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Concepts Of Operations for the Bifrost Instrument

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1. INTRODUCTION

The purpose of this ConOps is to provide a brief description of Bifrost, and its basic concept. The description includes a high-level introduction to the science case of the instrument as well as the framework and context within which the instrument will be designed, operated and maintained through its life cycle. As the scope for the instrument is not finally set, the document is to be regarded as preliminary.

The intended audience for this document includes everyone involved in the construction and operation of Bifrost, i.e. all central stakeholders. It will also serve the function as a quick overview of the instrument's purpose, construction and operation for both those familiar with neutron spectroscopy and those that are not.

The ConOps is intended to be updated several times to ensure its actuality.

1.1 Definitions, acronyms and abbreviations

ABBREVIATION	EXPLANATION OF ABBREVIATION
PBS	Product Breakdown Structure
NOSG	Neutron Optics and Shielding Group
BTS	Beam Transport and Conditioning System
SES	Sample Exposure System
SCS	Scattering Characterization System
GUI	Graphical user interface
CLI	Command line interface
EPICS	Experimental Physics and Industrial Control System
PSS	Personnel Safety System
PSI	Paul Scherrer Institute
LLB	Laboratorie Leon Brillouin
IFE	Institut for Energiteknik
KU	University of Copenhagen
DTU	Technical University of Denmark

1.2 References

[1] CAMEA - Proposal

[2] Bifrost – Preliminary Systems Design Document

[3] Bifrost – System Requirements

[4] F. Groitl, et. Al., “CAMEA—A novel multiplexing analyzer for neutron spectroscopy” Rev. Sci. Instrum. **87**, 035109 (2016)

[5] F. Groitl. Et al., “A combined radial collimator and cooled beryllium filter for neutron scattering”, NIM-A, **819**, 99 (2016)

[6] L.C. Chapon, et. al, Neutron News, 22, 2 (2011)

[7] F. Issa, et. al., “Characterization of Thermal Neutron Beam Monitors”, in review

[8] Bifrost, table of motion. Attached to the Indico page.

2. HIGH LEVEL SCIENTIFIC REQUIREMENTS (HLSR)

As indirect ToF spectrometer, Bifrost is able to use the full ESS neutron pulse and optimize flux on the sample. As a high flux instrument, Bifrost has the unique opportunity to sacrifice flux for high resolution. Hence, the scientific requirements are also based on the versatility of the instrument resolution and coverage in momentum and energy transfers. The requirements are as follows:

I. **Flux optimization for small samples and weak signals** is the most important feature of Bifrost. Small sample mass is still the main limitation in single crystal neutron spectroscopy today. Bifrost should offer at least an order of magnitude improvement *in flux alone* compared to high flux options today and in the near future. This will produce a new understanding of this broad range of materials unobtainable elsewhere, and give ESS a clear advantage when new game-changer materials are discovered, as Bifrost will be the first feasible option for dynamic studies when single crystals start to become available.

II. **Resolution optimization for complex dynamics in the entire whole cold-to-thermal dynamic range.** The unprecedented flux at Bifrost allows for entirely new options for detailed investigations of complex multimode dynamics, hybrid modes, electro-magnons, spin wave continua and gap studies. If the signals are weak or samples small, such cases are not suitable for classic ToF spectrometers. Triple-axis spectrometers on the other hand offers little flexibility in terms of resolution. Here, this is done by either reducing the final energy (limiting Q-range end high resolution E-range) or by introducing collimators (greatly reducing flux for only minor improvements in energy resolution). The resolution of Bifrost should be efficiently tuneable within an order of magnitude in energy resolution width in the 0-15 meV energy transfer range, while retaining a sample flux competitive with high flux triple axis spectrometers. This will open up a new range of science cases that lies in the terra incognita between the capabilities of ToF and TAS spectrometers.

III. **Single exposure mapping capabilities for continuous parametric studies** is another unique option that the Bifrost flux opens up. Due to the high flux, a coarse-grained overview of the dynamics of a system can be obtained in less than a minute in most cases. Bifrost should have a broad enough single exposure (Q,E) range to probe qualitative changes in dispersion relations. This allows for continuously changing a control parameter, like temperature, pressure or magnetic field, while mapping the main features of an excitation. This cannot be done today in neutron scattering since TAS' perform too localized measurements and ToF spectrometers have insufficient flux on the sample.

IV. **Strong magnetic fields on the sample** is one of the ideal uses of Bifrost. The standard split-coil magnet geometry limits the performance of direct ToF spectrometer, by reducing the spatial angle coverage and introducing background from the unavoidable sample surroundings. Bifrost compresses the capabilities of a direct ToF spectrometer into the horizontal scattering plane, and is thus ideally suited for both vertical and horizontal magnets. In addition, spurious elastic scattering events from the sample surroundings do not have an impact on the inelastic signal due to the long primary flight path. Field strength is a central control parameter in the entire field of magnetism, one of the main uses of neutron scattering now and in the future. Bifrost should be designed with the anticipation of a breakthrough in High-Tc superconductor technology in mind. Bifrost should be able to allow 35 T vertical and horizontal field on the sample. When this technology becomes available, Bifrost will immediately take the lead.

V. **The option for accessing the thermal energy transfer range** becomes an option by using the second order reflections off the analysers. This will give Bifrost access to large energy transfers at small momentum transfers and vice versa. Bifrost should allow simultaneous use of first and second order reflections from the analysers to tailor a measurement for maximum coverage in (Q, E)-space. This will give Bifrost unprecedented resolution in the thermal range, of crucial importance for a number of science cases. These include hour-glass excitations in high-Tc superconductors, and phonons in functional materials.

VI. **Polarization analysis in inelastic measurements** is still very much a flux-limited technique in neutron scattering. Here, Bifrost could excel in the future as polarized inelastic measurements become much feasible. Bifrost should plan for a future upgrade allowing polarized measurements and include for this in its initial design.

VII **Time-resolved measurements** can be possible on Bifrost. Detectors, detector electronics and software should allow event mode data and a method for synchronization with sample parameters (e.g. electrical field) should be prepared.

3. HIGH LEVEL SYSTEM REQUIREMENTS

ID	Requirement
13.6.14.r1	Using the full ESS pulse in the coarsest resolution mode, Bifrost shall have an energy resolution better than 4 % below 5 meV energy transfer
13.6.14.r2	Bifrost shall have a tuneable resolution down to 0.02 meV in the finest resolution mode
13.6.14.r3	Bifrost should be able to usefully employ an incoming wavelength band of 1.7 Å taking up the full time interval between pulses at the sample position.
13.6.14.r4	For incoming wavelengths between 2.5-4 Å, Bifrost shall have a neutron flux larger than 10^{10} n/s/cm^2 in coarse resolution mode, and 10^8 n/s/cm^2 in the finest resolution mode – at 5 MW
13.6.14.r5	Bifrost shall allow cold spectroscopy studies on samples smaller than 1 mm^3 and up to 20x20x20 mm^3.
13.6.14.r6	For an incoming wavelength of 1.2 Å, Bifrost shall have a neutron flux larger than 5 % of the peak flux in all modes
13.6.14.r7	Bifrost shall be able to measure at least 4 scattered energies from the sample in a single setting
13.6.14.r8	Bifrost should fully cover a 90 degree scattering angle interval for all analyzer energies in two settings, and be able to reach scattering angles between 10-135 degrees
13.6.14.r9	Bifrost shall have an angular resolution down to 0.7 degrees
13.6.14.r10	Bifrost shall be able to accommodate a maximum magnetic field of 35 T at the sample position
13.6.14.r11	Bifrost shall have an inelastic background of the less than 5 cts/min pr channel, for a single E_f-analyzer/detector channel.
13.6.14.r12	Bifrost should serve the user and science and instrumental development program without interruptions during source operation.
13.6.14.r13	Bifrost shall allow a safe operation for both users and bystanders

4. SYSTEM CHARACTERISTICS

4.1 System purpose

Neutron spectroscopy is the main tool for investigating low energy dispersive dynamics in materials. Cold neutron spectroscopy is the only tool in existence for probing such dynamics in the 0-40 meV range. Due to the intrinsically low signal-to-noise in neutron spectroscopy, it remains a flux limited technique, requiring large sample mass for feasibility. However, many species of materials are only grown with techniques that intrinsically yield small crystals in the milligram range, like for instance flux growth techniques or electrocrystallization. Low temperature dynamics in many of these systems are currently unobservable for this reason alone. In addition, some of the most interesting crystalline systems currently under investigation have inherently weak signals. Neutron spectroscopy today suffers from the partitioned choice between the low flux/large coverage capabilities of ToF spectrometers and the high flux/low coverage capabilities of triple axis spectrometers. These choices are united in the Bifrost spectrometer while increasing flux on the sample by an order of magnitude compared to the best options today. This allows for Bifrost to function both as a workhorse instrument and as a first feasible option to study low energy dispersive dynamics when small single crystals start to become available of the materials to be discovered in the future – a clear competitive advantage for the ESS. The science scope of Bifrost contains - but are not limited to – the following cases:

- **Excitations in unconventional superconductors:** Weak spin fluctuations in the high-T_C cuprates, nesting vectors in pnictides, excitations in heavy fermion superconductors. Suffering from intrinsic weak cross sections, they will benefit greatly from Bifrost flux.
- **Excitations in frustrated magnets.** Many frustrated magnets have reduced moments and/or intrinsic disorder like spin liquids, resulting in weak signals. Some frustrated magnets cannot form large single crystals using known techniques. Bifrost will greatly impact this important field of magnetism.
- **Low dimensional magnets/quantum magnets** are systems with the main dispersive features residing in a single scattering plane, and which is usually investigated in applied fields and/or pressure. Bifrost is an ideal tool for these problems.
- **Strongly correlated electron systems** exhibiting for instance charge order and spin density waves, often suffer from weak scattering cross sections. Flux is paramount to investigate these materials with neutron spectroscopy
- **The study of materials under extreme pressure in geoscience** becomes possible at Bifrost. With the high flux, elegant screening of background from sample environment close to the sample and the good elastic resolution, Bifrost can study quasielastic dynamics in the GPa pressure range.
- **Functional materials** are also of interest to Bifrost. Many multiferroic materials of interest have many different phases and the fast aquisition rate of Bifrost makes it ideal for parametric studies.

4.2 System Life-Cycle

The figure below shows the life cycle of Bifrost on a high level schematic and without the details of the corresponding further detailed development phases. Each phase of the instrument development is concluded with a TG review, with accompanying design review.

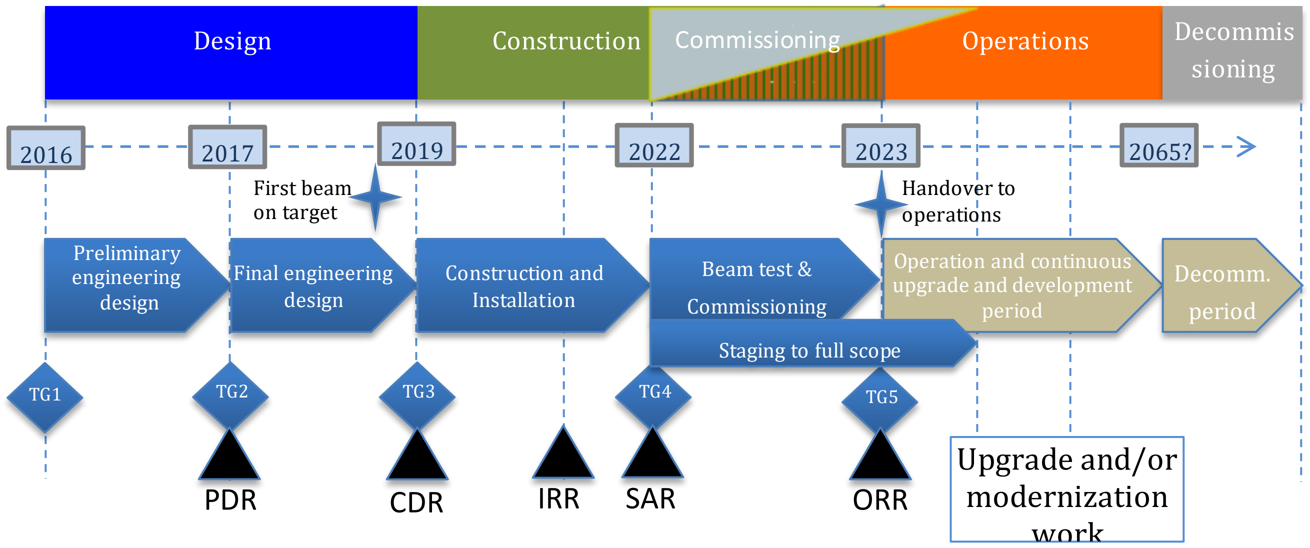

Figure 1. Schematic Bifrost Instrument Development process and its related life-cycle

The schematic process above is a simplified depiction, as in reality, there are overlaps between the seemingly distinct separations of the phases. For example, the design of details lingers on until very late, if not until the end of the construction and long lead-time items have to start tendering and production in the design phase and have to be developed with companies hand in hand with the final design. The Instrument Development process provides the framework within which the instrument will be developed with timely milestones in order to measure progress, still allowing the overlap to exist. The controlling document for the instrument development is: Process for Neutron Instrument Design and Construction: ESS-0051706.

The commissioning for Bifrost is an extended process specific for this instrument, as the basic design is completely new. The reach out to the user community and achieving full scope has to be a process, where a gradually better understanding of the instrument precedes gradually more challenging experiments. As Bifrost aims for experiments infeasible anywhere else, it is important to keep track of and develop feasibility and present working solutions to the user community. The central commissioning challenges are the following:

- **Understanding the background:** As the flux is unprecedentedly high at Bifrost, sources of background insignificant anywhere else, become important. A thorough and systematic examination of the background, and the resulting shielding decisions, are essential for an excellent instrument.

- **Understanding the flux/resolution relationship:** The achievable resolution needs to be verified, and the trade-off between resolution and flux needs to be verified to allow users to evaluate feasibility precisely. This is a challenge at Bifrost due to the unconventional design of both the primary and secondary spectrometer. Accurate feasibility estimates are paramount for Bifrost, as the instruments serves to move the feasibility boundary for neutron spectroscopy in general.
- **Understanding and suppressing spurious signals:** Spurious signals will be present at Bifrost, but many can be suppressed by proper shielding and the BE-filter. Nevertheless, spurions need to be identified and handled before the most challenging experiments.

Commissioning of Bifrost is to be overlapped with user operation as the most feasible and straightforward experiments will improve the understanding of the instrument further.

4.3 System overview

4.3.1 General

Bifrost is subdivided into the following generic main functional blocks:

- Neutron guides
- Shielding
- Chopper system
- Shutters
- Cave
- Beam stop
- Secondary spectrometer tank
- Collimators
- Magnet
- Personnel Safety System, PSS
- Control hutch
- Instrument control

All of these have to be defined and designed to enable the high level requirements as the basis for the detailed functional and non-functional instrument and component requirements (See Bifrost system requirements description).

For a detailed description of the preliminary systems design, consult the preliminary systems design report.

4.3.2 Neutron Optics System (PSI)

The neutron guide system has to transport a large bandwidth in the cold-thermal range 160 m to the sample position, while still accepting a large divergence. While beam symmetry is important, beam homogeneity is desirable but not paramount. To optimize chopper performance and reduce shielding costs we have chosen a guide with a virtual sources at the first chopper, followed by a curved narrow guide that looses LoS within the bunker. Before the first chopper at 6.45 m, there is a feeder in the monolith insert, taking in an appropriate phase space and creates a 25x50mm^2 VS for the first chopper. . In the bunker, we surround the guide with copper collimator blocks in the guide housing, which drastically reduces the prompt pulse flux at the bunker wall interface. As a whole, this design reduces gamma-shielding costs outside the bunker. Upon exiting the bunker, the guide ballistically expands into a straight wide section with low m-value and low divergence. This wide straight section continues in most of the E02 hall. 15-20 meters before the sample there is a parabolic focusing section. See figure 2. As a whole, this design reduces gamma-shielding costs outside the bunker.

The guide system is dependent on precise alignment and stable coating in the fierce high radiation environment near the monolith. The guide is a static installation not requiring heavy maintenance, although gold foil measurements needs to be done to check guide throughput at regular intervals on at least a bi-yearly basis.

Other parts of the optics systems include:

The divergence jaws. These variable slits are placed near the last focusing section to control the divergence of the incoming beam.

The get-lost tube. This is an evacuated flight tube after the sample position to transport the direct beam to the beam stop. This is to minimize the air scattering from the unprecedentedly intense direct beam creating increased background on the detectors.

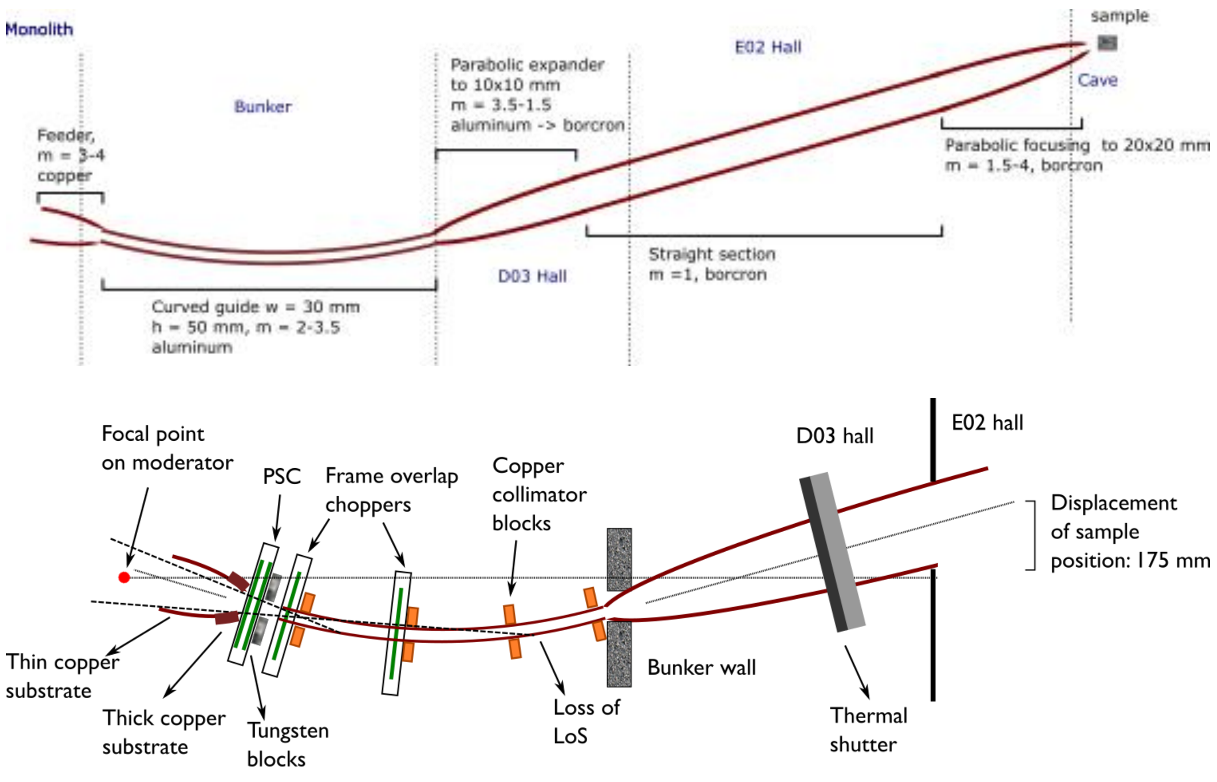

Figure 2, Guide and prompt pulse suppression in Bifrost

4.3.3 Prompt pulse suppression

Since we employ a narrow curved guide losing LoS in the bunker, we are able to employ the prompt pulse strategy utilized at NMX and validated by Valentina Santoro in a recent work. Here, a set of copper collimators less than 500 mm in length are placed in strategic places surrounding the guide in the vacuum housing. This allows for a drastic reduction in prompt pulse flux at the bunker wall, and hence removes the need for a heavy shutter. The only serviceable component downstream of the bunker is at 80 m's, which is far enough away from the last copper block for it to be safe from a large fast neutron dose.

4.3.4 Shielding (IFE)

The shielding for Bifrost can be divided into 4 categories designated from the monolith to the sample position

Within bunker: This includes shielding for choppers, for neighbouring instruments and the steel for the bunker wall insert.

Fast neutron shielding: Just outside the bunker, the fast neutron flux is expected to be high enough to need considerable shielding. This will be mainly steel and concrete and most of the material will be concentrated between 30-50 m from the moderator, constructed in hall D03

Gamma shielding: Gamma shielding of the guide is necessary all the way to the last curved section. However, due to the parallel beam in the long straight section and the low m-value, the neutron loss will be low, and hence the gamma flux in the E02 hall limited. Hence, the gamma shielding can be made entirely out of concrete. Small modular blocks of concrete is preferable due to craning limitations and mold prices. This shielding will be constructed in the guide hall, E02.

Secondary spectrometer shielding: At the last curved section of the guide, the gamma intensity will be extremely high due to the high m-value. This needs dedicated shielding efforts to reduce the gamma flux on the secondary spectrometer, possibly a combination of steel (or lead) and concrete. The magnetic impact of this shielding is paramount due to the forces of a possible high field magnet.

4.3.5 Chopper System (LLB)

The chopper system is central to the Bifrost instrument as it determines the energy resolution of the instrument and provides sets of clean, white and non-overlapping pulses to the sample. The chopper system as a whole is one of the most important parts of the instrument and the most vulnerable.

The choppers are classified by their function into Pulse Shaping Chopper (PSC), Frame Overlap Choppers (FOCs) and a Bandwidth Chopper (BW). Their respective function is as follows.

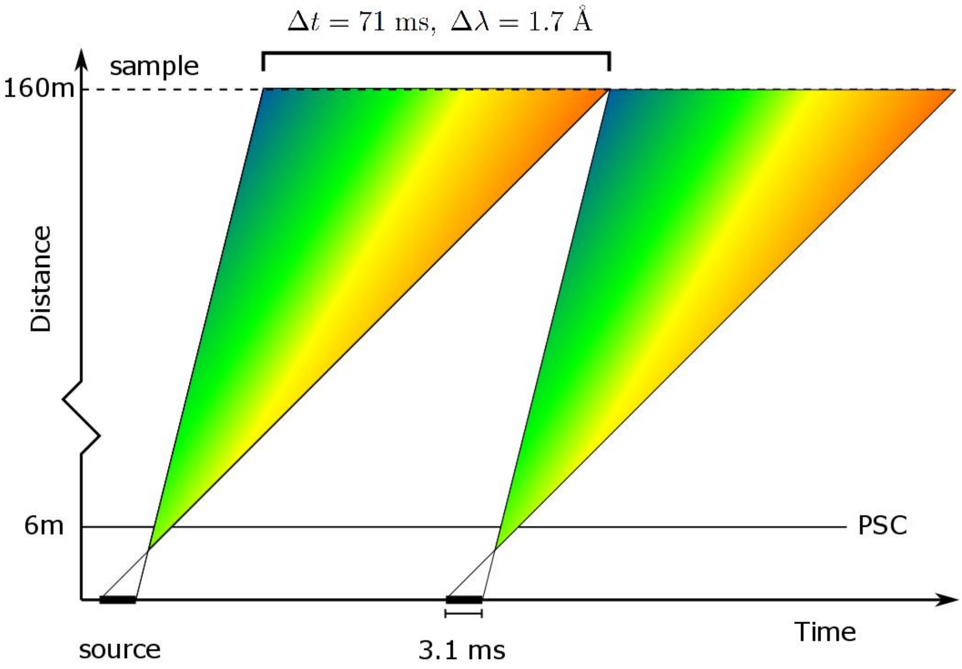

Figure 2. Basic principle of the chopper relevant for the resolution of the Bifrost primary instrument.

Pulse Shaping Chopper (PSC): The PSC is paramount for the energy resolution of Bifrost, as it determines the wavelength uncertainty at the sample. The PSC can allow the full ESS pulse of 3.1 ms to reach the sample, but also reduce the pulse width by a factor of 30 – to match the best analyser resolution – down to 0.1 ms. In order to achieve this, we employ a co-rotating double disc chopper where the relative phase and speed of rotation can be varied, to allow for full flexibility. The opening of each disc should be 170 degrees, and the frequency range 14-210 Hz. This allows for flux flexibility in terms of flux/resolution optimization.

Frame Overlap Choppers (FOCs): If the PSC spins with a high frequency, there will be a contamination from the slow part of the neutron velocity distribution. To remove this, we place 2 slow boron choppers in the first guide ellipse rotating at 14 Hz. In unison, these can remove the slow neutron contamination completely.

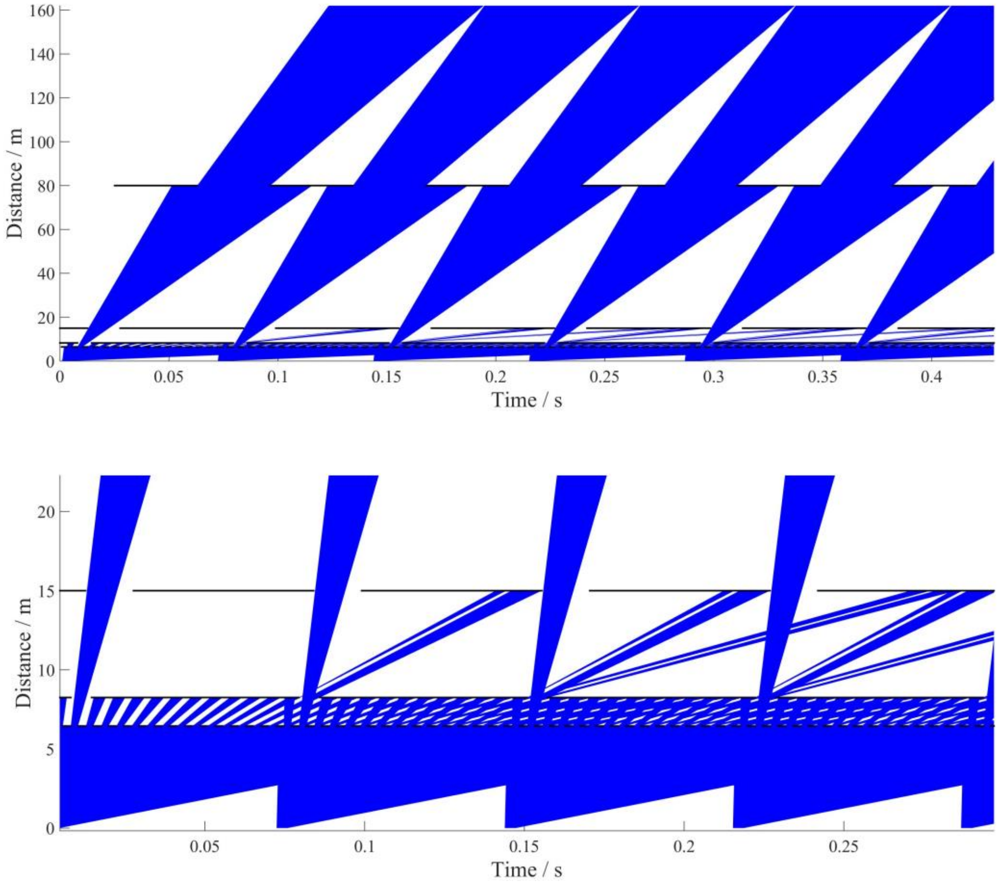

Figure 3 ToF diagram for the chopper system in a worst case setting of maximum speed (210 Hz), maximum opening (2.25 ms). (Top) Full beamline. (Bottom) Bunker and frame overlap

Bandwidth chopper (BW): To ensure non-overlapping frames, a slow boron chopper is placed 100 m downstream from the moderator. The placement is placed this far downstream to minimize shadow effects, affecting the resolution at the pulse edges. The BW should run at 14 Hz.

In total, we have a simple chopper system, controlling the wavelength interval and temporal resolution of the white beam on the sample, ensuring clean a non-overlapping frames, see figure 3. The risk of this chopper system is mainly carried by the PSC, being the most crucial and most challenging component, which sits close to the moderator in a high radiation environment. The PSC CHIM will be a single evacuated component, but the FOCs are foreseen to be connected with their vacuum housings with no windows to the guide system, hence sharing the same vacuum system. The BW chopper will not share vacuum with the guide system as it is not foreseen to save vacuum windows. For shared vacuum, we employ a horizontal split CHIM.

4.3.6 Shutters

Due to the loss of LoS in the bunker, no heavy shutter is needed for prompt pulse suppression. 10-15 m’s downstream of the bunker wall, we place a thermal neutron shutter allowing access to the BW chopper pit in the E02 hall. In addition, a minor lead gamma shutter is envisioned before the cave, to ensure safe operation during the many sample changes on Bifrost.

4.3.7 Cave (IFE)

The cave for Bifrost poses a challenge. It needs to be able to shield a very large flux of neutrons or gammas if the primary beam is scattered or absorbed by accident. In addition, no large quantities of steel are to be used, as a magnetization of such steel would impair performance when a polarization option is realized. The cave has to be large enough to allow access to the magnet – including magnet replacement - and full access to the analyser tank for maintenance. Since the analyser tank is placed on one side of the primary beam path, the cave is displaced to that side with respect to a centring on the beam axis.

4.3.8 Beam stop (IFE)

The unprecedented flux of Bifrost allows a unique option to increase the signal-to-noise, since fast neutron background will not necessarily be the main contributor. To achieve this, we employ a beam transport vacuum tube from the guide end point to the sample and from the sample to the beam stop. The beam stop is large and placed outside the cave. It consists of a conically shaped borated BE piece shielded with lead. The reflected neutrons from the boron insert is reduced by a Gd2O3 coated aluminium grid in from of the insert. This beam handling reduced air scattering from the intense beam and the gamma count rate in the detectors. If a magnet is properly shielded, the fraction of the direct beam producing inelastic background can be reduced by an order of magnitude.

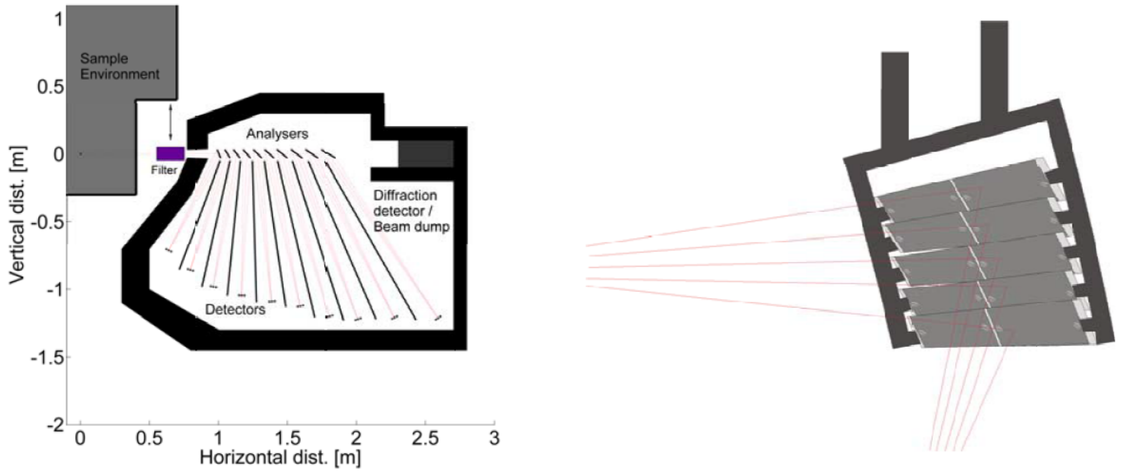

Figure 4 Outline of the spectrometer tank and the analyser setup of Bifrost

4.3.9 Secondary spectrometer tank (DTU)

The secondary spectrometer tank (SST), contains the entire energy analysis apparatus after the sample. These consist of the Beryllium filter, the analysers and the detectors. To reduce noise from air scattering, the SST is to be evacuated. To accommodate most magnet geometries, the SST is at its widest below the sample with the analysers scattering downwards. To identify Bragg peaks, a diffraction detector/monitor in the line-of-sight of the sample could be implemented. The three sub-components are elaborated below:

Pyrolytic graphite analysers (PSI): The PG analysers utilizes Bragg's law to reflect a single wavelength onto the detector, which is placed at the appropriate angle. The take-off angles and therefore the accepted wavelengths of the analysers are fixed. Due to the transparency of PG at long wavelengths, several analysers are placed behind each other, downstream from the sample, each accepting a different wavelength. This fixed multianalyzer approach is stable – with no moving parts – and very efficient. For each scattering angle, six scattering triangles are measured simultaneously, as the Ef varies and exhaustive information is recorded in the horizontal scattering plane. The various PG analysers in the same channel is dimensioned as to cover the same spatial angle, which leaves the analysers furthest from the sample the largest. Since the analyser positions are fixed, mechanical prealignment is necessary.

Table 1 Analyzer specifications for Bifrost

Analyser energy	Distance from sample [m]	Take-off angle [deg]	2-Theta coverage [deg]	Total area of analyser [mm^2]
2.7 meV	1.05	55.11	4.6	6075
3.0 meV	1.13	51.09	4.85	7360
3.4 meV	1.21	46.97	5.1	8840
3.9 meV	1.32	43.04	5.35	10738
4.4 meV	1.42	39.98	5.6	13230
5.0 meV	1.52	37.07	5.85	15960

Detectors (LLB): The standard He-3 tube detectors are placed entirely in a horizontal plane near the bottom of the tank. The detectors need at least 1D position sensitivity perpendicular to the sample-analyser axis to allow the prismatic analyser concept to be implemented. A possibility is to cover an entire tank section with radially arranged detector tubes for full coverage. The detector electronics are placed outside the SST. The detector electronics carries some risk. The main risk is failing vacuum pumps increasing the pressure inside the tank. Due to the high voltage on the detector, sparking may occur. Another risk are strong Bragg peaks, overloading the detectors. This could result in anode wire breakdown and fast detector wear. To remedy this, we implement either a failsafe mechanism in the detector electronics or a mechanical attenuator system.

Beryllium filter (PSI): The nature of Bragg's law allows not only the desired wavelength to be accepted by the system but any fraction of it as well. This can be exploited directly when an upgrade allows for an order-sorting chopper. However, since the raison d'etre of Bifrost is cold neutron spectroscopy, the high-energy neutrons emitted from the sample need to be blocked to minimize background and remove the so-called second-order signal. Since the transmission function of a Be filter is a step-function with a cut-off at 5 meV, Be-filtering is an ideal method to achieve this. Large beryllium blocks of minimum 10 cm depth downstream from the sample are necessary. To allow for a future, order-sorting upgrade, the Be-filter needs to be translatable out of the beam path. Either the Be-filter is placed inside the vacuum tank to exploit the vacuum efficiently or an external Be-filter is built. The beryllium need to be cooled to liquid nitrogen temperatures to function properly.

4.3.10 Personnel Safety System, PSS (ESS WP)

A PSS system will be designed and provided by ESS and the instrument team to allow safe operation concerning access to the instrument and its components.

4.3.11 Control Hutch (DTU)

A control hutch will host remote control equipment, computers and the experimentalists during measurement times. Close to the control hutch there should also be a sample preparation area with the most common tools in neutron scattering.

4.3.12 Instrument control (DTU)

Most instrument components will require remote control through specific electronics placed outside the shielding but connected to the components inside and to the control computers. The main parts of the instrument control include: Control of sample environment, control of sample and analyser tank rotation and control of chopper system.

4.3.13 Future upgrade possibilities

At present three potential major upgrade options have been identified:

Order sorting:

When the fixed set of measured wavelengths in the SST are in the long wavelength regime, instrument performance is impaired at very large energy transfers. This is due to an imbalanced scattering triangle that reduces the Q-range to relatively limited intervals centred on the incoming neutron momentum. Since the Bifrost guide transports a useable flux of thermal neutrons to the sample, efficiently utilizing the thermal neutrons is an ideal upgrade for Bifrost. This allows for both low- and high-Q measurements at large energy transfer. In order to achieve this, we can make use of the second order low wavelength reflections off the analysers to balance the scattering triangle at high energies. This rules out the use of a Be-filter, which should be translatable out of the scattering plane. Since the analyser system now effectively accepts two wavelengths per analyser, an order-sorting chopper just before the sample is mandated. This chopper serves to create gaps in the time structure of the primary beam, so the short and long wavelength neutrons scattered from the sample can be separated into two non- overlapping frames. This upgrade requires the following investments: Order sorting chopper, additional chopper shielding and additional PG analysers. Furthermore, labour is needed to handle the spurious signals at short wavelengths. To allow for this upgrade, we need to build a large SST to accommodate additional analysers and design the guide and shielding to accommodate the order sorting chopper and accompanied shielding.

Polarization analysis:

With the unprecedentedly large flux of Bifrost, an obvious and powerful way to upgrade is to build a polarization analysis option. Polarization analysis usually reduces the recorded signal intensity by an order of magnitude, which drastically reduces the feasibility range of polarized spectroscopy in the majority of cases. Bifrost can provide a feasible option for polarized spectroscopy in a plethora of cases infeasible today. Many options remain for implementing this, including S-bender polarizers, He-3 polarizers and removable Heussler polarization analysers. The details of this upgrade are to be worked through in Phase 2. However, the cave needs to be designed in a way such as minor magnetization of shielding material and impurities therein does not affect the polarization in a major way.

High field magnet:

Since the minor technical revolution of high-Tc superconducting wire occurred in 2007, high temperature superconducting magnets have started to surface as a possibility for scattering experiments. Already, 25 T split coil versions have started to appear in technical design studies. These magnets are currently very expensive, and requires dedicated design studies spanning many years of research. However, a split coil magnet for Bifrost with a maximum field of 25 T or above will have an enormous impact on the field of magnetism and superconductivity. Not only is the parameter space almost doubled compared to previous options, but also Bifrost will be the most powerful neutron spectrometer in the world and it can accommodate such a magnet with no loss of functionality whatsoever.

4.4 Key system interfaces

Key interfaces have to be considered carefully in order to embed Bifrost in an environment and context, which enables its optimisation and finally operation and efficient operation. Key interfaces to the following systems are outside the scope of Bifrost.

4.4.1 Target system

This interface concerns the beam extraction guide system and its interplay with the monolith in terms of geometry, cooling and atmosphere, the utilized moderator and its influence on performance and guide optics. In addition, the service shutter as part of the target monolith hosting a piece of the guide system performs a vital function for the operation and maintainability of Bifrost.

4.4.2 Bunker

A large number of key instrument components will be placed in the shared bunker, which in Bifrosts instrument sector (west) extends from the monolith wall at 6m out to 28m with a wall thickness of 3.5m, which implies that no choppers can be positioned between 24.5 and 28m from the source. Interfaces with the structure, floor, columns, construction time plan etc. have to be considered and clarified with the bunker system in the design and construction phase.

4.4.3 CF

This interface and external system defines parameters like the floor and ceiling heights, crane access, space for paths and infrastructure of the instrument, which are all of significant importance for the construction, operation and maintainability of the system.

4.4.4 Neighbouring instruments

There are significant physical interfaces with neighbouring instrument systems in terms of space occupation, which in particular close to the monolith and in the area of the end station have potential impact on the performance, availability and maintainability as well as operational access of the involved systems.

4.4.5 ICS

ICS is an important provider of key input and services for the instrument operation and in the current planning is hence vital to the instrument operation as it provides the source timing input as well as it records and transports key instrument data, without which the instrument becomes non-operable.

4.4.6 DMSC

The data management and software centre also provides key services and systems for the instrument in the form of control, reduction and analyses software, without which the instrument cannot be operated and exploited for its central mission. Hence, it has to be guaranteed that the provided software and data solutions meet the requirements of the system to function in the foreseen and useful way also for third party users. For Bifrost in particular, the data analysis and visualization is a challenge – close collaboration and possibly additional contributions are foreseen.

4.4.7 SAD

The SAD provides the instrument with the indispensable services of the user office handling user requests and beam time proposals, hence organizing the access of users required for the scientific productivity of the system according to its purpose. In addition, SAD is administrating and maintaining the common sample environment, which is especially indispensable at Bifrost. As Bifrost might employ a limited geometry magnet in the future, such equipment will be coordinated and maintained by the SAD group.

4.4.8 Maintenance and service groups

The integration and application of standards and corresponding solutions as well as access strategies and maintenance requirements and schedules have to be agreed with technical groups to the extent possible. In order to enable the services needed or best possible enabled through these for a high availability of the instrument system.

4.4.9 Radiation protection

The samples to be used at Bifrost have often taken months or even years of manpower to produce, and are non-disposable. The very high flux at Bifrost will render may samples very active, for hours after the experiments and possibly for years. A key interface of Bifrost is to the radiation protection team. Partly to ensure a good protocol for handling user samples and for identifying possible problems in advance.

For a preliminary safety analysis, see the preliminary systems design document, chapter 12.

4.4.10 Others

Other interfaces of the system in construction (c) and operation (o) are amongst others with users (o), industry (c,o), public relations (c,o) and other instruments (c,o). Of special importance for Bifrost is a local sample characterization lab near the ESS, capable of measuring heat capacity, magnetization and electric polarization at low temperatures and high fields. Such support labs are central for attracting users with high impact projects, but limited local infrastructure.

5. SYSTEM STAKEHOLDERS

This paragraph is dedicated to the stakeholder analysis. The governance structure for the Bifrost instrument is outlined in the Work Package Specification. It is not unlikely that a general level Stakeholder Analysis is more suited to be incorporated in a higher level ConOps, especially for parts of the analysis that are common for all instruments. The ConOps at the instrument level could instead focus on the unique areas of the instrument in the stakeholder analysis.

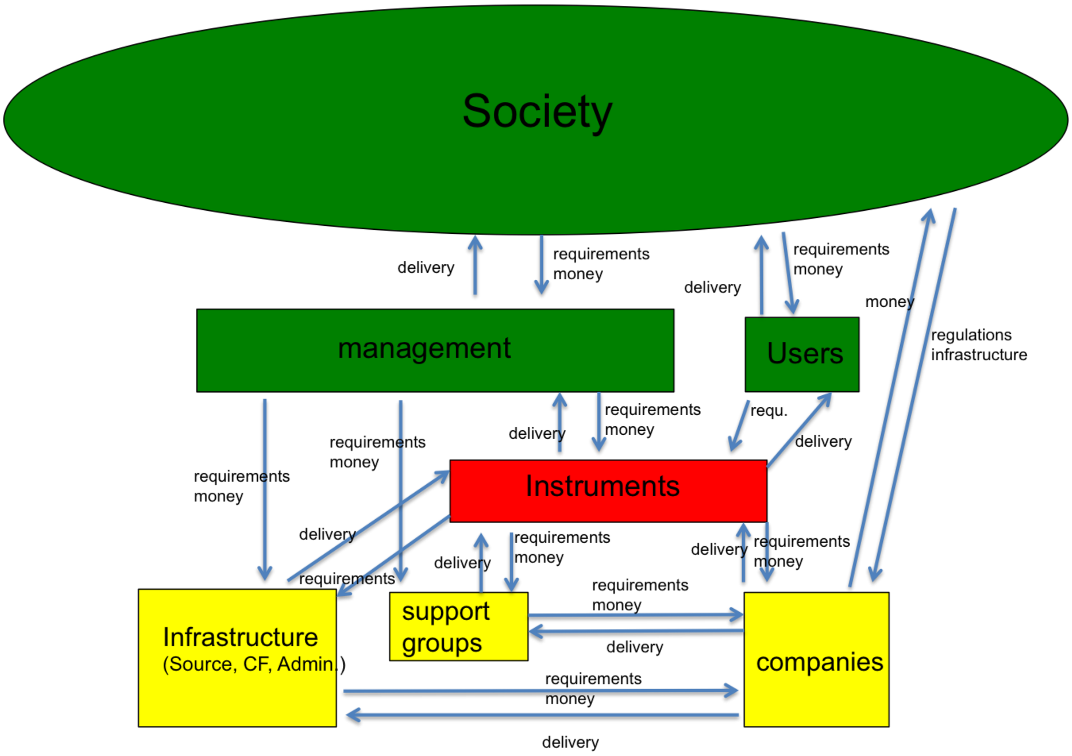

Figure 5. Generic stakeholder schematic overview

Table 2. Draft generic stakeholder list with respect to the three main life-cycle phases

Stakeholder classification	Stakeholder	design and construction		operation		decommissioninhg		Related, as applicable, NSS system requirement/-s	Comments
		Involvement/provides	Involvement/receives	Involvement/provides	Involvement/receives	Involvement/provides	Involvement/receives		
stakeholders of system purpose	Society/Government/Funding Organisation	requirements of progress and development, new materials; money to enable corresponding research to construct large scale research infrastructure (ESS)	research infrastructure	requirements of progress and development, new materials; money to enable corresponding research to universities (users) and large scale research infrastructure (ESS)	operational research infrastructure and research results, new materials and know-how				
	Management	efficient use of budget for addressing agreed science case to funding body, requirements to fullfill respective defined needs and corresponding shares of money to parts of organisation	budget from society/government, functional and productive cutting edge user instrument from instrument scientist, infrastructure requirements from instruments, required infrastructure from corresponding parts of organisation	efficient use of budget to funding body, requirements to fullfill respective defined needs and corresponding shares of money to parts of organisation	budget from society/government,scientific poductivity, stable operations, upgrades to keep up with development and needs				
	User	scientific requirements, cutting edge science case, corresponding advice	cutting edge instrumentation made available for their science case	scientific requirements, cutting edge science case and measurement plan	beamtime, high performance and reliabilit and scientific and technical support, high quality data				
Instrument scienists (stakeholder of purpose and with support function)	Instrument scientists	system (construction to agreed specifications, performance and reliability), support requirements and pays for necessary support and production	budget from management and support from supporting stakeholders (partly against payment)	operation, user service, upgrades, support requirements, availability, payment for support, scientific results	support required for operation, budget required for operation (including required support) and agreed system upgrades				
stakeholders with support function only	Instrument engineer(s)	engineering support to the construction process	functional and non-functional requirements from instrument scientist and standards, boundary conditions from support groups and other systems at interfaces	n.a.	n.a.				
	Technology and other Support Groups (e.g. vacuum)	support infrastructure and capacity development, standards, technical advice, technical support	budget and requirements from management to build up support infrastructure and develop standards, budget from instruments for technical support	maintain support infrastructure and capacity, provide maintenance and support	budget from management to maintain infrastructure and cpacity, potentially budget from instrument to provide maintenance and support (tbc), maintainability and access full documentation and specification of systems to be maintained when required for support				
	DMSC	software development required for instrument control, data reduction and analyses, and development of data transfer storage strategies and capacities	requirements from management and instrument, budget from management	maintain and further development software required for instrument control, data reduction and analyses, and maintain data transfer and storage capacities	requirements from management and instrument, budget from management				
	RAMI	policy targets for availability	support from management						
	ES&H	policy targetsand standards concerning health and safety, PPS system design	budget and requirements from management and regulatory authority, budget from instrument for PPS	maintenance and control of PPS and savety relevant systems	budget from management, requirements from management and instruments				
	Facility Infrastructure (including source, administration, CF, user office etc.)	sufficient planning and performance as well as interface coordination with respect to the requirements of the facility in general and the instrument system in particular	requirements, budget	sufficient performance and availability of all required systems for instrument operation and efficient exploitation	requirements and budget				
	suppliers	components, products and services, to facility and instrument; taxes and jobs to society	requirements, specifications, payment by facility and instrument; infrastructure etc. from society	components, products and services	requirements, specifications, payment				
	regulatory authority	safety and other relevant requirements, licenses	budget from government, system and process specifications from ESS as required	controls	budget				

*partners are not specifically mentioned, as depending on the partnership they take one or several of the stakeholder roles

6. OPERATIONAL CONCEPTS

6.1 Operational environment

It is envisaged that Bifrost is allocated the beam port W4 in building designation E01.

The instrument will be operated in a controlled environment with a temperature of 22±2 °C all year round. The floor height in E01 is 3 meters below target centerline. Free height to lifting hook of the overhead gantry crane is maximum 10 meters. Floor loading in E01 must not exceed 20 ton/m^2. Floor stability in the hall is specified to be maximum 3 mm w.r.t elastic movement and another maximum 3 mm due to creep/deformation.

In D03, utilities and media are brought to the instrument from the service gallery, while in E01/E02 this is available on the wall between E01 and E02. Media include: N2, instrument grade compressed air, cooling water low. Utilities include: office IT, office comms, Power, PSS, DMSC and ICS. For detailed and updated listing of requirements and/or specifications related to operational environment see ref xx. Details for e.g maintaining the stable temperature in the experimental hall are still in development but one suggested solution could be to place ventilation hoods directly above instrument equipment generating most heat. Which then could have an impact on selection of location of such equipment and thus considerations for this need to be made.

The ESS facility has 5 different operating modes, ref [ESS-0003640 Conops]: Shutdown, Studies, Studies on Target, Startup and Production. These modes have various impact on instrument operations. Pure experimental work can only be conducted during ESS-mode Production. Access to instrument equipment for maintenance, calibration, cold commissioning is mainly done during shutdown, studies and studies on Target – naturally after due safety assessment - is still possibly with some restrictions. During start-up instrument operations is limited to alignment, commissioning and calibration runs.
When ESS has entered into a steady-state operations phase the following principal schedule is currently expected to apply:

- 200 days/year of neutron Production for the ESS users after 2026,
- Proton beams will be on target for ~225 days/year,
- Two long Shutdowns, one in winter (~6 weeks) and the other in summer (~10 weeks) followed by Studies and Studies on Target periods,
- 3 Optional Studies Days every second week to avoid long down time of instruments due to failures of activated components, followed by 2 days for Studies and Studies on Target,
- A series of Studies days to allow for fine-tuning of accelerator and target systems.
- 160 days/year of user operation

One goal of ESS is to ensure that at least 90% of the users receive a neutron beam allowing them to execute the full scope of their experiments. This is in accordance to the availability and reliability assessments made in ref [ESS-0017709 and ESS-0008886].

The Bifrost instrument is foreseen to be managed and operated by a team of 3 scientists and 1 engineers. ESS will be manned 24 hours/day, 7 days a week in neutron production mode. This manning of the instrument will ensure flexibility, enough manpower for analysis participation and many different experiments with different scope.

6.2 Operational scenarios

Although Bifrost can be operated in a vast variety of modes the following principal generic steps are required performing a measurement:

Scenario 1: Instrument preparation and sample environment installation (beam on or off, shutter closed, cave accessible)

- Setting the primary instrument parameters for a specific experiment including choppers, slits, pinhole etc. remotely via control computer and software
- Mounting the sample environment through the roof with the E01 Hall crane, and move it inside the cave with an internal crane.
- Setting up sample environment power supplies to the instrument control, checking sample rotation motor, test ramping of field, temperature or pressure
- Checking filter temperature, tank rotation and removing possible beam obstruction.

Required staff: instrument scientist & technician (if available), SAD scientist

Scenario 2: Hot characterization (cave closed, shutter open, beam on)
- Elastic mode measurement with attenuation and standard vanadium sample, double check of energy resolution and intensity – possibly resulting in a count normalization file.
- Powder sample measurement with attenuation, check tank rotation calibration check sample rotation reproducibility and check the Bragg peak overload safety system.
- Allow for short time to customize magnet shielding to reduce inelastic background.

Required staff: instrument scientist & technician

Scenario 3: Prepare sample for measurement (Shutter closed, cave accessible)
- Double check sample mount, apply extra shielding for sample holder if needed.
- Consult with SAD scientist regarding temperature range if dilution stick is used.
- Consult with SAD scientist when pressure cell is used
- Mount the sample in sample environment and prepare for beam.

Required staff: Instrument scientist, SAD scientist, user

Scenario 4: Sample set-up and alignment (cave closed/opened, shutter open/closed, beam on/off)
- Measure with attenuator in elastic mode, to find Bragg peak and align the sample.

- Possibly pull out the filter, go to 2nd order elastic mode and use 2nd order for alignment and record many Bragg peaks, with attenuator
- Setup and prepare visualization and analysis software
- If possible/desirable, measure high temperature phonons for normalization

Required staff: User and instrument scientist

Scenario 5: Measurement (cave closed, shutter open/closed, beam on)

- Perform test measurement to determine optimal scan time
- Decide on scan range, either in rotation angles or sample environment parameters, and prepare appropriate script to run automatically.
- Perform on the spot analysis of test measurement to identify possible spurions and check fitability of the recorded dispersion surface.
- Sample environment variable are monitored automatically, and the instrument responsible is automatically notified if the parameters are outside specified tolerances.
- During the experiment, the instrument responsible is present and participates in the analysis – to make sure the data is of the sufficient quality and to help the users with invariably unconventional analysis tools.
- At the end of the experiment, the data is transferred to the user cluster and remote access given to the user – instrument responsible makes sure at least 1 member of the user team can employ the Bifrost analysis package

Required staff: User, instrument scientist

Scenario 6: Sample removal (cave open, shutter closed, beam on/off)

- Sample dose is monitored in the minutes/hours after beam off by the instrument scientist following guide lines from the radiation protection.
- After cooling down, the sample is removed by the instrument scientist
- Upon agreement with radiation protection, very hot sample are removed by specialized staff.
- Sample is labeled and stored in a centralized lab or cabinet.

Required staff: user, instrument scientist

Scenario 7: Data analysis

- The Bifrost on-site analysis package give the user an overview of the data, unrefined results, data quality, etc
- The user prepares an experimental report to be submitted internally
- The user employs the ESS cluster from his/her home institution to analyze the data in greater detail – with the help of the instrument scientist – to achieve publication worthy results.
- The instrument scientist is available for the use to consult regarding analysis and data evaluation

Required staff: User, instrument scientist

6.3 Maintenance Concepts

6.3.1 Levels of maintenance

Within ESS, there are three identified levels of maintenance, see ref [ESS-0003640]:

1. Organizational maintenance: maintenance performed on site where the element is normally being operated,
2. Intermediate maintenance: maintenance performed on site at a dedicated workshop,
3. Supplier maintenance: maintenance performed off site at the supplier premises.

The term supplier includes In-Kind partners.

6.3.2 Maintenance categories

Maintenance can be divided into two categories: Corrective and Preventive. By utilising condition based monitoring, taking into account the overall ESS operational schedule, preventive maintenance on instruments is aimed to be conducted during the planned facility shutdown periods unless instrument reliability and availability are sacrificed. This will minimise disruption to user operation.

Preventive maintenance is part of scheduled maintenance which also include maintenance work to be conducted on equipment where condition based monitoring cannot be achieved. Performed instrument reliability analysis, part of RAMI work, aims to ascertain that preventive maintenance on this type of equipment/components could be limited to periods of scheduled shutdown of the facility. Maintenance and monitoring requirements of critical components will be taken into account in design and procurement of equipment from the beginning.

Corrective maintenance will mainly apply when an event occurs, forcing unscheduled maintenance. This occurs when either a component failure or detection of an issue that requires immediate action during user operation. The instrument will have to stop user operations for the duration of repairs or maintenance.

Another key categorisation of maintenance is the distinction regarding to access requirements and limitations. Components can hence be categorized into *easy maintenance access, limited maintenance access* and *difficult maintenance access* devices. In the first category all devices and components can be placed in areas, which are located outside the radiation shield of the primary instrument, including such devices placed in the end station. These devices can be serviced anytime when required, though downtimes are used for preventive maintenance in order not to interfere with the scientific utilisation of the instrument. In the second category are the limited number of hardware components installed in instrument shielding between the bunker shield and the end station (cave) downstream of the heavy shutter system of the instrument. These components shall be accessible during source operation in case of required corrective maintenance. The third category are components installed in the bunker area where access currently appears to be possible only during source downtimes and through remote handling. Access to components within the last two categories requires removal of shielding with the corresponding implications of crane use, space requirement and scheduling. This might involve a required cool down time of components due to activation, which increases times required for the maintenance.

As yet another category of practically no access the components of the extraction system in the monolith could be defined, which are practically non-accessible, as access requires removal of significant parts of the instrument and its neighbours. Hence, no moving parts and components requiring maintenance can be placed there and the design of the components installed there has to be especially robust.

6.3.3 Maintenance philosophy

Bifrost's maintenance philosophy is in line with the approach of the facility to utilize condition based preventive maintenance as much as possible. In order to minimize resource requirements and potential instrument downtimes, inspectability and accessibility, but also failure-mode instrument operation and application of facility standards are in the focus of a sustainable instrument design. However, performance and in particular cost against the background of a very limited instrument budget are major constraints also in this regard and hence balanced cost-benefit solutions are indispensable.

For Bifrost, the most critical components are the choppers (especially the PSC chopper), the main shutter, the detectors, the SST and the BE-filter. To these components, the following philosophies apply.

Choppers:

- Choppers are accessible and removable vertically from above, and when required by remote handling; however, up to date there is no information available on expected activation and radiation situation within the bunker, which follows a new concept of large free space, i.e. with limited material to get activating and posing an irradiation source apart from the beamline components themselves. Better knowledge of the situation to be expected is essential in order to plan accordingly and under the correct assumptions. This is important in particular with respect for the remote handling requirements that have to be met, designed and which affects cost, complexity, space demand etc.
- Choppers are removable without impact on the guide system; this implies a state of the art split housing approach for choppers, which are connected, to the guide vacuum system, which is a design driver with respect to performance in order to keep guide interruptions as small as possible.
- Choppers are removable independently. For Bifrost, useful operation may be envisaged using only one FOC for instance.
- Chopper solutions with minimum maintenance requirement (magnetic bearings) are preferred where affordable, final choice requires cost-benefit analyses; failure mode operation enables maintenance with certain frequency.
- The PSC double disc chopper has to be inspected as often as practically possible.

Main shutter:

- The main shutter is situated in the DO3 hall. Although not a complicated piece of equipment, it can only be serviced and maintained during shutdown periods.
- Maintenance includes removal of fast neutron shielding, which makes the operation expensive and time consuming.
- This shutter should be designed to be as simple and robust as possible, yet also maintenance free.

Detectors (maintainable in production mode):

- The high flux of Bifrost makes Bragg peaks strong enough not only to attenuate He-3 detectors but to cause considerable damage as well.
- A failsafe safety system is to be implemented, at either the electronics level or mechanical attenuators.
- The detectors need to be monitored and calibrated at regular intervals

Secondary spectrometer tank vacuum (maintainable in production mode):

- The vacuum in the SST is critical for the detector electronics. If vacuum is broken, the breakdown voltage decreases, and the high voltage electronics of the detectors become vulnerable.
- If the filter is placed within the tank, a broken vacuum will reduced filter performance and render the secondary spectrometer unusable.
- The breakdown of vacuum can also cause spurions via air scattering.

Beryllium filter (maintainable in production mode):

- The Be-filter needs to be translatable out of the neutron path to allow for alignment.
- The filter needs to be cold to work.
- Both cooling and translation stage of the filter should be designed in a robust way.

The guide system should not require maintenance, but in case of failures, partial removal follows similar principles as for the choppers. Partially choppers might need to be removed as well. Realignment requirements of the guide are to be considered in the general design of the system. The guide design shall be robust against misalignment, to the extent possible in terms of cost and performance. The hard radiation environment inside the bunker requires metal guide substrates.

All other components are accessible, should be fast replaceable as possible (standards) or allow failure mode operation, partly through replacement by alternative components (e.g. different detector to be used). Regular maintenance and check shall prevent failure.

7. CONSEQUENCES OF THE CONCEPTS

7.1 General design considerations

General design considerations concern all functional and non-functional requirements and are/will be documented in detail in the corresponding documentation.

7.1.1 Upgrade options

Identified upgrade options shall be considered and be catered for as much as possible in the design solutions, see 4.3.10.

7.1.2 Robust design

The current preliminary design can be considered robust with respect to the scientific and technical aspects raised. The prompt pulse suppression is static, and most of the critical components are maintainable in target production mode. The Bifrost chopper system and the thermal shutter are the only moving parts difficult to access. However, careful provisions have to be made in particular also during final design and especially the performance and respective corresponding issues of the extraction guide and the main shutter have to be considered carefully. The final design of the guide including its alignment and support as well as choices still to be made on details of choppers and their support will be of significant importance.

However, robustness has to take the viable systems that Bifrost is connected to and relying on into account. This concerns particularly the ICS and data streaming functions coupled with it. In order to guarantee best possible availability it is foreseen that Bifrost is able to operate in a stand-alone mode in case of difficulties of the ICS and data streaming systems. All choppers can usually, just like other motion control, be addressed locally either through internal hardware connection or in the worst case by directly approaching the specific electronics or controls. The detector area of Bifrost is limited, and the count rate low enough for local data storage at least for some days. Standalone versions of analysis software is preferable as well as options for data reduction into intermediary files to be analysed on desktop or laptop devices.

Better knowledge of the operational environment and interfaces like with the target but in particular, also the conditions during access in the bunker are key boundary conditions to enable optimum choices and design. This information is subject to change, and design iterations keeping robustness in mind are paramount.

7.2 Training of personnel

The operational model for the instruments has not yet been defined, so it is not possible to specify the exact roles for the personnel involved in the instrument operations. The smooth operation of the instrument in the user program will likely require 2-4 PhD level scientists knowledgeable in neutron spectroscopy for day-to-day scientific support of the users, as well as technicians and or engineers in mechanical, electronic and
software engineering who are familiar with the instrument and its components. The technical personnel can be fully or partly organized in teams that are shared between instruments.