NMX a macromolecular crystallography diffractometer at ESS

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Instrument Project Engineer NMX

www.europeanspallationsource.se

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Summary

- The project structure
- NMX Scientific case
- NMX project status
- Baseline layout
  - Shielding
  - Wavelength selection Chopper
  - Endstation
  - Detectors

Project structure

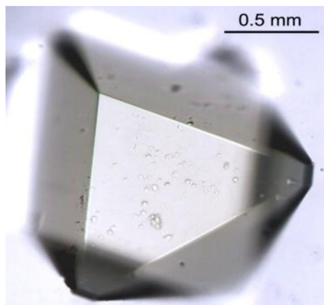
Instrument Project Leader: Esko Oksanen, ESS

Instrument Project Engineer: Giuseppe Aprigliano, ESS

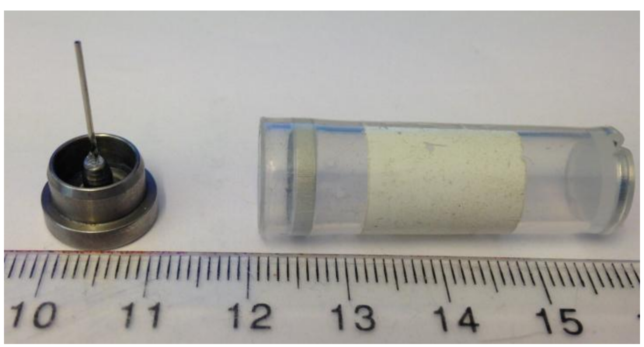
Zoe Fisher	(ESS-SAD)
Anders Pettersson	(ESS-SAD)
Richard Hall Wilton	(ESS -Detector group)
Dorothea Pfeiffer	(ESS- Detector group/CERN)
Phillip Bentley (ESS-NOSG)	
Valentina Santoro	(ESS-NOSG)
Damian Martin Rodriguez	(ESS-NOSG)
Iain Sutton	(ESS-NCG)
Markus Olsson	(ESS-NCG)
Stuart Birch	(ESS-PSS)
Peter Ladd	(ESS-Vacuum Group)
Marcelo Juni Ferreira	(ESS-Vacuum Group)
Thomas Gahl	(ESS-MCA)
Paul Barron	(ESS-MCA)
Thomas Holm Rod	(ESS-DMSC)
Jonathan Taylor	(ESS-DMSC)
Peter Sångberg	(ESS-SPD)
Magnus Israelsson	(ESS-Programme office)
Jean-Luc Ferrer	(IBS – GSY Group)
Márton Markó	(Wigner research centre)

NMX Scientific case

“Small” crystals : 0.2mm to 5mm



Oksanen, E *et al.* *J. R. Soc. Interface* **2009**, *6 Suppl 5*, S599-610.



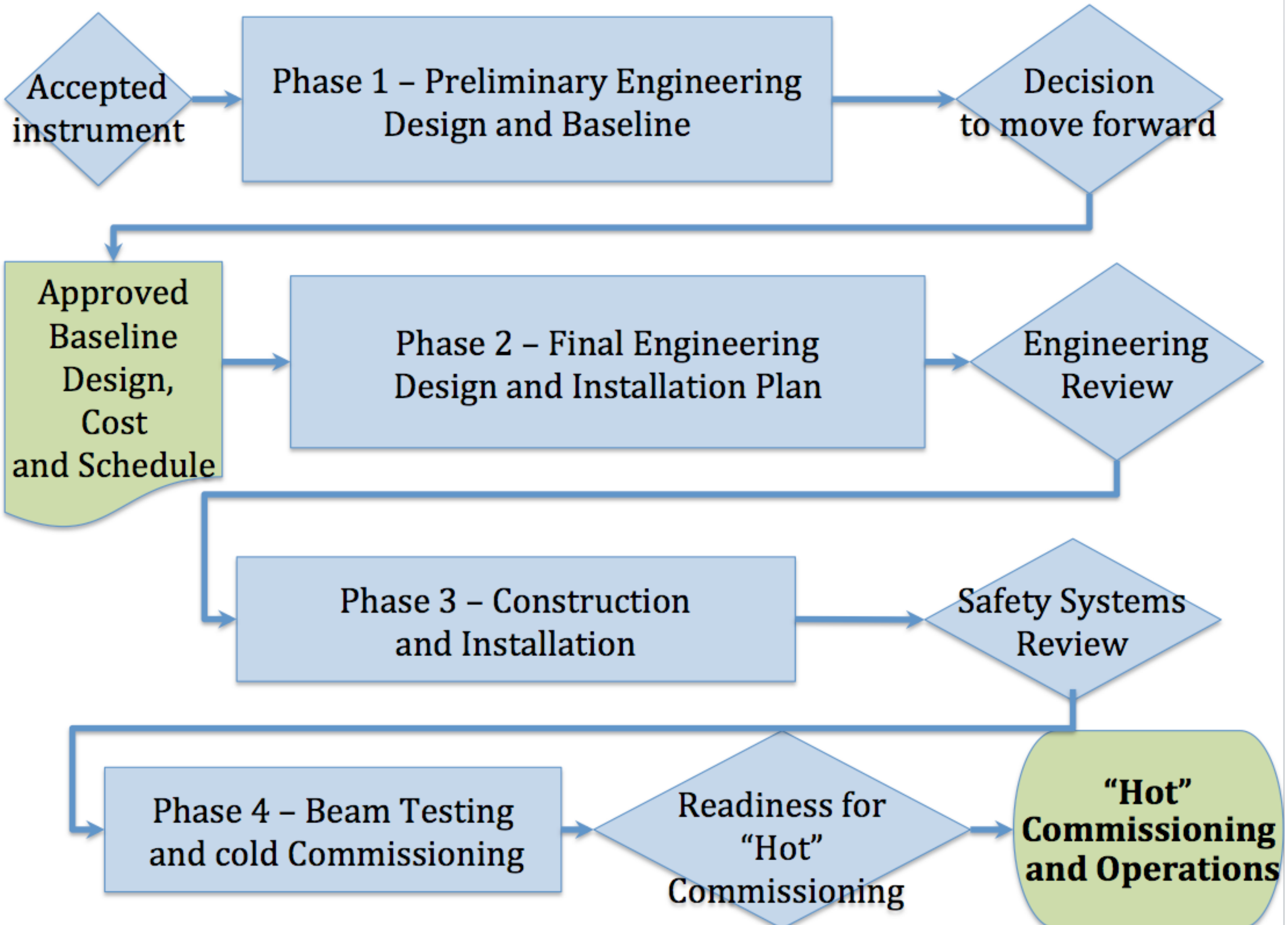
Quasi-Laue time of flight diffractometer

Primary scientific case: Macromolecular crystallography

Compared to X-ray:
☺ Hydrogens are visible
☺ No radiation damage
☹ Large crystals needed
☹ Data collection takes weeks
☹ Few instruments available

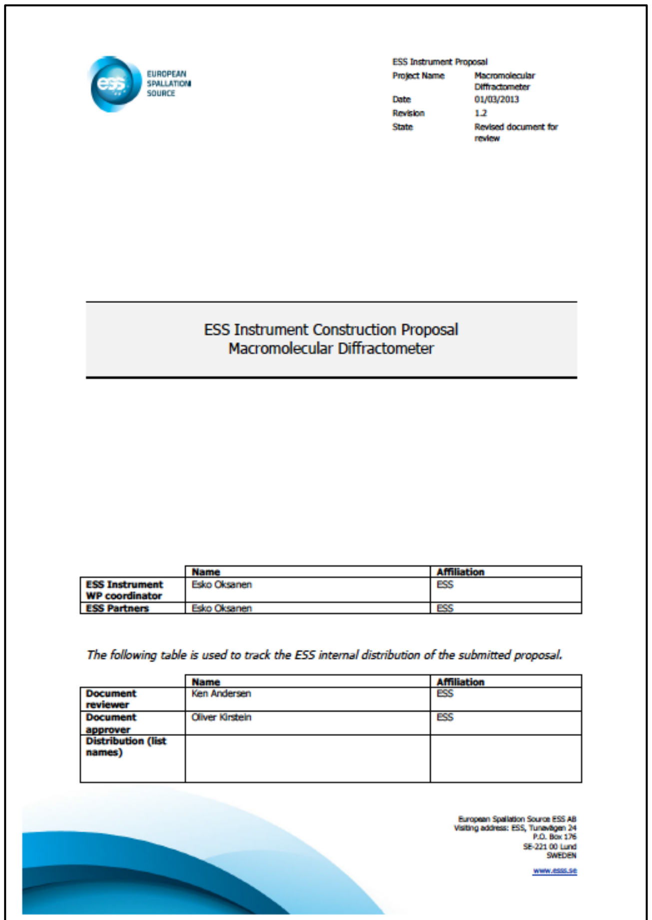
Beam property	min	max
Beam size	0.2mm x 0.2mm	5mm x 5mm
Wavelength	1.8Å	3.55Å
Max divergence	±0.2°	
Sample-Source distance	157.6m	

NMX project status



Courtesy : Rob Connatser

NMX project status: Phase 1



ESS Instrument Proposal

Project Name	Macromolecular Diffractometer
Date	01/03/2013
Revision	1.2
State	Revised document for review

ESS Instrument Construction Proposal
Macromolecular Diffractometer

	Name	Affiliation
ESS Instrument WP coordinator	Esko Oksanen	ESS
ESS Partners	Esko Oksanen	ESS

The following table is used to track the ESS internal distribution of the submitted proposal.

	Name	Affiliation
Document reviewer	Ken Andersen	ESS
Document approver	Oliver Kirstein	ESS
Distribution (list names)		

European Spallation Source ESS AB
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P.O. Box 176
SE-221 00 Lund
SWEDEN
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Baseline Documents:

Instrument Work Package Specification
- P&ID of Instrument
- Schedule
- Budget

3D CAD model of instrument envelope
Technical Group design documents
Work Unit documentation
Product Breakdown Structure
Concept of Operations for the instrument
Requirements List
Staging Plan
Draft Commissioning Plan

High level scientific requirements

1. The instrument shall allow data collection from crystals with unit cell repeats > 300Å.
2. The instrument shall allow data to be collected to a d_{min} of 1.5 Å.
3. The instrument shall match the size of the neutron beam to the size of the sample.
4. The instrument shall match the divergence of the neutron beam to the mosaicity of the sample.
5. The instrument should maximise the signal-to-background (S/B) ratio of the Bragg reflections.
6. The instrument should allow data collection from crystals of < 0.01 mm^3 volume

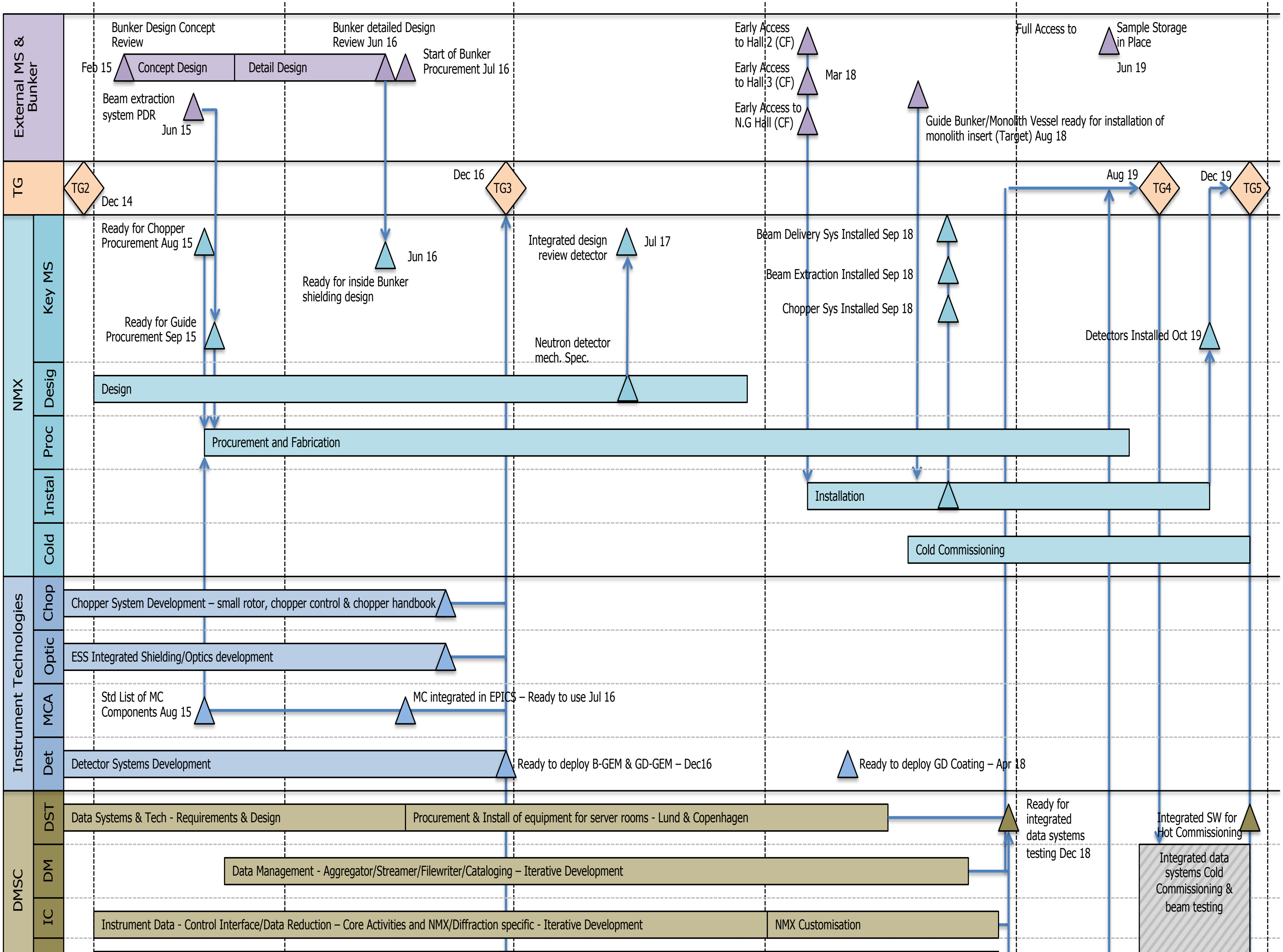
10. Sample alignment stroke

10.1. The SPS shall have ±10 mm stroke to position the sample in intersection of the sample rotation axis and the neutron beam axis.

10.2. **Rationale**: Samples can be mounted on pins and capillaries of widely varying length (see ConOps) and they need to be positioned at the beam center (see 13.6.4.2(1).

10.3. **Verification**: Test

NMX – Summary Construction Schedule Key – Key Milestones and Tasks



Partner institutes:

Wigner Research Centre for Physics

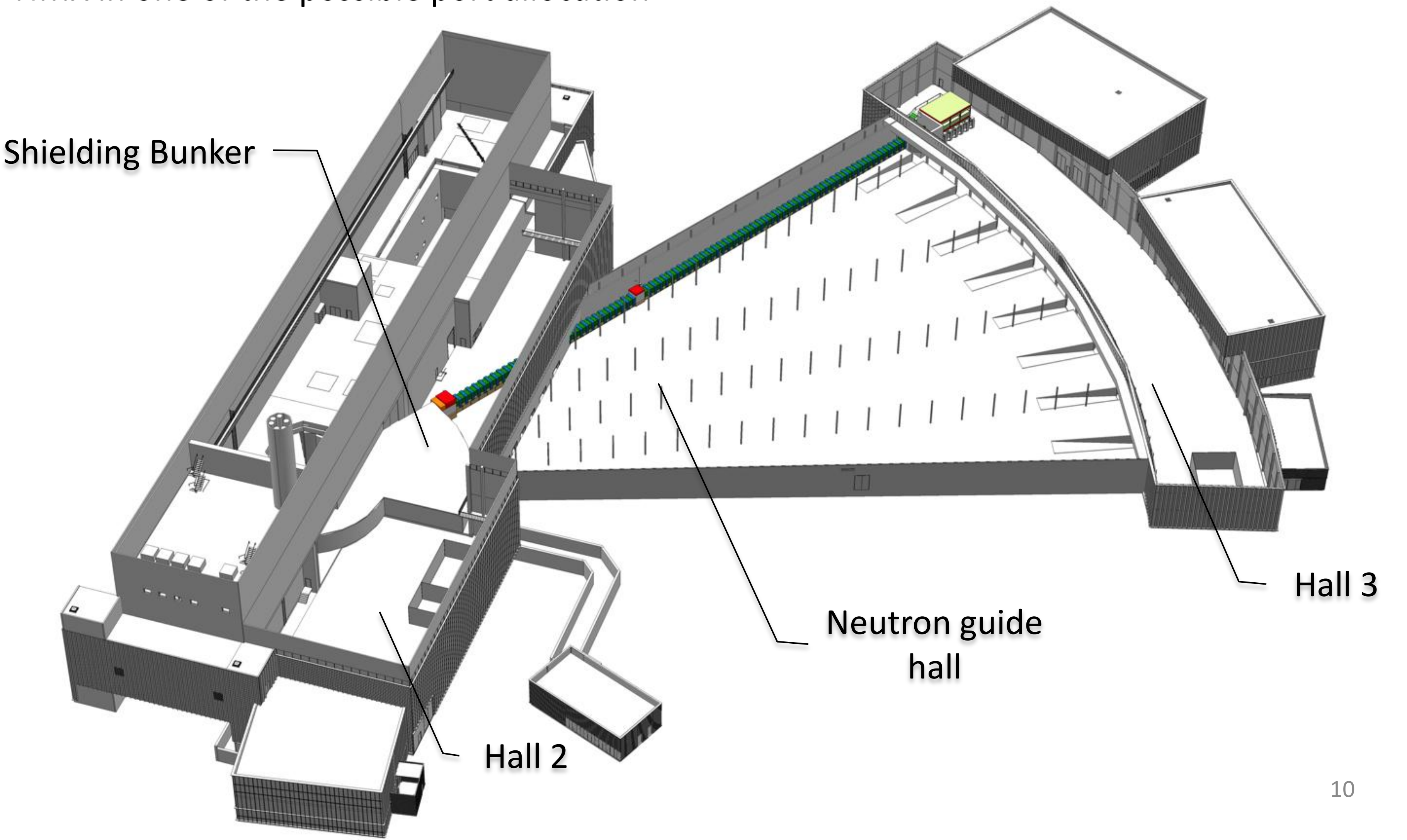
Neutron guide system (Through NOSG)
Chopper system (Through NCG)
Secondary Shutter
Manpower

LLB/CEA/CNRS IBS Grenoble

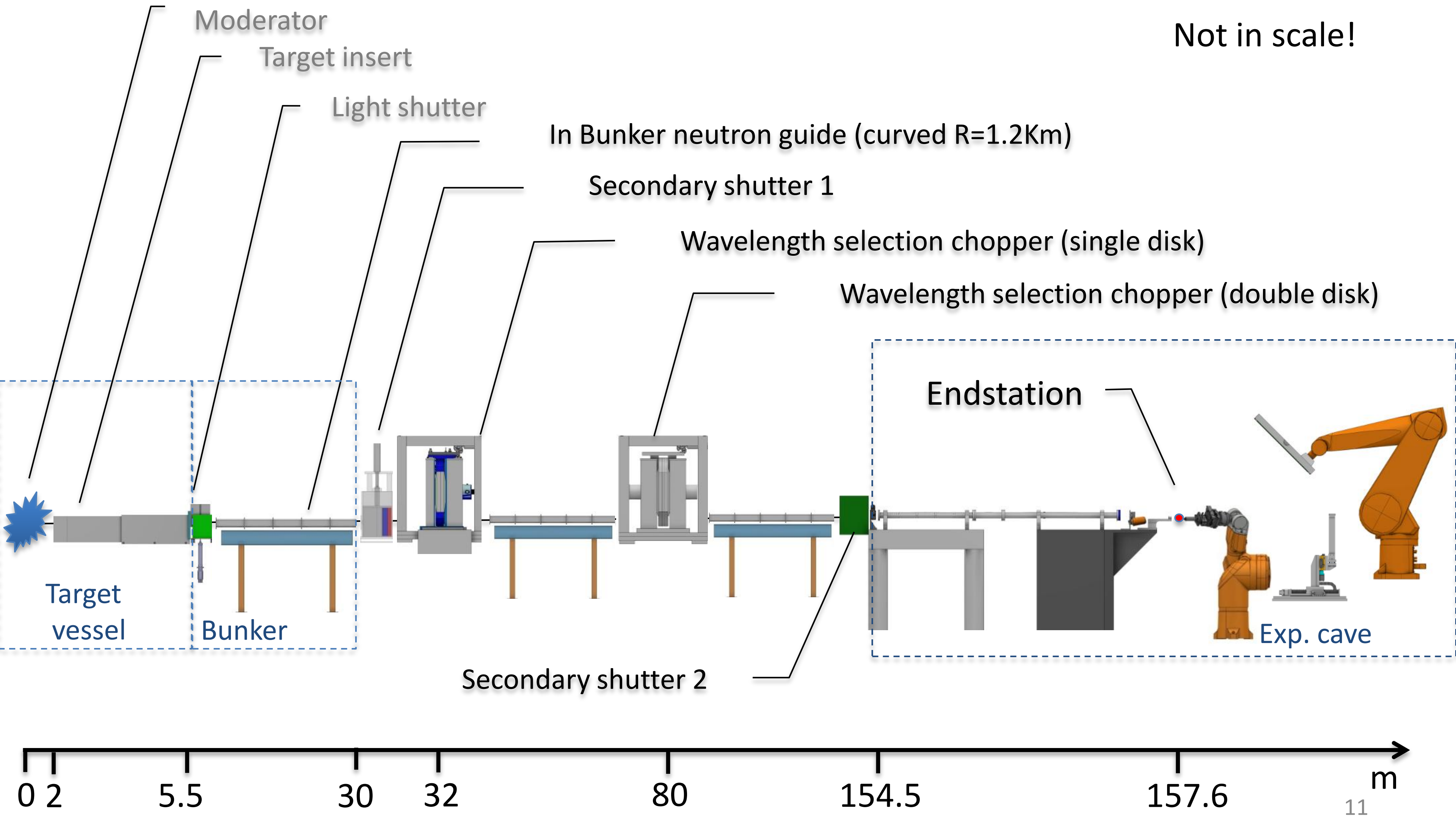
Detector positioning system

Baseline Layout

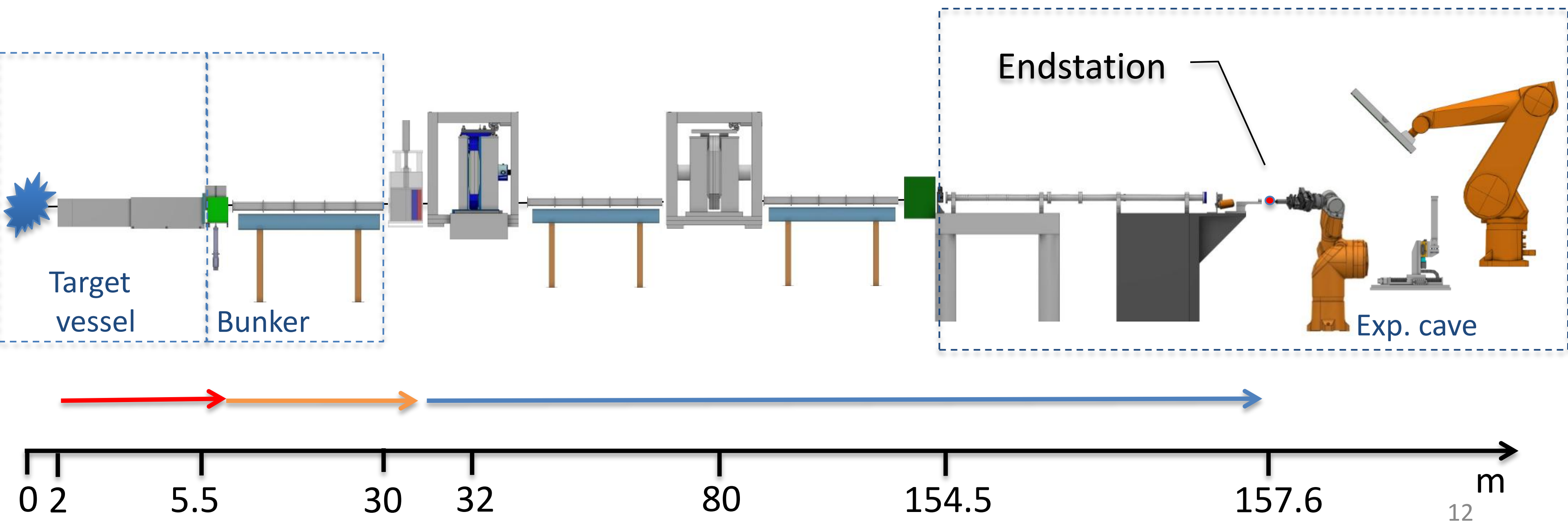
NMX in one of the possible port allocation



Baseline Layout

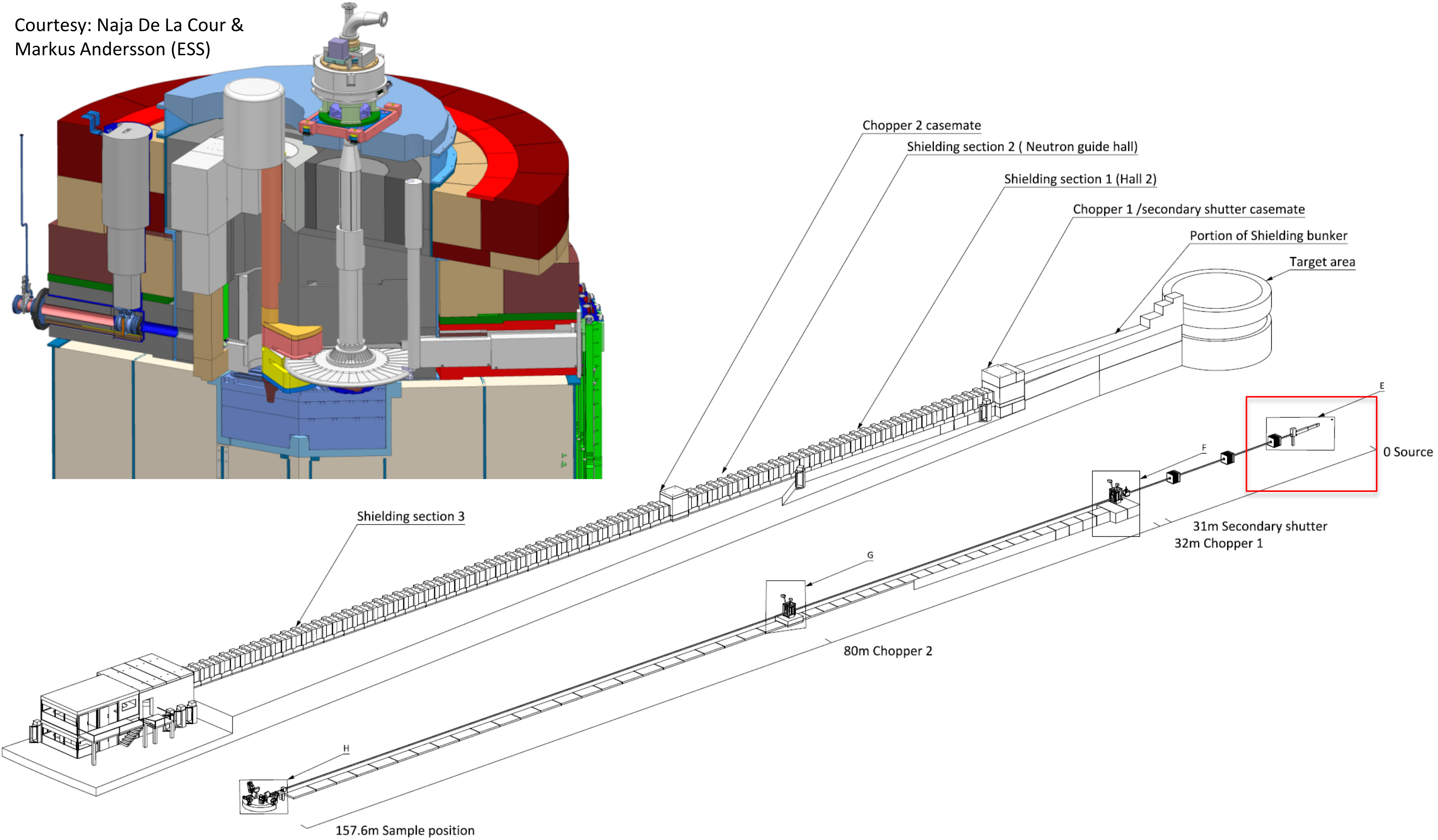


System	Description						
Beam properties at sample position	Wavelength band			Beam size		Divergence	
	1.74 Å (1.8-3.55 Å)			5mm x 5 mm (max)		± 0.2˚ (max)	
Neutron Guides	Start (m)	End (m)	Height (mm)	Width (mm)	Horizontal Geometry	Vertical Geometry	Coating
Extraction	2.0	6.0	30 to 45	30	Straight	Lin. tapered	m=1 sides; m=2 top/bottom
Inside Bunker	6.0	31.5	45	30	Curved R1.2Km	Straight	m=1; m=2.2 only outer side,
Outside Bunker	31.5	154	45	30	Straight	Straight	m=1
Frame overlap mirror	1.2˚ inclination in vertical plane, m=1, substrate						



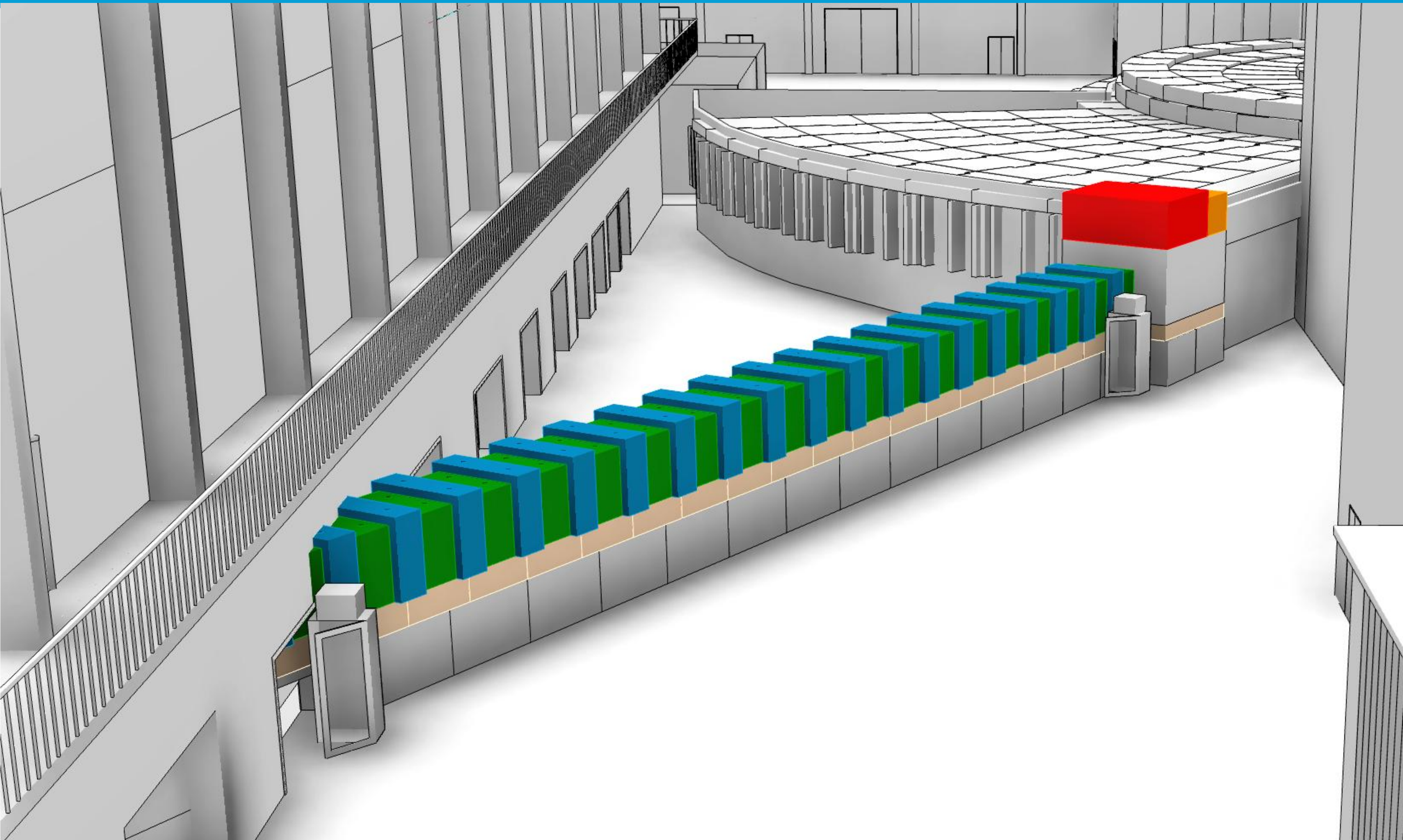
Baseline Layout

Courtesy: Naja De La Cour & Markus Andersson (ESS)

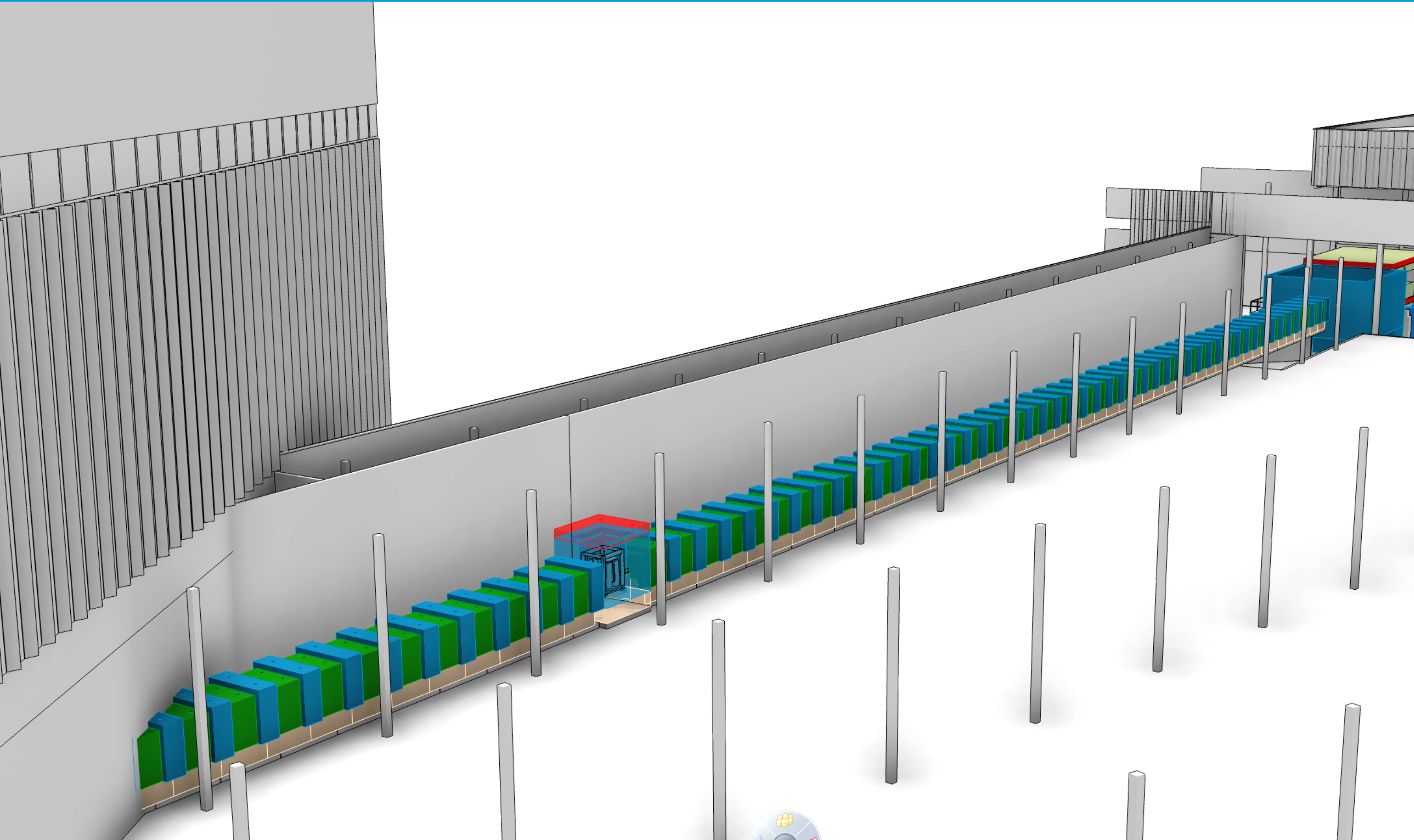


Baseline Layout

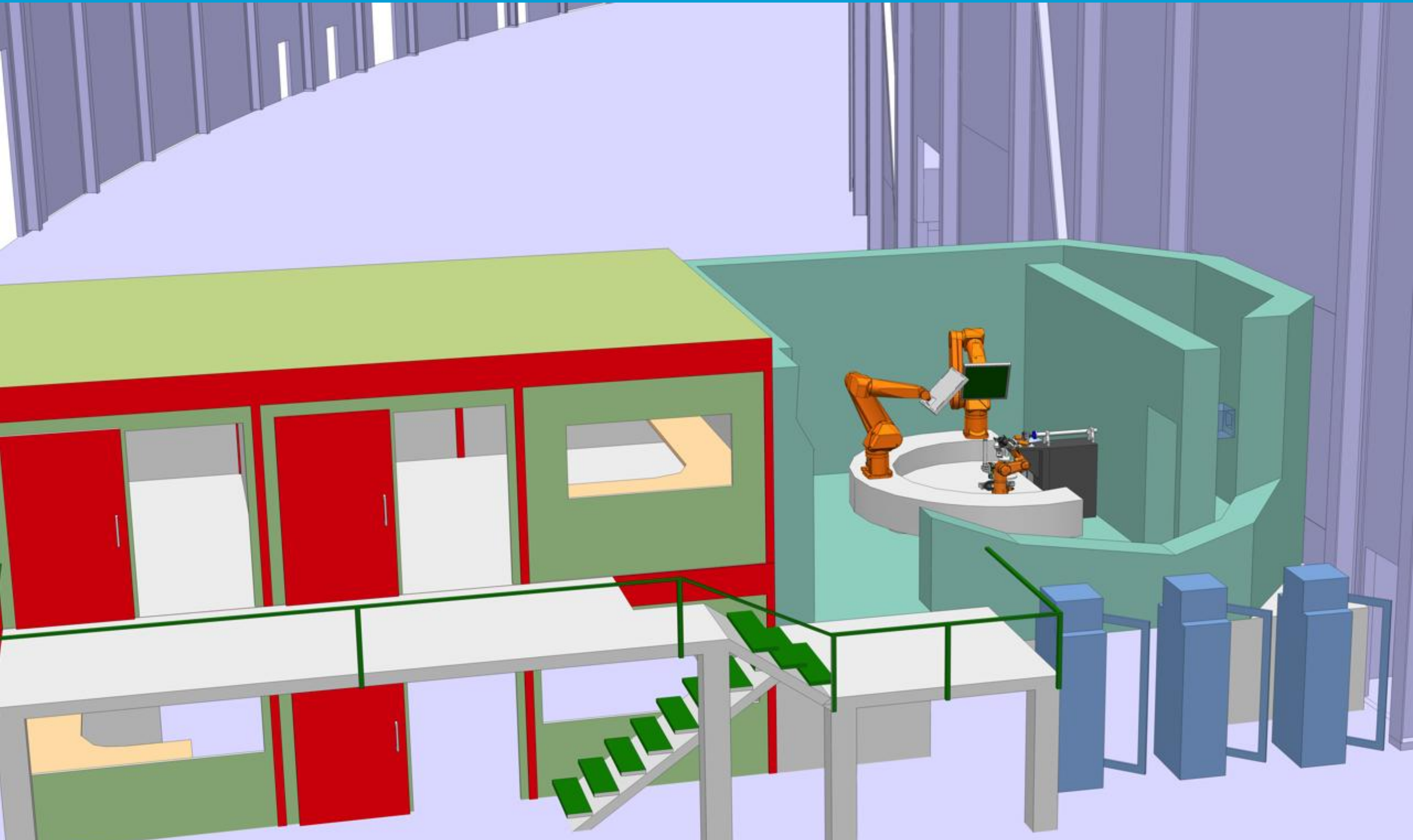
EUROPEAN
SPALLATION
SOURCE



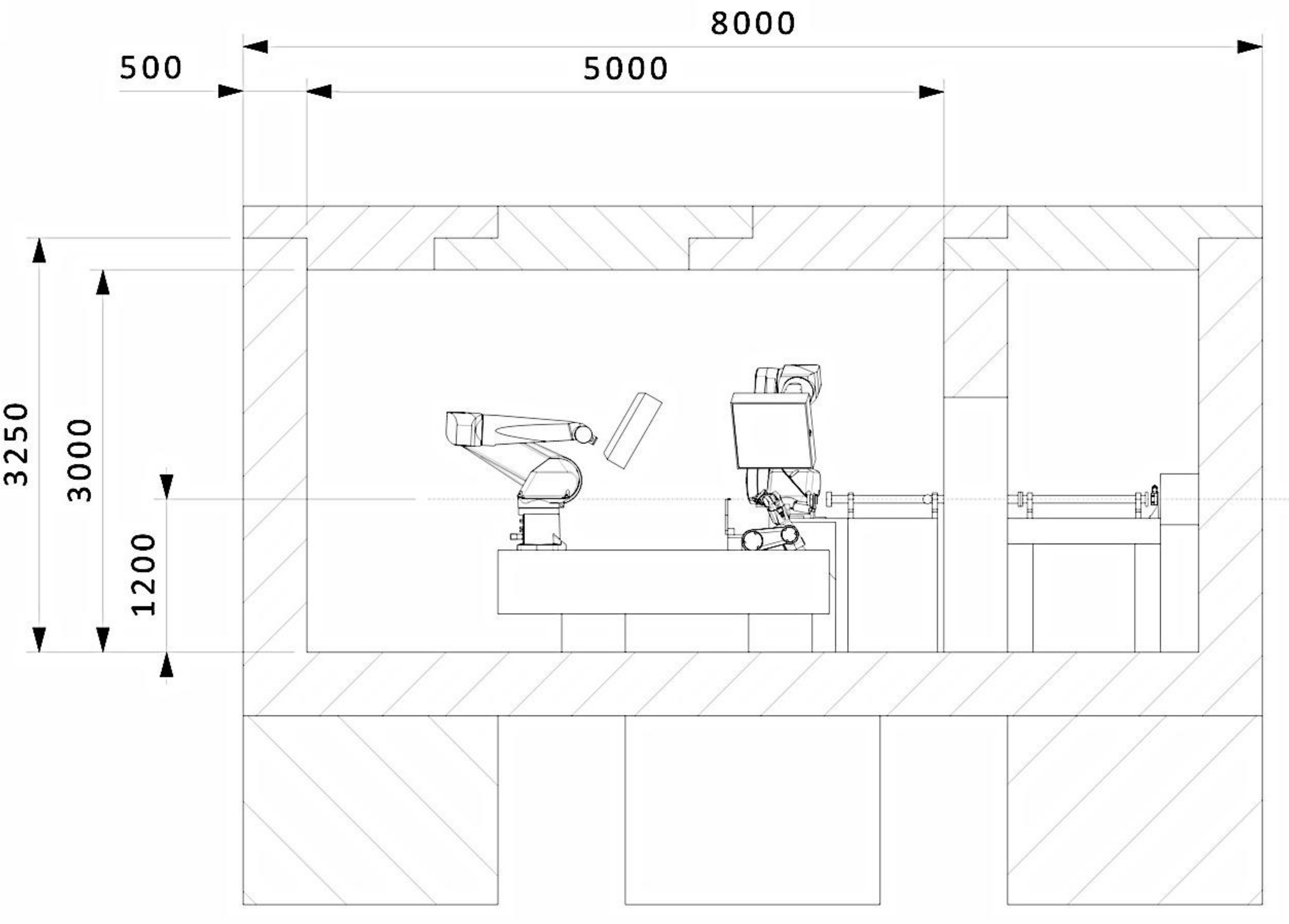
Baseline Layout: Shielding



Baseline layout: Experimental cave

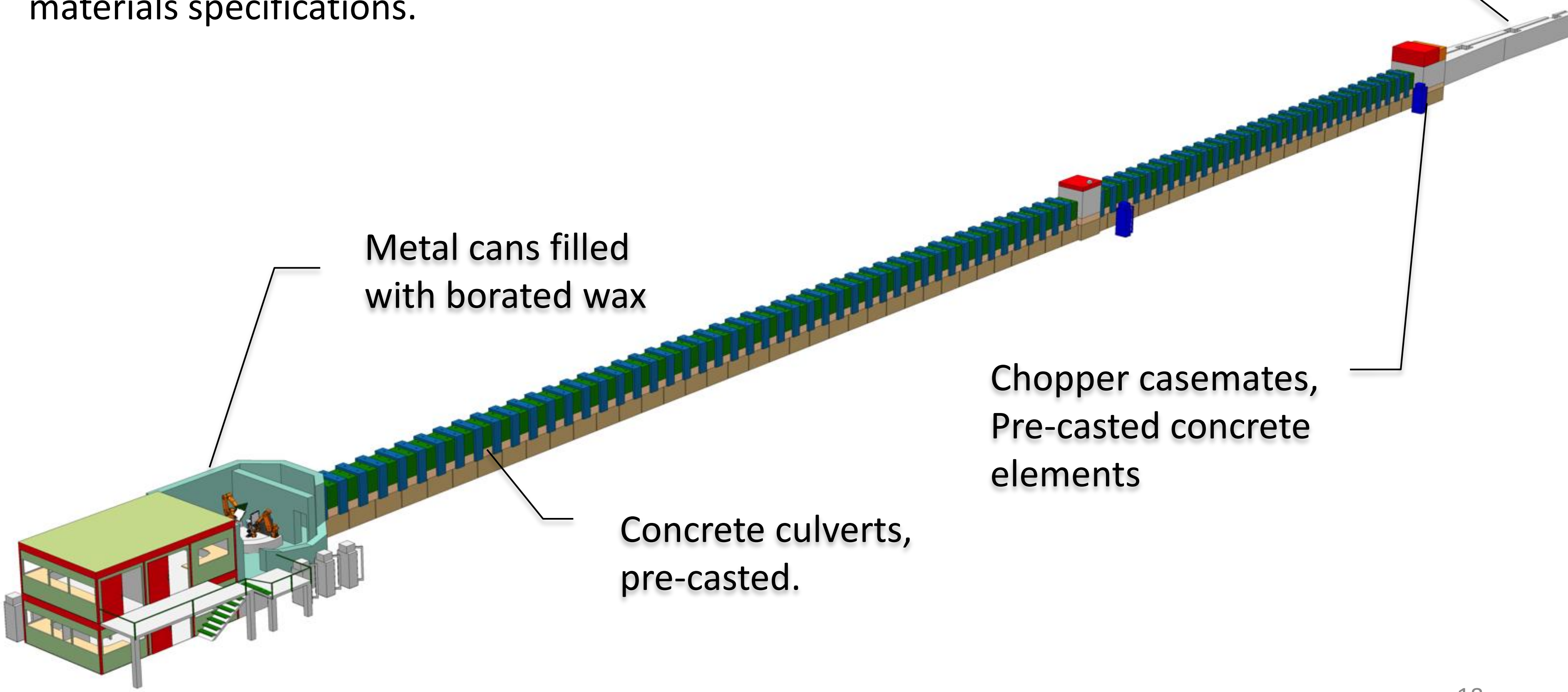


Baseline layout: Experimental cave



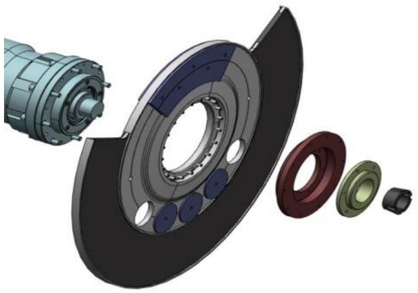
Baseline layout: Experimental cave

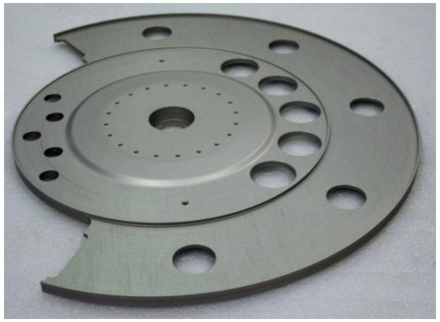
Simulations are being carried on by Valentina Santoro of the ESS NOSG To properly specify thicknesses and materials specifications.

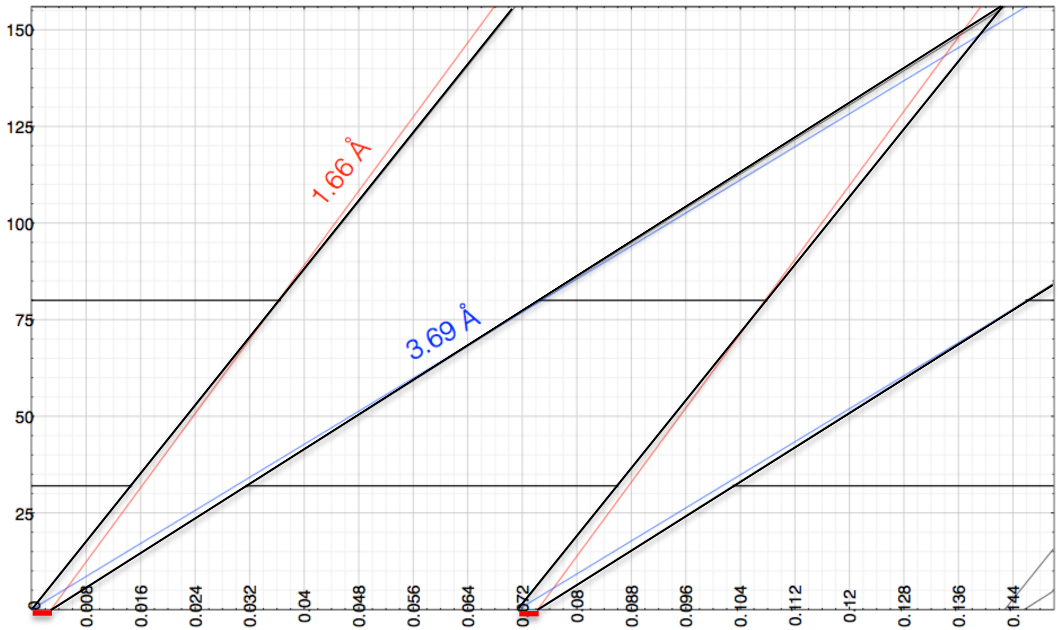


Wavelength Selection Choppers

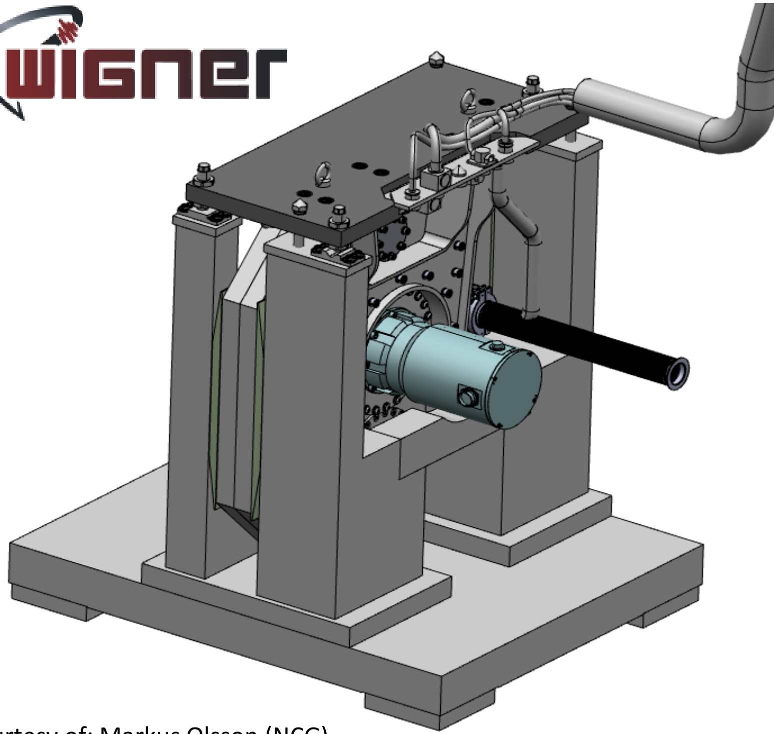
- Disk diameter 700mm
- Rotating frequency 14 Hz
- B4C resin-epoxy coating.
- Single disk at 32m
- Double, co-rotating disk at 80m





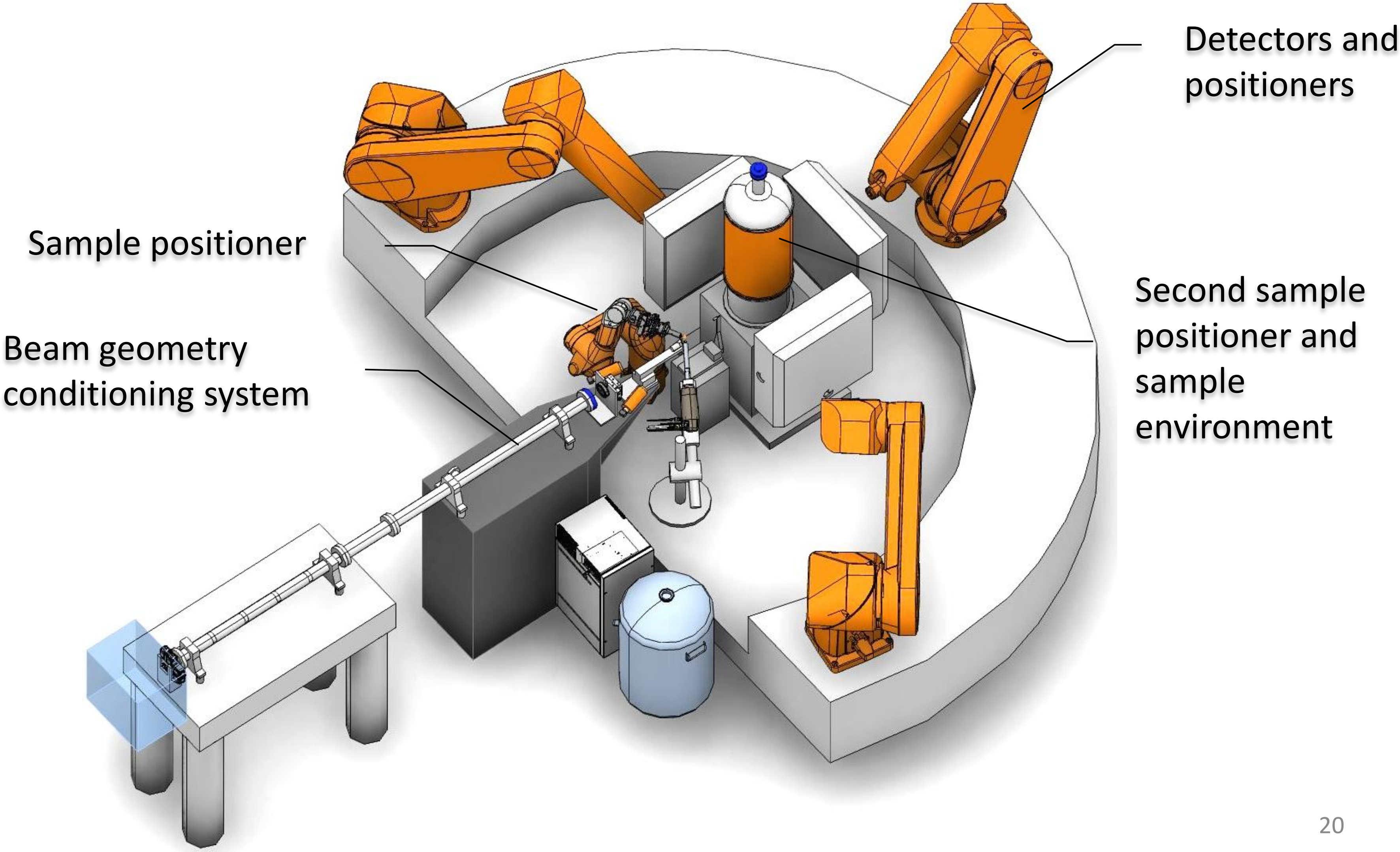


1.8-3.55 Å nominal bandpass



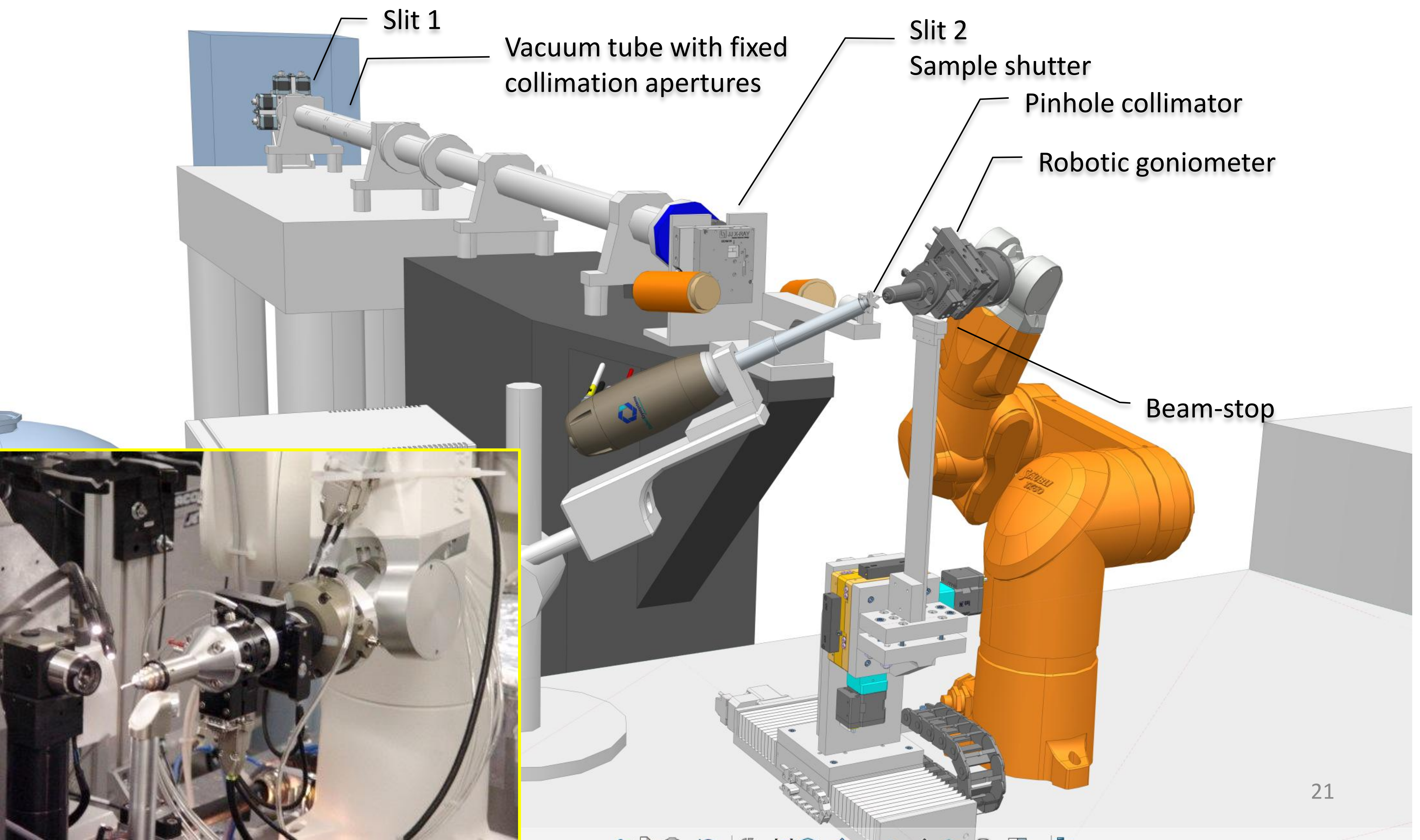
Courtesy of: Markus Olsson (NCG)

Endstation



Detectors and positioners
Sample positioner
Second sample positioner and sample environment
Beam geometry conditioning system

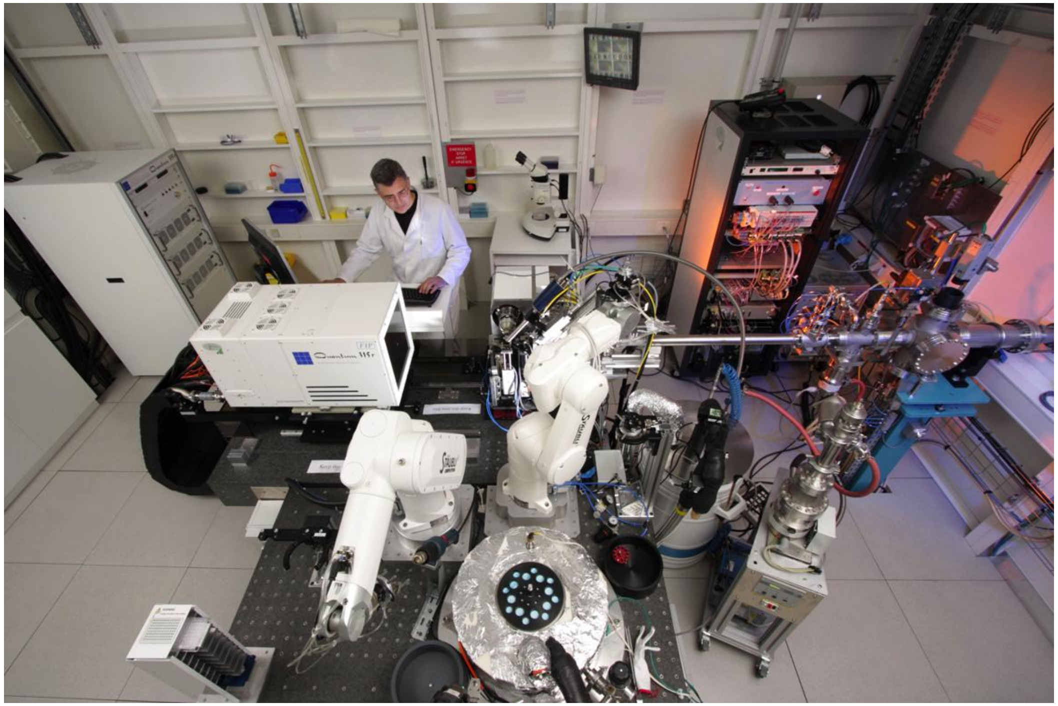
Endstation

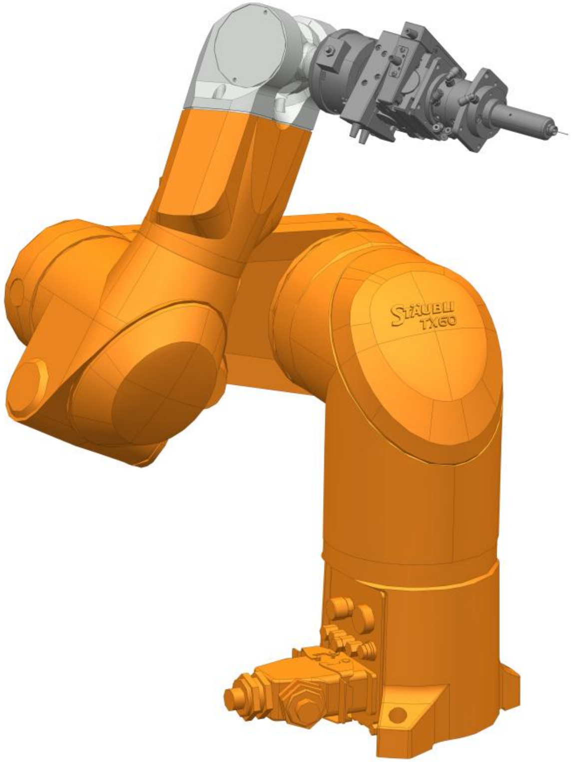

Slit 1
Vacuum tube with fixed collimation apertures
Slit 2
Sample shutter
Pinhole collimator
Robotic goniometer
Beam-stop

Endstation

Arbitrary orientation of spindle axis in the lower hemisphere.
Limited S.O.C. <0.04 mm rms during rotation.
Sample changer capability
Minimized user interaction with Exp cave hardware.

G-Rob at BM-30A FIP (ESRF)



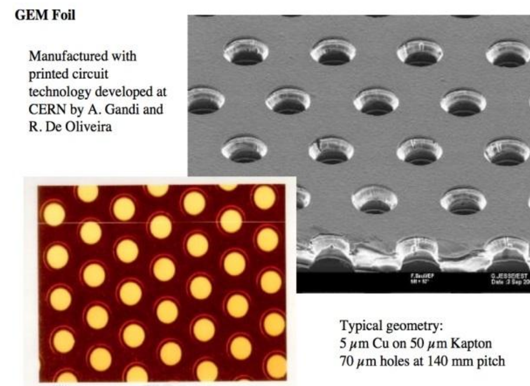


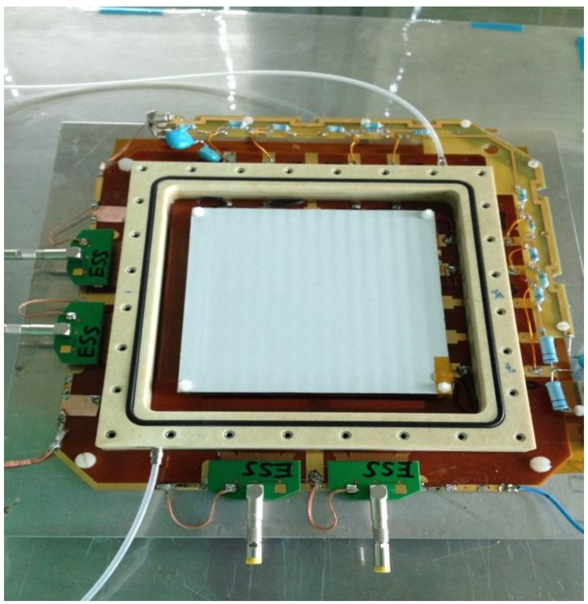
Contact: Jean-Luc Ferrer (IBS Greoble)

Detectors

- Dorothea Pfeiffer (ESS/CERN), Richard Hall Wilton(ESS)

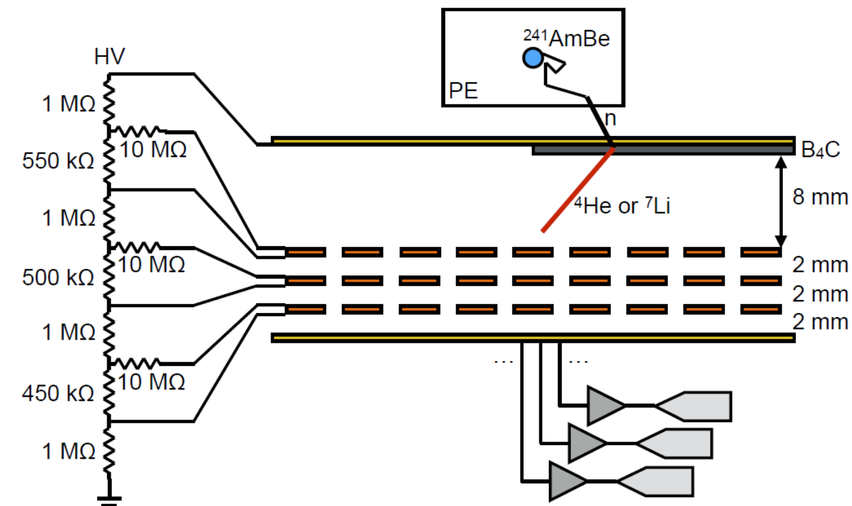
Three detectors of 600 mm x 600mm active surface.
Expected spatial resolution 200µm using µTPC





Triple GEM with Gd2O3 coated cathode 100mmx100mm prototype

Courtesy of: Dorothea Pfeiffer



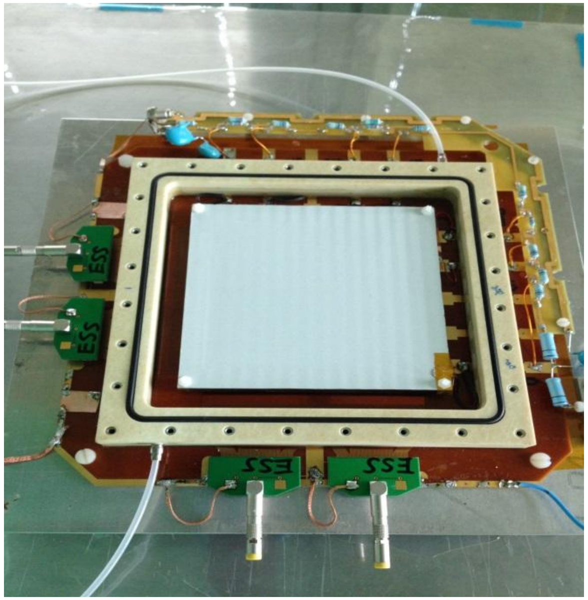
The µTPC method: improving the position resolution of neutron detectors based on MPGDs
D.Pfeiffer et al. 2015 JINST 10 P04004 doi:10.1088/1748-0221/10/04/P04004

Detectors

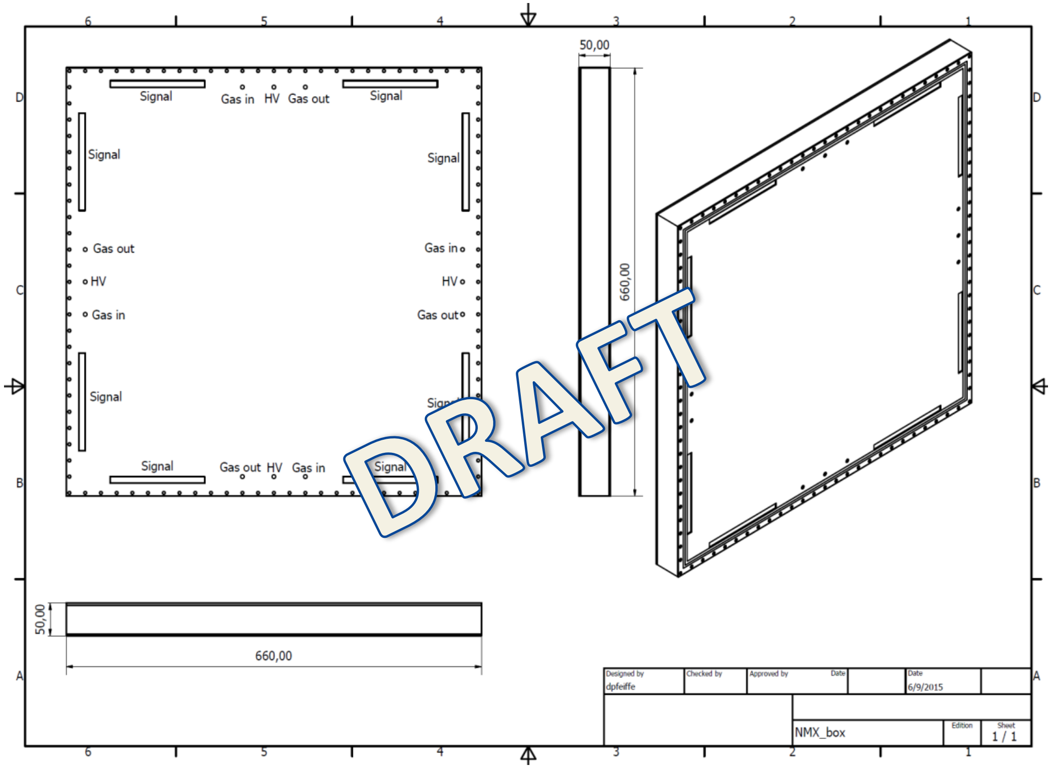
EUROPEAN SPALLATION SOURCE

- Dorothea Pfeiffer (ESS/CERN), Richard Hall Wilton(ESS)

Three detectors of 600 mm x 600mm active surface.
Expected spatial resolution 200µm using µTPC

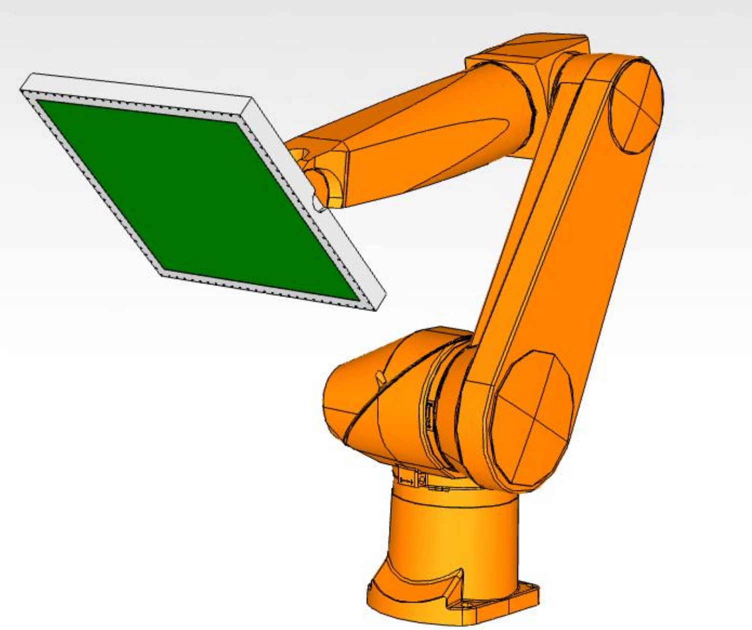


Triple GEM with Gd2O3 coated cathode



Courtesy of: Dorothea Pfeiffer

Detectors



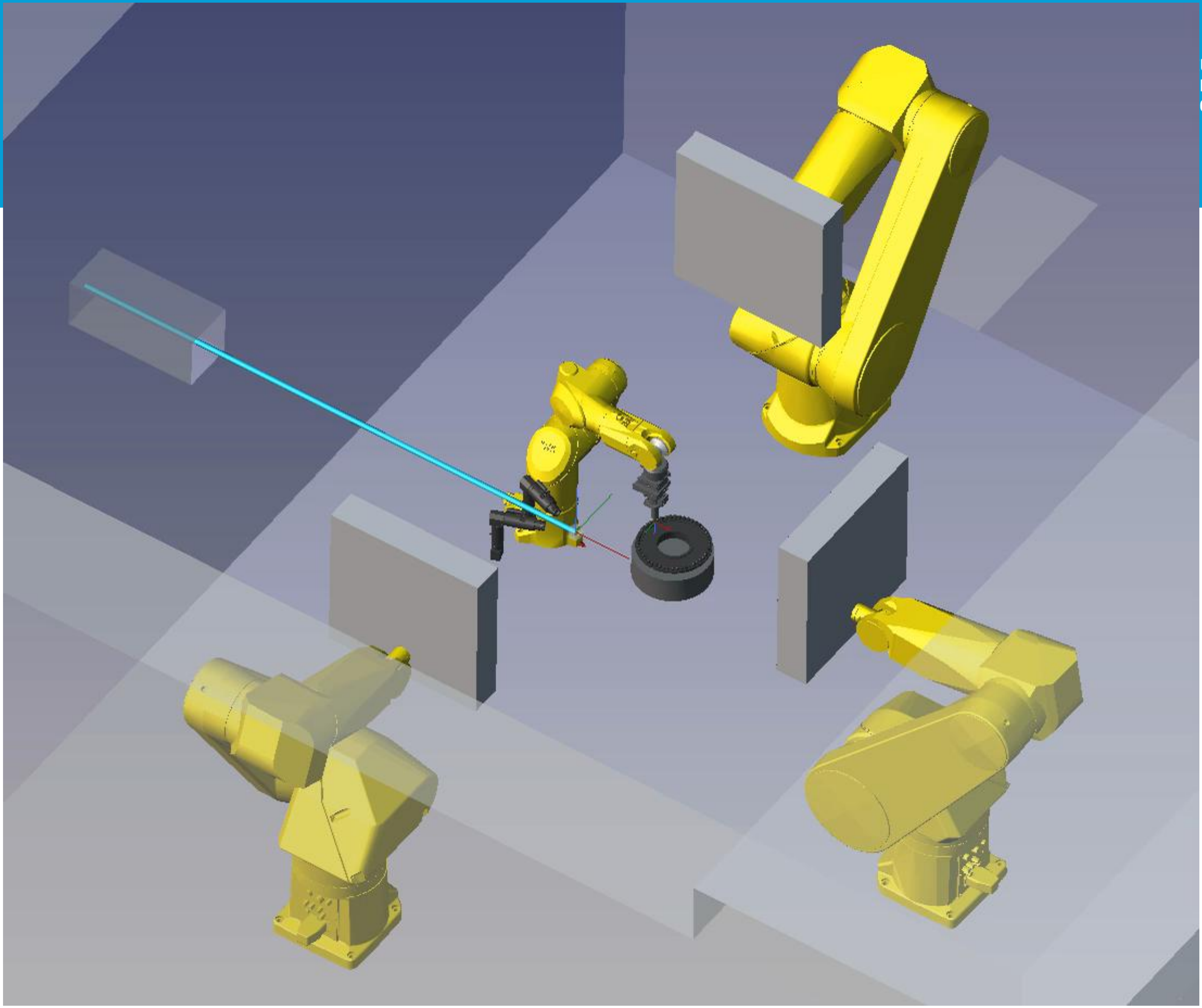
Example of detector positioner based on Stäubli robot

Performance	Min	Max
Sample detector distance	0.2 m	1m
Hor. Plane 2θ angle	-165°	165°
Vert. Plane	Upper hemisphere	

- Collection only on upper hemisphere.
- Industrial components with high reliability
- Scalable system (more detectors / heavier detectors).
- Technical risks are compensated by large flexibility

Preliminary design to start in September 2015

In



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Thank you for your attention