LoKI Hot Commissioning

Commissioning Workshop ESS-JPARC: Instrument Session

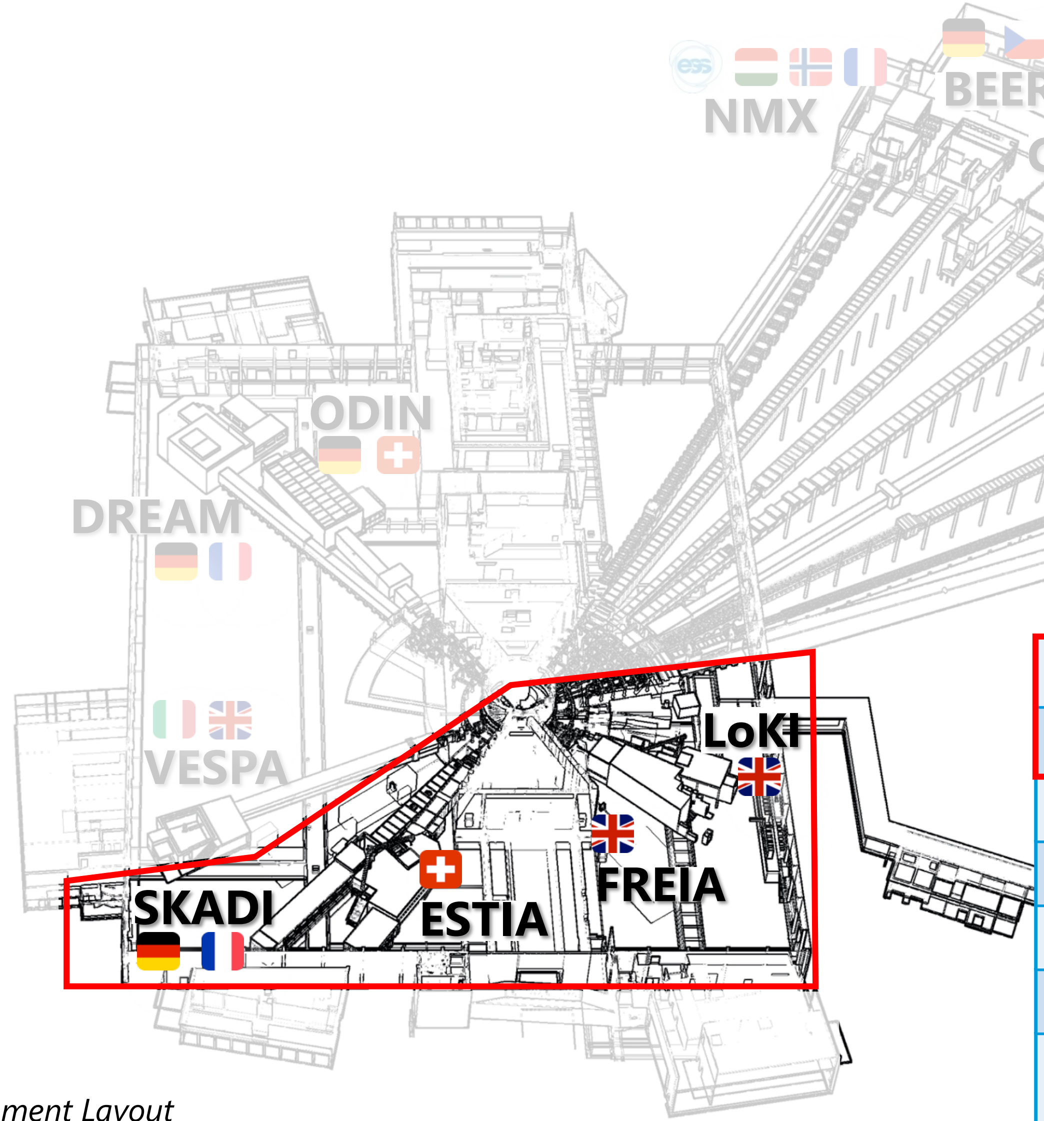
JUDITH HOUSTON

2022-10-10

1

Instrument class: Large-Scale Structures

ESS Instrument Suite: Large-Scale Structures



ESS Instrument Layout (September 2017)

SANS	**LoKI**, *SKADI*
Reflectometry	**ESTIA**, FREIA
Powder Diffraction	**DREAM**, HEIMDAL
Single-Crystal Diffraction	**MAGIC**, *NMX*
Imaging & Engineering	**ODIN, BEER**
Direct-Geometry Spectroscopy	**CSPEC**, *T-REX*
Indirect-Geometry Spectroscopy	**BIFROST**, MIRACLES, VESPA

2

Neutron reflectometers

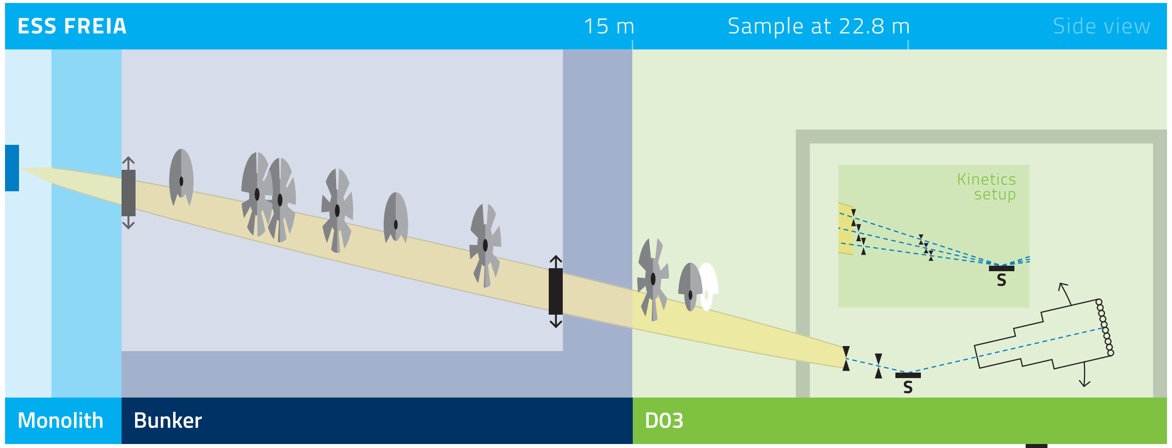
FREIA Horizontal Reflectometer

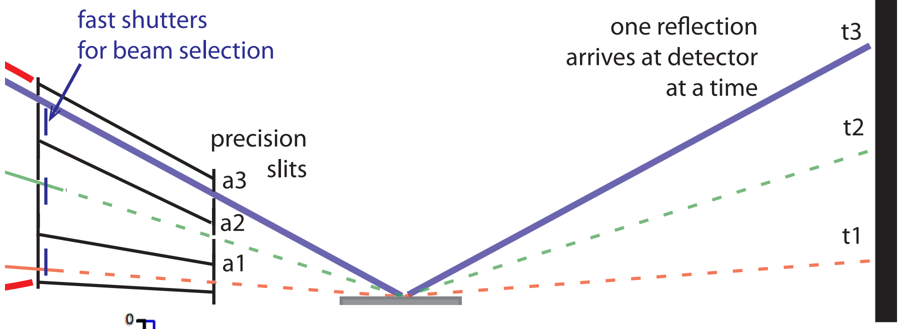
T. Arnold (ESS), J. Nightingale (ISIS), J. Elmer (ISIS)

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 res. (dλ/λ < 3%) modes

Wide ranging science case in **soft matter & biosciences**

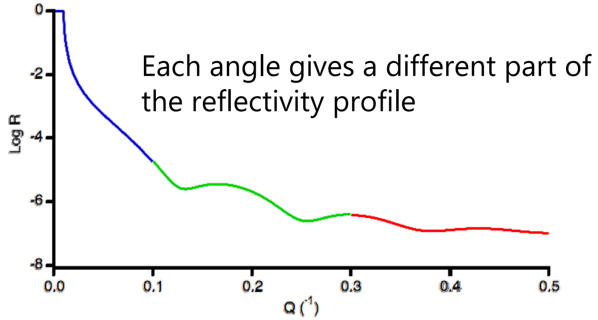



fast shutters for beam selection

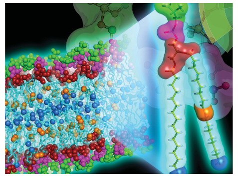
precision slits

one reflection arrives at detector at a time

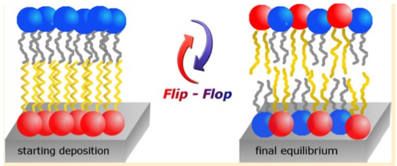
Each angle gives a different part of the reflectivity profile



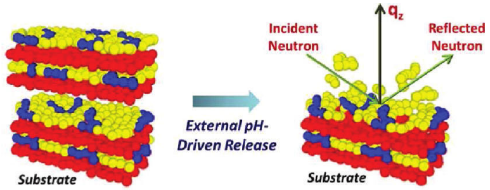
Structure



Kinetics



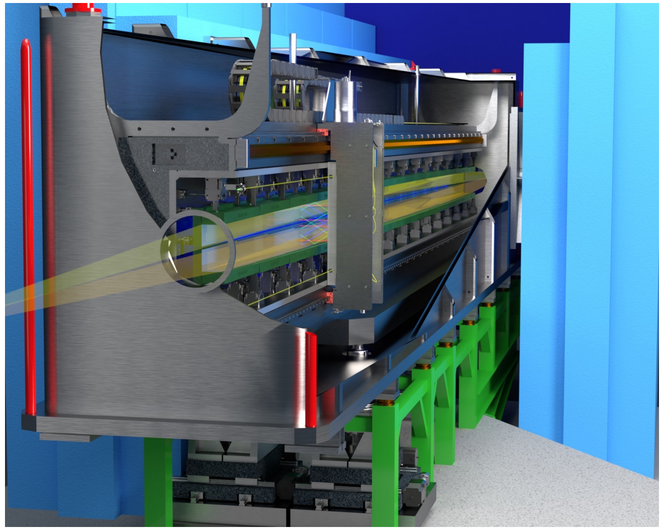
Function



ESTIA Small Sample Polarised Reflectometer

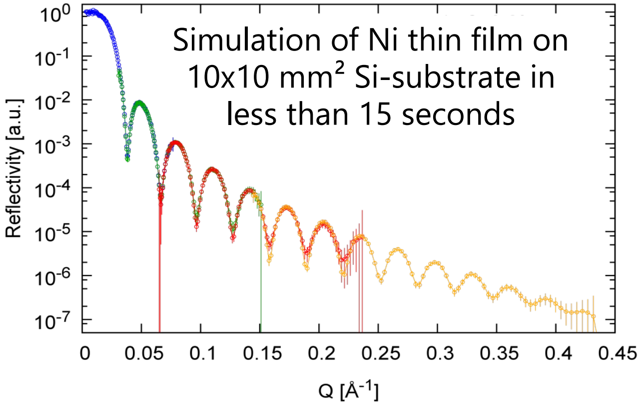
A. Glavic (PSI), S. Schütz (PSI), T. Arnold (ESS)

- The investigation of the **chemical and magnetic** depth-profile near surfaces and of **lateral correlations and structures**
- **Selene neutron guide** projects tiny beam from Virtual Source
- **Small samples:**
  - Large divergence (1.5°x1.5°)
  - Samples down to 1x1 mm²
- **Polarization >99%** for curved transmission polarizer and analyser
- Simultaneous measurement of two polarization states



Selene Neutron Guide

ESTIA is optimised for small samples and polarisation analysis:



Quick Facts	
Moderator	Cold
Length	35 m
Q-Range (solid samples)	10^{-3} – 3 $Å^{-1}$
Sample orientation	Vertical
Standard Mode (14 Hz)	
Min. Wavelength Band	7 Å
Min. Wavelength Range	3.5 – 28 Å
Min Q Resolution	ΔQ/Q < 2-7 %

3

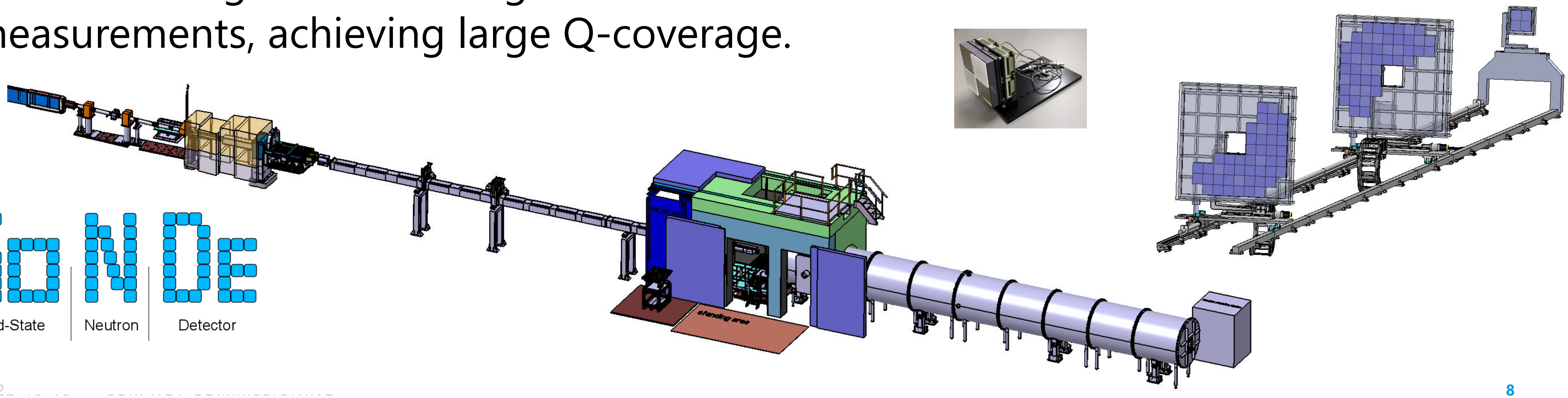
Small-angle neutron scattering

SKADI High Resolution SANS

S. Jaksch, H. Frielinghaus (JCNS), J. Jestin (LLB), R. Hanslik (FJZ), S. Desért (LLB)

- High-flux neutron extraction by optimized deflector
- Separate long/short wavelength polarization with supermirrors
- 4, 8, 14 and 20 m collimation settings
- VSANS: Down to ~10^{-5}Å^{-1}
- SoNDe : Dedicated detector development for best use of high-flux and single shot measurements, achieving large Q-coverage.

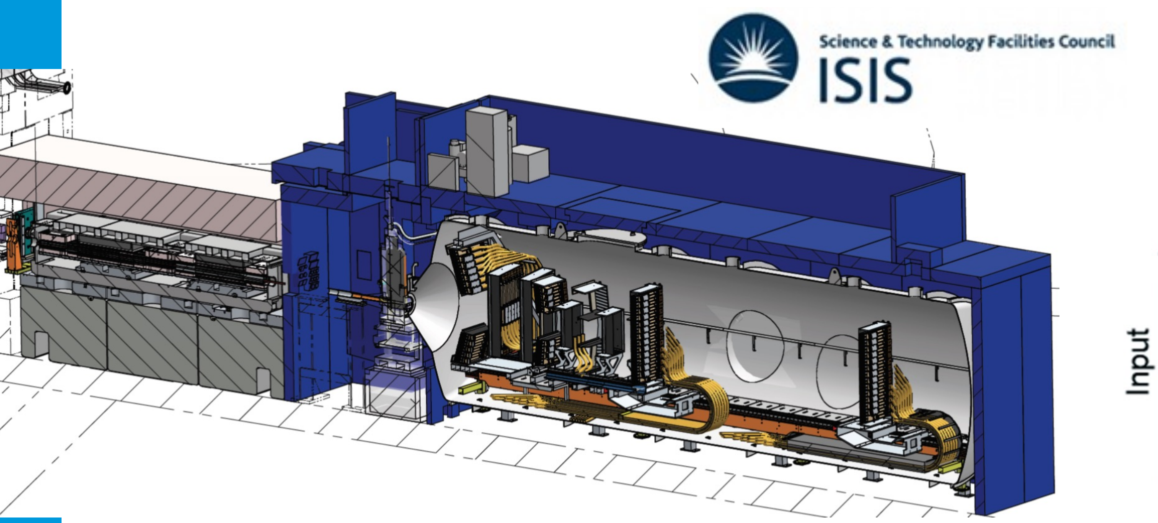
Quick Facts	
Moderator	Cold (max @ ~3 Å)
Length	58 m
Q-Range	10^{-4} – 1 Å^{-1}
Flux at sample position	7.7 × 10^8 n s^{-1} cm^{-2}
Standard Mode (14 Hz)	
Wavelength Band	5 Å
Wavelength Range	3 – 21 Å
Momentum Resolution	ΔQ/Q= 2-7 %



SoNDe

Solid-State | Neutron | Detector

LOKI Broad Band SANS

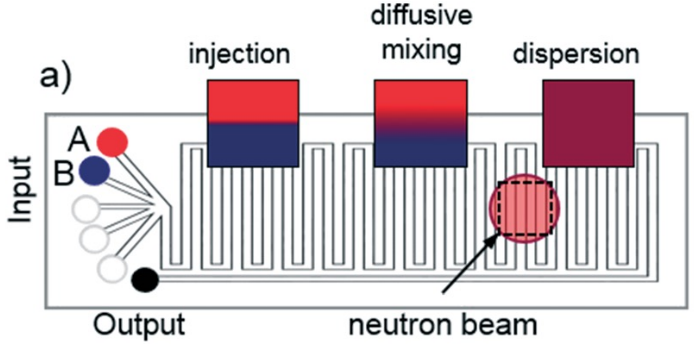


→ high flux, wide simultaneous size range, and a flexible sample area.

ABILITIES:

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

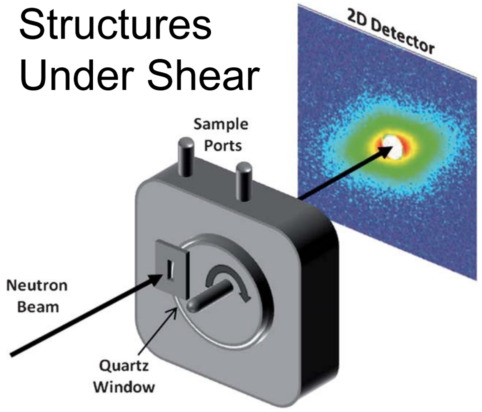
Microfluidic SANS:
High Throughput Mixing &
Tailored Flow Geometry



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

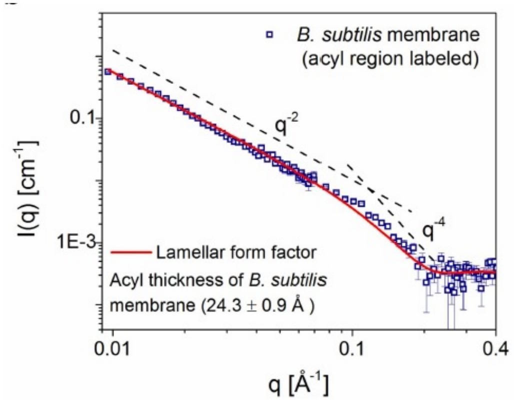
Rheo-SANS:

Structures
Under Shear



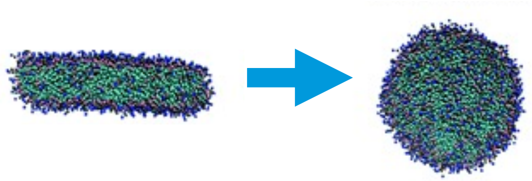
Soft Matter, 2011, **7**, 9992

Biological Samples:
Weak Scatterers &
Dilute Solutions



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

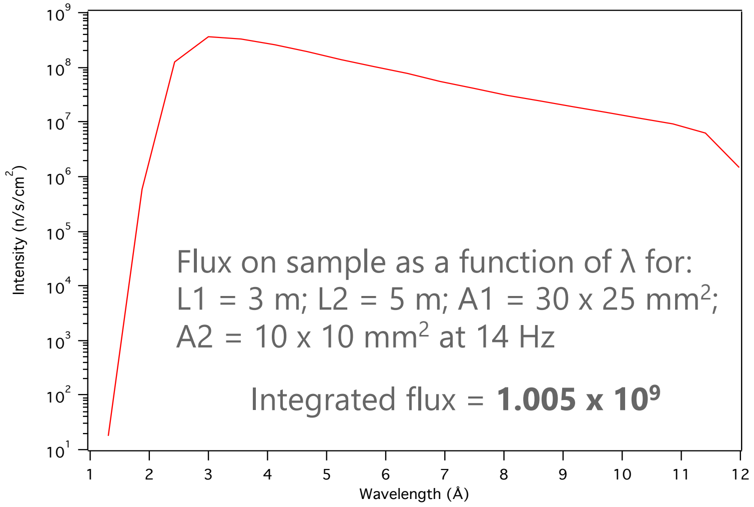
Non-Equilibrium Studies:
Self-Assembly & Kinetics

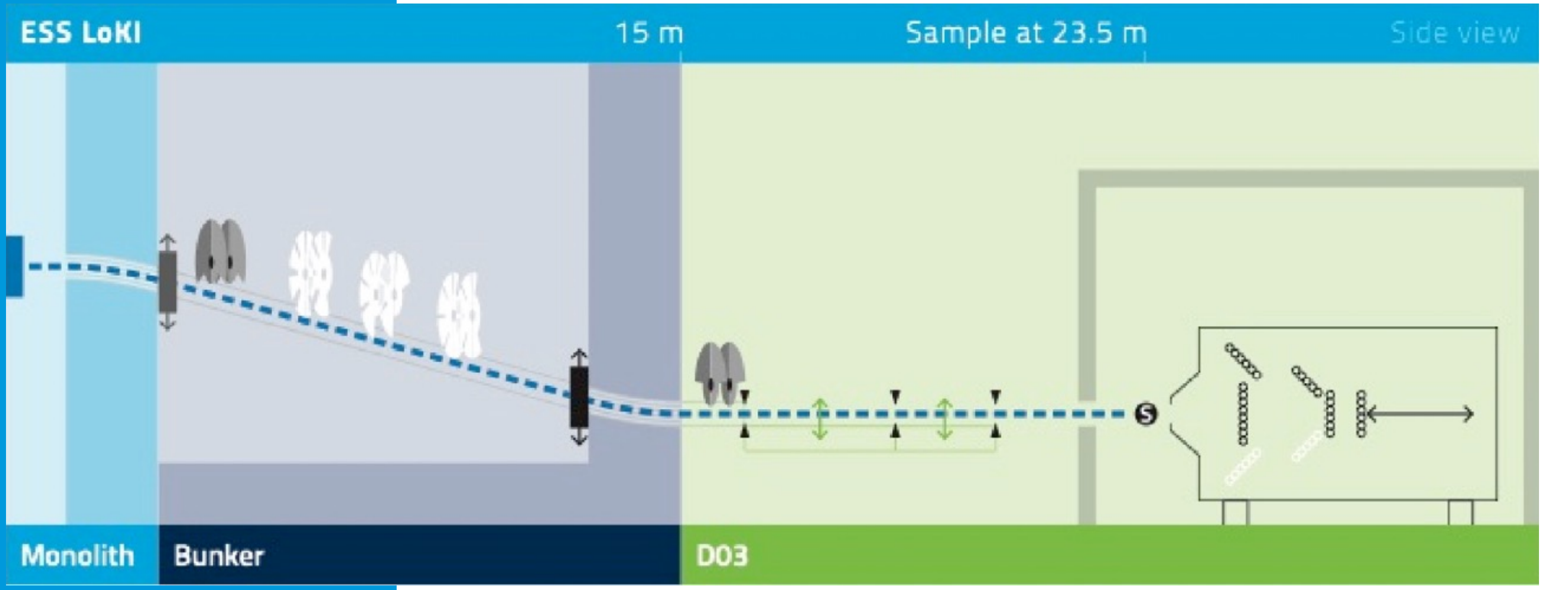


Colloid Polym Sci, 2010, **288**, 827

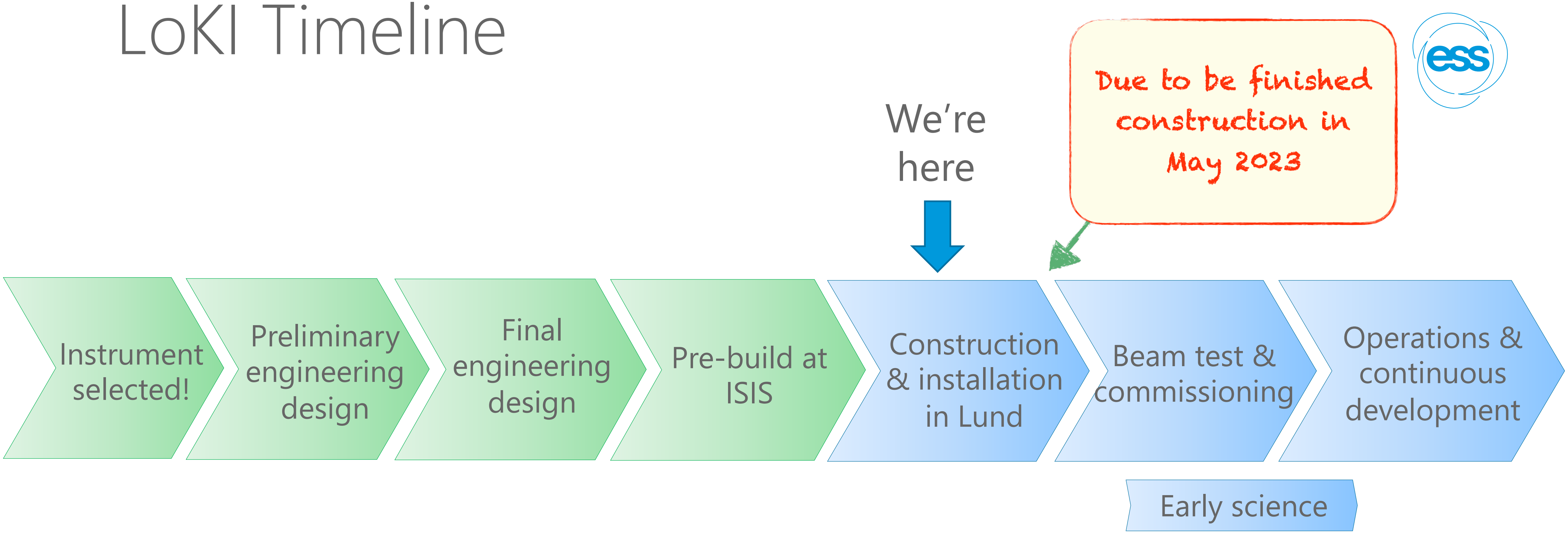
4

LoKI: SANS for Soft Matter, Materials & Bioscience





LoKI Timeline



Instrument selected!

Preliminary engineering design

Final engineering design

Pre-build at ISIS

Construction & installation in Lund

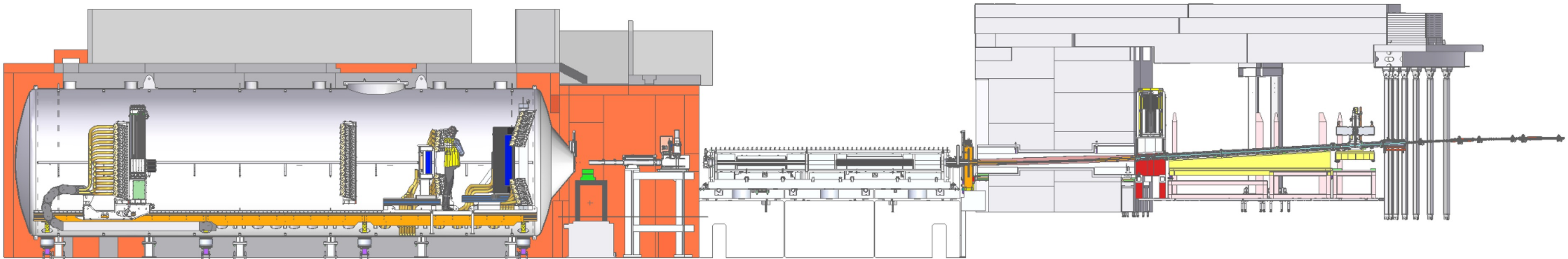
Beam test & commissioning

Operations & continuous development

Early science

We're here

Due to be finished construction in May 2023



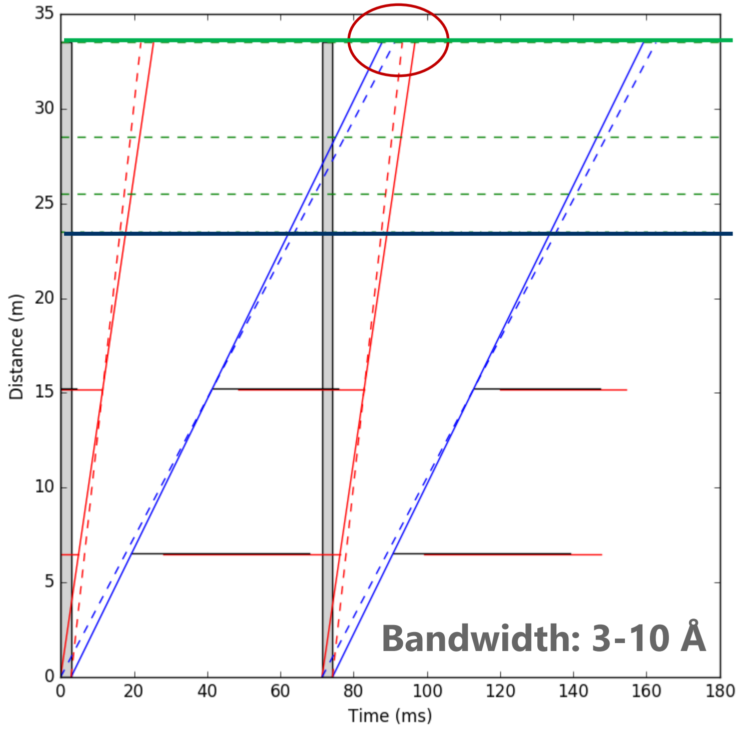
Defining our beam : Choppers

Requirements

- Cut the bandwidth down from 0.4 Å and 20 Å to a defined wavelength band of up to 10 Å at 14 Hz and up to 20 Å at 7 Hz (pulse-skipping)
- Operate in monochromatic mode

*Option for resolution enhancing choppers

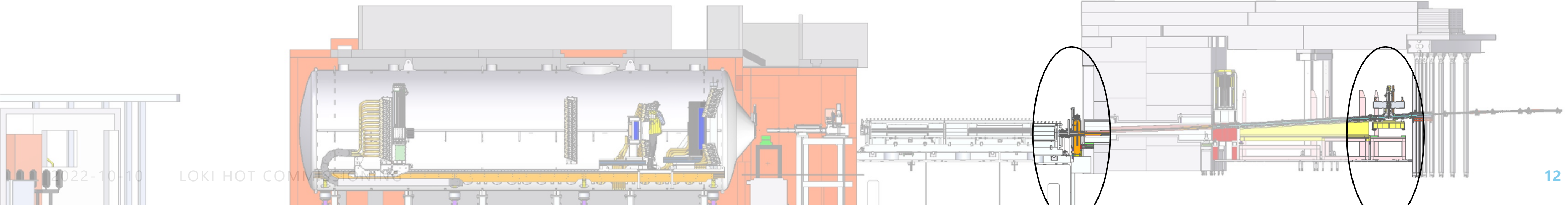
No frame overlap



10 m detector distance

Sample position

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

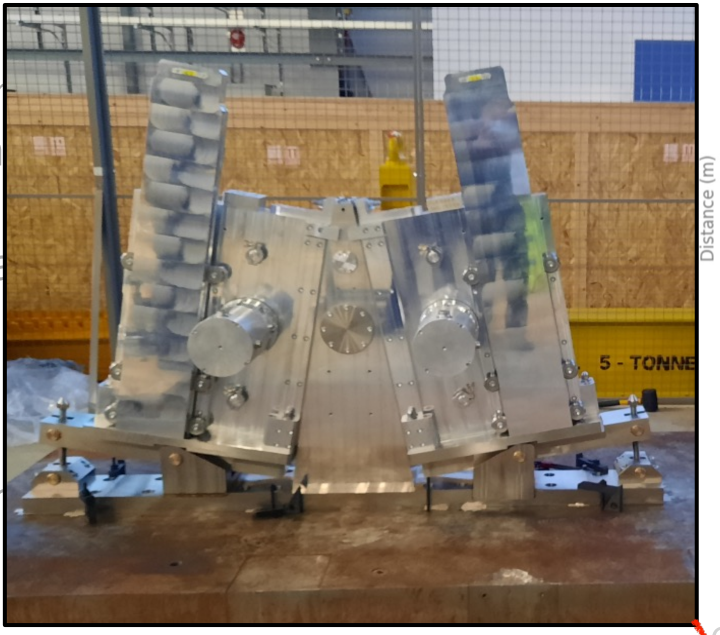


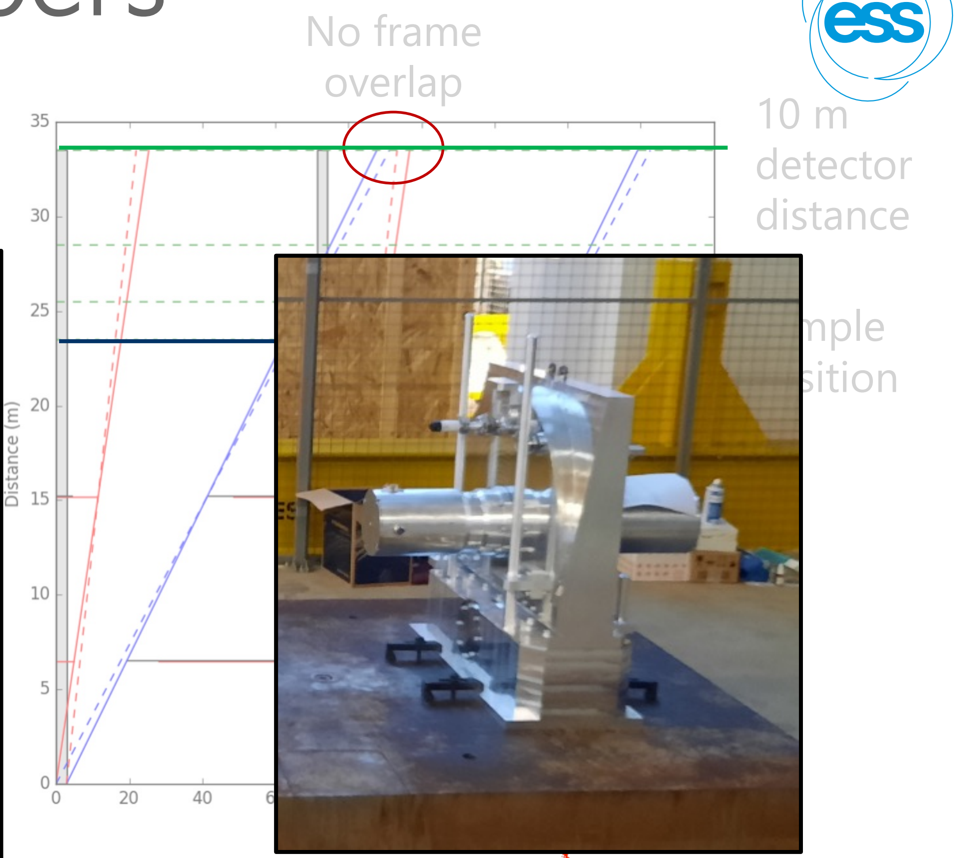
Defining our beam : Choppers

Requirements

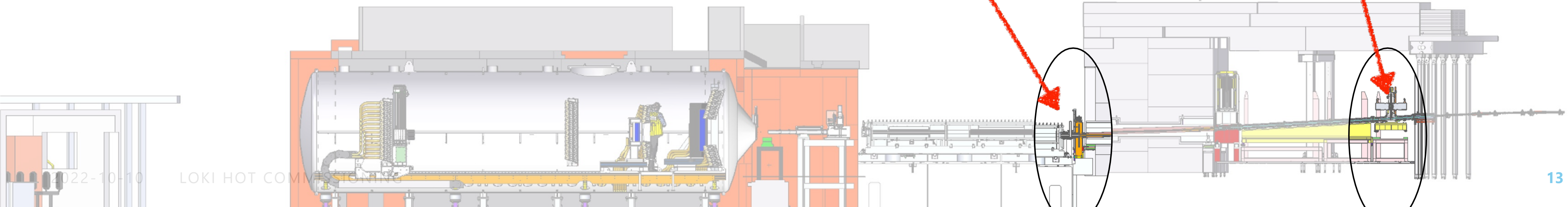
- Cut the bandwidth dow
  to a defined wavelength
  14 Hz and up to 20 Å at
- Operate in monochroma

*Option for resolution enhan





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



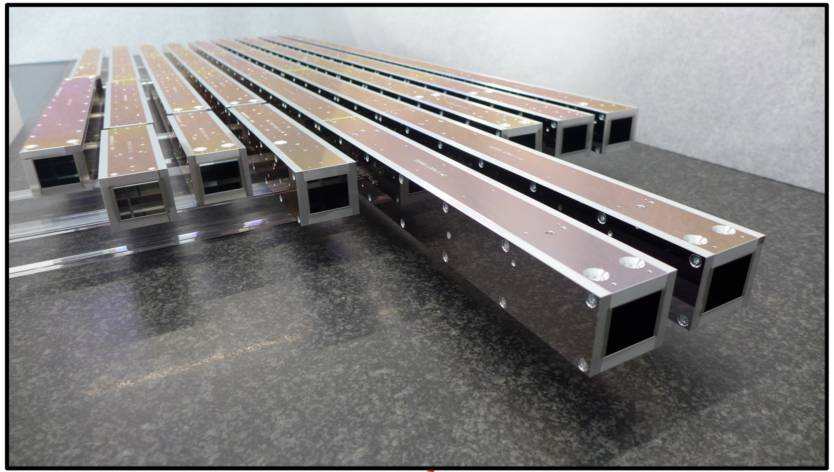
Defining our beam : **neutron guide**

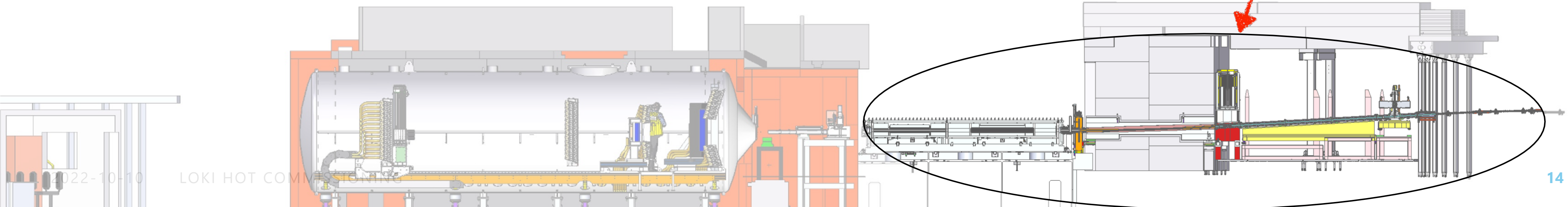
Requirement:

- **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
- Minimise **signal-to-noise**

What we have:

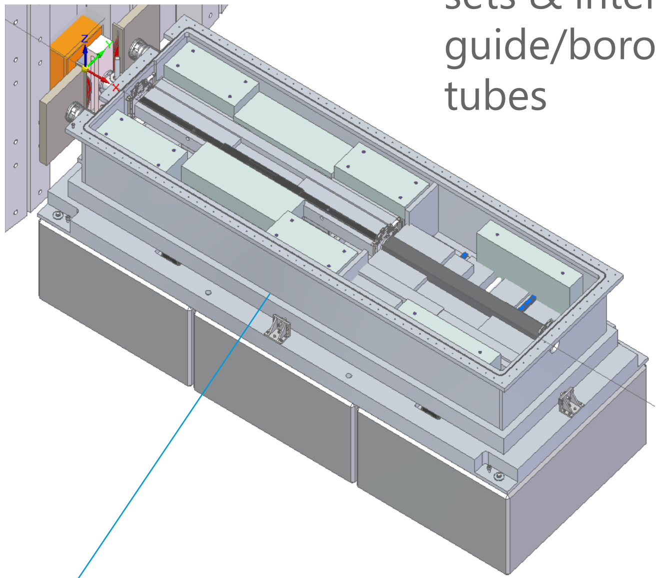
- Use straight highly reflective guide (m=2) under vacuum
- Two multichannel benders (m=3) = **twice** out of line-of-sight
- Smaller beam size (25 mm × 30 mm (V × H)) to minimise transport of background





Defining our beam : **Collimation**

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

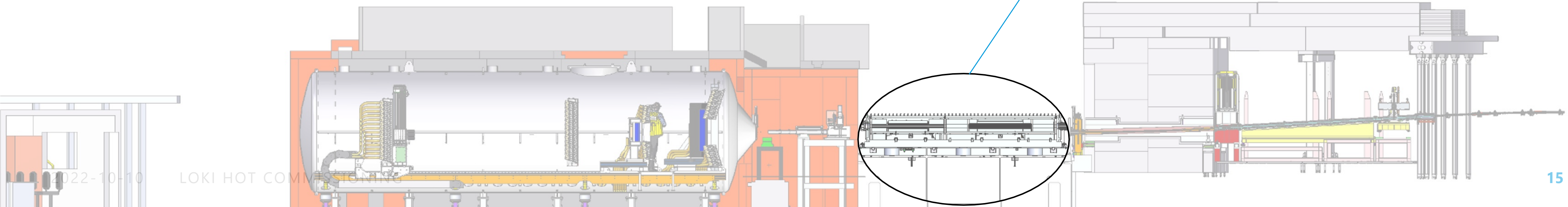


Requirements

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

What we have:

- 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



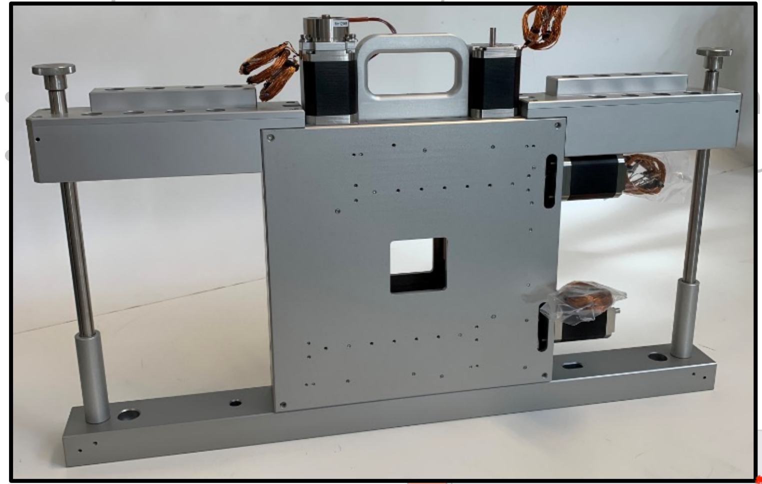
Defining our bear on

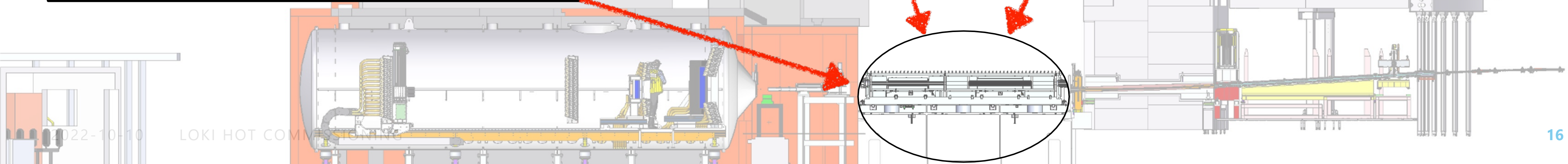
Requirements

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

What we have:

- 4-jaw slit sets at 8, 5 & 3 m before t
- mple position
- uated boron-lined m=2 guide





Shielding

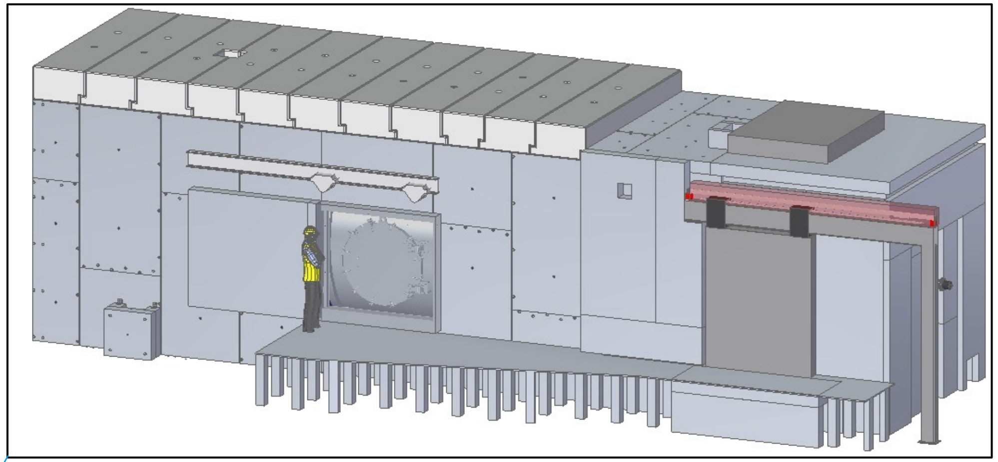
Crucial for personal protection as well as background reduction

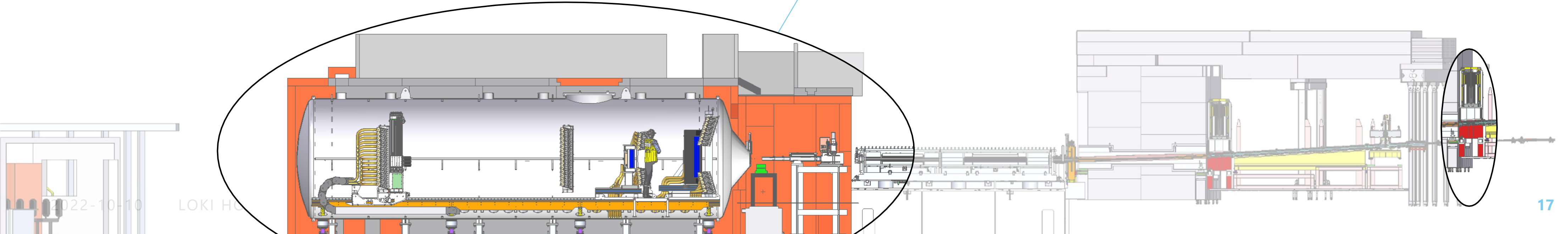
Requirements

- Fulfill radiation requirements
- **Improve background**: Best signal-to-noise possible

To do this, we:

- Steel and concrete caves around the entire instrument
- Heavy shutter to allow access to the sample area to change samples





Shielding

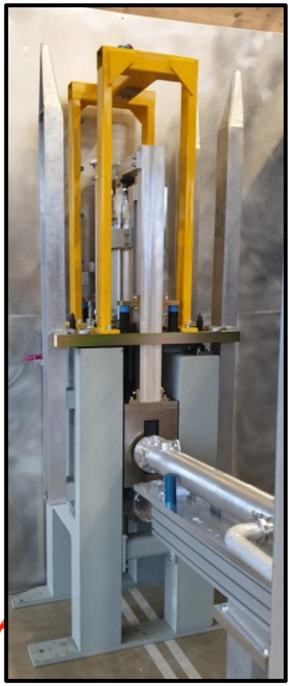
Crucial for personal protection as well as background reduction

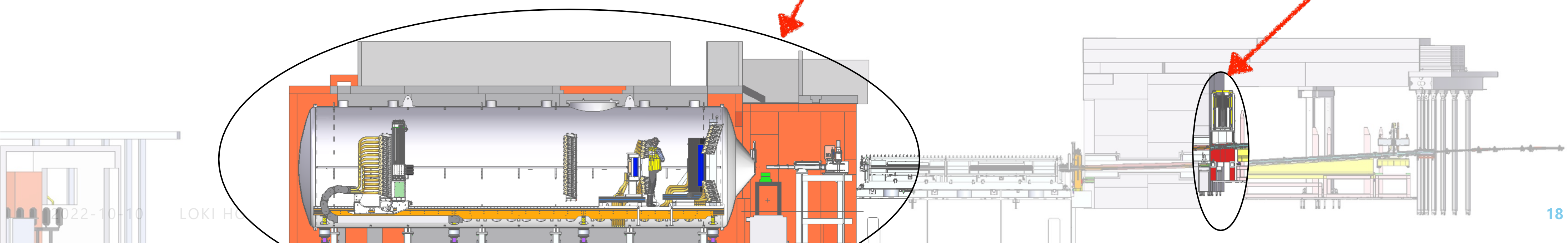
Requirements

- Fulfill radiation requirements
- **Improve background**: Best signal-to-no

To do this, we:

- Steel and concrete caves around the entir instrument
- Heavy shutter to allow access to the samp area to change samples



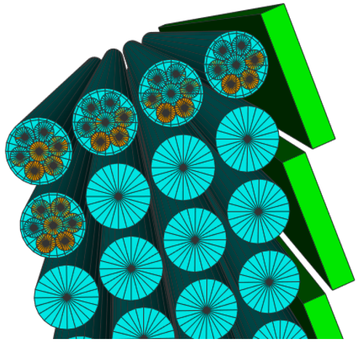


Detector System

Novel ^{10}B-based straw tubes design typically used in security

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

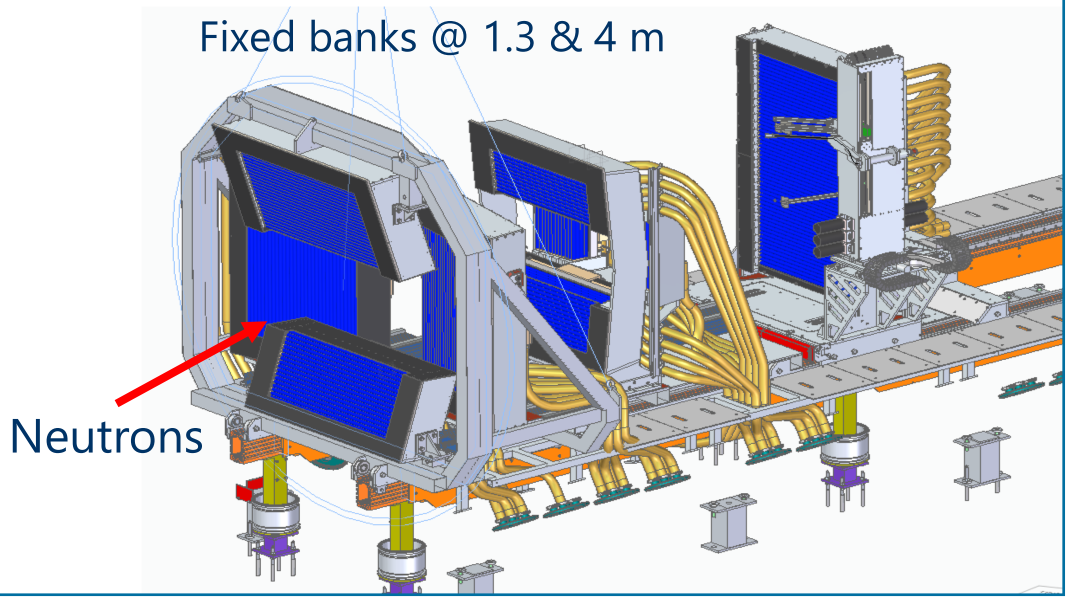
4 layers of Al tubes, each containing 7 boron-coated straws

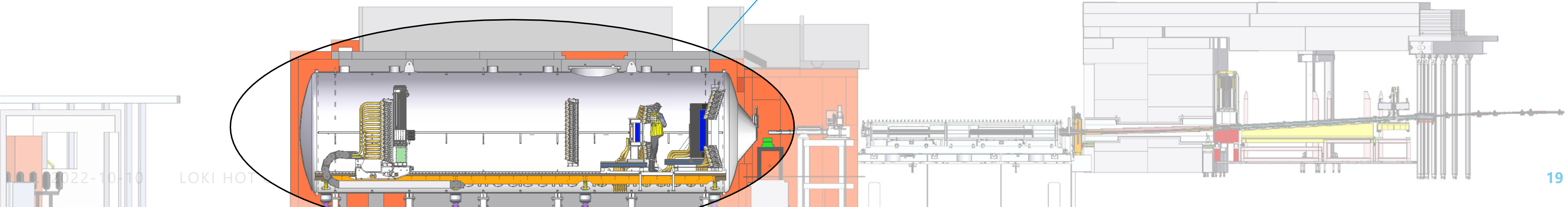


880 tubes x 7 straws x 256 pixels
= **1,576,960 pixels**

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

Rear detector moveable between 5 & 10 m

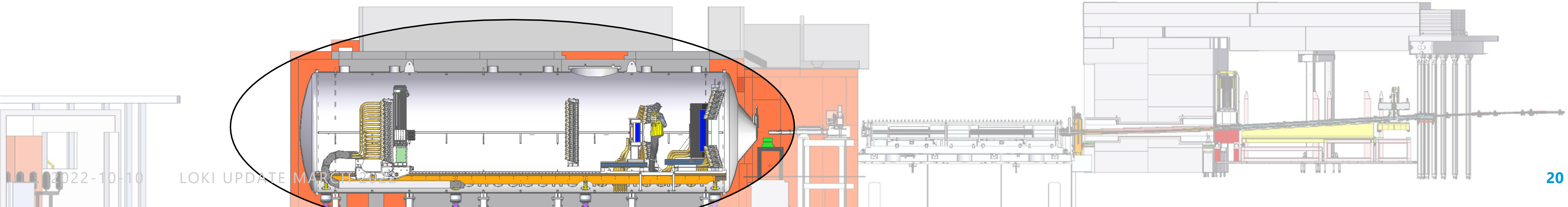




Detector System

Detector vessel installed at ESS

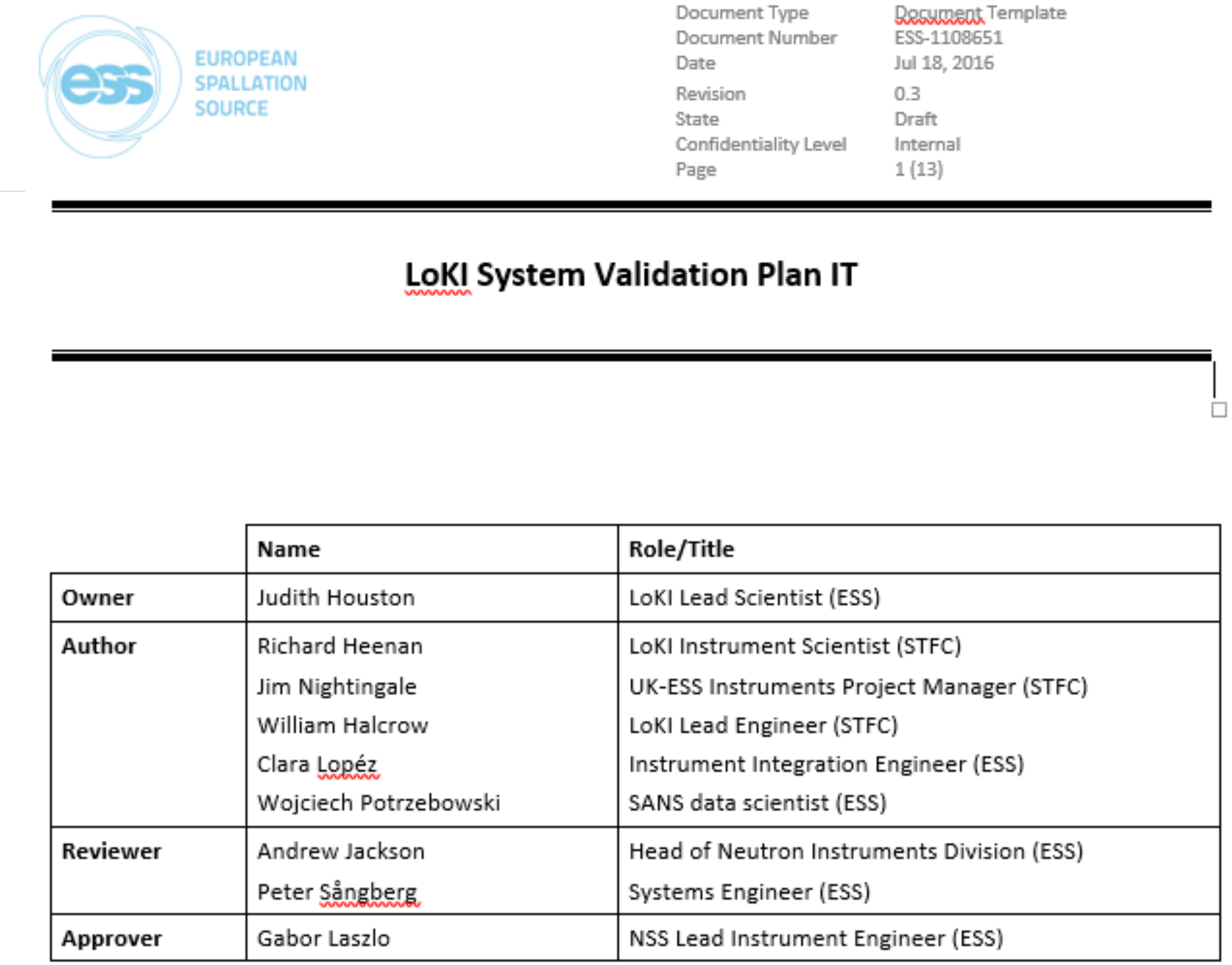
Detector mechanics prebuild at ISIS



5

Hot commissioning Day 1

LoKI Hot Commissioning Plan



EUROPEAN SPALLATION SOURCE

Document Type	Document Template
Document Number	ESS-1108651
Date	Jul 18, 2016
Revision	0.3
State	Draft
Confidentiality Level	Internal
Page	1 (13)

LoKI System Validation Plan IT

	Name	Role/Title
Owner	Judith Houston	LoKI Lead Scientist (ESS)
Author	Richard Heenan Jim Nightingale William Halcrow Clara Lopéz Wojciech Potrzebowski	LoKI Instrument Scientist (STFC) UK-ESS Instruments Project Manager (STFC) LoKI Lead Engineer (STFC) Instrument Integration Engineer (ESS) SANS data scientist (ESS)
Reviewer	Andrew Jackson Peter Sångberg	Head of Neutron Instruments Division (ESS) Systems Engineer (ESS)
Approver	Gabor Laszlo	NSS Lead Instrument Engineer (ESS)

Activities for a successful hot commissioning:

1. Fulfil radiation protection requirements
2. Hot Commissioning of beam monitors
3. Gold foil measurement
4. Choppers phases verification
5. Characterize beam profile
6. Flight path calibration
7. Characterization of position and tilt of detectors
8. Calibration of detector efficiency and resolution
9. Commissioning of sample environment

Many of these steps will be continuously repeated during the ramp-up of the proton beam.

Commissioning linked to source ramp-up

Accelerator power

BOT + 3 months
Fulfil radiation requirements
HOLD POINT
Accelerator power <100 kW

BOT + 3-9 months
Fulfil radiation requirements
HOLD POINT
Gold foil
Beam monitors
Chopper phases
Beam profile using ID
Flight path calib

Background characterisation
Detector calibration
Sample environment
Standard samples
Accelerator power 100 kW

BOT + 9-12 months
Fulfil radiation requirements
HOLD POINT
Gold foil
Beam monitors
Chopper phases
Beam profile using ID
Flight path calib

Background characterisation
Detector calibration
Sample environment
Standard samples
Accelerator power 300 kW

BOT + 12-18 months
Fulfil radiation requirements
HOLD POINT
Gold foil
Beam monitors
Chopper phases
Beam profile using ID
Flight path calib

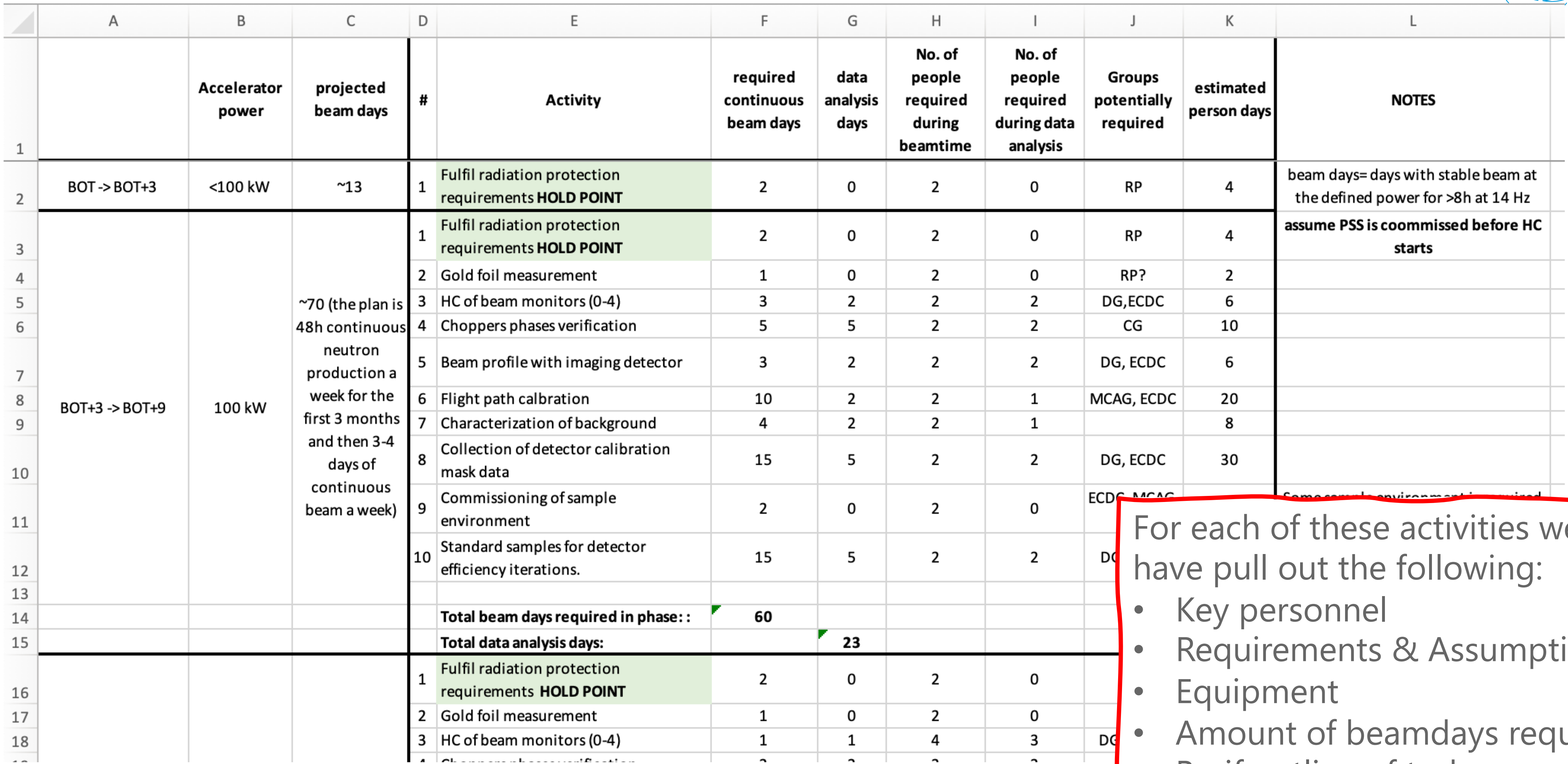
Background characterisation
Detector calibration
Sample environment
Standard samples
Accelerator power <500 kW

Commissioning linked to source ramp-up

For each of these activities we have pull out the following:

- Key personnel
- Requirements & Assumptions
- Equipment
- Amount of beamdays required
- Brief outline of tasks

LoKI Hot Commissioning Plan



	A	B	C	D	E	F	G	H	I	J	K	L
1		Accelerator power	projected beam days	#	Activity	required continuous beam days	data analysis days	No. of people required during beamtime	No. of people required during data analysis	Groups potentially required	estimated person days	NOTES
2	BOT -> BOT+3	<100 kW	~13	1	Fulfil radiation protection requirements **HOLD POINT**	2	0	2	0	RP	4	beam days= days with stable beam at the defined power for >8h at 14 Hz
3	BOT+3 -> BOT+9	100 kW	~70 (the plan is 48h continuous neutron production a week for the first 3 months and then 3-4 days of continuous beam a week)	1	Fulfil radiation protection requirements **HOLD POINT**	2	0	2	0	RP	4	**assume PSS is coommissed before HC starts**
4				2	Gold foil measurement	1	0	2	0	RP?	2	
5				3	HC of beam monitors (0-4)	3	2	2	2	DG,ECDC	6	
6				4	Choppers phases verification	5	5	2	2	CG	10	
7				5	Beam profile with imaging detector	3	2	2	2	DG, ECDC	6	
8				6	Flight path calbration	10	2	2	1	MCAG, ECDC	20	
9				7	Characterization of background	4	2	2	1		8	
10				8	Collection of detector calibration mask data	15	5	2	2	DG, ECDC	30	
11				9	Commissioning of sample environment	2	0	2	0	ECDC, MCAG		Some sample environment is required
12				10	Standard samples for detector efficiency iterations.	15	5	2	2	DG		
13												
14					**Total beam days required in phase: :**	**60**						
15					**Total data analysis days:**		**23**					
16				1	Fulfil radiation protection requirements **HOLD POINT**	2	0	2	0			
17				2	Gold foil measurement	1	0	2	0			
18				3	HC of beam monitors (0-4)	1	1	4	3	DG		
19				4	Choppers phases verification	[illegible]	[illegible]	[illegible]	[illegible]			

For each of these activities we have pull out the following:

- Key personnel
- Requirements & Assumptions
- Equipment
- Amount of beamdays required
- Breif outline of tasks

e.g. Flux and Beam Profiles

Key personnel: instrument team, detector group, DMSC, and RP for the Au-foil measurements

6

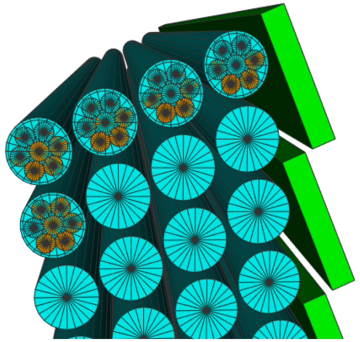
Challenge with detectors

Detector System

Novel ^{10}B-based straw tubes design typically used in security

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

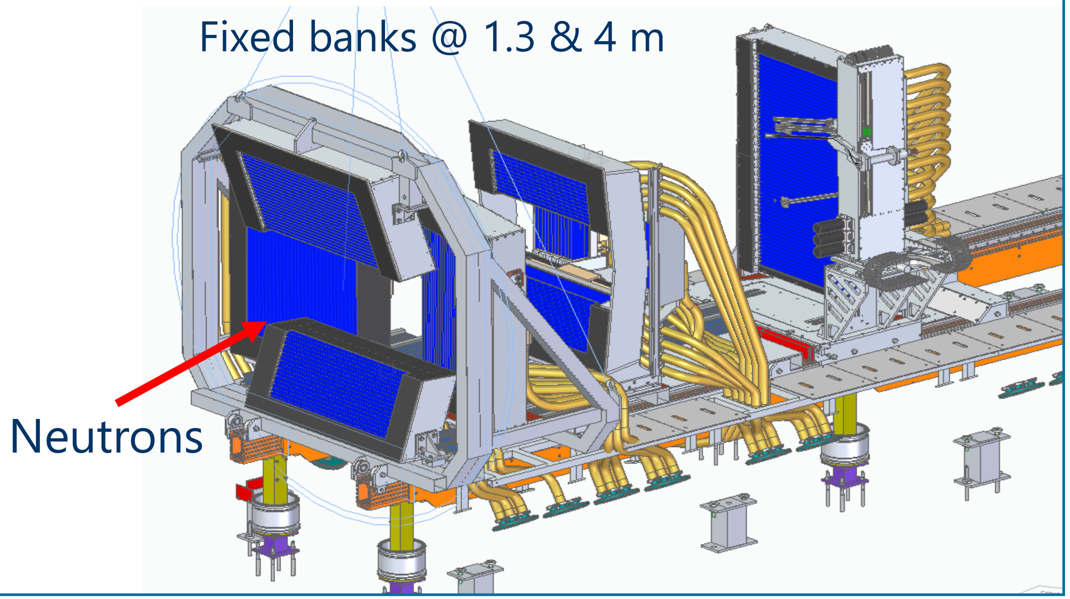
4 layers of Al tubes, each containing 7 boron-coated straws

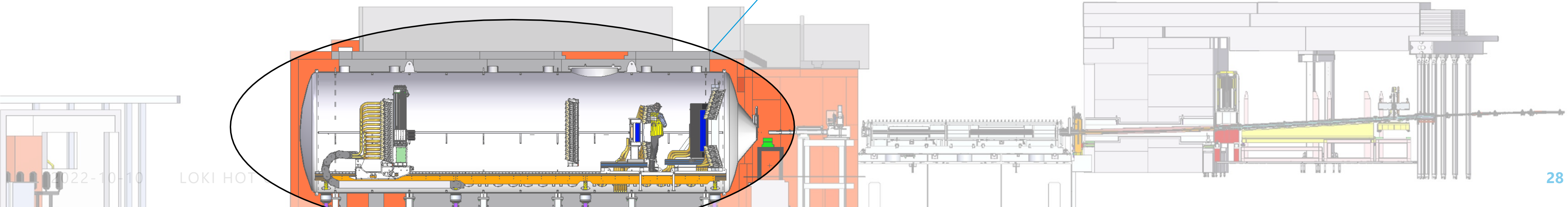


880 tubes x 7 straws x 256 pixels
= **1,576,960 pixels**

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

Rear detector moveable between 5 & 10 m



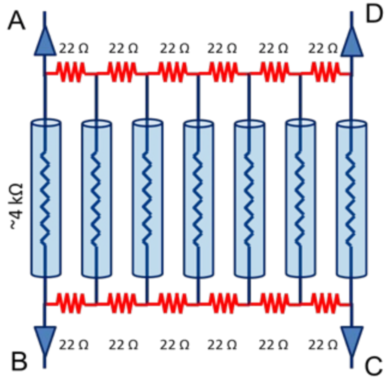


Detector System

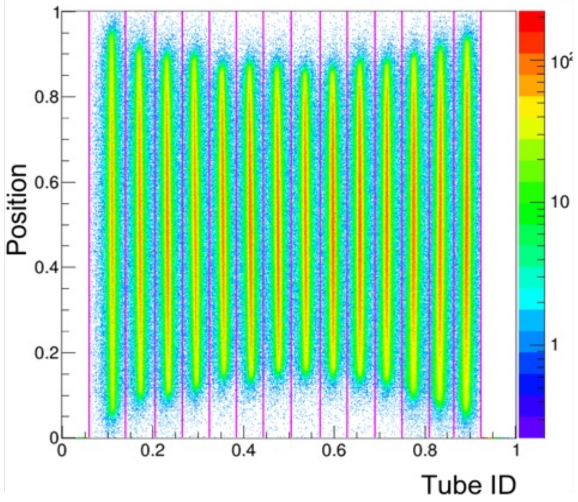
Novel ^{10}B-based straw tubes design typically used in security

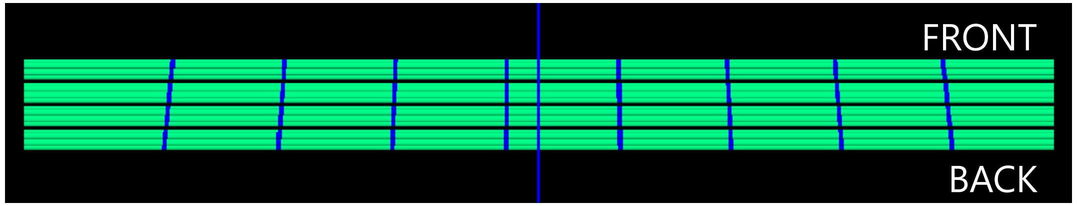
Challenges:
- ~1.6 million pixels
- Detector multiplexing corrections
- Parallax effects through the depth of the detector
- High angle banks (up to 45º)
- Self-screening through the detector panel

(a) 7 straw multiplexing



(b) Before correction



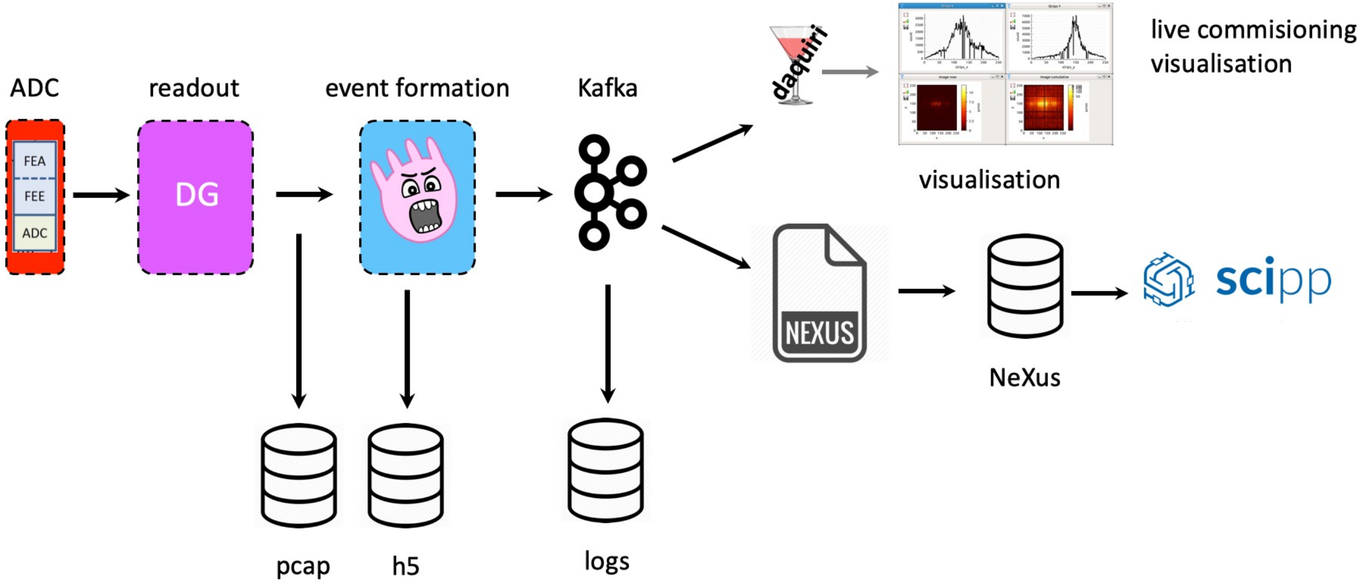


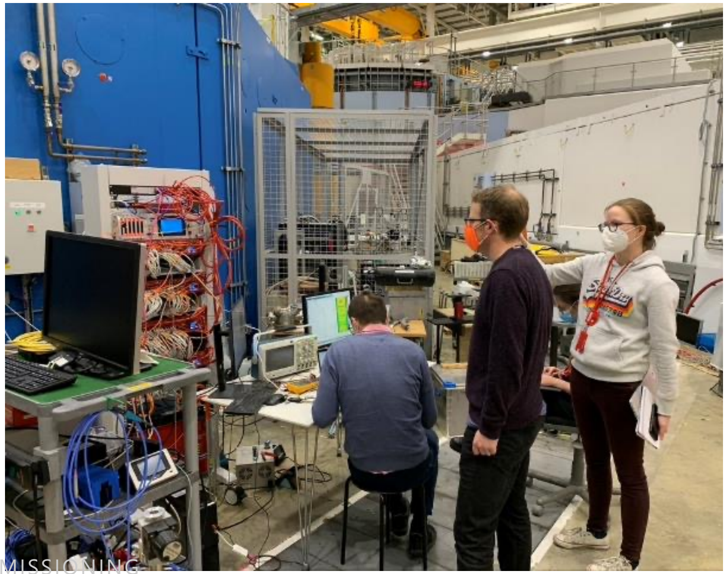
Detector Verification Stages

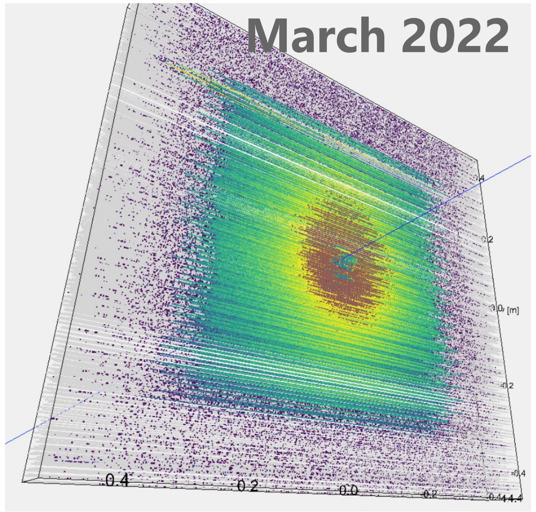
Key personnel: instrument scientist and data scientist, DMSC*, detector group*

Detector Tests on Larmor (ISIS, UK)

Collected calibration data on the LoKI rear detector using the **full ESS software stack:** Excellent test for Hot Commissioning


ADC
readout
event formation
Kafka
live commisioning visualisation
visualisation
NeXus
pcap
h5
logs




March 2022

NeXus file displayed in scipp

Sample measured:
1. Cd stripped mask
2. Silver behenate
3. SDS powder
4. empty beam
5. blocked beam
6. ISIS standard polymer
7. Silica particles
8. Vanadium

Geant4 Simulations

Support the development of calibration and data reduction routines:

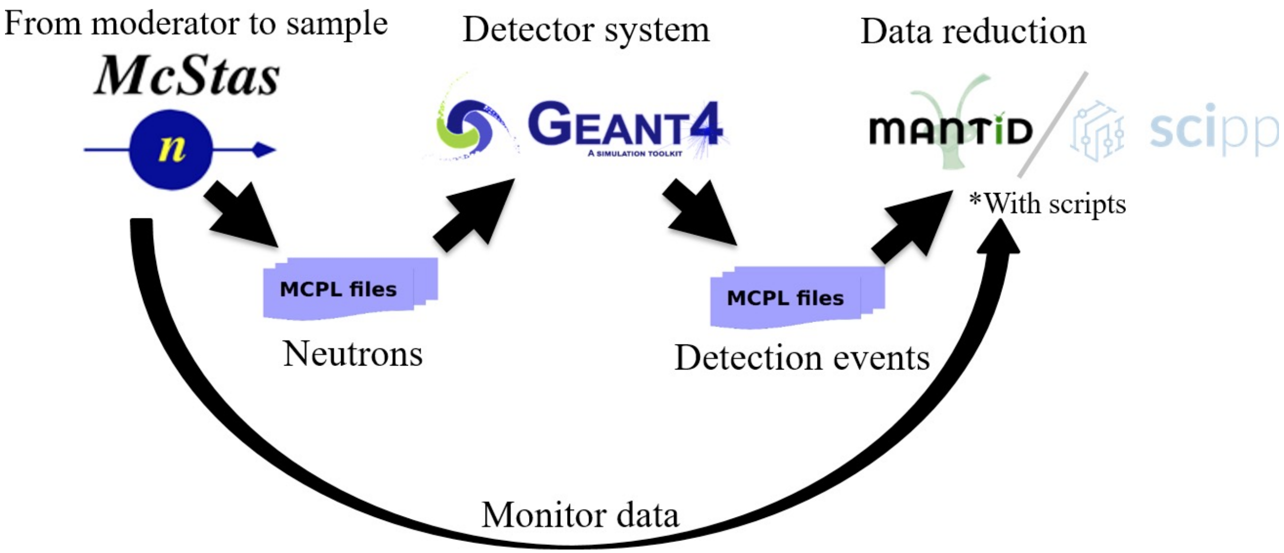
- Replicate measured data on other beamlines with simulation, and generate realistic data (for LoKI) for processing in Mantid/Scipp, to test calibration procedures and data reduction routines
- Provide data to generate calibration files to be used at the beginning of the LoKI hot commissioning phase

Using multiple simulation/software tools:

- Using a chain of Monte Carlo simulations to carry out the full simulation of a neutron scattering instrument using the adequate software at each part of the system

1. *McStas* for the beam transport and conditioning system
2. *Geant4* through the *ESS Detector Group Simulation Framework* for the detector system
3. *Mantid* (later *Scipp*) for data reduction

Simulation and data workflow from moderator to data reduction



Simulations vs. real tests

Simulate and visualise the expected readout of the real detector modules

Real tests

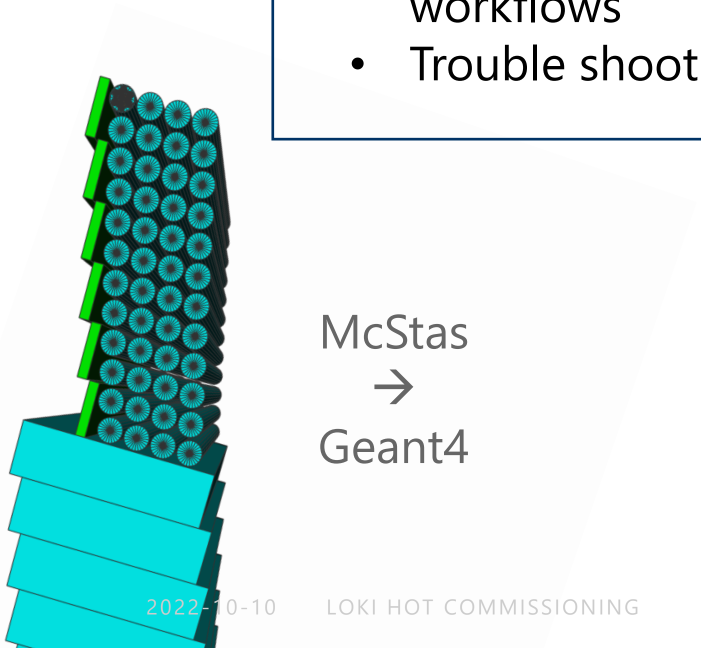
- Full tests of the detector technology and data chain from detection to reduction software.
- Real data for testing calibration & data processing workflows
- Trouble shooting

Simulations

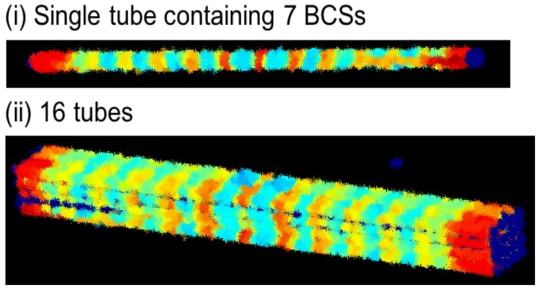
- Data for the Mantid *team to test capability for data streaming/reduction*
- Idealised data for data processing and reduction
- Bug finding
- Calibrating challenging wide angle detectors

Ready for hot commissioning:

1. Data processing workflow from detector to Mantid
2. Calibration plan
3. Data reduction workflow



McStas → Geant4



7

Standard Samples

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

Thanks for listening!

Any questions?