Large Scale Structures Division

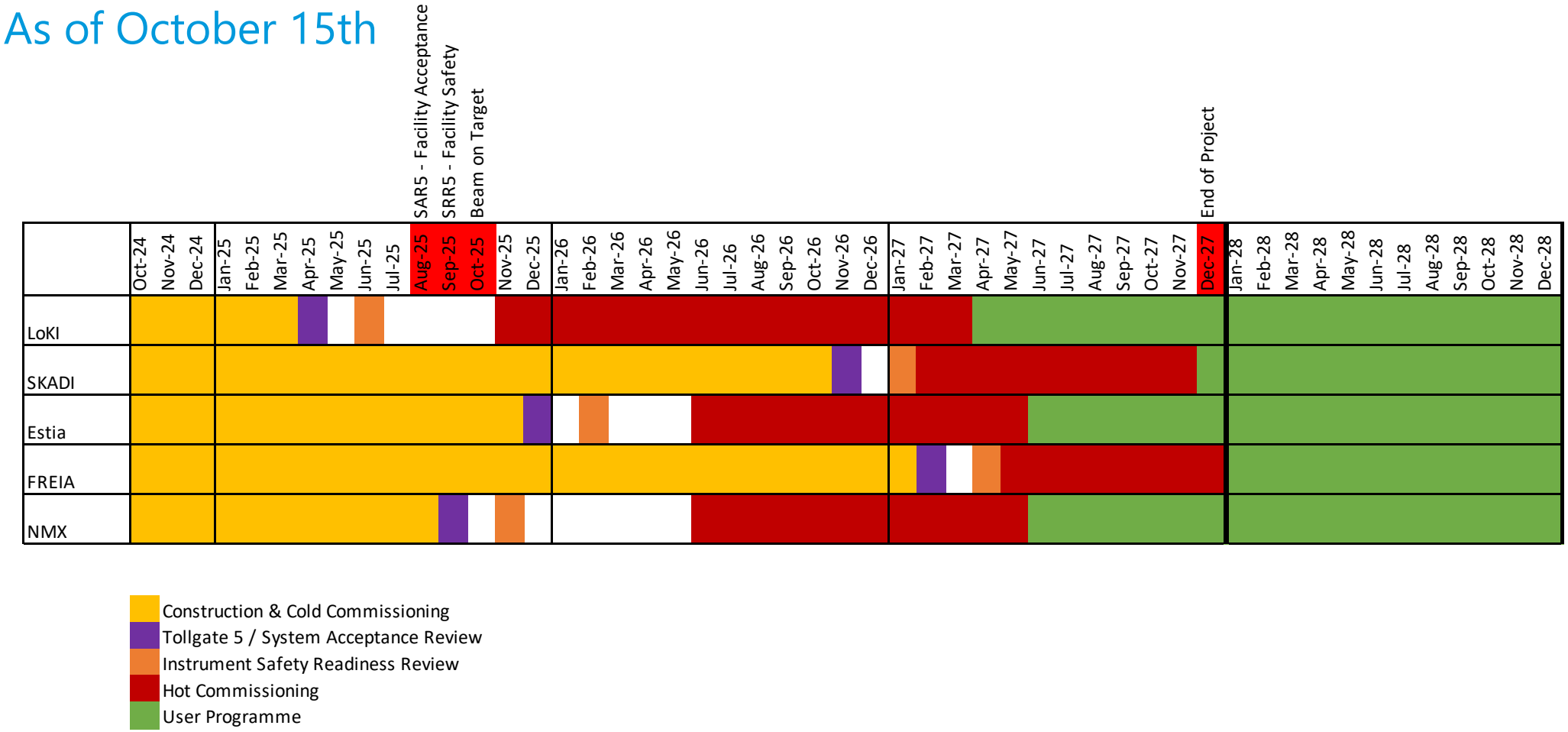
SAC 33, October 24th-25th 2024

ANDREW JACKSON

2024-10-23

Instrument Timelines

As of October 15th



On the current schedule only LoKI will be ready before BOT. Instruments after BOT are subject to notification to SSM (Swedish Radiation Authority) before hot commissioning can start – time for this is unknown. Acceleration measures needed to get Estia and NMX ready before BOT – we are reviewing the activities to see where we can speed up or defer until after BOT.

LoKI Progress

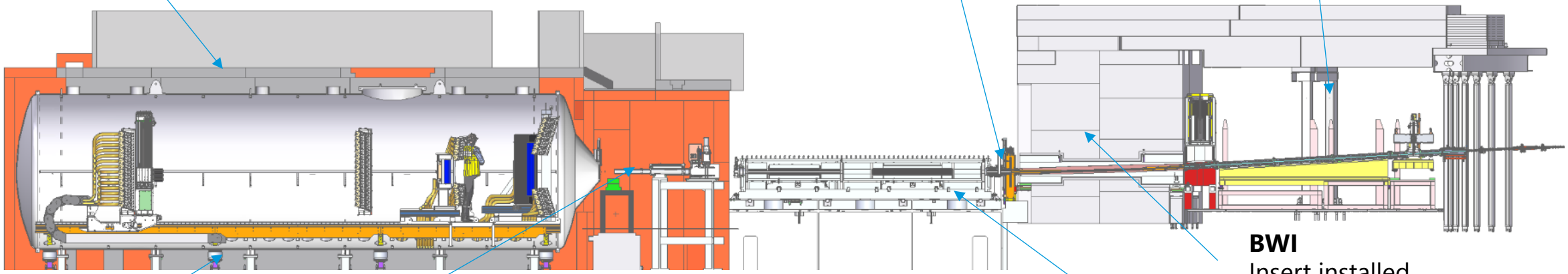
Items which are concerns to the timeline

Detectors
Vessel, **mechanical frames and most modules** installed
All detector components, including beamstop installed, *awaiting cable connections and testing*

Utilities
Electrical services, utilities, PSS and network being installed and almost complete in all cases
Energisation is imminent – *although causing delays to commissioning*

Chopper 2
Installed

In-bunker
All components installed, awaiting final alignment checks



BWI
Insert installed

Cave Shielding
- Steel is installed
- Concrete roof is installed

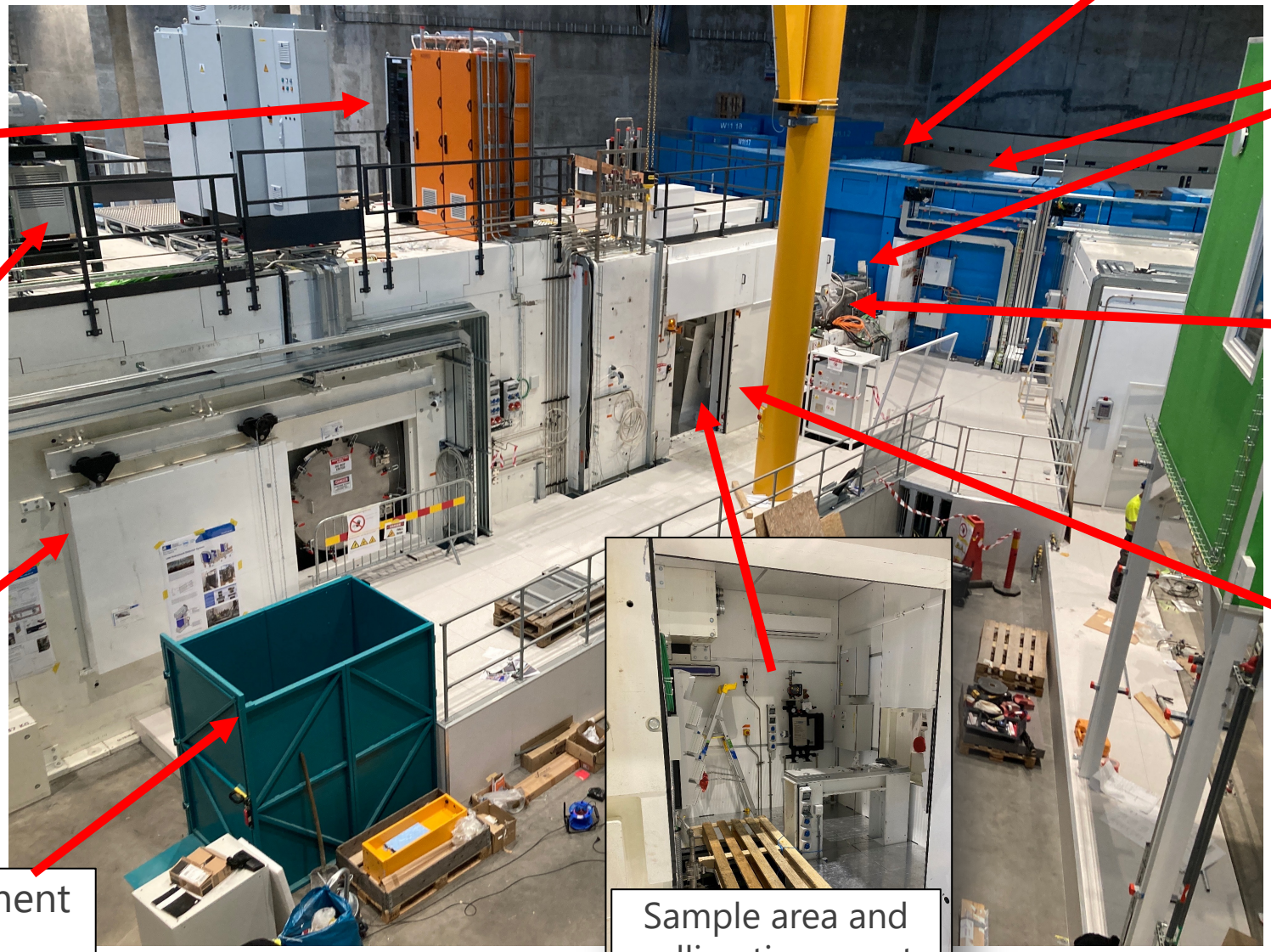
Sample Area
- Stack awaiting installation
- Snout system about to begin installation
- Door and roof installed

Beam monitors
- First 2 monitors installed last week
- *Other 3 monitors awaiting final assembly (risk to timeline)*

Bunker-to-cave
- Collimation tank installed and vacuum tested
- Collimation selectors and slits installed and undergoing final testing before commissioning

- TG3 (design) milestone passed
- All TG4 (final manufacture) documentation submitted by ISIS
- Current installation complete date (TG5) is **Spring 2025**

LoKI Progress



In bunker equipment

Racks for motion, choppers, PSS, ICS, vacuum installed

Choppers

Collimation including selectors with guides and slit sets

Pumps and racks installed

All detector mechanical structures including beamstop installed

Door and roof mechanism installed

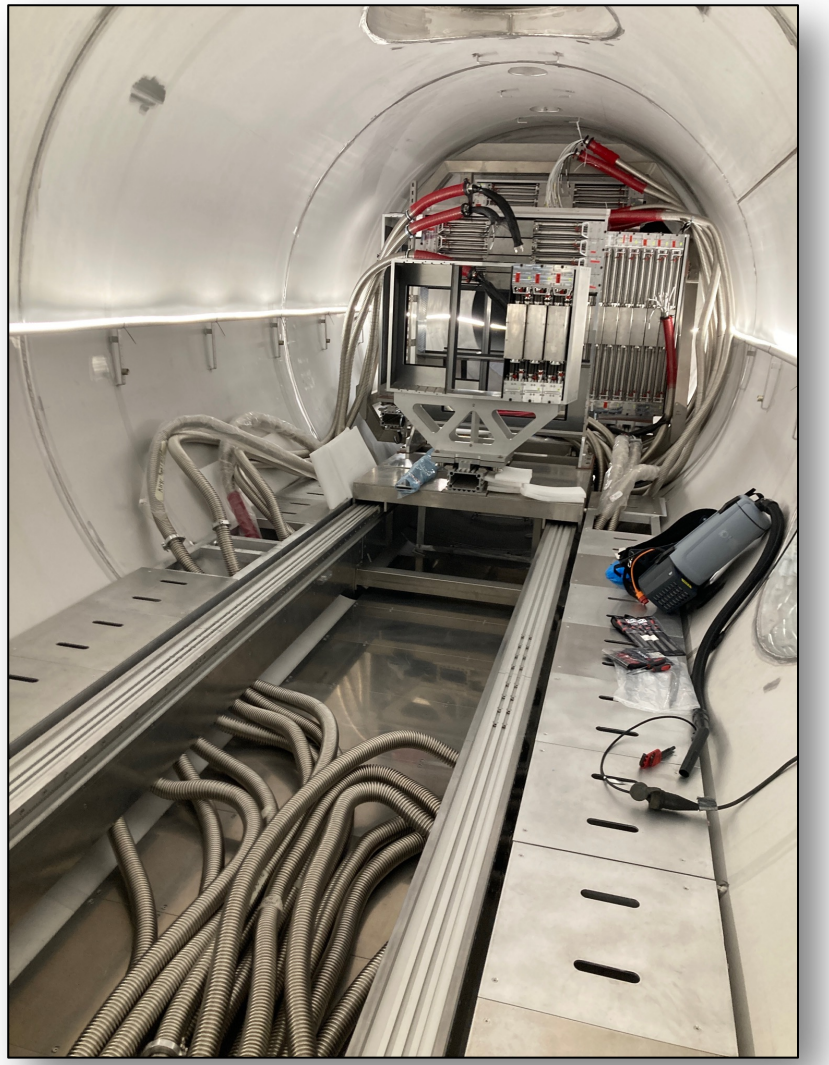
Utilities and electricial

Goods/Equipment Lift

Sample area and collimation snout

LoKI Progress

Detectors

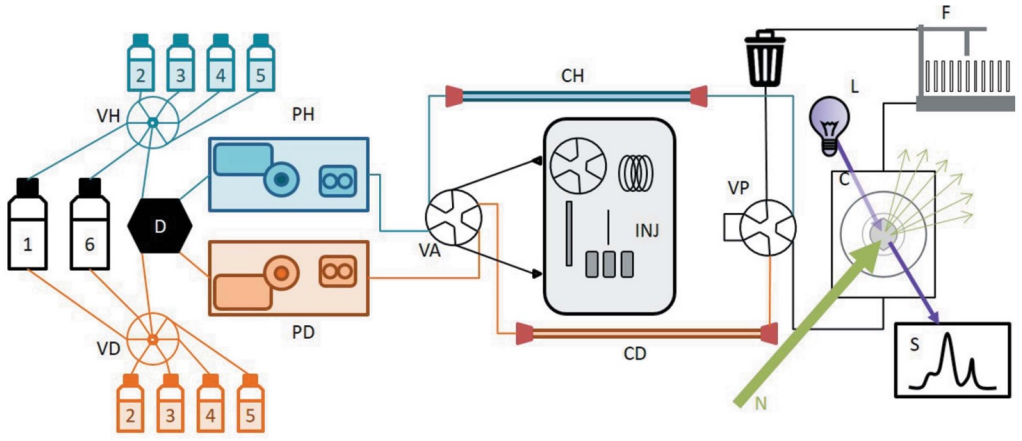


- Almost all mechanical infrastructure installed including: all the frames, most of the modules, beamstop mechanism, air hoses, racks on hutch roof
- Detector group are now completing cable connections to patch panels, models and racks.
- Detector carriage and beam stop mechanism undergoing motion testing

LoKI Progress

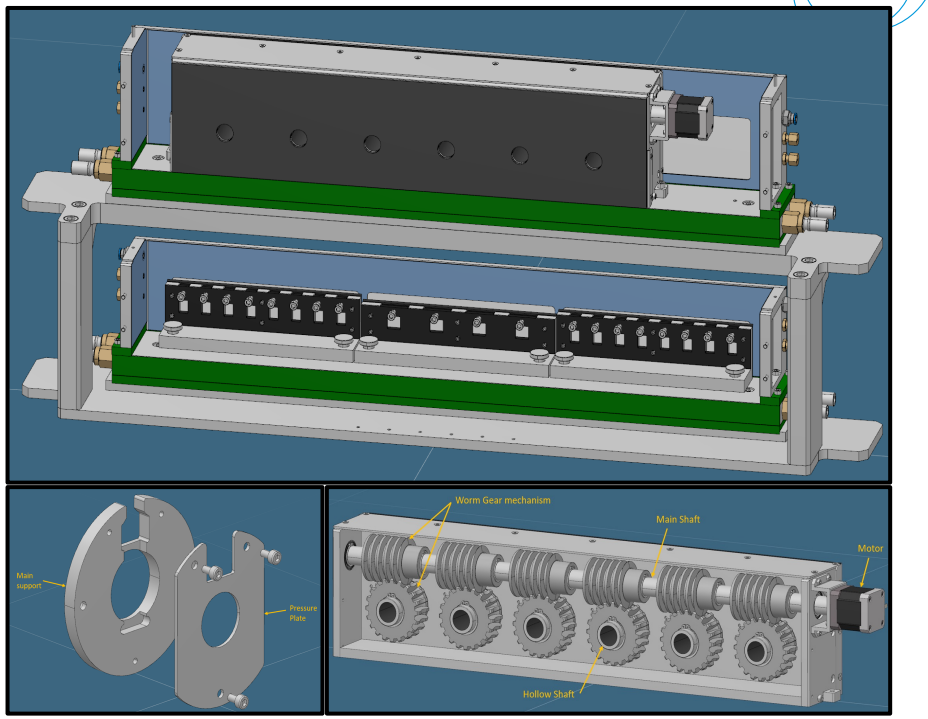
Sample Environment

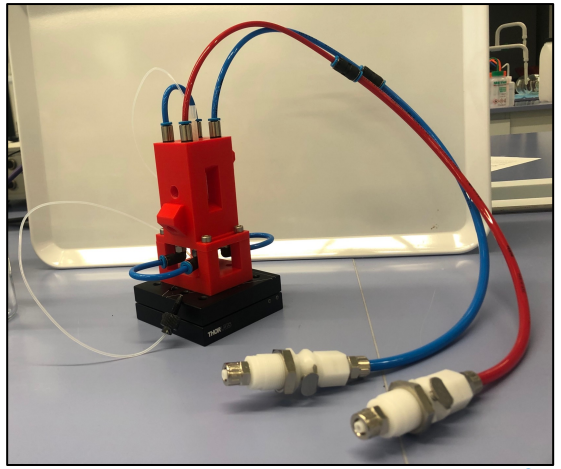
- **Thermostated cell holder** and **rotating cell holder** components manufactured and about to begin assembly.
- **Rheometer** integration is underway and making progress (ESS pool equipment). Sub-pulse project with Uppsala on-going with ISIS
- **Size-exclusion chromatography** set-up delayed due to loss of post-doc.
- **NURF (in situ spectrometers and continuous flow cell)** cell prototyped and devices integrated.



(a)

Ann Martel's SEC set-up (J. Appl. Cryst. (2023). 56)

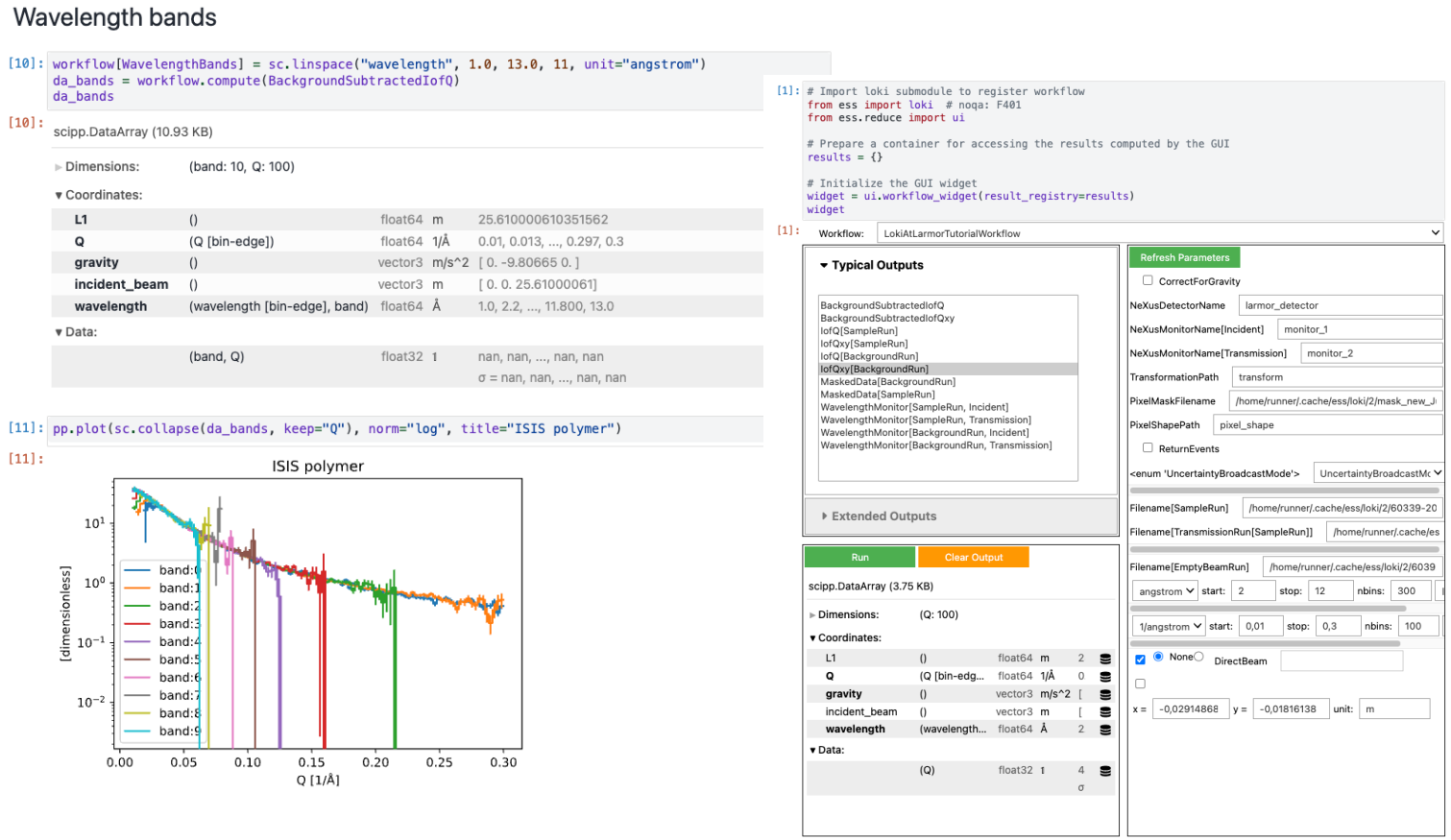




LoKI Progress

Data Processing

- New IDS **Oliver Hammond** started mid-September and is getting up to speed
- Data reduction and direct beam script in Mantid have been transferred to SCIPP, and the workflow optimised
- DMSC have been working on the GUI for the data reduction interface for LOKI
- The GUI (made of widgets) are generated from the workflow (sciline) graph. This means that if we change something in the workflow, the GUI will automatically follow/be updated.



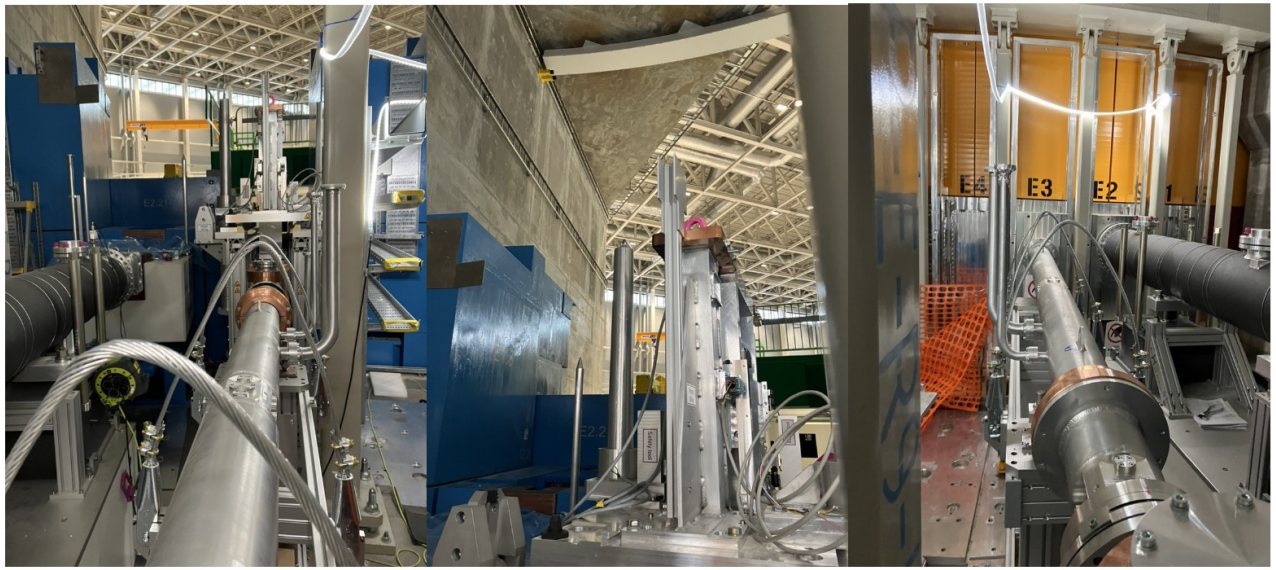
Data reduction scripts available online : https://scipp.github.io/esssans/user-guide/loki/loki-iofq.html

Data reduction GUI available online : https://scipp.github.io/esssans/user-guide/loki/workflow-widget-loki.html

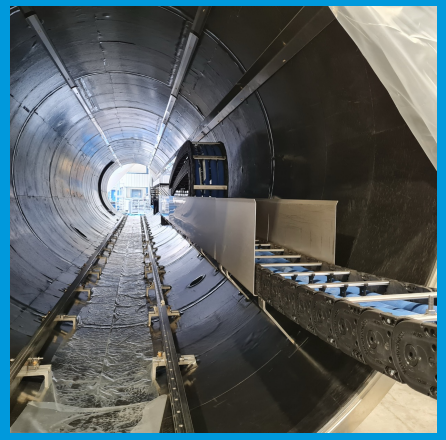
SKADI Progress

Installation

In bunker components



Cave and Collimator Shielding

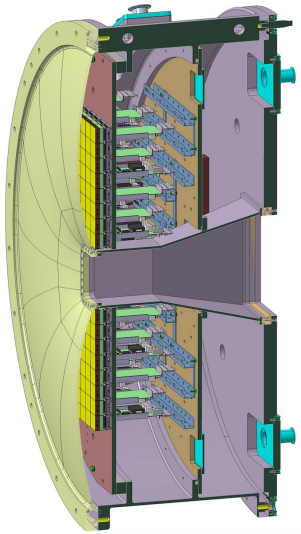


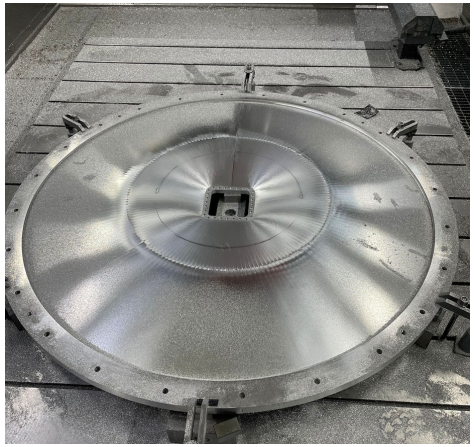
Detector vessel in manufacturing at vendor

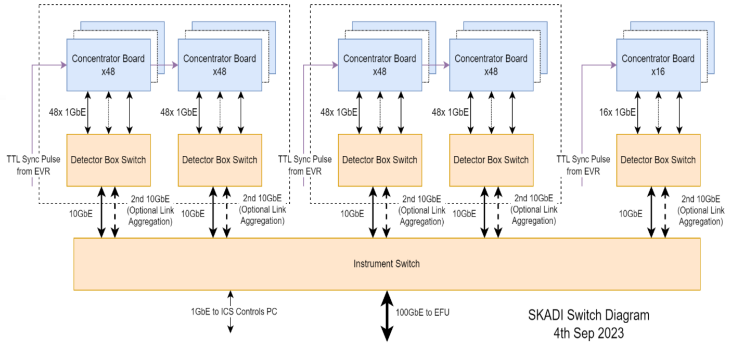
Out of bunker guides in manufacturing at vendor

SKADI Progress

Detectors





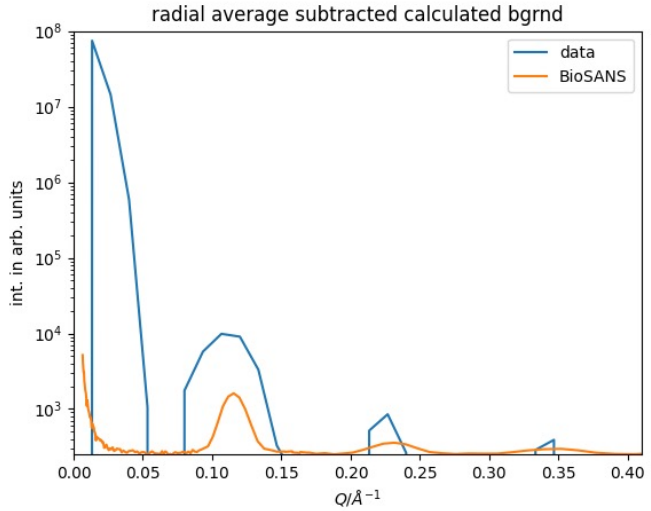


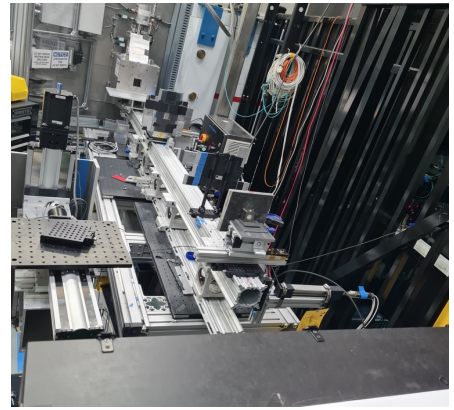
- Detector air box construction under way
- Plan developed for integrating SoNDE into ESS readout chain:
  - Bespoke solution – not using the RMM as other instruments
  - Challenges remain with code development, hardware testing, and scale up to 200+ detector modules – both technical and manpower

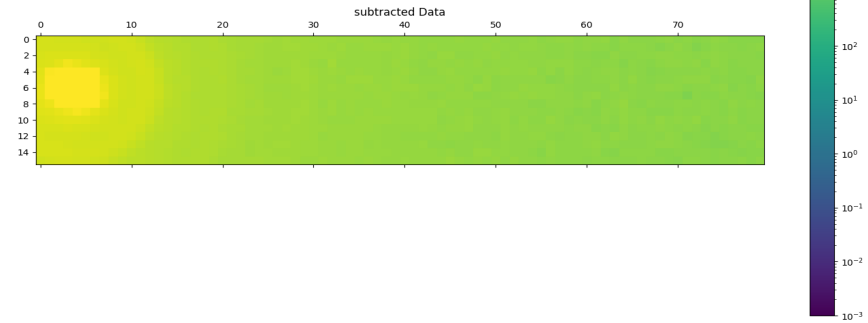
1x5 (10x50 cm) detector tested at HFIR measuring AgBeh

Poor signal to noise due to rudimentary collimation, running in air, no shielding and no beamstop

Proof of principle - full testing with ESS electronics still needed.
Waiting on updated firmware from supplier

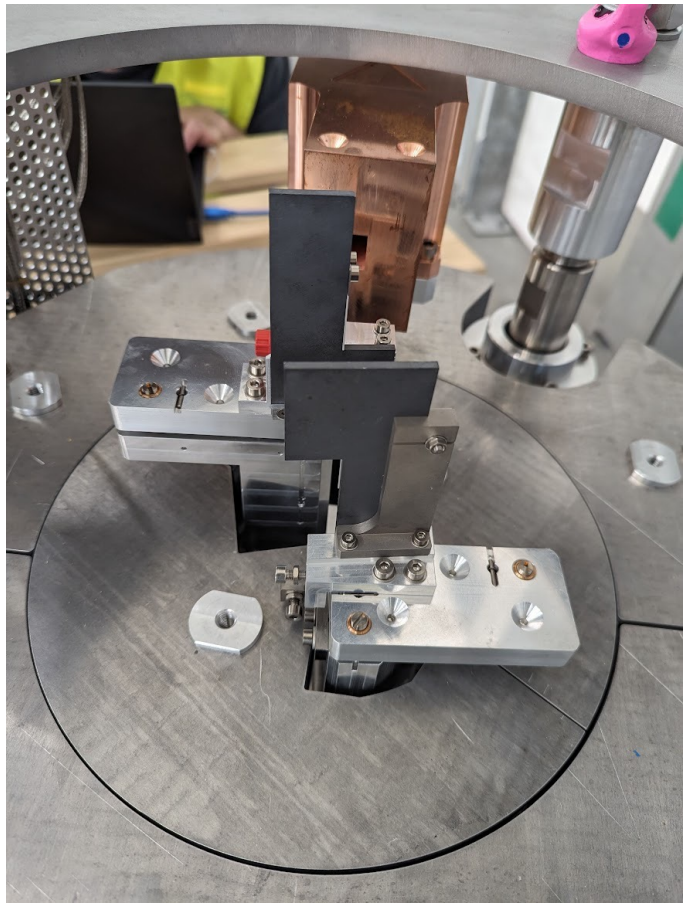


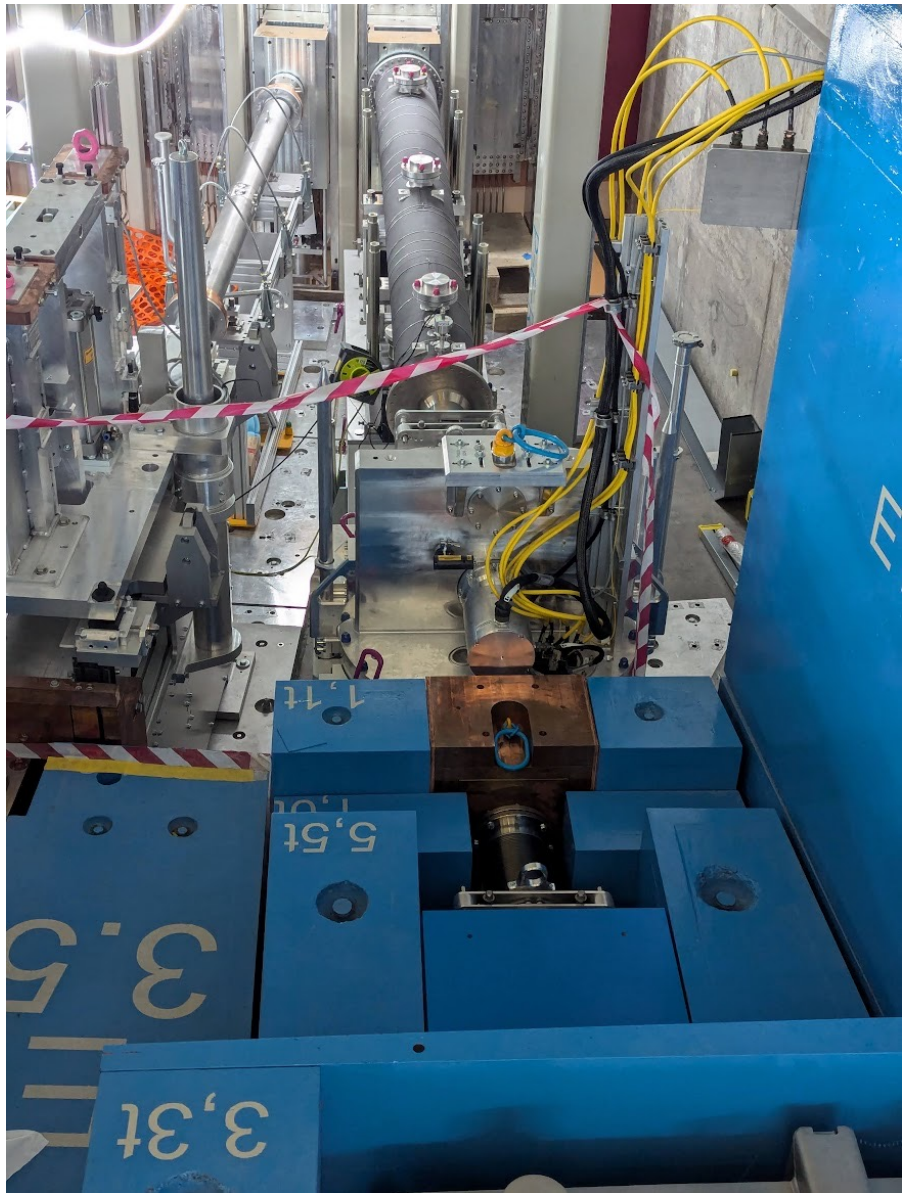




Estia Progress

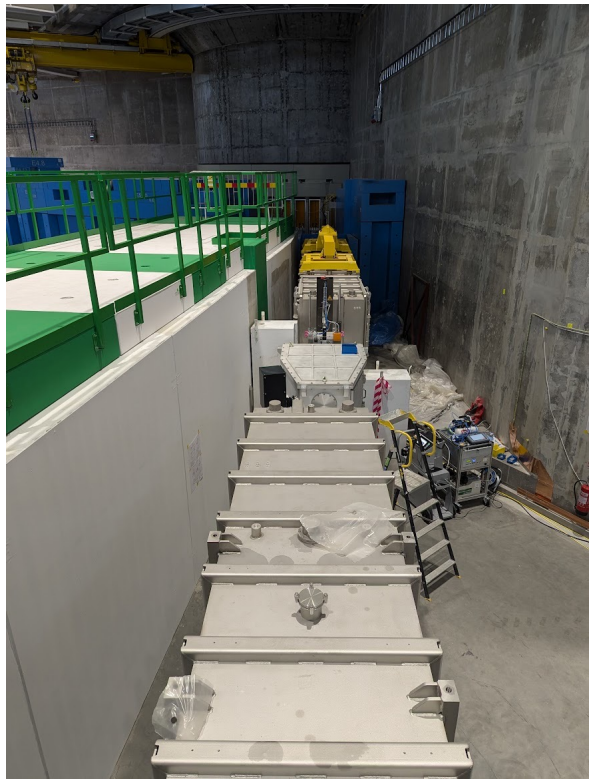
Installations





Estia Progress

Installations



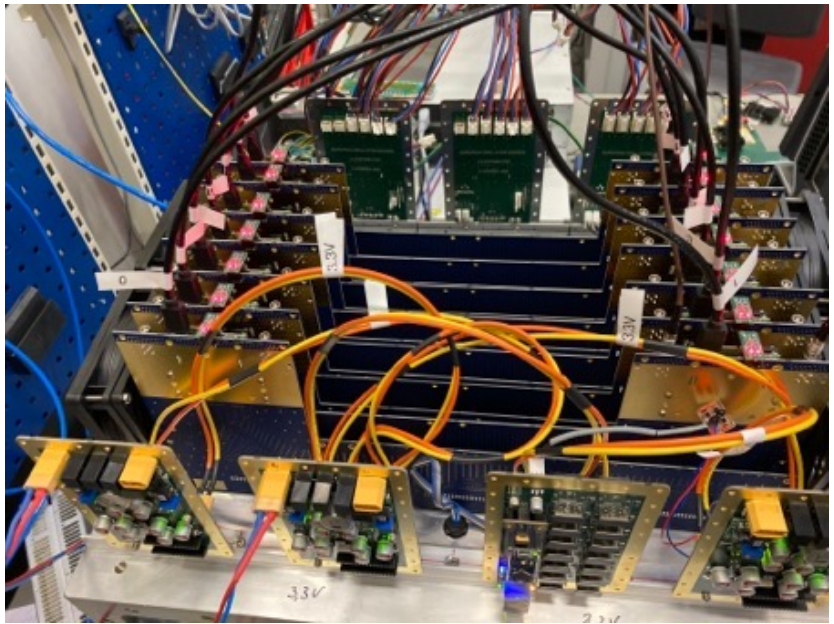
Estia Progress

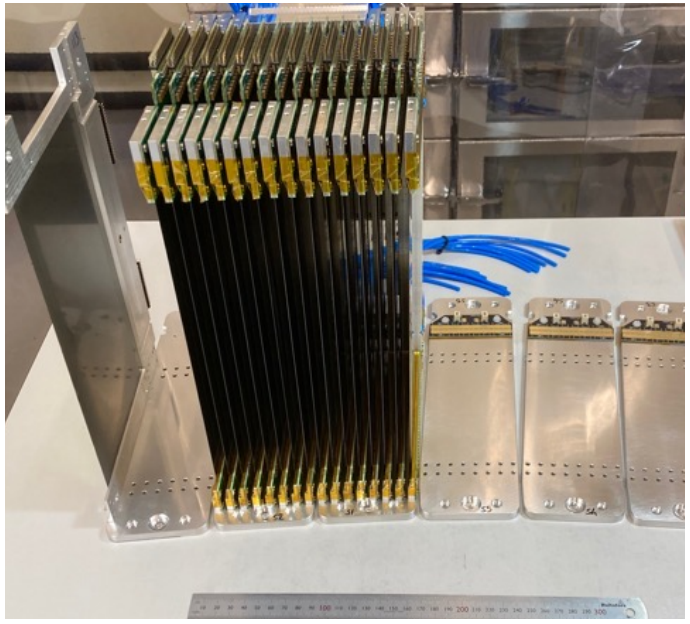
Installations

Multiblade Detector

- Multiblade detector permanently installed at AMOR (PSI) and running smoothly since November 2023 in their user programme.

- For Estia:
  - Vessel assembled and leak tested
  - Awaiting alignment system manufacture to complete assembly and final testing
  - Electronics under test in Utgard





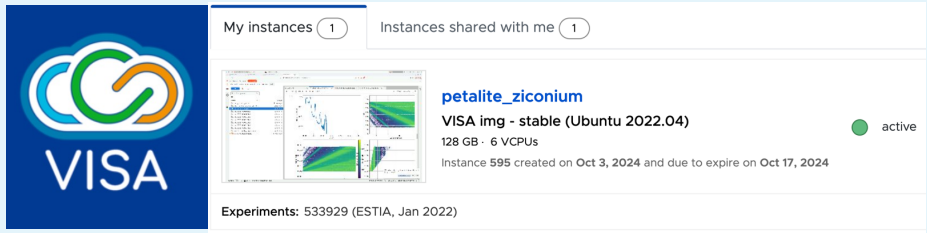
Estia Progress - Data

ESS User office

EUROPEAN SPALLATION SOURCE User Office

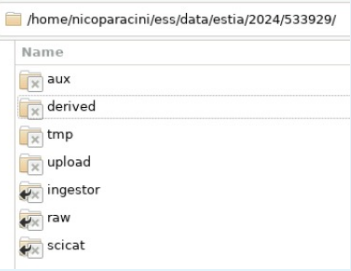
✓ Estia proposal submitted

VISA



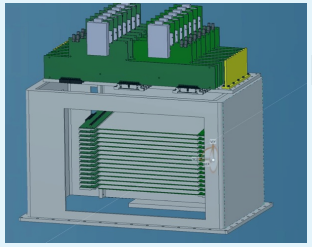
✓ VISA session created & shared

Experiment Folder



✓ Experiment folder created

Data collection



MultiBlade detector @AMOR

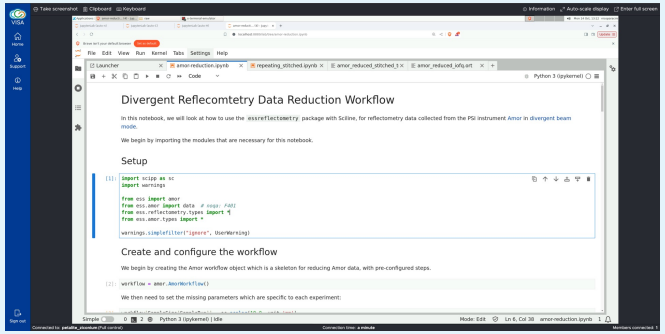
✓ Detector electronics

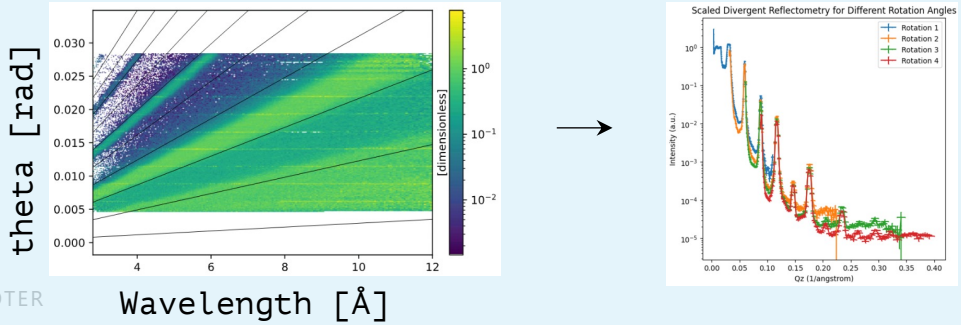
✓ Event formation unit (EFU)

↓

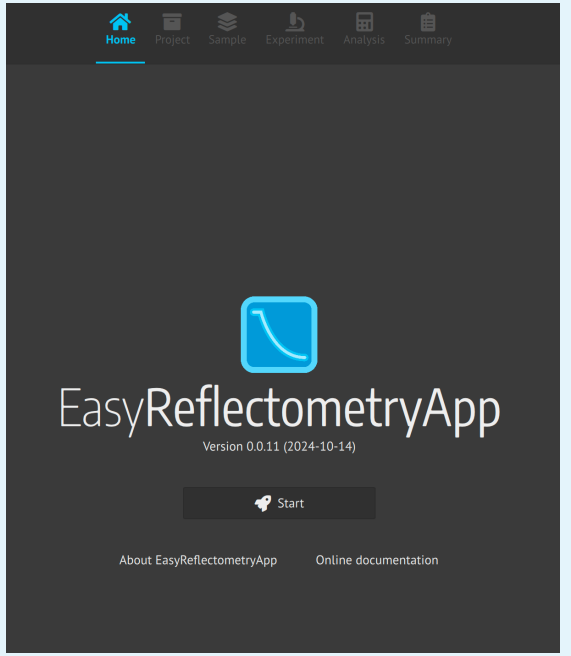
.hdf

Data Reduction and Analysis on VISA





Dedicated Analysis Software



FREIA Pre-build at STFC

NMX Progress

Installation

Cave and Hutch

Guide

Shutter and Choppers

Collimator and pinholes

NMX Progress

Robots

Robots ready – Factory Acceptance scheduled for November 2024

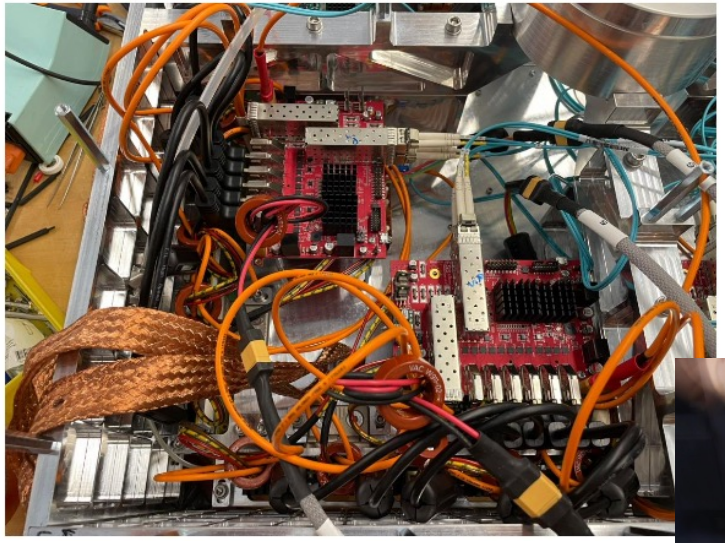
Installation scheduled for January 2025

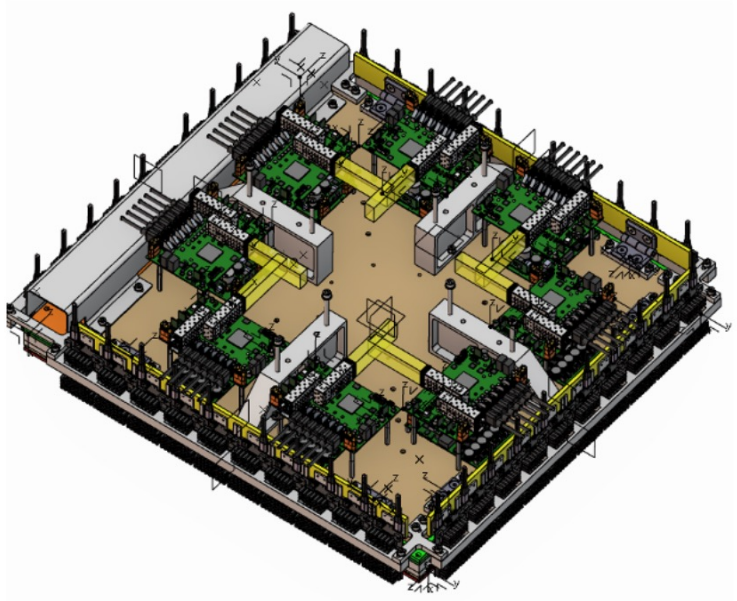
NMX Progress

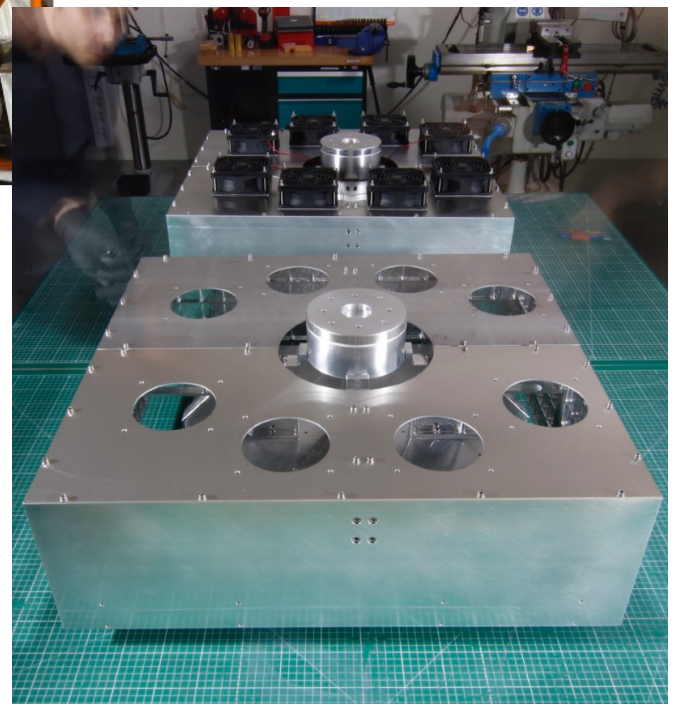
Detectors

Module 0 (Day 1 scope) scheduled to be available in Lund for testing in December 2024

Module 1-3 to be installed after BOT during shutdowns and are expected to all be delivered by end of 2025







Progress Risks

LoKI : energisation of racks, testing of motion controls

SKADI : detectors

Estia : installation and energisation of racks, testing

FREIA : design effort (CEP/CUP/MCA/BM)

NMX : detectors, energisation of racks

Energisation : We now have a co-ordinator for Energisation and Testing (Hannes Larheden) who is working to speed up energisation and manage resources for testing of equipment.

Detectors : we are working closely with the SKADI team to solve integration issues; for NMX we will start the instrument with only one detector and add the others after BOT.

LSS Team

LoKI

Judith Houston (ESS, Instrument Scientist)

Hannah Burrell (ESS, Instrument Ops Engineer)

Estia

Jos Cooper (ESS, Instrument Scientist)

Felipe Lopes (ESS, Instrument Ops Engineer)

NMX

Esko Oksanen (LU/ESS, Instrument Scientist)

Justin Bergmann (ESS, IOE/Instrument Scientist)

Swati Aggarwal (LU/ESS, IOE/support scientist)

SKADI

Sebastian Jaksch (ESS/FZJ, Instrument Scientist)

Annika Stellhorn (ESS, Instrument Scientist Polarization)

FREIA

Tom Arnold (ESS, Instrument Scientist)

Ellen Wilson (LU/ESS, Postdoc)

Instrument Data Scientists (matrixed from DMSC)

SANS : Oliver Hammond

Reflectometry : Nicolo Paracini

NMX : Aaron Finke

Currently Recruiting
Instrument Scientist for Estia
Instrument Scientist for LoKI

Future Recruitments
Instrument Scientist for FREIA - 2026
Instrument Ops Engineer for SKADI - 2026
Instrument Ops Engineer for FREIA - 2026

First LoKI Early Science Workshop

25-30 scientists mostly expert users or international neutron facility scientists, as well as contributors from the ESS Science Directorate

1. Provide an overview of the instrument capabilities, expected performance as a function of facility start-up, keys dates, and currently planned sample environment and data analysis abilities.

2. Brainstorm early science experiments within the instrument's target themes: soft matter, materials and bioscience.

3. Ensure we have identified the necessary infrastructure (sample environments, utilities, data analysis, etc) in order to take best advantage of the early beam at the ESS.

ECIS 1-6 SEPTEMBER 2024

38th Conference of European Colloid & Interface Society

SCANDIC FALKONER, COPENHAGEN, DENMARK

Finding the right samples…

Path from hot commissioning to early science

Stage 1:
Compulsory calibration tests

Standard calibrating samples for SANS:
Vanadium
SDS Powder
Silver Behenate
Latex nanoparticles
Gratings?

Round robin samples:
Glassy carbon (NIST)
Mesoporous silica (FSM-16)

Stage 2:
Early science tests - Samples selected to match the available instrument set-up

INSTRUMENT SET-UP	SCIENTIFIC CAPABILITY	POTENTIAL SAMPLES (using the regular cell holder or pre-commissioned sample environments)
Only the rear detector	Low Q only, length scales of 10-300 nm	Nanogels, surfactant self-assemblies, photoluminescent materials, e.g. conjugated polymers
Wide-angle detector banks	High Q only, length scales of 0.5-50 nm	Crystalline/mesoporous materials, e.g. templated organosilica
Full detector coverage	Simultaneously probe multiple length scales (0.5-300 nm)	Liquid crystal nanoparticles, e.g. hexasomes, cubosomes Wormlike micelles

* Samples should be stable for storage & readily available at the instrument
** Samples will be provided by the instrument team or close collaborators

Stage 3:
Early science - more complex samples/sample environment & full instrument set-up

Work with collaborators and expert users to:

- Investigate multiple length scales
- Perform experiments using flow e.g. rheology & microfluidics
- Use pre-commissioned in situ sample environments

LOKI Early Science (0.5 MW)

Taking advantage of the wide simultaneous q-range & moderate flux

Performance @~0.5 MW:
- Comparable to SANS2D

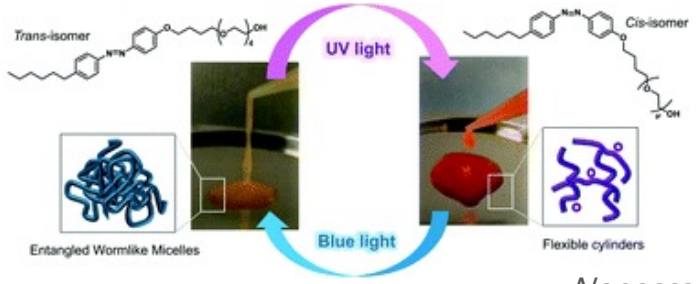
Performance @2 MW:
- ~5x compared to D22 (LoKI@14 Hz)
- ~20x SANS2D (LoKI@7 Hz)

Work with collaborators and expert users to:
- Investigate multiple length scale systems (simultaneously 0.5-300 nm)
- Perform experiments that use flow e.g. rheology & microfluidics
- Carry out work-horse SANS measurements with higher throughput
- Take advantage of pre-commissioned in situ sample environments

Some current ideas…

Photoswitchable worm-like micelles

R. Evans in Cambridge, UK

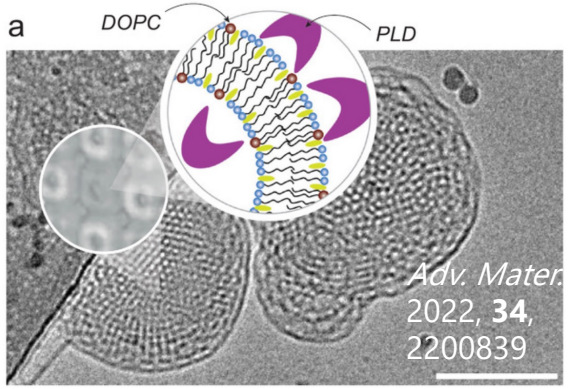


Nanoscale, 2020,**12**, 6300

System under flow ✓
Multiple length-scales ✓
In situ sample irradiation (adaptive sample environment) ✓

Lipid nanoparticles

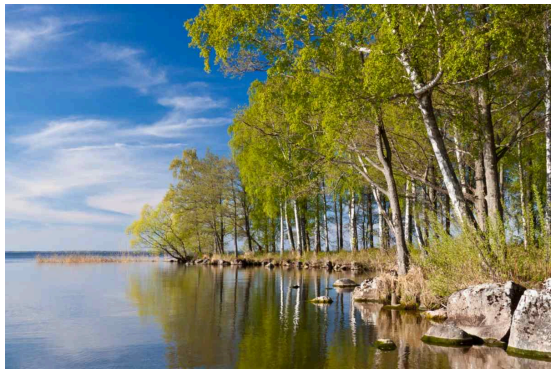
H. Barriga & M. Holme



Potential to involve ESS DEMAX ✓
Multiple length-scales ✓
Work-horse SANS experiments ✓

Dissolved Organic Matter

U. Olsson in Lund



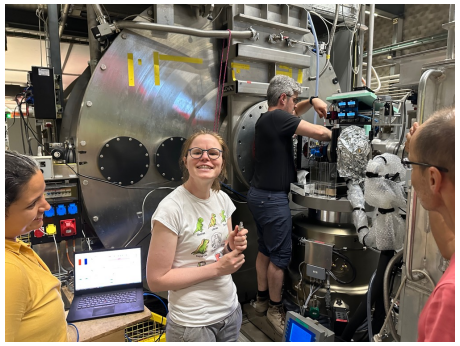
JCIS Open, 2023, 11, 100091

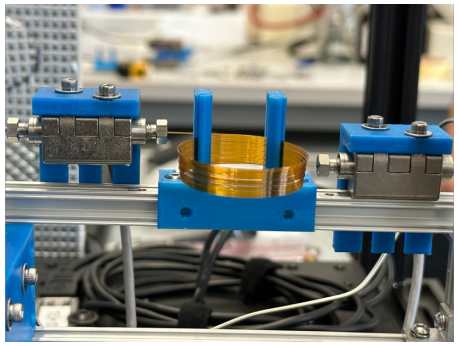
Multiple length-scales ✓
Workhorse SANS experiments ✓
Potential to involve ESS DEMAX ✓

LOKI Future Science (full detector coverage & 2 MW)

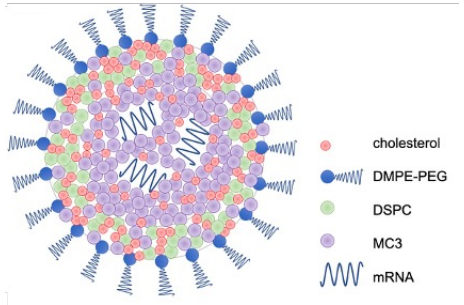
Taking advantage of the wide simultaneous q-range & great flux

Systems under shear

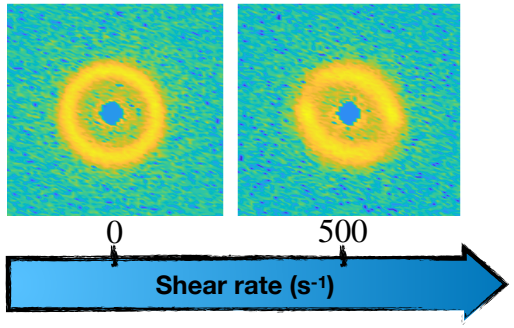




Faster timescales and smaller beam sizes ✓
Multiple length-scales ✓

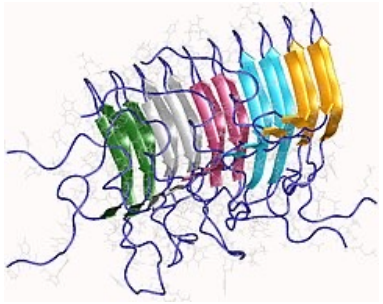


Structural effects due to the shear stress upon intravenous administration

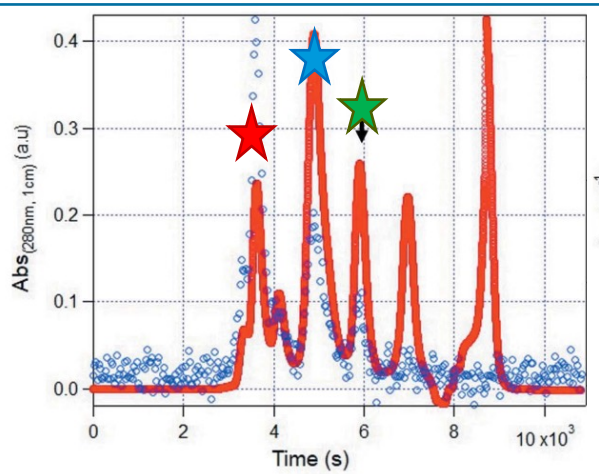


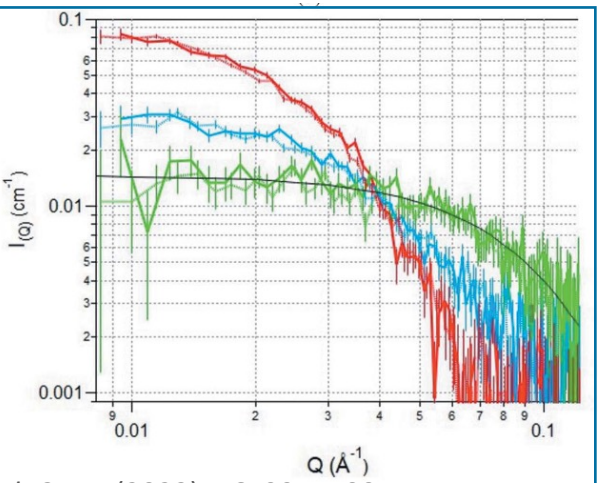
How different parameters affect the flow behavior of soft colloidal systems, e.g. microgels

BioSANS with a size-exclusion chromatography



Studying the suppression of Amyloid β-protein formation into fibrils with molecular chaperone proteins





Better resolution due to smaller cell size ✓
Potential to involve ESS DEMAX ✓

A. Martel et al., *J. Appl. Cryst.* (2023). 56, 994–1001

Major discussion points

- **Ramp-up of ESS:**
  - **Gradual ramp of ESS** will limit flux of LOKI in the early science period (12 months after BOT). Flux on par with SANS2D (ISIS), so not fantastic but certainly reasonable.
  - Potentially **unreliable stability of the target/accelerator** should be taken into account when planning precious and/or expensive samples.
- **Sample environment:**
  - Plan for the **generic sample environments**, e.g. 48 position cell holder, rheometer, stopped flow, rotating cell holders
  - Plan for the more **specialist set-ups**, e.g. in situ setups such as SEC, spectroscopies and DLS, crystats (*all currently in plan*)
  - Items currently **not in the plan**, e.g. high temperature furnaces, high pressure cells, super high temp
- **DEMAX and bio-labs:**
  - **Deuteration capabilities** and how they useful for early science
  - There will be labs equipped for bio-sample prep, to L1 - no decision yet made on L2 lab availability
  - There may be possibilities for users with the necessary skills (organic synthesis/protein expression) to spend time at DEMAX learning deuteration methods and strategies.
  - Samples may also be available through **DeuNet collaboration** (there will be a satellite @ ICNS)
- **Discussion of Early Science experiments:**
  - "Low hanging fruit" experiments. There are samples and studies that will have been performed elsewhere that can be complimented and completed on LOKI
  - Aim for good publicity experiments that are interesting from a press release perspective, e.g. food studies, vaccines, etc
  - Take advantage of DEMAX
  - Take advantage of vicinity to MaxIV (CoSAXS and ForMAX).

Overall Feedback

- Workshop was well-received by the attendees, who were all people who were aware of ESS and SANS. No new users, although this it is probably too early in the timeline of ESS to be getting them involved.
- Attendees generally happy to have another meeting closer to actual early science (realistically still 2 years away)
- Approach for the community to get involved in early science on LOKI, is firstly to approach the instrument team for very early science (real commissioning experiments), and then there will be a proper system introduced by ESS with reviews etc for the first user call.

All slides from the workshop are available here:

https://indico.ess.eu/event/3478/

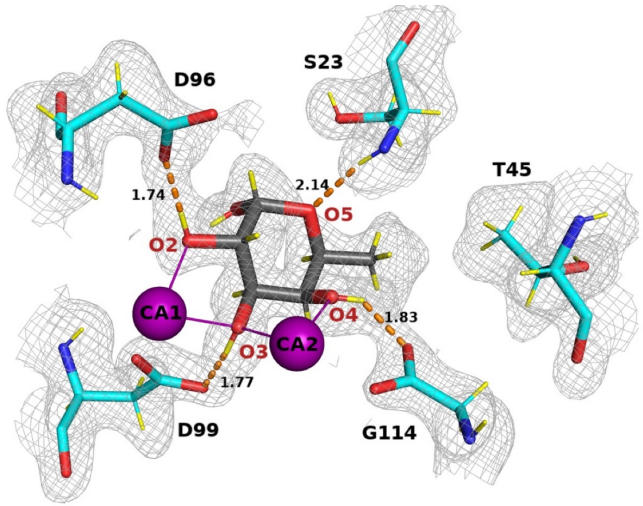
First NMX Early Science

26th August 2024

- **Satellite to European Crystallographic Meeting (ECM34) in Padua**
  - **Speakers from ESS, STFC, MRC LMB & ILL**
  - **Attended by ~20-25 protein crystallographers**

- **Presentations** (available at https://indico.ess.eu/event/3459/) **:**
  - ESS introduction & overview of NMX capabilities
  - Deuteration and crystallisation support from DEMAX
  - Data processing and refinement
  - Recent science example from ILL

- **Conclusion:**
  - NMX is well positioned for relevant early science on *e.g.* enzyme catalysis and ligand binding
  - More challenging systems (membrane proteins) would be feasible when ESS power is higher
  - Further outreach to expand neutron MX user community is needed



Gajdos et al. (2022)
Nat. Commun.

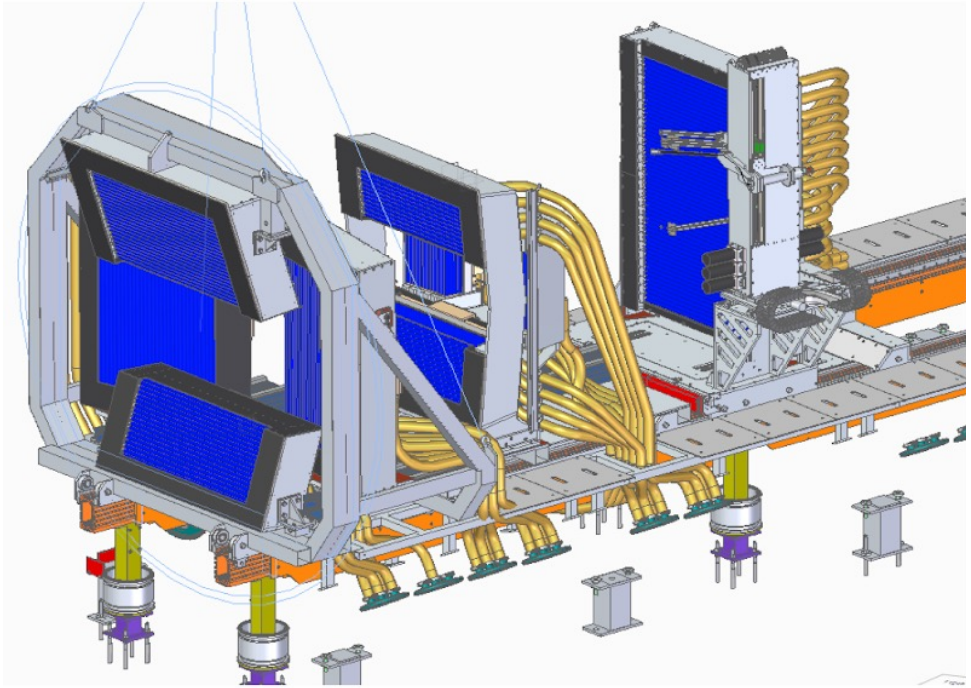
LSS Rescoping Priorities

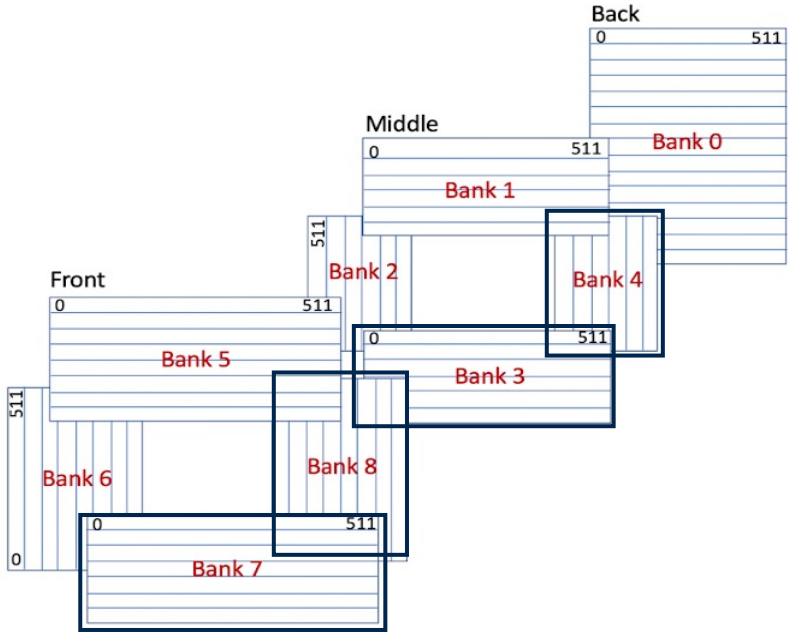
Highest Priority Items based on impact and readiness

1. LoKI detector area completion (1.04 M€) – key for meeting world leading performance - detectors procured, installation pending
2. FREIA fast shutter system (0.35 M€) – key for meeting world leading performance for kinetics measurements, development work done (via grants) – final design and procurement can be done now.
3. Estia add-ons (1 M€) – enhancement to capabilities - can be executed mostly as small procurements procurements over time (spin-resonance flipper, space-time collimator, GISANS re-focusing, in-situ MOKE, ultra-focus+imaging, various dedicated SEE)
4. NMX isotopic Gd for detectors (1 – 4M€) – key to world leading performance (detector efficiency from <15% to >30%), supply chain issues, needs to wait for detector system to be complete and tested.
5. NMX extra detector (< 1 M€) – enhancement of data quality or increase in throughput, needs to wait for NMX to be commissioned and operated for some user cycles.
6. SKADI detector area completion (2.5 – 4 M€) – key for meeting world leading performance, needs to wait for detector system to be tested and performance validated.

LoKI Detector upgrade update

- All cables and mechanical structures are at ISIS, and tubes are arriving from PTI (USA).
- 65% of modules are complete at ISIS.
- Electronics already at ESS. External cables from detector vessel to racks are already in place
- On target to made March 2025 delivery.



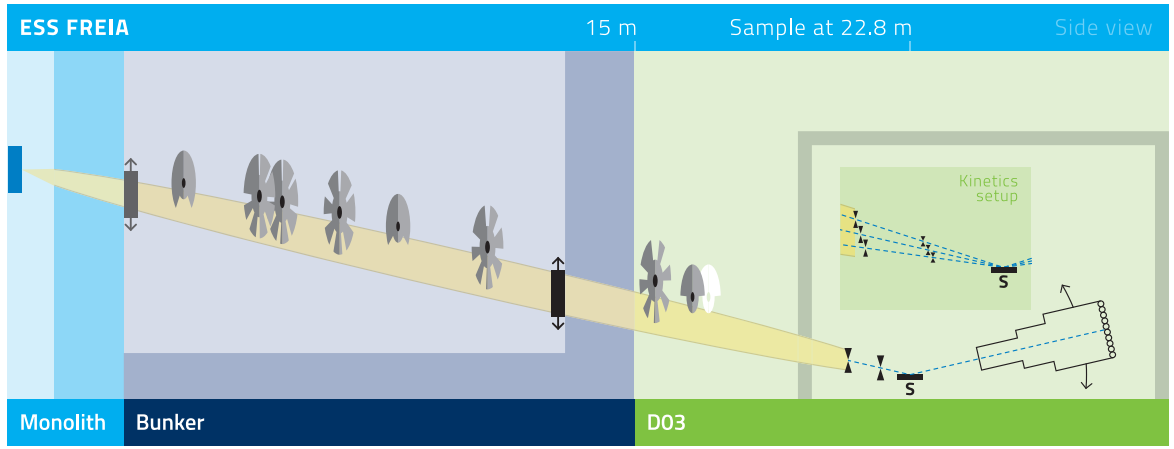


FREIA Fast Shutters

FREIA is a flexible instrument optimised for **time-resolved** and high throughput studies:

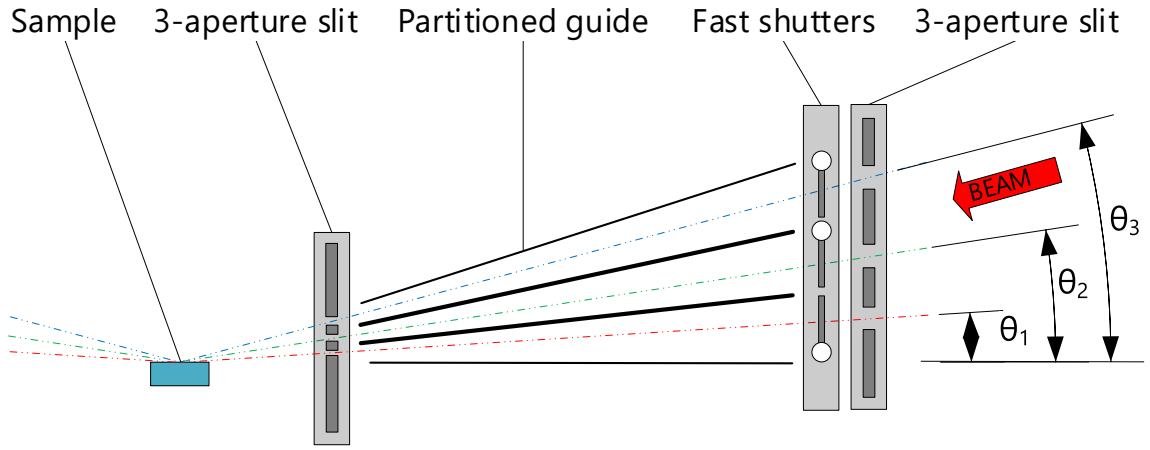
- Wide vertical divergence; **extended simultaneous Q range** & avoids slow sample movements
- Downward orientation for **liquid interfaces**
- **Flexible** Collimation options
- High flux (dλ/λ = 3-20 %) or high resolution (dλ/λ < 3%) modes

Wide ranging science case in **soft-matter and biosciences**



The Unique feature of FREIA design is the ability to **change angles without moving sample**

- allows full Q-range measurement with collimated beam without positioning overaheads

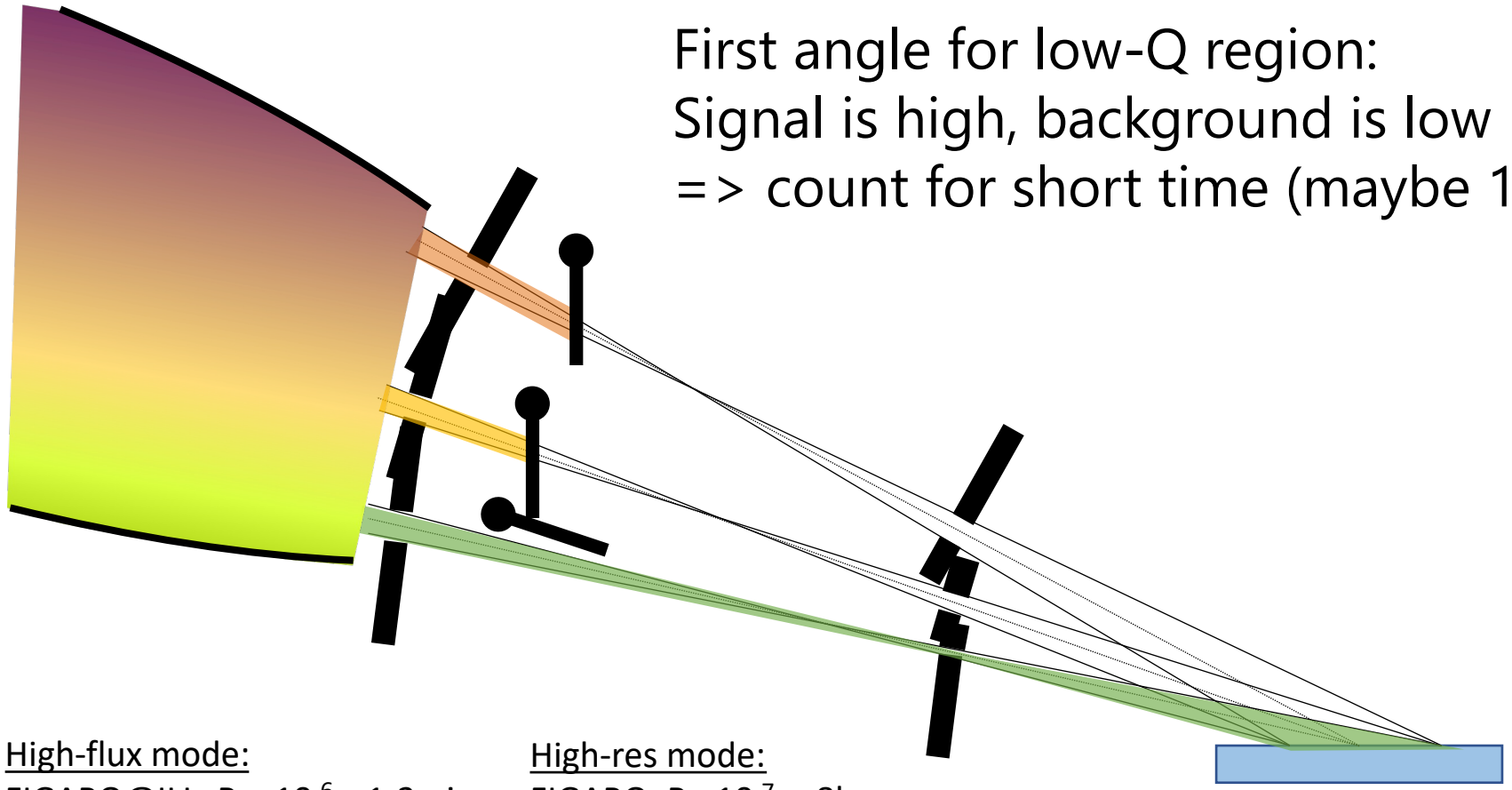


Fast Shutter development

Significantly increases the speed for angle changes to sub-second time resolution

FREIA Fast Shutters

Concept



First angle for low-Q region:
Signal is high, background is low
=> count for short time (maybe 1 pulse)

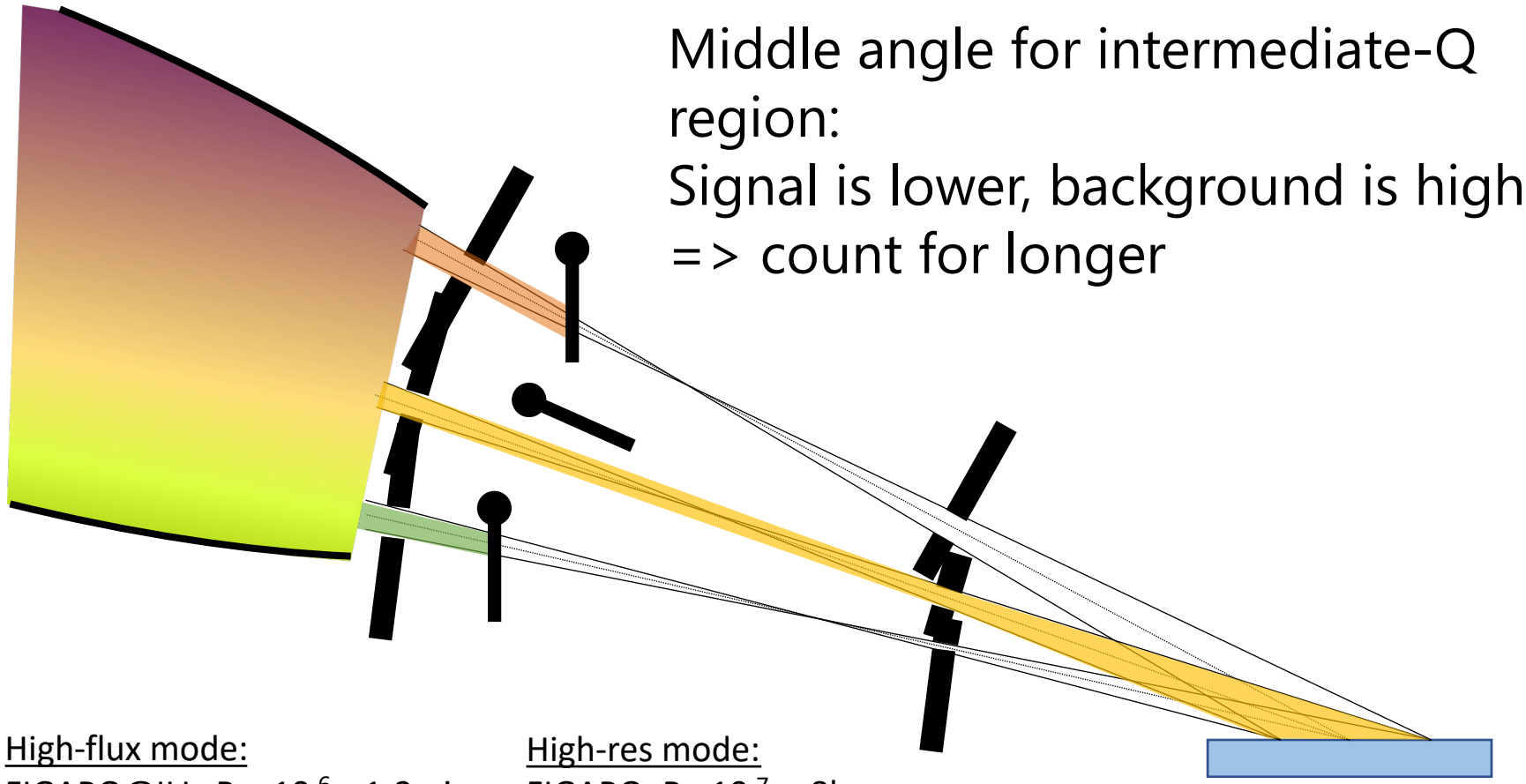
<u>High-flux mode:</u>
FIGARO@ILL: R = 10^{-6} – 1-2min.
FREIA @2MW: 3.75s
FREIA @ 5MW: 1.5s

<u>High-res mode:</u>
FIGARO: R =10^{-7} ~ 8h
FREIA @ 2MW = 15 min.
FREIA @ 5MW: 6 min.

*comparison is quite old, current instruments have been getting faster

FREIA Fast Shutters

Concept



Middle angle for intermediate-Q region:
Signal is lower, background is higher
=> count for longer

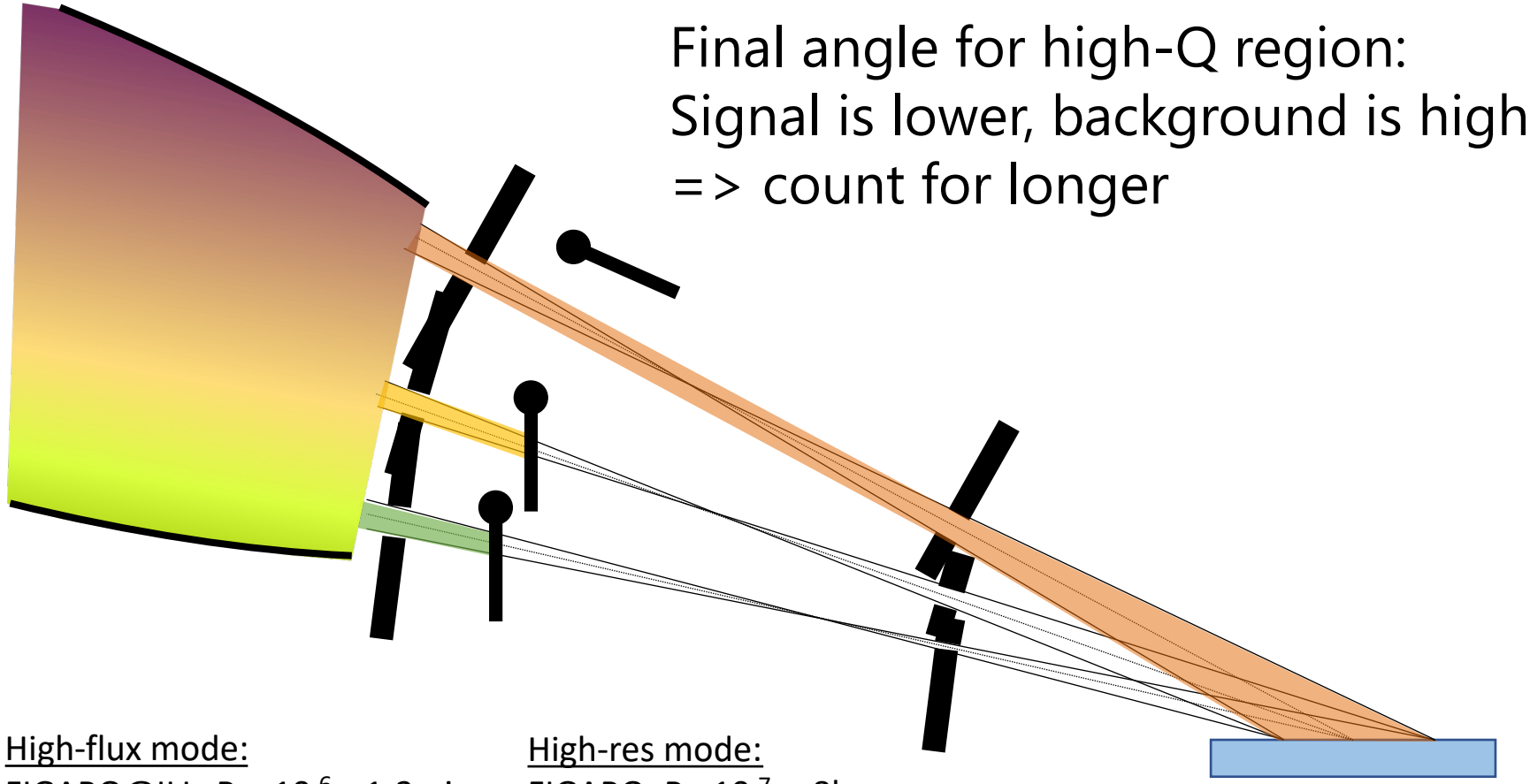
<u>High-flux mode:</u>
FIGARO@ILL: R = 10^{-6} – 1-2min.
FREIA @2MW: 3.75s
FREIA @ 5MW: 1.5s

<u>High-res mode:</u>
FIGARO: R =10^{-7} ~ 8h
FREIA @ 2MW = 15 min.
FREIA @ 5MW: 6 min.

*comparison is quite old, current instruments have been getting faster

FREIA Fast Shutters

Concept



Final angle for high-Q region:
Signal is lower, background is higher
=> count for longer

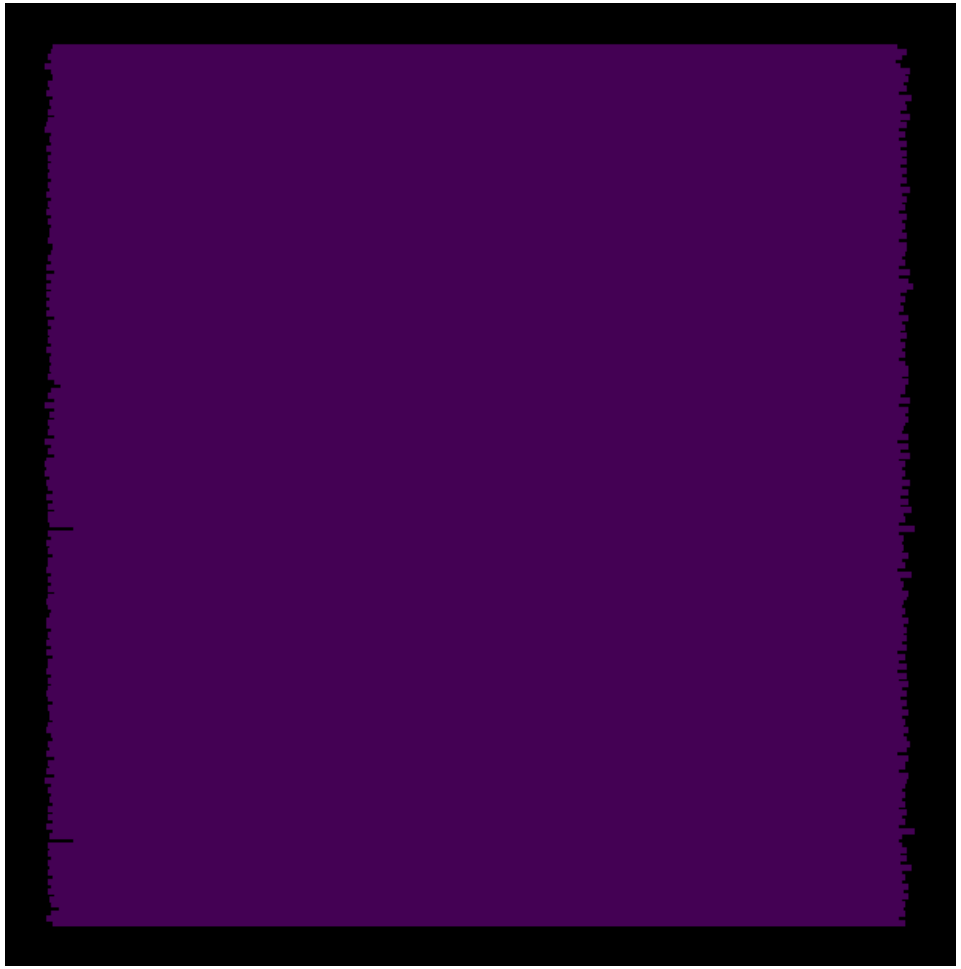
<u>High-flux mode:</u>
FIGARO@ILL: R = 10^{-6} – 1-2min.
FREIA @2MW: 3.75s
FREIA @ 5MW: 1.5s

<u>High-res mode:</u>
FIGARO: R =10^{-7} ~ 8h
FREIA @ 2MW = 15 min.
FREIA @ 5MW: 6 min.

*comparison is quite old, current instruments have been getting faster

FREIA Fast Shutters

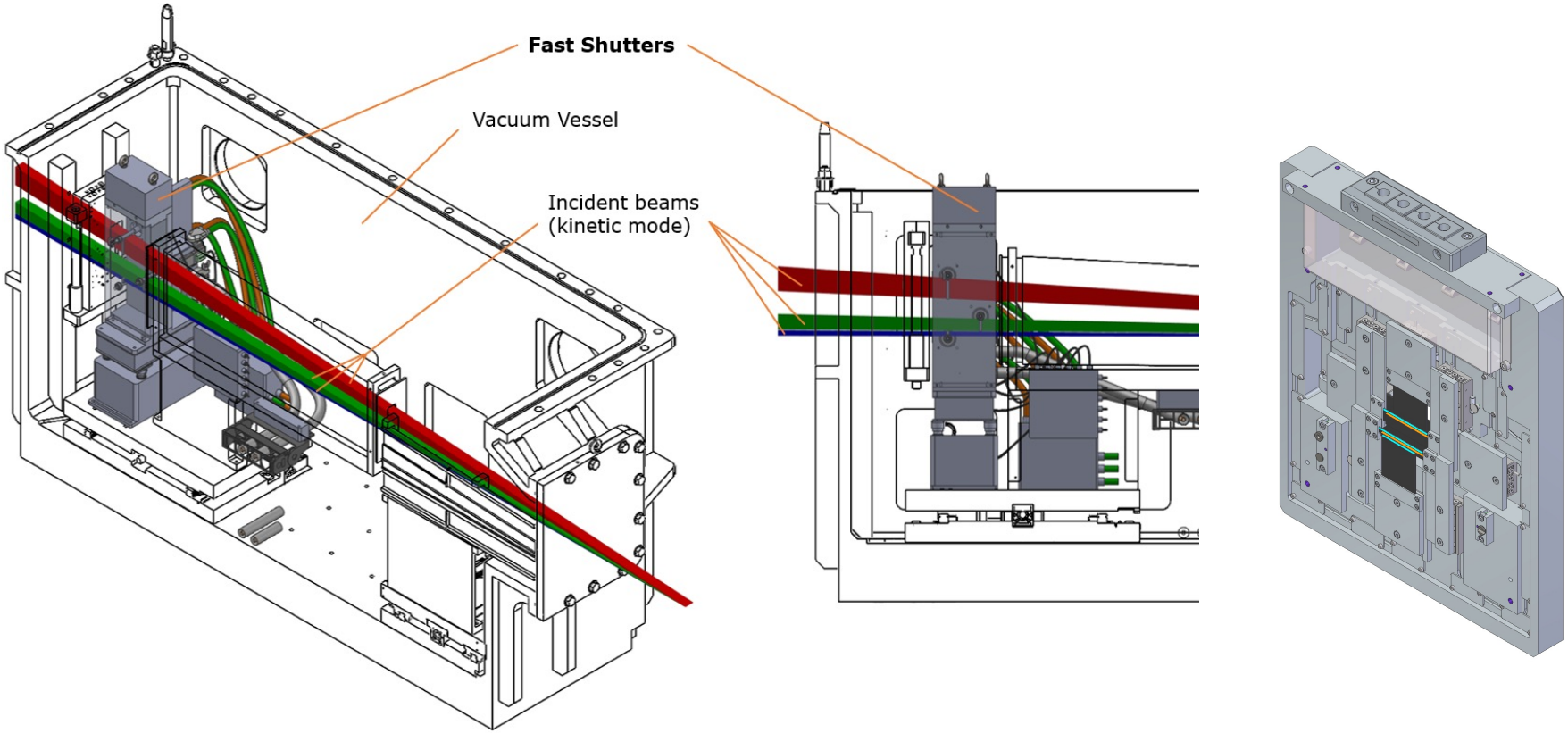
Test Experiments



A prototype was tested with neutrons at ISIS: https://doi.org/10.1016/j.nima.2023.168556

FREIA Fast Shutters

Conceptual Design



Full design concept integrated with FREIA collimation system has been designed… likely to be first “upgrade” to FREIA

Note these compact slits are not trivial: solution based on piezo stages has been designed

Questions?