# Estia - Scope Setting Report

## Version 1.1

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# Summary

The purpose of this document is to describe the possible baseline options for the *Estia* project and how the instrument performance will be upgraded over time after the construction project to get from the day one scope to the full scope as envisaged in the instrument proposal.

*Estia* has been assigned to cost category A (9M€). The conclusion from analyzing the costs is that it is not possible to build *Estia* within cost category A in a manner that delivers expectable day one performance for most of the experiments in the instrument scope. This was also pointed out by the Scientific and Technical Advisory Panel (STAP), that states in their report that *Estia* seems to have be put in the wrong cost category.

Two possible baseline options are presented, both with the same full-scope after upgrade; (1) within cost category limits, (2) world leading instrument following the STAP advice.

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# 1 Overview

## 1.1 Science Case

(Polarized) Neutron Reflectometry (PNR) is a surface scattering technique used across a wide range of scientific disciplines including physics, chemistry, materials science, engineering and biology. The method allows the determination of depth sensitive structural and magnetic information present in thin film samples, with direct access to the scattering length density (SLD) of the materials and the average in-plane magnetic moment. The explored science ranges from fundamental investigations of interface and surface effects to functional devices. For this reason the reflectometers at ESS will need to be flexible enough to accommodate this wide range of experiments.

In the following we'll describe the main areas outlined by the STAP committee that are addressed with the technique:

**Soft Matter and Life Sciences** NR provides unique possibilities for the investigation of nanoscale structure and chemical composition of multicomponent thin film systems. Modern instrumentation may be used to routinely probe the air-liquid, solid-liquid and liquid-liquid interfaces all of which are relevant to the study of soft matter. Since the first dedicated instruments were constructed three decades ago soft matter studies have been a driving force in the development of the technique. The NR user base continues to grow and the largest sections of the community today are interested in soft condensed matter, polymers and life science systems. Although the ESS *FREIA* instrument will be dedicated to these kind of studies, especially build for horizontal air-liquid and liquid-liquid studies, there are several cases where *Estia* could be used for solid-liquid investigations with comparable performance:

- The possibility to study the solid biological/solid inorganic interface (implants, biosensors).
- In-situ environmental studies (polymer coatings, weathering). Such measurements require enough flux for kinetic studies, small spot sizes to scan across samples and may potentially also require space for sample environment.
- Lubricants or additives for systems on metal surfaces such as fuel additives.

- Materials science at solid-solid interfaces (other than electronics) i.e. concretes, polymer-polymer layering, joining etc., metal-metal (brazing, welding).
- Studies of surfaces such as artificial skin which would greatly benefit from small beam sizes.
- Forensic science, probing changes to interfaces when they interact with e.g. fingerprints, explosion residue, bio-weapon residue, shockwaves.
- Initiation of surface or near-surface reactions via stop flow/microfluidics chambers or triggered e.g. by laser flash, following switchable/responsive surfaces as they respond to stimuli.
- The measurement of nanoparticle concentration profiles in polymer based solar cells.
- Study of interfaces under "extreme conditions" for applications in food science (high pressure processing) as well as in marine biology.

The need for complimentary measurements such as X-ray reflectometry, ellipsometry, Brewster angle microscopy or spectroscopy measurements that may be carried out in-situ or simultaneously will become increasingly important. It is frequently seen that sample preparation is affected by transportation and increasing complexity leads to increasing problems in this area. It will therefore be critical to the success and reproducibility of experiments that secondary characterisation of samples is possible at or very close the time of the neutron measurements.

**Hard Condensed Matter and Magnetism** PNR remains a unique probe for the study of numerous characteristics of thin magnetics films. The ability of the neutron to probe buried magnetic interfaces and to investigate the detailed magnetic interactions in complex artificial magnetic nanostructures is a unique strength of the technique. All other probes are limited in some way or another by their lack of magnetic sensitivity or are dominated by surface or bulk averaging effects.

The proportion of NR experiments that study hard condensed matter has reduced when compared to soft condensed matter but there has still been a general increase in the number of user groups taking advantage of the technique. The type of measurements have changed, as in many cases, such investigations are now often just one part of a complex array of experiments that have been used to obtain incredibly detailed knowledge of a particular system. Hence the users tend to only rarely perform PNR experiments to answer specific questions, but they often perform some of the most technically challenging and intensive types of measurement.

The fields associated with hard condensed matter and magnetism are currently dominated by studies of multifunctional materials, complex heterostructures that are intended for use in data storage, diffusion processes and complex magenetic effects at the interfaces between layers in multilayer structures.

These are generic terms that cover an extremely broad range of physics and materials science. The direction that sample preparation and experimental demands are likely to push measurements in the future are:

- Sample sizes will continue to become smaller. It is already commonplace to see maximum sample sizes of $<10\text{x}10\,\text{mm}^2$.
- Patterned structures with 2 and 3d engineered structures will become more and more commonplace significantly enhancing the need for off-specular and GISANS measurements.
- In-situ complementary measurements of conductivity and other properties of the films will be increasingly demanded, leading to much more complex sample environment equipment. This will be made significantly easier if small beam sizes are available.
- A broad range of resolutions 1, 3, 5 and 10% $\Delta q/q$ are essential for the wide variety of requirements in this field.
- Low backgrounds are essential even with the ESS's enhanced flux. Reflectivities $<10^{-7}$ will be needed to further increase the techniques ability to study finer magnetic structural detail.
- High throughput and kinetic studies that necessitate large incident intensity and broad q-ranges.

## 1.2 Requirements

The top level requirements for *Estia*, following the scientific case, define the target scope for the instrument construction project. They have been formulated to capture the key aspects of the instrument proposal science case and are:

1. The instrument shall allow specular reflectivity measurements from samples between $1\text{x}1\,\text{mm}^2$ and $10\text{x}10\,\text{mm}^2$.
2. The instrument shall provide neutron polarization analysis with at least 95% polarization over the whole wavelength and divergence range.
3. The beam size at the sample position shall be controllable to minimize over illumination and concentrate on specific sample areas.
4. The instrument should minimize the background from high energy neutrons and other non-sample intrinsic sources.
5. The instrument should allow fast sample changes within $\approx$10 min or less.
6. The instrument should provide options for the measurement of off-specular and Grazing Incidence Neutron Scattering.

7. The instrument should provide a higher resolution option for investigations of thick samples.

## 1.3 Configuration Options

The special instrument configuration and optics of *Estia* have implications for a possible staging of upgrades, that distinguishes it from other ESS instruments. Mirror optics and most other in-beam components are spatially separated, allowing a later installation without changes to the initial design. On the other hand, the high precision necessary for the optical system alignment can hardly be upgraded at a later stage without total rebuild of the whole components.

Due to these facts we present the two configurations that all allow upgrade to the same full instrument scope. The presented configuration are:

1. A configuration almost within cost category A (9M€). Here all components not absolutely essential to transport a beam to the sample are removed.
   **Cost: 9.8M€**
2. A configuration meeting the most important scientific requirements with world leading performance following the STAP advice. In addition to allowing full-scope beam intensity PNR experiments with simultaneous spin-up and spin-down channels will be measurable.
   **Cost: 15.4M€**

## 1.4 General Assumptions

The budget presented hereafter is based on certain assumptions about the ESS contribution to the instruments and some boundary conditions imposed on the instruments, some of which could have significant impact on the costing if changed after the budget decision. In the following we will outline the most important aspects that the *Estia* team used and where additional costs need to be accommodated by ESS if significant changes occur.

- Biological shielding is based on the assumption that 200 mm of steel plus 500 mm of normal concrete will be sufficient outside the bunker wall. This falls in-line with the LoKi instrument, which is already in phase 2 of the instrument project.
- The bunker wall design is not finalized at this point and it therefore can't be estimated by the instrument team, what additional spending will be necessary for the instrument specific changes for the beam path through the bunker wall. These costs are not included in the options proposed here.

- Cost estimates for ESS delivered items are as provided by ESS groups up to July 5th 2016.
- All vacuum equipment, although defined by ESS vacuum groups, are included in the *Estia* costing.
- Design and construction of the monolith insert including cooling for insert and guides will be provided by ESS.
- The installation efforts of early instruments and bunker will be coordinated by ESS, the *Estia* construction estimates therefore the availability of the main crane of 50% during installation.
- No heavy shutter will be installed for *Estia*, this presumption includes that there will be no ESS rule for including these shutters.
- No additional ESS constrains will be added at a later point that require design changes or additional cost points.
- All software development including data storage, visualization, data analysis, EPICS integration, *Selene* adjustment and instrument controls will be provided by ESS and DMSC for no charge and is therefore not part of the instrument budget.
- To be able to approach the 9M€ goal for option 1, the probable extra cost (600k€) for hiring contractors to do e.g. machining work not possible at the ESS site during installation have been removed (Installation Infrastructure). The budget therefore assumes that only working hours for machining components have to be paid out of the instrument budget. This means for option 1 a full workshop and support stuff needs to be available at ESS from the beginning of installation to avoid any additional cost.

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

## 2.1 Scope

- Full feeder for two separate beam paths
- Full heavy collimation (necessary for shutter concept)
- No chopper, bandwidth will be limited by special frame-overlap mirror (fixed 3-10Å band)
- The virtual source will be of fixed size (10x10 $mm^2$), only rotatable
- Selene guides only equipped with a set of mirrors for one beam path and a single segment for horizontal divergence (0.1°x1.5°)
- Only one detector, as only one beam path will be installed initially
- No polarizers or analyzers will be installed, polarization will be done with the horizontal divergence segment of Selene 2
- No instrument specific sample environment will be available
- The adjustment of the sample to the beam must be done with manual stages

These limitations result in extreme reduction of the experimental capabilities as well as in the initial intensity (≈3% of full-scope).

This scope does **not** meet the top level requirements with respect to:

- Measure small sample sizes (#1), due to low initial intensity
- Polarization analysis (#2) will not be possible as well as most polarized studies due to missing control of magnetic field
- Beam size at the sample (#3) will only be partially controllable horizontally by the virtual source rotation
- Fast sample changes (#5) won't be possible due to lengthy manual alignment
- Although off-specular experiments will be possible, GISANS will not (#6)

- No higher resolution option (#7) will be avialable.

In addition to the high level requirements not fulfilled by this option there are additional practical limitations following from removing some components. Replacing the chopper with the frame-overlap mirror fixes the available wavelength band. On one hand this reduces usable intensity further, as the band needs to start at the lowest wavelength transmitted by the Selene guide. On the other hand it removes the flexibility to use longer wavelength for improved resolution or pulse-skipping for improved bandwidth. In addition, using one Selene mirror as polarizer removes the possibility of using unpolarized neutrons for higher intensity.

Thus, this scope **does not fulfill** the science case for *Estia*.

## 2.2 Costing

| | | **Cost [k€]** | | | **Work Units [person-years]** | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | **PBS Item** | Labor | Non-Labor | Total | 02 P. Management | 03 Design | 04 Construction | 05 Installation | 06 Commissioning | Total Work |
| 1 | Beam Transport and Conditioning System | 1 822.4 | 3 351.5 | 5 173.9 | 0.425 | 1.774 | 1.276 | 2.018 | 0.645 | 6.138 |
| 2 | Sample Exposure System | 173.8 | 88.4 | 263.1 | 0.088 | 0.177 | 0.057 | 0.155 | 0.141 | 0.618 |
| 3 | Scattering Characterization System | 139.0 | 365.0 | 504.0 | 0.155 | 0.286 | 0.270 | 0.163 | 0.136 | 1.541 |
| 5 | Experimental Cave | 309.9 | 657.0 | 966.9 | 0.188 | 0.672 | 0.155 | 0.962 | 0.044 | 2.021 |
| 6 | Control Hutch | 45.3 | 71.0 | 116.3 | 0.074 | 0.044 | 0.066 | 0.180 | 0.008 | 0.373 |
| 7 | Sampe Preparation Area | 21.6 | 11.2 | 32.7 | 0.038 | 0.031 | 0.000 | 0.105 | 0.000 | 0.174 |
| 8 | Utilities Distribution | 8.6 | 28.0 | 36.6 | 0.017 | 0.033 | 0.000 | 0.000 | 0.000 | 0.050 |
| 9 | Support Infrastructure | 88.5 | 145.0 | 233.5 | 0.026 | 0.195 | 0.000 | 0.288 | 0.133 | 0.642 |
| 10 | Control Racks | 558.1 | 146.3 | 704.3 | 0.221 | 1.163 | 0.088 | 1.944 | 0.605 | 4.022 |
| | Travel | 81.0 | 0.0 | 81.0 | | | | | | |
| | Phase 1 | 700.0 | 50.0 | 750.0 | 0.000 | 0.000 | 0.000 | 0.000 | 0.000 | 3.250 |
| | *Contingency* | | | *984.7* | | | | | | |
| | Sum | | | 9 847.2 | 1.232 | 4.375 | 1.913 | 5.814 | 1.713 | 18.827 |

## 2.3 Upgrade/Staging Plan

As with the option, this scope could be upgraded to the full scope by adding the necessary components without the need for large changes to the existing instrument.

At first it is envisioned to install affordable systems with large impact on the science case, including the full virtual source motorization, automatic sample positioning and the basic instrument specific sample environment (magnet, cryostat, hexapod). Following these components the bandwidth chopper will be a necessary component to install.

At any time with available resources the two Selene guides could be gradually upgraded for full horizontal divergence and the second beam path. This will also require an increase of shielding, that was taken out of the budget initially due to the reduced beam intensity. The later extension of beamline shielding will probably increase the total cost for this upgrade path. In parallel the polarization analyzers can be installed.

For the later upgrades common to both options see 4.

## 2.4 Risk

The major risk associated with this configuration is the loss of reputation for the ESS and in-kind partners due to the strongly reduced scientific performance. This option not only reduces the instrument capability to that of typical reflectometers at other sources but with missing SE achieves much less than is possible at any of the current instruments.

In addition to the global risks listed at the end of this document, option 1 has the following risks associated with the limited scope:

| Risk Level | Risk | Treatment Name | Treatment | Category | Treatment Plan |
|---|---|---|---|---|---|
| High 5x5 | Loss of reputation | Lower expectations | Mitigate | budget, quality and function | Communicate lower performance expectations to stakeholders. Begin early upgrade and seek funding. Responsible: ESS management |
| High 5x5 | Loss of support from in-kind partner | Get founding and expand scope | Mitigate | all | Communicate with stakeholders the minimum scope acceptable by PSI and try to get larger funding to expand scope or seek different in-kind partner, which might increase phase 1 cost significantly. Responsible: ESS management |
| | | Stop project | Observe | | *Estia* is a very unique instrument and it might be complicated to find a new in-kind partner to build it if PSI pulls back it's support. Responsible: ESS management |
| High 5x5 | Component failure or increased cost | Seek additional funding | Mitigate | all | Option is already minimal to deliver neutron beam to sample, leaving no flexibility for unforeseen design issues. A later increase of budget might become necessary. Responsible: *Estia* team, NSS technical |
| High 5x5 | No R&D | lower expectations | Mitigate | budget, quality and function | Foreseen R&D work for Selene adjuster implementation not included in option. Reduced beam quality and maybe delays and component failure with additional costs could be the result, so expectations need to be lowered. Additional funding could be sought out to support early tests of the adjuster system. Responsible: ESS management |

# 3 Option 2: World-leading Capability Following STAP Advice

## 3.1 Scope

- Full feeder for two beam paths
- Full heavy collimation (necessary for shutter concept)
- Bandwidth chopper
- Complete virtual source with rotation and size absorber positioning
- Complete Selene guide with two beam paths (2 x ($1.5^\circ$ x $1.5^\circ$) divergence)
- Both detectors will be installed initially
- Polarizers and polarization analyzers and normal frame-overlap mirrors available
- Instrument specific RT bore cryomagnet (>2T), flow cryostat (<5K) and sample changer
- Sample positioning with hexapod, alignment support with laser adjustment system

In contrast to the other option, this scope includes the full available intensity at the initial commissioning of the instrument, when the source intensity is lowest. The additional benefit of the two beams is the option to measure all 4 polarization analysis channels simultaneously (up-down incident beams and separation of scattered beams onto different areas of detector by the analyzers).

This scope does **not** meet the top level requirements with respect to:

- Although off-specular experiments will be possible, GISANS will not (#6)
- High resolution (#7) will only be accessible through the use of longer wavelengths with largely reduced intensity

Thus, this scope **does fulfill** most of the science case for *Estia*. The STAP has pointed out the absolute necessity of having the high intensity option together with polarization analysis and a minimum set of sample environment available for day 1 at *Estia*. This option therefore follows their top 3 priority items pointed out in the STAP report. The increased initial cost should be weighted against an intensity gain of factor 30 with respect to option 1, which will be very valuable in the initial ESS operation to allow larger number of users, especially if *Estia* will be one of the first beamlines in operation.

## 3.2 Costing

| | | Cost [k€] | | | Work Units [person-years] | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | **PBS Item** | Labor | Non-Labor | Total | 02 P. Management | 03 Design | 04 Construction | 05 Installation | 06 Commissioning | Total Work |
| 1 | Beam Transport and Conditioning System | 2 190.8 | 6 074.5 | 8 265.3 | 0.973 | 4.362 | 3.077 | 3.111 | 2.012 | 13.535 |
| 2 | Sample Exposure System | 184.4 | 451.4 | 635.8 | 0.088 | 0.376 | 0.194 | 0.225 | 0.252 | 1.136 |
| 3 | Scattering Characterization System | 213.8 | 907.0 | 1 120.8 | 0.199 | 0.419 | 0.402 | 0.296 | 0.224 | 1.541 |
| 5 | Experimental Cave | 309.9 | 657.0 | 966.9 | 0.188 | 0.672 | 0.155 | 0.962 | 0.044 | 2.021 |
| 6 | Control Hutch | 45.3 | 71.0 | 116.3 | 0.074 | 0.044 | 0.066 | 0.180 | 0.008 | 0.373 |
| 7 | Sampe Preparation Area | 21.6 | 11.2 | 32.7 | 0.038 | 0.031 | 0.000 | 0.105 | 0.000 | 0.174 |
| 8 | Utilities Distribution | 8.6 | 28.0 | 36.6 | 0.017 | 0.033 | 0.000 | 0.000 | 0.000 | 0.050 |
| 9 | Support Infrastructure | 88.5 | 145.0 | 233.5 | 0.026 | 0.195 | 0.000 | 0.288 | 0.133 | 0.642 |
| 10 | Control Racks | 558.1 | 146.3 | 704.3 | 0.221 | 1.163 | 0.088 | 1.944 | 0.605 | 4.022 |
| | Travel | 81.0 | 0.0 | 81.0 | | | | | | |
| | R&D Selene Guide | 150.5 | 209.5 | 360.0 | | | | | | |
| | Installation Infrastructure | 0.0 | 600.0 | 600.0 | | | | | | |
| | Phase 1 | 700.0 | 50.0 | 750.0 | 3.250 | | | | | |
| | *Contingency* | | | *1 544.8* | | | | | | |
| | Sum | | | 15 448.2 | 1.973 | 7.279 | 3.895 | 7.078 | 3.323 | 26.799 |

## 3.3 Upgrade/Staging Plan

As with the other option, this scope could be upgraded to the full scope by adding the necessary components without the need for large changes to the existing instrument.

At first it is envisioned to install the spatial spin resonance (SSR) flipper to increase wavelength resolution for a small cost. A test device build at SNS could already be tested at the beamline before the design and implementation is optimized for *Estia*.

For the later upgrades common to both options see 4.

## 3.4 Risk

In addition to the global risks listed at the end of this document, option 3 has the following risks associated with the limited scope:

| Risk Level | Risk | Treatment Name | Treatment | Category | Treatment Plan |
|---|---|---|---|---|---|
| Med. 3x3 | Unforseen shielding/optics costs | Reduce second beam path and seek funding | Mitigate | budget, quality and function | Unforseen additional cost for larger shielding or neutron mirrors might force the reduction of the initial scope. Reduced initial intensity will be accepted. Responsible: *Estia* team |

# 4 Full Scope Instrument

## 4.1 Upgrade Scope

Additional options that will be part of all upgrades are:

- Space-Time collimator (moving aperture) for $\lambda - \theta$ encoding and increased wavelength resolution
- Re-focusing mirror to the detector allowing high performance GISANS and incoherent background reduction measurements
- Ultra-focusing options, reducing minimal beam size to $\approx 10\,\mu$m for neutron microscopy and scanning local probe PNR
- Additional SE equipment for e.g. liquids handling and other non-magnetism related studies
- A spatial-spin-resonance flipper, only flipping a small wavelength range at a time, will be installed as second high resolution option.
- Two additional cryostats to allow sample change and cool down while experiment is running.
- Pulsed laser for pump-probe experiments.
- Kerr-effect add-on for laser adjustment system.
- Pressure cell capable of low temperatures.

## 4.2 Costing

The following lists a rough estimate of the costs of each component, adding 10% contingency to the total cost for the upgrade. Total cost for the full scope instrument is indicated at the bottom.

| | Component | Cost [k€] Labor | Non-Labor | Total |
|---|---|---|---|---|
| 1 | Space-Time collimator | 47.0 | 200.0 | 247.0 |
| 2 | Re-focus for GISANS | 100.0 | 250.0 | 350.0 |
| 3 | Ultra-focus option + Imaging | 150.0 | 300.0 | 450.0 |
| 4 | SSR Flipper | 50.0 | 20.0 | 70.0 |
| 5 | Pump-Laser SE | 50.0 | 150.0 | 200.0 |
| 6 | Liquids SE | 150.0 | 150.0 | 300.0 |
| 7 | Additional Cryostats | 20.0 | 30.0 | 50.0 |
| 8 | Kerr-effect | 50.0 | 10.0 | 60.0 |
| 9 | Pressure cell | 100.0 | 50.0 | 150.0 |
| | *Contingency* | | | *189.5* |
| | Sum | | | 1 894.7 |
| | Sum full-scope instrument | | | 17 342.9 |

## 4.3 Global Risks

The following summarizes general risks to the instrument project, that hold for all two staging options previously described.

| Risk Level | Risk | Treatment Name | Treatment | Category | Treatment Plan |
|---|---|---|---|---|---|
| High 4x3 | Delay in monolith or bunker project | Insert and in-bunker installation | Observe | schedule and budget | Follow the progress of the design and project schedule. *Estia* team. Responsible: target |
| High 2x5 | Conventional Facilities Delay | CF LEVEL ESS-0019533 | Observe | schedule, budget, quality and function | Access to hall 1 is a milestone for *Estia* schedule. *Estia* team. Responsible: CF |
| | | External areas like labs and workshops | Mitigate | | External areas will give the opportunity to start pre-installations Responsible: CF |
| High 3x5 | Significant changes to bunker | Shielding update plan | Mitigate | schedule, budget, quality and function | If ESS changes the bunker design significantly at a later stage this might have strong impact on *Estia* cost. An adjustment of funding should be through out. Responsible: *Estia* team and ESS group |
| High 3x4 | Detector solution development late | Detector action plan and schedule with mitigation plan | Mitigate | schedule, budget, quality and function | Detector technical group is following an action plan and schedule plan for developments. Responsible: Detector Group |
| Med. 2x4 | Increased ground sinking | Adjust heights | Mitigate | schedule and budget | If the ground sinking at vital point in the experimental hall exceeds expected values, it might be necessary to install new shims or different adjuster. The detailed design will try to minimize this risk by supplying large enough adjustment range, if feasible. *Estia* team |
| Med. 3x3 | Late delivery of key components | *Estia* schedule | Mitigate | schedule and budget | Properly assess delivery time and transportation, order most important components at early stage. Responsible: *Estia* team |
| Med. 2x4 | VS solution not suitable for rad. level | VS design change | Mitigate | budget | If the stage based solution of the preliminary design cannot sustain the radiation level in the bunker, a different one needs to be found, which likely will increase the cost. This is, however, expected to be much lower then the 10% contingency. |
| Low 3x2 | Mirror segment shape does not fulfill accuracy requirement | Imaging quality lost | Mitigate / Observe | quality | Regular communication with vendor and quality control of segments will be of large priority. If the degree of quality cannot be achieved some minor possibilities of *Estia* might show reduced performance. |
| Low 4x1 | Not enough coffee during commissioning phase | Self Brewing | Mitigate | quality and function | Bring own coffee brewing equipment. Responsible *Estia* |