

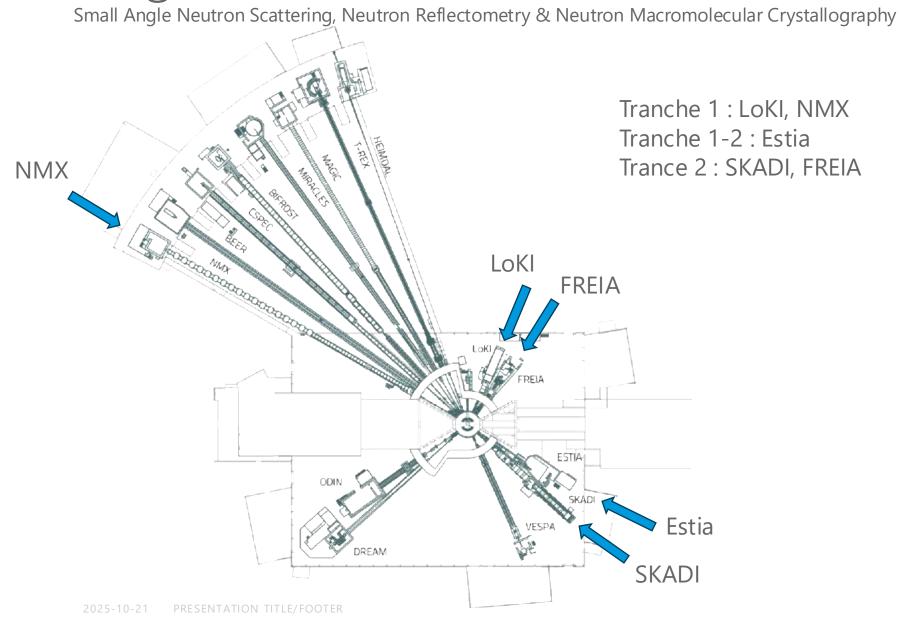
## Large Scale Structures Division

Common STAP Meeting – October 2025

ANDREW JACKSON HEAD OF LARGE SCALE STRUCTURES DIVISION

## Large Scale Structures Instruments





## Deuteration and Crystallisation

Previously ...





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



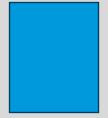
## Biological Deuteration At Lund University (Biol. Dept)

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



## Protein Crystallization 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)



New Deuteration Chemist starting soon



Hanna



Jia-Fei



0.75 RE @ LU 0.2 analysis @ ILL



Zoë

## Deuteration and Crystallisation

Now







Science Support Division



**Chemical Deuteration** At ESS

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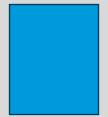
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- Deuterated biomass from E. coli, B. braunii, P. pastoris
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### LSS Division



- 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)



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0.2 analysis @ ILL



Zoë



Swati

### Teams on site

**LoKI (Partner: STFC)** 

Judith Houston (ESS, Instrument Scientist)

Santiago Bordin (ESS, Instrument Scientist – Jan 2026)

Hannah Burrall (ESS, Instrument Ops Engineer)

Clara Lopez (ESS, Engineer - NSS)

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)

Sylvain Desert (LLB, Engineer – NSS)

**Instrument Data Scientists** (DMSC)

**SANS**: Oliver Hammond

Reflectometry: Nicolo Paracini

NMX: Aaron Finke

Judith & Ellen are on parental leave.

Andrew is filling in for Judith on LoKI



**Estia (Partner: PSI)** 

Jos Cooper (ESS, Instrument Scientist)

Grace Causer (ESS, Instrument Scientist)

Felipe Lopes (ESS, Instrument Ops Engineer)

Nicolae Popescu (ESS, Engineer – NSS)

FREIA (Partner: STFC)

Tom Arnold (ESS, Instrument Scientist)

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

*Instrument Operations Engineer (Position advertised)* 

Clara Lopez (ESS, Engineer – NSS)

**NMX** 

Esko Oksanen (LU/ESS, Instrument Scientist)

Justin Bergmann (ESS, Instrument Scientist)

Swati Aggarwal (LU/ESS, Support Scientist)

Zoë Fisher (ESS, Crystallisation and Biodeuteration Scientist)

Daniel Lundström (ESS, Engineer – NSS)

## LoKI Progress

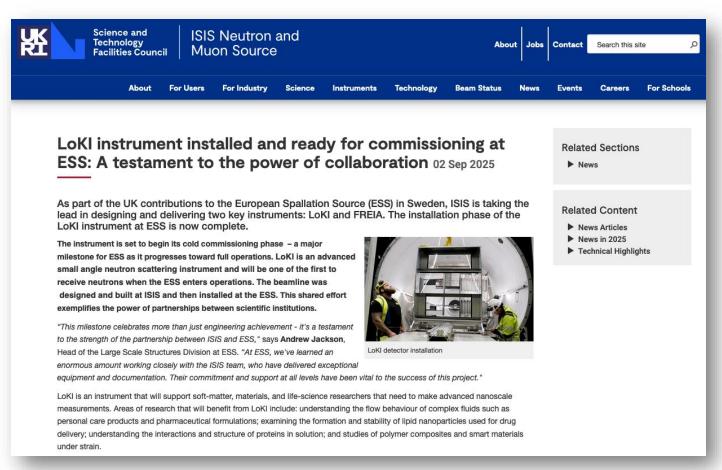
### Installation Complete – June 2025







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://www.isis.stfc.ac.uk/Pages/News25\_Lokl.aspx

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

## LoKI Progress

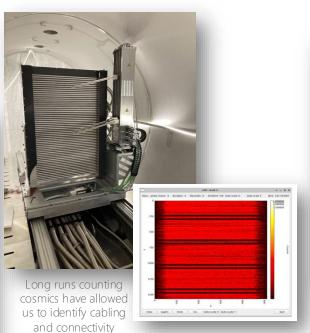
### **Installation Complete**



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



Hannah and Clara inspecting slit system cabling before closing shielding



issues on the detectors. All now resolved



PSS Installed



Sample stack in place



Andrew pretending to be useful by fixing 4 bolts

## LoKI Progress

# ess

### Getting ready for Hot Commissioning

Integrated Testing Completed – June to September System Acceptance Review held – 19<sup>th</sup> 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 – 3<sup>rd</sup> or 4<sup>th</sup> December

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

## SKADI Progress

Installation well under way







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

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





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

### 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





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

## FREIA Progress

### Installation started





Base for cave installed

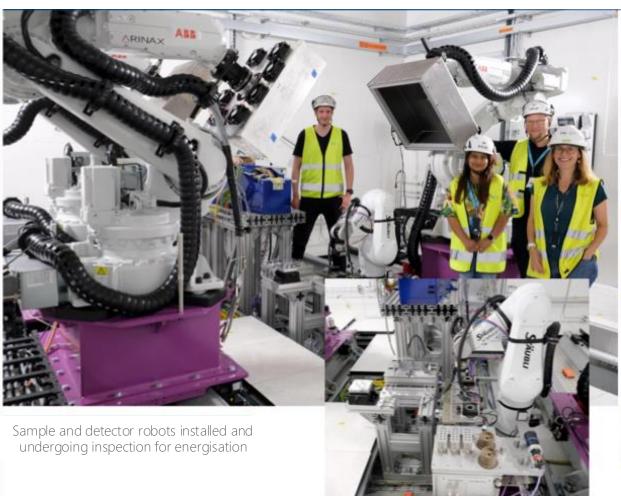
Installation of cave ongoing

Delivery of components from ISIS/STFC ongoing

## NMX Status

### Installation almost complete









Sample prep lab fitted out and operational



Control Hutch fitted out and awaiting IT equipment

## 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

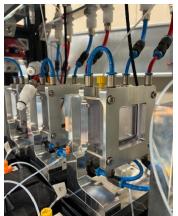




### Estia

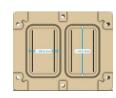
- 7 position solid-liquid cell changer
- Small footprint / low volume solid-liquid cells











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)

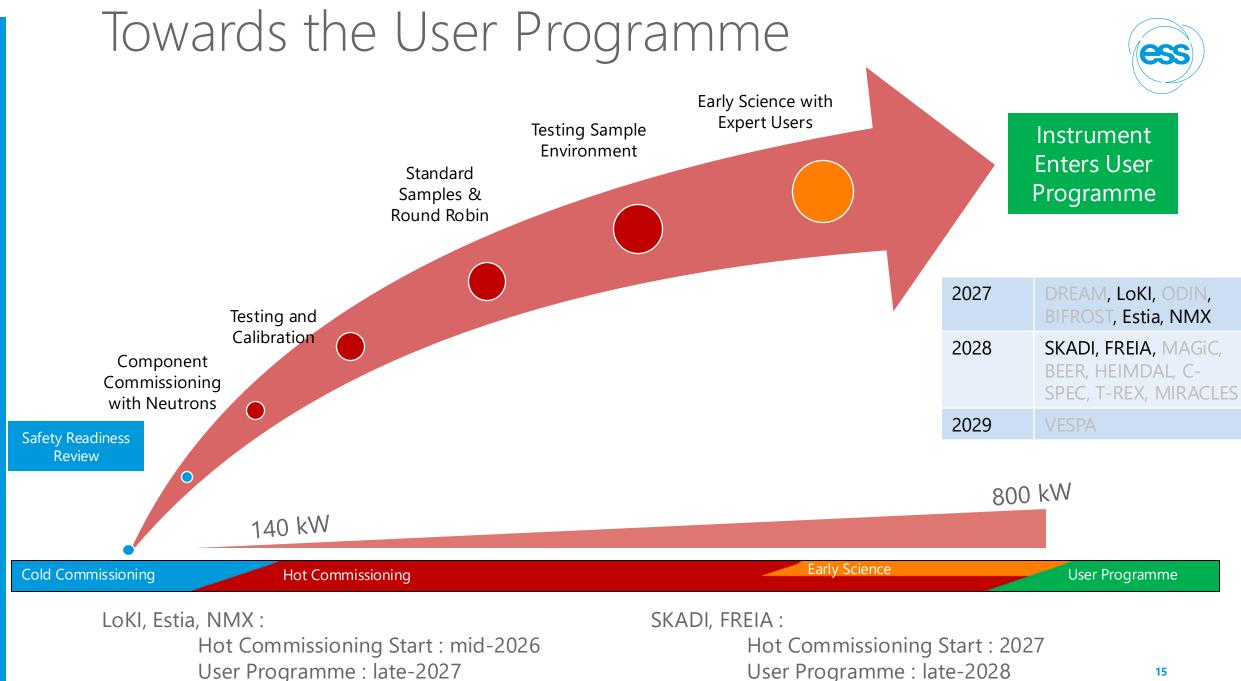
- Additional solid-liquid cells and Langmuir troughs
- •in-situ ellipsometry/ATR-FTIR
- multiwell troughs
- •small volume/cooled troughs

#### · 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



## ESS Early Science Postdocs

### Estia and LoKI



### **Estia**

*In-operando Studies of Lithium-Ion Batteries* ESS: Jos Cooper, Grace Causer

Collaborators : Robert Weatherup (Oxford)

Using the unique capabilities of Estia to enable new studies of the solid-electrolyte-interphase in lithium-ion batteries.

Development of small-footprint battery cell for use with neutrons and comparison of this cell with existing coin cells used for x-ray studies.

Postdoc to start in mid 2026

#### LoKI

Rheology of microgels

ESS: Judith Houston

Collaborators: Emanuela Zaccarelli (La Sapienza) and

Marco Laurati (Florence)

Using the capabilities of LoKI to understand the rheology of concentrated microgel suspensions.

(Project proposal in preparation and subject to review and approval)

Postdoc will start in late 2026/early 2027 if approved

### Swedish Science Initiatives at ESS



### VR Funded Early Science Consortia (2026-2029) – proposals under evaluation

### **Lifecycle of a Lipid Nanoparticle** (PI: Margaret Holme, Chalmers)

- Examining the production, delivery, and biological interactions of lipid nanoparticles used as drug delivery agents
  - LoKI and Estia
  - Three postdocs based at ESS:
    - Lipid particles under flow (working with Judith Houston and Andrew Jackson)
    - Biological interactions of LNPs (working with Tom Arnold and Sebastian Jaksch)
    - Modelling of data from LNPs (working with Oliver Hammond and Andrew Jackson)

### **Quantum Horizons at ESS: From Synthesis to Scattering** (PI: Elizabeth Blackburn, LU)

- Looking for skyrmion-vortex coupling and altermagnetism driven by interfaces
  - Estia (and possibly GISANS on SKADI)
  - One postdoc based at KTH (working at ESS with Jos Cooper and Grace Causer)



## Questions?