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| Scope Setting ReportInstrument : FREIA Reflectometer |
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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 not 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, would cost 16.34M€.

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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# OVerview

## 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 1Å-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.

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.

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).

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.

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.

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.

## 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 = 1Å-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 = 0.2Å-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%.

## 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. **Cost : 16.348M€**
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€**

# Option 1: Scope within Cost Category A (9M€)

## 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 stack for mounting one sample
* 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 reflectivity.* 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. ***The limitation to a single detector makes this 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 requires the high-resolution option, without which 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 changers means that the instrument throughput 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 would not provide the fast kinetics capability*** and 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 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.**

## 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€.

## 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 |

# Option 2: world class Scope meeting REFLECTOMETRY requirements

## 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 counter-rotating at ~6.5 m
	+ 1m Double disk counter-rotating at ~10 m
	+ 1m Double disk counter-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
	+ 1.3m FOC single disc at ~15.5 m
* 30cm x 30cm 0.5mm x 2.5mm resolution 10Bdetector 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
* Sample environment**: 392k€**
	+ water bath (0 C to 100 C) **17K€**
	+ vibration isolated sample table **10k€**
	+ Laser interferometer for liquid surface alignment **35k€**
	+ Temperature/humidity controlled air-liquid troughs **40k€**
	+ Temperature/humidity controlled Langmuir trough (small) **55k€**
	+ Temperature controlled sample changer and rack for solid-liquid and liquid-liquid cells **30k€**
	+ Set of solid-liquid and liquid-liquid cells **60k€**
	+ Aspirator pump for liquid surface cleaning **5k€**
	+ HPLC pump/syringe pumps for automated contrast and sample changes **55k€**
	+ Integration costs for sample environment (ESS) **50k€**
	+ **From the ESS pool: electromagnet, humidity chamber, rheometer, vacuum chamber, furnace**
* All necessary associated infrastructure (shielding, cabling, cabins etc)

**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.

The specular reflectometry science case will mostly be met by this configuration. 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.

## 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

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|   | **01 Phase 1** | **02 Project Management & Integration** | **03 Design** | **04 Procurement & Fabrication** | **05 Installation** | **06 Cold Commissioning** | **Total** |
|
| **01 Shielding** | € 0 | € 0 | € 0 | € 1,821,000 | € 0 | € 0 | **€ 1,821,000** |
| **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 | € 392,000 | € 0 | € 0 | **€ 392,000** |
| **05 Detector and Beam Monitors** | € 0 | € 0 | € 0 | € 952,000 | € 0 | € 0 | **€ 952,000** |
| **06 Data Acquisition and Analysis** | € 0 | € 0 | € 0 | € 0 | € 0 | € 0 | **€ 0** |
| **07 Motion Control and Automation** | € 0 | € 0 | € 0 | € 1,010,000 | € 0 | € 0 | **€ 1,010,000** |
| **08 Instrument Specific Technical Equipment** | € 0 | € 0 | € 0 | € 172,000 | € 0 | € 0 | **€ 172,000** |
| **09 Instrument Infrastructure** | € 0 | € 0 | € 0 | € 1,201,000 | € 0 | € 0 | **€ 1,201,000** |
| **10 Vacuum** | € 0 | € 0 | € 0 | € 0 | € 0 | € 0 | **€ 0** |
| **11 PSS** | € 0 | € 0 | € 0 | € 133,000 | € 0 | € 0 | **€ 133,000** |
|  |  |  |  |  |  |  |  |
| **Labour & Travel (Cost)** | € 367,965 | € 320,790 | € 1,294,260 | € 0 | € 1,929,180 | € 148,629 | € 4,060,824 |
|  |  |  |  |  |  |  |  |
| **12 Contingency** |   |   |   |   |   |   | **€ 1,485,582** |
|  |  |  |  |  |  |  |  |
| **Total** | **€ 367,965** | **€ 320,790** | **€ 1,294,260** | **€ 10,795,000** | **€ 1,929,180** | **€ 148,629** | **€ 16,341,406** |

Upgrade/Staging plan

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€.

## 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 |

# Option 3 : Full Scope

## 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 counter-rotating at ~6.5 m
	+ 1m Double disk counter-rotating at ~10 m
	+ 1m Double disk counter-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 10B detector at 3m from sample, movable ±400mm vertically
* 1m2 10B 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.

## 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.

## 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 |
| High5 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 topicsImprove 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 requirements of the design - Complexity in design for monolith insert and light shutter | Schedule for external milestone | Observe | Schedule, budget, Quality and function | Follow the progress of the design and project schedule. FREIA TeamResponsible: Target |
| ***TARGET LEVEL ESS-0003739*** | Observe | Focus on Safety, feasibility, operability and requirementsResponsible: 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 3He 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 |

# References

[1] FREIA instrument proposal

[2] Reflectometry STAP report July 2016

[3] ESS Technical Design Report 2013