THE ESS INSTRUMENT SUITE – A CAPABILITY GAP ANALYSIS

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Abstract

The 15 instruments currently under construction at ESS represent a subset of the full 22-instrument suite needed for the facility to reach its full scope, as defined in the ESS statues. In order to guide the selection of the remaining 7 instruments, we here provide an analysis of the missing capabilities.

We have identified that the two most important missing capabilities in the current instrument suite are:

- Particle Physics
- High-Resolution Neutron Spin-Echo

The particle physics community is not at all addressed within the current 15 instruments, while the addition of a spin-echo instrument will greatly increase the kinematic coverage of the ESS spectrometer suite.

An analysis of the remaining capability gaps results in the following highlight areas:

- High-Pressure Diffraction
- Grazing-Incidence SANS
- Very Fast Spectroscopy
- Wide Bandwidth Spectroscopy
- High Magnetic Fields

where the first four are new instruments, specialised in areas not adequately covered by the current 15 instruments, and the fifth capability need is for sample environment equipment.

At the present time, lower priority is given to the following capability gaps:

- Bio-SANS
- Hydrogenous-Sample Diffraction
- Wide-Angle Spin-Echo

The construction of instruments 16-22 should progress in parallel with the Completion of instruments 1-15, so as to optimise the ramp-up to full scientific output. When combined with an increase in accelerator power from 2 to 5 MW, investing another 9% of the current ESS construction budget will result in an increase of the scientific output of ESS by 100%.

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1. Introduction

The scope of ESS, as defined in the ESS statutes [1], is to build and operate 22 world-leading instruments in an open user programme. Of these, the first 15 are funded by the construction budget and will be brought on-line by the end of 2025. Given that it typically takes about 8-9 years from first idea to completion of an instrument, it is therefore timely to start considering which instruments to build as numbers 16-22. This document aims to deliver an analysis of the capability gaps remaining after construction of the first 15 instruments, as requested by the ESS Scientific Advisory Committee (SAC) [2] and the ESS Council. It is expected that it can serve as a guide in selecting the next instruments.

A reference suite of 22 instruments was assembled for the ESS Technical Design Report (TDR) [3] in 2013, based on a set of science drivers identified at the time. The 15 instruments currently under construction were identified in an instrument selection process, consisting of annual competitive proposal rounds. Instrument concepts were developed around their science case, resulting in instrument proposals being submitted over three proposal rounds: 2013, 2014, 2015. In each proposal round, the submitted proposals were reviewed by Scientific and Technical Advisory Panels (STAPs) associated with each instrument class. The proposals and STAP reviews were presented at annual extraordinary meetings of the SAC, which ranked the proposals in order of scientific interest for ESS. Guided by the Early Success Strategy [4] and SAC advice, ESS management then made recommendations to the ESS Council on which instruments to move into the construction programme. The 22-instrument TDR reference suite and the 15 instruments selected for construction are shown in Figure 1.

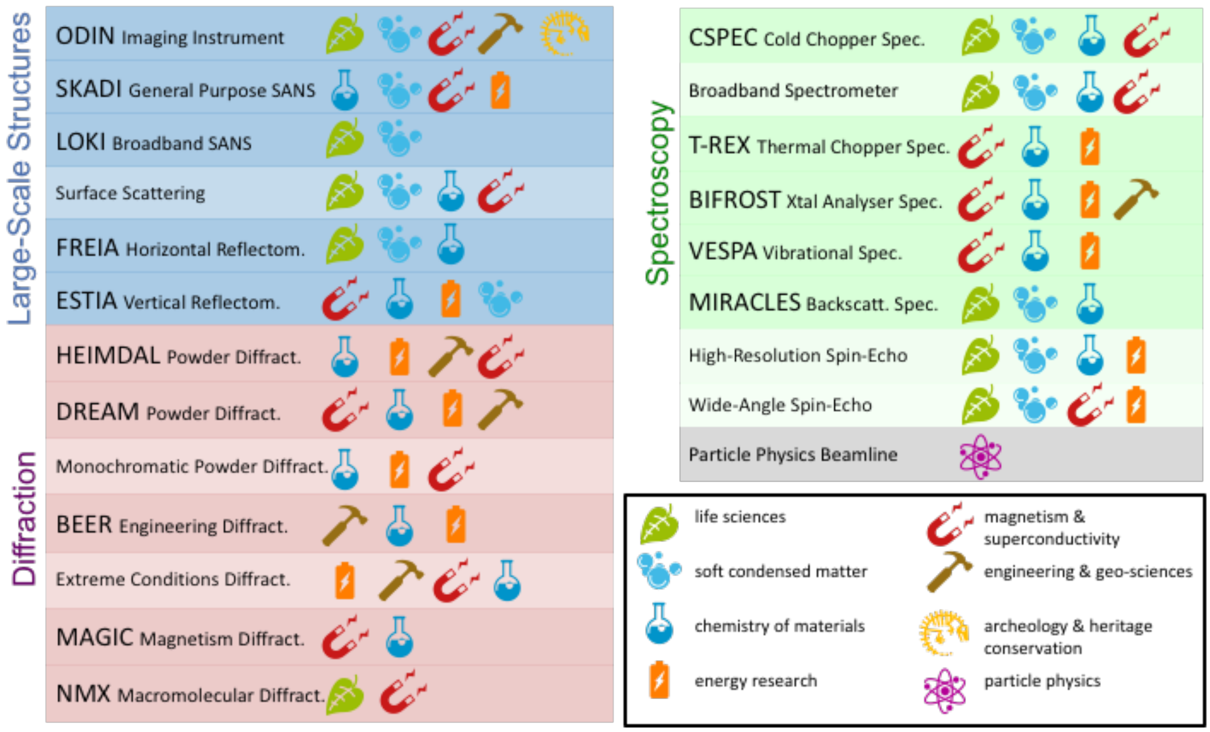

Figure 1: TDR Reference Suite. Named instruments (e.g. ODIN) are those which are currently in construction. The scientific communities addressed by the instruments are indicated with the symbols shown.

2. The First 15 Instruments

The selection of the first 15 instruments was guided by the ESS Early Success Strategy [4] which prioritises instruments falling within the following categories:

- World-class instruments that address the needs of the bulk of the user community and as such bring in our community and ensure early high-impact science.
- Instruments that build on the unique strengths of the ESS source, providing transformative new capabilities.
- Instruments catering to science communities with limited neutron usage today, but with clear potential to bring large scientific impact.

Between them, they cover a broad range of science with some trade-offs between overlapping and complementary capabilities, as detailed in the following.

Of the two SANS instruments, LOKI is optimised for broad bandwidth, while SKADI can access lower Q. Both use the full ESS pulse and thereby provide very high flux over a broad instantaneous Q-range.

The two reflectometers are strongly complementary: ESTIA being able to measure vertical samples below 1 mm^2 in size, while FREIA can measure free liquid surfaces and is optimised for fast kinetics.

The two single-crystal diffractometers are specialised instruments: NMX will address the very large synchrotron x-ray protein crystallography community, allowing them a much more sensitive handle on proton positions, while MAGIC is aimed at the existing neutron community for single-crystal magnetism.

ODIN is a general-purpose imaging instrument with several operational modes, ranging from white-beam to high-resolution monochromatic, with a range of add-on options.

The BEER engineering and materials diffractometer addresses the large engineering community with an interest in the measurement of local strain fields, texture and macroscopic structure in engineering components.

The two powder diffraction instruments, DREAM and HEIMDAL, have overlapping capability, but with different areas of specialisation. Both are general-purpose diffractometers with a flexible trade-off between flux and resolution. DREAM can offer a wide instantaneous Q-range with high resolution, while HEIMDAL is optimised for in-situ and in-operandi measurements, with an upgrade path for covering multiple length scales.

There are two chopper spectrometers – general-purpose inelastic instruments with flexible resolution and large solid-angle coverage. CSPEC uses cold neutrons with a focus on soft matter and in-situ applications, while T-REX extends the coverage to thermal neutrons with a focus on magnetism and a polarisation-analysis capability.

The three other inelastic instruments are strongly complementary. BIFROST is designed for very efficient coverage of single-crystal excitations, particularly in geometries restricted by extreme environments. MIRACLES is a multi-purpose backscattering instrument which extends the resolution coverage into the μeV range, and VESPA measures predominantly incoherent molecular vibrations, complementing optical spectroscopy techniques.

The 15-instrument suite thereby includes many workhorse, general-purpose instruments addressing wide and varied user communities, while also including a number of more specialised instruments, consistent with the early success strategy.

As part of an ongoing value-engineering exercise, the scope of each instrument project has, in most cases, been scaled back with respect to the instrument capability outlined in the original proposal. This effort is a trade-off between maximising the scientific capability and output of the ESS as a whole, while keeping within the budgetary limits. In all cases, a requirement was maintained that each instrument should remain world-leading in performance at an accelerator power of 2 MW.

As a result, many instruments will not have their complete capabilities and detector coverage available when they first come on-line. Each instrument is designed to allow the addition of these features in as straightforward and cost-effective a manner as possible, through the process known as Instrument Completion.

The science on the instruments is supported and enabled by a number of activities related to sample environment, user labs, instrument technologies, control and analysis software, and so on, which we have largely not included within the scope of this analysis, with the exception of where they directly impinge on a decision on whether or not to build a particular instrument.

One area which is worth highlighting is the provision of Polarisation Analysis (PA) capabilities using polarised-^{3}He gas. The equipment needed for PA Systems is not included in the construction budget, but we consider it a high priority to set up the required infrastructure in the early years of operation.

3. Missing Capabilities and Opportunities

The high-level case for building ESS has always been to make new capabilities available to researchers, addressing both existing neutron user communities and seeding the emergence of new areas which can be addressed using neutrons, rather than only providing additional capacity. Identifying and addressing capabilities which ESS should provide is therefore an essential part of the core scope of ESS as a facility.

The process by which the 15 instruments were selected ensures a clear link between the science case and the particular technical solutions proposed, with care taken to ensure coherence of instruments across proposal rounds. It also links the instrument proposal with an identified instrument team, which often has backing from a partner institute to deliver the instrument as an in-kind contribution to the ESS. The process, however, was stopped before reaching the full suite of 22 instruments. The list of 15 instruments was therefore never intended to be a complete instrument suite, addressing the full ESS science case as outlined in the TDR. As such, there are a number of missing capabilities, corresponding to scientific communities which ESS does not cater for with the 15 instruments currently under construction.

In the following, a number of capability gaps are listed, for complementing the capabilities of the first 15 instruments. It is not a complete list of which instruments could be built, nor of the instrument proposals which have been submitted for construction but were rejected (for reference, the complete list of instrument construction proposals can be found in the Appendix). What is provided here is a list of the capabilities which we currently consider to be important to add to the ESS instrument suite. It has its origins in the TDR reference suite, but does not map directly on to it. Some of the instruments listed have some ESS history behind them, in which case this is briefly outlined. The areas are arranged in three categories: high priority, other significant capability gaps, and lower-priority areas.

In addition to the areas described in the following sections, there are two particular areas which we consider as given: Instrument Completion and Polarisation Analysis Systems.

Instrument Completion, the process of approaching the full capability of each instrument, as outlined in the instrument proposal before value-engineering, is regarded as a high priority, and should proceed in parallel with the construction of new instruments. It is a straightforward and very cost-effective way of increasing the capability and scientific output of the full instrument suite. A first round of prioritisation on completion options was performed with the instrument STAPs in 2016-17, and should continue during initial operations in order to determine the most cost-effective way of maximising scientific output by balancing Instrument Completion and construction of new instruments.

Polarisation Analysis Systems, the provision of polarised-^{3}He infrastructure to support the instruments, is needed for T-REX to fulfil its project scope of delivering polarisation analysis. It will also greatly enhance the scientific capability of many other instrument, both for magnetism and for coherent-incoherent separation.

4. High-Priority Capability Gaps

Particle Physics

The scientific community which is most obviously not catered for is particle physics, as can be seen in Figure 1. Cold neutrons can be used for making high-precision tests of the standard model (SM) and ESS has received proposals and expressions of interest for such beamlines, which so far have not been approved for construction.

The ANNI proposal, submitted in 2015, was for a neutron beta-decay beamline to study new physics models beyond the SM at mass scales from 1 to 100 TeV, far beyond the threshold of direct particle production at accelerators, and providing a systematically different access to the fundamental properties related to matter formation in the universe or the unification of fundamental forces.

Compared to other neutron facilities, ESS is particularly interesting to use for such applications, firstly because it will provide the world's highest time-average neutron flux of cold neutrons, but also, importantly, because the source time structure can be used to suppress systematic errors which are usually at least as important a source of error as the random errors associated with the limited counting rate. This is expected to result in an accuracy gain of an order of magnitude in neutron beta decay measurements.

The ANNI proposal was strongly supported by the relevant STAP and the SAC, but was not prioritised at the time due to the limited number of available instrument slots within the (then) 16 instruments to be funded within the construction budget.

At the same time as the ANNI proposal, a letter of intent was submitted for an Ultra-Cold Neutron (UCN) facility for experiments addressing the neutron electric dipole moment and gravity spectroscopy. The scientific impact was judged by the STAP to be very high, but the concept maturity was not sufficient for the instrument to be evaluated at the same level as the construction proposals.

An expression of interest was also submitted that year for a beamline to search for neutron – anti-neutron (n-nbar) oscillations. This would be a major project, costed in the several 10s of M€, and as such outside the funding envelope enabled by the ESS construction project. The beamline is envisioned as a single ~5-year experiment rather than a permanent facility. It would have a sensitivity of at least 1000 times greater than the previous experiment, performed at the ILL. A possible location for the beamline has been identified, with the target monolith designed to allow the extraction of the required very large (~1m^2) cold-neutron beam and downstream space reserved for the >200m length needed. The instrument concept has since evolved into the HIBEAM concept, to include the search for mirror neutrons (a dark matter candidate), and the consortium continues work on progressing the instrument design and organises regular workshops.

The HIBEAM and ANNI teams have recently started discussions on integrating some aspects of the HIBEAM science case into the ANNI beamline, as a first step towards building a dedicated beamline.

Of these various projects within fundamental and particle physics, the ANNI beamline remains the most mature and the one with the clearest technical design. Its construction cost is expected to be the same as that of a "normal" neutron scattering instrument, which makes it a good candidate for one of the slots in instruments 16-22.

The prioritisation of the instruments for condensed matter science has left the particle physics community without a current stake in the operation of ESS. It is our view that this situation should be remedied by including a particle physics beamline, such as ANNI, as one of the first instruments within the remaining seven slots.

High-Resolution Neutron Spin-Echo

In the TDR reference suite there are two spin-echo instruments: a high-resolution instrument, pushing the limit in Fourier times up to about 1µs, and a wide-angle instrument designed to cover a broad simultaneous Q-range with good Q-resolution. A superconducting version of the high-resolution instrument was submitted as an instrument proposal in 2014, under the name of ESSENSE. It was strongly supported by the relevant STAP, but the SAC advised that ESS make a decision on which of the two TDR spin-echo instruments should be built first, before deciding on any particular spin-echo proposal.

A topical workshop was then held [5], in which it was established that the first spin-echo instrument at ESS should be the high-resolution version. In 2015, the ESSENSE proposal was resubmitted, but this time in competition with the RESPECT proposal, which aimed to deliver the same long spin-echo times using the alternative Longitudinal Neutron Resonance Spin-Echo (LNRSE) technique. This is a developing technique which has not yet demonstrated its ability to reach long spin-echo times, but could potentially do so with greater flux and fewer restrictions on sample environment and sample size. The Spectroscopy STAP recommended that ESSENSE go ahead and RESPECT should not, due to its technical immaturity. The SAC, on the other hand, recommended that a decision on spin-echo at ESS be postponed for a time, to allow the LNRSE technique to demonstrate its potential, allowing a better-informed decision between the two instrument proposals. ESS management concurred.

The ESSENSE and RESPECT teams subsequently worked on a joint instrument concept, incorporating both conventional and resonant spin-echo techniques into a single instrument. The conceptual design and performance were evaluated by the spin-echo STAP in 2016, which concluded that work on the hybrid instrument design should not go ahead due to the levels of compromise needed between the two techniques, and recommended that the original ESSENSE and RESPECT concepts be pursued separately.

We thereby find ourselves without a spin-echo instrument in the ESS instrument suite. This despite the strong scientific case, the well-adapted time structure and spectral properties of the ESS neutron source, and the very large increase in dynamic range which such an instrument would add to the ESS spectroscopy suite, as shown in Figure 2.

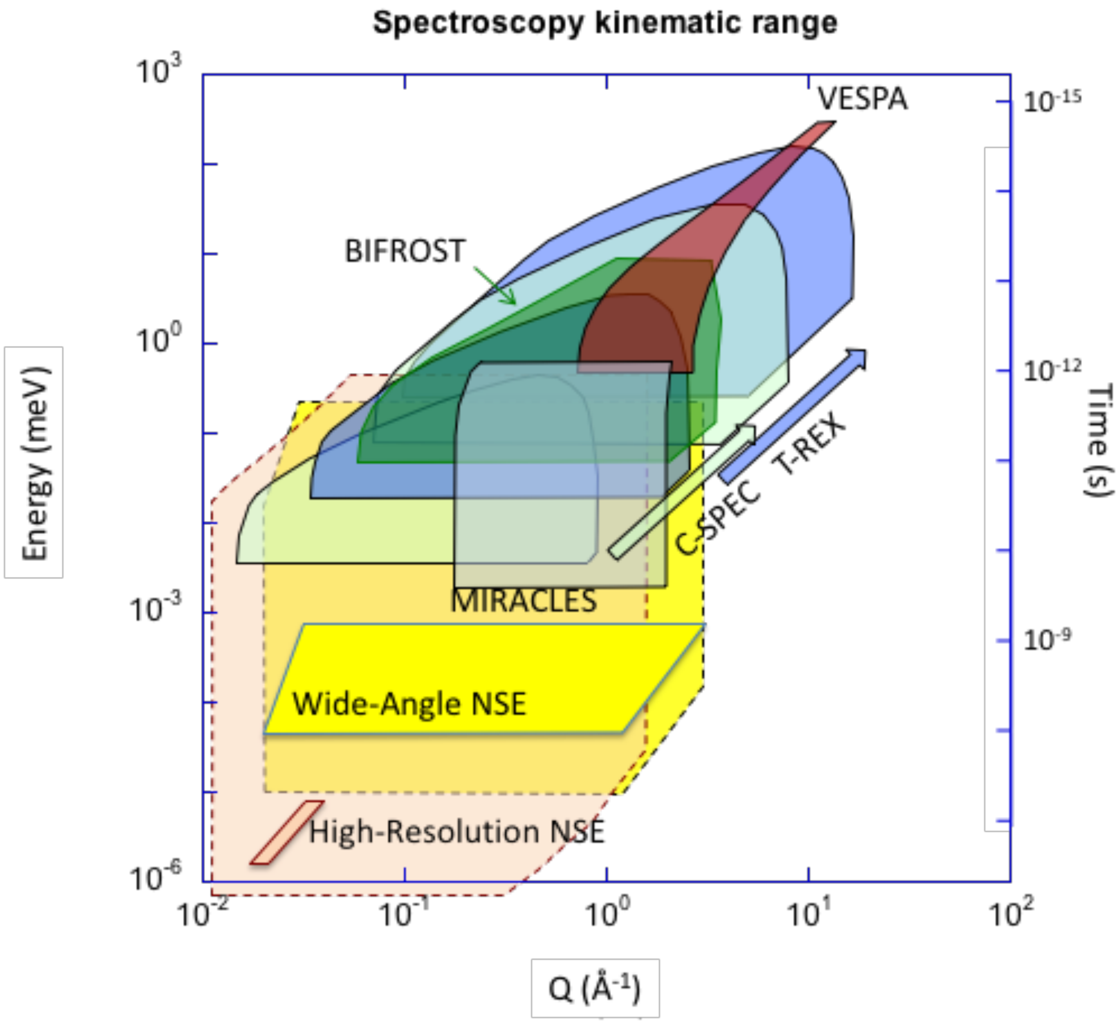

Figure 2: Kinematic range of the various spectroscopy instruments. CSPEC and T-REX can shift their Q-E coverage by rephasing their choppers, as indicated by the arrows, while VESPA, BIFROST and MIRACLES typically cover the similar kinematic ranges at any one time. The high-resolution spin-echo instrument typically covers the area shown by the solid pink parallelogram in a single measurement, but can access the full area delineated by the dashed pink line, by changing wavelength range, precession field, and/or scattering angle. The wide-angle spin-echo instrument covers the area shown by the solid yellow area in a single measurement, and can cover the larger yellow area enclosed by the dashed line by scanning through wavelength range and precession field.

The kinematic range accessed by ESS instruments would be greatly increased by the addition of a high-resolution spin-echo instrument. The following science highlights illustrate the communities which would be addressed by the addition of a high-resolution spin-echo instrument [5].

- Life science, protein dynamics and drug design: Understanding molecular micromechanics and dynamics in proteins to enable rational computer aided drug design. The move from discussing molecular biology purely in terms of structure to the characterisation of the dynamics of the intrinsically disordered proteins making up these systems using molecular dynamics (MD) simulations requires direct measurement of these correlated motions, which only neutron spin-echo can provide.

- Interface and surface dynamics, tribology and lubrication: Wear and friction are ubiquitous in machines and vehicles, as well as in biological systems, such as joints. Understanding the role of solid-surface fluid boundary on the molecular scale is essential to optimise or develop new lubrication systems. Only spin-echo can access the relevant time scales.
- Functional and self-healing polymers: The recovery of fracture and barrier properties or improvements in corrosion resistance are the hallmarks of this emerging class of functional materials. The recovery process depends sensitively on the mobility and diffusion of the polymers within these dense polymeric networks.
- Proton dynamics in fuel cell membranes: localised proton motions and the nature of proton traps.
- Relaxation of ion-polymer dynamics in battery electrolytes.
- Leading-edge studies of high-resolution neutron spin-echo and MD simulations are moving in parallel and need each other to progress. MD will soon be routinely reaching the µs timescale, requiring a corresponding evolution of spin-echo capability.

In addition, the large gain in intensity which ESS will offer is expected to be a game-changer for neutron spin-echo, making it more available to non-expert users and tapping into a potentially even larger user community than currently addressed.

In conclusion, there is a vast range of scientific problems which can only be addressed using high-resolution neutron spin-echo. The large increase in count rate offered by such an instrument at ESS will be transformative in a number of areas, and is needed to validate MD simulations as they evolve to cover larger systems.

5. Other Significant Capability Gaps

High-Pressure Diffraction

An instrument proposal for a dedicated high-pressure beamline, called ESPRESSO, was developed in-house and submitted for approval in 2015. Its science case and design were strongly endorsed by the Diffraction STAP [6], which ranked it at the same level as MAGIC for inclusion within the first instruments. The SAC, however, ranked it slightly lower, due to its higher degree of specialisation, and recommended that it should be included within the full suite of 22, but not within the first 16 (the number of instruments envisaged at the time).

The instrument is designed to measure accurate structural information at pressures exceeding 120 GPa (=1.2Mbar) at temperatures from 4K to 4000K. This would be achieved by optimising the diffractometer around specialised sample environment, known as diamond anvil cells (DACs). Not only are DACs the only means to statically maintain such conditions, but they are familiar tools to the majority of the high-pressure community, thereby allowing researchers to easily pivot from existing synchrotron programmes towards neutron science.

The P-T range offered by ESPRESSO is unprecedented in neutron scattering. The nearest competitor, SNAP at SNS, holds a current pressure record of ~60 GPa, and has 1-2 orders of magnitude lower flux, impacting both data quality and experimental scope. Therefore, ESPRESSO will be a transformative instrument for high-pressure structural science, both because of the much larger P-T range it can cover, and the significant improvements in data quality due to its much higher counting rate and reductions in background afforded by new detector and guide technologies.

Europe has a diverse high-pressure community of about 3,000 scientists, working in materials and earth sciences, chemistry, and physics (including magnetism). This is a highly active and productive community, in terms of high-impact publications, using over 500 days/year of synchrotron beamtime for DAC experiments. The proposers estimated that about 40% of these users would benefit from neutrons if the higher-pressure and temperature capabilities of ESPRESSO were available. We are confident that this community will guarantee high-quality productive use of a dedicated high-pressure instrument at ESS.

The instrument would impact on many areas of solid-state research, ranging from materials, planetary and earth sciences, to fundamental chemistry. High pressures can be exploited to make structure itself the experimental variable. It can either subtly tune or dramatically change chemical bonding, even creating entirely new phases; sometimes with highly interesting physical properties, and sometimes recoverable to normal pressures.

There is currently a large gap in this field between what can be done at synchrotron x-ray sources and what is accessible to neutrons, which would be considerably narrowed. Highlight areas which only neutrons can address include:

- Light elements, notably metallic H2 (D2) and other H(D)-rich materials, such as ices, clathrates, ammonia, methane and silanes at pressure.
- Correlated electron and magnetic systems, such as superconductors (e.g. the new hydrogen-sulphide based high temperature systems) and electronic distortions in functional materials.

- New materials generated by structural changes or reactions at high pressure, e.g. nanophase carbons, ultrahard and ultra-strong materials, high-low spin state changes, metallic glasses and ferroelectrics and multiferroics.
- Geosciences, allowing conditions in earth's lower mantle and outer core to be reproduced in neutron scattering experiments for the first time, enabling studies of water in minerals, element partitioning, volatiles in the core and melts.

Some high-pressure diffraction can be performed on the current diffraction instruments. However, experience at existing synchrotron sources clearly demonstrates the benefits of dedicated instruments for high-pressure experiments, which are in general far more challenging to conduct than other measurements.

The lack of high-pressure optimisation will compromise set-up time and data quality, and severely curtail maximal P-T capabilities. Such work would inevitably be competing for beam-time with experiments which fall within the mainstream of these instruments' remit, and which are usually shorter and more straightforward. The likelihood is, therefore, that high-pressure experiments with DACs would struggle to make an impact on these instruments.

A further argument in this direction relates to the instrument staffing, whose scientific areas should ideally match those of the users on their instruments, in order to achieve a good and productive level of scientific collaboration. This would be more difficult to achieve on a general-purpose diffractometer, or one specialised in another area.

We are of the opinion that a dedicated high-pressure instrument is needed if ESS is to fulfil the potential of the technique. ESS is currently the only pulsed spallation source not to have a dedicated high-pressure diffractometer in its suite.

Grazing-Incidence Small-Angle Neutron Scattering (GI-SANS)

Understanding the self-assembly of nanostructures at surfaces and interfaces is a topical challenge for both soft and hard condensed matter. Such interfacial nanostructures play a key role in many medically and technologically important areas, ranging from biological cell signalling, and functional coatings, to the performance of organic solar cells, as well as data-storage and energy materials. These structures, with dimensions ranging from a few nanometres up to micrometres, are often difficult to study due to their small size and because they are often found at buried interfaces between two materials. Grazing incidence neutron scattering has a unique ability to reveal the structure of surfaces in complex multi-component nanostructures. Due to the sensitivity of neutrons to nuclear isotopes (deuterium labelling) and magnetic structures (polarised neutrons), neutrons offer a highly complementary surface probe to synchrotron X-ray studies (GISAXS/GIWAXS) and other surface-sensitive methods. Neutrons have been very successful for specular reflection experiments that elucidate the one-dimensional depth profile of surfaces, but the development of grazing incidence scattering methods to detect lateral nanoscale interface structure lags behind due to the low flux of current neutron sources. The high source brightness of ESS has the potential to offer a step-change in surface studies, and consequently calls for the development of new techniques and instrumentation. For this reason, a dedicated beam line for Time-of-flight (TOF) GISANS was already envisaged in the TDR reference suite, under the name of the Surface Scattering beamline.

Time-of-flight (TOF) GISANS has the unique advantage that it can probe nanostructures at different distances from an interface using the wavelength-dependent penetration depth of neutrons. This allows the 3D structure of surfaces and thin films to be determined. A few experiments have been demonstrated successfully at existing neutron sources, but current measurement times are often prohibitively long. Wide-spread use and broad application of neutrons in this area are still missing in the absence of dedicated high flux instruments that are optimised to use the time-of-flight method in a surface geometry.

The main motivation for grazing incidence neutron scattering at ESS is to perform experiments that are impossible using other techniques, and to exploit the advantages of neutron scattering, such as isotopic labelling to identify particular components of complex interfacial structures, the ability to probe buried interfaces between bulk phases, and to determine magnetic structures. In soft and biological materials, the non-damaging low energies of neutrons are also important for functional and in-operando studies as a function of time. Key applications are organic photovoltaic materials and organic light emitting diodes, in which case grazing incidence neutron measurements have been valuable to relate the interfacial structure to device performance and stability. A vast number of other applications utilising polymers and surface-active molecules in, for example, drug delivery, food packaging, biomedical materials, and anti-corrosion coatings depend on understanding how interfaces influence the material properties. In biological and biomedical sciences, a wide range of potential applications are waiting for high-flux instrumentation applicable to surface aggregation of membrane lipids and proteins to elucidate the functions of healthy and diseased cells.

The overlaps of these fields with current major societal challenges and with both industrial and academic research are clear.

The ESS peak cold moderator intensity will give a gain of ~90 at 5 Å compared to the highest time-averaged neutron flux available today (ILL cold source). This means that experiments that are now between 3h and 48h, depending on sample size, scattering, and background conditions, will be reduced to measurement times of a few minutes or a few hours under the same experimental conditions. This significant difference makes it feasible for the first time to develop TOF-GISANS into a mainstream technique for interface characterisation. An ESS instrument designed to combine reflectivity and GISANS from the outset will bring 3D characterisation of interfaces to kinetic and parametric studies of, for example, temperature, chemical composition and magnetic/electric fields within reasonable timescales for many systems, and has applications across most of the ESS materials science case.

None of the currently foreseen SANS or reflectometry instruments at ESS are well-optimised for such studies, due to their particular collimation, bandwidth, and resolution requirements. In addition, even for the subset of possible GI-SANS experiments which would be technically feasible on these instruments, their very large existing user communities in the x-ray world, and their generally high throughput, would make it very difficult for grazing-incidence techniques to gain a foothold without a dedicated instrument at ESS.

A dedicated TOF GI-SANS instrument is needed to allow the technique to fulfil its potential, and ESS is uniquely placed, due to its high brightness, to provide this breakthrough capability.

Very Fast Spectroscopy

A new concept for a very rapid cold-neutron spectrometer, providing similar resolution to CSPEC but with an increase in counting rate of up to two orders of magnitude, was recently proposed [7]. Though less flexible in terms of adjusting resolution or dynamic range, such an increase in sensitivity would provide breakthrough capability for experiments probing coherent excitations in single crystals. Chopper spectrometers and triple-axis spectrometers excel in these measurements and have seen rapid development over the last years, but are intrinsically limited by their low flux (chopper spectrometers) or low solid-angle coverage (triple-axis spectrometers).

The machine uses graphite crystals arranged on a quasi-ellipsoidal surface, at a distance of about 1 m from the sample, covering a significantly larger solid angle than achieved at current chopper spectrometers. By Bragg-reflecting the neutrons through a shielded aperture on to an array of position-sensitive detectors below the sample position, the instrument should provide good signal-to-noise conditions and 3D **Q**-resolution, albeit with a somewhat relaxed resolution compared to a chopper spectrometer with the same energy resolution.

Such an instrument would extend the measurement of coherent excitations to much smaller samples than currently achievable. This would allow inelastic neutron scattering to become part of the materials discovery pipeline, measuring new materials that can only be grown as single crystals in small volumes, such as hydrothermal and solvothermal synthesis of metal-organic magnets, intercalated Fe-based superconductors, as well as epitaxially grown systems, such as the iridium-based pyrochlores. Coupled with the high brightness of the ESS source, it would allow the measurement of excitations in thin-film materials, opening up new fields of study to neutron scattering.

It would also greatly extend the applicability of parametric studies of coherent excitations, allowing careful tracking of phase diagrams as needed when following critical scattering phenomena. Studies as a function of pressure or strain would be able to probe new parts of the phase diagram on systems such as the strain-induced nematic phases of Fe-based superconductors or pressure-driven phase transitions in quantum magnets. Accessing extreme environments, such as high strain or pressure, invariably restrict the available sample volume, making such measurements very challenging with today's instruments.

This instrument does not feature in the TDR reference suite as the idea has only recently been developed. It would, however, offer an increase in counting rate of three orders of magnitude compared to existing instruments, which would be transformative for neutron spectroscopy.

Wide-Bandwidth Spectroscopy

This is an instrument concept based on the proposal for the Versatile Optimal Resolution (VOR) chopper spectrometer, submitted in the 2014 proposal round. This was strongly supported by the relevant STAP, which deemed VOR an essential instrument for the ESS instrument suite, ranking it just below CSPEC. It was also recommended for construction by the SAC, but since there were no immediate in-kind partners involved in the design phase, the instrument ended up being cut from the project when it became clear that the funding level was insufficient to build more than 15 instruments.

The instrument is a short chopper spectrometer, designed to use extensive repetition rate multiplication (RRM) to provide instantaneous access to a broad range of incident energies of 1-80 meV from each ESS pulse. Its short length allows a very large scope for increasing flux by relaxing resolution, and its novel chopper system allows the energy resolution to be freely tuned across the full range of incident energies simultaneously.

VOR is specialised in rapid mapping of S(Q,ω) over a broad energy range. Coupled with its high flux, this will allow it to make spectroscopic in-operando and in-situ measurements in the timeframe of a few seconds. This is vital for the study of complex and hierarchical states of matter, as found in soft matter, and, for example, to study the interplay between phonon and magnon excitations in functional materials. It would be possible to visualise the effect of trapping hazardous CO_2 by a porous material on the dynamics of the crystal lattice and gas molecules, thereby providing the opportunity to optimise the process. In addition, the flux gains on VOR will enable fast scanning of the relevant dynamics in samples that are currently too small to address with neutron scattering. Fast scanning of samples provides a broad overview of a range of materials enabling key phenomena to be determined. Further, more detailed energy resolution studies can then be carried out using the complementary narrow bandwidth spectrometers CSPEC, T-REX and BIFROST.

By covering a wide range of energy scales quasi-simultaneously, VOR is well-suited to studying non-equilibrium states of matter. We inhabit a world in which we are perpetually out of equilibrium, note, for example, the irreversibility of transitions between microscopic states in biomolecular processes. Non-equilibrium states are believed to lead to particular cell polarities, differences in shape, structure and dynamics within a cell that allows them to carry out specialised function. Equally, non-equilibrium physics are of the utmost importance in reaction-diffusion systems, such as in many chemical reactions, but also recently demonstrated in magnetic order with interacting spatial and temporal fluctuations to provide a wide variety of dynamical phenomena. However, very little progress has been made in understanding the laws that govern the statistical fluctuations leading to non-equilibrium states of matter. VOR will enable the neutron scattering community to probe the dynamics of non-equilibrium physics.

High Magnetic Fields

Neutron scattering has many intrinsic advantages over other techniques in the field of magnetism. The quantum mechanical atomic interactions that drive magnetic phenomena can generally be rather strong. In normal iron, the magnetic field strength felt by the individual atomic magnetic moments, which are due to interaction with their neighbours, can exceed several hundred Tesla. Functional magnetic materials working at room temperature, therefore, have inherently strong magnetic couplings.

Applying an external magnetic field to a material is a commonplace way of perturbing the magnetic ground state in order to learn more about the material under investigation. However, since the best sample environment magnets for neutron scattering currently reach a field strength of only 15-17 T, they can apply only a weak perturbation to strong magnets, thereby limiting the scientific relevance of such experiments.

Strongly coupled materials lie at the heart of many subtopics in magnetism. Room temperature multiferroics serve to allow control of the magnetic state of a material using electrical fields, with potential high impact in information processing and data storage. Strong magnetic interactions seem to drive superconductivity in the so-called high temperature superconductors, working above liquid nitrogen temperatures, though as of now still not completely understood. Quantum magnets – the study of which have major basic scientific relevance – are inherently weakly coupled. However, even they sometimes require fields exceeding the current state of the art to be fully understood.

Since the full study of functional and many other materials lies outside current capabilities using neutron scattering in applied fields, increasing magnet field strength is of the utmost importance to further the understanding of many strongly coupled magnetic materials.

There are two main routes to reach fields beyond the capabilities of current Nb-based cryomagnet technology. One is the use of pulsed fields, which can reach ~60T with pulse durations of a few milliseconds, ideally matching ESS's time structure. Due to the short duty cycle of these experiments, which require time to recover after each pulse, the high flux of ESS is especially important.

The second is to use high-T_c superconducting (HTSC) magnet coils, on their own or in combination with traditional low-T_c coils, to produce DC fields of the order of 25T. Recent advances in HTSC tape manufacture and the use of non-insulated coils have brought significant improvements to the manufacture of this type of magnet. The costs remain an order of magnitude larger than that of traditional cryomagnets, but are already an order of magnitude lower than that of the currently world-leading DC high-field magnet at the Helmholtz-Zentrum Berlin, and even greater when taking operating costs into account, making this the technique of choice for DC magnetic fields.

The majority of instruments at ESS are being designed to accommodate the use of large cryomagnets. Requirements on the instrument designs have been imposed on space and robustness to stray fields, which will enable the use of unshielded magnets beyond the current state-of-the-art on most instruments. Several instruments (e.g. MAGIC, BIFROST) are specifically dedicated to magnetic measurements. BIFROST in particular is very well suited to vertical field split coils with a small vertical aperture, which will enable the highest DC fields in this geometry. MAGIC will be able to accommodate both static and pulsed field magnets, as will other instruments, such as DREAM.

The current plans for sample environment will allow the user programme to access magnetic fields of up to approximately 15T, the current state-of-the-art at neutron facilities. The instrument suite is well placed to allow the use of hybrid DC magnets with fields of the order of 25T, as well as pulsed magnets, going up to ~60T. Therefore, in this case, a new instrument is not needed to fill this capability gap. Instead, ESS should ensure that it invests in high-magnetic-field sample environments in time to make full use of the game-changing capabilities of its suite, also in this field of science.

6. Lower-Priority Capability Gaps

Bio-SANS

This is a concept for a SANS instrument dedicated to biological systems in solution, modelled on the highly productive Bio-SAXS beamline at DESY. It was submitted as an instrument proposal in the first proposal round in 2013 under the name of Compact SANS. At the time, it was judged to be too specialised an instrument to build before the more general-purpose SANS beamlines. It was modified and resubmitted in 2014 with a more general science case, but retaining the same essential characteristics, and was given the name SLEIPNIR at the time. It was rejected for similar reasons, while the LOKI instrument, which had meanwhile been approved for construction, was encouraged to update its design so as to allow some of the capabilities of Compact SANS.

While a large part of the capability of this instrument would be equally well covered by LOKI, and to some extent SKADI as well, the thrust of the argument for building this instrument sits in its focus on the life-sciences community. By having an instrument dedicated to this science area, ESS would provide capacity and expertise for successful and very productive scientific collaborations. This would finally allow the life-science community a clear path into neutron scattering, allowing an opening towards a potentially huge community which is currently not strongly engaged with neutrons but has long been presented as an area of future growth.

Hydrogenous-Sample Diffraction

Many of the most important scientific challenges which can be addressed with neutron powder diffraction relate to the structural chemistry, physics, and biochemistry of hydrogen. These cover energy and functional materials, geo- and planetary sciences, as well as health and life sciences. Despite playing to one of the key strengths of neutrons, i.e. their ability to see hydrogen atoms, there are no instruments worldwide which are optimised for determining hydrogen positions in polycrystalline materials.

The Hydrogen Observation Diffractometer (HOD) was proposed in 2014 in order to address this science case. It is a novel concept for a pulsed neutron source, using a compound crystal monochromator to select an array of monochromatic neutron pulses in order to provide a set of diffraction patterns, each one equivalent to a data set taken on a continuous-source diffractometer. It features a polarisation analysis mode for separating the coherent (structural) signal from the incoherent (largely background) scattering, and a chopper system for separation of the elastic and inelastic scattering. At the time, the relevant STAP approved the more general-purpose instruments DREAM and HEIMDAL, while encouraging the HOD team to take the time to further develop their scientific case and technical design. As a result, the instrument team decided to delay submission of their proposal to the SAC until the following year.

Upon resubmission in the 2015 proposal round, the Diffraction STAP recommended that ESPRESSO and MAGIC should go ahead, and that HOD should be considered for a later slot within the full 22-instrument suite. The SAC concurred with this view, as did ESS management.

Though the science case is felt to be very strong, it is our judgement that the technical implementation of a hydrogenous-sample powder diffraction capability can also be performed on the existing powder diffractometers DREAM and HEIMDAL, with a performance which is similar to that of HOD. This can be done by installing polarisation analysis on one or both of these instruments, using polarised-^{3}He spin-filter cells. The infrastructure needed to support such a capability is planned to be made available in time for the first 15 instruments. We would therefore recommend that the DREAM and HEIMDAL instrument teams study how such a capability could be implemented on their instruments, once an early science programme has been established.

Wide-Angle Neutron Spin-Echo

The wide-angle spin-echo concept is based on the SPAN instrument which operated briefly at HZB, and the WASP instrument which is about to start user operation at ILL. It allows the coverage of a much larger detector solid angle (up to two orders of magnitude) than the high-resolution spin-echo instrument, at the cost of a reduced spin-echo time by about an order of magnitude. As can be seen in Figure 2, this would still represent a significant extension of the dynamic range accessible by ESS instruments. The increase in detector coverage is particularly interesting for systems which exhibit important Q-dependence to the relaxation times measured, such as in crystalline systems, where relaxations need to be probed away from Bragg peaks that swamp the inelastic signal, and for systems with smaller macromolecules, such as glass-forming polymers and magnetically-frustrated materials.

Given that ESS does not yet have any spin-echo instruments in its instrument suite, and due to the fact we propose to build the high-resolution spin-echo instrument first, as it is the one which will address a broader scientific case and allow a larger extension of the ESS dynamic range, we feel that there is no immediate urgency for the wide-angle instrument to go ahead. In addition, with the WASP project at ILL nearing completion, it will take a number of years of user operation before the full impact of this instrument type is understood, both with regard technical uncertainties and scientific impact.

7. Summary and Conclusion

We have identified two areas we consider to be the most significant omissions from the ESS capabilities and which need to be filled.

The first of these is particle physics, specifically the community working on correlation effects in neutron beta decay, at the precision frontier in particle physics. Major existing neutron sources, such as ILL, SNS, NCNR and J-PARC, include one or more fundamental physics beamlines as part of their scientific programme. A particle physics beamline at ESS will be world-leading; pushing sensitivity by an order of magnitude in neutron beta decay experiments, providing more stringent tests of the standard model, resolving the effects of the hadronic weak interaction, and improving the measurement of fundamental physics parameters, which underlie matter formation and the unification of fundamental forces. It is essential that ESS addresses this community.

The other serious omission from basic ESS capability is neutron spin-echo. The addition of high-resolution spin-echo capability to the ESS spectroscopy suite will vastly increase the area of kinematic space which ESS accesses. It will bring in user communities in soft matter, life sciences, and energy materials, and provide a unique and essential support to the evolving capability of molecular dynamics simulations in order to understand and design macromolecular systems. Some of these user communities already use neutron spin-echo, but we expect that the large increase in instrument capability at ESS will attract many new users.

After filling these two areas, there remain a number of other significant capability gaps in the ESS instrument suite. Of these, we consider the following five would have the highest scientific impact:

- High-Pressure Diffraction
- Grazing-Incidence SANS
- Very Fast Spectroscopy
- Wide Bandwidth Spectroscopy
- High Magnetic Fields

Most of the instruments within the current first 15 are workhorse instruments addressing wide user communities, in order for ESS to cater to as large a fraction of the existing neutron community as possible. In addition to these general-purpose machines, there are already a number of more specialised instruments included in the 15. The first four areas listed above all represent other instruments with specialised capabilities which it is timely for ESS to consider adding. The fifth area, we believe, is best addressed by providing appropriate sample environment equipment for use on the existing instruments.

In addition to these areas, a number of other capability gaps have been identified:

- Bio-SANS
- Hydrogenous-Sample Diffraction
- Wide-Angle Spin-Echo

These originated as concepts for specialised instruments, and our feeling is that the case for building these instruments is less compelling at the current stage. Many of their capabilities can equally well be addressed on other instruments.

While the strongest selling point of the first two instruments is in their potentially very significant new user communities, we feel that these communities could also be well served on the existing instruments by adequate staffing and the implementation of auxiliary facilities, such as biological user labs for biological SANS, or polarisation analysis on an existing powder diffractometer for the structural measurement of hydrogenous samples.

The major part of the science case for spin-echo will be addressed with the high-resolution spin-echo instrument which needs to be built before the wide-angle instrument. Experience from WASP at ILL and high-resolution spin-echo at ESS should signal if and when a wide-angle instrument spin-echo is to be built at ESS.

As such, in order to bring ESS to the full scope of 22 instruments, six of the remaining seven instrument slots are recommended to be pursued further, with the highest priority placed on a particle physics beamline and a high-resolution spin-echo instrument. A first call for proposals could focus on those two, while one or two later calls could address the other significant capability gaps. Since new ideas may yet emerge, the later call(s) should be open for these as well. At the present stage, the seventh slot should be kept open for new ideas or for one of the additional lower-priority capability gaps discussed above.

A possible layout, including the six new instruments ranked as the highest priority, is sketched in Figure 3. The GI-SANS, HR-NSE, ANNI and VOR instruments can straightforwardly be allocated beam ports in the east and north sectors. ESPRESSO was originally proposed for a slot in the 165m west hall, but subsequent analysis has indicated that a beam port in the south hall would be advantageous, providing a larger Q-coverage at the expense of slightly lower flux. The technical design for MUSHROOM is not sufficiently mature to clearly identify an optimal length. Preliminary studies indicate that an instrument length of 80m or 160m would suit it well. Since there are no free spaces in the long-instrument hall, we have placed it on a beam port providing an instrument length of 80m, adjacent to ESPRESSO.

The layout shown here does not require any modifications to the buildings or the layout of the bunker, allowing the required funding to go into the construction of instruments and sample environment equipment, rather than infrastructure.

The three instruments ranked as lower priority can also all be optimally located within the existing instrument halls.

Beyond the instruments shown in Figure 3, there remain a number of unused positions in the north, east and south sectors within the existing instrument halls, which can be used for future instruments. Positions for additional >160m instruments can be created by extending the 165m hall in the west sector on its north side, and by building a new 165m hall in the south sector. In the long term, it is expected that approximately 35 of the 42 beam ports in the target monolith can be used for instruments.

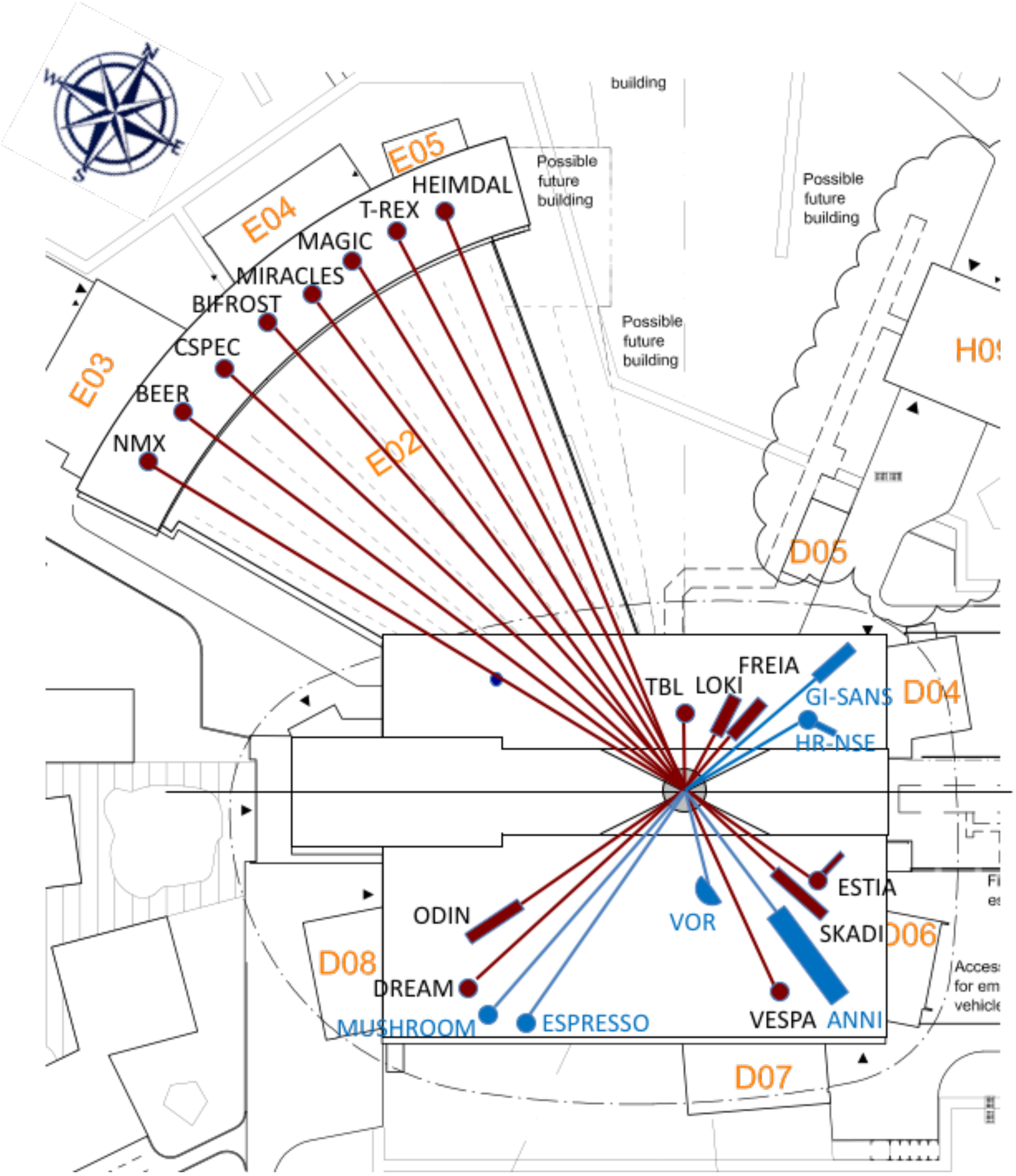

Figure 3: Tentative schematic instrument layout with the current 15 instruments shown in purple and the six highest-priority instruments listed above shown in blue.

The impact of continuing the build-out of new instruments and other capability at ESS is illustrated in Figure 4 below.

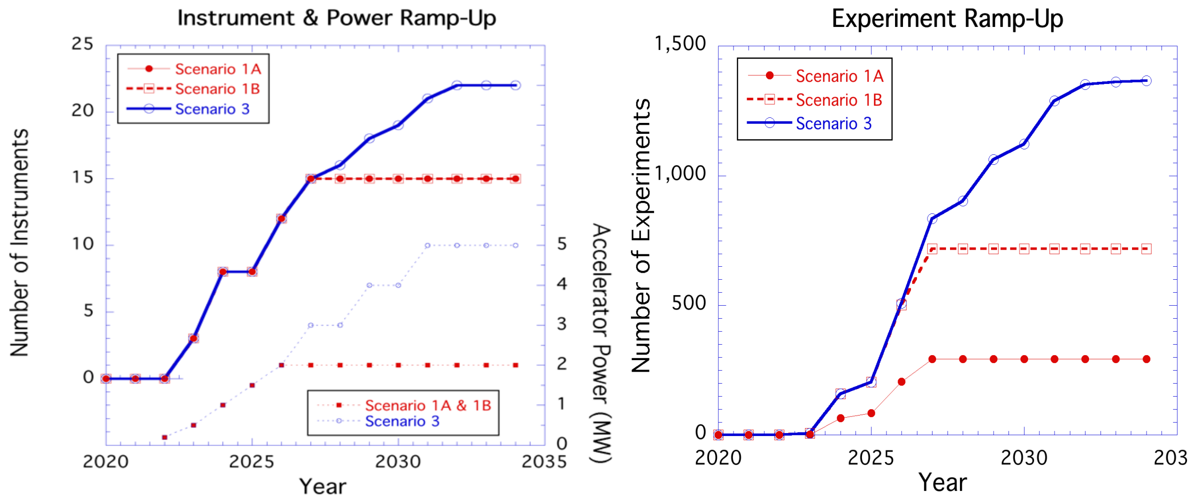

Figure 4: Evolution of various ESS parameters with time for three different funding scenarios. Left: number of instruments and accelerator power. Right: number of experiments.

These figures are based on figures from a report submitted to the ESS Council in September 2017 [8], which have been updated according to the new baseline schedule approved in the summer of 2018. They show the expected evolution of the high-level parameters and scientific output of ESS for a number of different funding scenarios:

Scenario 1A: lowest funding level: sufficient to finish construction of instruments 1-15, but insufficient to upgrade the accelerator power beyond 2MW, or to operate it reliably. Instruments 1-15 are not brought up to full-scope capability, and instruments 16-22 are not built.

Scenario 1B: same as 1A, except that sufficient operational funding is available to operate the accelerator reliably.

Scenario 3: ramp-up of Instrument Completion and new instruments, consistent with the 2018 baseline for project completion. Sufficient funding for reliable accelerator operation.

The right-hand frame of Figure 4 shows how the number of experiments performed increases with time for the various funding scenarios. As long as the accelerator is operating reliably, the number of experiments scales roughly with the number of instruments. It also uses experience from ILL to estimate how the duration of experiments is reduced when the counting rate increases, due to accelerator power increases and completion of instrument scope.

The present capability gap analysis identifies which areas the new instruments and sample environment should address. By suitably filling these gaps, ESS needs to continue to ramp up its capability and hence scientific output beyond completion of the construction project in 2025, and well into the 2030s. The construction of the additional seven instruments and the completion of the first 15 instruments, combined with an increase in accelerator power from 2 to 5 MW, will roughly cost another 9% of the current ESS construction budget. This will result in an increase of the scientific output at ESS by 100%, making this an excellent investment.

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4. An Early Success Strategy for ESS, ESS-0060903, S. Petersson Årsköld, 2013 *(this document has recently been updated)*
5. Report from NSE workshop in Copenhagen Airport Hilton 5/8/2014, Dimitri Argyriou and Dieter Richter (Chairs), 2014
6. Diffraction STAP Report, Paul Attfield (Chair), May 2015
7. R.I. Bewley, ISIS Facility, presentation at ECNS 2015
8. Report to ESS ERIC Council on Completion of Construction, ESS-0122911, September 2017

Appendix: Complete list of ESS instrument construction proposals

2013 instrument proposal round		
Compact SANS	SANS optimised for biological systems in solution	Rejected
LOKI	Broadband SANS	Approved
NMX	Macromolecular crystallography	Approved
ODIN	General-purpose imaging	Approved
2014 instrument proposal round		
BEER	Engineering materials diffractometer	Approved
Compact SANS	SANS optimised for biological systems in solution	Rejected
CSPEC	Cold chopper spectrometer	Approved
BIFROST	Extreme-conditions crystal-analyser spectrometer	Approved
DREAM	General-purpose bispectral powder diffractometer	Approved
ESSENSE	High-resolution superconducting conventional spin-echo	Rejected
ESTIA	Vertical-sample focusing reflectometer	Approved
FREIA	Horizontal-sample reflectometer optimised for fast kinetics	Approved
HEIMDAL	Hybrid powder diffractometer for in-situ studies	Approved
HOD	Crystal-monochromator diffractometer for hydrogenous systems	Rejected
SKADI	High-resolution SANS	Approved
Tempus Fugit	Rotating-crystal monochromator spectrometer	Rejected
T-REX	Bispectral chopper spectrometer	Rejected
THOR	General-purpose horizontal-sample reflectometer	Rejected
VERITAS	General-purpose vertical-sample reflectometer	Rejected
VOR	Wide-bandwidth chopper spectrometer	Approved
2015 instrument proposal round		
ANNI	Cold-neutron particle-physics beamline	Rejected
ESPRESSO	High-pressure diffractometer	Rejected
ESSENSE	High-resolution superconducting conventional spin-echo	Rejected
HERITAGE	General-purpose horizontal-sample reflectometer	Rejected
HOD	Crystal-monochromator diffractometer for hydrogenous systems	Rejected
MAGIC	Single-crystal diffractometer for magnetism	Approved
MIRACLES	High-resolution backscattering spectrometer	Approved
RESPECT	High-resolution longitudinal resonant spin-echo	Rejected
T-REX	Bispectral chopper spectrometer	Approved
VESPA	Vibrational spectroscopy	Approved

The list above covers all instrument proposals submitted in the three ESS instrument proposal rounds. In addition, the following instrument concepts were studied as part of the ESS Design Update, or submitted as Expressions of Interest or Letters of Intent:

- Small-sample SANS
- Horizontal focusing reflectometer
- Extreme environments beamline
- Thermal powder diffractometer
- Bispectral chopper spectrometer
- Wide-angle spin-echo
- Chip-irradiation facility
- n-nbar experiment
- UCN facility