



# LoKI STAP Report

April 2021

2021-04-09

# Overview



Even in the current circumstances, the progress of the LoKI project remains good, with manufacturing complete for some major components and underway for most of the rest. In the next six months we will begin installation activities and components will be starting to arrive from the UK.

In this report we will give a brief update on:

- The engineer, design and installation progress
- Current progress with simulations (McSTAS, Geant4), and data reduction (Scipp)

Following requests from the STAP review in October 2020 we also have a few slides on:

- List of the sample environment systems planned for LoKI including “need by” dates and current status
- An overview of the instrument control software NICOS and the (prototype) implementation for LoKI

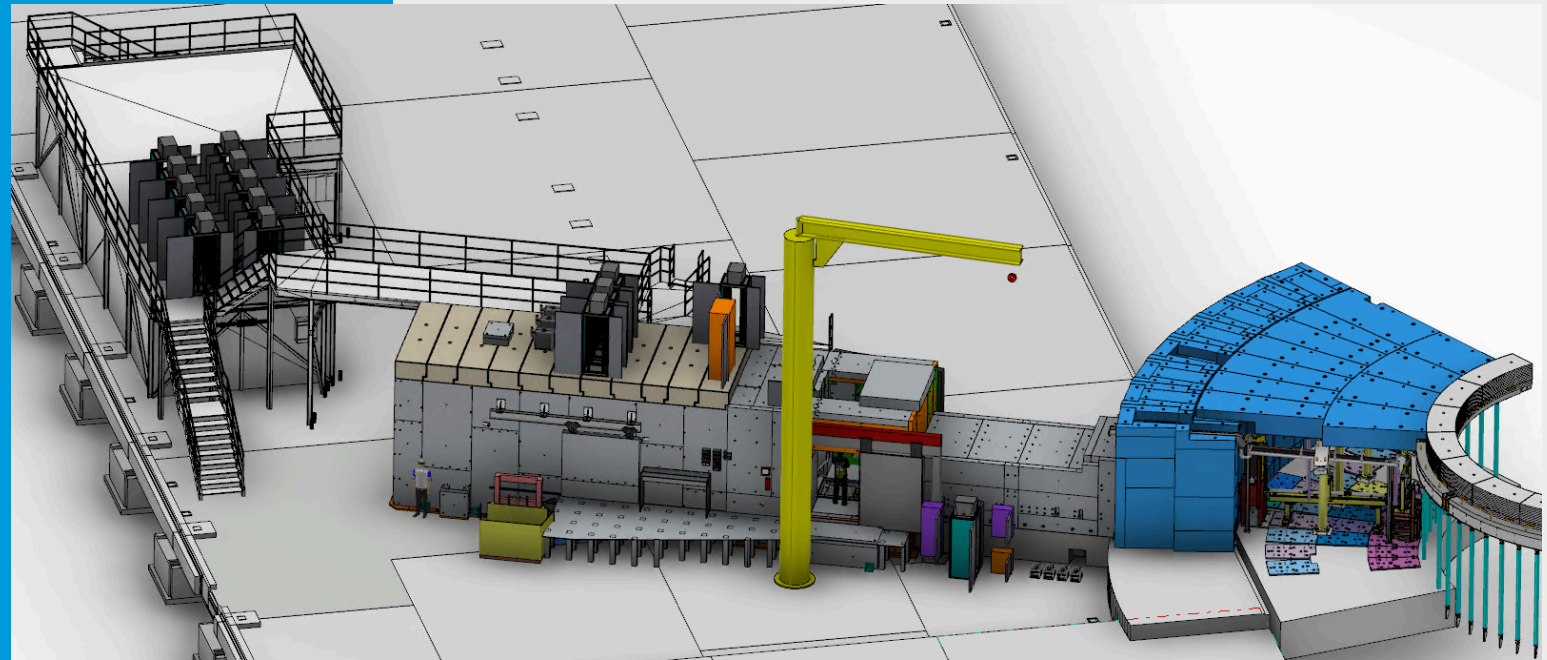
While there has been a lot of progress in many areas, two major activities still require a lot of attention over the next 6 months:

- Hot commissioning plan, including physical measurements and coordination of software deliverables
- Streamlined data reduction procedure, including wavelength slices



# Engineering update

Will Halcrow, Clara Lopez,  
Judith Houston and Richard  
Heenan



# Covid impact



- ISIS design team working from home, with intermittent access to site (when gov guidelines allow & when work activities require it) working at ~85% efficiency due to remote access limitations.
- Pre-build work progressing but fragmented due to lack of engineering support. Opportunity for pre-build activities and remaining design work to hit 110% efficiency not realized due to remote working.
- Suppliers have largely progressed in-spite of the challenges
- Guide continues to be delayed due to technical challenges and an unavailability of neutrons

# In bunker assemblies

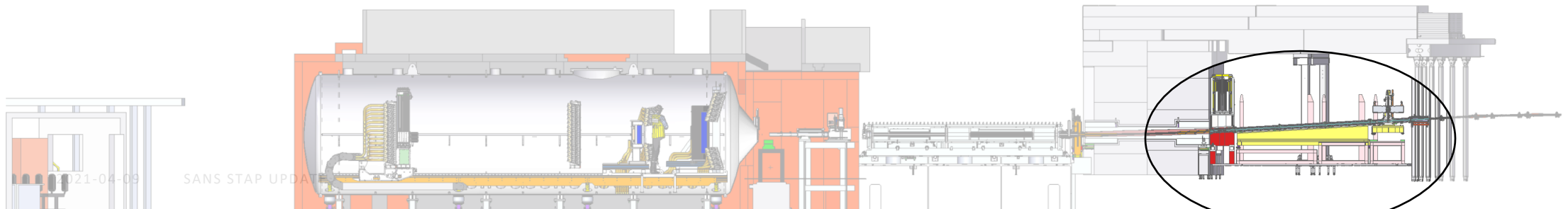
## In-Bunker Remote Handling Structures

- Manufacture complete
- Testing underway



## Heavy Shutter

- Re-work underway – resolving some issues identified during initial testing
- Primary performance requirements regarding motion verified



# Guide and Vacuum Vessels (in-bunker and bunker-cave)

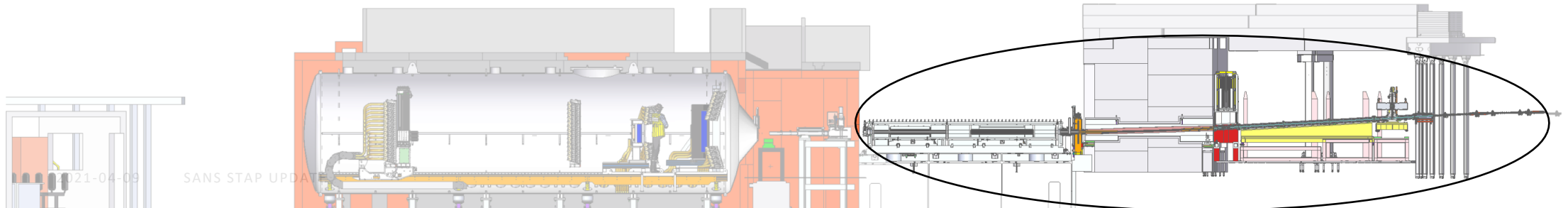


## NBOA

- FAT testing carried out – ~all parts accepted
- 1x Si wafer damaged during testing, awaiting resolution before FAT approved

## Guide and Vacuum Vessels (in-bunker and bunker-cave)

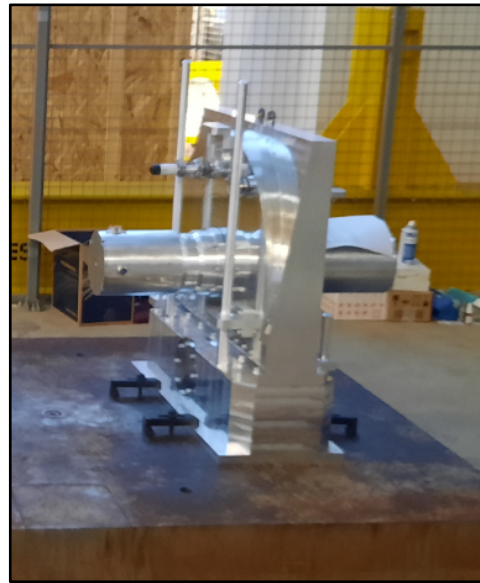
- BWI Vessel Manufactured
- BWI vessel integration into plug tested
- Aluminum vessels manufactured
- Guide segments in manufacture – significantly delayed due to COVID & technical issues at SNAG



# Choppers

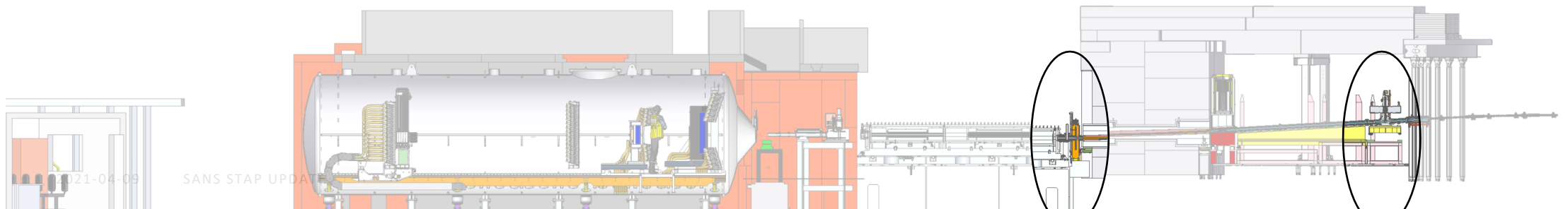
## Chopper 1

- Fully manufactured and assembled
- Fully tested at ISIS
- Awaiting integration checks on RH frames



## Chopper 2

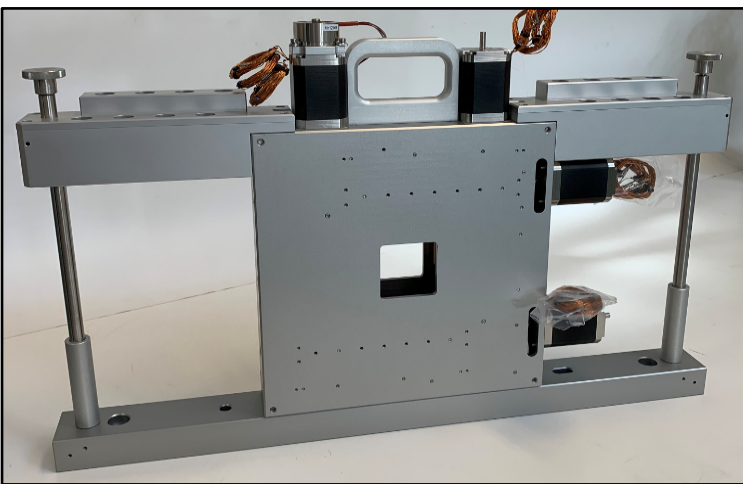
- Fully manufactured and assembled
- Fully tested at ISIS



# Collimation vessel

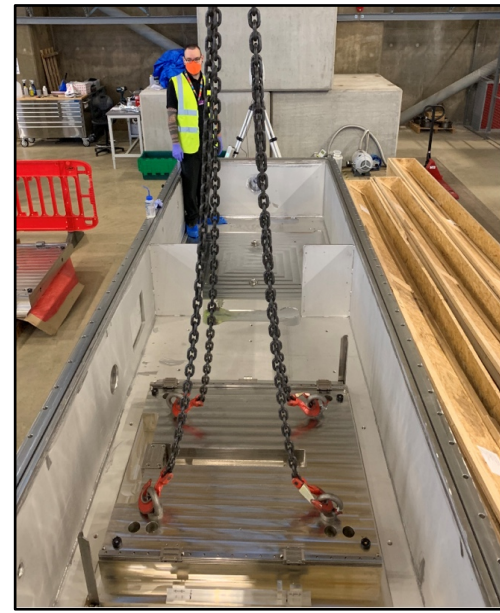
## Jaw Sets

- Manufacture complete
- Significant issues found with motors – re-work underway
- 1x jaw set assembly delivered, but issues found during SAT and so now returned to JJ

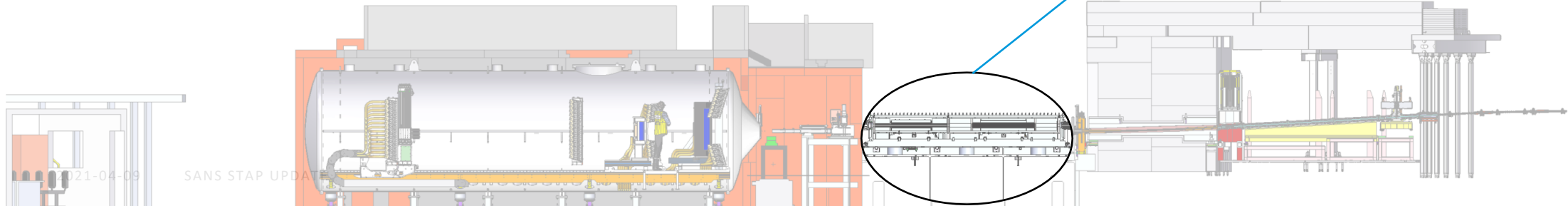
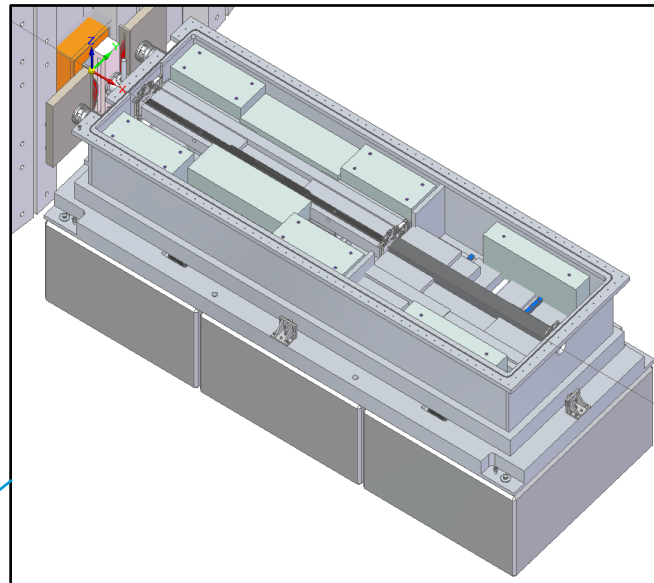


## Collimation Selector Vessel

- Manufacture & assembly underway
- Provisional motion testing completed



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



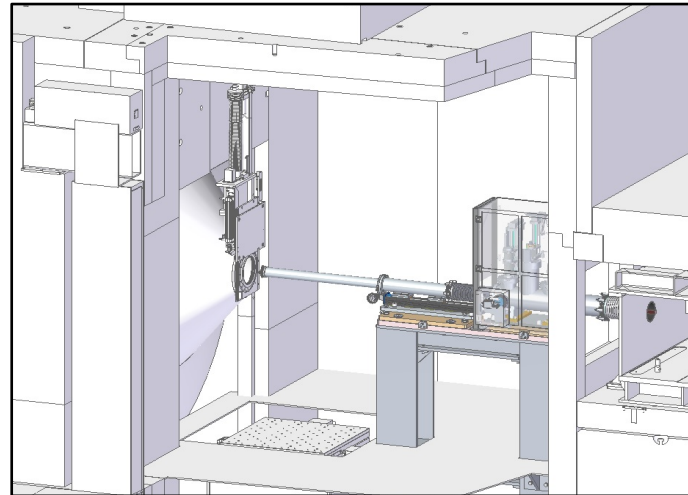




# Sample area

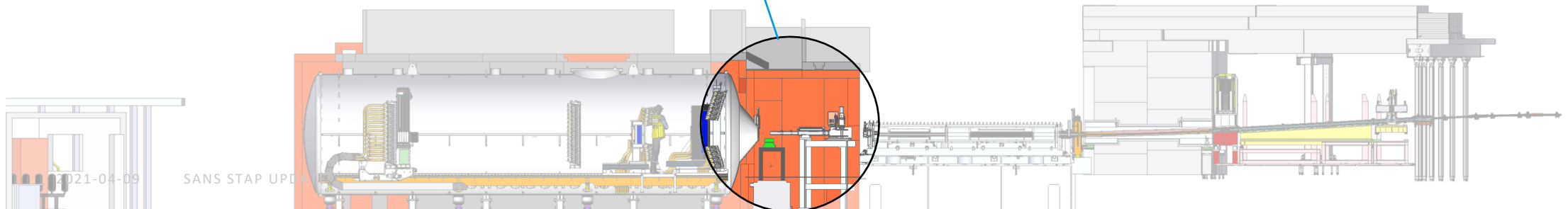
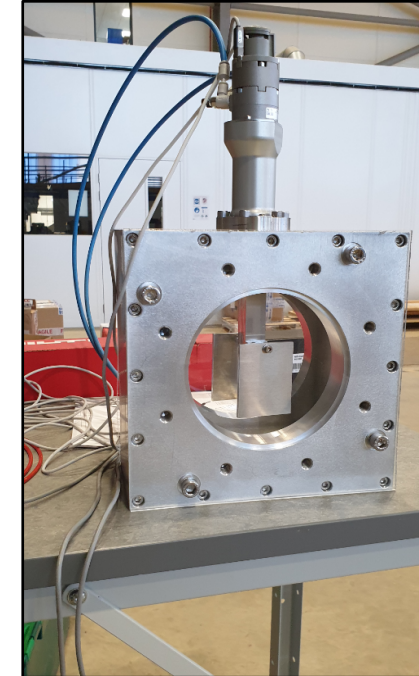
## Sample Stack (underfloor translation stage)

- Design complete and TG3 approved
- Manufacture underway



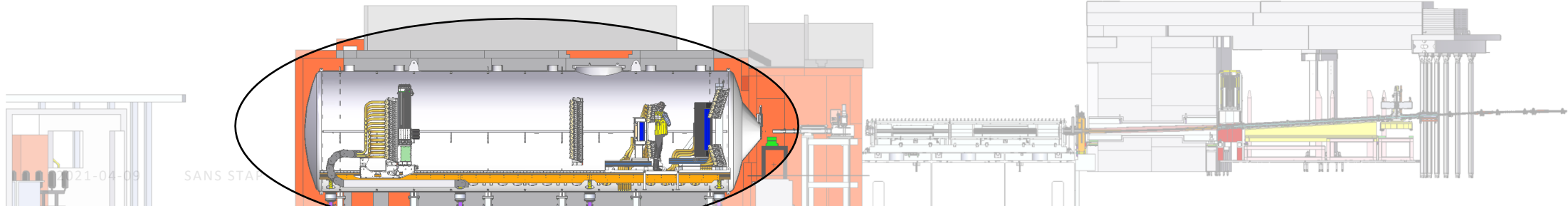
## Sample Snout

- Design complete and TG3 approved
- Manufacture underway



# Detector vessel

- Manufacture complete
- FAT approved
- In-storage awaiting delivery to the ESS in June 2021



# Detector

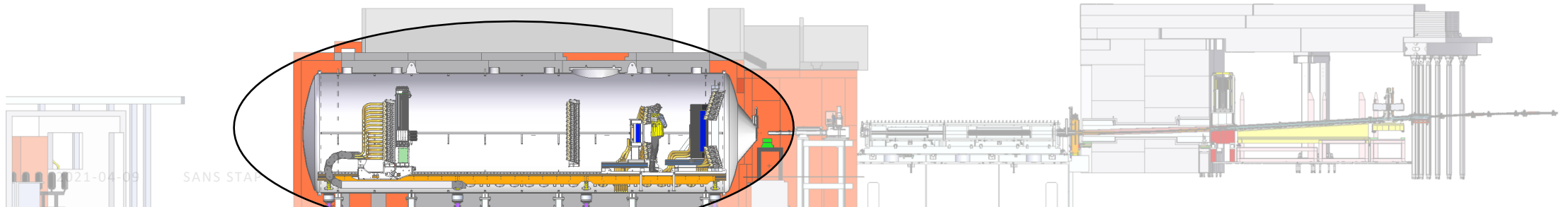


## Detector Mechanical Systems

- Manufacture & assembly largely complete
- Awaiting testing and integration checks
- Hoses not yet ordered

## Straw Tubes

- Deliveries on-going (90% complete) – delays due to COVID, but progressing largely on track
- Straw tube testing at ISIS (SAT) progressing well with few issues found
- Detector module assembly 80% complete



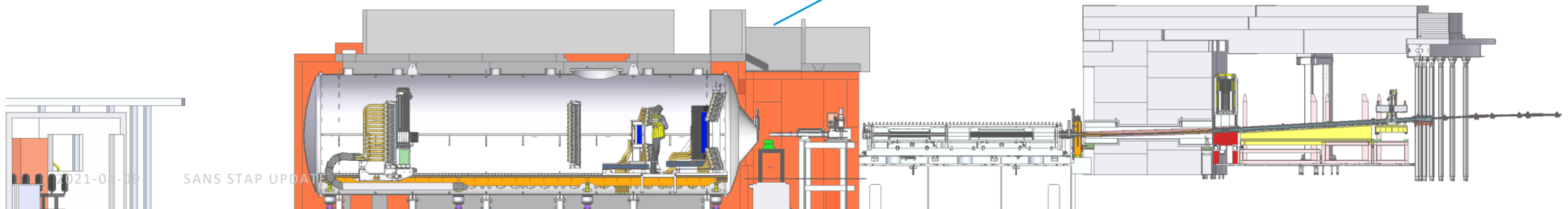
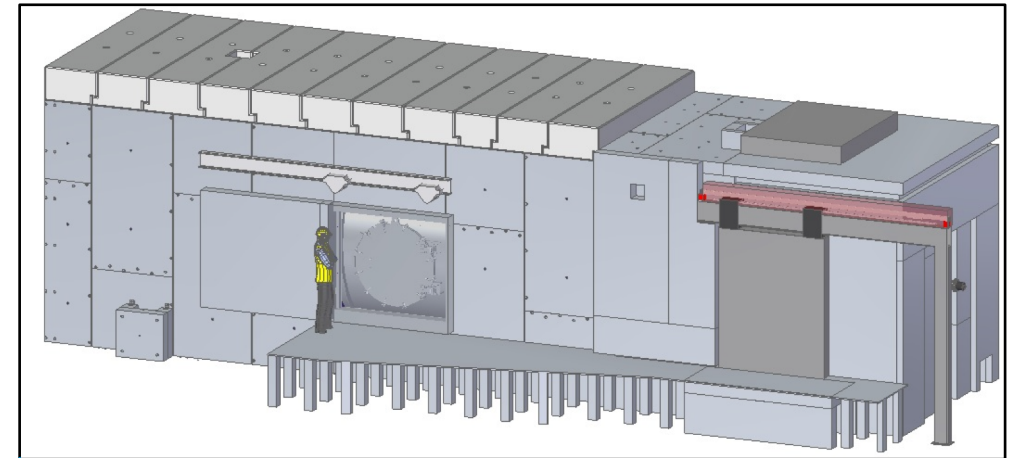
# Shielding

## Bunker to Cave Shielding

- Design complete and TG3 all but approved
- Tender underway

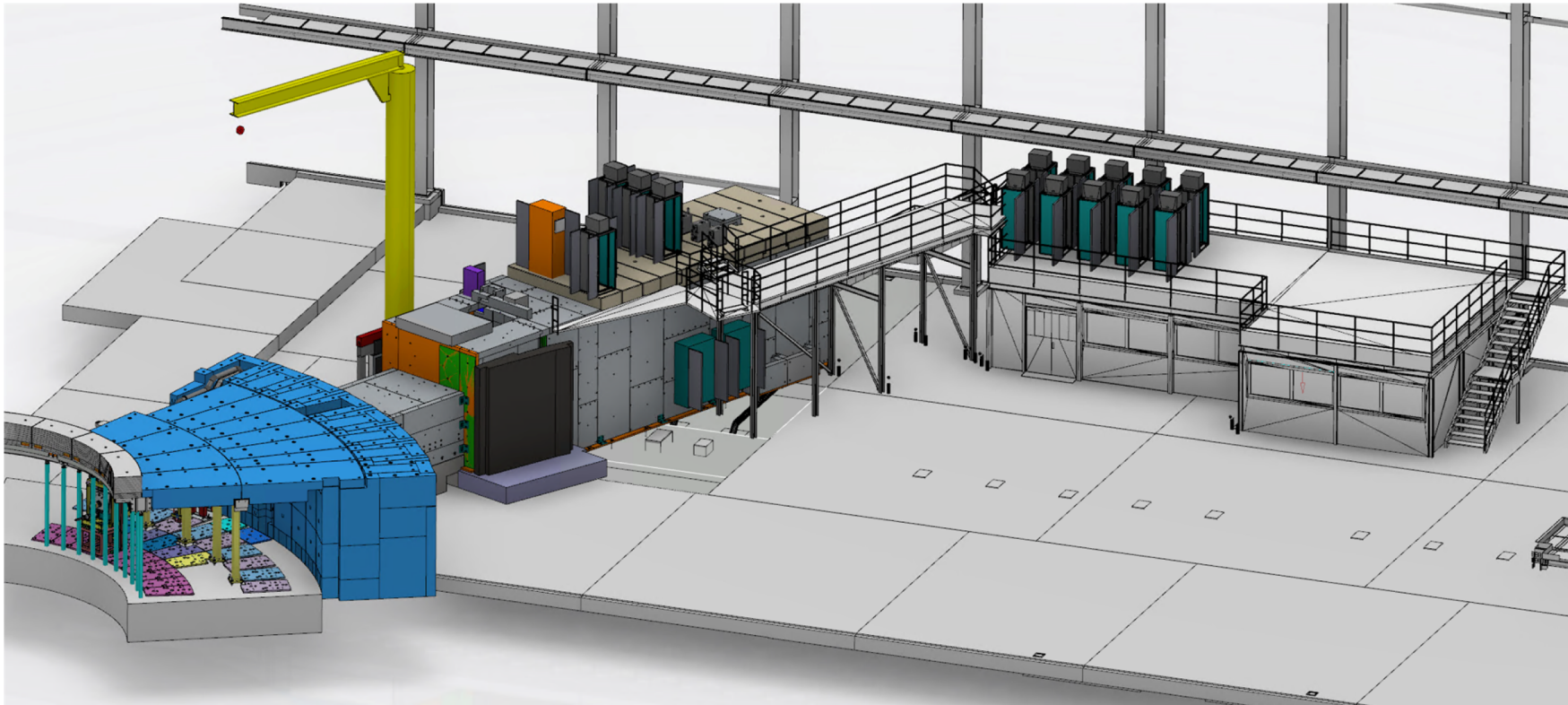
## Cave Shielding

- Design revised due to floor loading issue
- Awaiting final review of neutronics
- Power operated door and roof contract placed, PDR completed



# Hutch

- Contract awarded (mico)
- Preliminary design review completed
- Installation July/August





# Other Progress

## External Access & Supporting Systems (crane, goods lift, suspended floor)

- Concept layout drafted
- Local crane: market engagement started – floor drilling issues require resolution before contracts can be placed

## Service Routes & Racks

- Instrument requirements, provisional routes & concept layout generated and issued to the ESS
- ESS workpackages (CEP & CUP) now ramping up well (if a little late)

# ESS workpackages



A number of key ESS workpackages are now progressing well:

- Vacuum system – TG3 review imminent. Availability of kit for FAT & SAT requires further planning
- PSS concept and interface definitions issued – Technical challenges seem to be under control
- Chopper controller design progressing well – no obvious risk to instrument project progress
- Detector software in development (see later slides)
- Bunker design and manufacture progressing well – now very few unknowns that effect instrument project progress
- Out of Bunker mechanical & electrical utilities – though late getting started, now ramping up well

A number of key ESS workpackages are behind schedule:

- In-bunker mechanical & electrical utilities
- Motion control racks
- Motion safety
- Sample environment
- Detector Racks
- Bunker procedures and concepts of operation (particularly for maintenance and alike)
- General procedures and concepts of operation (particularly for maintenance and alike)



# LoKI Installation

Activities Q2-Q4

Clara Lopez



# Installation progress 2021



Date	Activity	Component	Teams	Required documentation
April	Marking and drilling	Baseplates in bunker	LoKI team/SAG	Work orders/work request/documentation
May	Reception at arrival	NBOA	LoKI team/Hansdieter/QA	Logistics Jira kanban/Fill in records/storage
July	Reception at Arrival	Bunker Wall Insert BWI	LoKI team/QA	Logistics Jira kanban/Fill in records/storage
July	Reception at Arrival	Guide optics	LoKI team/QA	Logistics Jira kanban/Fill in records/storage
July – August	Unloading	Detector vessel	LoKI team / rigging team	Work order/work request/Quality documentation
July-August	Site Acceptance test -SAT	Detector vessel	LoKI team/Vacuum team/CEP	Installation binder/documentation
July-August	Reception at Arrival & Site Acceptance Test -SAT	LoKI choppers	Loki team/Chopper group/QA	Logistics Jira kanban/Fill in records for Reception at arrival and Site acceptance test
July/August	IRR/ Installation	Hutch	LoKi Team/Supplier (MICO)	Installation binder/documentation
August/Sep tember	Casting in place	Concrete plinths for collimation vessel	Loki team/Supplier	Installation binder/documentation
September	Grouting and drilling	Bases for cave and detector tank	LoKI team	Installation binder/documentation
October	Installation	Bunker wall insert	LoKI team/rigging team/Survey team/Hansdieter	Installation binder/work requests/documentation
November	Installation	Detector vessel	LoKI team/rigging team/Survey team	Installation binder/work requests/documentation



# Sample environment

Judith Houston

# LoKI sample environments



Priority	Sample Environment System (SES)	Phase	Date Needed*	Status
1	Thermostated sample changer for quartz cuvettes	HC	Q3 2022	Prototype design underway based on ISIS set-up
1	Cell tumblers/rotating sample holders	HC	Q3 2022	Evaluating existing set-ups, e.g. Adrian Rennie design versus ESS
1	Flow cell (including HPLC pumps)	HC	Q3 2022	Integration underway, direct purchase (Knauer)
2	In situ techniques, as spectrometer attachments to the flow-through cell	ES	Q1 2023	Integration underway, direct purchase (Ocean Optics)
2	Rheometer	ES	Q1 2023	Procured (Anton Paar) and awaiting delivery Integration yet to begin
3	Stopped-flow cell	ES	Q3 2023	In-kind device from Estonia (Biologic) and awaiting delivery
4	Individually thermostated cuvette rack	ES	Q2 2023	Prototype exists and integrated at ESS
4	Goniometer(s)	ES	Q3 2021	ISIS to purchase in ~6 months
4	Dismountable 'sandwich'-style cells (ESS)	ES	Q2 2023	Designs exist. Just to be sent for manufacture
4	Warm Bore Cryomagnet 2.5T	ES	Q2 2023	Procurement underway
4	Stress/stretching rig (ESS)	ES	Q1 2023	ESS colabation(s) to develop different rigs
4	Cryostat – dilution fridge less than 1K	ES		
4	Cryostat wet	ES	Q4 2022	



# Geant4 Simulations

Milán Klausz

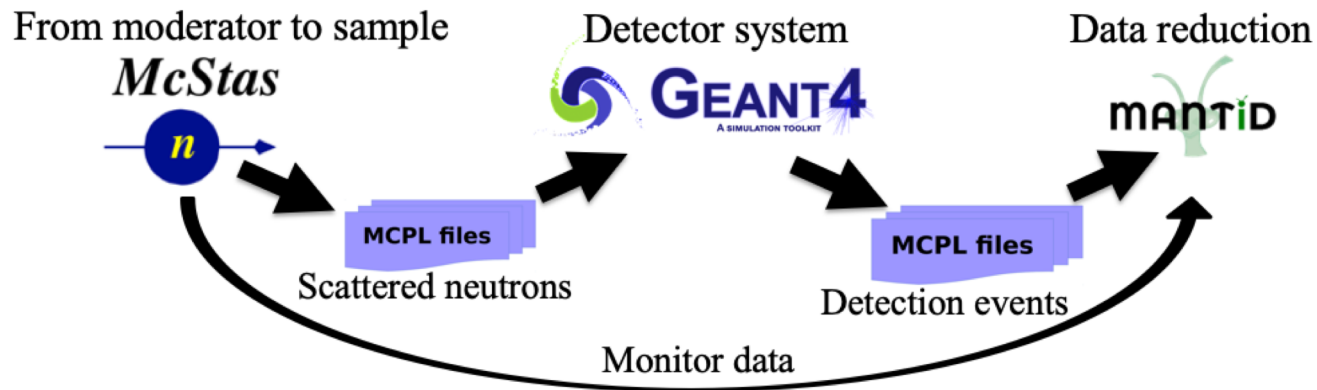
# Aims

## Detector characterisation:

- Improve Geant4 model and optimise simulation and data workflow
- Perform analysis with monochromatic and predicted profile of the LoKI beam

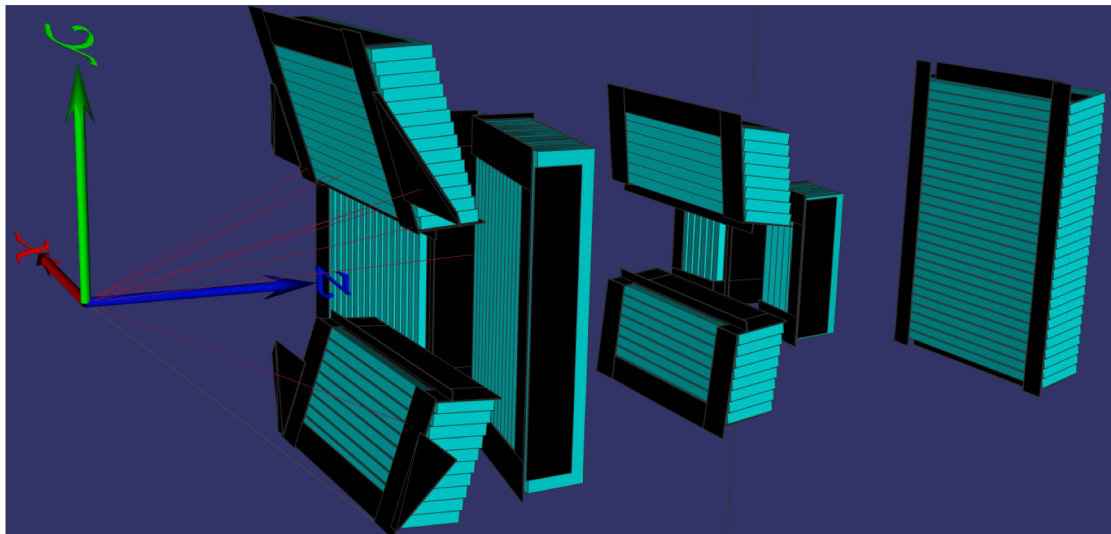
## Support the development of calibration and data reduction routines:

- 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

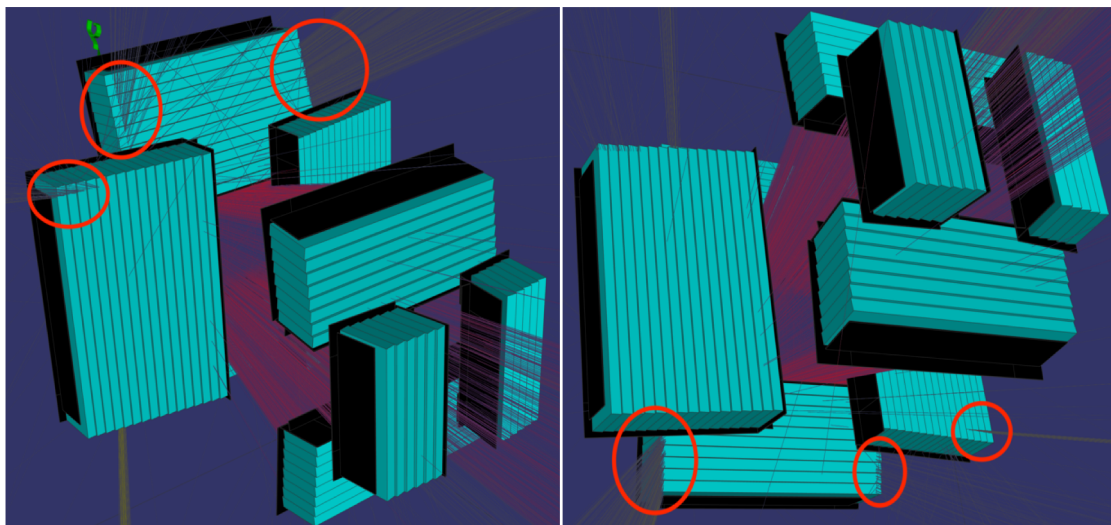


*Simulation and data workflow from moderator to data reduction*

# Preliminary results & work in progress

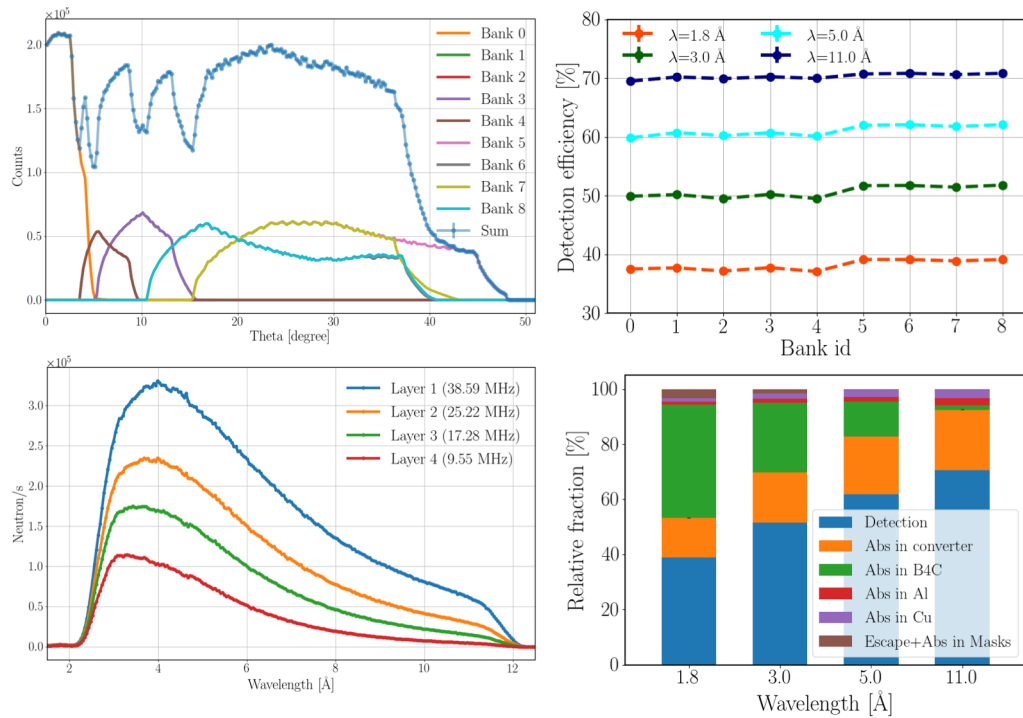


- A (greatly improved) detailed Geant4 model of the detector system is implemented based on CAD models - including B4C masks

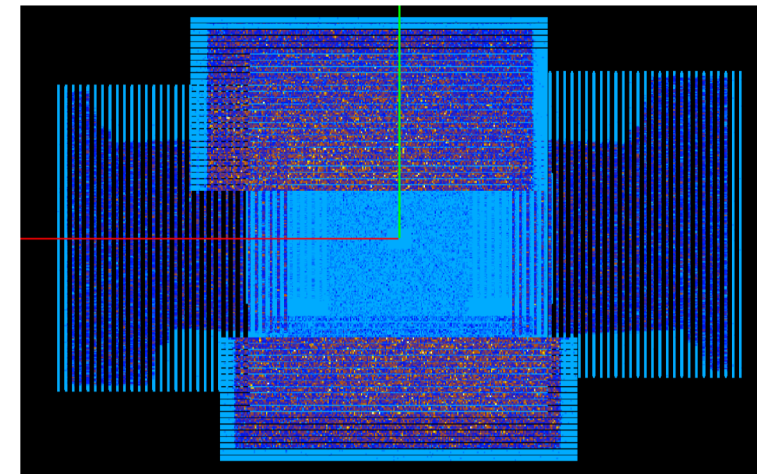
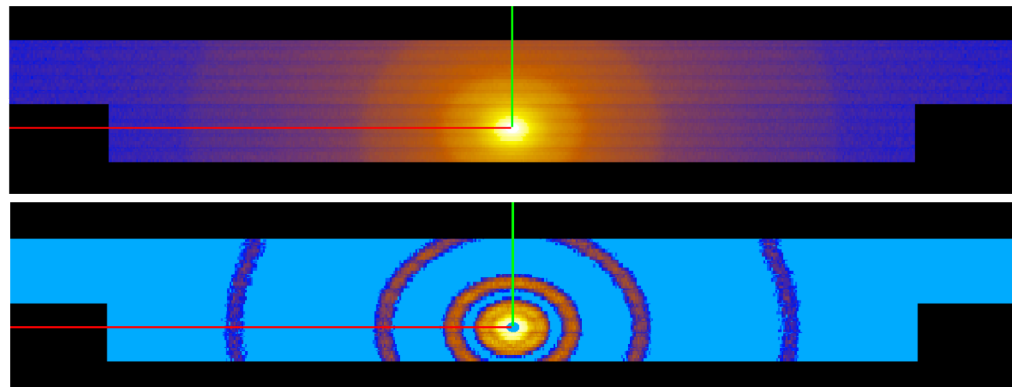


- The model helped to identify and prevent neutron streaming issues

# Preliminary results & work in progress



- Studied aspects include:
  - Efficiency
  - Coverage/uniformity
  - Absorption/transmission
  - Scattering effects
  - Hardening of spectra
- First simulated data of the LoKI/Larmor ISIS tests and for the full LoKI detector array has been provided in nexus format for data reduction in Mantid/Scipp
- Work continuing to analysis this data (progress has been much slower than we'd like on this)





# Data Reduction, McStas Simulations

How to interrogate /  
optimize the details of data  
reduction Scipp?

Wojciech Potrzebowski, Torben Nielsen  
and Judith Houston





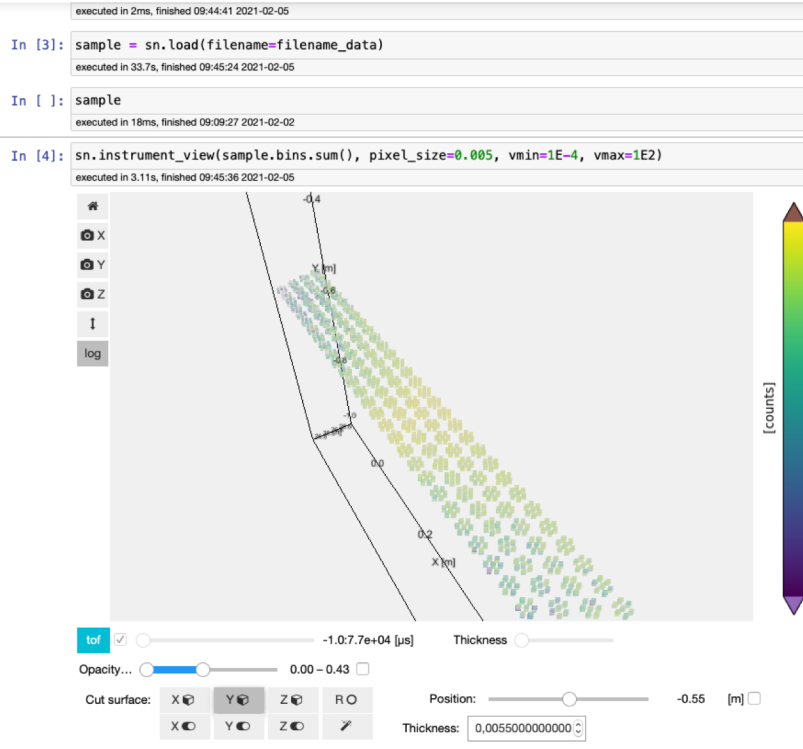
# Scipp on ISIS SANS2D data

## Exploring core functionality

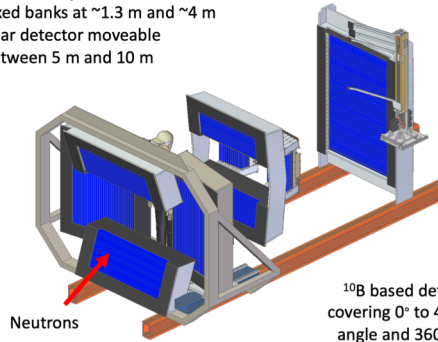
- Proof of concept for LoKI detector demonstrated at the last STAP
- "Debugging" with better understood SANS2D data
  - Easy control of variables in scipp (plotting/printing intermediate results)
  - Easy version update using conda
  - Improved data reading/writing, instrument view and plotting in recent versions of scipp
  - Scaling difference between scipp and Mantid to be confirmed
  - Wavelength slicing to be fully explored
- Scipp data reduction from SANS2D McStas simulations agrees with Mantid

# Scipp – Instrument View

McStas LoKI data can be read directly into Scipp



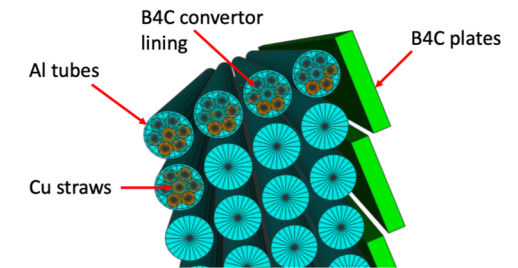
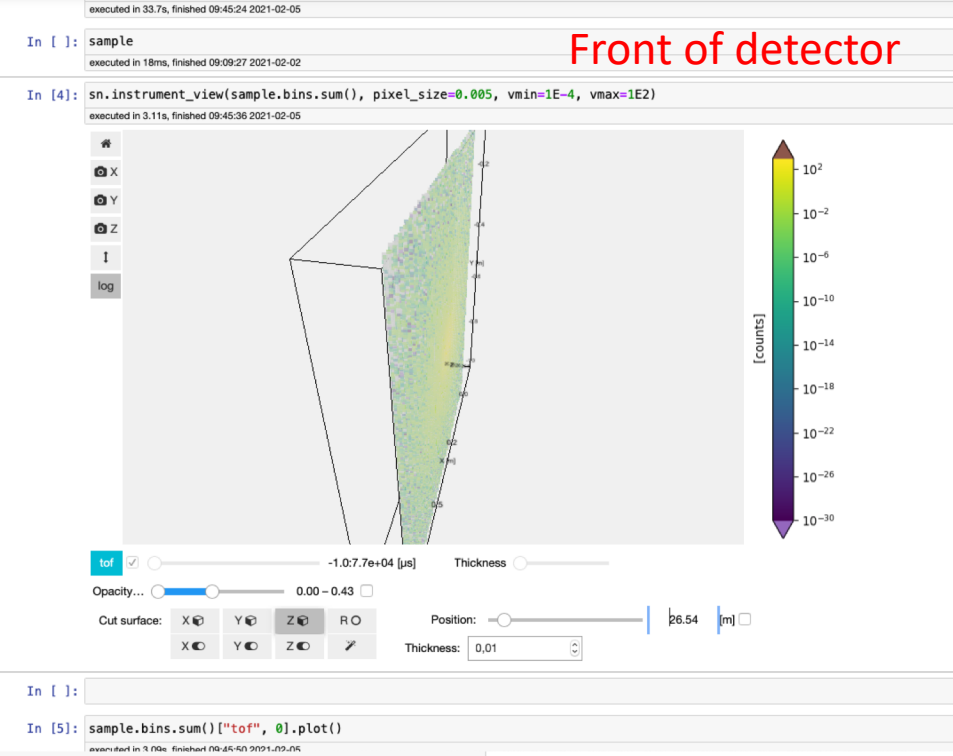
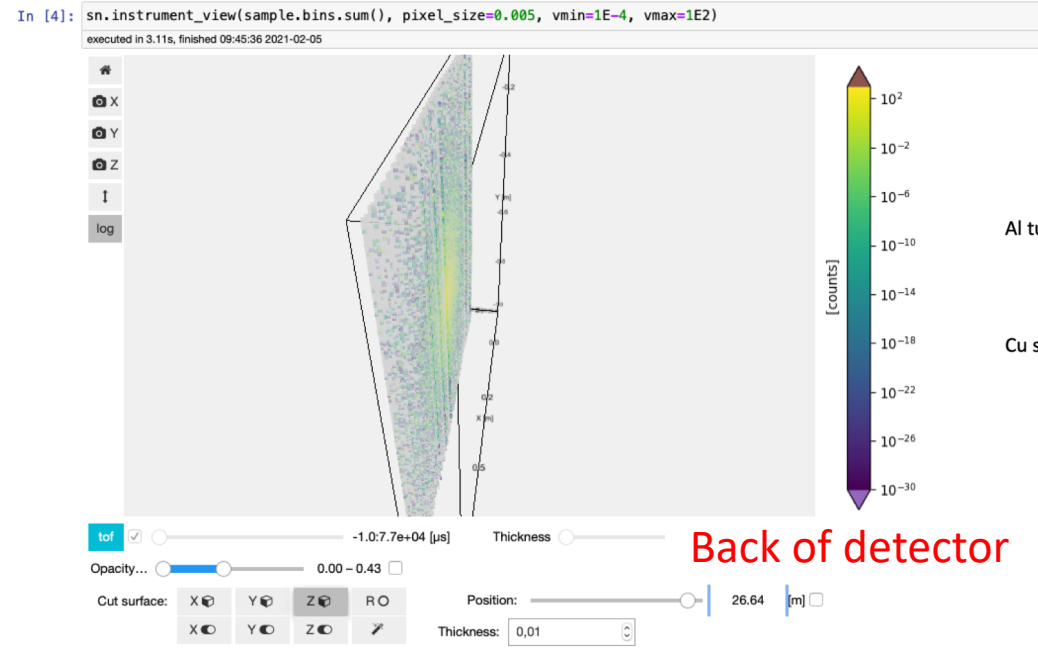
- Large detector array:
- Fixed banks at ~1.3 m and ~4 m
  - Rear detector moveable between 5 m and 10 m



<sup>10</sup>B based detector system covering 0° to 45° in scattering angle and 360° in azimuthal angle (180° Day 1).

```

executed in 33.7s, finished 09:45:24 2021-02-05
In [ ]: sample
executed in 18ms, finished 09:09:27 2021-02-02
    
```



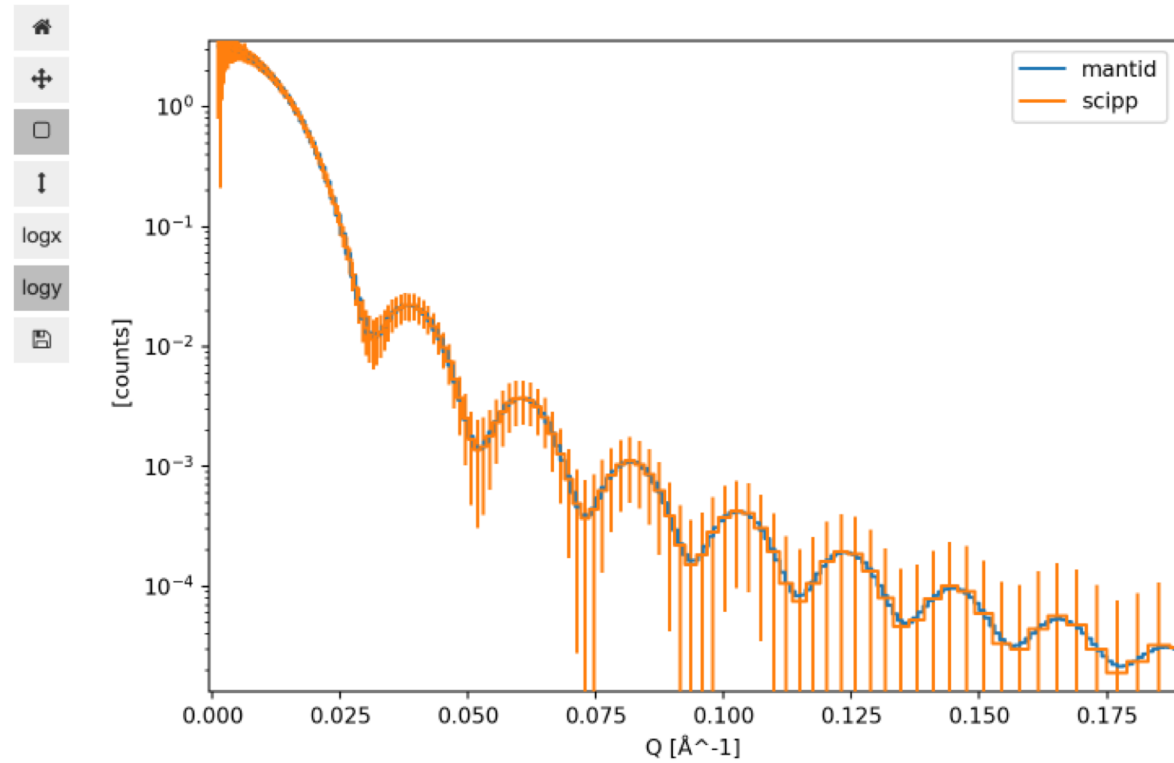


# Scipp – Data reduction

## Scipp and McStas event data

```
In [34]: sc.plot.plot({'scipp':I, 'mantid':sample_iq})
```

executed in 170ms, finished 08:40:40 2021-02-12





# Scipp user interface

## Exploring details of data reduction at different levels

- Scipp code becomes more and more mature and easier to understand
- Scipp widgets provide programable interface in Jupyter notebook

```
In [3]: from scipp_widgets import ProcessWidget
        ProcessWidget(sc.sum, [data_input, dimension_input])
```

var                      x                      summed

sum

scipp.Variable (160 Bytes)

(z: 10)	float64	45.0, 46.0, ..., 53.0, 54.0	☰
		$\sigma^2 = 0.29, 0.31, \dots, 0.57, 0.64$	

- Plotting, manipulating and comparing many data sets and their fits to be streamlined
- McStas/scipp pipeline provides easy setup to explore detector features
- User experience workshop to be organized by IDS in Q3 2021
- Scipp demos and training for future ESS users (regularly at IKONs)



# NICOS-LoKI Prototype

Instrument control  
software

Ümit Ali Cemal Hardel, Matt  
Clarke, Tobias Richter

# NICOS-LoKI Prototype



The NICOS software developers have been working closely with the LoKI team for the past few months to develop the instrument control software.

Still in the prototype stage, some key areas still to be developed next include:

- How we input the sample lists and what relevant information is saved
- How we select and set-up different pieces of sample environments

In general though, the interface is progressing, as can be seen from the next few slides.



New - NICOS editor

Instrument: LOKI Experiment: Demo Experiment

✓ Connected

Experiment

Setup

Samples

Experiment Configuration

Instrument interaction

Script Editor

Prototype

Detector Image

History

Logs

Finish Experiment

### Current experiment

Proposal number:

Experiment title:

Users:

Local contact:

Notifications  
(one email address  
per line):

Do not continue scripts after fatal errors

Apply changes

The "Experiment" tab holds the basic information about the experiment.



New - NICOS editor

Instrument: LOKI Experiment: Demo Experiment

✓ Connected

Experiment

Setup

Samples

Experiment Configuration

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Script Editor

Prototype

Detector Image

History

Logs

Finish Experiment

Select basic instrument configuration:

<keep current>

Select optional components:

- beamstop
- chopper\_1
- chopper\_2
- collimator\_1
- collimator\_2
- detectors
- gate\_valve
- laser
- monitors
- sample\_changer\_a
- sample\_changer\_b
- sample\_stack
- shutters
- slit\_set\_1
- slit\_set\_2
- slit\_set\_3

Show all plug & play components

Apply Reload current setup

In "Setup" tab, a user can decide and select additional components for the experiment. These devices will show up in the "Instrument Interaction" tab and can be controlled via Nicos.





Instrument: LOKI Experiment: Demo Experiment

Experiment Configuration

Experiment Setup Samples Experiment Configuration Instrument interaction Script Editor Prototype Detector Image History Logs Finish Experiment

List selection

Select a sample list:

Sample definition

New sample configuration

Sample name:

Comment:

Thickness:  mm

Device positions:

Device	Position
--------	----------

In "Samples" tab users provide the necessary information about the samples and device positions.



NICOS Instrument: LOKI Experiment: Demo Experiment

Output Scan Plot Detector Image Script Status

```
[09:16:55] >>> [guest 2021-04-07 09:16:55] NewExperiment(proposal='1', localcontact='J. Houston <judith.houston@ess.eu>', title='Demo')
[09:16:55] Exp : experiment directory is now /opt/nicos-data/2021/p1
[09:16:55] Exp : script directory is now /opt/nicos-data/2021/p1/scripts
[09:16:55] Exp : data directory is now /opt/nicos-data/2021/p1/data
[09:16:55] Exp : New experiment p1 started
[09:16:55] >>> [guest 2021-04-07 09:16:55] SetMailReceivers('J. Houston <judith.houston@ess.eu>')
[09:16:55] WARNING: general email notification is not configured in this setup
```

Devices

Name	Value	Status
slit_set_1	5.00 x 0.00 ...	idle
slit_set_2	0.00 x 0.00 ...	idle
slit_set_3	0.00 x 0.00 ...	idle
system		
Exp		
lastpoint	0	
lastscan	0	
LoKI		
Sample		
Space	354.209 GiB	354.21 GiB free

”Instrument Interaction” tab provides a user friendly interface to control devices. Any (valid) command can be typed to change a desired property of a device.

Similarly one can double-click the device on the right hand side and change the property without doing it programmatically if it is supported.

>>  + New Cmd ▶ Run



A screenshot of the Nicos software interface. The top header bar is dark blue and contains the Nicos logo, the text 'Instrument: LOKI Experiment: Demo Experiment', and a 'Connected' status indicator with a close button and a settings gear. On the left, a vertical sidebar lists various tabs: 'Experiment', 'Setup', 'Samples', 'Experiment Configuration', 'Instrument interaction', 'Script Editor' (which is highlighted), 'Prototype', 'Detector Image', 'History', 'Logs', and 'Finish Experiment'. The main area above the 'Script Editor' tab shows a 'New command:' section with four dropdown menus labeled 'Device', 'Scan', 'Other', and 'Measure'. Below this is a toolbar with icons for file operations (new, open, save, print, undo, redo, cut, copy, paste) and execution (dry run, run, get, update). The 'Script Editor' window itself shows a single line of text '1' on a yellow background, indicating the start of a script.

”Script Editor” tab provides a basic interface to create/save/load scripts.



**NICOS** Instrument: LOKI Experiment: Demo Experiment ✓ Connected ✕ ⚙️

**Experiment**  
Setup  
Samples  
Experiment Configuration  
Instrument interaction  
Script Editor  
Prototype  
Detector Image  
History  
Logs  
Finish Experiment

**Settings**  
TRANS order: **TRANS First** ⌵  
Do SANS:  time(s)  
Do TRANS:  time(s)  
duration type: **Mevents** ⌵  
duration type: **Mevents** ⌵  
Optional  
 Temperature  
 Pre-comman  
 Post-comma

	Position	Sample	Thickness (mm)	TRANS Duration (Mevents)	SANS Duration (Mevents)
1					
2					
3					
4					
5					
6					
7					
8					
9					
10					
11					
12					
13					
14					
15					
16					
17					
18					
19					
20					
21					
22					
23					
24					
25					

**Prototype** tab holds the relevant information and settings for the sample and experiment. The tables can be loaded or saved for later use.

Generate

Bulk update:  Apply Copy Cut Paste Add Row Above Add Row Below Delete Rows Load Table Save Table Clear Table