Scope Setting Report for T-REX Instrument

	Name	**Role/Title**
Owner	T-REX instrument team, represented within the ESS project by: Nicolò Violini Hans Kämmerling	 Lead Scientist of T-REX project phase 1 Lead Engineer of T-REX project phase 1
Reviewer	Ken Andersen	Science Directorate
Approver	Shane Kennedy	Science Directorate

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1. OVERVIEW

This document is written to facilitate the Scope Setting Meeting of T-REX, scheduled for the 28th of October 2016 in Lund. It describes three potential instrument configurations and, as a consequence, various upgrade scenarios to reach the full scientific scope and performance.

An instrument configuration within the cost category C (15 M€) is presented. We stress that our conclusion from the budget analysis is that IT IS NOT POSSIBLE TO DELIVER a world class instrument within the cost category C, in a way that it matches the expectation of the wider scientific community, by delivering adequate performance and meeting the scientific requirements, in the context of a reliable and reasonable upgrade path.

Two more potential configurations are described: the “Competitive” one achieves the minimum detector coverage and shows competitive performance when comparing to world class existing instruments and the “Full Scope” configuration achieves performance anticipated in the instrument proposal. Since a reduced scope has an impact on the scientific capability, a rational description of the effect is provided and the analysis of every configuration is complemented with the proposed upgrade path and strategy to reach wider and full scope.

We stress here that the cost addressed in the instrument proposal is outdated, since new information came about the most expensive components: shielding, detectors, neutron optics, infrastructures. Labor cost has been reviewed and a smaller contingency has been applied, according to the ESS request.

According to ESS-0063538 various items in the budget are provided by the ESS-NSS free of charge to the instruments. In particular for the vacuum system, it has been proposed a budget of 326.7 k€, which includes development, integration design, procurement and installation. The instrument team considers it sufficient, so that no additional cost is added. Various items might be subject to change, when new information will come about: (i) ICS, for which the instrument budget should include non-standard components, but the standards are not issued yet; (ii) it seems that enough resources are allocated to DMSC scope to deliver data analysis software for INS in time for cold commissioning, (iii) the present cost information for infrastructures might change once a more detailed analysis is run during the final design, (iv) the cost for shielding has been calculated according to the calculation process proposed by the NOSG of ESS, (v) the cost for MG detectors are determined by the ESS Detectors Group and considered preliminary, subject to review once the design will be finalized. A very rough estimate of installation cost is possible at this stage, while logistics has been neglected because of the various uncertainties and unknowns.

The proposed timeline for the project is briefly analyzed stressing the key dates for time-critical components of T-REX. In particular we analyze in Section 4.1 a proposed strategy for mitigation of risks regarding the critical decision on detector technology.

1.1 Science case

1.1.1 Spectroscopy for a broad user community

Exploiting both thermal and cold ESS moderators, T-REX will allow measurements in a wide energy range (from 20 μeV to 140 meV), with good energy-wavevector resolution, with Polarization Analysis (PA) option and in repetition rate multiplication mode. As such, it will have the flexibility to satisfy the needs of a very wide user community. Polarized neutrons will allow the separation of magnetic and nuclear scattering, the analysis of polarization and eigenvectors of magnetic excitations, and the separation of coherent and nuclear spin-incoherent scattering (i.e. in hydrogen containing samples). Non-polarized neutrons will enable more traditional investigations on coherent excitations, spin correlations and fluctuations, relaxations and diffusion processes, in a broad range of samples and applications. By tuning the choppers frequencies and phases, the users can match the requested energy resolution. The use of a polychromatic beam allows the optimization over a relatively narrow energy transfer range for an individual wavelength, still covering a wider energy range with all the other wavelengths available in a single band. By choosing the beam collimation, the Q-resolution can be tailored to the needs of the users and proper background conditions can be achieved to perform clean measurements down to the lowest detection angles (1°). In view of the wide user community, the sample area will host various sample environment equipment, enabling high/low temperature, pressure, magnetic/electric fields. More complex studies, such as *in-operando* or levitation experiments, will be allowed by easy (top and side) access to the sample area and by auxiliary characterization tools in parallel to the scattering experiment.

1.1.2 Quantum phenomena

Excitations in quantum condensed matter range from tenths of μeV to hundreds of meV. Typical samples are low-dimensional, topological and frustrated materials, quantum magnets, unconventional superconductors, multi-functional oxides, molecular magnets. Often neutrons are the only means to study magnetic excitations throughout the Brillouin zone. Neutrons are also unique to study low energy excitations at temperatures in the mK range, e.g. quantum critical systems. In these fields, single crystals provide the most stringent information, but often only small specimen are available, rendering the observation of weak features difficult or even impossible. Such investigations will become readily possible thanks to the flux increase achieved by T-REX. In single-crystal studies, position sensitive detection is a must. In most cases, the relevant samples need to be measured in severe thermodynamical conditions, such as temperatures below few mK or above 1000 K, magnetic fields up to 10 T, pressures of several tens of GPa. PA is an essential asset in this context, as it allows separating different cross sections in a manifold of complex systems, ranging from heterogeneous magnetic thin films to multiferroics with chiral magnetic structures or magnetostriction effects.

1.1.3 Functional Materials

Functional materials, such as catalysis metals, ion-transport materials, fuel cell membranes, nanoporous or metal-organic frameworks for hydrogen storage, nanomembranes for filtration, thermo-electric and magneto-caloric materials promise applications for sustainable energies, environmental pollution, or water purification, with high impact on society. Their functional capabilities are often governed by a coupling mechanism between phonons and spin waves (e.g. magneto-calorics), or phonons and ion diffusion (e.g. ion-transport materials). PA and high incident energies are simultaneously necessary to separate phonon and spin waves. High energies and high energy resolutions are both needed to measure phonons along with the quasielastic signal of diffusion processes. The latter often occur in complex spatial geometries, thus requiring access to a wide Q-range. In hydrogen storage materials, position, lineshape and Q-dependence of the quantum rotational peak of H_2 at low temperatures provide rich information about number, strength and nature of the hydrogen binding sites. Again, this requires high incident energies, very good energy resolution and wide Q-range simultaneously. Finally, *in-operando* studies of prototype membranes, for fuel cells or nanofiltration, are nowadays severely limited by the reduced volumes of the working devices that can be installed in the neutron beam and will strongly benefit from the increased flux of T-REX. Functional materials are a typical field needing simultaneously all the capabilities of T-REX.

1.1.4 Disordered systems, Soft matter and Life Sciences

Neutron spectroscopy is nowadays a widespread tool for studying disordered materials, soft matter and life sciences. The number of such systems studied with neutrons ranges from simple and complex liquids to glassy systems; from natural and artificial polymers to proteins, nucleic acids and lipid membranes; from gels of all kinds to complex biological molecules, like chromatin in the cell nucleus or entire living cells. More recently new artificial polymers have been engineered to mimic the functional behaviour of real proteins, bringing the two fields of soft matter and life sciences even closer. In all such systems, it is clear nowadays that “functionality” is governed by *ps* and *ns* dynamics, where low-energy single-particle diffusional motions and high-energy collective modes play equally important roles, and are often entangled with each other. Such scientific fields obviously need the very wide dynamical range of T-REX, capable of measuring both quasielastic and inelastic scattering, independently of the specific kind of sample under investigation.

Moreover, soft matter and life science samples, where hydrogen atoms are ubiquitous and abundant, will greatly benefit from the availability of PA that will provide a clean way to separate coherent and incoherent scattering. Finally, recent cutting-edge experimental results are suggesting that functional vibrational motions have often an anisotropic character. Therefore a more stringent need to study oriented single-crystal samples is emerging also in the field of soft matter and life science. These will be pioneering experiments that future neutron sources will have to face. The high flux combined with the 4D-mapping capabilities of T-REX make the instrument ready for such scientific challenges.

1.2 Requirements

The top level scientific requirements for T-REX define the target scope for the instrument construction project. They have been formulated to capture the key aspects of the science case described in the proposal and are:

1. The instrument shall allow data to be collected to min en. transfer of 20 μeV.
2. The instrument shall allow data to be collected to max en. transfer of 140 meV.
3. The instrument shall allow data to be collected to minimum Q of 0.05 $Å^{-1}$.
4. The instrument shall allow data to be collected to maximum Q of 10 $Å^{-1}$.
5. The instrument shall match the size of the neutron beam to the size of the sample, assuring the homogenous illumination of rotating samples.
6. The instrument shall allow data to be collected to min scattering angle of 1°.
7. The instrument shall allow the analysis of neutron spin polarization.
8. The instrument shall allow the E resolution to be optimized for the experiment.
9. The instrument should allow the Q resolution to be optimized for the experiment.
10. The instrument should be capable of providing elastic energy resolution of 1% at incident energy of 2 meV.
11. The instrument should be capable of providing energy resolution of 3% for an energy transfer of 100 meV.
12. The instrument should be capable of providing a Q resolution in elastic scattering condition of 0.05 $Å^{-1}$ at incident energy 80 meV.
13. The instrument should allow data collection from samples < 10^2 mm^3 volume.
14. The instrument should maximize the S/B ratio in the scattering pattern.
15. The instrument shall allow the control of the physical and thermodynamical condition of the sample.
16. The System’s design shall provide the space and flexibility necessary to host and drive the staging process to achieve the full scientific scope.
17. T-REX should serve the user, science and instrumental development program without interruptions during source operation.

1.3 Full Scope Instrument Layout

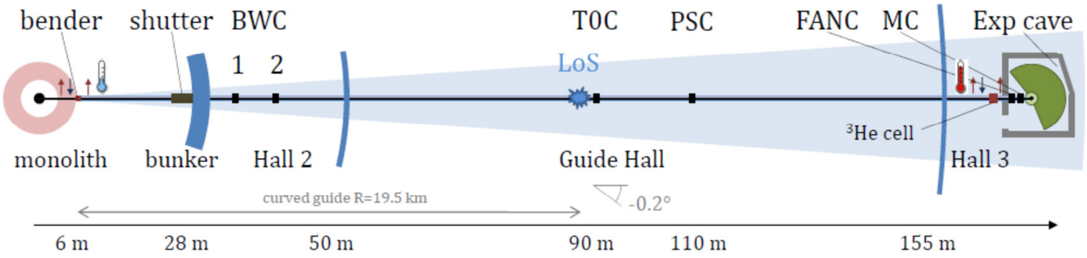

Fig.1 Schematic Full Scope instrument layout of T-REX.

The main building blocks of the T-REX instrument that are relevant to ensure its operation and functionalities, are: neutron optics systems, shielding, chopper systems, shutters, experimental cave, detectors, Beam Stop, Personnel Safety System (PSS), control hutch.

2. PROJECT TIMELINE

Phase 1 of the T-REX project started in May 2016 in collaboration between JCNS, Forschungszentrum Jülich and CNR and University of Perugia, Italy. The partners aim at delivering the instrument project for entering the hot commissioning in 2022, therefore as part of the first eight instruments of the ESS.

Many critical components are relatively advanced in their design as they can be based on the experience from a similar instrument project (TOPAS, MLZ, Garching), therefore delivering those components will involve a limited engineering effort. For some components engineering development is not needed and can be simply adapted

A major item is the detector system which could already be specified in many details, like the chamber, including its vacuum system, whose design is based on the TOPAS design. At the moment of writing a decision has not been taken on which technology shall be used for detectors of T-REX. A critical decision is expected to happen by the end of 2017 to guarantee stability of the development and detector construction.

High-speed choppers are crucial for T-REX. With adaptions based on work in phase 1, the experts from the Jülich chopper group are confident to deliver the chopper system for T-REX and plan for cold commissioning for end of 2021. The chosen neutron optics is rather simple and efficient, and according to a leading company, it can be produced in time. Simulations of the fast neutron transport are still pending, but we do not expect that conceptual changes will be necessary, since shielding issues can be covered at reasonable cost. The development of T0 choppers is taken by the ESS in agreement with our requirements. Even if this new development would not be available for hot commissioning or start of user operation, a safe fall back option is to work without T0 choppers and sacrificing ~10 % of the TOF frame.

The project timeline of the basic instrument for user operation is essentially independent of the choice of configuration that will be made. The full scope configuration can also be reached via upgrades of the other configurations.

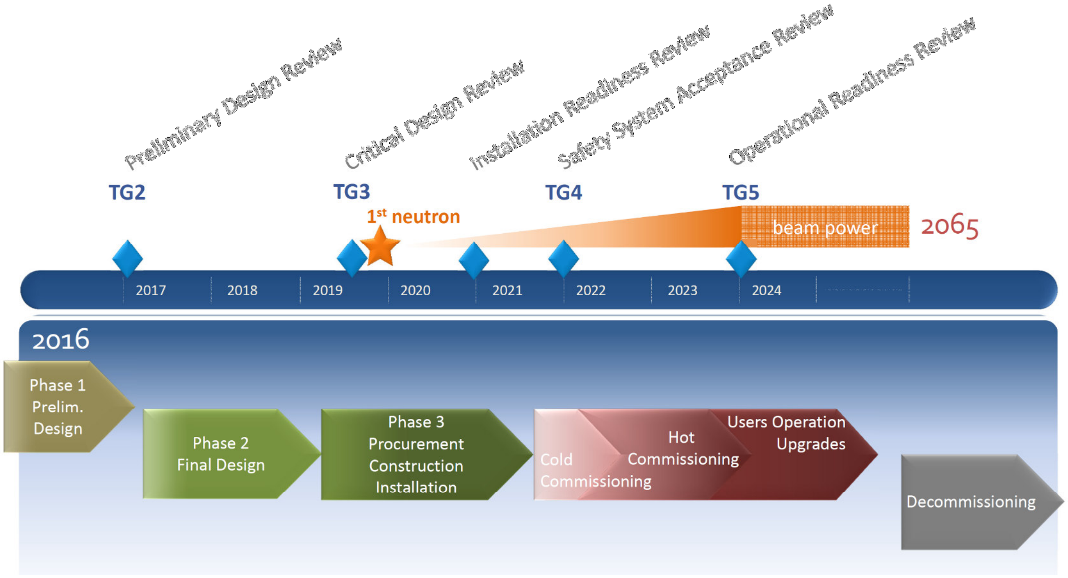

Fig. 2 Timeline of the T-REX project

3. CONFIGURATIONS

We present three configuration options:

1. A configuration within the given **Cost Category C** (15.0 M€).
2. A configuration termed **"Competitive"** that meets prioritized scientific requirements with a competitive performance aiming at a world-class instrument (with full upgrade capabilities to the full scope). Cost: 19.5 M€.
3. A configuration that provides **"Full Scope"** and is named as such. Cost: 22.6M€.

10 % contingency is included in all configurations.

13.6.15 T-REX	**within cost category C**	**competitive**	**full scope**	**proposal**
13.6.15.1 Beam transport and conditioning system	6260	7361	7731	7110
13.6.15.2 Sample exposure system	70	289	1737	200
13.6.15.3 Scattering characterization system	2408	5090	6085	4220
13.6.15.5 Experimental cave	725	725	725	650
13.6.15.6 Control Hutch	25	25	25	30
13.6.15.7 Sample preparation area	26	26	26	0
13.6.15.8 Utilities distribution (Infrastructure)	185	185	185	0
13.6.15.9 Support infrastructure	44	44	44	0
13.6.15.10 Control racks	0	0	0	0
13.6.15.12 Integration control and monitoring	56	94	94	0
labor	3711	3711	3711	4080
contingency	1501	1950	2262	2642
consumables				1000
total cost in k€:	**15010**	**19499**	**22624**	19932

Table 1 The total cost breakdown for three different configurations of T-REX is compared to the table of cost from proposal (Apr '15).

Configurations 2 and 3 are identical for most components and differ mainly by the detector coverage and sample environment equipment. An upgrade path from configuration 2 to 3 is possible. T0-chopper has been included equally in the two options, one more chopper is included in configuration 3. The oscillating radial collimator is included equally in the two options, following the STAP advice.

In order to avoid redundancy in description of each option, we focus on the key differences between them. For an easier comparison, the cost breakdown, the budget and schedule for the three configurations are given in the summary table.

While the most of instrument components have the same costs in all three configurations, the variation in price is related to detector coverage and sample environment (Tab. 1). It is clear from Table 1 that the detector system and the shielding are the greater cost items for the instrument.

In view of expected current budget limitations we have analyzed possible detector modifications for a best performance to cost ratio.

Table 2. The cost breakdown of three different options

		phase 1	phase 2	phase 3	phase 4	phase 5			
13.6.15 T-REX	**config**	**Preliminary Design**	**Detailed Design**	**Procurement Construction**	**Installation**	**Cold Commissioning**	**Total**		
13.6.15.1 Beam transport and conditioning system	base	0	0	6179	81	0	6260		
	comp	0	0	7280	81	0		7361	
	full	0	0	7650	81	0			7731
13.6.15.2 Sample exposure system	base	0	0	0	70	0	70		
	comp	0	0	0	289	0		289	
	full	0	0	0	1737	0			1737
13.6.15.3 Scattering characterization system	base	0	0	2408	0	0	2408		
	comp	0	0	5090	0	0		5090	
	full	0	0	6085	0	0			6085
13.6.15.5 Experimental cave		0	0	538	187	0	725		
13.6.15.6 Control Hutch		0	0	0	25	0	25		
13.6.15.7 Sample preparation area		0	0	0	26	0	26		
13.6.15.8 Utilities distribution (Infrastructure)		0	0	0	185	0	185		
13.6.15.9 Support infrastructure		0	0	0	44	0	44		
13.6.15.10 Control racks		0	0	0	0	0	0		
13.6.15.12 Integration control and monitoring		0	0	56	0	0	56		
labor		398	1104	663	994	552	3711		
contingency	base	0	0	751	300	450	1501		
	comp	0	0	975	390	585		1950	
	full	0	0	1131	452	679			2262
total cost in k€	base	398	1104	10593	1913	1002	**15010**		
	comp			14639	2221	1137		**19499**	
	full			16160	3732	1231			**22624**

3.1 CONFIGURATION 1: COST CATEGORY C

In the first configuration, we tried to include the following recommendations of the STAP:

- emphasis is given to thermal neutrons,
- as much as possible detector coverage on day one, where 70 deg is the absolute minimum advice by the STAP,
- priority in detector coverage should be given to forward scattering, on the left side as seen from the neutron path, so that any SEE could be shared with C-SPEC,
- sample environment equipment includes only the Orange cryofurnace.

In order to limit the instrument budget within the cost category C, the following budget items are **NOT INCLUDED**:

- the bender for extraction of cold neutrons,
- the T0 chopper and the FAN chopper,
- collimators of the incident beam,
- radial oscillating collimator.

Moreover the configuration does not provide any polarization capability, because the polarization related devices are NOT INCLUDED in the cost category.

We note that the STAP recommendations for a basic and minimal version of the instrument cannot be fulfilled within the category C budget, independent from the chosen detector technology, MG (or ^{3}He 6 bars tubes), in particular the detectors would cover nearly 19% (or 16 %) of the anticipated active area, maximum angle 34° (or 29°).

3.1.1 Configuration 1: Impact on Science Case

The modular structure of detectors enables an upgrade path to cover a larger angular range, but in the basic configuration the instrument will keep only its basic features by detection limited at small angles, below 34°. The instrument will be still able to provide inelastic neutron scattering patterns with high energy resolution, by using only incident energy from 16 meV to 160 meV and exploring the range of energy transfer from 0.5 meV to 140 meV in a limited Q range (max Q: 5.1 $Å^{-1}$ at 160 meV and 1.6 $Å^{-1}$ at 16 meV incident energy). The instrument won't be able to provide efficient measurements using incident energies from 2 meV to 16 meV, because it will use the brightness generated by the thermal moderator in this energy range. The guide system will still provide 10 fold increased flux on sample compared to existing thermal instruments even at a reduced source power of 2 MW, but only a small fraction of the scattered neutrons can be detected. The signal to noise ratio won't be optimal because of the absence of the T0 chopper and the radial oscillating collimator.

The limited (Q,E) coverage concerns the entire science case, but particularly the core experimental investigations on single crystals in magnetism and material science.

According to the scope setting guidelines, we anticipate that, assuming an ESS power of 2 MW, the detected intensity falls severely below its full potential, down to a level of about 8 % taking into account the reduced power and detector coverage. Reducing (Q,E) space and lowering the overall efficiency make the instrument NOT competitive with existing thermal only instruments, like 4-SEASONS (J-PARC), MAPS and MERLIN (ISIS), HYSPEC, ARCS and SEQUOIA (SNS).

Without Polarization Analysis the instrument can run only using non-polarised neutrons, therefore missing a significant fraction of the scientific scope (see below for further discussion).

Configuration 1 will have a **STRONG** negative impact on the scientific scope:

- **Magnetism**: low detector coverage and energy band limited to the thermal range would severely limit the capability to measure small energy gaps, magnetic excitations in high temperature superconductors and multi-functional oxides and spin correlations in molecular magnets. Basically the entire area of frustrated magnetism and quantum criticality will be missing. Without PA it will not be possible to realize the fundamental separation of magnetic and phonon scattering cross sections and disentangle the various contributions to neutron cross sections, therefore compromising the capability to investigate the nature of excitations, like e.g. chiral dynamics.
- **Functional Materials**: the low detector coverage and the resulting upper limit of momentum transfer prevent even basic investigations of lattice dynamics including the mapping of phonon dispersions. Diffusive motions could not be addressed due to both too coarse energy resolution using only thermal neutrons and too small Q-range. The absence of PA removes new opportunities offered to study the coupling mechanism between phonons and diffusive motions or to distinct incoherent motions addressing the spin-incoherent cross section. Without PA this instrument configuration will not be able to make significant new contributions to this highly active and very fast developing field of research, e.g. for the study of incoherent motions of elements such as H or Na.
- **Soft-matter and Life Science:** low detector coverage and energy band limited to the thermal range would severely limit the capability to study low-energy diffusions and relaxation motions. Without PA the separation of coherent and incoherent scattering cross section would not be possible, therefore compromising this peculiar feature.

3.1.2 Configuration 1: Impact on High Level Scientific Requirements

The following High Level Scientific Requirements CANNOT be matched by this configuration:

1. The best energy resolution of 20 μeV CANNOT be achieved if the cold extraction is not optimal, because the flux won't be high enough. Therefore also the HLSR number 10 CANNOT be achieved.
4. The covered Q range is limited to 5.1 Å^{-1}.
6. The absence of collimators in the incident beam DOES NOT allow optimization of the Q resolution for small detection angles, whereas the absence of the radial

oscillating collimator DOES NOT allow measurements with optimised collimation of the scattered neutron beam. Therefore also the HLSR number 12 CANNOT be achieved.

14. The signal-to-noise ratio is not optimal because of the absence of T0 chopper and radial oscillating collimator.
15. Missing essential Sample Environment Equipment DOES NOT enable to achieve the control of physical and thermodynamical conditions of samples according to science case for full scope.

3.1.3 Configuration 1: Upgrade Options

According to STAP recommendation the highest priority should be given to increasing the detector coverage, in order to make a world-class instrument, and finally the full detector coverage should be achieved.

Here it's worth to address a basic difference between MG and ^{3}He detectors, which is analysed in more detail in the risk section:

Upgrade path description	MG detectors	^{3}He PSD tubes
Increasing detector coverage from Configuration 1 to "Competitive"	2.35 M€	2.35 M€
Increasing detector coverage from Configuration 1 to "Full Scope"	3.48 M€	6.06 M€

We expect to collaborate with other instrument teams to share the cost of development and possibly procurement of new sample environment, which can be used by the instruments of the same class, in particular C-SPEC. The additional SEE (CCR, ILL furnace, clamp cells, HV supply) with additional funding of 219 k€, will bring the instrument to have the same equipment of the "Competitive" configuration.

Even though polarization capabilities can be added later in an upgrade path, it will be extremely difficult and expensive to integrate at a later stage the polarizing bender and the guide field over the entire guide length, because it is part of the guide structure. As alternative to the solution proposed so far, the polarization of cold neutrons could be obtained through a SM cavity placed further downstream (to reduce cost/impact of the upgrade). Nevertheless the configuration with the cavity will provide a polarized flux reaching only 60 to 70% of the proposed option with the combined cold extraction/polarization bender. The cost of the upgrade, to bring the instrument at the "Competitive" configuration, should not exceed the cost of the entire PA equipment, which is estimated in 547 k€.

To the best of our knowledge, at the moment of writing, the process for a later installation/integration of components inside the bunker is not defined in detail. First of all this affects any considerations regarding the future installation of the benders (i.e. polarizing and non-polarizing) for extraction of cold neutrons. A potential solution is under investigation in collaboration with the NOSG of ESS, which is based on the integration of the bender in the light shutter system. Moreover the T0 chopper could be installed either inside the bunker or further downstream outside the LoS. The installation inside the bunker could be facilitated by the pre-installation of the support structure at the anticipated position.

The FAN chopper, the collimators of the incident beam and the radial oscillating collimator could be installed at a later stage, given that an accurate provision is made regarding space requirements. For instance, the installation of the FAN chopper can be facilitated by adequate planning of the space around its position. For the installation of the collimators, provision must be taken in the design of the vessel around the sample position.

3.1.4 Configuration 1: Risk

A brief analysis of risks related to delivering this configuration is given in chapter 4.

Here we want to point at the risk that the required upgrades of the insufficient detector coverage may take too long time (see examples at other facilities) and frustrate potential users of the ESS.

3.2 CONFIGURATION 2: COMPETITIVE

The aim of this configuration is to make T-REX competitive with instruments at other facilities. While the flux gain as shown in the proposal will be realized, the increased detector coverage assures that the thermal performance of the instrument will be world leading. The flux at the sample increases with the ESS power and at 2 MW reaches 2/5 of the numbers in T-REX proposal, making the instrument gain at least one order of magnitude, when comparing to existing instruments configured at similar resolution conditions. We confirm gain factors already shown with respect to other instruments. Anyhow, following the request to emphasize the thermal performance, we discuss here briefly the expected gain, when compared to the world class instrument MERLIN at ISIS. When operating at 5% elastic energy resolution at 45 meV, T-REX will have 10 times greater monochromatic flux at the sample and nearly 5 times greater detected intensity. These are obtained from the flux numbers available for MERLIN and scaling down according to the smaller solid angle covered by T-REX, nearly 2 times less than MERLIN. Once more we stress that with the design of T-REX we aim at performing INS differently and not simply faster because of the increased flux, by combining the use of polychromatic experiments with Polarization Analysis over a wide dynamic range. This characteristic is not available nowadays at any instrument.

The realization of the "Competitive" configuration requires increasing the category C budget by more than 4 M€. This additional budget will help us build a very competitive instrument with a scientific scope that covers much of the original proposal. The major difference to configuration 1 is the increased detector coverage to reach the 70 deg scattering angle in the horizontal plane, which the STAP considered as the minimum to have an instrument to cover the 'thermal' and the magnetic science case. The upgrade to full scope will be straightforward.

One may notice here that the budget of "Competitive" configuration is independent from the chosen detector technology, because of including two equally costed solutions: MG with all the mechanical components for the first day and upgrading only the electronics and ^{3}He PSD tubes (6 bars ^{3}He filling pressure) full height covering 50% of detection area. Therefore the upgrade to full coverage comes for different prices, whereas the cost within this configuration is the same.

Moreover the instrument includes a T0 chopper unit, the Fan chopper, the radial collimator and additional SEE (CCR, clamp cells, HV supply, for additional 219 k€), which benefits most from the unique capabilities of T-REX, e.g. high flux to measure small sample volumes or PA for multiferroics.

3.2.1 Configuration 2: Impact on Science Case

With the increase of the detector coverage T-REX will be a competitive instrument. At high neutron energy, the momentum transfer up to 10 Å^{-1} can be accessed to allow the measurement of vibrations/lattice dynamic up to large Q. With the provision of bispectral extraction and polarization analysis unique investigations of spin excitations will become possible. The higher signal-to noise-ratio will enable to study weak inelastic signals.

Configuration 2 will have a **MODERATE** negative impact on the scientific scope of T-REX because the absence of detectors at large angles limits significantly the available Q range only when using cold neutrons.

- **Magnetism:** Investigations requesting ultimate energy resolution, i.e. by use of long wavelength neutrons, will have too small Q-range. Typical examples include frustrated magnets and molecular magnetism.
- **Functional Materials:** studies of diffusive or relaxational processes and potential interactions with lattice dynamics rely on the combination of ultimate energy resolution and large available momentum transfer range.
- **Soft-matter and Life Science**: the use of polarization analysis for the distinction of coherent and incoherent scattering will be limited by the reduced Q-range in studies of diffusive motions.

3.2.2 Configuration 2: Impact on High Level Scientific Requirements

The configuration has an impact on High Level Scientific Requirements number 4, in that the maximum wavevector transfer CANNOT be achieved when using cold neutron energy. The configuration will have limited capability to control physical and thermodynamical conditions of the sample (HLSR n. 15).

3.2.3 Configuration 2: Upgrade Options

According to STAP recommendation the critical upgrade is to bring detector to completion, i.e. increase the coverage up to 100%. This can be done stepwise. We refer to the risk analysis section for a discussion about comparing upgrade path of MG and ^{3}He detectors.

Upgrade path description	MG detectors	^{3}He PSD tubes
Increasing detector coverage from “Competitive” to 75% coverage	0.5 M€	1.9 M€
Increasing detector coverage from “Competitive” to “Full Scope”	1.1 M€	3.7 M€

Every additional SEE provided by the ESS can be used on T-REX to expand the scientific scope towards the full scope capability. Additional funding of 1448 k€ will bring the instrument to have the full scope SEE. We anticipate that part of full scope SEE could be shared with other instruments, so that a share of the cost is also possible. The SEE to be included in the upgrade path is listed here in order of priority. Priority should be given to SEE not included in the ESS pool: ^{3}He sorption stick and humidity chamber. Moreover the following SEE should be procured in order of priority, according to the expected demand: vertical cryomagnet (7T), Paris-Edinburgh cell, gas cells and gas handling system, IR furnace, ES levitator, pump&probe set-up.

A second unit of the T0 chopper could be installed at a later stage, assuming that an accurate provision is made regarding space requirements. For instance, the installation can be facilitated by adequate planning of the space around its position, including shielding design.

3.2.4 Configuration 2: Risk

A brief analysis of risks related to delivering this configuration is given in chapter 4.

There is the risk that the upgrade of the full detector coverage may take too long time (see examples at other facilities) and that the full scientific scope of the proposal will not be delivered according to user needs and expectations.

3.3 CONFIGURATION 3: FULL SCOPE

The “Full Scope” configuration includes full detector coverage of 2.5 sr. The world-class sample environment includes: ^{3}He sorption stick, humidity chamber, vertical cryomagnet (7T), Paris-Edinburgh cell, gas cells and gas handling system. This configuration includes more expensive bender and polarizing bender, which are based on a lamellar design providing higher accuracy.

3.3.1 Configuration 3: Impact on Science Case

The “Full Scope” configuration represents how T-REX can be a world-leading Direct Geometry Chopper Spectrometer addressing the entire scientific scope of the instrument, which was endorsed by SAC and STAP.

3.3.2 Configuration 3: Impact on High Level Scientific Requirements

The “Full Scope” configuration will match all the High Level Scientific Requirements of T-REX listed in this document.

3.3.3 Configuration 3: Upgrade options

Despite the “Full Scope” configuration will address the very broad scientific case of T-REX, it is flexible enough to provide more capabilities through the upgrades described below.

1 The state-of-the art SEE. Considering that magnetism is one of the main science drivers of T-REX, availability of various magnets in the sample environment pool is important, either being instrument specific or in shared efforts with other instruments. The availability of IR furnace, pulsed magnet, pump and probe set-up is also important to develop the user program efficiently.
2 An additional T0 chopper to improve the background level could be installed inside the bunker, to further reduce the background noise due to the prompt pulse.
3 The resolution limits considered in the present proposal are determined by the maximum chopper speed available nowadays. Future developments can provide a higher resolution with very similar flux, as the reduction of intensity in an individual pulse is compensated by a higher pulse density. Additionally the realization of an optically blind four chopper system, as introduced in the VOR proposal, would allow a continuous optimization of the energy transfer region of interest as compared to the discrete choice offered by the combination of different windows on the PSC and MC discs.
4 A supermirror analyser array could be considered as an alternative analyser. Filtering high final neutron energies, it would be efficient for deep inelastic scattering with low final neutron energy. As it would cut out the high neutron energies it would avoid frame overlap from the subsequent pulse and therefore enable higher repetition rates with the respective flux gains. However the cost of such a device is much higher and the flexibility is lower compared to a wide angle ^{3}He spin filter cell and this is the main reason for keeping this device as part of the upgrade path.

3.3.4 Configuration 3: Risk Analysis

A brief analysis of risks related to delivering this configuration is given in chapter 4.

4. RISK ANALYSIS

4.1 Detector technology

The major risk for T-REX project is related to detector technology: it involves technical, schedule and cost risks.

The MG detectors tests performed, and still running, on CNCS are very promising and show a significant effort made to provide an alternative to ^{3}He, at least for longer wavelength. Following the STAP advice, our concern is the characterization of efficiency and background of the multigrid detector for high energies, which should fairly compare with ^{3}He. T-REX emphasizes the use of high energy neutrons and low efficiencies of the multigrid would be a concern for performance, so that it should reach the benchmark of ^{3}He tubes 6 bars at least. The construction and test of a prototype with the characteristics suitable to T-REX (i.e. designed to achieve higher efficiency for thermal neutrons) would be an asset in the critical path towards the decision. Therefore we envisage following up with the ESS Detectors Group the progress with the development at a scientific level. A technical risk is associated with the MG integration with the vacuum chamber. As part of phase 1 we are investigating a conceptual engineering design, which would need continuation: final engineering design, FEM calculations, procurement, construction and tests on a prototype before proceeding to final construction, vacuum and mechanical tests and installation. Engineering work is included in personnel cost, whereas the cost for materials and construction has been estimated in 97.5 k€, independent from the instrument configurations.

The decision on the detector technology to be used for T-REX is a key milestone towards the delivery of the project and is expected to happen by the end of 2017, without compromising the schedule.

There is a basic difference between MG and ^{3}He detectors approaches to the upgrade, which is worth to take into consideration as part of the cost risk:

- MG detectors are to be constructed in house at the ESS, therefore one may note that the development costs for the specific detector modules are covered by first detector segments only and not by the serial production. Moreover any future upgrade needs restarting the coating production with exactly the same settings, which requires many calibration runs, re-installation of holders for the blades. Likely new technicians will be trained for coating production, grid assembly and wiring. The entire process can be pointed out as rather complex and shows hidden costs, which are now difficult to establish, therefore cost risky. All new parts must be procured in smaller quantities, therefore at somewhat higher rates. The cost of any upgrade has been estimated neglecting this unknown. The ESS Detectors Group proposed a potential mitigation of the cost risk that comes from production of all the hardware components for the first day and upgrading only the electronics, when resources are available. The instrument configuration “Competitive” includes this solution.

- At the moment of writing it is fair to assume that enough ^{3}He gas is available on the market, so that ^{3}He tubes can be procured off-the-shelf, with the requested specifications. GE Oil & Gas provided the instrument team with price information for ^{3}He detectors at various pressures of 6 bar, 8 bars, 10 bars, including also mounting frames and front-end electronics. Therefore any future upgrade is a comparably straightforward procurement process, which might happen at any time resources are allocated, even in small amount. Of course the upgrade process will be subject to risk of price fluctuations, pending on the availability of gas on the market. Moreover we can't rule out that procurement of small amount of tubes might result in higher rates per tube, so one may envision several steps in increasing detector coverage.

4.2 Risk categories for main building blocks

Three different categories of risks are identified: technical, cost and schedule related. The analysis is limited to major building blocks and budget items. We considered major risks which may impact significantly the instrument project. The probability was assigned to each potential event. The risk level then was calculated by multiplying probability by estimated effect. As a result, the high, medium and low risk levels were identified.

Low (1-4)
Medium (5-6)
High (7-15)

Technical related risks

Risk	Probability (1-5)	Effect (1-5)	Risk level	Mitigation strategy
Detectors may not meet requirements	2	4	8	Close follow up development with Detectors Group, plan tests
T0-chopper failure	2	4	8	Operate without, if beam not blocked
Bi-spectral switch misaligned	2	3	6	Radiation hard alignment mechanism
Insufficient shielding (for background)	2	3	6	Add shielding, accept background level
Settlement of buildings	2	3	6	Re-align optics
M-chopper failure	1	5	5	Use established technology / vendor
Bandwidth chopper failure	1	5	5	Use established technology / vendor
Heavy shutter failure	1	5	5	Choose simple reliable components
Software may not meet requirements	1	4	4	Plan additional resources
Neutron optics may not meet requirements	1	3	3	Accept lower performance / contract with vendor

Polarization Devices may not meet requirements	1	3	3	Accept lower performance / contract with vendor/ Use contingency

Cost related risks

Risk	Probability (1-5)	Effect (1-5)	Risk level	Mitigation strategy
Increase of personnel costs due to delays	3	3	9	Use contingency, Assign other jobs
Detectors cost underestimated	2	4	8	Reduce detector coverage, Use contingency
Cost of any component underestimated	2	3	6	Use contingency
Shielding cost has to be increased (because of background or safety)	1	3	3	Use contingency

Schedule related risks

Risk	Probability (1-5)	Effect (1-5)	Risk level	Mitigation strategy
Delay in choppers delivery	2	5	10	Select reliable vendors, early procurement
ESS infrastructure not yet ready	2	4	8	Plan accordingly
Delay in detector delivery	2	3	6	Early procurement, start with lower coverage
Design and manufacturing of T0-choppers are delayed	3	2	6	Operate without T0-choppers
General procurement delays	2	3	6	Early procurement
Delay in neutron optics delivery	1	5	5	Early procurement
Sample preparation lab at T-REX is not ready for day one operation	4	1	4	Temporary use sample preparation labs available at ESS