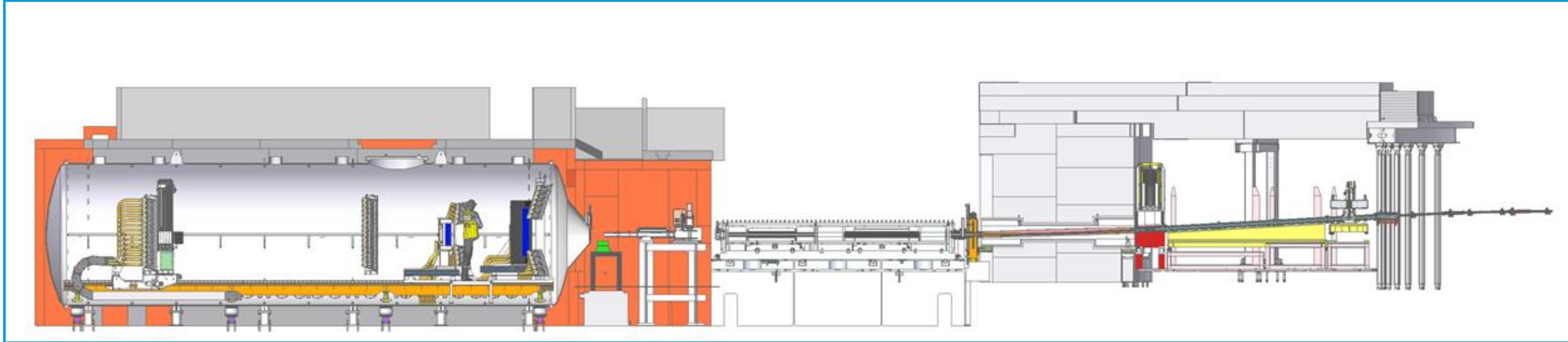
Scientific Overview of LoKI



System Acceptance Review
2025-09-19

ANDREW JACKSON FOR THE LOKI TEAM

12/09/2025

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

The extended LoKI team over the years

2012-2025

Core Team at ESS

Current
Judith Houston
Clara Ines Lopez
Hannah Burrall
Oliver Hammond
Andrew Jackson

Former
Kalliopi Kanaki
Gergely Nagy
Milán Klausz
Wojciech Potrzebowski

ISIS
Richard Heenan
William Halcrow
Davide Raspino
Jim Nightingale
Sean Langridge
Kevin Jones
David Turner
Rob Dalgliesh
Anton Orzulik
Gabor Nafradi
Chris Cornall
Federico Masi
Simon Cooper
Peter Galsworthy
Ben Hicks
Jacob Simms
John Crawford
Nick Webb
Steven Cox

ESS

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Markus Olsson

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Nathaly De La Rosa

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Volodymyr Zhovtovskiy
Safaa Zaki

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Jessia Lastlow
Ahmed Abujame

ECDC:
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Nikolce Andonovski

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Harald Schneider

RP:
Ana Cintas

CUP/PowerHeat:
Jesper Ringnér
Kristofer Falkland
Jonnie Sipikari
Sebastian Malmqvist

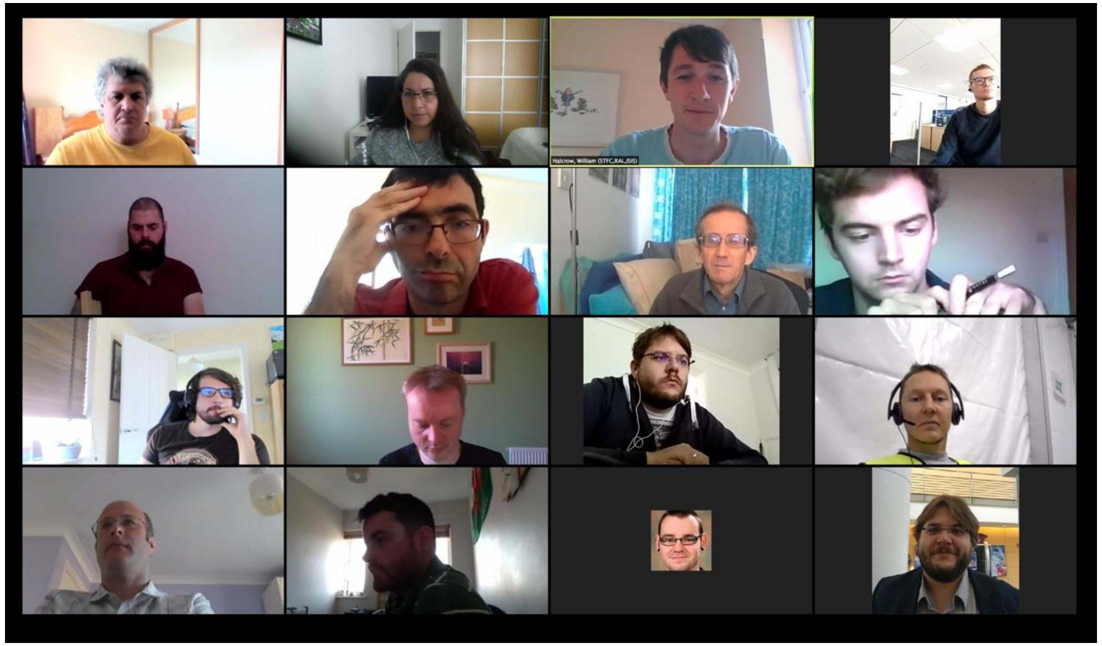
NSS Techs:
Dennis Vedelgart
Adriano de Morais
John Flannery
Hans Ekmark

Rigging:
Fredrik Lundström
Hampus Ivesköld
Anders Cederholm

Workshops:
Andreas Malmquist
Guillaume Barthet
Javier Fores
Patrik Andersson

In-Kind:
Nataliia Cherkashyna

And everyone else who has contributed!

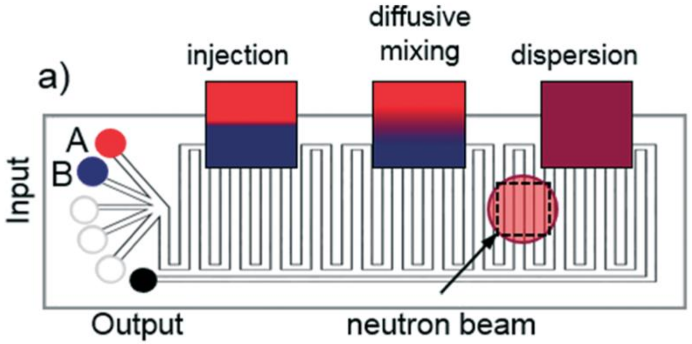


(we are generally much happier than this photo suggests…)

Thanks to all for the hard work and collaborative spirit!

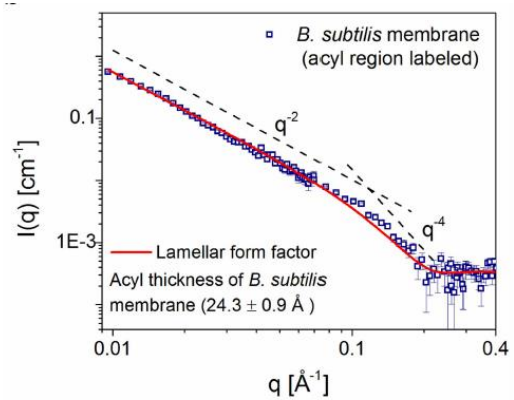
LoKI : SANS for soft matter, materials & bioscience

Microfluidic SANS:
High Throughput Mixing & Tailored Flow Geometry



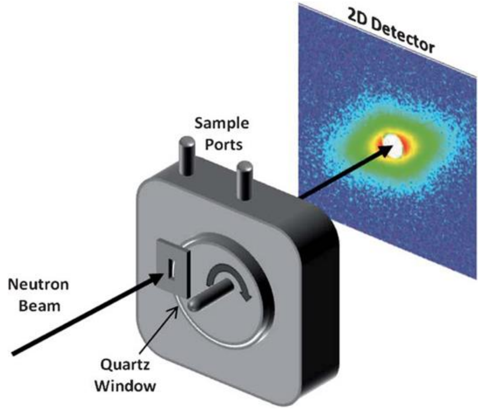
Lab Chip, 2017, **17**, 1559

Biological Samples:
Weak Scatterers & Dilute Solutions



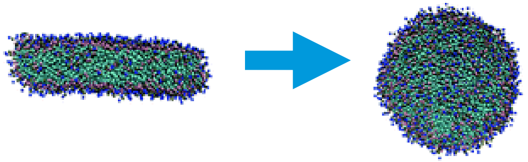
PLoS Bio, 2017, **15**, e2002214

Rheo-SANS:
Structures Under Shear



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

Non-Equilibrium Studies:
Self-Assembly & Kinetics



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

Our goals:

- Small beams for flow-through, scanning & microfluidic experiments.
- Perform "single-shot" kinetic measurements on sub-second timescales.

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

LoKI Requirements

A broad Q range, high flux SANS instrument for soft matter, materials, and bio-science

Science Based Goals

- Rapid data collection / short counting times to enable kinetics
- Probe broad size range to examine hierarchical structures
- Small sample volumes for scanning, biological and complex samples
- Integrated flexible sample environment for non-equilibrium studies
- Integration of complementary techniques experimentally and in data analysis
- Simplicity of operation to allow users to focus on science

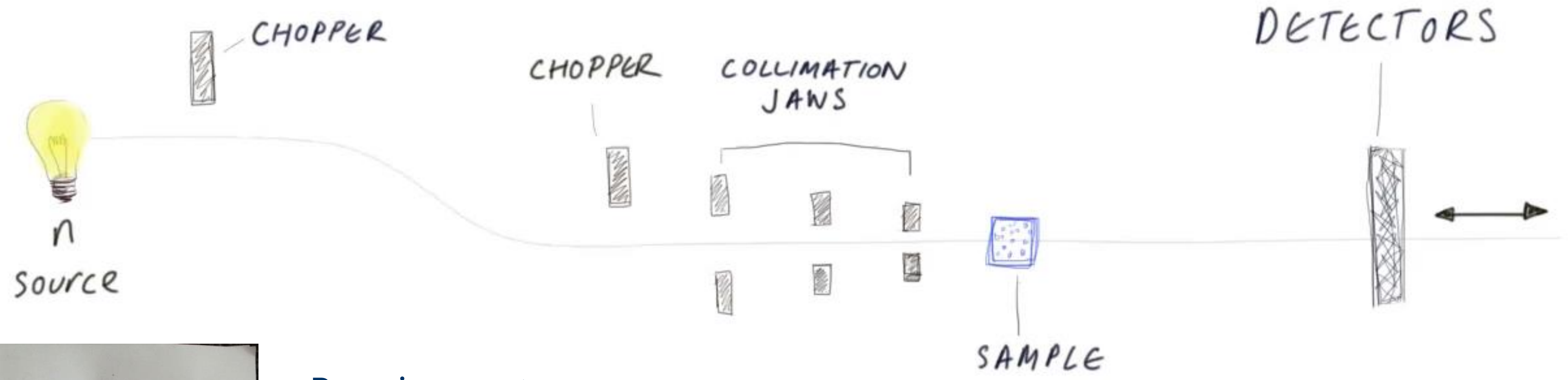
Technological Goals

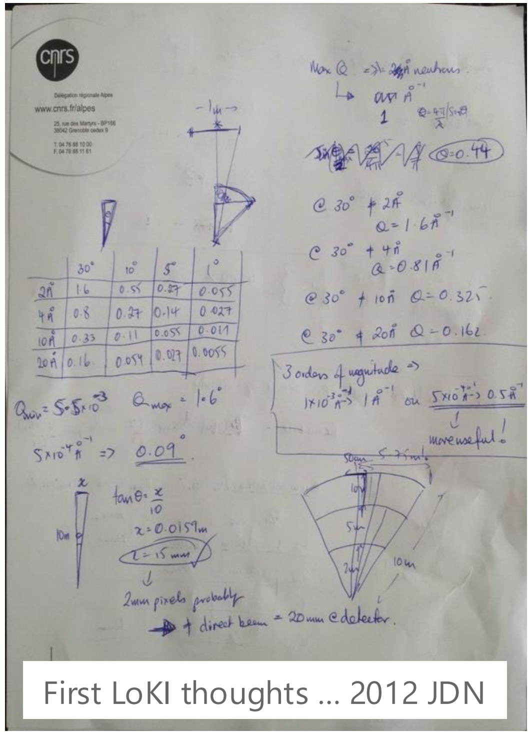
- Broad simultaneous Q range with Q_{max}/Q_{min} = 1000
- Good Q resolution over the whole Q range
- High flux making best use of ESS source
- Single pulse scattering measurements
- Optimized use of new detector technologies

High-level Scientific Requirements for the Instrument

- The instrument shall allow data to be collected to a Q_{min} of < 0.001 Å^{-1}.
- The instrument shall allow data to be collected to a Q_{max} of > 2 Å^{-1}.
- The instrument shall allow data to be collected simultaneously over a continuous Q range with Q_{max}/Q_{min} > 1000.
- The instrument shall match the size of the neutron beam to the size of the sample.
- The instrument should allow the Q resolution (dQ/Q) to be optimised for the experiment.
- The instrument should be capable of providing a Q resolution < 10% dQ/Q over the whole Q range.
- The instrument should allow data collection from samples < 8 mm^3 volume
- The instrument should maximise the signal-to-background (S/B) ratio of the small angle scattering.

The Design




First LoKI thoughts … 2012 JDN

Requirements

1. Super bright **source** & cold moderator
2. **Guide** to tunnel the neutrons down to our sample position
3. **Choppers** to shape and define our neutron profile
4. **Collimation** jaws (pinholes) to “shape” our beam
5. **Environments** to support our samples
6. Efficient **detectors** with good resolution and wide coverage to measure our scatter

Other considerations

1. Vacuum
2. Shielding (in **and** out)
3. Speedy electronics and state-of-the-art software

Defining our beam : **neutron guide**

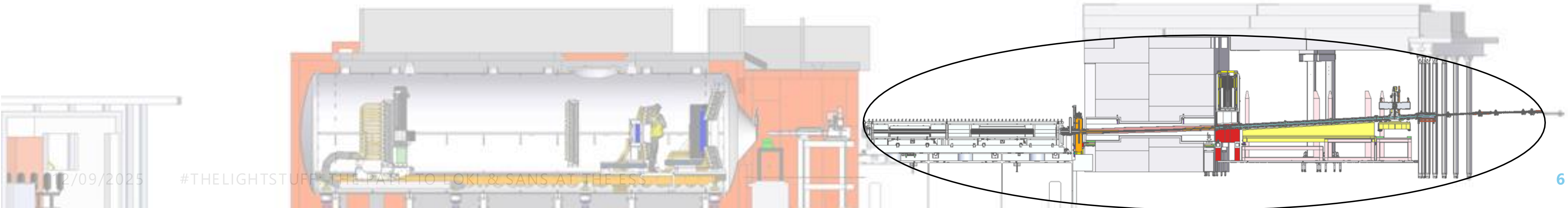
Transporting the good neutrons, removing the "bad" ones

Requirement:

- **Transport neutrons** from the moderator to the sample with 100% brilliance transfer within the selected wavelength and divergence range
- **Prevent the transport** of high energy neutrons
- **Signal-to-noise** to be the best it possibly can possibly be

What we can do:

- Use straight highly reflective guide (m=2) under vacuum
- Two multichannel benders (m=3) = twice out of line-of-sight
- Smaller beam size (25 mm × 30 mm (V × H)) to minimise transport of background



Defining our beam : **Choppers**

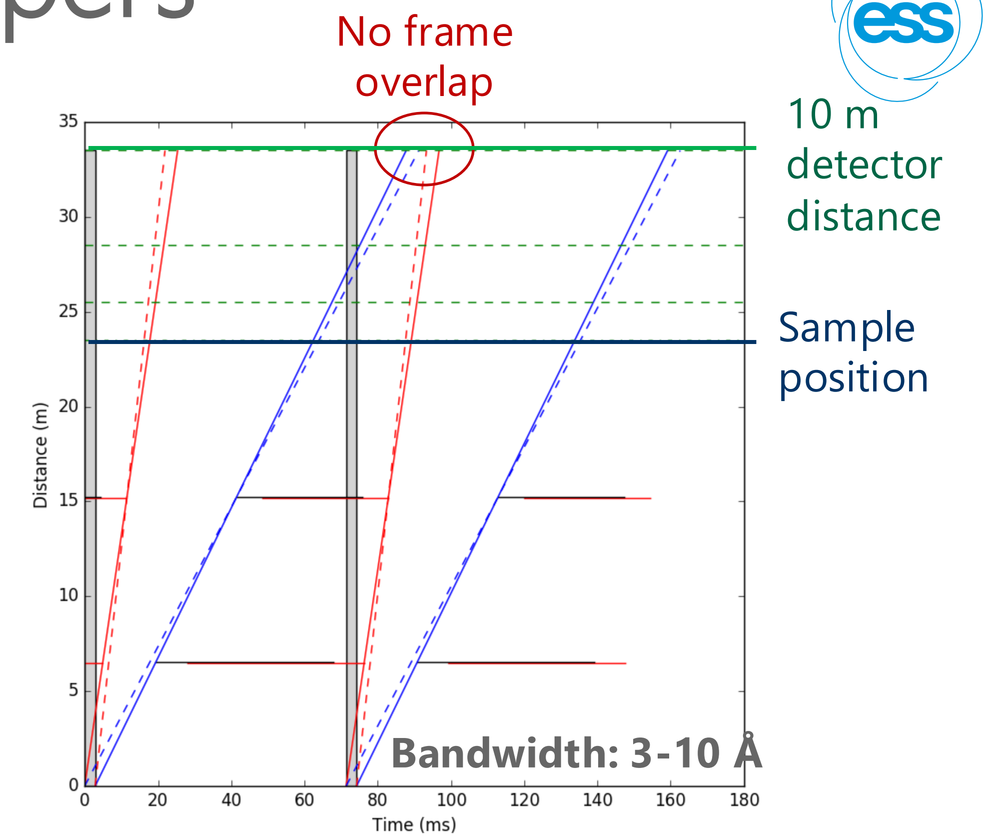
Select the wavelength band for an experiment

Requirements

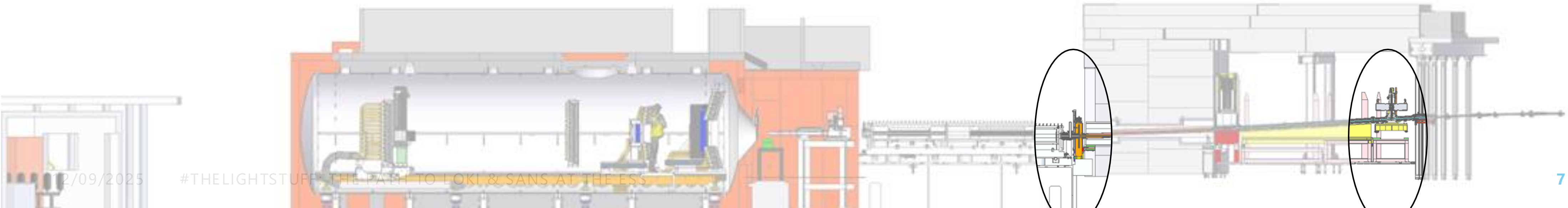
- Cut the bandwidth down to a defined wavelength band
- Maximise bandwidth – 7Hz option
- Prevent overlap between sequential pulses
- Operate in pseudo-monochromatic mode

To do this, we define:

- Disk openings
- Rotation speed
- Position along the beam



e.g. Time-distance diagram for 14 Hz operation with rear detector at 10 m from sample



Defining our beam : **Collimation**

Controlling the size and divergence of the beam

Generally, the biggest challenge in the design of any SANS instrument is to separate the direct beam from the scattered radiation at small angles (<0.1°).

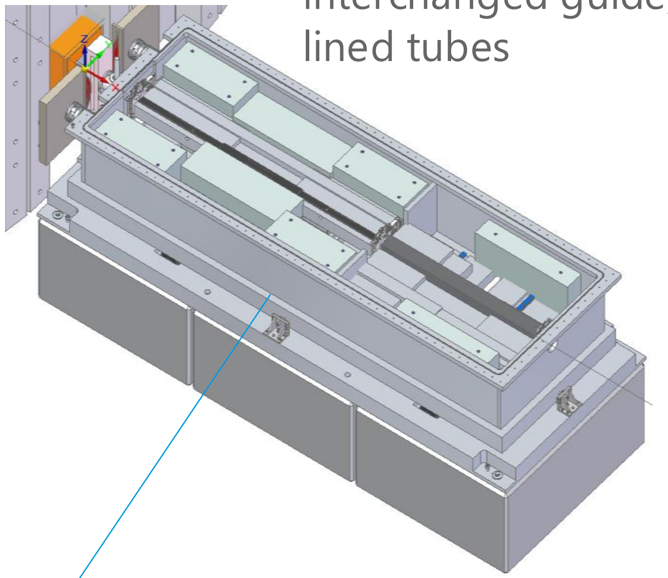
Requirements

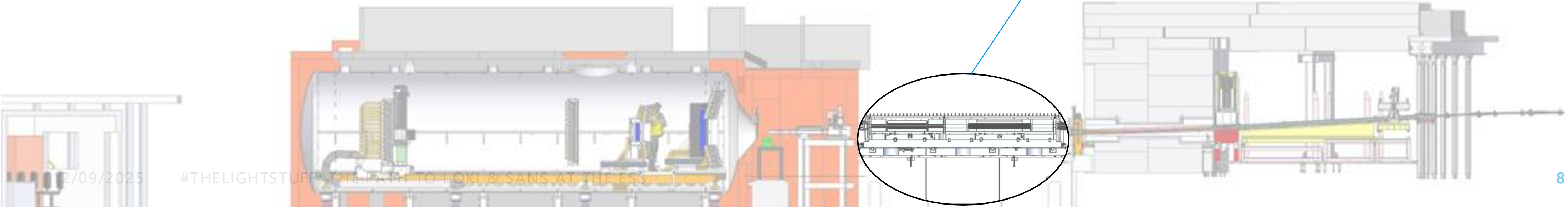
- Control the **size** and **divergence** of the beam

To do this:

- 4-jaw slit sets at 8, 5 & 3 m before the sample position
- Variable-sized apertures at the sample position
- Platform to switch between evacuated boron-lined tubes (collimation) or sections of m=2 guide

Collimation vacuum tank containing slit sets & interchanged guide/boron-lined tubes

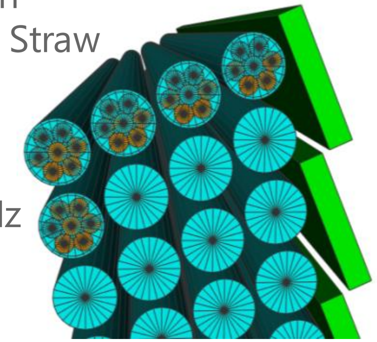




Detectors

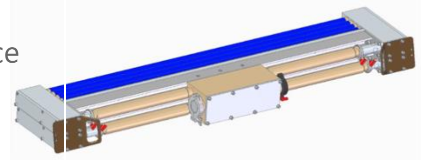
Maximising the neutrons we count – make the most of the source

Various different options were considered : 3He tubes, Boron blades (BandGEM) and Boron Straw Tubes. On balance of performance, cost and complexity Boron Straw Tubes were chosen



Efficiency: ~50%-60% at LoKI wavelength
Position resolution: FWHM is ~6 mm up to 350 kHz
Rate capability: 15% rate lost at 2.3 MHz

4 layers of 1" Al tubes, each containing 7 x 8mm boron-coated straws



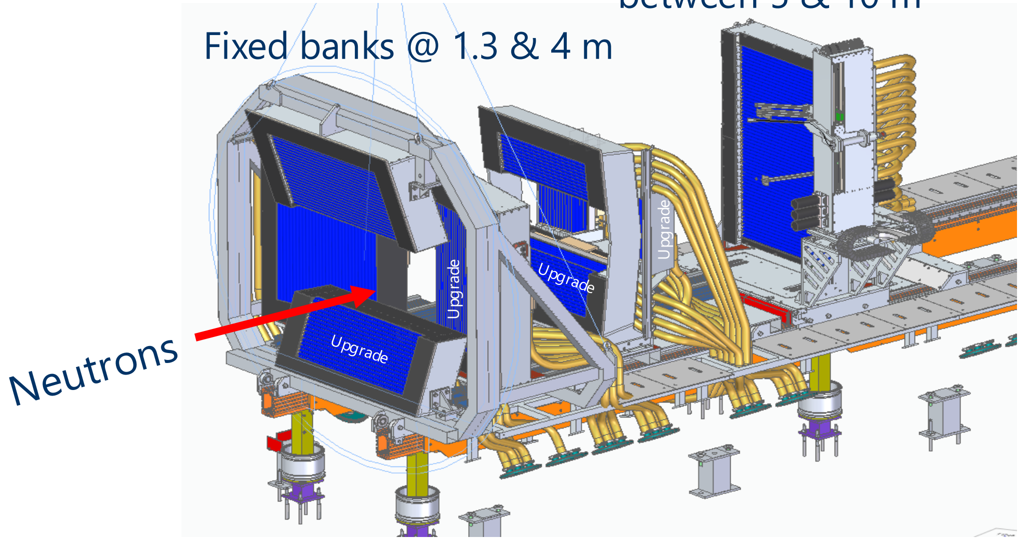
Signal is read out via 4 wires per tube with multiplexing resistance chain.

Detectors assembled as modules of 16 tubes.

Preamp and power board in airbox on ends of tube assemblies

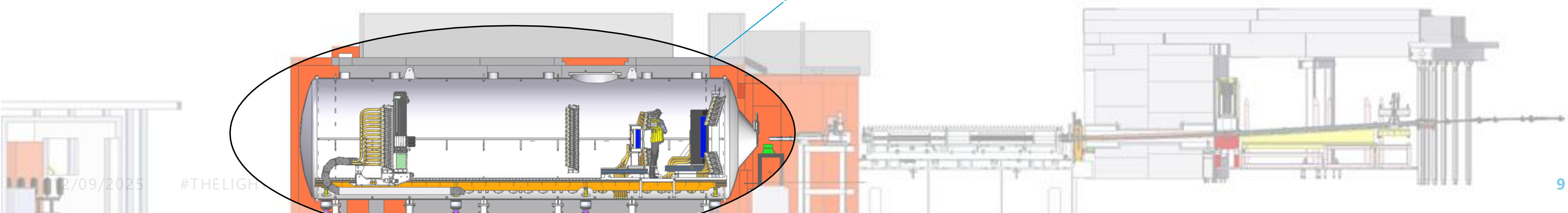
Covering 0º to 45º in scattering angle and 360º in azimuthal angle (180º Day 1).

Rear detector moveable between 5 & 10 m



Day 1 scope : 576 tubes x 7 straws x 256 pixels
= **1,032,192 pixels**

Full scope : 880 tubes x 7 straws x 256 pixels
= **1,576,960 pixels**



Detector Realities

Cables … lots of cables …

Support for Day 1 Detector Scope

576 tubes x 4 preamp channels = **2304 readout channels**

2304 readout channels / 128 channels per ADC = **18 R5560 ADC units**

576 tubes / 16 = **36 modules**

(16 tubes per module x 4 readout channels / 4 channels per cable) + 2 spares = 18 signal cables per module

18 signal cables x 36 modules = 648 signal cables

36 modules x 1 HV = 36 HV cables

36 modules x 1 LV = 36 LV cables

Total of 720 cables

Support for Full Detector Scope

880 tubes x 4 preamp channels = **3520 readout channels**

3520 readout channels / 128 channels per ADC = **28 R5560 ADC units**

880 tubes / 16 = **55 modules**

(16 tubes per module x 4 readout channels / 4 channels per cable) + 2 spares = 18 signal cables per module

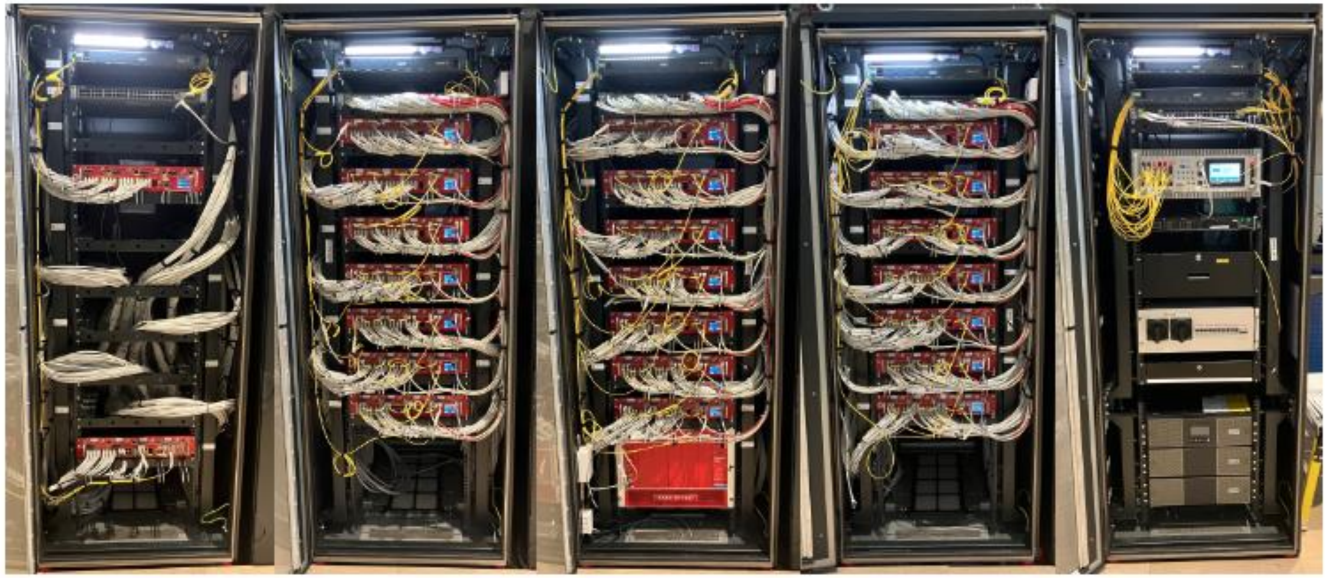
18 signal cables x 55 modules = 990 signal cables

55 modules x 1 HV = 55 HV cables

55 modules x 1 LV = 55 LV cables

Total of 1100 cables

Slave Rack 4 Slave Rack 2 Slave Rack 1 Slave Rack 3 Master Rack



Cabling for full detector scope has been installed as part of initial scope.

Detector and electronics hardware for full scope have been delivered and will be installed later

See Irina's presentation on testing

Sample environment

How best can we support our science case and take advantage of the wide simultaneous q-range and high flux?

The "off-the-shelf" variety

Needed for Hot Commissioning (LoKI Scope)
- **Thermostated cell holder**
- **Rotating cell holder**
- **Flow cell with HPLC pumps**

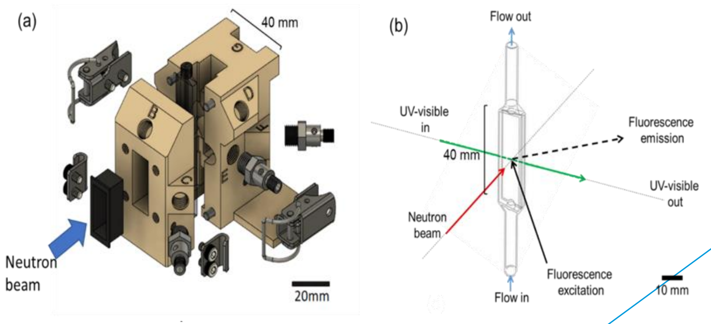
Needed for Early Science/SOUP
- Rheometer
- 2.5T electromagnet
- Stopped-flow equipment

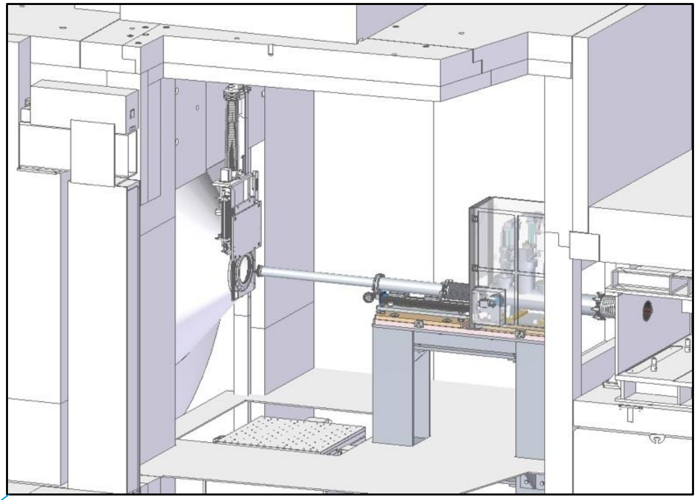
Needed later …
- Humidity chamber
- Couette shear (higher shear rates)
- Plate-plate shear (for e.g. polymers)
- Stress/strain rig (load capacity for stretching polymers)
- Cryostats

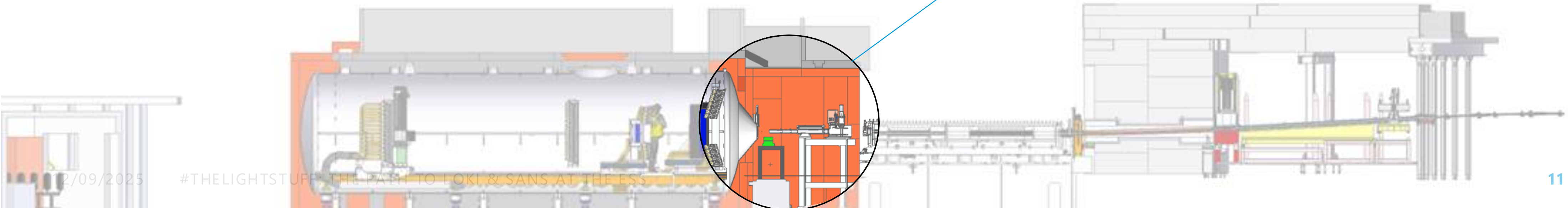
Custom-built sample environments

NuRF (Swedish VR collaboration)

In situ fluorescence, UV/vis absorption spectroscopies, densitometry on a continuous flow cell







12/09/2025