neutron sources. Hugin-Munin can open neutron scattering to these questions in materials synthesis, quantum materials and earth & planetary sciences that would require neutrons but currently cannot be probed due to lacking sample environments.

Neutron spin polarisation is already the core feature of the MAGIC single crystal diffractometer and is not an obvious must-have feature for Hugin-Munin. However, it can be easily introduced as a removable add-on option for a timely preparation for the exciting case of Dynamical Nuclear Polarisation (DNP) of macromolecular crystals which is currently under development [52,57]. This would enable the determination of hydrogen atom positions not only from smaller crystals than before, but also at lower crystallographic resolution. This would allow neutron structures of e.g. membrane proteins that are not sufficiently ordered for today's methods. This includes many important drug targets such as many proton pumps. Thinking ahead, it may become a general method for hydrogenous, organic and inorganic materials with much higher and tuneable contrast.

2.4. Potential user community

A substantial fraction of the user community will come from the quantum and functional materials community, as well as the chemistry community, which currently faces a dearth of neutron instruments optimised for structural studies of small single crystals; where such instruments exist, they are typically high quality but low throughput compared with the potential of Hugin–Munin at the ESS. A strong component will come from synchrotron facilities, where samples and science cases to benefit immediately from Hugin–Munin. In fact, the capability of operating with the same sample sizes as routinely possible at the synchrotron, will allow Hugin-Munin to attract new users to neutron who previously avoided neutrons due to sample size barriers. This provides a large pre-established, multidisciplinary user base. This unique capability of Hugin-Munin also includes complementary measurements of the same samples at high pressure with X-rays and neutrons to maximise analytical power and thus naturally provides a collaborative space to engage with existing high-pressure single crystal beamlines at the various synchrotrons. Further, existing high-pressure neutron users will find Hugin–Munin a powerful and complementary resource for its specialised capabilities not accessible at other high-pressure diffractometers. The high throughput and broad scientific remit of the twin diffractometers will create an excellent training environment for a new generation of neutron users across the physical sciences. A well-established X-ray DAC-based high-pressure community already

exists, enabling rapid knowledge transfer and a fast ramp-up in scientific productivity. Furthermore, MAX IV with SYNCRIS, its new single (micro)crystal X-ray diffraction beamline set to come online in 2026, is next door. Bringing these users together with (high pressure) neutron diffraction experts at ESS will strengthen the scientific ecosystem and ensure broad access to state-of-the-art methods. The reduced entry barriers associated with small sample requirements and the adoption of synchrotron-like workflows, such as the users' ability to use their own pressure cells, will significantly enhance the diversity and accessibility of neutron science, while the worldwide-unique capabilities of Hugin–Munin will foster increased international collaboration and exchange.

3. AN INITIAL TECHNICAL OVERVIEW OF THE PROPOSED INSTRUMENT, DISCUSSING TECHNICAL FEASIBILITY

The instrument scheme and allocation at beam port S4 is shown in the figure below. Both of the twin instruments use a medium length of ~65 m to 70 m, which provides a broad wavelength band of ~4 Å width and sufficient time resolution to separate Bragg peaks with the long pulse. The instrument **Hugin** has a direct view on the thermal moderator, while the cold moderator spectrum is added by the inflection of a bi-spectral switch, - a short Si-wafer stack -, in a focus point close to a pulse shaping chopper system at 7 m. The following neutron guide consists of opening and closing ~15 m long half-ellipses with a straight ~30 m long section in between, and focal points at the pulse shaping chopper and sample positions. In the low divergence straight section, still in the bunker, we introduce a kink to deflect the beam by 0.6°, firstly suppressing fast neutron background at the sample and secondly separating further the sample positions of the twin instruments. The neutron guide is optimised for small beam cross-sections of few mm size and less at the sample and relatively small divergence. The half axes of the elliptical parts are a~15 m and b~15 mm. A typical divergence of ~0.5° (FWHM) at the sample is obtained by terminating the reflecting guide end 75 cm before the sample. The interchangeable absorbing end places a flexible pinhole size close to the sample, e.g. from 35 cm for illuminating 3 mm of a powder sample to few mm distances close to a diamond anvil cell, illuminating tenth of µm size of a crystal, as used in X-ray and synchrotron studies. The instrument **Munin** is built with a very similar concept, with the difference of using only the undisturbed cold moderator view with a wavelength band of 1.8 Å to 5.8 Å. The beam paths of the twins cross already in the NBOA system in the monolith shielding and are 8 cm apart at the pulse shaping chopper positions. The chopper systems are optional and offer a capability for powder diffraction or whenever good resolution in wavelength and time is required. The closeness of the beam lines requires small disk size of ~25 cm diameter. Two disks with counter-rotating slits may offer flexible time resolutions and generate also the sub-pulses for wavelength frame multiplication, which are

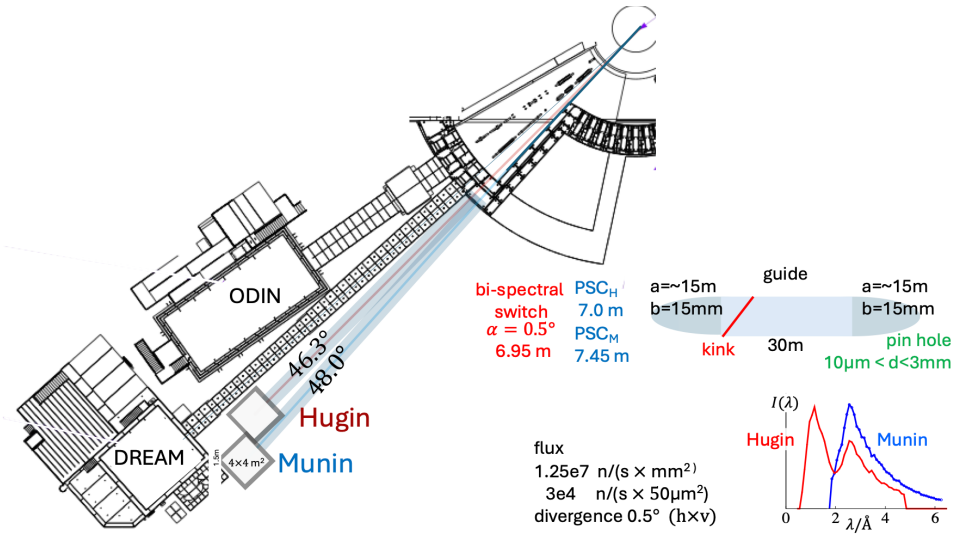

Fig 3. Scheme of the twin instruments Hugin and Munin and their location at S4 in the South Hall.

terminated by an integrated 14 Hz overlap chopper. Flux reductions for work with powders at a medium resolution would be approximately a factor of 20 for a window of 140 µs, with a resolution at $\lambda = 2$ Å of $\frac{\Delta t}{t} \approx \frac{\Delta d}{d} \approx 4 \times 10^{-3}$. The shape of the neutron guide is similar, as is the final beam definition at the sample position. These instrument twins will deliver the highest flux density for single crystal diffraction worldwide. Feasibility and performance of the are verified by VITESS simulations.

The cold instrument **Munin**, using $\lambda > 1.8$ Å, is best suited to magnetic structure determination and large unit cells, while **Hugin** is better suited for nuclear, or combined nuclear and magnetic structure determination. For both, we propose a new measuring method which should achieve an equivalent data quality to the monochromatic single crystal diffractometers at reactor sources.

The secondary part of the instruments is relatively compact with small sample to detector distances of 10cm to 30cm. We propose a recently developed 2D detector system the LumaCam [58], with an optical detection from a scintillation screen with single neutron event detection in the ns region [59]. The several photons generated by a neutron absorption are used to localise the event with better than 100 µm resolution. Therefore, it appears to be a favourable new technique particularly for diffraction from small samples and further enhancing significantly the signal to background ratio.
For standard magnetic structure determination, we propose an unpolarised beam. A possible add-on is a polarising kink in the initial part of the straight section, especially for macromolecular crystallography of samples with dynamical nuclear polarisation of hydrogen [60][52]. Here, the challenge remains on the practicability of the nuclear polarisation.

4. AN EXPLANATION OF HOW THE CONCEPT MAKES USE OF THE ESS LONG-PULSE SOURCE

The ESS long pulse provides a sufficient time resolution to separate by neutron time-of-flight Laue diffraction the Bragg peaks of different Laue orders. This concept is used by the ESS instrument NMX for macromolecular crystallography, providing a superior flux density for the smallest protein crystals. For smaller unit cells, the instrument can be even shorter, which allows to extend to a broader wavelength band including the peak fluxes of the thermal and cold source in bi-spectral extraction. Therefore, the instrument can make use of the full average flux for time-of-flight measurements and so will have a superior performance not only compared to the possibilities at existing other neutron facilities but further to those of upgrade plans and projects like ISIS-2 at Rutherford and STS at Oak Ridge (Fig. 4). The option of shaping the long pulse can be used for a flexible choice in resolution benefitting from the high brilliance of the ESS source.

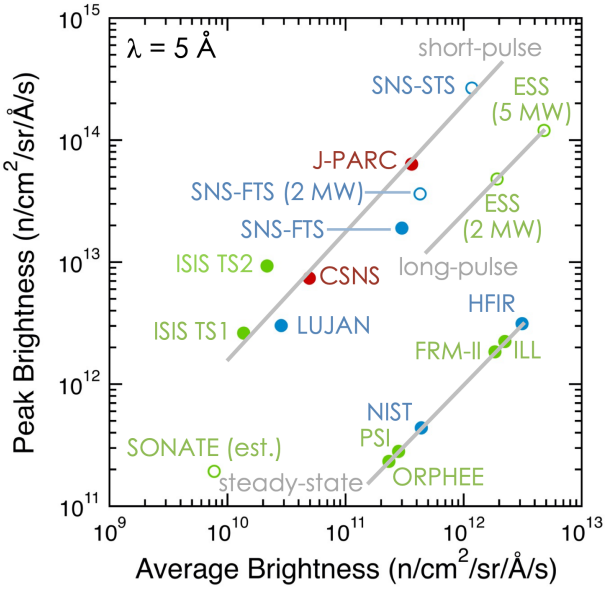

Figure 4 Comparison of brightness at different neutron sources **[64].**

5. PLANS OR REQUIREMENTS FOR SAMPLE ENVIRONMENT AND LABORATORY ACCESS

General technical aspects for sample environments are already well met in the present concept. Some advanced cases would require targeted optimisation and development during the project. For the

structure determination and magnetism programme standard equipment such as gloveboxes, high-magnification microscopes and precision micromounting will be necessary. Sample environment will include cryogenic capability with low background, high-field magnets compatible with the tight detector geometry, furnace capability and gas handling for in-situ processes. A dedicated micro-focus/rotating anode X-ray diffractometer would support the high-throughput aspect by verifying single/multigrain nature of samples, allowing prioritisation work that is often not available at home institutions beforehand. The location of S4 next to the diffraction labs is highly convenient. The high pressure capability would require standard DAC laboratory equipment (gasket drillers, ruby fluorescence for pressure measurement, ideally with Raman spectroscopy, laser-heating for the DAC, and a glovebox loading environment. Furthermore, sufficient expert support personnel will be critical. The potential biochemistry-focused DNP experiments on Munin would require a dedicated high-field magnet, dilution refrigerator and a radio-frequency system to pump the spins.

6. PROPOSED LOCATION OF THE INSTRUMENT AT THE ESS FACILITY, INCLUDING MOTIVATION

The proposed location is S4, which is highly valuable and attractive for building an instrument of a medium length of about 70 m. It is an otherwise unused beam port, adjacent to DREAM and the diffraction lab. The section of beam port S4 offers sufficient space and two views to the thermal and cold moderator which are taken by the proposed slim twin instrument Hugin and Munin. Both are operated independently with pulse shaping choppers. In view of a possible future ESS upgrade to a medium pulse source, the position is perfect to benefit from the natural ultimate peak brightness [61]. The twins need relatively small caves that both fit into the angular section of S4 leaving the neighbouring section undisturbed. The cold view is currently running closely along the inner side wall of the bunker shielding. It is possible to reduce the wall thickness by using heavy concrete, or to move the side wall further similarly to the original plan for the bunker shielding.
Do we have to build both twins at the same time? They are very cost-efficient and needed, as we think, just as Odin needed his two raven birds for gathering information. A common birth is an essential feature of twins. The final optimal realisation depends on a comprehensive planning when using a common beam port. Obviously, a detailed design and building is required for the initial part with the NBOA insert. Furthermore, both twins need their space allocations from the start, and building common guide shielding would be cost beneficial. There is also significant complementarity of the two instruments, meaning concurrent construction and usage optimises the output of the user programme from the outset. But, it would be possible to build bispectral Hugin first, while leaving Munin for later construction if the beam port architecture is properly considered from the beginning.

7. GAP ANALYSIS IN TERMS OF BOTH CAPABILITY AND CAPACITY, IN RELATION TO ESS AND THE GLOBAL FACILITY LANDSCAPE.

A wide range of single crystal diffractometers exist, including e.g. **ILL**: D3 (polarised, hot), D9 (hot), D10 (thermal), D23 (thermal) **PSI**: ZEBRA (thermal), DMC (cold) **MLZ**: HEIDI (hot), POLI (polarised) **HFIR**: WAND (thermal), HB-3A (thermal, extreme conditions), IMAGINE (cold) **SNS**: TOPAZ (cold), MANDI (cold), CORELLI (diffuse scattering), SNAP (cold, high pressure) **JPARC**: SENJU (cold, extreme environments), PLANET (high pressure) **ISIS**: WISH (cold), WISH-2 (current project), SXD (thermal) **ESS:** MAGIC (polarised cold/thermal), NMX (macromolecular)

The capacity of a dedicated 'workhorse' single crystal diffractometer is still missing at ESS. MAGIC with its specialised polarised neutron capability is more like a "racehorse" for complex magnetism but less suited for standard crystal structure determination, while NMX is highly specialised for biology-related macromolecular studies.

There are two groups of single crystal diffractometers, neutron TOF Laue diffractometers at pulsed spallation sources and the traditional monochromatic 4-circle diffractometers used at reactor sources. The difference in performance is dramatic. For usual structure determination, the peak-by-peak collection on 4-circle instruments takes about a week of measuring time for a sample of cube mm size, while many more peaks are collected on TOF diffractometers within short times of minutes, or less than an hour. The case for very small samples is clearly most favourable for time-of-flight diffraction using the intense full wavelength spectrum. **In such cases, the world leading average peak brightness of the ESS source offers the highest flux density among the pulsed neutron sources for studying tiny samples and to further reach out to most extreme conditions.** Considering standard structure determination, however, there is a prevailing competitiveness of monochromatic instruments due to the much better data quality. For TOF instruments, the phase space of the incoming white spectrum is quite inhomogeneous and rough due to extinction in the primary beam. Multiple Bragg excitations may further occur in the sample and extinction effects severely increase with wavelength. In view of standard structure determination, the time-of-flight data needs an improved strategy of data acquisition and analysis. By continuous sample rotation, each Bragg peak will be measured with a variation of wavelengths, see right Figure, which allows to measure and correct for the extinction effects in systematic detail on each Bragg peak.

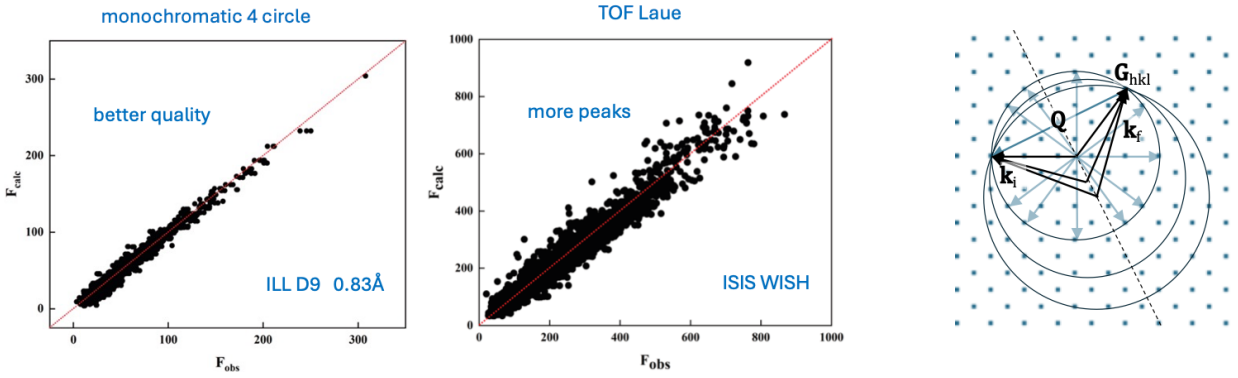

Figure 5 Comparison of typical data quality from measurements at a monochromatic 4 circle instrument (left) **[62]** and at TOF diffractometer (middle) **[63]**. Right: variation of k-vectors for a Bragg condition $\mathbf{k}_f - \mathbf{k}_i = \mathbf{G}_{hkl}$.

8. COMPARISON TO OTHER SIMILAR INSTRUMENTS IN THE WORLD, IF POSSIBLE

With respect to other time-of flight diffractometers or monochromatic instruments, the superior competitiveness of Hugin and Munin relates to huge average and peak brightness, respectively, of the ESS source, see Figure 4. As outlined in section 7, above, this instrument pair inhabit a unique situation within the global single crystal diffraction landscape. As 'workhorse' instruments for materials discovery and development this could be transformative in terms of capability and capacity of the single crystal neutron community as a whole, opening up an area of truly high-throughput characterisation highly complementary to the other existing instruments.

When comparing to instruments applied for the challenging cases of smallest samples, as typical for the high-pressure experiments, we note all are located at pulsed sources and focus on powder diffraction, while SNAP at SNS offers also single crystal capabilities. A common feature is that full crystallographic analysis is still very limited by sample size, limiting pressure regimes, compatibility with other extreme conditions and true synergy with complimentary synchrotron X-ray instruments. With the flux of ESS, the proposed instrument Hugin-Munin and realising the potential for method development, crystallography of tiny crystals at Megabar pressures appears to be a fair stretch goal. The full strength of Hugin-Munin can be achieved when tackling real-world multi-grain crystals in a routine workflow of exploration and analysis as already done in experiments at synchrotrons. Obviously, such capabilities will serve the whole science case of the instrument.

NOTE: Support letters follow references.

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