Opportunities for Large Scale Structures Research at the European Spallation Source

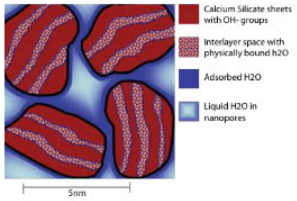
1st Workshop on Research & Innovation in Poland

ANDREW JACKSON
HEAD OF LARGE SCALE STRUCTURES DIVISION

2025-07-07

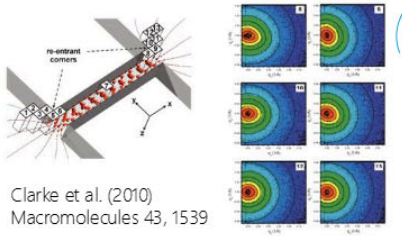
LSS Science Areas

Multi-Component



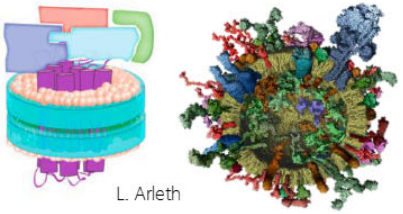
Allen AJ, Thomas JJ, Jennings HM. Nature Materials, 6(4), 311 (2007)

Non-Equilibrium



Clarke et al. (2010) Macromolecules 43, 1539

Bio-molecular Complexes

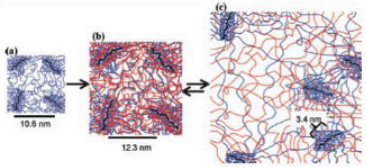


L. Arleth

Operating Devices

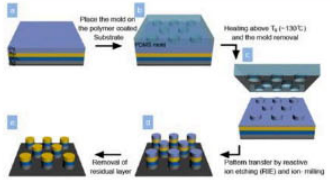
Alfred Hicks/NREL

Hierarchical Structures



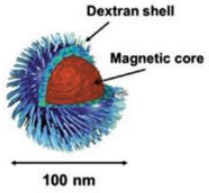
Waters et. al (2011) Macromolecules 44 5776

Patterned Materials



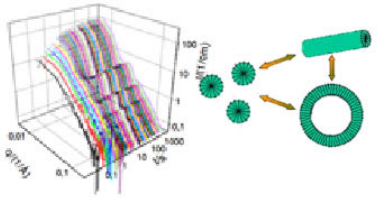
Kim et al. (2012) Nanotechnology **23** 315302

Hybrid Soft-Hard



Krycka, K. L., et al. *J. Appl. Phys.* **2011**, *09*, 07B513

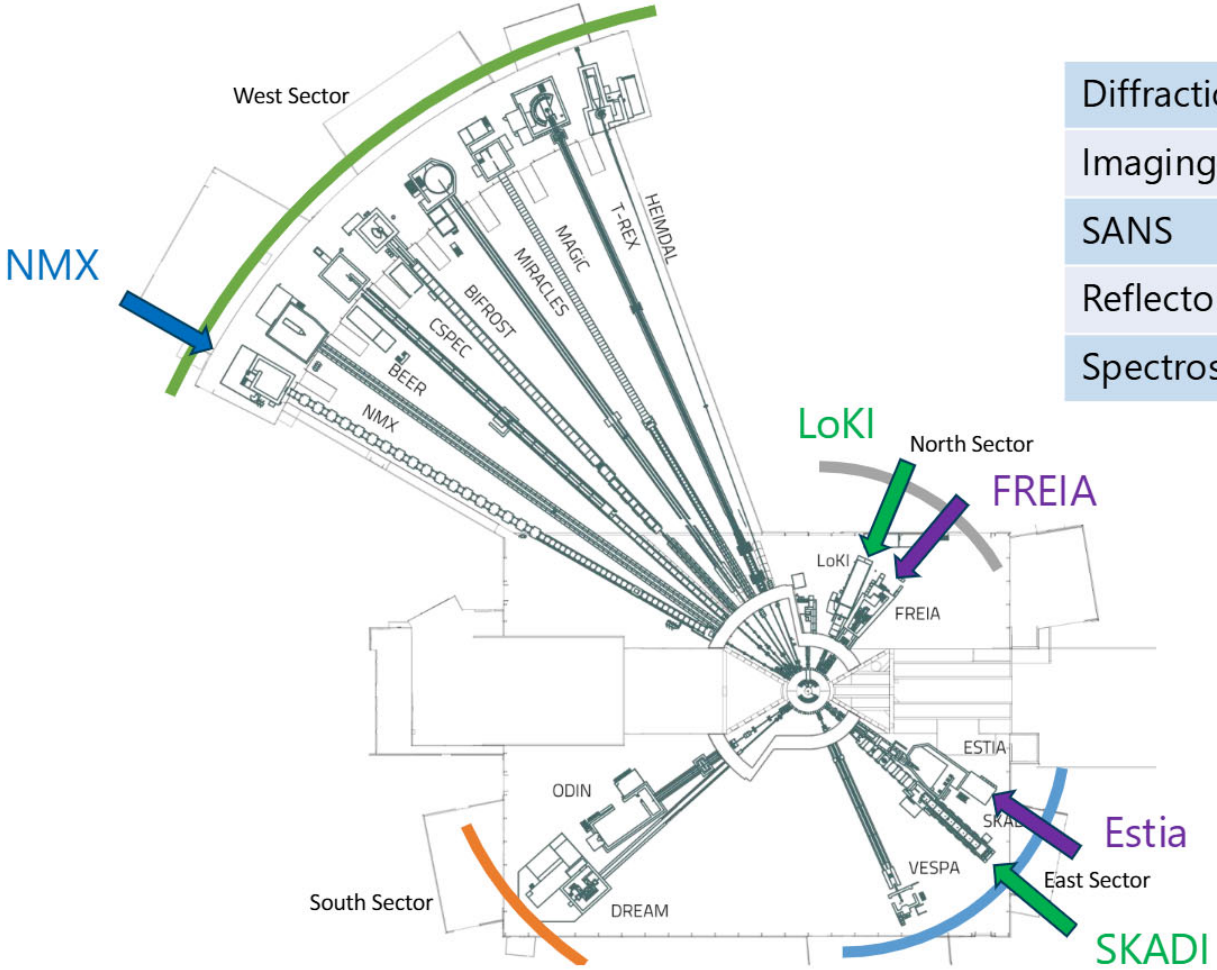
Kinetics



Bressel et al. (2010) Coll. and Polym. Sci. 288, 827

Large Scale Structures Instruments

Small Angle Neutron Scattering, Neutron Reflectometry & Neutron Macromolecular Crystallography



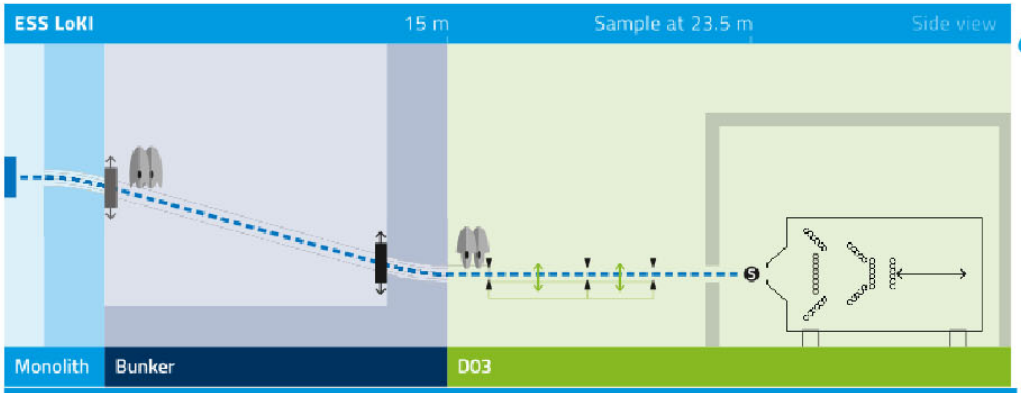
Diffraction	DREAM, HEIMDAL, BEER, MAGiC, NMX
Imaging	ODIN, TBL
SANS	LoKI, SKADI
Reflectometry	Estia, FREIA
Spectroscopy	BIFROST, CSPEC, T-REX, MIRACLES, VESPA

SANS
Reflectometry
Macromolecular Crystallography

LoKI

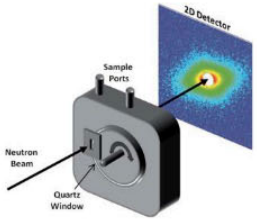
SANS for Soft Matter, Materials, & Bio-Science

Science and Technology Facilities Council



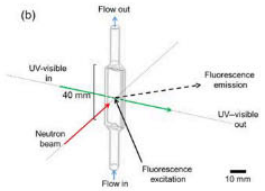
high flux, wide simultaneous size range, and a flexible sample area.

Changes over Multiple Length-Scales:
Structures Under Shear



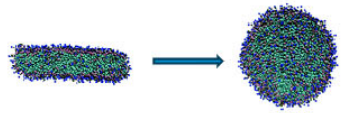
Soft Matter, 2011, **7**, 9992

Automated and Autonomous SANS:
Flow cell with complementary techniques



Rev Sci Instruments 91, 075111 (2020)

Non-Equilibrium Studies:
Self-Assembly & Kinetics



Colloid Polym Sci, 2010, **288**, 827

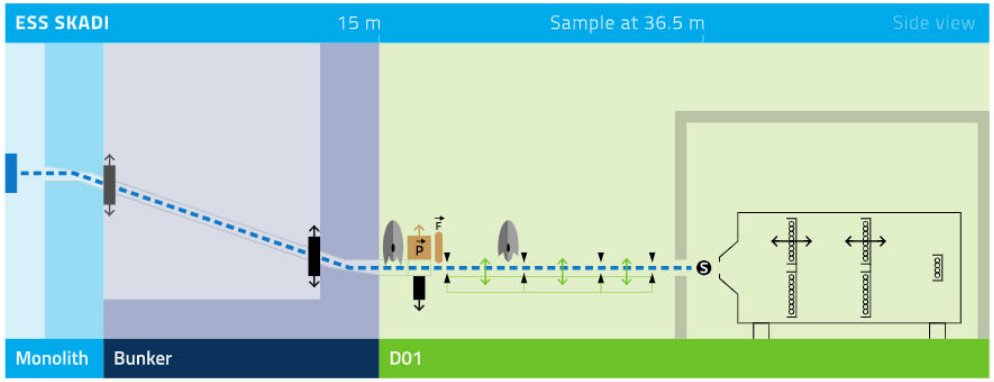
Goals:

- Investigate **multiple length scale** systems (simultaneously 0.5-300 nm)
- Aim to perform **"single-shot" kinetic measurements** on sub-second timescales. (5MW)
- Perform experiments that use flow e.g. rheology & microfluidics **with small beam sizes**
- **High throughput** of regular SANS measurements

LoKI Quick Facts	
Instrument Class	SANS
Moderator	Cold
Primary Flightpath	23.5 m, L_1 = 3, 5, 8 m
Secondary Flightpath	L_2 = 1.5 m, 3 m, 5–10 m
Wavelength Range	2–22 Å
Standard Mode (14 Hz)	
Bandwidth	7.5 Å [L_2 = 10 m] 10 Å [L_2 = 5 m]
Flux at Sample at 2 MW	4×10^8 n s^{-1} cm^{-2} [L_1 = 3 m] 5.6×10^7 n s^{-1} cm^{-2} [L_1 = 8 m]
Q-Range	0.01–2 $Å^{-1}$ [L_1 = 3 m, L_2 = 1.5, 5 m] 0.005–2 $Å^{-1}$ [L_1 = 8 m, L_2 = 1.5, 10 m]
Pulse Skipping Mode (7 Hz)	
Bandwidth	15 Å [L_2 = 10 m] 20 Å [L_2 = 5 m]
Flux at Sample at 2 MW	2×10^8 n s^{-1} cm^{-2} [L_1 = 3 m] 2.8×10^7 n s^{-1} cm^{-2} [L_1 = 8 m]
Q-Range	0.005–2 $Å^{-1}$ [L_1 = 3 m, L_2 = 1.5, 5 m] 0.002–2 $Å^{-1}$ [L_1 = 8 m, L_2 = 1.5, 10 m]

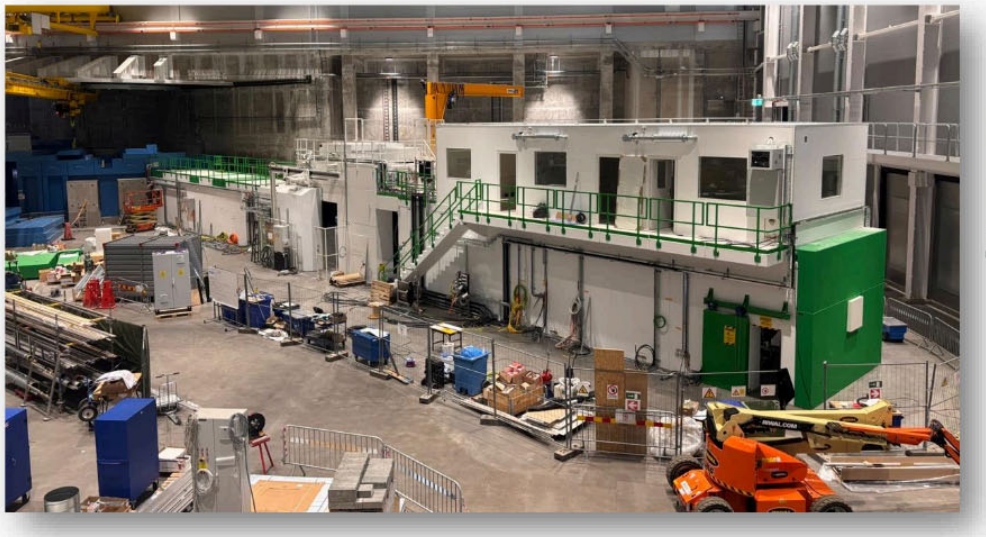
SKADI

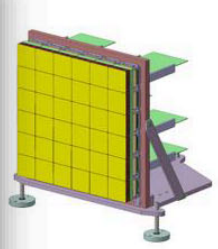
Small-K Advance Diffractometer – Polarised SANS for Materials Science

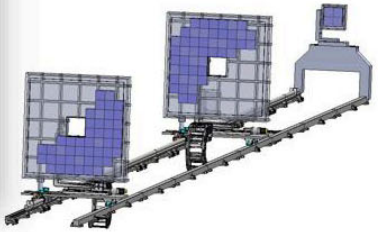


- Separate long/short wavelength polarization with supermirrors
- 4, 8, 14 and 20 m collimation settings
- VSANS: Down to ~10^{-4} Å^{-1}

Quick Facts	
Sector	East
Beam Port	E03
Class	Polarized SANS
Moderator	Cold
Length	58 m
Q-Range	10^{-4} – 1 Å^{-1}
Flux at sample position	7.7×10^{8} n s^{-1} cm^{-2}
Standard Mode (14 Hz)	
Wavelength Band	5 Å
Wavelength Range	3 – 21 Å
Momentum Resolution	ΔQ/Q= 2-7 %
Pulse Skipping Mode (7 Hz)	
Wavelength Band	10 Å
Wavelength Range	3 – 21 Å
Momentum Resolution	ΔQ/Q = 1-7 %





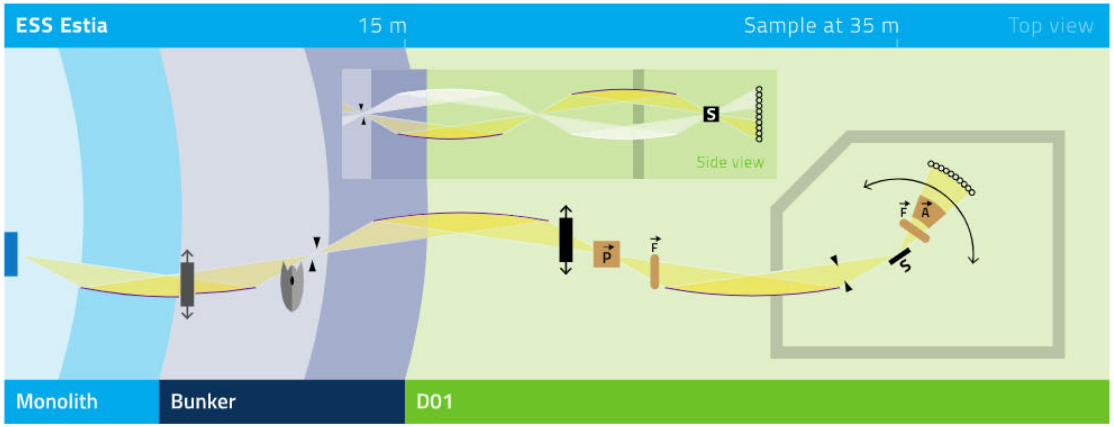


Orphée Laboratoire Léon Brillouin

JÜLICH FORSCHUNGSZENTRUM

ESTIA

Polarised Reflectometry with a very small beam footprint



Estia Quick Facts.

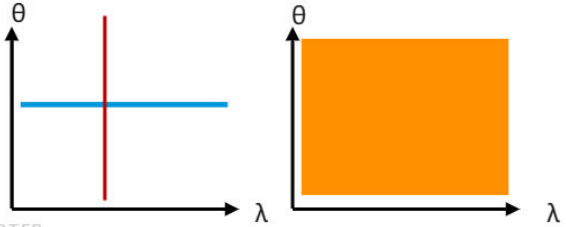
Estia Quick Facts	
Instrument Class	Reflectometry
Moderator	Cold
Primary Flightpath	35 m
Secondary Flightpath	4 m
Wavelength Range	3.75–28 Å
Polarised Incident Beam	Optional
Polarisation Analysis	Optional
Sample Orientation	Vertical
Total Q-Range	0.001 to 3.15 $Å^{-1}$/−0.001 to −0.3 $Å^{-1}$
Standard Mode (14 Hz)	
Bandwidth	7 Å
Flux at Sample at 2 MW[a]	6×10^8 n s^{-1} cm^{-2}
Relative Q-Range	$Q_{max} = 2.85 \times Q_{min}$
Q-Resolution $\Delta Q/Q$	7.8%–3.0% over Q-range
2-Pulse Skipping Mode (4.7 Hz)	
Bandwidth	21 Å
Flux at Sample at 2 MW[a]	2×10^8 n s^{-1} cm^{-2}
Relative Q-Range	$Q_{max} = 6.6 \times Q_{min}$
Q-Resolution $\Delta Q/Q$	7.8%–1.3% over Q-range

[a]Full-divergence beam averaged over 5(H) × 10(V) mm^2.

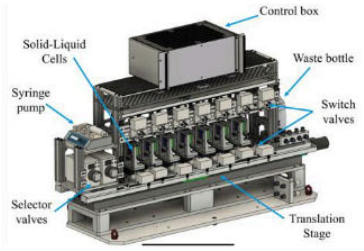
Reflectometers explore Q using either ToF at a fixed angle, or multiple angles at a fixed wavelength

$$Q = \frac{4\pi \sin\theta}{\lambda}$$

ESTIA uses a Selene guide to focus the neutrons, along with time of flight to look at both!

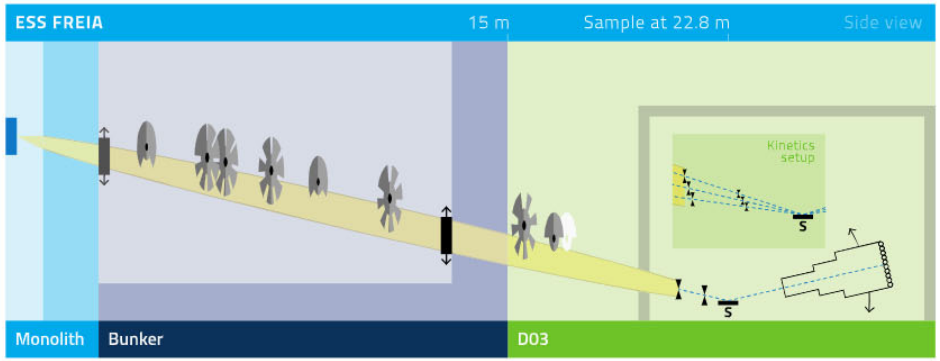


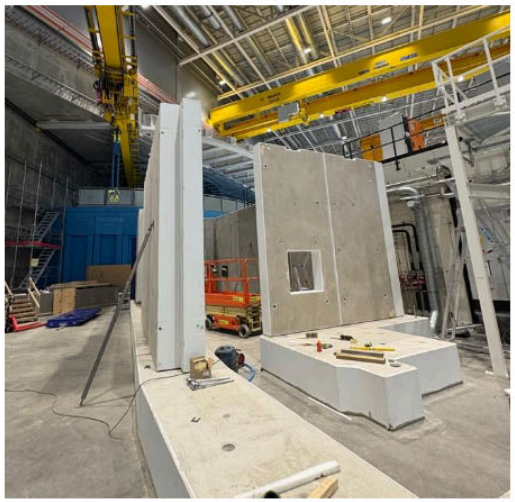
- **Selene neutron guide** projects tiny beam from Virtual Source
- **Small samples:**
  - Large divergence (1.5°x1.5°)
  - Samples down to 1x1 mm^2



FREIA

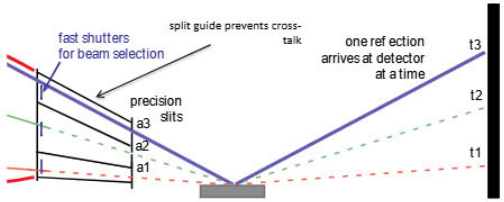
A fast neutron reflectometer for soft matter and life science.



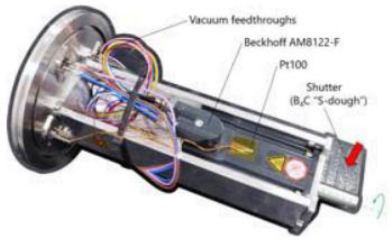


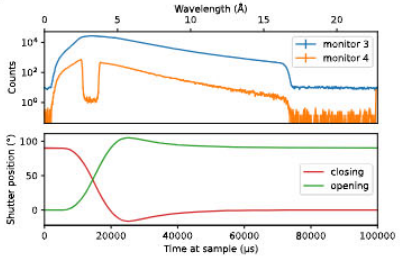
Fast-shutter project

Collaboration with Marek Jacewicz, Niklas Johansson & Tord Ekelöf (FREIA lab, Uppsala University), James Doutch (ISIS, STFC) and Tommy Nylander & Ben Humphries (Lund University)



- used to rapidly change angles in between source pulses
- prototype tested with beam at ISIS (ZOOM)





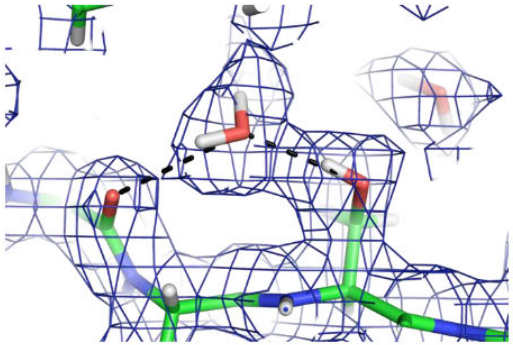
LUND UNIVERSITY

UPPSALA UNIVERSITET

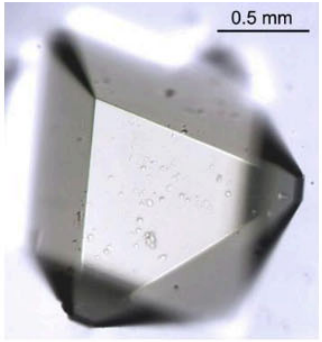
FREIA Quick Facts	
Instrument Class	Reflectometry
Moderator	Cold
Primary Flightpath	22.8 m
Secondary Flightpath	3.0 m
Polarised Incident Beam	Available as a foreseen upgrade
Sample Orientation	Horizontal
Representative Incident Beam Angles*	0.45°, 0.9°, 3.4° (full range 0.2 - 3.7° depending on angular resolution)
Standard Mode (14 Hz)	
Wavelength Range	2-10 Å
Flux at Sample at 2MW*	1×10^5, 5×10^5, 7×10^6 n s^{-1} cm^{-2} [high res (WFM) mode] 1×10^6, 4×10^6, 6×10^7 n s^{-1} cm^{-2} [high flux mode]
Q-Range	0–1 Å^{-1} (solid samples) 0.0045 –0.38 Å^{-1} (free liquids)
Q-resolution*	3–3.5% [high res (WFM) mode] 5–23% (across free-liquid Q-range) [high flux mode]
Pulse Skipping Mode (7 Hz)	
Wavelength Range	2-18 Å
Flux at Sample at 2MW*	5×10^5, 2×10^6, 3×10^7 n s^{-1} cm^{-2} [high flux mode]
Q-Range	0–1 Å^{-1} (solid samples) 0.002–0.38 Å^{-1} (free liquids)
Q-resolution	3–23% (across free-liquid Q-range) [high flux mode]

NMX

Macromolecular Crystallography



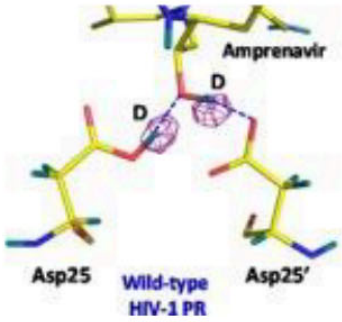
- 👍 Hydrogens are visible
- 👍 No radiation damage
- 👎 Large crystals needed
- 👎 Data collection takes weeks
- 👎 Few instruments available

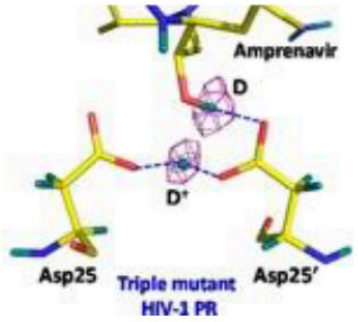


Oksanen, E *et al. J. R. Soc. Interface* 2009, ***6*** *Suppl 5*, S599-610.

- Where are hydrogens important?
- Enzyme mechanisms
- Protein-ligand interactions
- Proton transport across membranes

Sample and detector robots installed and undergoing inspection for energisation





Sample Environment

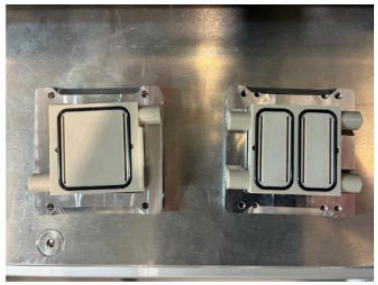
Sample Changers

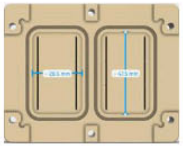
LoKI/SKADI

- Up to 48 narrow rectangular cuvettes
- Various options for different sizes/styles of cuvette
- Independent top and bottom temperatures
- Optional rotating sample holder for sedimenting samples
- *Future* : Peltier augmented sample racks for precise temperature control

Estia

- 7 position solid-liquid cell changer
- Small footprint / low volume solid-liquid cells





Hannah Burrall, Nico Paracini, Adrian Rennie

Large Scale Structures

Sample environment priorities

LOKI

- **HC (May 2026)**
  - Sample Changer
  - Circulating baths (Julabo)
  - Temperature readout box
- **First/Early Science (April 2027)**
  - Rheometer
  - NURF set up
    - HPLC Pumps and Switches
    - Syringe Pumps
  - Stopped Flow cell
- **SOUP (November 2027)**
  - SEC-SANS
  - AF4 (grant?)
  - Electromagnet
  - Humidity chamber (?? Which one)
  - Microfluidics
- **Later**
  - Liquid/gas mixing supercritical
  - EC cell
  - Humidity cell extreme condition
  - Vapor sorption (liquids)
  - In-situ reaction corrosive
  - Hydrostatic pressure cell
  - Soft matter stress rig
  - User/Grant led SEE

SKADI

- **HC (Jan 2027)**
  - Sample Changer
  - Circulating baths (Julabo)
  - Temperature readout box
- **First/Early Science (December 2027)**
  - Warm bore magnet
  - Flow cryostat
  - Electromagnet
  - Rotation stick
  - Rheometer
  - Stopped Flow cell
  - Syringe pump
  - HPLC pump
  - Flexiprob : DLS
  - Flexiprob : Foam Column
- **SOUP (March 2028):**
  - SANS Magnet
  - Cryostat or CCR
  - Humidity chamber
- **Later:**
  - SANS Magnet with PA
  - Dilution insert
  - He insert
  - EC cell
  - Vacuum furnace Niobium
  - DAC high P cells
  - Soft matter stress rig
  - UHT furnace
  - User/Grant led SEE

ESTIA

- **HC (June 2026)**
  - Warm bore magnet
  - Flow cryostat
  - Ambient sample changer (Estia)
  - Solid-Liquid cells + changer (manual cell loading)
  - Electromagnet (maybe)
- **First/Early Science (May 2027)**
  - HPLC/syringe pumps
  - 6.5T magnet
- **SOUP (December 2027)**
  - in-situ ellipsometry/ATR-FTIR
  - EC cell (batteries, potentiostat)
  - Environmental cell (humidity/temperature)
- **Later**
  - User/Grant led SEE

FREIA

- **HC (May 2027)**
  - Langmuir trough
  - Air-liquid troughs
  - Solid-Liquid cells + changer
- **First/Early Science (March 2028)**
  - Temperature controller
  - HPLC/syringe pumps
- **SOUP (May 2028)**
  - Additional solid-liquid cells and Langmuir troughs
  - in-situ ellipsometry/ATR-FTIR
  - multiwell troughs
  - small volume/cooled troughs
- **Later**
  - Sample changing robot
  - Shear/confinement cells
  - Rheometer
  - Environmental chamber (humidity/temperature)
  - User led SE including Liquid-liquid cells, Electrochemical cells + potentiostat, Overflowing cylinder, Humidity cell, WLS, GISANS (Flexiprobe).

NMX

- Provided by NMX

Deuteration and Crystallisation

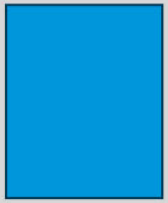
Science Support Division

Chemical Deuteration
At ESS

- Small organic molecules, monomers
- Lipids (e.g. POPC, SOPC, POPE)
- Surfactants (e.g. sugar-based)
- Novel organic molecules for various applications

Biological Deuteration
At Lund University (Biol. Dept)

- Deuterated biomass from *E. coli*, *B. braunii*, *P. pastoris*
- Recombinant soluble proteins, plasmid DNA, "other"
- Yeast-derived lipids (total,p-lipid)



New Deuteration Chemist starting soon

Hanna

Jia-Fei

\+ 0.75 RE @ LU

\+ 0.2 analysis @ ILL

LSS Division

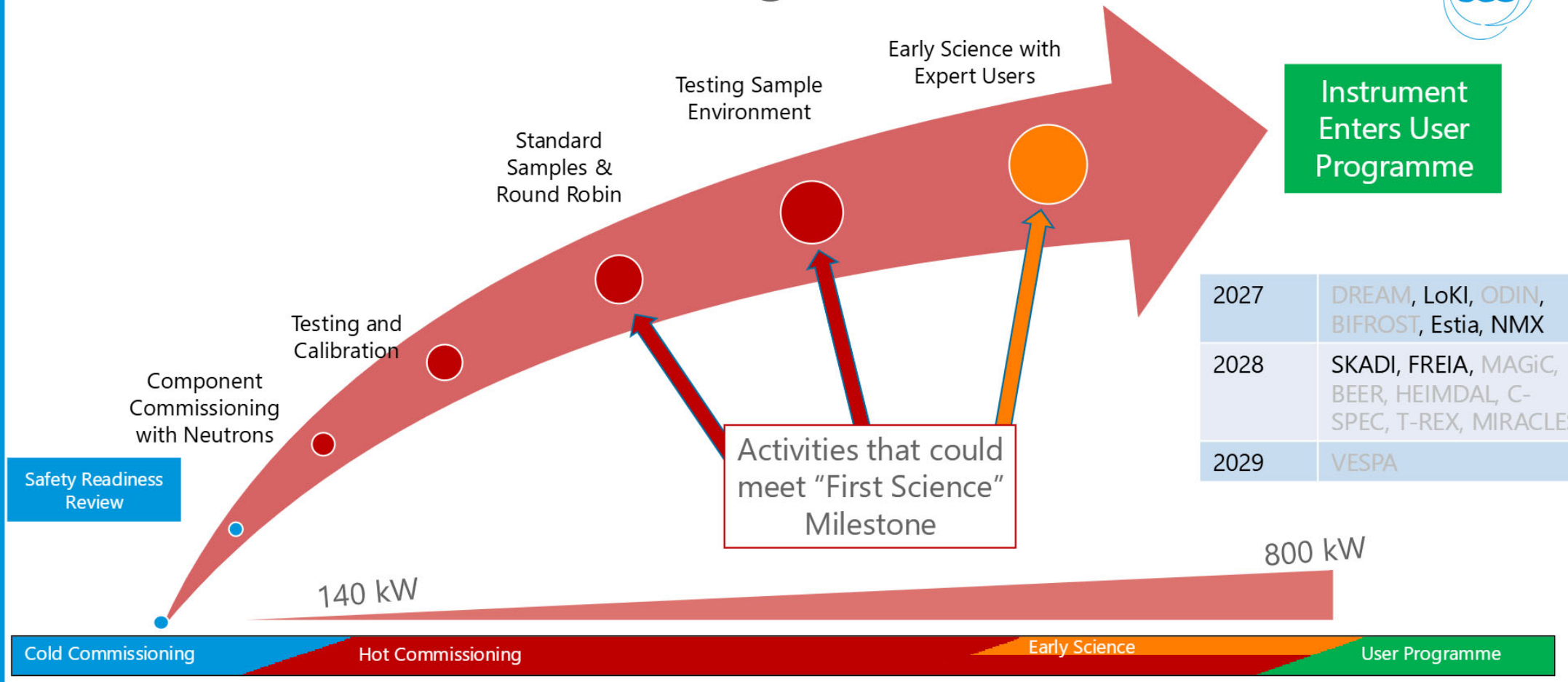
Protein Crystallization
NMX team at ESS & Lund University

- High- and low-throughput screening
- Fine screening in large volumes
- Support for room temperature crystal mounting & data collection
- X-ray testing (LU BAG at MAX lab)

Zoë

Swati

Towards the User Programme



2027	DREAM, LoKI, ODIN, BIFROST, Estia, NMX
2028	SKADI, FREIA, MAGIC, BEER, HEIMDAL, C-SPEC, T-REX, MIRACLES
2029	VESPA

LoKI, Estia, NMX :
Hot Commissioning Start : mid-2026
User Programme : late-2027

SKADI, FREIA :
Hot Commissioning Start : 2027
User Programme : late-2028

Large Scale Structures Team

LoKI (Partner : STFC)

Judith Houston (ESS, Instrument Scientist)

Santiago Bordin (ESS, Instrument Scientist – Jan 2026)

Hannah Burrall (ESS, Instrument Ops Engineer)

SKADI (Partners : LLB & FZJ)

Sebastian Jaksch (ESS/FZJ, Instrument Scientist)

Annika Stellhorn (ESS, Instrument Scientist Polarized SANS)

Tamires Gallo (ESS, Instrument Operations Engineer)

Milan Klausz (HUN-REN, Postdoc Detector Simulations)

Instrument Data Scientists (DMSC)

SANS : Oliver Hammond

Reflectometry : Nicolo Paracini

NMX : Aaron Finke

Estia (Partner : PSI)

Jos Cooper (ESS, Instrument Scientist)

Grace Causer (ESS, Instrument Scientist)

Felipe Lopes (ESS, Instrument Ops Engineer)

FREIA (Partner : STFC)

Tom Arnold (ESS, Instrument Scientist)

Ellen Wilson (LU/ESS, Postdoc XRR + FREIA support)

Instrument Operations Engineer (to recruit this year)

NMX

Esko Oksanen (LU/ESS, Instrument Scientist)

Justin Bergmann (ESS, Instrument Scientist)

Swati Aggarwal (LU/ESS, Support Scientist)

Zoë Fisher (ESS, Senior Scientist Protein Biochemistry & Crystallography)

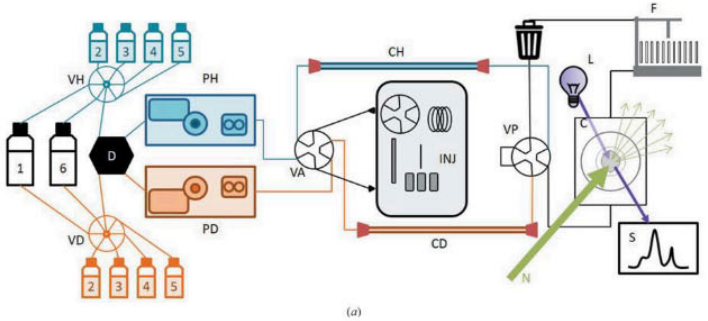
Future Upgrades and New Instruments …

Instrument Scope Completion

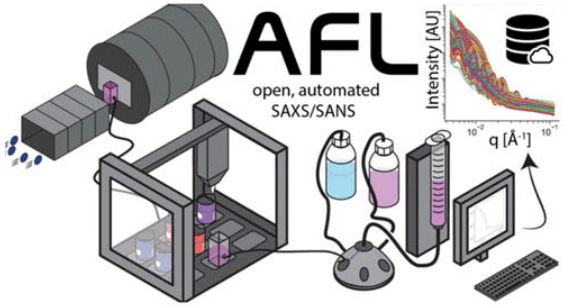
- LoKI detector area completion
- FREIA fast shutter system
- Estia add-ons
  - spin-resonance flipper, space-time collimator, GISANS re-focusing, in-situ MOKE, ultra-focus+imaging
- NMX isotopic Gd for detectors.
- NMX extra detector
- SKADI detector area completion

Sample Environment & Software

SEC, AF4, Magnets, Rheology, Autosamplers, Humidity, Autonomous ML-driven measurements, …



D22 SEC-SANS (J. Appl. Cryst. (2023). 56)



Chem. Mater. 2023, 35, 3, 846–852

Future Upgrades and New Instruments …

Science Thenes

Integrated Structural Biology and Biophysics

Bringing together multiple neutron techniques with computational methods and complementary techniques to answer complex structural biology and biophysics questions.

Amorphous/Semi Crystalline Materials

Extending Q range towards diffraction.

Formulations and Food

Complex multi-component systems require large parameter space studies with high throughput.

Surfaces and Interfaces

In-situ and in-operando 3D structural analysis of surfaces and interfaces

Environment

Molecular interactions within complex mixtures on surfaces and in bulk

Geology and Geomaterials

Connecting with imaging and microscopy length scales to enable the study of structures from nanometres through micrometres to millimetres

Industrial Research

Providing capacity and optimised instrumentation for industrial usage

Future Upgrades and New Instruments …

Shaping the Future of ESS https://indico.ess.eu/category/110/

- **SAGA –** Dedicated surface scattering instrument for 3D studies of interfaces
- **Structural Biology Cluster** – 2nd NMX with DNP and a dedicated Bio-SEC-SANS
- **SMÅ -** High throughput SANS for industry and parametric studies
- **Yggdrasil –** Polarised SANS/WANS – targeting high Q / overlap with DREAM
- **ULL –** Membrane/Partially Ordered Systems Diffractometer
- **MIMER -** Solid-Liquid Bio-Reflectometer
- **Estib –** Small sample footprint reflectometer for in-situ and in-operando studies
- **SANS at very low Q –** VSANS/SEMSANS/USANS – possible upgrades to SKADI

Most concepts at early stages of development – ideas and input on science cases welcome!

Questions?

LoKI Progress

Installation Complete – June 2025

About ESS | Science & Instruments | Technology | Building ESS | Partnerships | Careers

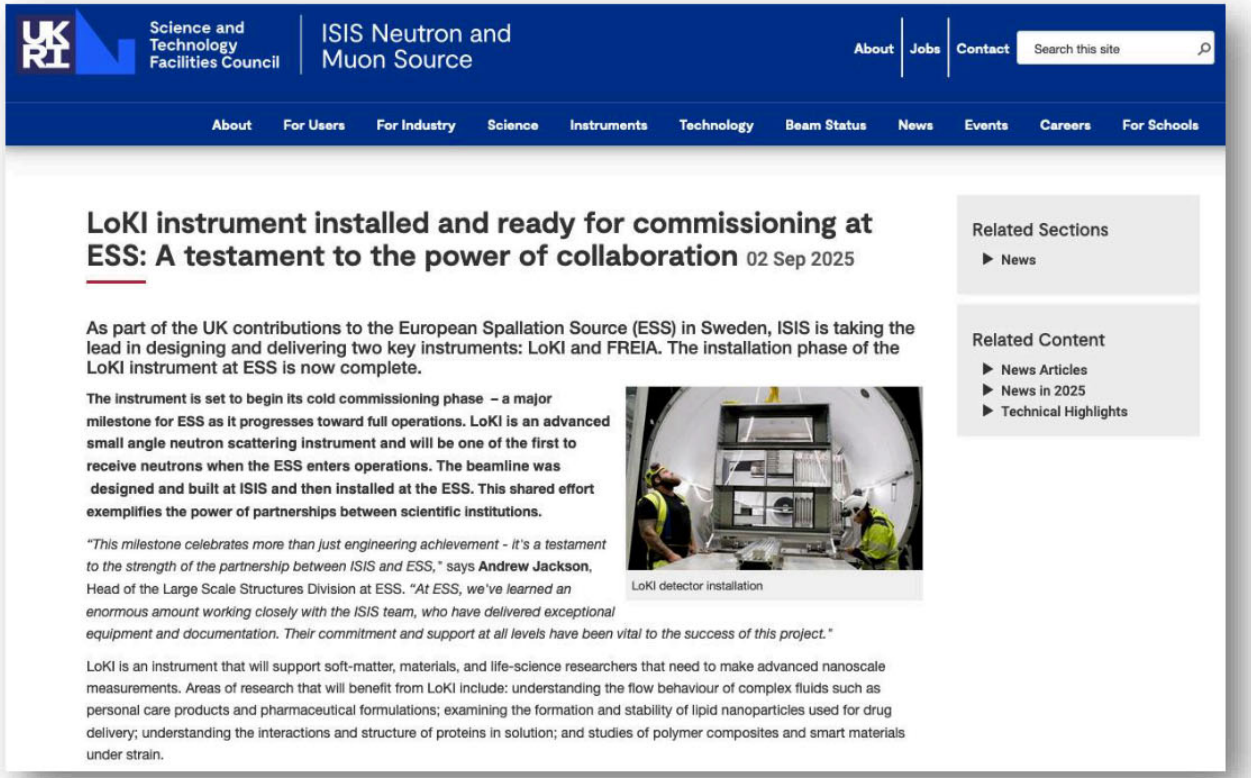
LoKI instrument installed and ready for commissioning at ESS: A testament to the power of collaboration

SEPTEMBER 2, 2025

LoKI is getting ready for neutrons. Image: Ulrika Hammarlund/ESS

The installation phase of the LoKI instrument at ESS is now complete, and the instrument is set to begin its cold commissioning phase – a major milestone for ESS as it progresses toward full operations. LoKI, an advanced Small Angle Neutron Scattering (SANS) instrument, has been developed and delivered through a close collaboration between ESS and its UK In-Kind Partner, ISIS Neutron and Muon Source. This shared effort exemplifies the power of partnerships between scientific institutions.

https://ess.eu/article/2025/09/02/loki-instrument-installed-and-ready-commissioning-ess-testament-power



UKRI Science and Technology Facilities Council | ISIS Neutron and Muon Source

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LoKI instrument installed and ready for commissioning at ESS: A testament to the power of collaboration 02 Sep 2025

As part of the UK contributions to the European Spallation Source (ESS) in Sweden, ISIS is taking the lead in designing and delivering two key instruments: LoKI and FREIA. The installation phase of the LoKI instrument at ESS is now complete.

The instrument is set to begin its cold commissioning phase – a major milestone for ESS as it progresses toward full operations. LoKI is an advanced small angle neutron scattering instrument and will be one of the first to receive neutrons when the ESS enters operations. The beamline was designed and built at ISIS and then installed at the ESS. This shared effort exemplifies the power of partnerships between scientific institutions.

LoKI detector installation

"This milestone celebrates more than just engineering achievement - it's a testament to the strength of the partnership between ISIS and ESS," says **Andrew Jackson**, Head of the Large Scale Structures Division at ESS. *"At ESS, we've learned an enormous amount working closely with the ISIS team, who have delivered exceptional equipment and documentation. Their commitment and support at all levels have been vital to the success of this project."*

LoKI is an instrument that will support soft-matter, materials, and life-science researchers that need to make advanced nanoscale measurements. Areas of research that will benefit from LoKI include: understanding the flow behaviour of complex fluids such as personal care products and pharmaceutical formulations; examining the formation and stability of lipid nanoparticles used for drug delivery; understanding the interactions and structure of proteins in solution; and studies of polymer composites and smart materials under strain.

Related Sections
- News

Related Content
- News Articles
- News in 2025
- Technical Highlights

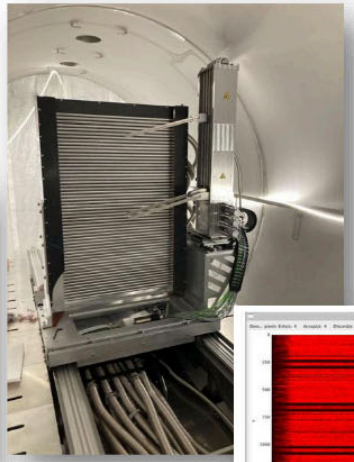
https://www.isis.stfc.ac.uk/Pages/News25_LoKI.aspx

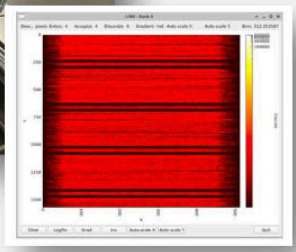
LoKI Progress

Installation Complete

*Rear wall will be last thing we do, but it has been test fitted

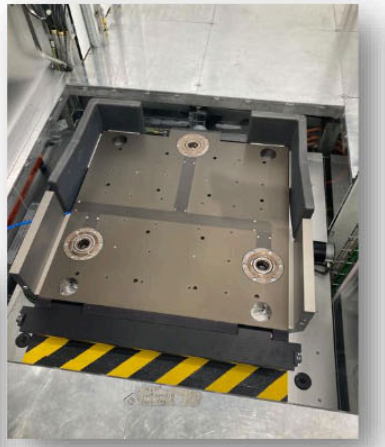
Hannah and Clara inspecting slit system cabling before closing shielding





Long runs counting cosmics have allowed us to identify cabling and connectivity issues on the detectors. All now resolved

PSS Installed



Sample stack in place

Andrew pretending to be useful by fixing 4 bolts

LoKI Progress

Getting ready for Hot Commissioning

Integrated Testing Completed – June to September

System Acceptance Review held – 19th September

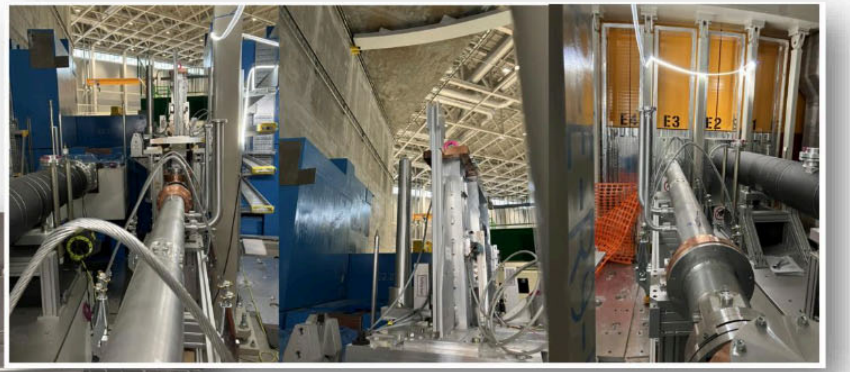
- Not approved due to outstanding issues arising from testing
  - Mostly controls issues
  - Detector module failure that has now been diagnosed and determined to be “expected” failure mode and the module is removed and awaiting maintenance.
- Review of completion of issues to be held by early December

Safety Readiness Review to be held – 3rd or 4th December

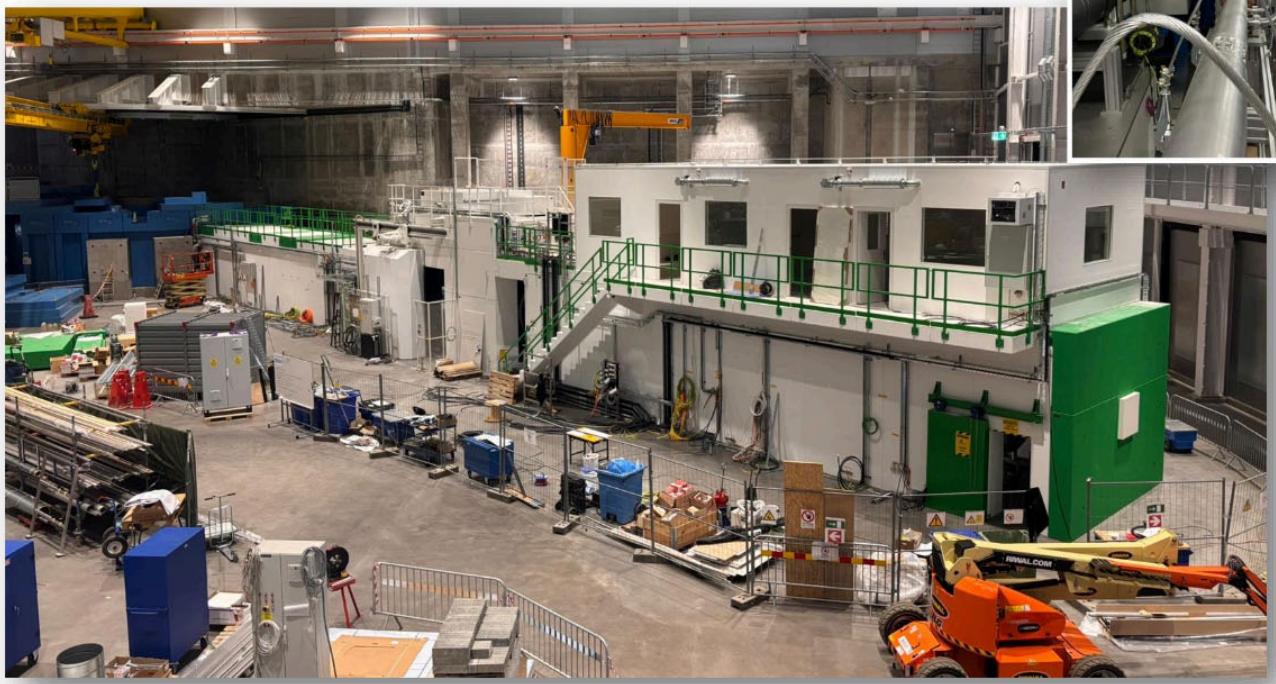
- PSS integration test completed
- Motion safety installation and integration to be done
- Quality and compliance process ongoing

SKADI Progress

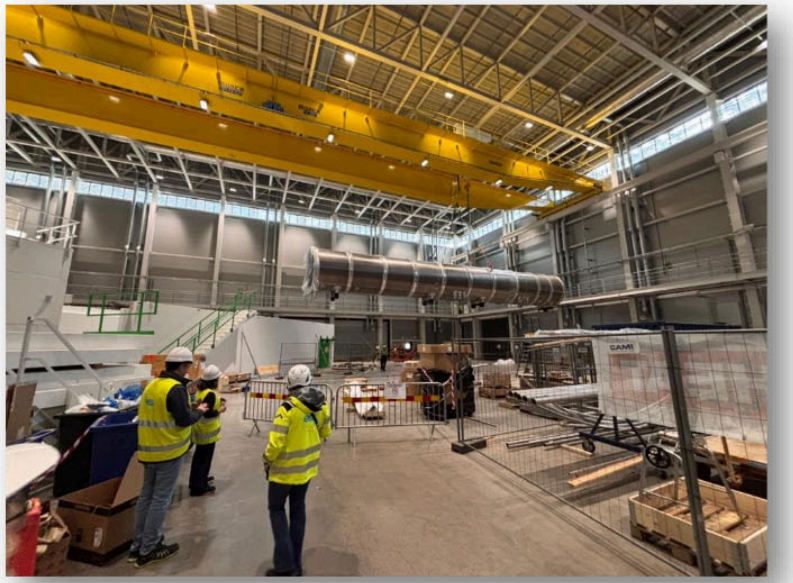
Installation well under way



In bunker components installed



Cave, Collimator Shielding, and Hutch Installed
Electrical and Utility installation started

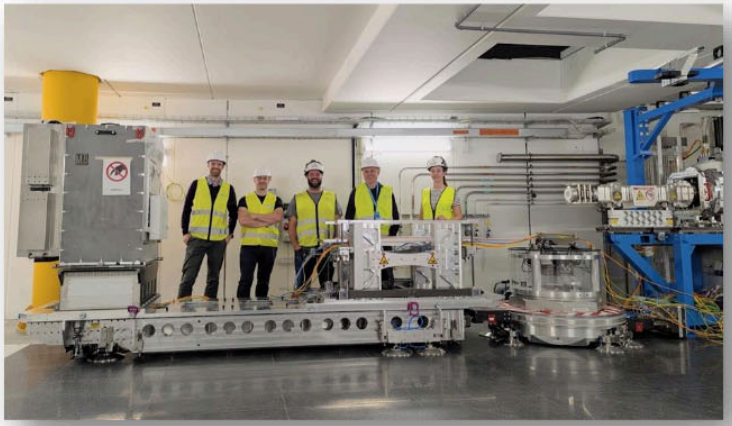


Detector vessel delivered and installed,
undergoing mechanical integration,
alignment, and testing.

TG3 before end of 2025
TG5/SAR before end of 2026

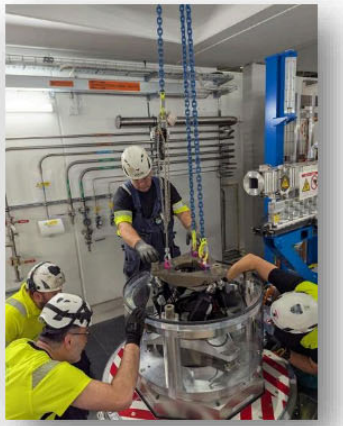
Estia Status

Installation almost complete



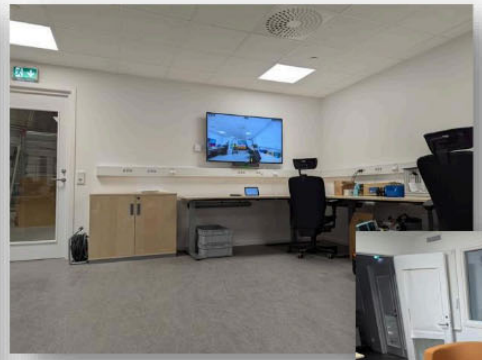
Estia team after completion of testing of detector arm

Detector complete, installed, and initial testing with cosmics done



Hexapod installed

Felipe testing the microscope and wire-bonder in the sample prep area

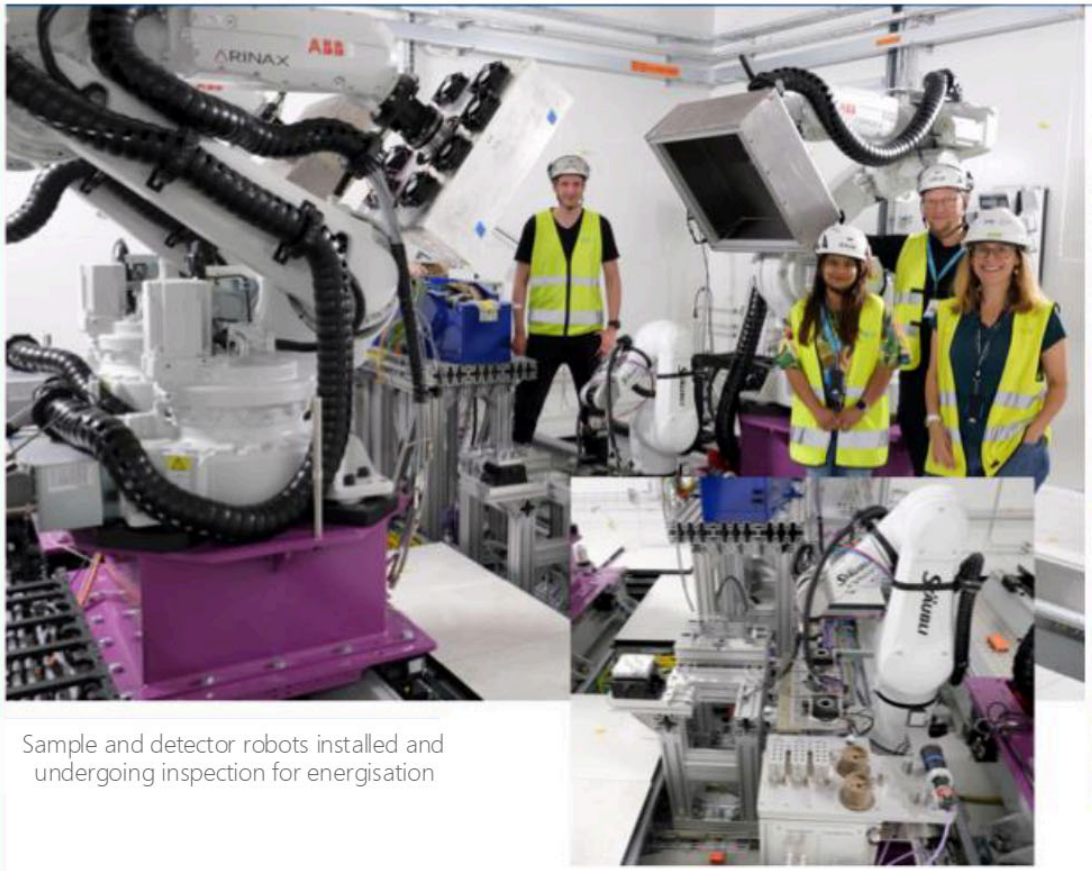


Control Hutch fitted out

TG3 completed 3rd October 2025
TG5/SAR due in Q1 2026

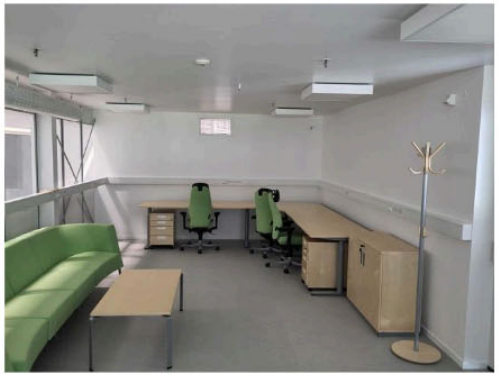
NMX Status

Installation almost complete



Sample and detector robots installed and undergoing inspection for energisation

Sample prep lab fitted out and operational



Control Hutch fitted out and awaiting IT equipment