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LoKI Overview and Progress

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Outline

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- Brief Science Case
- Instrument Goals
- Top Level Requirements
- Instrument Components
    - Line of sight and Benders
    - Wavelength selection and frame overlap
    - Sample position
    - Detectors
- Performance
- Software
- Sleipnir Options
- Tollgate 2

Fluid Flow

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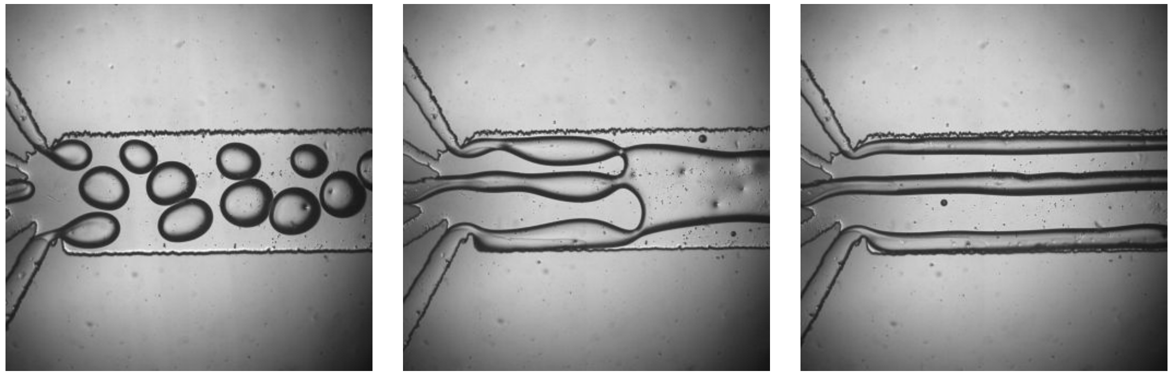
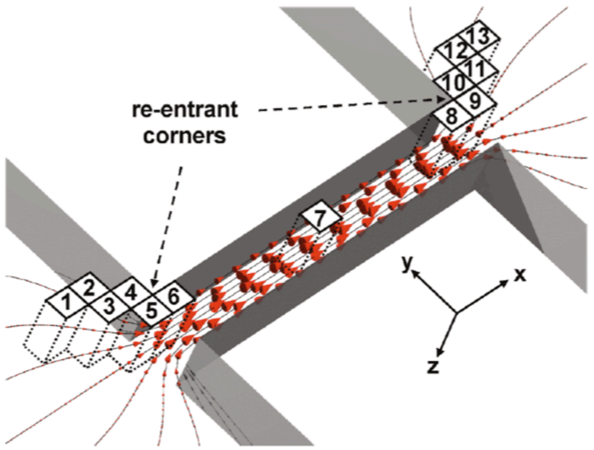
The flow of **complex fluids** through **complex geometries** is relevant to many industrial processes including polymer processing and oil recovery.

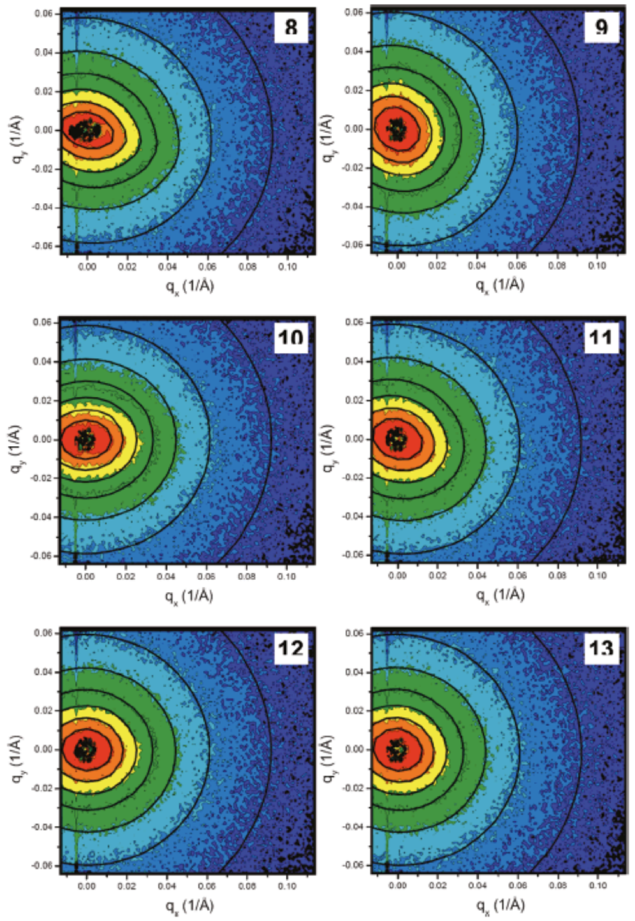
Microfluidic devices are increasingly used for chemical and pharmaceutical discovery, production and processing.

There is a need to understand **structural effects of flow** both for practical puroposes and to compare with fluid flow models.

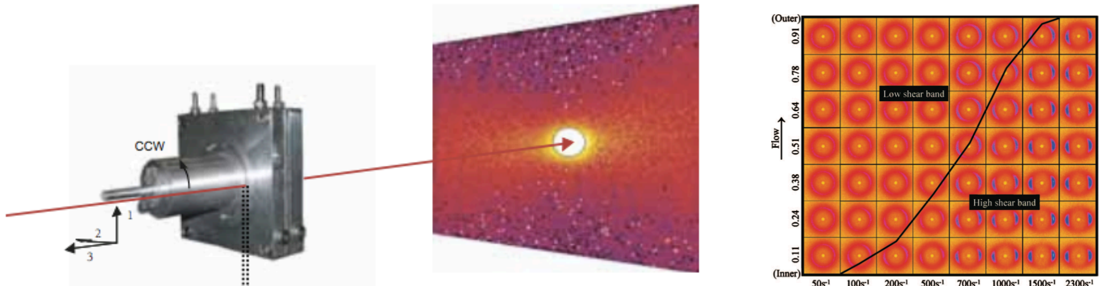


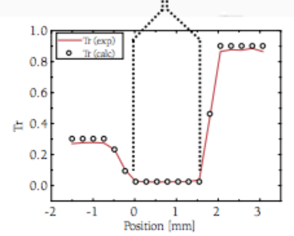
Fluid thread breakup under microfluidic confinement (Cabral group, Imperial College)





Measuring the deformation of polymer chains allowing development of new models of polymer flow (Clarke et al. (2010) Macromolecules 43, 1539)





Shear Banding in CTAB wormlike micelles providing confirmation of rheological model. (Helgeson et al. (2009) J. Rheol 53, 727)

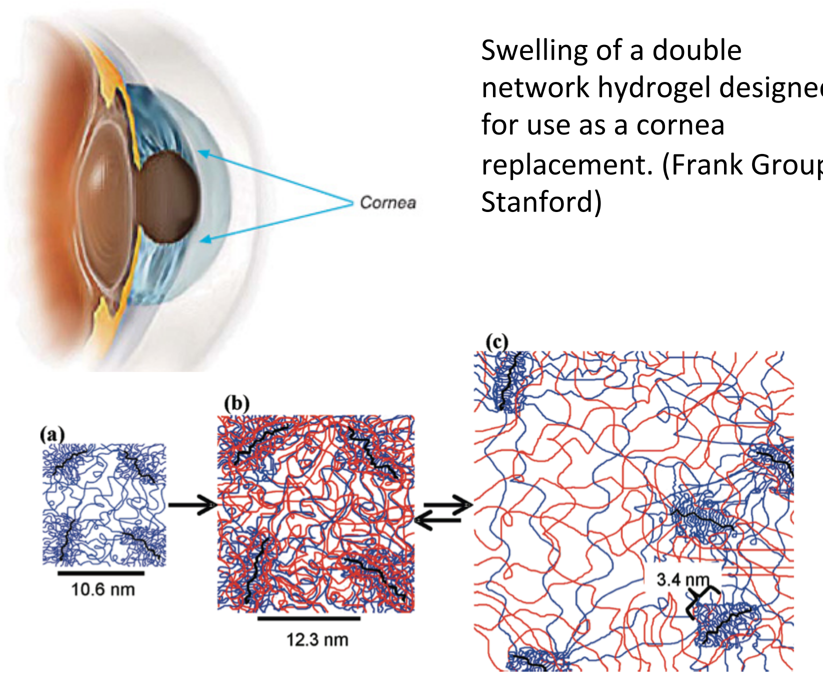
Multiple Length Scales & Kinetics

Double network hydrogels provide strength and resiliance together with high water content.

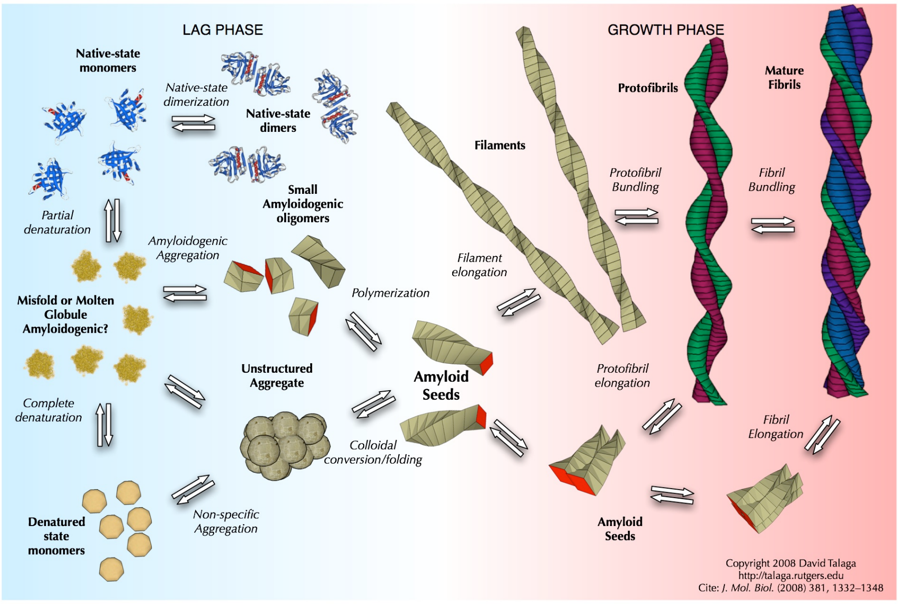
Gel structure forms over **multiple length scales.**

Kinetics of gelation can be rapid needing **sub-second** time resolution.

Neutrons provide the structure of each component in the presence of the other.



Swelling of a double network hydrogel designed for use as a cornea replacement. (Frank Group, Stanford)



Amyloid fibrils have been associated with more than 20 human diseases including Alzheimer's and Parkinson's diseases and rheumatoid arthritis.

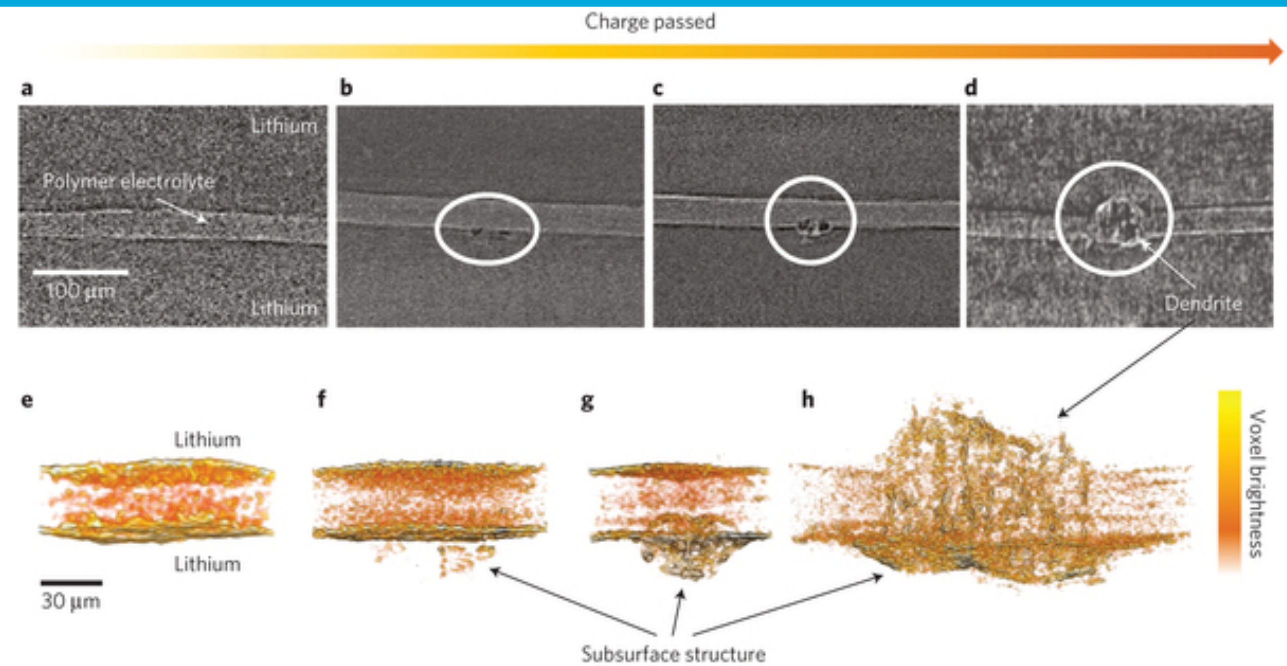
Fibril formation and growth is a multi-length scale problem and to understand methods of formation and inhibition the structural evolution must be observed.

In-Operando Behaviour

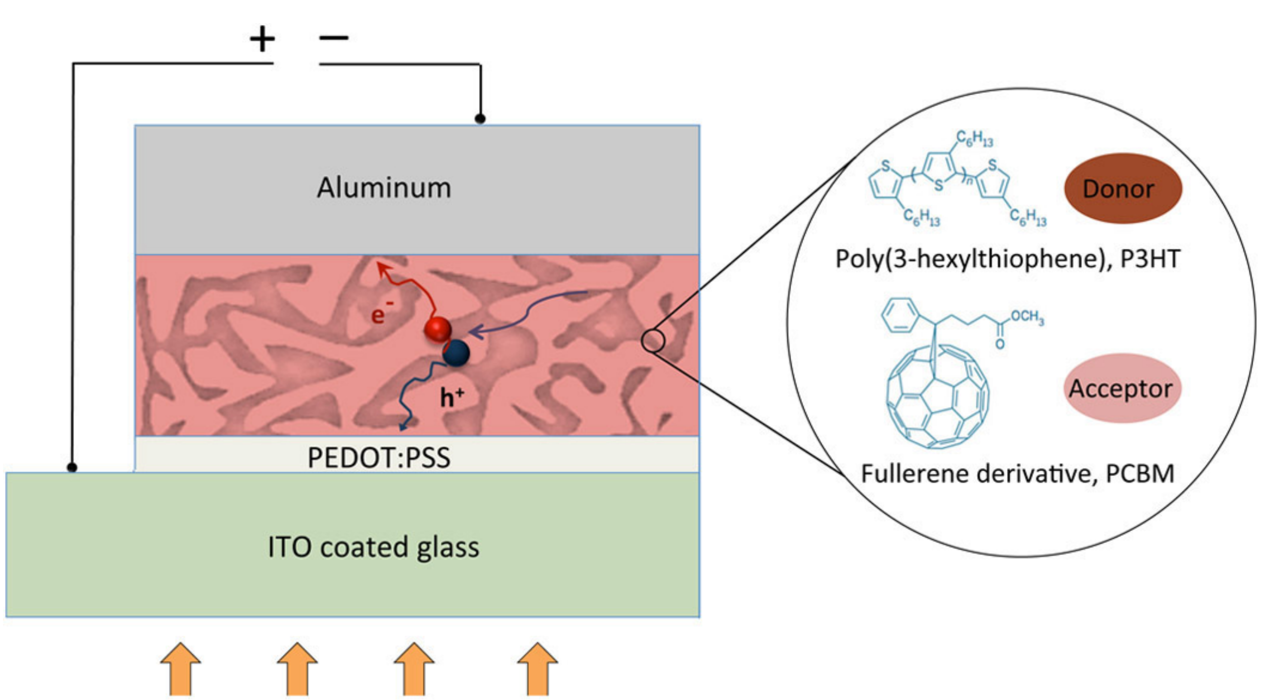
Lithium Ion Batteries are a crucial technology for the expansion of electric vehicle use and for mobile computing.

Higher energy densities could be achieved with **alternative anode materials** and **new electrolytes**.

Analysis of **operating devices** allows the monitoring of **nano- and micro-structural change.**



Dendrite growth in lithium metal anode batteries observed by x-ray microtomography. (Harry et al. (2013) Nature Materials 13, 69)



Organic Solar Cells promise to provide cheap and accessible solar energy.

The **lifespan** and **efficiency** of the devices depends on the **nano-structure** of the bulk heterojunction polymer mixture.

Understanding the **structural evolution** under operation guides development of new devices.

Goals

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

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

Goals

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

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

Requirements

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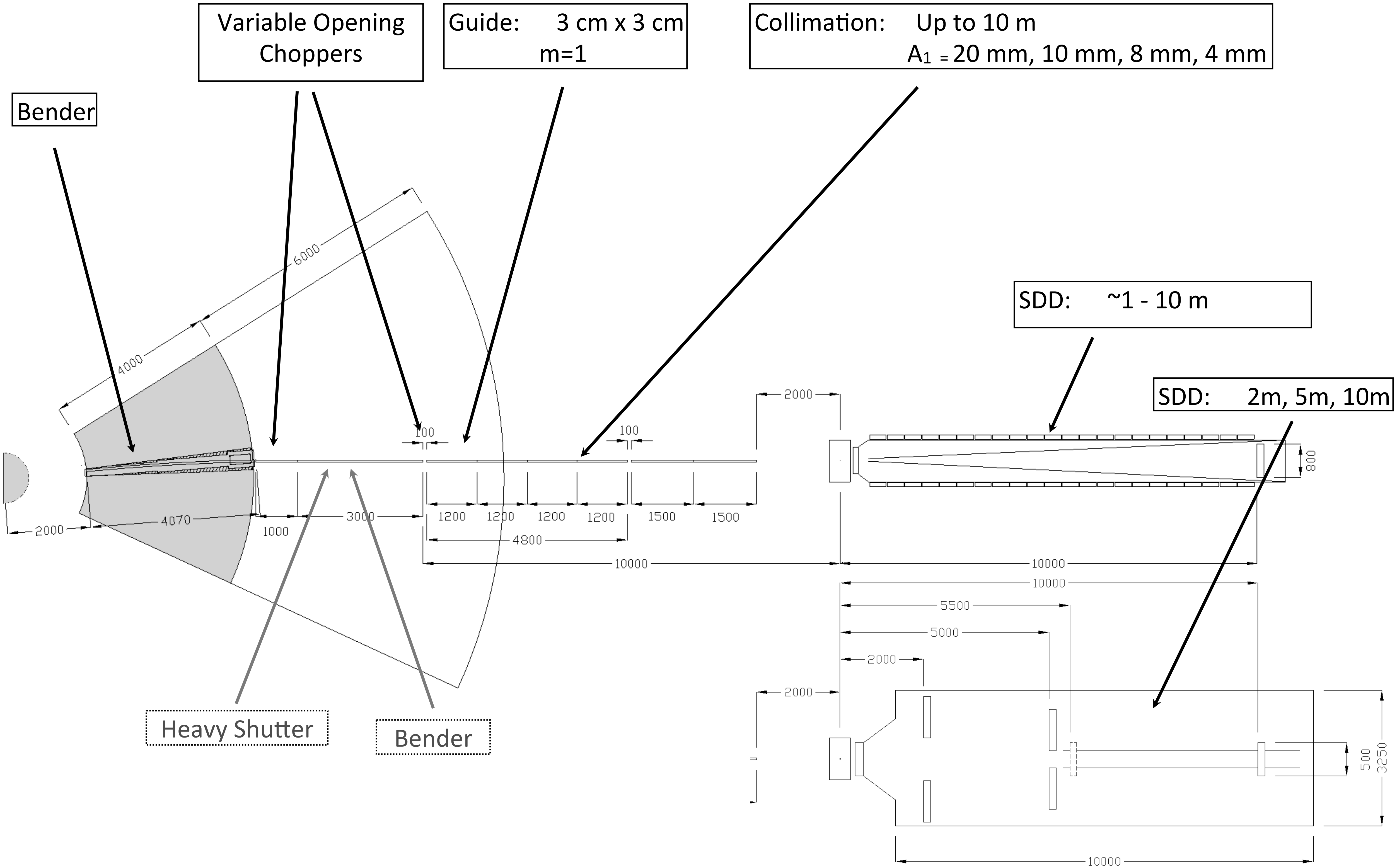
A broad Q range, high flux SANS instrument for materials science and soft matter

High-level Scientific Requirements for the Instrument

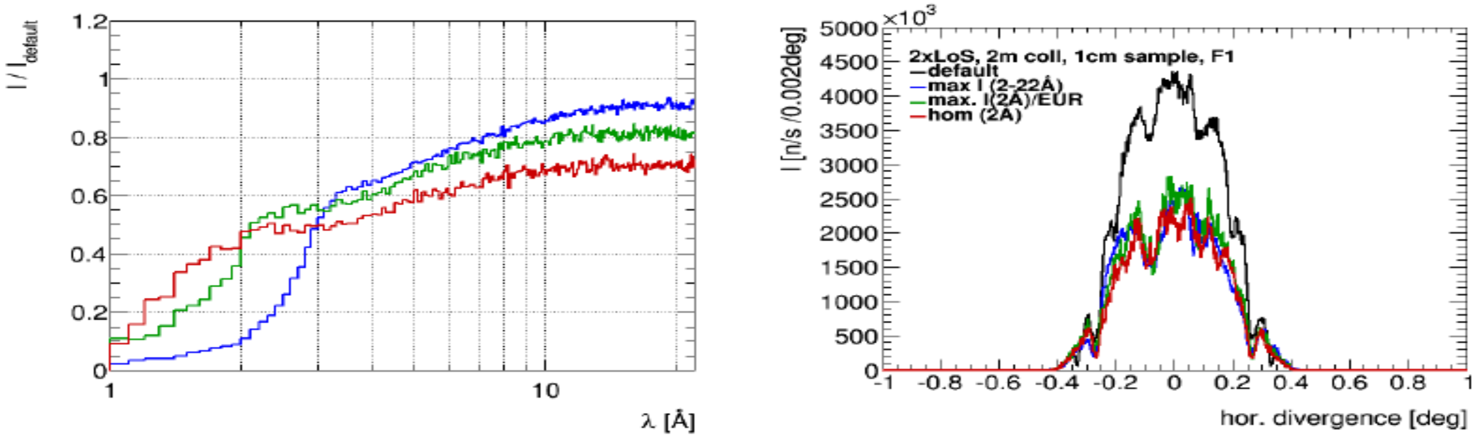
- The instrument shall allow data to be collected to a Q_{min} of < 0.001 $Å^{-1}$.
- The instrument shall allow data to be collected to a Q_{max} of > 1 $Å^{-1}$.
- The instrument shall allow data to be collected simultaneously over a continuous Q range with Q_{max}/Q_{min} > 1000.
- The instrument 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 < 9 mm^3 volume
- The instrument should maximise the signal-to-background (S/B) ratio of the small angle scattering.

Overview

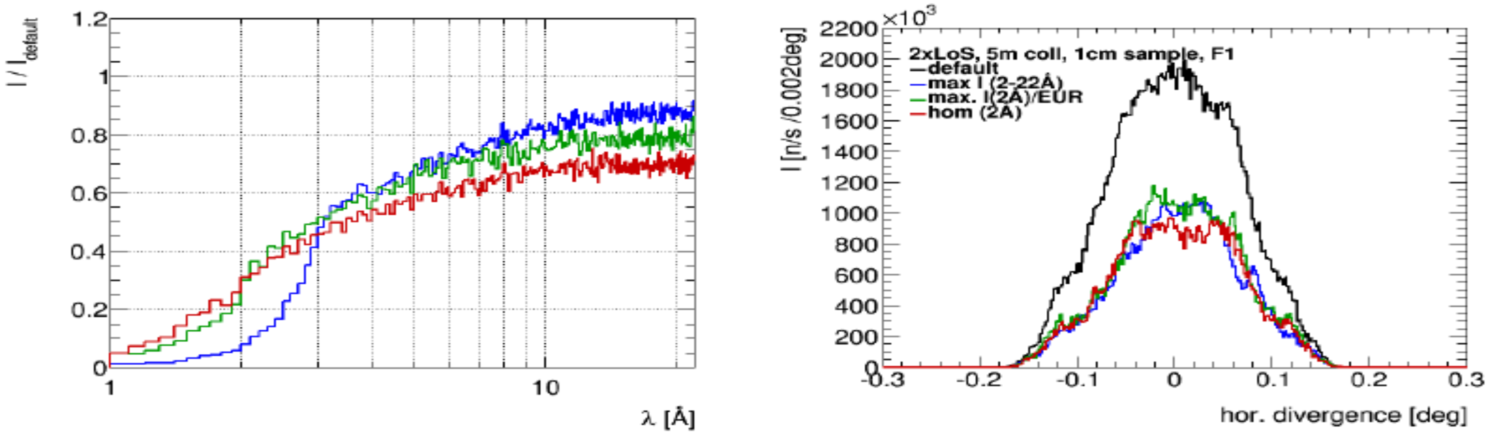

Variable Opening Choppers
Guide: 3 cm x 3 cm
m=1
Collimation: Up to 10 m
A1 = 20 mm, 10 mm, 8 mm, 4 mm
Bender
SDD: ~1 - 10 m
SDD: 2m, 5m, 10m
Heavy Shutter
Bender
6000
4000
2000
4070
1000
3000
100
1200
1200
1200
1200
1500
1500
4800
10000
2000
800
10000
10000
5500
5000
2000
2000
500
3250
10000

Line-of-sight and Bender

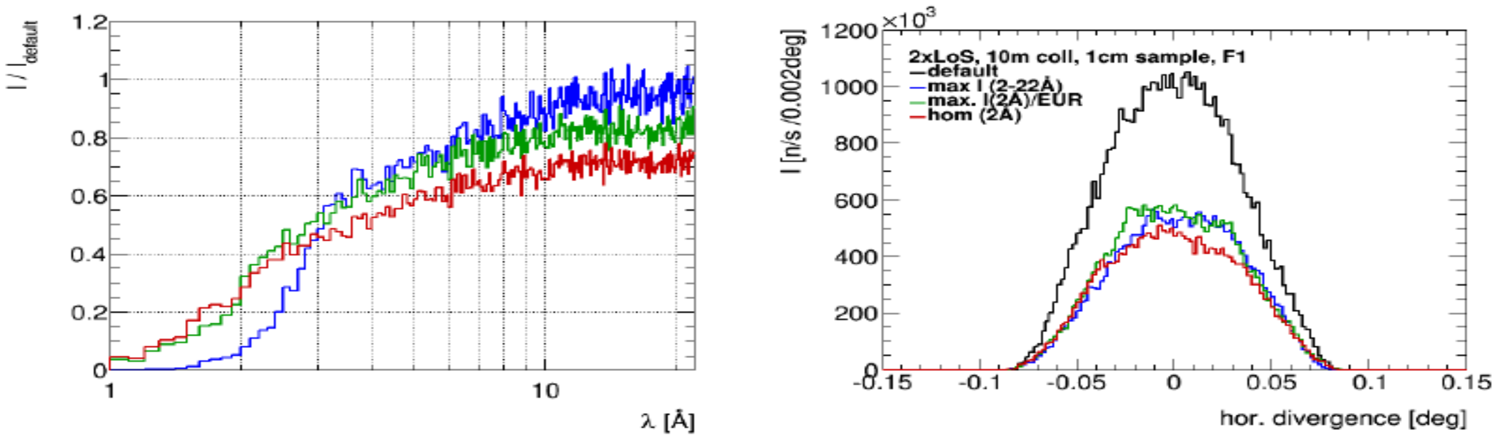
LoKI Bender optimization summary



(a) 2 m collimation length



(b) 5 m collimation length

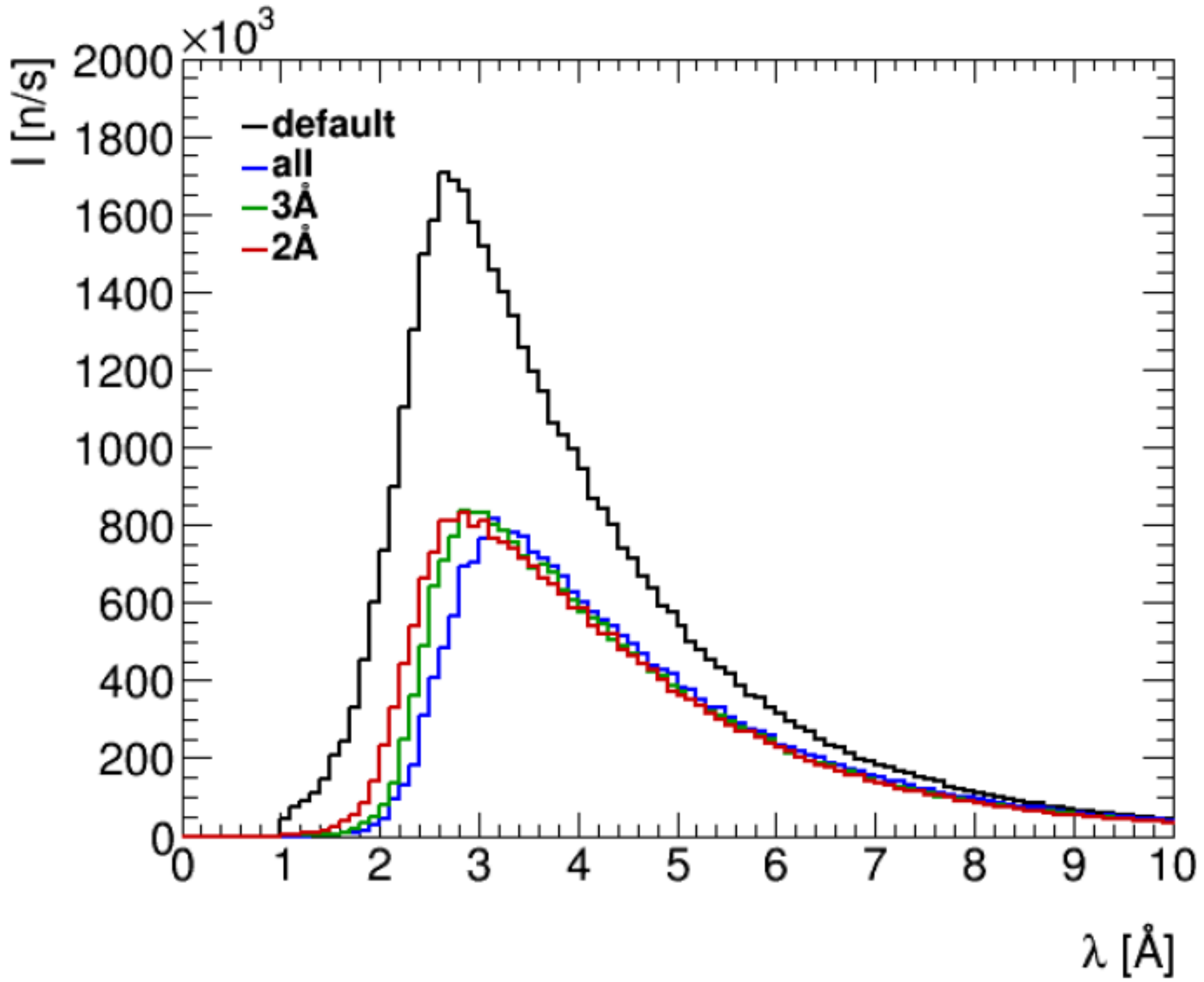


(c) 10 m collimation length

- Simulations of instrument performance with various bender options for 2x line-of-sight curvature, including cost.
- Result : 2x line-of-sight leads to approx. 50% reduction in flux
- Now need shielding simulations to see whether 2x line-of-sight is required – cost/performance ratio.
- 2x LOS has repercussions on space requirements

option	optimized wavelength	Bender 1 m	Bender 1 N	Bender 1 k€	Bender 2 m	Bender 2 N	Bender 2 k€	Bender 2	sum k€
1	2-22 Å	6	1	59	3	5	75	same curv.	134
2	3 Å	6	1	59	3	9	126	s-bender	185
3	2 Å	6	2	99	3	10	139	s-bender	238
default		4	4	162	-	-	-		162

Line-of-sight and Bender



10m collimation

	I [n/s]	F [n/scm²]
2 m collimation		
default	$8.6 \cdot 10^8$	$1.1 \cdot 10^9$
option 1	$5.6 \cdot 10^8$	$7.2 \cdot 10^8$
option 2	$5.4 \cdot 10^8$	$6.8 \cdot 10^8$
option 3	$5.5 \cdot 10^8$	$7.0 \cdot 10^8$
5 m collimation		
default	$1.7 \cdot 10^8$	$2.1 \cdot 10^8$
option 1	$8.8 \cdot 10^7$	$1.1 \cdot 10^8$
option 2	$9.3 \cdot 10^7$	$1.2 \cdot 10^8$
option 3	$9.7 \cdot 10^7$	$1.2 \cdot 10^8$
10 m collimation		
default	$4.7 \cdot 10^7$	$5.9 \cdot 10^7$
option 1	$2.5 \cdot 10^7$	$3.1 \cdot 10^7$
option 2	$2.5 \cdot 10^7$	$3.2 \cdot 10^7$
option 3	$2.6 \cdot 10^7$	$3.3 \cdot 10^7$

Wavelength Selection

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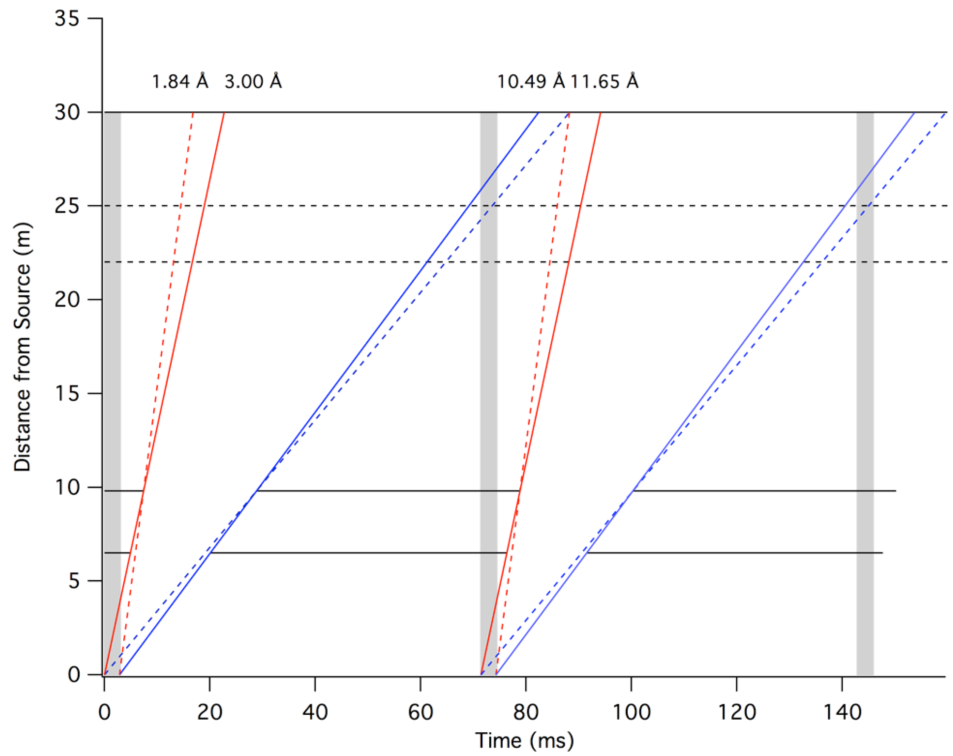
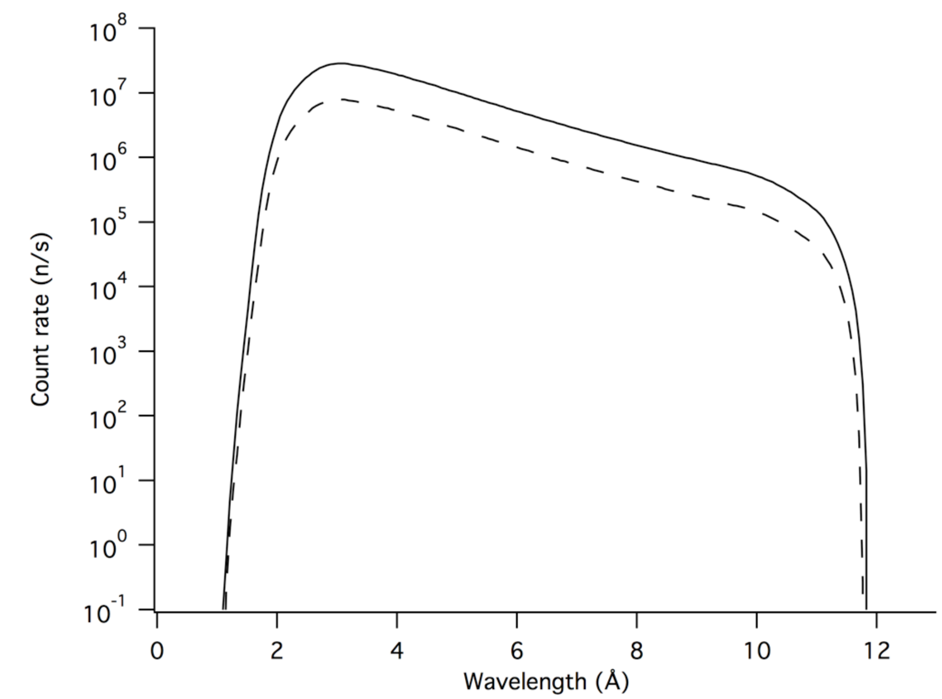
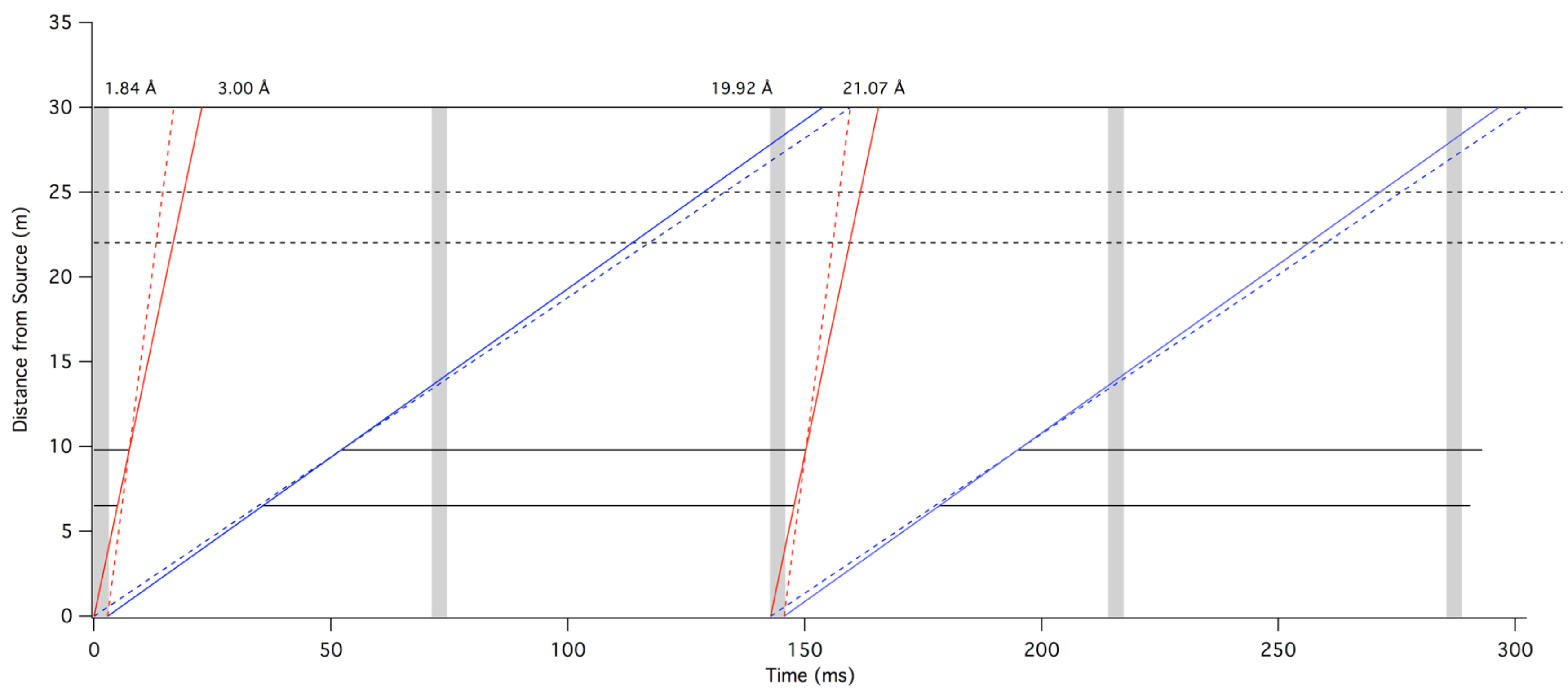
Variable opening double disc choppers at 6.5 m and 9.5 m



14 Hz

3 - 10.5 Å



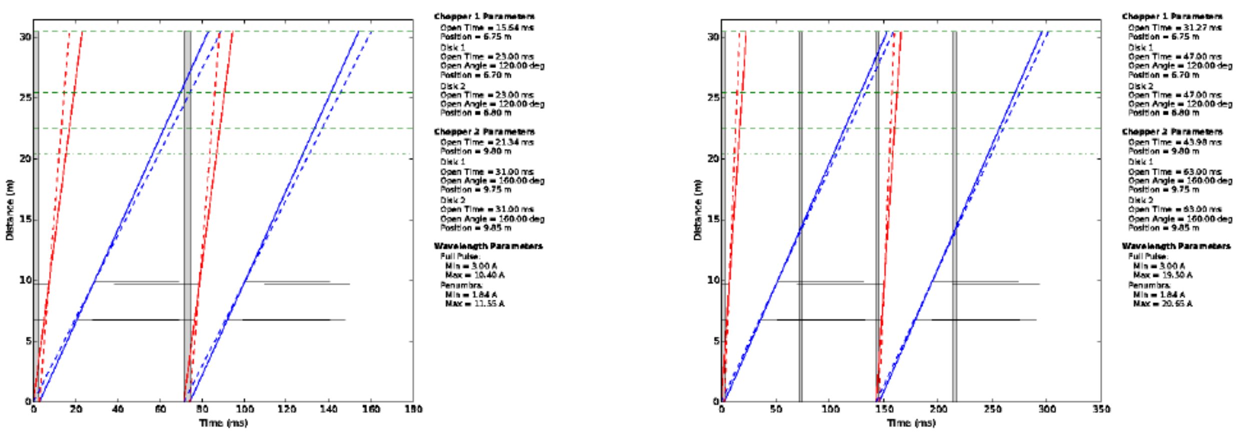


7 Hz

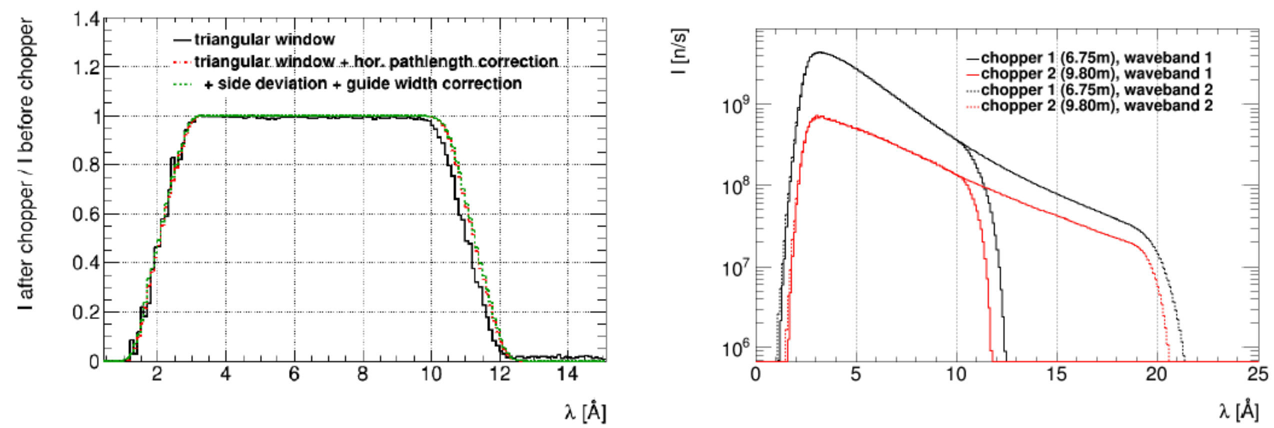
3 - 20 Å

Frame Overlap Contamination

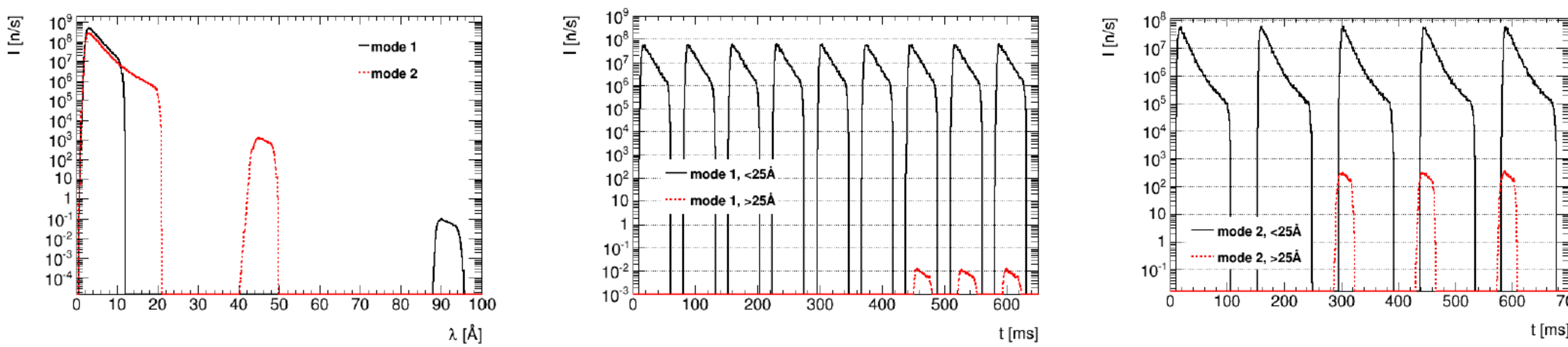
LoKI Chopper simulations report



(a) wavelength band 1 (b) wavelength band 2



(a) chopper 1, waveband 1 (b) Spectrum after choppers 1, 2 in modes 1 (3-10.4 Å) and 2 (3-19.5 Å)



(a) wavelength spectrum (b) time-of-flight, mode 1 (c) time-of-flight, mode 2

- Simulations to assess issue of long-wavelength frame overlap
- Worst case is 10^{-5} contamination at 7Hz

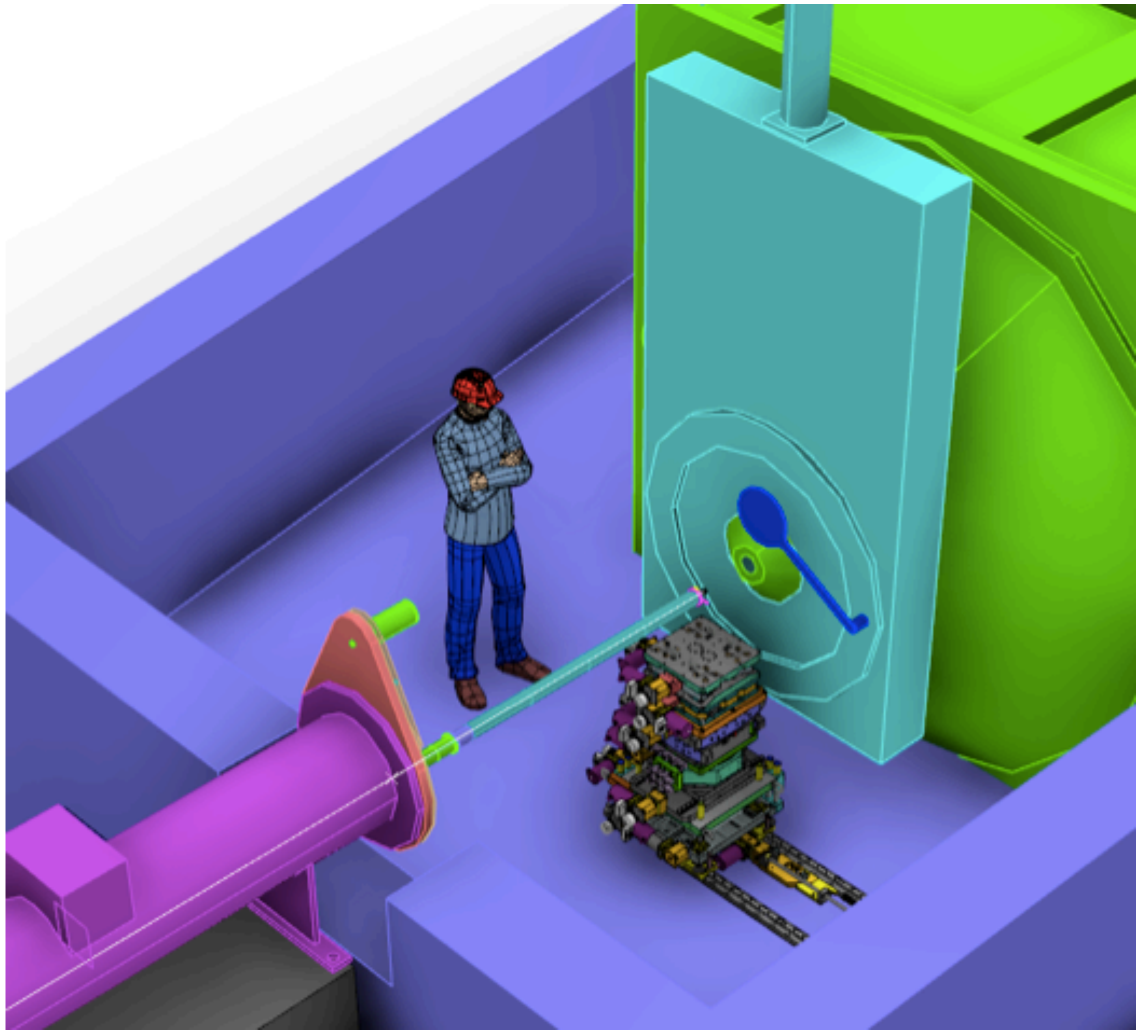
Sample Position

A **flexible** space with **2.5 m** along the beam and **3 m** perpendicular to the beam

A system of sample environment pallets that can be quickly interchanged allowing offline setup of equipment

Space for magnets, rheometers and shear cells, pressure cells, sample changers, auto-sampling robots, flow-through cells ... whatever the user can think of!

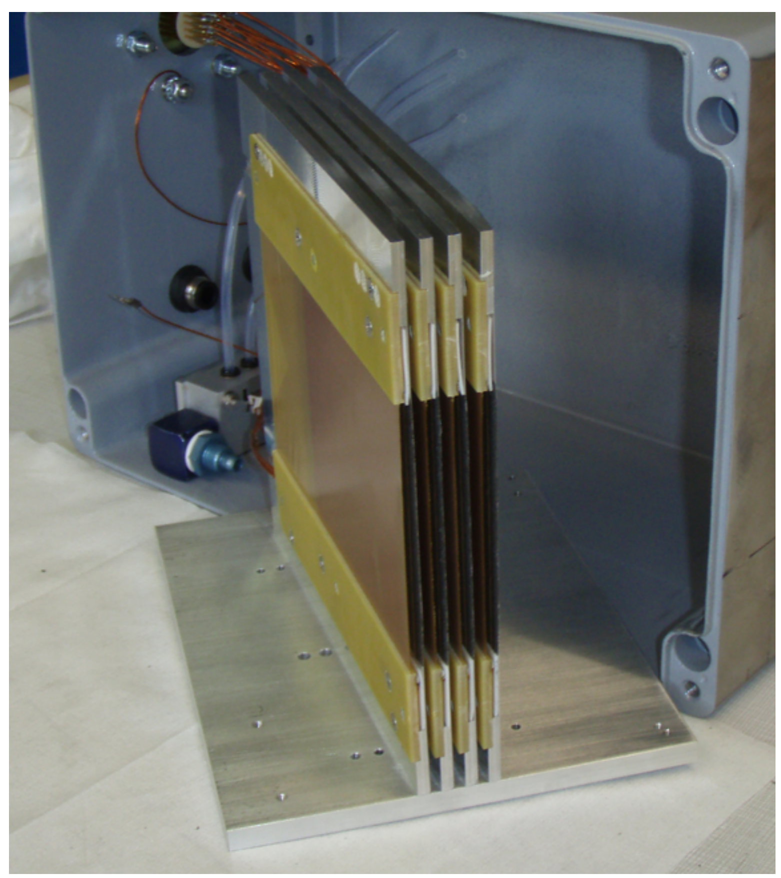
Space for complementary measurement techniques

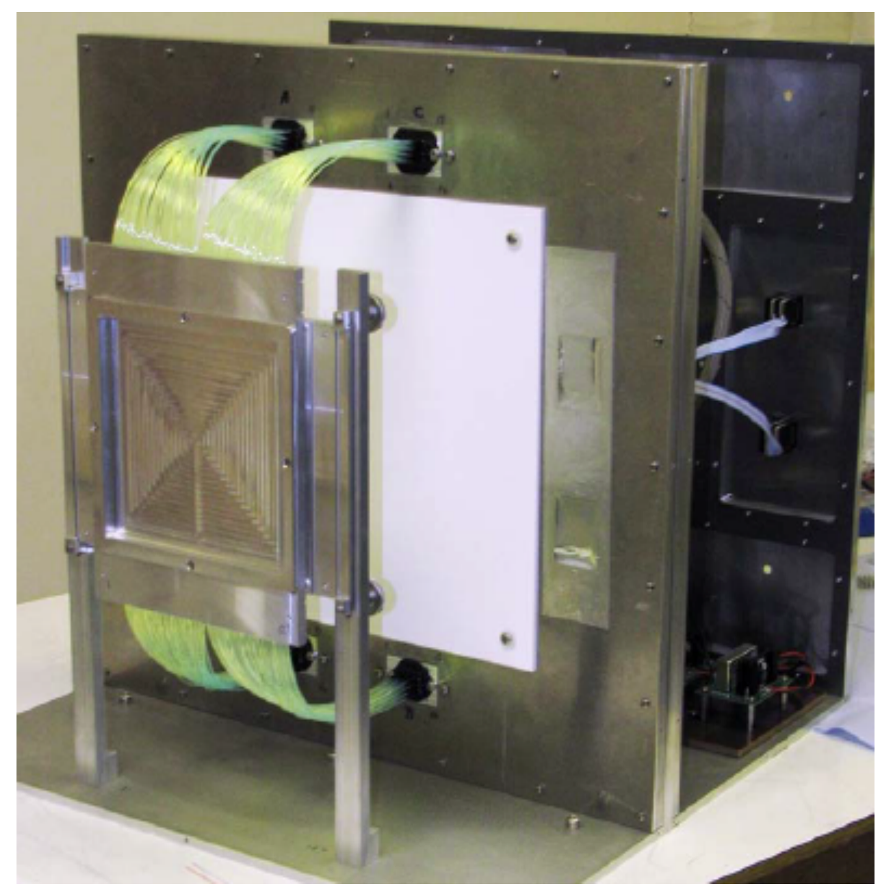


Detectors

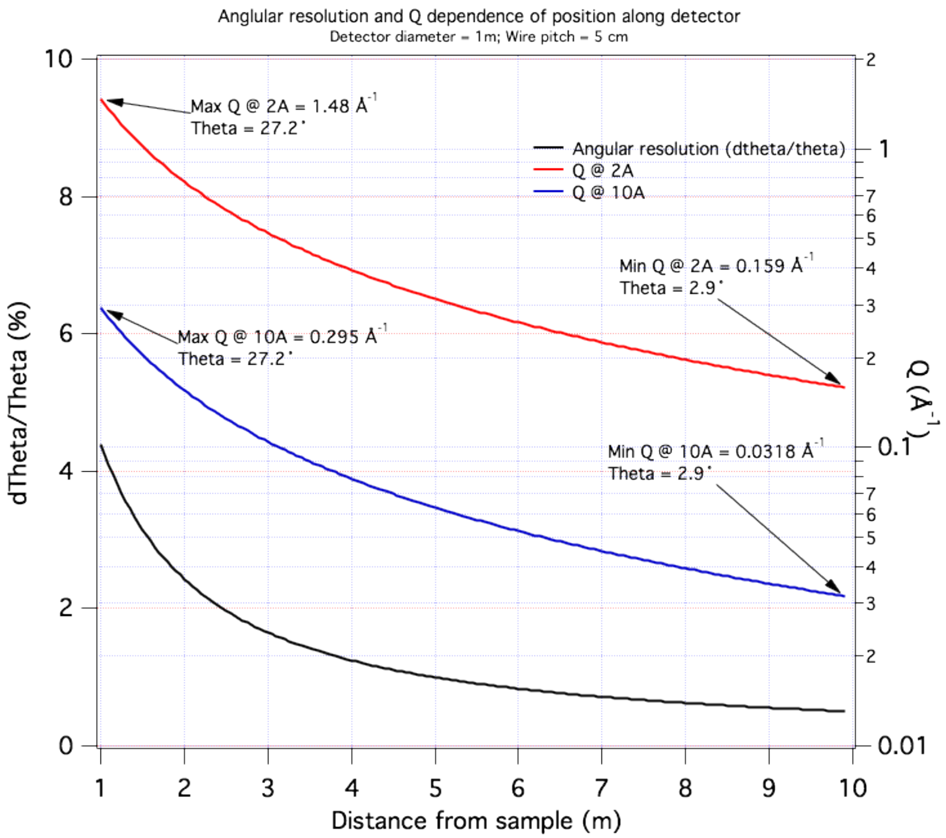
Evaluation of the different technologies for detectors

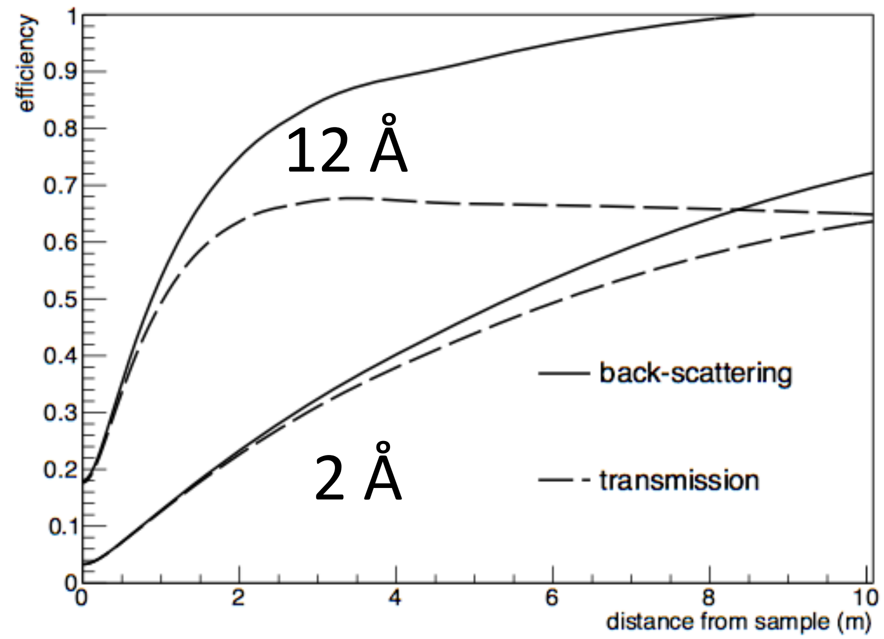
- Inclined Geometry ^{10}B Detectors
  - Multi-Blade
  - ^{10}B barrel
- Micro-Pattern Gaseous Detectors (MPGD)
- Scintillator detector
- ^{3}He detector
- Semiconductors





“Lined Tube” Detectors

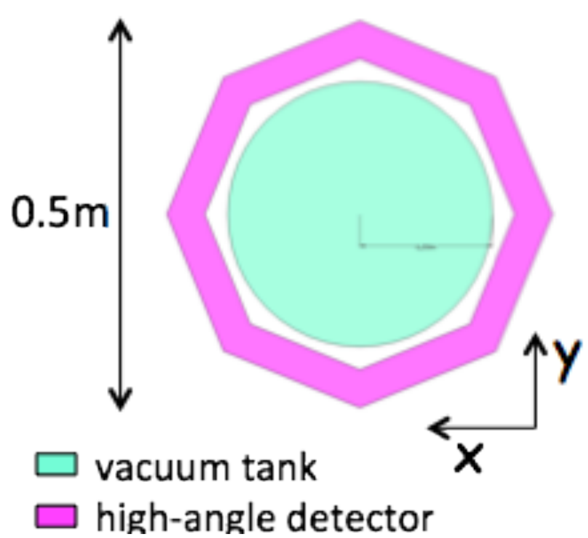


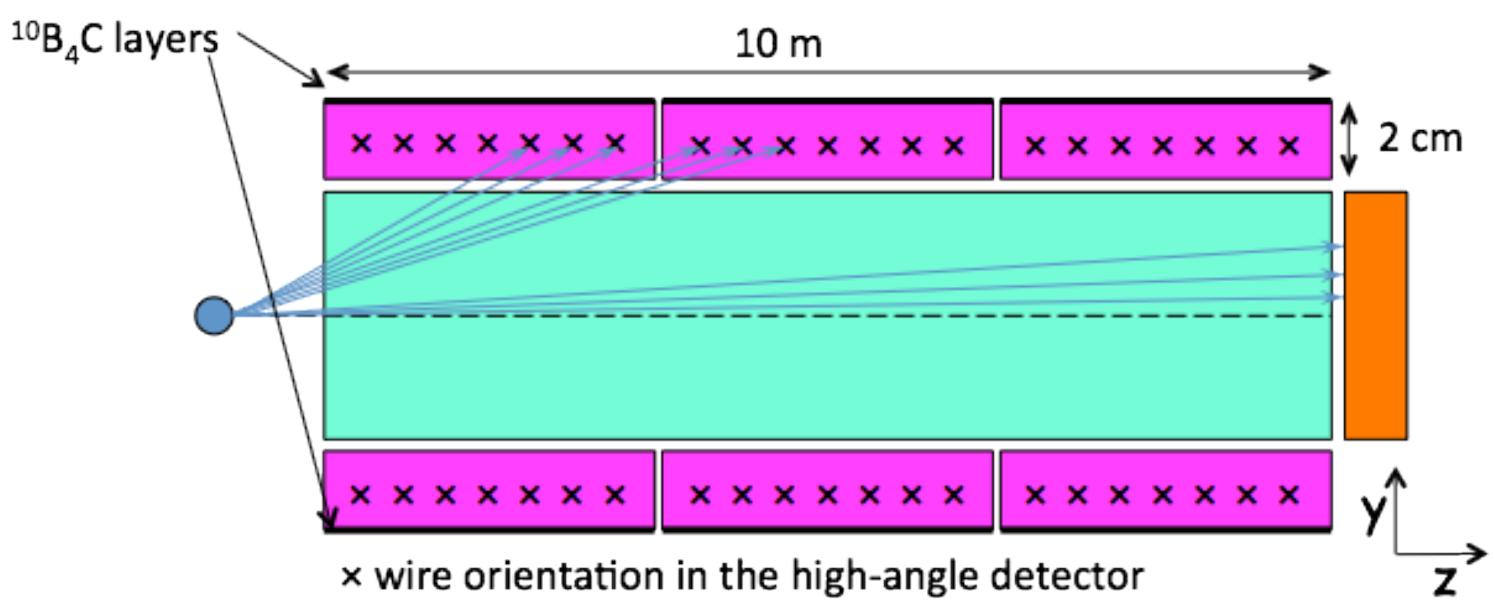


Q range of 1m diameter high angle detector

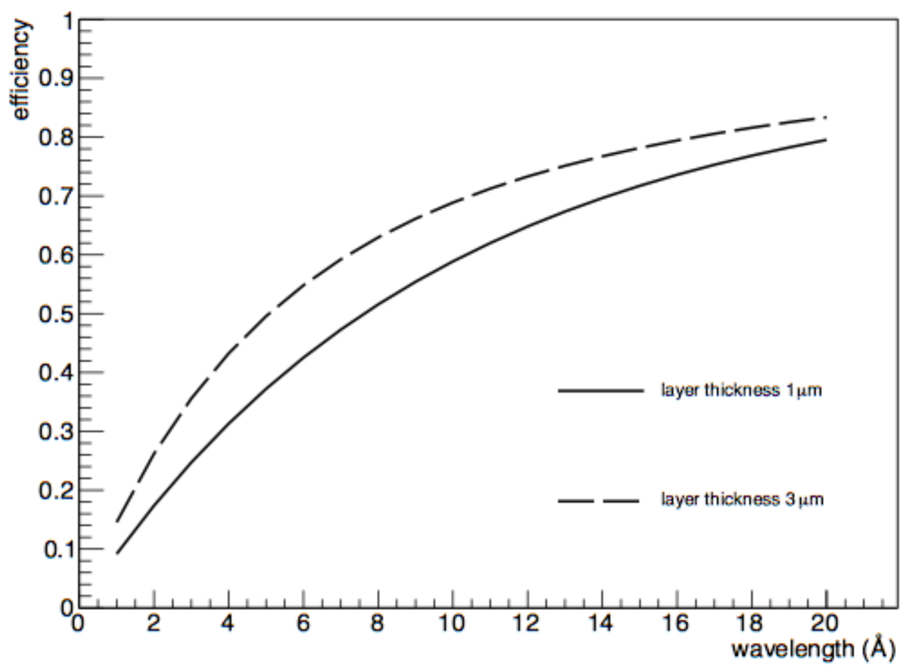
$0.03\ \text{Å}^{-1} < 1.0\ \text{Å}^{-1}$

using 3Å - 10.5 Å neutrons



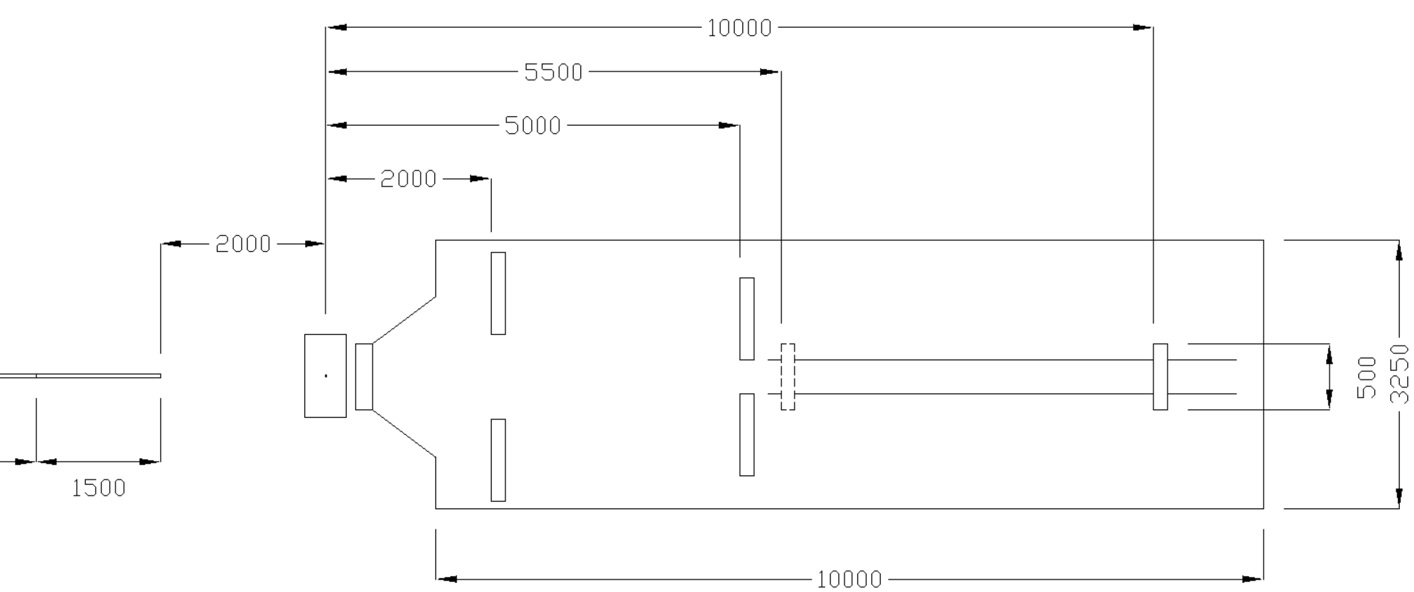


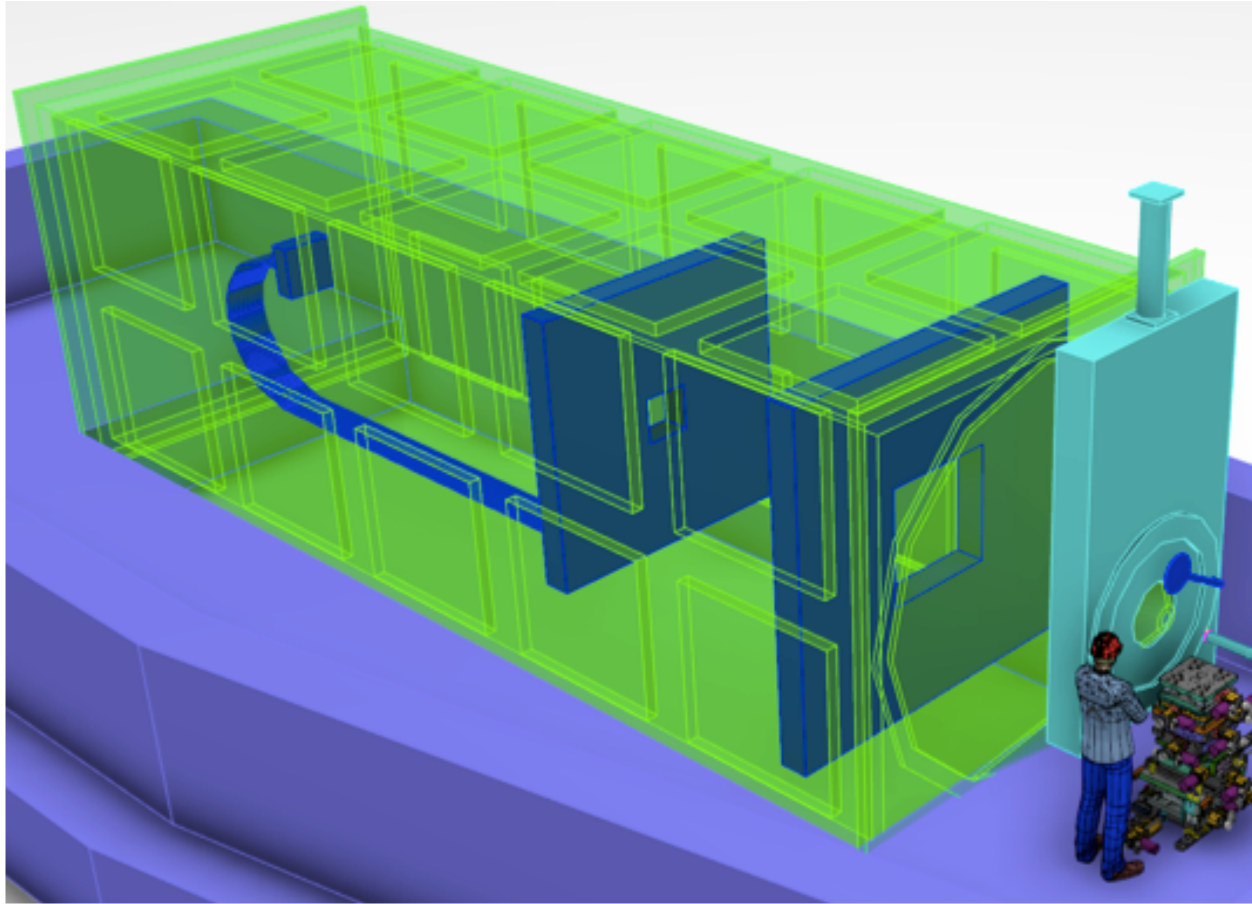
“Window Frame” Detectors



Ap2 Diam (mm)	L1 (m)	L2 (m)	$Q_{min}(\times10^{-3}Å^{-1})$	Q_{max} ($Å^{-1}$)	Q_{max}/Q_{min}
10	2	5	7.63	1.66	218
5	2	5	3.82	1.66	435
4	2	5	1.53	1.66	1085
10	5	5	3.59	1.66	462
5	5	5	1.79	1.66	927
4	5	5	0.72	1.66	2305
10	10	10	1.79	1.66	927
5	10	10	0.90	1.66	1844
4	10	10	0.36	1.66	4611

Accessible Q ranges with 3 Å - 10.5 Å neutrons





Front: 3 m x 3 m with 1 m x 1m hole
Middle: 2.4 m x 2.4 m with 0.5 m x 0.5 m hole
Back: 0.5 m x 0.5 m

Detectors: Current status of technology options

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	spatial resolution	rate capability	cost	maturity
zero-angle				
gaseous detectors	ok	maybe	ok	development
scintillators	ok	maybe	ok	development
semiconductors	ok	ok	maybe	concept
fission chambers	ok	maybe	ok	development
micromegas	ok	ok	ok	concept
low-angle				
Multi-Blade	ok	ok	ok	prototype
MPGD	ok	ok	ok	concept
A1-CLD	ok	maybe	maybe	prototype
scintillators	maybe	maybe	maybe	development
^{3}He	no	no	no	mature
high-angle (WF)				
Multi-Blade	ok	ok	ok	prototype
MPGD	ok	ok	ok	concept
scintillators	ok	ok	no	N/A
^{3}He	ok	ok	no	N/A
high-angle (B)				
MWPC	ok	ok	ok	development
GEM	ok	ok	ok	development
scintillators	ok	ok	no	N/A
^{3}He	ok	ok	no	N/A

Performance

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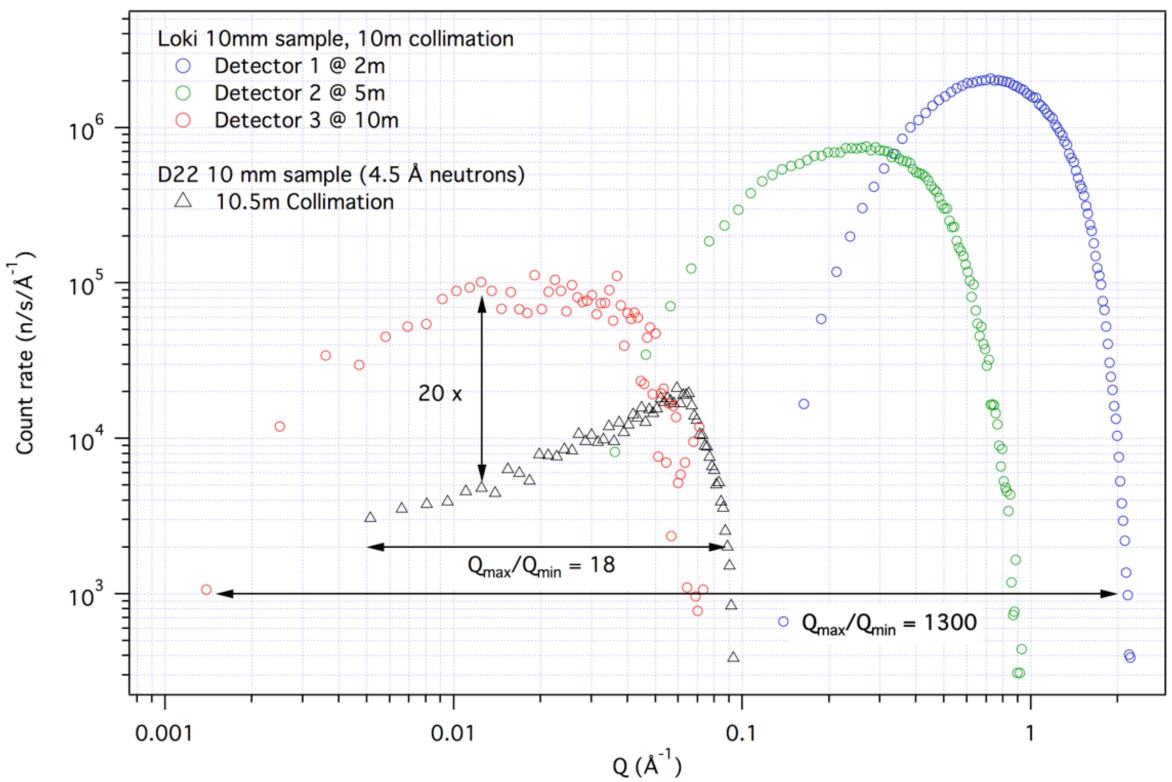
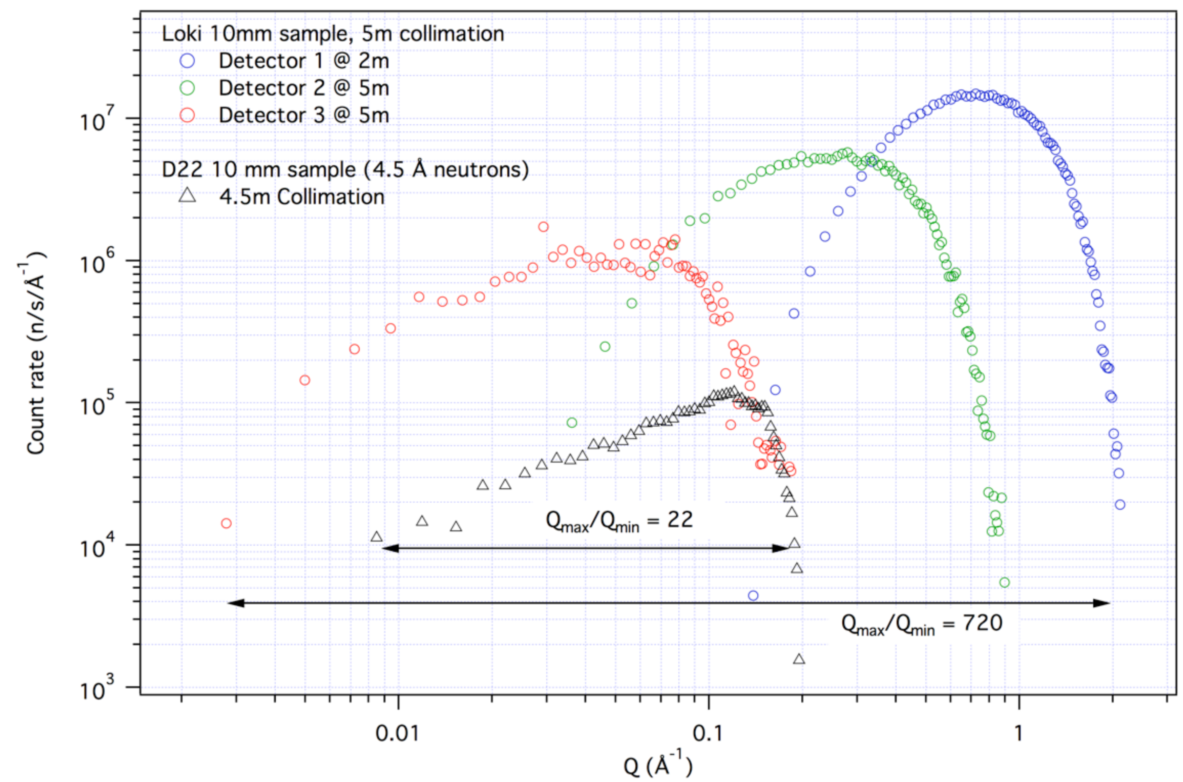
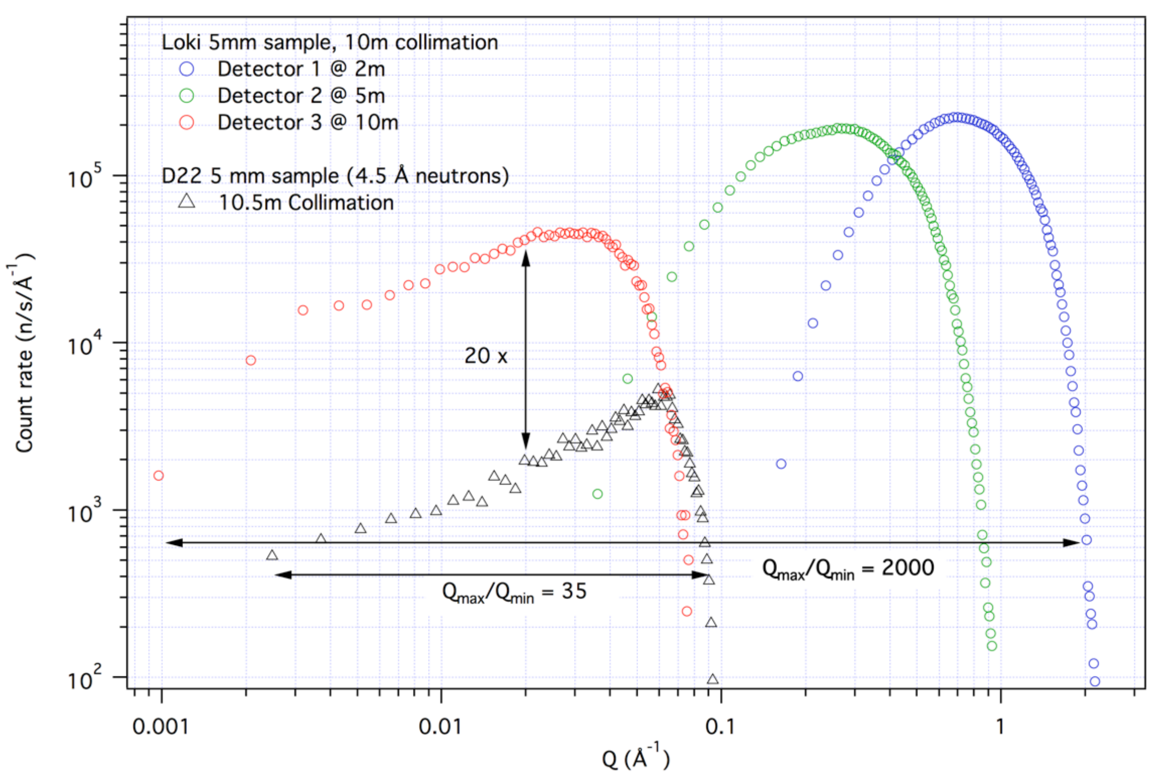
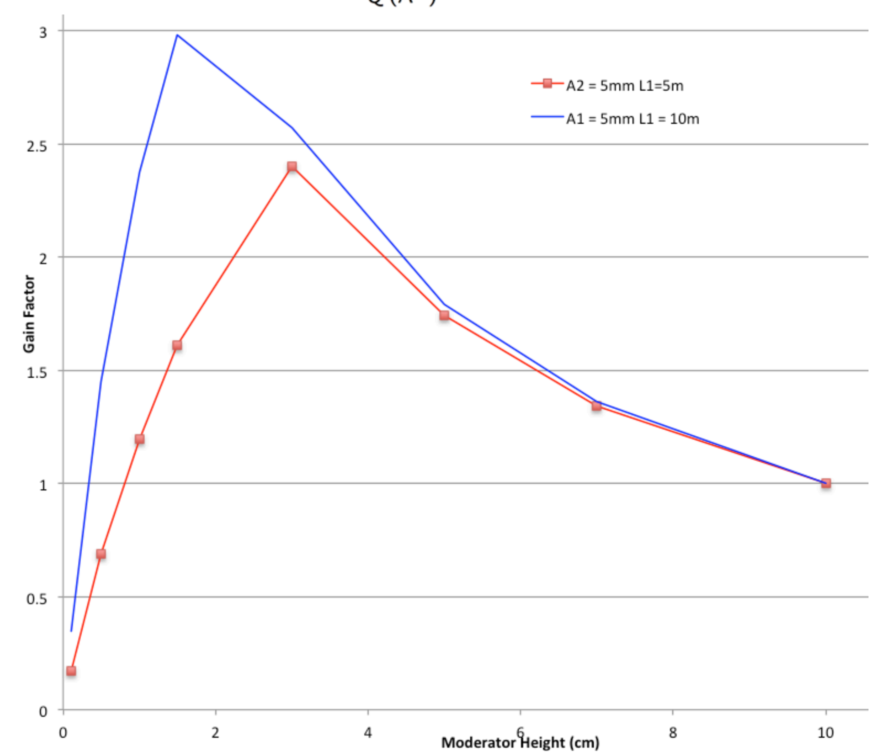
Scattering from 1mm H_2O using “Window Frame” detector layout









Sleipnir Option

SAC Recommendation to incorporate Sleipnir into LoKI

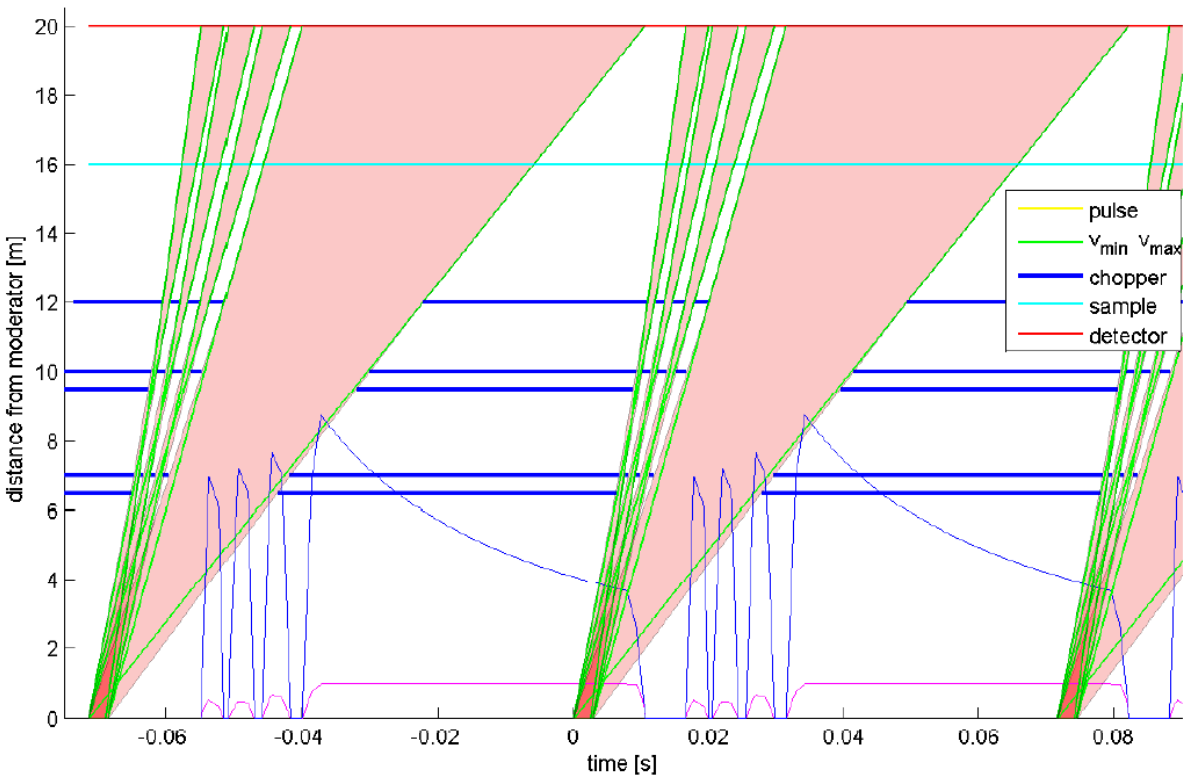
Two Possible Approaches

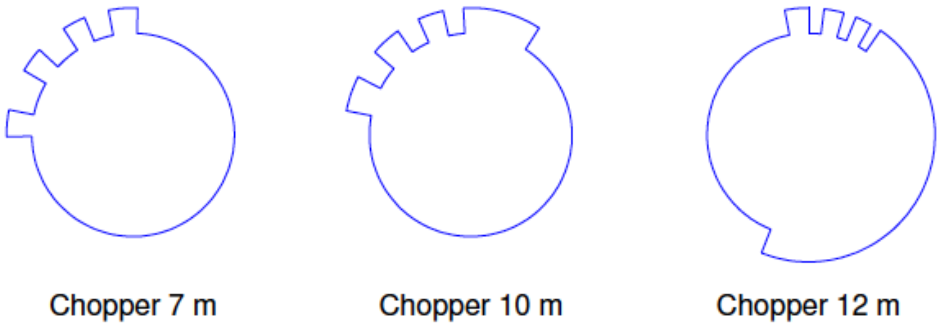
Supporting science case of Sleipnir as far as possible. → Sample Environment & Software

Incorporating specific aspects of the design → ~~Short collimation~~ & Resolution Enhancing Choppers

Resolution Enhancing Choppers

- Choppers at 7m, 10m and 12m.
- 3x, 2x and 1x source frequency
- Provide short pulses for short wavelengths to improve resolution
- Can be thought of as enhanced flux at a given resolution compared with not using short wavelength bins in data processing
- Calculations being done by G Nagy at PSI to adapt to LoKI
- Will be costed as add-on with design accommodating future addition of choppers





42 Hz 28 Hz 14 Hz

Sleipnir Option

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SANS-LOKI v2

L	6.5		9.8		20
#	1	2	3	4	
FUNCTION	PULSE SHAPING	PULSE SHAPING	PULSE SHAPING	PULSE SHAPING	
NOTES	7-14Hz, D700	7-14Hz, D700	7-14Hz, D700	7-14Hz, D700	

Sleipnir Option

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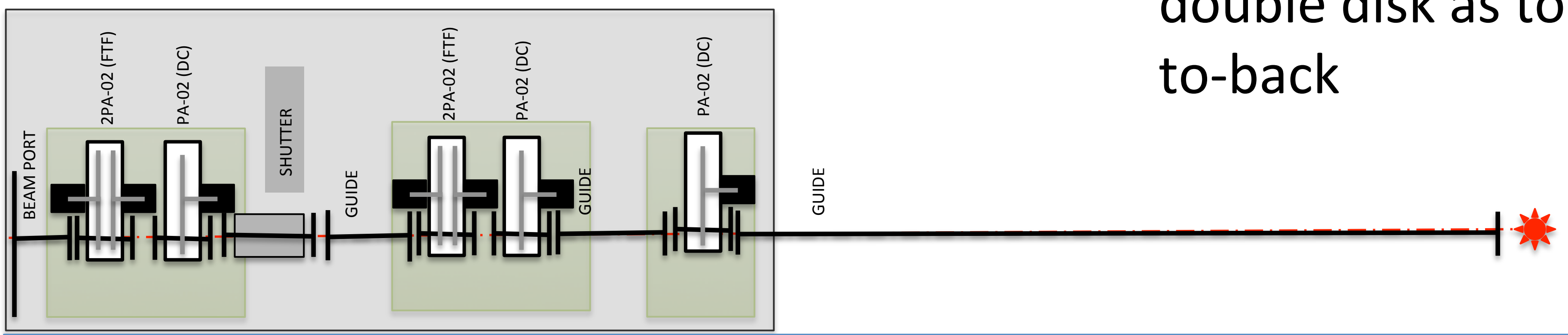
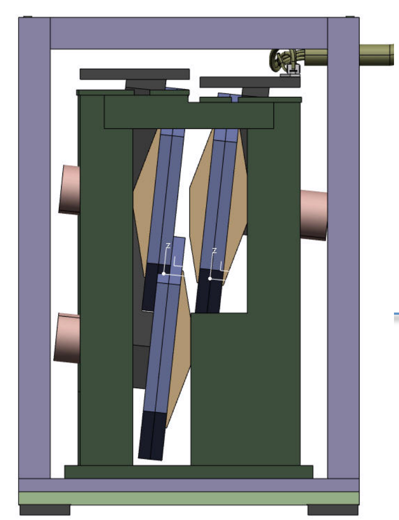
SANS-LOKI v3 (Sleipner merge)

- Instrument 2m longer
- Chopper pits 1 and 2 only slightly larger – put double disk as top/bottom rather than back-to-back



L	6.5	7	9,5	10	12	22
#	1/2	3	4/5	6	7	
FUNCTION	Wavelength selection Wavelength selection	Resolution improvement	Sub-frame overlap Sub-frame overlap	Resolution improvement	Resolution improvement	
NOTES	7-14Hz, D700 7-14Hz, D700	42Hz, D700	7-14Hz, D700 7-14Hz, D700	28Hz, D700	14Hz, D700	



Extra 2m

- Will reduce bandwidth from 7.5Å (9.5Å) to 6.8 Å (9.1Å)
- Can still meet Qmax/Qmin = 1000 requirement assuming necessary detector coverage
- Will clean up beam after second bender with straight section
- Will ease space problems at the sample position

Software

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DMSC work outside of instrument scope ....

... But we provide requirements.

Day One “Hot commissioning” we need:

- Command line / scriptable control of instrument motors and data acquisition
- Timestamped neutron event data being written to disk
- Instrument state data stored with neutron event data
- Visualisation of detector and monitor TOF spectra as a function of detector channel/channels
- Data reduction routines running such that instrument calibration tests and instrument debugging are possible (e.g. running scattering standards)

Day One "friendly users" we also need:

- GUI control of instrument configuration (motors, data acquisition, sample environment)
- Automated data reduction (at least minimal push button, no typing "run numbers", ideally fully automated pipeline)
- Live visualisation of data as it is collected ("raw" and reduced)

Day One "real operations" we also need:

- Automated pipeline for reduction and analysis
- Experimental control feedback from analysis of reduced data (e.g. "count until my errorbars are small enough”)

Tollgate 2

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Documents for TG2 include ...

- Conops
- Requirements
- PBS
- P&ID
- Preliminary System Design Description
- Instrument Work Package Specification
- Draft Commissioning Plan
- Budget
- Schedule
- CAD Model

Scientific Review

- Does the instrument meet its stated performance parameters?
- Has the science case evolved and how does that impact the instrument design?
- Does the instrument meet the needs of its science case?
- Does the layout of the instrument support the operation and use of the instrument?
- Does this instrument meet the users' needs for infrastructure, sample handling, sample manipulation, etc. ?
- ~~Can it be operated safely?~~
- Do the proposed sample environments and user support facilities meet the needs of the users and match the science case for the instrument?
- Does the draft commissioning plan sufficiently evaluate the instrument and prove that the instrument works as proposed?

Project/Engineering Review

- Is the proposal feasible to build?
- Has the team identified all of the appropriate interfaces?
- Has the team followed the ESS engineering and technical standards?
- Can it be operated safely?
- Are the cost and duration estimates reasonable?
- Has the team planned appropriately for the risks, both technical and otherwise?

Second Week of December