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Scope Setting Report

Instrument : FREIA Reflectometer

SUMMARY

The purpose of this document is to describe the possible baseline options for the FREIA project and a plan for how the instrument performance will be upgraded after the construction project from the day one scope to the full scope as envisaged in the instrument proposal[1].

Three baseline options are presented.

FREIA has been assigned to cost category A (9M€). The conclusion from analysing the costs is that it is not possible to build FREIA within cost category A in a manner that delivers a functional instrument capable of measuring specular reflectivity on day one, or that allows a reasonable, affordable upgrade path to world leading performance. This option is clearly not acceptable.

The minimum functional reflectometer capable of delivering a defined beam to a sample at grazing incidence and detecting one angle at a time would cost 11.35M€ if built by ESS without an in-kind partner. This option is not acceptable as it does not meet the key scientific requirements.

The minimum acceptable scope based on the advice of the reflectometry STAP[2], that is upgradable to the full scope, was originally estimated to cost 16.34M€. This costing has been revised according to the wishes of ESS management – the updated cost is **13.453M€.**

The configuration with the full technical scope described in the instrument proposal, taking into account changes in ESS design during Phase 1 and advice from the Reflectometry STAP[2] would cost: 21.35M€

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1. OVERVIEW

1.1. Science Case

Neutron reflectometry covers a very broad spectrum of science involving the growth, self-assembly, structure and interactions of a wide variety of thin films and has an impact on all the core areas of the ESS materials science case. This leads to a broad range of requirements on sample size, resolution and bandwidth in all types of reflectometry experiments.

The range of scientific challenges to be met in soft condensed matter and the life sciences is broad, and requires a number of different collimation options and specialist sample environments to carry out measurements at different types of interfaces. However, a common feature is that in order to be able to examine the relevant parameter space in increasingly complex materials, faster measurements, measurements on smaller sample volumes, and measurements with good signal-to-noise are required. Similar issues are equally relevant in a wide range of materials chemistry and hard condensed matter science. Consequently, the ability to match the experimental throughput to the ESS source performance in terms of the time needed for sample changes, data processing and analysis constitutes one of the key challenges in maximizing the scientific output of the instruments. While the sensitivity of neutrons to structural features offers a significant advantage in all types of multicomponent systems, there is a clear trend to follow time-dependent processes due to the development of time-of–flight reflectometers in the past three decades at facilities world-wide. These processes include, but are not limited to:

- Self-assembly of surfactants, polymers and proteins at solid and liquid interfaces
- Rearrangement processes in thin films: e.g. interdiffusion, inter-layer movement
- Encapsulation and release of components in e.g. plastics, polymer blends, drug delivery
- Switchable materials that respond to external stimuli (chemical, electrical, magnetic)
- Surface reactions e.g. enzyme catalysis, oxidation, surface functionalisation etc.
- High-throughput screening of e.g. biological/medical samples or industrial conditions
- Liquid-liquid interfaces: e.g. heavy metal extraction and oil-recovery processes

Time-of-flight (tof) neutron reflectometry offers the possibility to record a range of Q-values simultaneously, and determination of both structure and chemical composition as a function of time during such processes. The usefulness of tof-reflectometry critically depends on the ability to match both the time-resolution and the dynamic Q-range of the measurements to the structural changes investigated. The main challenge for kinetic measurements is to record the full range of interest simultaneously without need to move the sample or reconfigure the instrument. The length scales of interest for neutron reflectometry span 1Å-1000Å, so variable wavelength resolution options are required. For the majority of purposes in specular reflectometry a Q-range of 0.005 – 0.5 $Å^{-1}$ is sufficient, however, for surface diffraction experiments from multilayer samples, access to Q up to 1$Å^{-1}$ is often required. Liquid-liquid interfaces and many sample environments such as rheometers further require an inverted beam geometry in which the beam impinges on the interface from below.

Off-specular reflectometry and grazing incidence SANS are expected to become mainstream techniques at ESS. GISANS poses additional requirements on the collimation and detector distance/geometry, with Qy ranges between 10^{-4} and 1 $Å^{-1}$ of interest, and high resolution is needed (dλ/λ = 1-2%) to control the neutron penetration depth. Polarisation analysis is typically not required in soft matter experiments, but polarised reflection from magnetic reference layers for magnetic contrast variation is a popular method.

The operational modes supported by FREIA are based on the STAP advice [2] on the scientific case for the instrument which aims to cover the needs of the soft condensed matter surface science and chemistry, with an emphasis on enabling high throughput and fast kinetic measurements that make the best use of the ESS source performance. These experimental modes are:

I. **High-Intensity Specular and Off-specular Reflection** from thin films (< 150Å) at i) solid and (ii) liquid interfaces. Reason: The high ESS source intensity allows high-throughput characterisation of weakly scattering thin films/small samples. This will enable detailed, systematic studies of smaller samples and large chemical/biological and physical parameter spaces. This mode is required by approximately 50% of the science case.

II. **High-resolution Specular and Off-Specular Reflection** from thicker films (150 - 1000Å) at i) solid and (ii)) liquid interfaces. Reason: The ESS source and long pulse allow pulse-shaping to increase the resolution for investigations of thicker films and complex systems that exhibit structure at multiple length scales. This mode is required by approximately 50% of the science case.

III. **Fast kinetic measurements over a broad simultaneous Q-range** without moving the sample. Reason: the ESS source intensity allows very fast kinetic measurements (ms-s) over a wide simultaneous Q-range provided. The unique vertical divergence of FREIA will allow measuring three angles of incidence pseudo-simultaneously at this timescale, giving rise to an unprecedented dynamic Q-range (Qmax/Qmin = 70). It is expected that up to 50% of the scientific case will have kinetics experiments at these timescales.

IV. **Polarized time-of-flight (TOF) neutron reflection** for the investigation of magnetic thin films, particularly for use of magnetic contrast variation. Reason: the ESS pulsed source and TOF polarised mode of FREIA enable the use of polarised reflection in kinetic experiments using a broad wavelength band. This will enable the detailed characterisation of hybrid magnetic-soft materials, particularly their formation and interactions in applied systems such as sensors. Currently approximately 15% of the user community uses magnetic contrast variation but the figure could grow with the kinetic capability available on FREIA.

V. **Inverted Beam Geometry** for reflection from below the surface in i) liquid-liquid and other buried interfaces where beam attenuation can be controlled through selection of the more dense incident medium, ii) in-situ experiments requiring horizontal sample environments or complementary measurements to be performed above the sample surface (e.g. rheometry, microscopy, competition between two interfaces/effect of gravity). Reason: The ESS source intensity and the inverted FREIA configuration will allow detailed studies of a wide range of fundamental and applied systems using the full resolution/beam polarisation/collimation options at timescales inaccessible on existing instruments. This will for the first time enable kinetic studies at liquid-liquid interfaces. Liquid-liquid interfaces and rheology etc. make up approximately 25% of the user experiments on instruments where this is enabled, but most solid-liquid experiments would benefit from the geometry.

The expectation is that because the FREIA q-range is limited in this configuration, this will mainly used by the 25% who need it.

VI. **Grazing Incidence SANS** from horizontal samples to enable the observation of small angle scattering from 2D thin film structures. Reason: The ESS source intensity makes it possible to observe weak GISANS signals from thin films at experimentally accessible timescales, and the FREIA high-resolution TOF mode (ii) allows the collection of time-resolved GISANS patterns with good control of the neutron penetration depth. This, combined with specular reflection in the full Qz-range will enable depth-sensitive 3D profiling and time-resolved GISANS of complex thin film samples at both liquid and solid interfaces. Considering that the GISANS option on FREIA will be limited in Q-range and flux, approximately 30-40% of the science case would involve lateral structures in the accessible range.

1.2. Requirements

In order to support the above measurement modes, the following high level design requirements have to be met:

1. The central requirement of measuring specular reflectivity from free liquid surfaces without moving the sample or detector leads to the requirement of a vertically focused beam impinging at the sample surface. (Elliptical guide)

2. The requirement of covering the essential Q-range for free liquids with no more than three angles to minimize the time of angle changes and complexity data reduction dictates the required vertical beam delivered by the guide (divergence, wavelength bandwidth and vertical guide geometry/m-coating).

3. The requirement to measure reflectivities as low as 10^{-7} on liquids, and 10^{-8} on solids requires bending out of line of sight twice with efficient transport of 2.5Å neutrons as early as possible, which defines the horizontal guide geometry.

4. The resolution requirements follow from the length scales associated with the scientific case and determine the instrument length/intrinsic resolution as well as the need for a high-resolution option, which will be used by at least 50% of the experiments. The instrument length/WFM pulse length and wavelength band determine the working resolution range for the high-resolution choppers.

5. The sample size range is determined by the scientific case.

6. Time-resolved polarized neutron reflectometry requires the same wavelength band as non-polarised operation, which determines the method of polarisation. The requirement that this is an option determines that the polarised mode should not change the instrument design and should interfere as little as possible with the unpolarised operation/performance of the instrument.

7. The requirement for a GISANS option follows directly from the scientific case, and is determined by the length scales associated with the samples. These determine the resolution of the high-resolution chopper system (to control the penetration depth), the collimation lengths, detector size and distances.

8. The fast shutter system design is defined by the requirement to measure one pulse per angle of incidence, which gives the highest degree of flexibility, and the performance requirements of the shutters in turn define the arrangement of the 3-slit/shutter system.

9. The scientific case determines the types of interfaces and samples to be investigated which leads to a suite of specialist, custom made sample environments. The speed of the measurements implies that a high-level of automation in sample changes is required to match the ESS source performance.

Correspondingly the high level scientific requirements for FREIA are:

1. The instrument shall be capable of measuring specular reflection on free liquid surfaces without moving the sample or detector between Qmin = 0.0035 $Å^{-1}$ and Qmax = 0.44 $Å^{-1}$.
2. The instrument shall be capable of measuring specular reflection from solid samples in the range of Qmin = 0.005 and Qmax = 1$Å^{-1}$
3. The instrument shall allow the illumination of horizontal sample areas between 1cm(x) x 1cm(l) and 4cm (w) x 8cm (l).
4. The instrument shall be capable of providing a minimum angular resolution of dθ = 0.01°.
5. The instrument shall have a minimum wavelength band Δλ of 7Å without frame-overlap.
6. The instrument shall have a maximum wavelength resolution δλ/λ = 10.5% fwhm
7. The instrument shall have a high resolution option with δλ/λ = 1.5% fwhm
8. The instrument shall provide essential temperature-controlled sample environments for liquid and solid samples and mechanisms for changing samples automatically.
9. The instrument shall be able to skip every second source pulse (pulse-skipping)
10. The instrument shall allow fast collimation changes for kinetic experiments
11. The instrument shall be able to measure specular reflection from below the sample interface up to Q = 0.2$Å^{-1}$
12. The instrument shall be able to polarise the full wavelength band of 7Å.
13. The instrument shall provide a GISANS option for horizontal samples that is capable of detecting length scales of up to 190nm with resolution δQy/Qy = 5%.

Instrument Performance at 5MW and at 2MW

The instrument proposal[1] described the instrument performance with the TDR moderator in terms of a series of virtual experiments that were benchmarked against experimental data from FIGARO. In terms of measurement times, the gain factor for the TDR moderator was ~25 relative to FIGARO. Since the proposal, the ESS moderator upgrade and optimization of the bender configuration change have resulted in an additional gain factor of 3.5 over this, making the full gain factor 80 for 5MW operations. This is applicable for all of the FREIA operating modes relative to like-for-like conditions on existing instruments. At 2MW, FREIA can therefore be expected to perform with a gain factor of approximately 30.

The guide geometry of FREIA enables the fast kinetics mode without moving the sample or detector in a manner that is not available on any existing instrument. This geometry makes it possible to change angles at timescales appropriate for the measurements, and enables the use of the fast shutter system to record the full dynamic Q-range simultaneously, which is for the first time possible due to the high ESS source intensity.

The extremely fast measurements possible on FREIA will enable both kinetic and large parametric studies of complex systems not accessible with neutrons today and will also increase the experimental throughput by at least an order of magnitude, provided that the speed of sample changes and data-analysis can match the beam performance.

1.3. Configuration options

Three configuration options are presented:

1. A configuration that is within cost category A (9M€). The aim was to meet the cost category with 10% contingency and in order to do so, all components not required for safely delivering a beam of neutrons to the sample location were removed. This configuration is not functional as a reflectometer and not upgradable to Option 2 or 3. **Cost : 8.1 M€ + 0.9M€ contingency.**

2. A configuration that meets the scientific requirements for specular and off-specular reflectometry at reasonable performance, following the advice of the reflectometry STAP[2]. The aim was a world class instrument that is upgradable to the full scope. **Original Cost : 16.348M€ - Updated Cost: 13.453M€**

3. A configuration with the full technical scope including GISANS. This is the full scope presented in the instrument proposal[1], taking into account changes in ESS design during Phase 1 and advice from the Reflectometry STAP[2]. **Cost : 21.35M€**

2. OPTION 1: SCOPE WITHIN COST CATEGORY A (9M€)

2.1. Scope

- 2x line of sight benders (horizontal)
- Inclined elliptical guide focusing on sample position
- heavy shutter installed in the bunker wall
- Sample position at 22.2 m
- Collimation length of 2m with vertical/horizontal two slit collimation
- Basic sample x,y-table (no precision alignment)
- Single helium tube detector at 3m from sample, movable ±700mm vertically
- All necessary associated infrastructure for the above (shielding, cabling etc.)

The scope possible within cost category A does not meet any of the requirements*, as it cannot deliver a defined neutron beam to the sample or measure analysable reflectivity data.* As such this option meets none of the science case of FREIA . This configuration can not be cold-commissioned and can not be built as an in-kind collaboration, as the additional costs related to this also have to be removed to fit within the cost category.

A *minimal functional configuration that can deliver a defined beam to a sample and measure one reflection angle at a time would require the* bandwidth/frame overlap choppers (1354k€), a sample stack (372k€) and control hutch (178k€) to be included, and cost 11,325 M€ incl. 10% contingency, and would have to be built by ESS, as this does not include the collaborative costs (travel, logistics, manpower). However, this configuration still would not meet the following key requirements:

- **Measurements on liquids surfaces without moving sample/detector (#1)**
- The wavelength resolution (#7)
- Sample environment (#8)
- Pulse-skipping (#9)
- Fast collimation changes for kinetic experiments (#10)
- Specular reflection from below the sample interface (#11)
- Beam polarisation (#12)
- GISANS (#13)

The science case for FREIA is based on enabling high-through put and fast and kinetic measurements on a wide range of film thicknesses and types of interfaces, by not moving the sample or detector. Although this configuration would deliver the full intensity gain of 80 at 5MW or 30 at 2MW, ***the limitation to a single detector makes the kinetic experiments that make up to 50% of the science case impossible.***

***This option is not upgradeable* to include the high-resolution/pulse-skipping** requirements (#7/#9) by adding the WFM chopper system without replacement of the entire guide system. At least 50% of the science case requiring the high-resolution option could not be carried out with this configuration as the experiments will be limited to samples thinner than 150Å.

The lack of collimation options severely limits the scientific case and would require installation of a collimation changer system/vacuum flight path at a later stage.

The absence of sample environment severely restricts the experiments that can be performed to mainly solid samples, as the liquid sample environments, pumps and alignment equipment are not provided by users due to their large size, cost and maintenance requirements. ***The absence of sample environment means that the instrument could only perform a small fraction of the science case (20-25%)***. The experimental throughput also cannot match the source performance even at low beam power. All sample environment and changers need to be integrated into the instrument controls and as such need to be commissioned before the start of the user program. None of the essential sample changers or sample environment environments can be shared with the ESTIA reflectometer due to the difference in sample geometry.

The study of kinetics is a key part of the science case for FREIA and the reason for the chosen optical design. ***This day-1 configuration will be limited to measuring kinetics at one angle only for processes faster than 5 min. This represents no gain over existing instruments.***

This option is not upgradeable to do GISANS without a complete replacement of the instrument cave, cabling, detector vessel, and detector. This will be a costly and major disruption to the user programme may not be possible due to eventual safety or operational regulations at ESS.

Thus, the minimum functional scope even within 11,35M€ does not fulfil the science case for FREIA. It will not cover more than 20-25% of the experiments and is not upgradable.

2.2. Costing

The costing is based on bottom-up calculation of the procurement costs and manpower required for the tasks needed to deliver the higher level PBS items. Vacuum equipment is not included in the cost as this is expected to be delivered from outside the Freia budget.

Table 1 Costing for FREIA in Cost Category A

	01 Phase 1	02 Project Management & Integration	03 Design	04 Procurement & Fabrication	05 Installation	06 Cold Commissioning	Total
01 Shielding	€ 0	€ 0	€ 0	€ 1,743,490	€ 0	€ 0	**€ 1,743,490**
02 Neutron Optics	€ 0	€ 0	€ 0	€ 2,100,000	€ 0	€ 0	**€ 2,100,000**
03 Choppers	€ 0	€ 0	€ 0	€ 0	€ 0	€ 0	**€ 0**
04 Sample Environment	€ 0	€ 0	€ 0	€ 0	€ 0	€ 0	**€ 0**
05 Detector and Beam Monitors	€ 0	€ 0	€ 0	€ 128,400	€ 0	€ 0	**€ 128,400**
06 Data Acquisition and Analysis	€ 0	€ 0	€ 0	€ 0	€ 0	€ 0	**€ 0**
07 Motion Control and Automation	€ 0	€ 0	€ 0	€ 133,200	€ 0	€ 0	**€ 133,200**
08 Instrument Specific Technical Equipment	€ 0	€ 0	€ 0	€ 27,750	€ 0	€ 0	**€ 27,750**

09 Instrument Infrastructure	€ 0	€ 0	€ 0	€ 573,900	€ 0	€ 0	**€ 573,900**
10 Vacuum	€ 0	€ 0	€ 0	€ 0	€ 0	€ 0	**€ 0**
11 PSS	€ 0	€ 0	€ 0	€ 133,200	€ 0	€ 0	**€ 133,200**
Labour & Travel (Cost)							€ 3,342,000
12 Contingency							**€ 818,194**
Total	**€ 0**	**€ 0**	**€ 0**	**€ 4,839,940**	**€ 0**	**€ 0**	**€ 9,000,134**

Upgrade/Staging plan

The staging plan for this option would consist of installing the bandwidth/frame overlap choppers, the sample stack, detector and housing, instrument control hutch. It would not be possible to install the resolution enhancement choppers, and therefore it would not be possible to do GISANS with adequate control of the wavelength penetration depth. It would be possible to install the fast kinetics collimation, inverted beam option and beam polariser at a later stage. It would be possible to design, manufacture/procure/integrate and commission sample environments at a later stage. The choppers, sample stack and control hutch would have to be in place before the instrument can enter cold commissioning. The 300mm x 300mm detector for reflectivity would have to be in place for hot commissioning. The total cost of these upgrades would be approximately 10M€.

2.3. Risk

The main risk with this configuration is the failure to enter the user programme on schedule, and thereafter to deliver the science case that was presented to the SAC. This presents a clear reputational risk to ESS if it is not possible to perform any experiments on day 1, or any new experiments during the first 5 years of operation beyond that which is possible now. The minimal functional configuration would present steps backwards in terms of the instrument usability for science and the user experience offered. The later installations required to upgrade the detector and integrate the collimation options and sample environments would present continuous disruptions to the user programme and long delays in delivering the scientific output. Due to the limited upgradability, the resulting instrument would still only be applicable to less than 50% of the science case (<150Å thick films).

Below are top 5 risks rated high using ESS risk measures (impact x likelihood)

Table 2 Top risks for Option 1

Only the top risks relating specifically to this option are included here. The general project risks are common with options 2 and 3, and are listed in Table 6.

Risk level	RISK	TREATMENT NAME	Treatment	CATEGORY	TREATMENT PLAN

High 5x5	Failure to deliver functional instrument for cold commissioning	Extend project, Lower expectations	Mitigate	Budget, quality and function, Goodwill	Change schedule, communicate with stakeholders the lowered expectations. Begin planning for upgrade and seek funding. Responsible: FREIA Team, ESS management
High 5x5	Failure to deliver proposed scientific performance	Lower expectations	Mitigate	Budget, quality and function, Goodwill	Communicate with stakeholders the lowered performance expectations. Begin planning for upgrade and seek funding. Responsible: FREIA Team, ESS management
High 5 x 5	Failure to deliver successful user programme	Lower expectations	Mitigate	Reputation, quality and function, Goodwill	Communicate with stakeholders the lowered performance expectations and scheduling. Begin planning for upgrades and seek funding. Responsible: FREIA Team, ESS management
High 5x5	Failure to install GISANS upgrade	Build separate GISANS instrument.	Mitigate	Quality and Function, budget and schedule	Communicate with stakeholders the lowered expectations. Begin planning for GISANS instrument and seek funding. Responsible: FREIA Team, ESS management
High 5x5	Delay in chopper development.	Lower expectations	Mitigate	Quality and Function, budget and schedule	Communicate with stakeholders the lowered performance expectations. Begin planning for upgrades and seek funding. Responsible: FREIA Team, ESS management

3. OPTION 2: WORLD CLASS SCOPE MEETING REFLECTOMETRY REQUIREMENTS - UPDATED

3.1. Scope

The scope within this cost category is:

- 2x line of sight benders (horizontal)
- Inclined elliptical guide focusing on sample position
- heavy shutter installed in the bunker wall
- Sample position at 22.2 m
- Collimation length of 2m
- Vertical/horizontal two slit collimation
- Inverted beam option (m=6 mirror)
- Three-slit system for faster kinetics (10s-1min.)
- Evacuated collimation changer for the above
- Slit positions prepared for GISANS ~8m, ~6.5m and ~4m before sample.
- Bandwidth, frame overlap and pulse-skipping choppers:
  - 1m Double disk co-rotating at ~6.5 m
  - 1m Double disk co-rotating at ~10 m
- WFM/frame overlap choppers for high-resolution option
  - 1.3m WFM Double disk co-rotating at ~6.9 m
  - 1.3m FOC single disc at ~8.5m

    - 1.3m FOC single disc at ~11m
    - 1.3m FOC single disc at ~15.5 m
- 30cm x 30cm 0.5mm x 2.5mm resolution ^{10}B detector with 25cm x 25cm initial electronics coverage, at 3m from sample, movable ±400mm vertically
- Vacuum flight path for above
- Sample stage with ±200mm translation vertically and ±500mm horizontally
- Two goniometers at sample position
- All necessary associated infrastructure (shielding, cabling, cabins etc)

For this option, all sample environments and sample preparation area will be provided from the ESS operations budget and will be in place for hot commissioning in 2023. ISIS believes that the success of the instrument relies greatly on the availability of suitable sample environments and that Freia cannot be deemed as a world class instrument without it. The Priority list of SE includes (excluding ESS integration costs):

1. Sample translation table ±500mm 30k€
2. Vibration isolated sample table 10k€
3. A water bath + temperature probe 17k€
4. Aspirator pump 5k€
5. Laser interferometer 35k€
6. Sample preparation area 44k€
7. Atmosphere and temperature-controlled air-liquid troughs 40k€
8. Atmosphere and temperature-controlled Langmuir trough 50k€
9. a set of temperature controlled solid-liquid sample cells 30k€
10. a set of liquid-liquid troughs 30k€

Total: 291k€

Items 1-9 need to be in place for hot commissioning:

Items 10-11 could be temporarily borrowed from ESTIA until they start their user program, when FREIA needs a second set of these.

11. a 4-channel HPLC pump (preparative) with an automatic switch 55k€
12. a multichannel syringe pump 40k€

Total 95k€

In addition, the following pool equipment will be available from ESS:

1. electromagnet (<1T)
2. rheometer with cone-plate insert
3. vacuum chamber
4. humidity chamber
5. furnace

Provided that the essential sample environments (386k€) are provided from the operations budget in time for hot commissioning, this scope meets 11 of the 13 high level requirements for specular reflectometry and is upgradeable to a configuration that

provides the full scope by rebuilding the instrument cave and detector tank for a larger detector at a later stage. In all experiments that are enabled, the full gain factor of 80 (5MW) or 30 (2MW) will be achieved for like-for-like measurement conditions compared to the top-end liquid reflectometers covering the same science case (FIGARO, ILL; Inter, ISIS).

The specular reflectometry science case will mostly be met by this configuration (75%) and mainly excludes polarised experiments (15%) which are expected to be catered for by ESTIA to a large degree (except fast kinetics). The pulse-skipping chopper extends the simultaneously usable wavelength band to partly mitigate the lack of the fast shutter system for fast kinetics, which is required for kinetics faster than of the order of 10s.

The absence of the GISANS slits and larger detector at a longer distance means that GISANS experiments will not be possible, and the cost and effort to rebuild the entire cave will be significant, which will create a major disruption to the user programme. In the event that a dedicated GISANS instrument is not built at ESS; it will mean that no GISANS experiments will be possible at ESS.

The limitations in sample environments will lead to wasted beam time if no additional sets of the key sample holders are available for off-line preparation and fast changes at the start of the user programme. As a typical measurement time will be of the order of 5-10s per sample, the sample holders and changers for 5-10 samples included here will mean sample changes and cleaning will have to take place outside the beam every couple of minutes. ***Therefore the experiment throughput of this option will not meet the ESS source performance*** and will require users to bring in larger experimental teams to manage the sample changes. ***The lack of specialist SE for dynamic surfaces, electrochemistry, stopped-flow experiments etc. limits the study of non-equilibrium systems that form a key part of the FREIA science case*** and this configuration will not provide these capabilities on day one.

3.2. Costing

The costing is based on bottom-up calculation of the procurement costs and manpower required for the tasks needed to deliver the higher level PBS items. Vacuum equipment is not included in the cost as this is expected to be delivered from outside the FREIA budget.

Table 3 Costing for FREIA Option 2 - Updated

	01 Phase 1	**02 Project Management & Integration**	**03 Design**	**04 Procurement & Fabrication**	**05 Installation**	**06 Cold Commissioning**	**Total**
01 Shielding	€ 0	€ 0	€ 0	€ 1,737,844	€ 0	€ 0	**€ 1,737,844**
02 Neutron Optics	€ 0	€ 0	€ 0	€ 1,850,000	€ 0	€ 0	**€** 1,850,000
03 Choppers	€ 0	€ 0	€ 0	€ 2,832,720	€ 0	€ 0	**€** 2,832,720
04 Sample Environment	€ 0	€ 0	€ 0	€ 0	€ 0	€ 0	**€ 0**
05 Detector and Beam Monitors	€ 0	€ 0	€ 0	€ 831,800	€ 0	€ 0	**€ 831,800**
06 Data Acquisition and Analysis	€ 0	€ 0	€ 0	€ 0	€ 0	€ 0	**€ 0**
07 Motion Control and Automation	€ 0	€ 0	€ 0	€ 815,850	€ 0	€ 0	**€** 815,850

08 Instrument Specific Technical Equipment	€ 0	€ 0	€ 0	€ 144,000	€ 0	€ 0	**€ 144,000**
09 Instrument Infrastructure	€ 0	€ 0	€ 0	€ 901,320	€ 0	€ 0	**€** 901,320
10 Vacuum	€ 0	€ 0	€ 0	€ 0	€ 0	€ 0	**€ 0**
11 PSS	€ 0	€ 0	€ 0	€ 133,000	€ 0	€ 0	**€ 133,000**
Labour & Travel (Cost)				€ 0			€ 2,983, 000
12 Contingency							**€ 1,223,003**
Total				**€ 9,247,034**			**€ 13,453,037**

Upgrade/Staging plan

To enable pulse-skipping experiments, the third bandwidth chopper pair (1m double disk, co-rotating) would need to be installed at 16m, at a cost of approximately 200k€.

The additional fit out of the GISANS slits, larger detector, tank and cave rebuild, as foreseen in the full scope, would cost approximately 5M€. This is a large sum to be paid for from the operations budget and/or external grants. Furthermore, since a dedicated GISANS instrument is planned to be built later at ESS[3], it would in any case be optimised to cover the GISANS science case and requirements far better, and the operational/external funding would be better spent on this.

The costs to complete the fast shutter system cannot be reasonably estimated until further development is undertaken and is something that we could potentially envisage obtaining from external funding.

The additional sample environment could be paid for from an on-going programme using a operations funds (additional sets of SE and mechanisms for faster sample changes should be made available for the start of the user programme), external grants and collaborations with users could potentially provide some of the more specialist SE (electrochemical cells, potentiostat, overflowing cylinder etc.). Some of the items available from the ESS Sample environment pool are not funded through their initial scope (rheometer, electromagnet, humidity chamber) and would also require operational/external funding through SSS. The cost of the addition of key pieces of SE (overflowing cylinder, electrochemical cells, potentiostat, second Langmuir trough, second air-liquid and solid-liquid trough sets) is estimated to be 205k€.

3.3. Risk

The main risks for this configuration are delays in delivery of various ESS systems and FREIA components. The need for development of detectors is a risk that is not unique to FREIA but must be mitigated through schedule and planning for a backup solution. Technical risks include the delivery of new chopper sizes currently not in existence.

Below are top 5 risks rated high using ESS risk measures (impact x likelihood).

Table 4 : Top risks for Option 2

Only the risks specifically associated with this option are included here, the remaining project risks are common with Option 3, shown in Table 6.

Risk level	RISK	TREATMENT NAME	Treatment	CATEGORY	TREATMENT PLAN
5x5	Failure to install GISANS upgrade	Build separate GISANS instrument.	Mitigate	Quality and Function, budget and schedule	Communicate with stakeholders the lowered expectations. Begin planning for GISANS instrument and seek funding. Responsible: FREIA Team, ESS management
High 5 x 5	Major disruptions to user programme	Lower expectations	Mitigate	Reputation, quality and function, Goodwill	Communicate with stakeholders the lowered performance and operational expectations. Begin planning for upgrades and seek funding. Responsible: FREIA Team, ESS management
High 5 x 5	Wasted beam time due to lack of sample environments for fast changes	Lower expectations	Mitigate	Reputation, quality and function, Goodwill	Communicate with stakeholders the lowered performance and operational expectations. Begin planning for upgrades and seek funding. Responsible: FREIA Team, ESS management
High 5 x 5	Failure to develop large choppers	Early Development	Mitigate	Quality and Function, Budget and Schedule	ISIS have built 1.2m discs running at 10Hz. 1.3m discs at higher speeds will require technological development. Prototype discs should be built and tested as early as possible in order to validate technology. Responsible: FREIA team, STFC Chopper group
High 5 x 5	Failure of ESS to adequately provide equipment or services as agreed			Reputation, quality and function, Goodwill	Spend contingency
High 2x5	Weak integration process	Integration plan, Hall EPL (Included in FREIA planning), Checklist of activities, work package documentation, interface control document	Mitigate	Schedule, budget, quality and function	Keep a close contact with partner design, detail description of interfaces, involve ESS technical teams, Get more support from ESS integration and better efficiency of CAD tools. Responsible: FREIA team

4. OPTION 3 : FULL SCOPE

4.1. Scope

The full instrument scope consists of:

- 2x line of sight benders (horizontal)
- Inclined elliptical guide focusing on sample position
- heavy shutter installed in the bunker wall
- Sample position at 22.2 m
- Collimation length of 2m
- Vertical/horizontal two slit collimation
- Inverted beam option (m=6 mirror)
- Three-slit system for faster kinetics (10s-1min.)
- Evacuated collimation changer for the above
- Slit for GISANS at ~8m, ~6.5m and ~4m before sample.
- Bandwidth, frame overlap and pulse-skipping choppers
    - 1m Double disk co-rotating at ~6.5 m
    - 1m Double disk co-rotating at ~10 m
    - 1m Double disk co-rotating at ~16 m
- WFM/frame overlap choppers for high-resolution option
    - 1.3m WFM Double disk co-rotating at ~6.9 m
    - 1.3m FOC single disc at ~8.5m
    - 1.3m FOC single disc at ~11m
    - 1.5m FOC single disc at ~15.5 m
- 30cm x 30cm 0.5mm x 2.5mm resolution ^{10}B detector at 3m from sample, movable ±400mm vertically
- 1m^2 ^{10}B GISANS detector at 8m from sample, movable 300mm vertically
- Vacuum tank, beam stops and mechanism for changing detector used for the above
- Sample stage with ±200mm translation vertically and ±500mm horizontally
- Two goniometers at sample position
- Full suite of sample environment: **607k€ (**as for option 2 + the following)
    - overflowing cylinder **35k€**
    - electrochemical cells **5k€**
    - 50% of a potentiostat, shared with ESTIA **15k€**
    - second set of air-liquid, liquid-liquid and solid-liquid troughs **100k€**
    - second Langmuir trough **50k€**
    - integration costs **10k€**
- All necessary associated infrastructure (shielding, cabling, cabins etc)

This scope meets all the high level requirements and fulfils the science case.

4.2. Costing

The costing is based on bottom-up calculation of the procurement costs and manpower required for the tasks needed to deliver the higher level PBS items. Vacuum equipment is not included in the cost as this is expected to be delivered from outside the FREIA budget.

Table 5 Costing for FREIA Full Scope

	01 Phase 1	02 Project Management & Integration	03 Design	04 Procurement & Fabrication	05 Installation	06 Cold Commissioning	Total
01 Shielding	€ 0	€ 0	€ 0	€ 2,338,000	€ 0	€ 0	**€ 2,338,000**
02 Neutron Optics	€ 0	€ 0	€ 0	€ 2,100,000	€ 0	€ 0	**€ 2,100,000**
03 Choppers	€ 0	€ 0	€ 0	€ 3,014,000	€ 0	€ 0	**€ 3,014,000**
04 Sample Environment	€ 0	€ 0	€ 0	€ 607,000	€ 0	€ 0	**€ 607,000**
05 Detector and Beam Monitors	€ 0	€ 0	€ 0	€ 3,352,000	€ 0	€ 0	**€ 3,352,000**
06 Data Acquisition and Analysis	€ 0	€ 0	€ 0	€ 0	€ 0	€ 0	**€ 0**
07 Motion Control and Automation	€ 0	€ 0	€ 0	€ 1,343,000	€ 0	€ 0	**€ 1,343,000**
08 Instrument Specific Technical Equipment	€ 0	€ 0	€ 0	€ 980,000	€ 0	€ 0	**€ 980,000**
09 Instrument Infrastructure	€ 0	€ 0	€ 0	€ 1,240,000	€ 0	€ 0	**€ 1,240,000**
10 Vacuum	€ 0	€ 0	€ 0	€ 0	€ 0	€ 0	**€ 0**
11 PSS	€ 0	€ 0	€ 0	€ 133,000	€ 0	€ 0	**€ 133,000**
Labour & Travel (Cost)	€ 371,295	€ 321,567	€ 1,419,690	€ 0	€ 1,995,225	€ 197,469	€ 4,305,246
12 Contingency							**€ 1,941,225**
Total	**€ 371,295**	**€ 321,567**	**€ 1,419,690**	**€ 15,107,000**	**€ 1,995,225**	**€ 197,469**	**€ 21,353,471**

This configuration covers the full science case as described in the FREIA instrument proposal[1] and will have world-leading performance from day 1 in all experiments. This will cover up to 85% of the reflectometry user community's requirements, with the additional requirements on very small samples and polarisation analysis being provided by the vertical ESTIA reflectometer. This instrument will allow complementary GISANS measurements to be performed as part of standard reflectometry experiments, as recommended by the reflectometry STAP[2], but will not be able to reach the performance of a dedicated GISANS instrument in terms of the Q-range and intensity.

4.3. Risk

The main risks for all configurations are delays in delivery of various ESS systems and components. Technical risks specific to this option include: development of fast slits with unproven and highly risky technology, development of large area detector for GISANS.

Below are the top 3 risks relating to Option 3, followed by the top general project risks common to Options 1-3, rated high using ESS risk measures (impact x likelihood).

Table 6 : Risks for Option 3

Risk level	RISK	TREATMENT NAME	Treatment	CATEGORY	TREATMENT PLAN
High 5 x 5	Failure to develop large area detector for GISANS	Alternative technologies	Mitigate	Quality and Function, Budget and Schedule	Develop alternative using one alternative detector technologies and use 3He from detector pool as back-up solution. Responsible: FREIA Team, ESS management
High 5 x 5	Failure to develop large choppers	Early Development	Mitigate	Quality and Function, Budget and Schedule	ISIS have built 1.2m discs running at 10Hz. 1.3m discs at higher speeds will require technological development. Prototype discs should be built and tested as early as possible in order to validate technology. Responsible: FREIA team, STFC Chopper group
High 5 x 5	Failure to develop flexible and robust fast shutter system	Simplify design	Mitigate	Quality and Function	Develop alternative using one of the fall back options described in the instrument proposal. Responsible: FREIA Team, ESS management
High 5x3	-Lack of definition for instrument construction from NSS - Integration of components in bunker	Input information for detail design	Mitigate	Quality and Function, budget and schedule	Improve communications from instrument teams toward NSS and vice versa. Appoint a responsible team to clarify topics Improve decision making
High 4x4	Conventional Facilities Delay and deviations from expected design	***CF LEVEL ESS-0016466***	Observe	Schedule, budget, quality and function	Access to hall 2 is a milestone for FREIA schedule. Responsible: CF
		External areas like labs, instrument halls and workshops	Mitigate		External areas will give the opportunity to start pre-installations Responsible: CF
High 3x5	Target group not fulfilling the quality and safety	Schedule for external milestone	Observe	Schedule, budget, Quality and	Follow the progress of the design and project schedule. FREIA Team Responsible: Target

	requirements of the design - Complexity in design for monolith insert and light shutter	***TARGET LEVEL ESS-0003739***	Observe	function	Focus on Safety, feasibility, operability and requirements Responsible: Target
High 3x5	Late delivery of key components	FREIA schedule	Mitigate	Schedule, budget	Properly assess the delivery time and transportation, also the time that is required for installation and arriving at site. Define the critical path for every component. Responsible: FREIA Team
High 3x3	Detector development issues or late delivery	Detectors schedule and backup plan	Mitigate	Schedule, budget, quality and function	Detector technical group is following an action plan and schedule, and planning to provide two ^{3}He backup detectors for general use. Responsible: Detector Group
High 2x5	Weak integration process	Integration plan, Hall EPL (Included in FREIA planning), Checklist of activities, work package documentation, interface control document	Mitigate	Schedule, budget, quality and function	Keep a close contact with partner design, detail description of interfaces, involve ESS technical teams, Get more support from ESS integration and better efficiency of CAD tools. Responsible: FREIA team

5. POST SCOPE SETTING

With recommendations from the scope setting meeting the following updated costing has been created for Option 2 as described in this document. We have addressed all points suggested in the meeting to show what the cost for the instrument would be under these conditions. Risks should be considered the same as Option 2.

However, as stated in the scope setting meeting by ISIS, it is important for the team to review these recommendations to ensure that they fit with the delivery model envisaged, and ISIS would like to make clear the following points:

5.1. Sample Environment

UK-ESS considers Sample environment to be a crucial part of delivering a functioning instrument, the requirement for sample environment has been considered carefully and is the minimum required to deliver the science case. Therefore if ESS are stating that they will be paying for the sample environment from operations funding it will need to be delivered at the level stated in the scope document (386k€) and in time for hot commissioning. Until the operations budget for ESS is agreed and the funding for these items is earmarked within that budget, UK-ESS will need to set aside appropriate contingency.

5.2. Labour costs

ESS requested that we cost the instrument using the ESS Labour rates to make it easily comparable to other instruments. ISIS has done this, using 25 man years at ESS cost book rates, but we would like to make it clear that 25 man years of ESS time is equivalent to 31 man years of ISIS time plus £400k of contract installation labour. Therefore in order for ISIS to deliver the instrument, all future labour discussions should be agreed on a monetary value of 25 years at ESS rates, and not in ISIS man years so that this difference can be managed and the required amount of resource is paid for by the project. We have added an addition £150k installation labour to the budget to cover the remaining contract labour requirements we have estimated necessary for installation.

5.3. ESS Labour

From the outset ISIS has been clear that it is essential that it has a member of the project team who is embedded in the ESS facility. This person is in place to ensure the integration between the design work happening at ISIS and the ever-evolving situation at ESS. Without this person in place ISIS would find it incredibly difficult to deliver beamlines to ESS. Clara Lopez has been identified as this person for both Loki and Freia and we estimate that she will be required 100% of her time though the lifecycle of the two projects.

When ISIS installs the instruments at ESS, the installation plan is to send a team of contract installation engineers to Lund, and as experience has shown us, these engineers need to work with an engineer who knows the instrument and has been part of the design team of the project as well as the pre-build at ISIS. Clara has always been intended to be this person, as ISIS cannot send our engineer for long periods of time to do this work due to the ongoing work at ISIS.

During the scope setting meeting ESS made the request for the Freia to reduce the budget by the value of the ESS staff and that ESS would pay for these staff at the specified level. In order to deliver the project the required level is shown in the table below. In order to reduce the budget as the table above ISIS would require an agreement that ESS can allocate staff to the project as per this table.

	2016	2017	2018	2019	2020	2021	2022	2023	2024	Total Man years
People	Years	Years	Years	Years	Years	Years	Years	Years	Years	
Clara Lopez Engineer	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.2	0.0	3.7
scientist	0.6	0.4	0.1	0.1	0.1	0.1	0.1	0.1	0.0	1.6
Other technician	0.1	0.2	0.2	0.2	0.2	0.2	0.2	0.1	0.0	1.4
Grand Total	1.2	1.1	0.8	0.8	0.8	0.8	0.8	0.4	0.0	6.7
com total	1.2	2.3	3.1	3.9	4.7	5.5	6.3	6.7	6.7	

5.4. Other Assumptions

It was agreed during the scope setting meeting that the following costs, essential to delivering a successful instrument, would be covered by ESS:

1) Design and manufacture of chopper lifting and remote handling equipment

2) All vacuum services and equipment

3) All network cabling and hardware

5.5. Note

Please note that this sets the desired scope and budget for the instrument as defined by ESS. This does not constitute an agreement that UK ESS is able or willing to deliver the instrument to this scope or cost, and therefore it will require further work in Phase 1 before an agreement on the final scope and budget can be made between the partner organisations.

6. REFERENCES

[1] FREIA instrument proposal

[2] Reflectometry STAP report July 2016

[3] ESS Technical Design Report 2013