



Science and
Technology
Facilities Council

Planned Upgrade of the Primary Spectrometer of OSIRIS

Adrien Perrichon

Molecular Spectroscopy & NMIDG
ISIS Neutron and Muon Source

NDS 2023, ILL, Grenoble, July 11th

OSIRIS for low energy spectroscopy, quasielastic scattering, and long wavelength diffraction

Energy materials: electrode & electrolyte, barocaloric and solar cell materials

Condensed and soft matter physics, catalysis, advanced materials

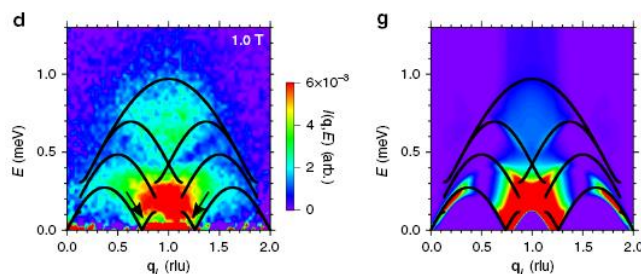


ARTICLE

<https://doi.org/10.1038/s41467-019-08715-y> OPEN

Spinon confinement and a sharp longitudinal mode in $\text{Yb}_2\text{Pt}_2\text{Pb}$ in magnetic fields

W.J. Gannon^{1,8}, I.A. Zaliznyak², L.S. Wu^{3,9}, A.E. Feiguin⁴, A.M. Tsvetlik², F. Demmel⁵, Y. Qiu⁶, J.R.D. Copley⁶, M.S. Kim⁷ & M.C. Aronson^{1,8}



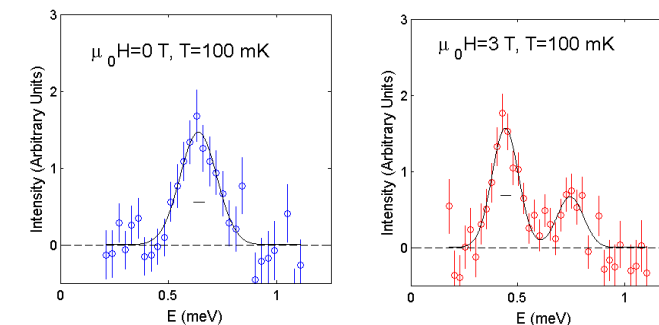
PRL 109, 167207 (2012)

PHYSICAL REVIEW LETTERS

week ending
19 OCTOBER 2012

Magnetic Field Splitting of the Spin Resonance in CeCoIn_5

C. Stock,^{1,2} C. Broholm,^{3,1} Y. Zhao,⁴ F. Demmel,⁵ H.J. Kang,¹ K.C. Rule,⁶ and C. Petrovic⁷



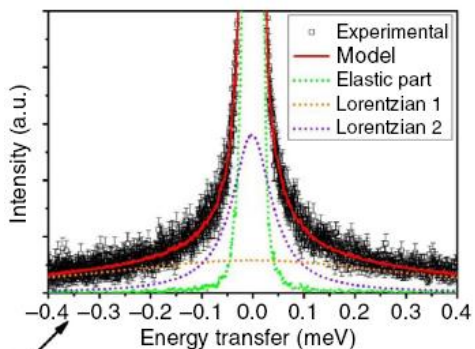
ARTICLE

Received 22 Dec 2014 | Accepted 7 Apr 2015 | Published 29 May 2015

DOI: 10.1038/ncomms8124 OPEN

The dynamics of methylammonium ions in hybrid organic-inorganic perovskite solar cells

Aurelien M. A. Leguy¹, Jarvist Moore Frost², Andrew P. McMahon¹, Victoria Garcia Sakai³, W. Kochelmann³, ChunHung Law⁴, Xiaoe Li⁴, Fabrizia Foglia⁵, Aron Walsh², Brian C. O'Regan⁴, Jenny Nelson¹, João T. Cabral⁵ & Piers R. F. Barnes¹



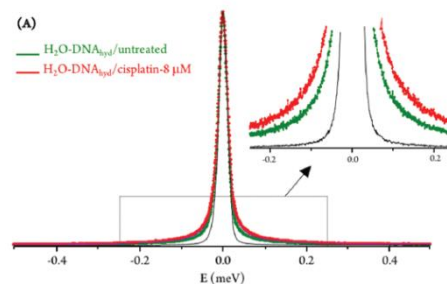
PCCP

PAPER

Check for updates

Anticancer drug impact on DNA – a study by neutron spectroscopy coupled with synchrotron-based FTIR and EXAFS†

Ana L. M. Batista de Carvalho,¹ Adriana P. Mamede,² Asha Dopplapudi,³ Victoria Garcia Sakai,⁴ James Doherty,^{5,6} Mark Frogley,⁷ Gianfelice Cinque,⁸ Peter Gardner,⁹ Diego Gianolio,¹⁰ Luis A. E. Batista de Carvalho,¹¹ and M. Paula M. Marques¹²



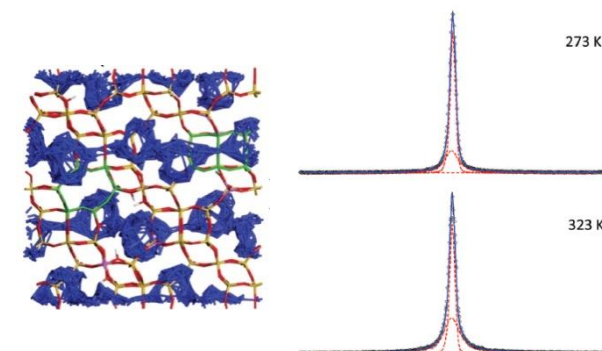
PCCP

PAPER

Check for updates
Cite this: Phys. Chem. Chem. Phys., 2018, 20, 11976

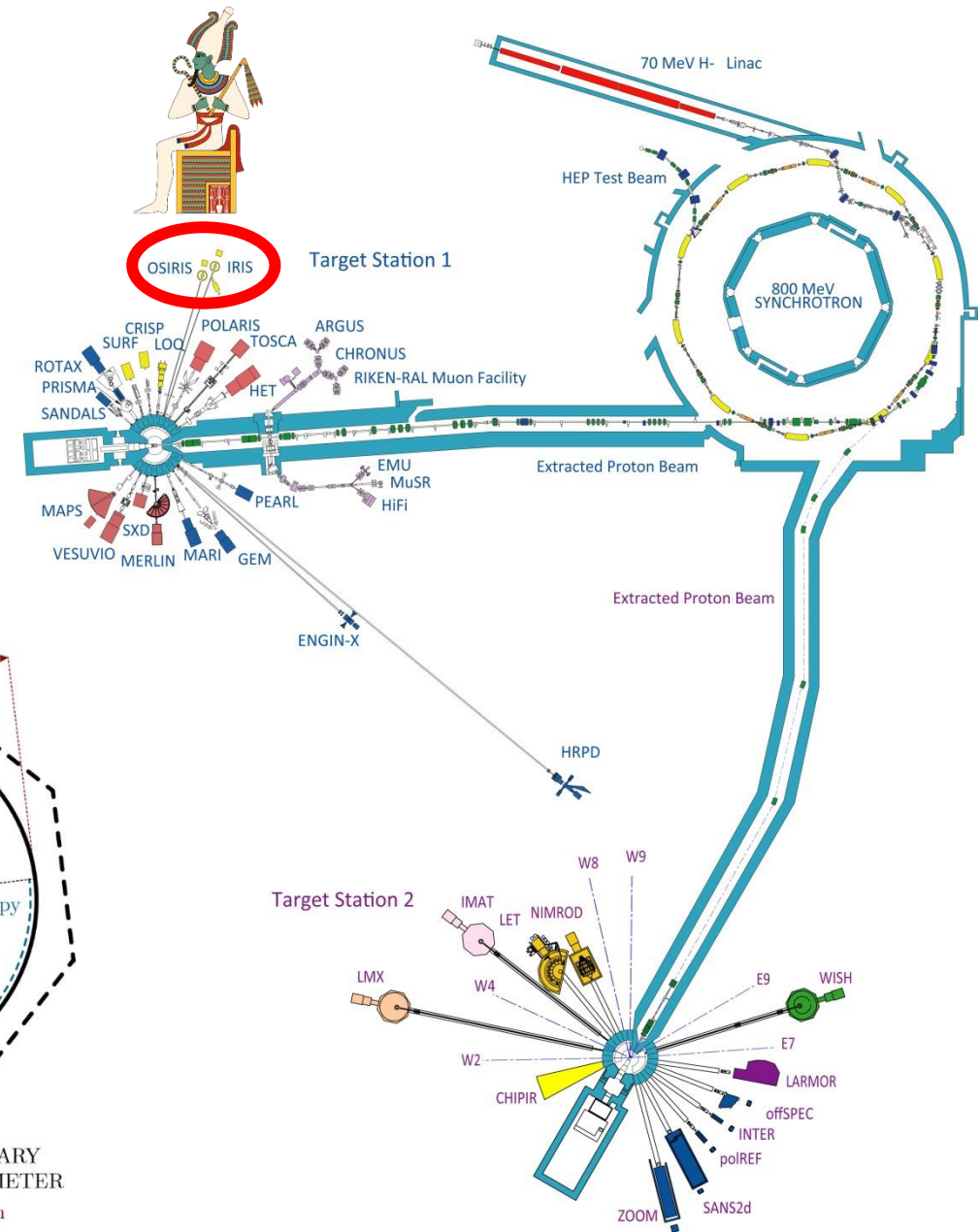
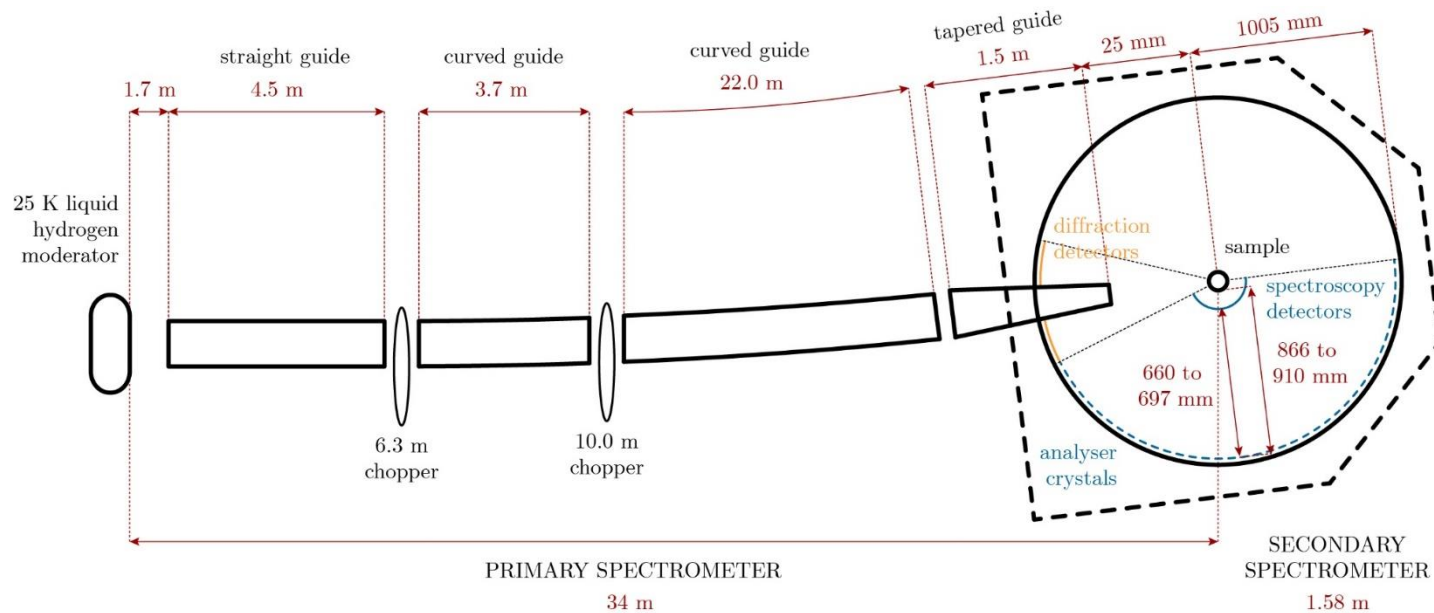
Comparing ammonia diffusion in NH_3 -SCR zeolite catalysts: a quasielastic neutron scattering and molecular dynamics simulation study

A. J. O'Malley,^{1,2,3} M. Sarwar,⁴ J. Armstrong,^{5,6} C. R. A. Catlow,^{6,7} I. P. Silverwood,^{8,9} A. P. E. York¹⁰ and I. Hitchcock¹¹

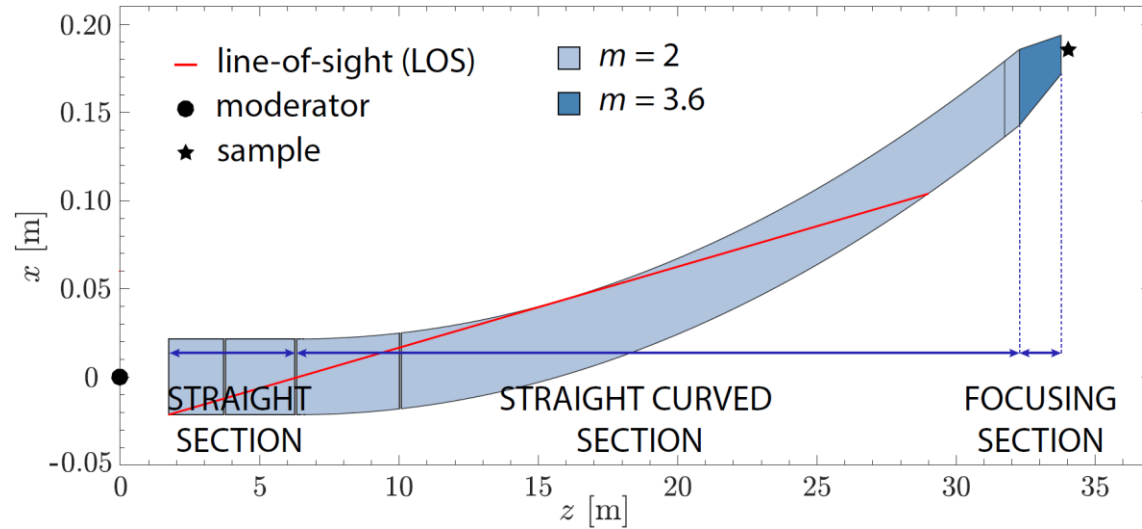


OSIRIS is a cold-neutron, indirect-geometry, time-of-flight spectrometer

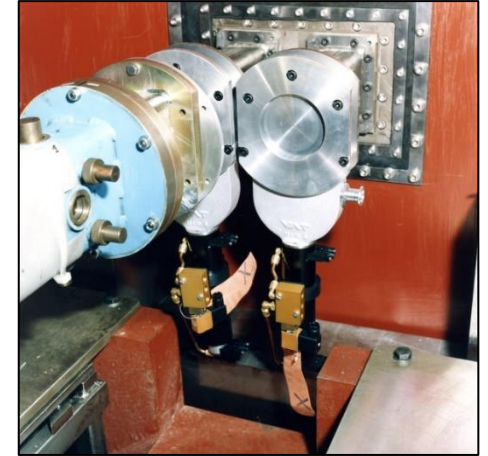
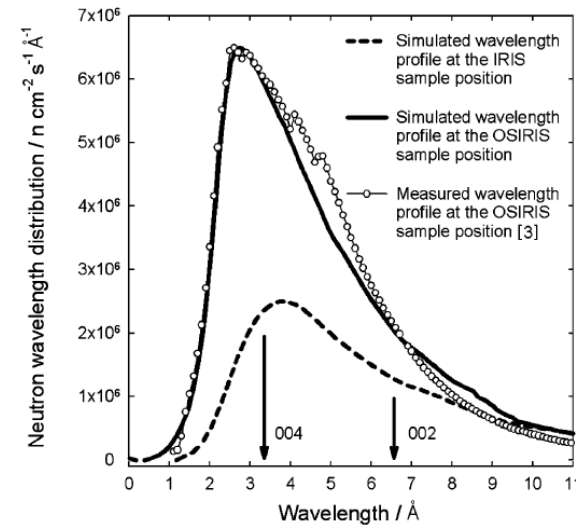
- Built in 1997
- Spectroscopy since 2002
- Beryllium filter in 2014
- North side of TS-1 (50 Hz repetition rate)
- H₂ moderator (incident wavelength 2–20 Å)



OSIRIS primary spectrometer



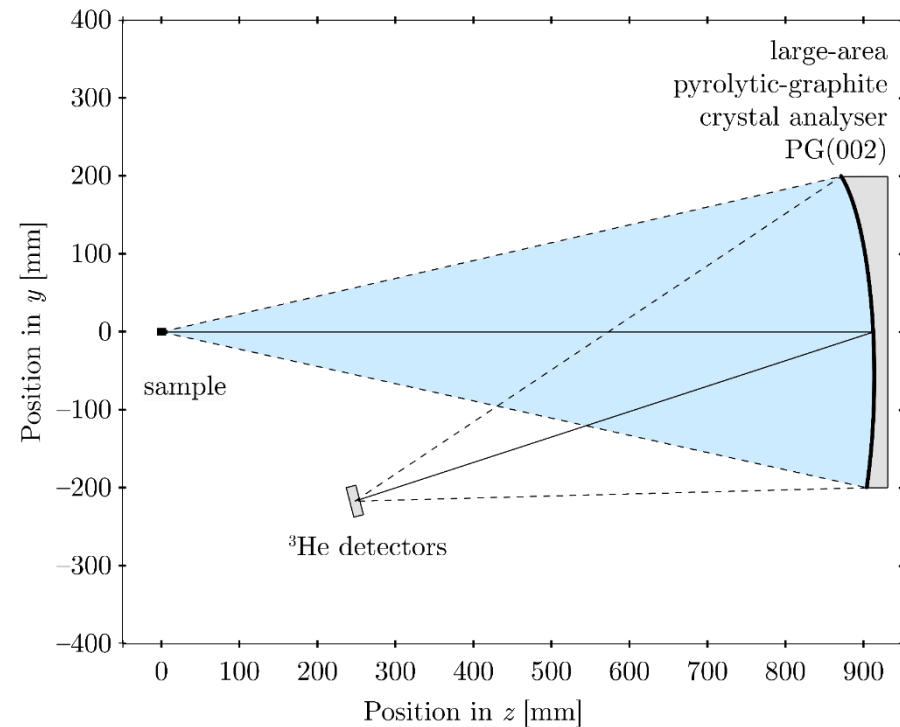
- 32 m long supermirror guide ($m = 2$)
- Curved to suppress direct line-of-sight (2 km radius)
- 1.5 m long tapered focusing section ($m = 3.6$)



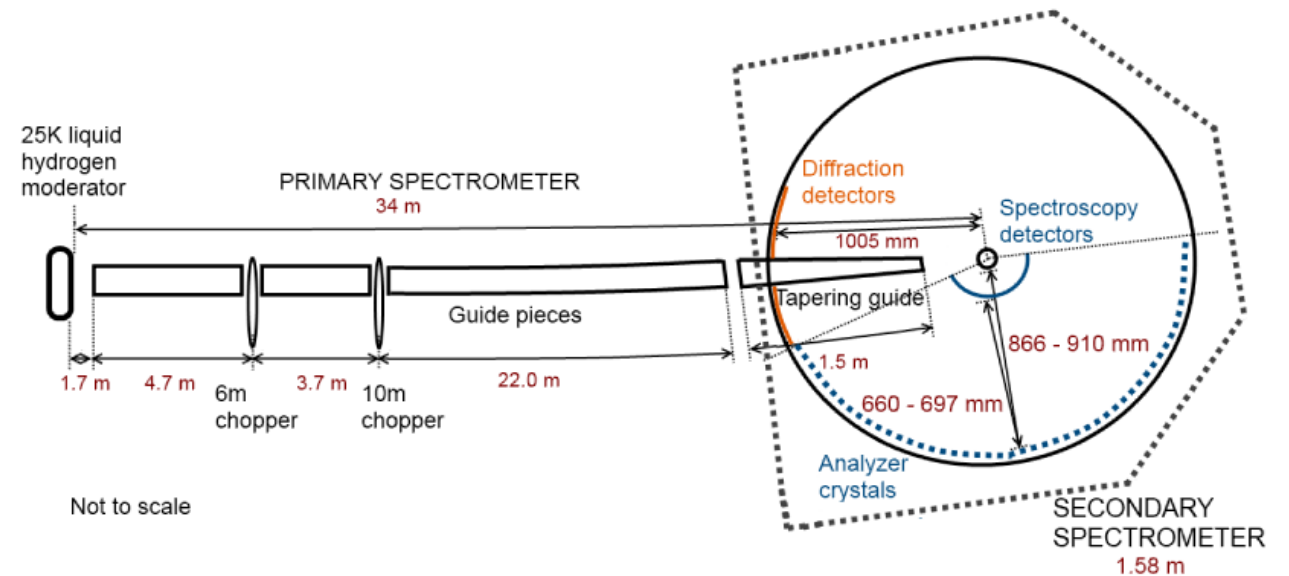
- Two disc-choppers (bandwidth, frame overlap) at 6.3 m and 10 m
- Shared shutter and insert sections with IRIS

OSIRIS secondary spectrometer

- Backscattering diffraction bank
- PG analyser (9000 1 cm² tiles) in near backscattering position (83–87°), radial collimator with moveable beryllium filter



	FWHM (μeV)	ΔE range (meV)	Q max (\AA^{-1})
PG002	24.5	± 0.5	1.8
PG004	99	± 4	3.6

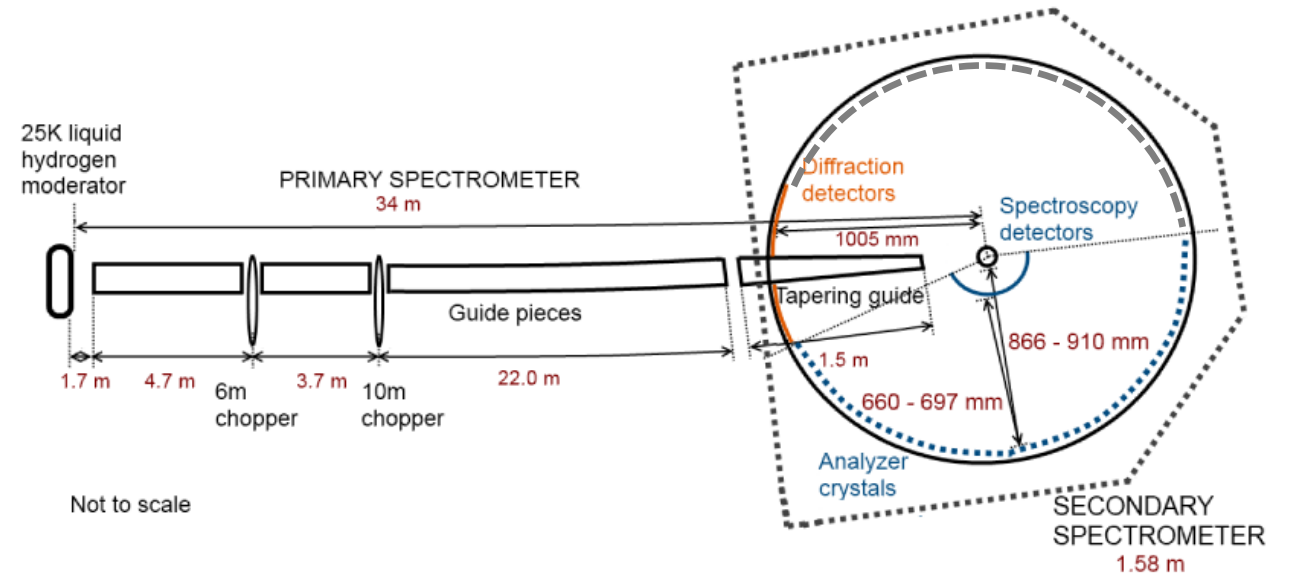
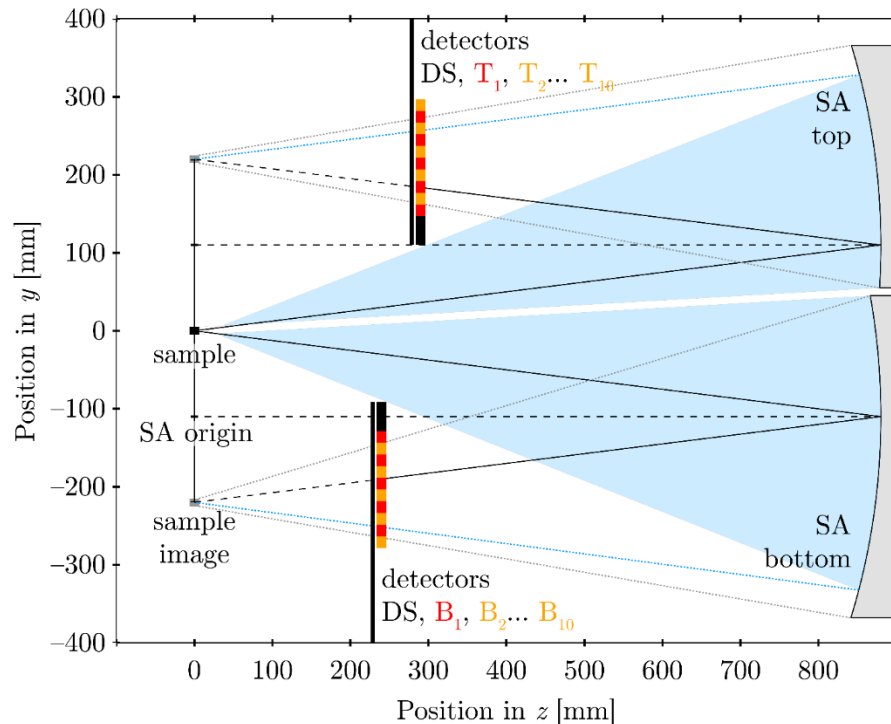


OSIRIS secondary spectrometer

- Backscattering diffraction bank
- PG analyser with beryllium filter
- Silicon analyser (in construction, fall 2024), for simultaneous operation with PG



	FWHM (μeV)	ΔE range (meV)	Q max (\AA^{-1})
PG002	24.5	± 0.5	1.8
PG004	99	± 4	3.6



	FWHM (μeV)	ΔE range (meV)	Q max (\AA^{-1})
Si111	11.1	± 0.6	1.9
Si333	78	± 15	5.8

Introduction

Key drivers & constraints

Design process

Performance comparison

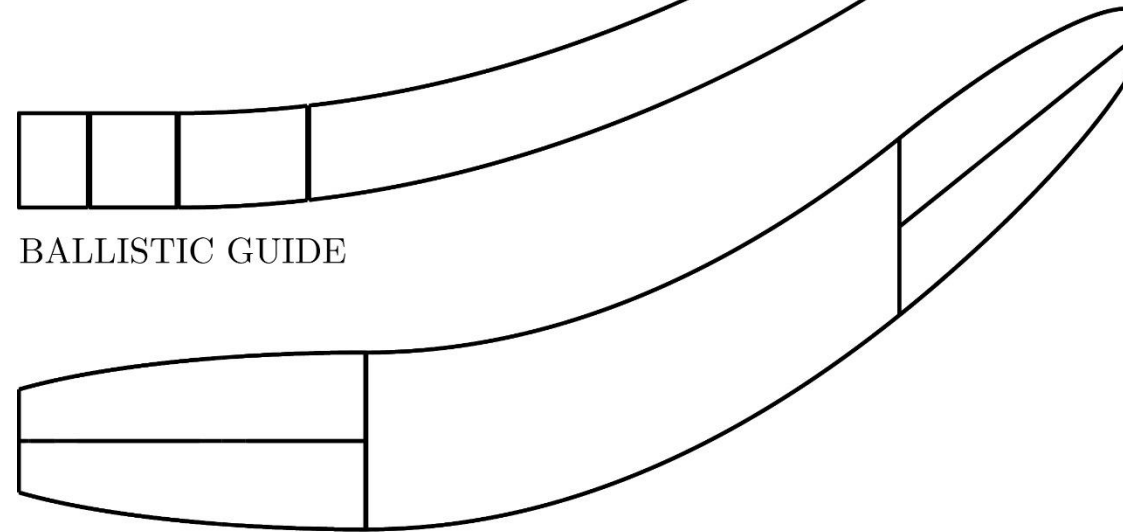
Slit system

Chopper system

Conclusions



BALLISTIC GUIDE



ELLIPTICALLY TAPERED GUIDE

Key drivers

- Maximise the flux at sample position for large ($2 \times 3 \text{ cm}^2$) and small ($1 \times 1 \text{ cm}^2$) samples

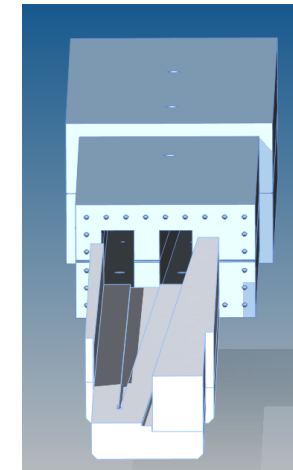
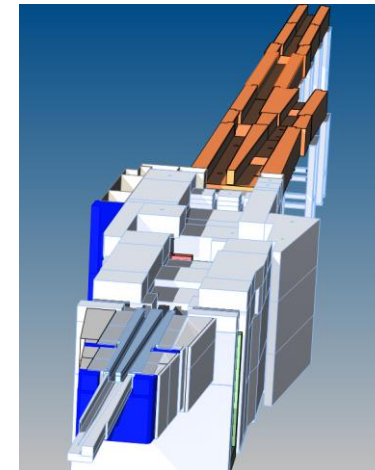
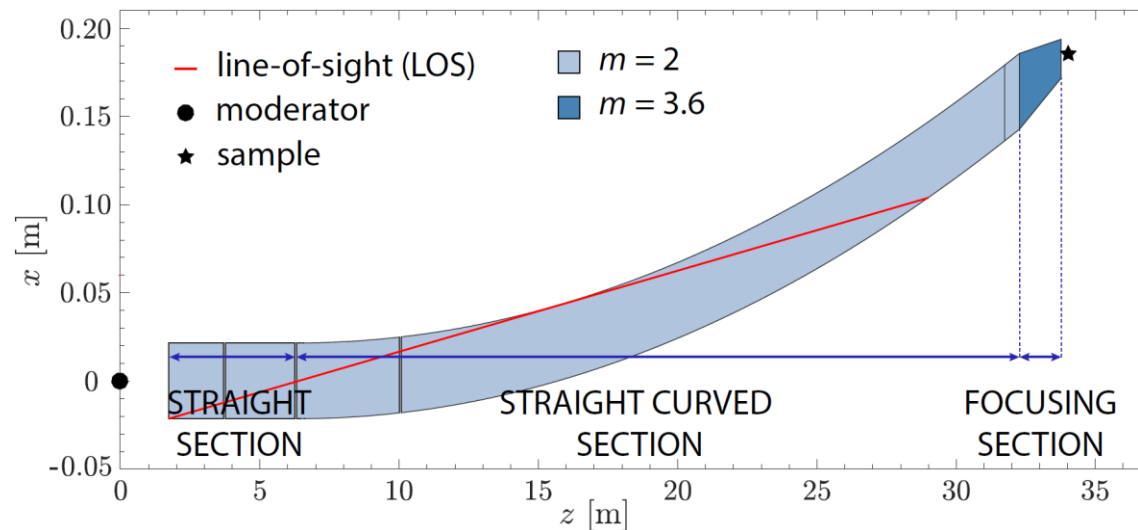
Constraints

- Fixed sample position
- No direct line-of-sight
- Guide height
- Shared insert with IRIS

*33.95 m total length, 18.6 cm deviation
curved guide section*

20 cm max height, 12 cm at entrance

full separation, or shortest possible shared section



Present OSIRIS guide

Total length 32 m, including

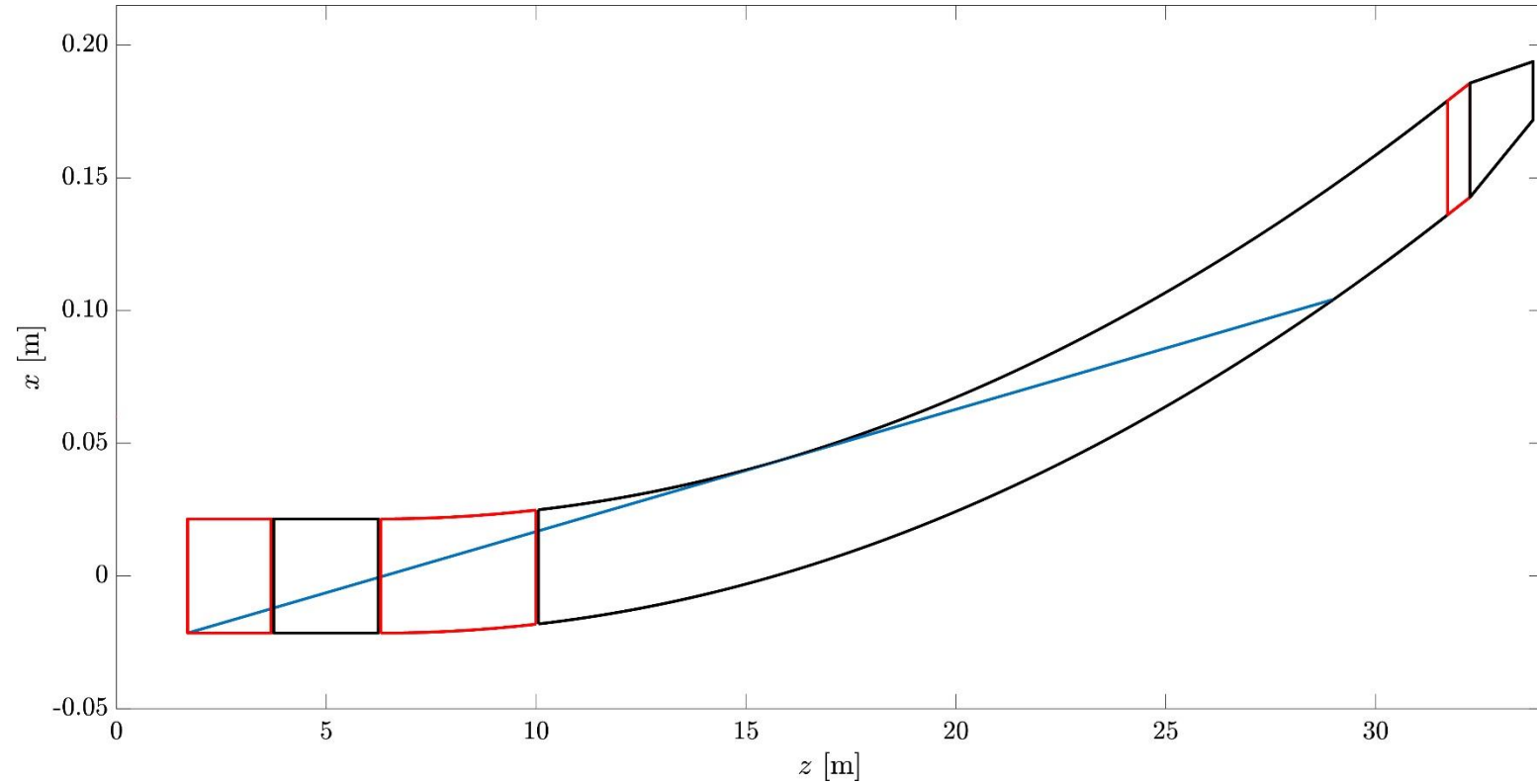
- straight section 4.5 m
- curved section 25.7 m (2050 m radius, cutoff $\lambda = 1.9 \text{ \AA}$)
- linear taper 1.5 m

Max. height 6.5 cm

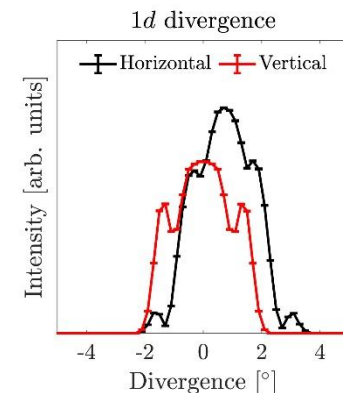
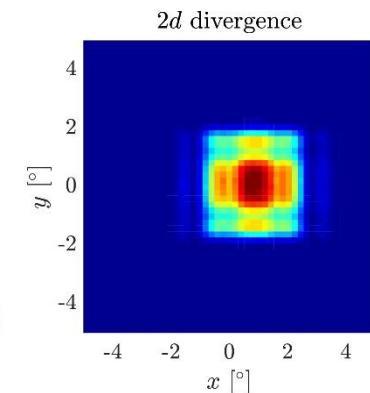
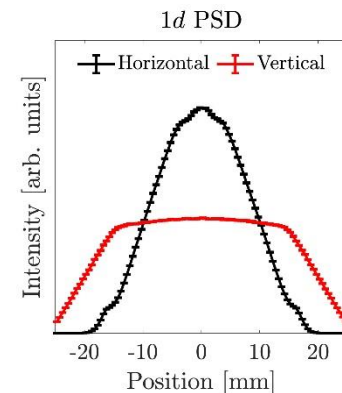
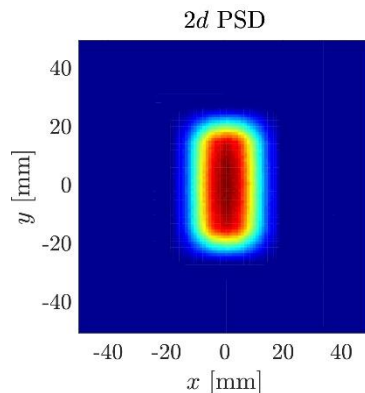
Max. width 4.3 cm

McStas simulation

- incident neutron energy
 $E_i = 1.4\text{--}4.0 \text{ meV}$ ($\lambda = 4.5\text{--}7.6 \text{ \AA}$)
- intensities on $1 \times 1 \text{ cm}^2$ and $2 \times 3 \text{ cm}^2$ monitors used as reference



id 737496.5146 413773.266(<0.078 %) counts / 10x10 mm² 3047276.620(<0.029 %) counts / 20x30 mm²



Guide geometry

Curved guides with various taper geometries

- Linear
- Elliptic (half ellipse or truncated ellipse)
- Parabolic

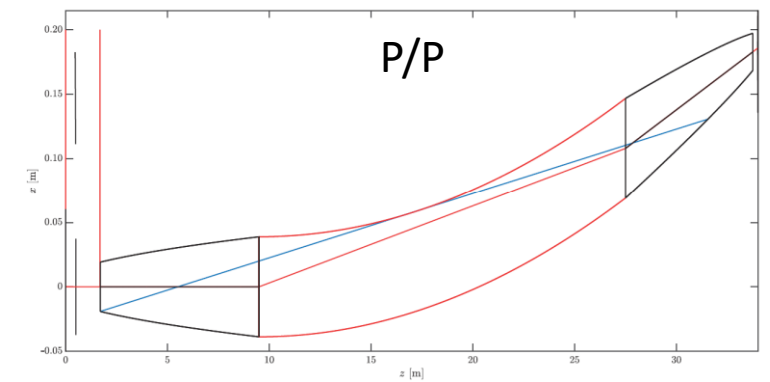
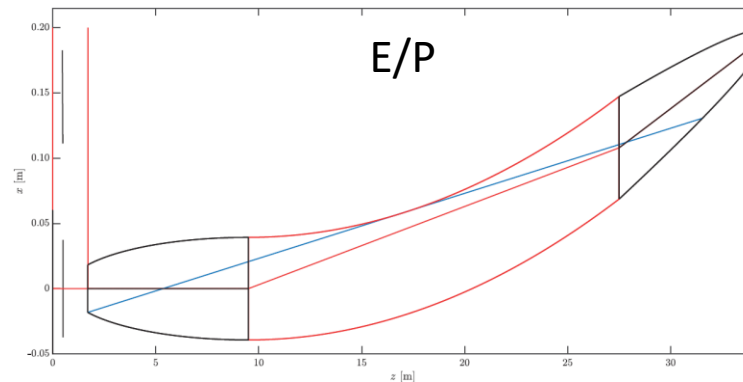
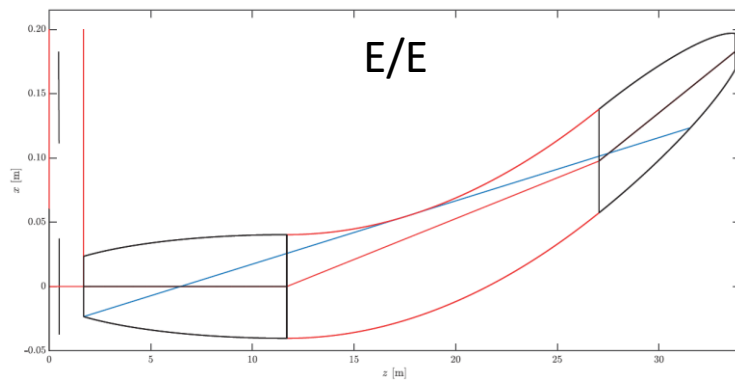
Curved guides with vertical/horizontal kinks

Double ellipse without curved section

Geometry

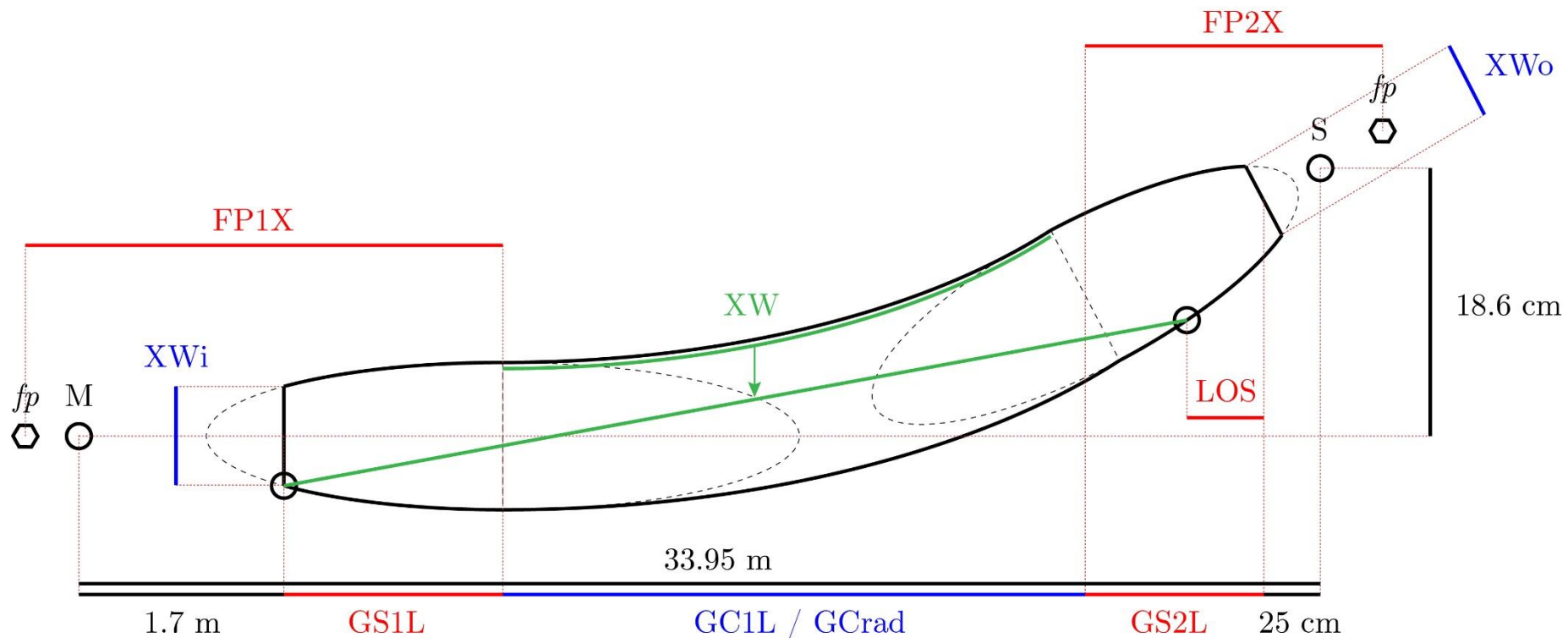
- Current OSIRIS guide
- Curved, elliptic/elliptic, default
- Curved, elliptic/elliptic, reduced height
- Curved, elliptic/elliptic, reduced R
- Curved, elliptic/elliptic, reduced LOS
- Curved, elliptic/elliptic, reduced height and R
- Curved, parabolic/parabolic
- Curved, parabolic/elliptic
- Curved, elliptic/parabolic
- Double-ellipse

Geometry	LOS (m)	Gain over $1 \times 1 \text{ cm}^2$	Gain over $2 \times 3 \text{ cm}^2$
Current OSIRIS guide	~ 4.0	1	1
Curved, elliptic/elliptic, default	2.2	4.3	3.9
Curved, elliptic/elliptic, reduced height	2.2	4.3	3.7
Curved, elliptic/elliptic, reduced R	2.2	4.5	4.2
Curved, elliptic/elliptic, reduced LOS	1.0	4.6	4.3
Curved, elliptic/elliptic, reduced height and R	2.2	4.5	3.9
Curved, parabolic/parabolic	2.2	2.6	2.4
Curved, parabolic/elliptic	2.2	3.3	3.1
Curved, elliptic/parabolic	2.2	3.1	3.0
Double-ellipse	0.8	3.6	3.3

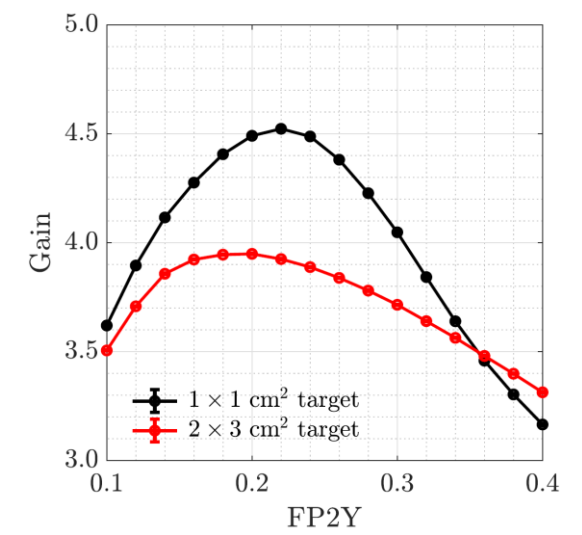
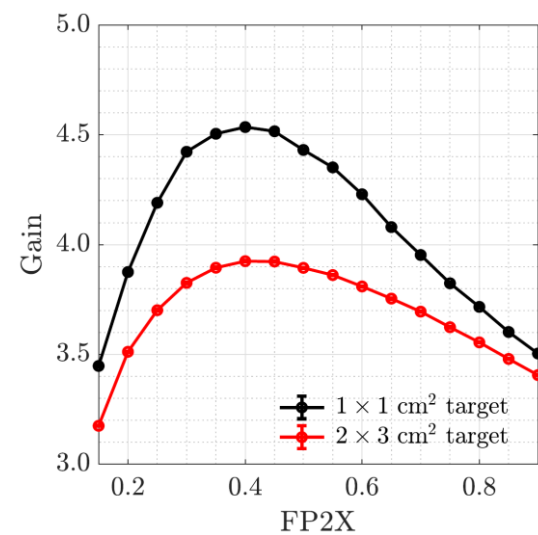
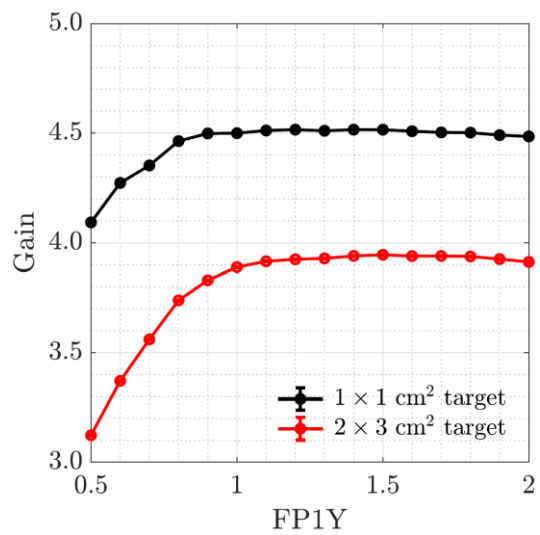
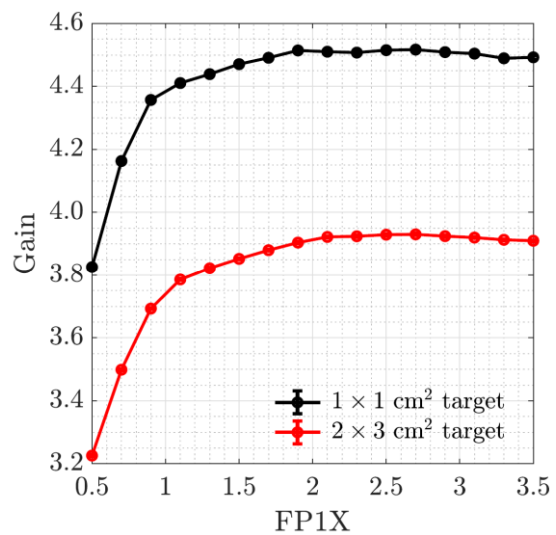
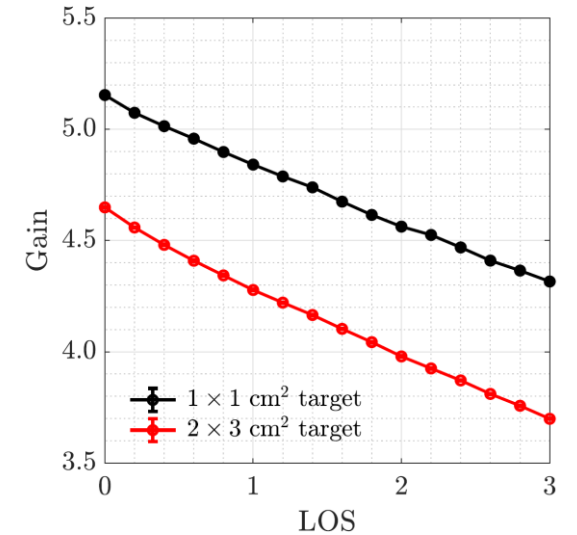
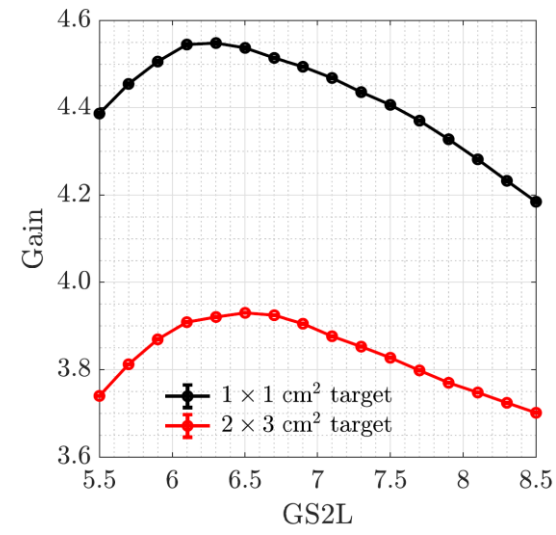
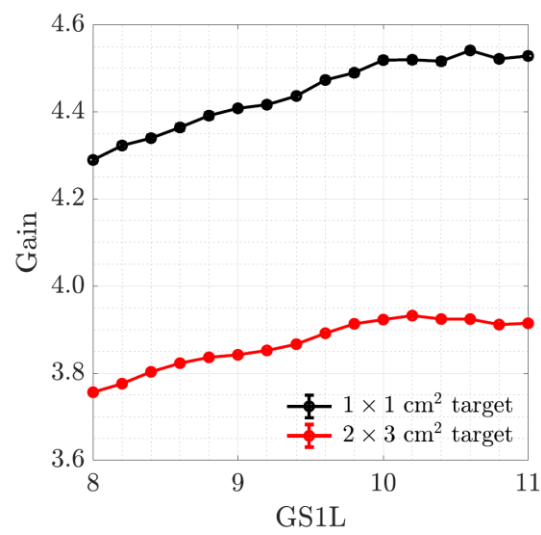
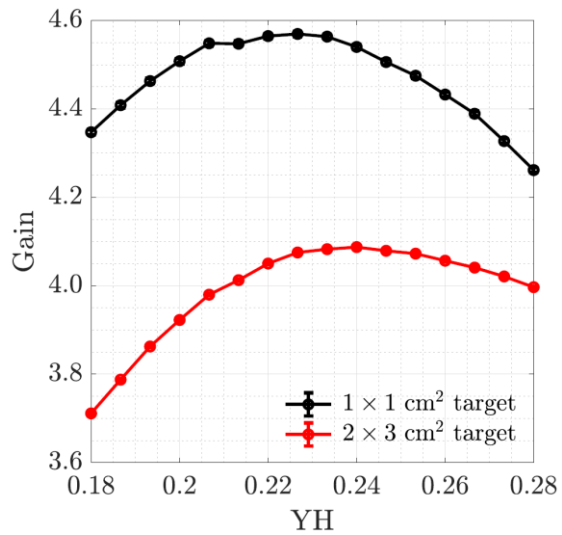


Elliptically tapered guide parameterisation

- (1) Constraints on guide entrance and sample positions, and length of elliptic sections (**GS1L** / **GS2L**), determines the curved section length (**GC1L**) and curvature radius (**GCrad**)
- (2) Elliptic sections defined by focal points along x and y (**FP1X** / **FP1Y** / **FP2X** / **FP2Y**) and guide width and height (**XW** / **YH**), defines guide width and height at entrance and exit (**XWi**, **YHi**, **XWo**, **YHo**)
- (3) Distance at which the line-of-sight is intercepted from the exit (**LOS**), and **XWi**, determines **XW**



Elliptically tapered guide parameter dependencies



Chosen design: Elliptically tapered guide

Total length 32 m, including

- defocusing section 10.0 m
- curved section 15.3 m (1.2 km radius, cutoff $\lambda = 1.7 \text{ \AA}$)
- focusing section 6.7 m

Max. height 20.0 cm

Max. width 8.1 cm

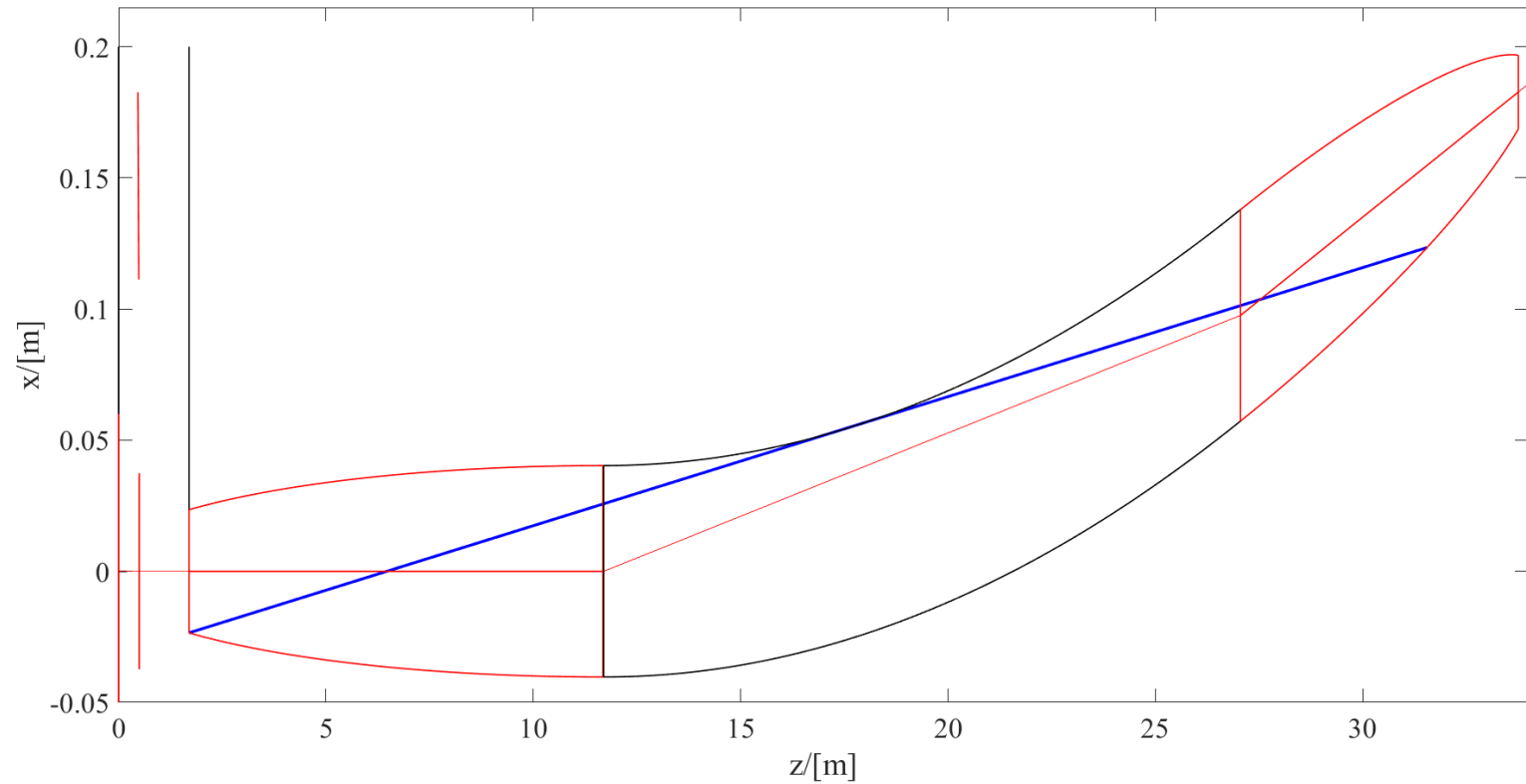
Similar line-of-site intercept point

Coarse coating

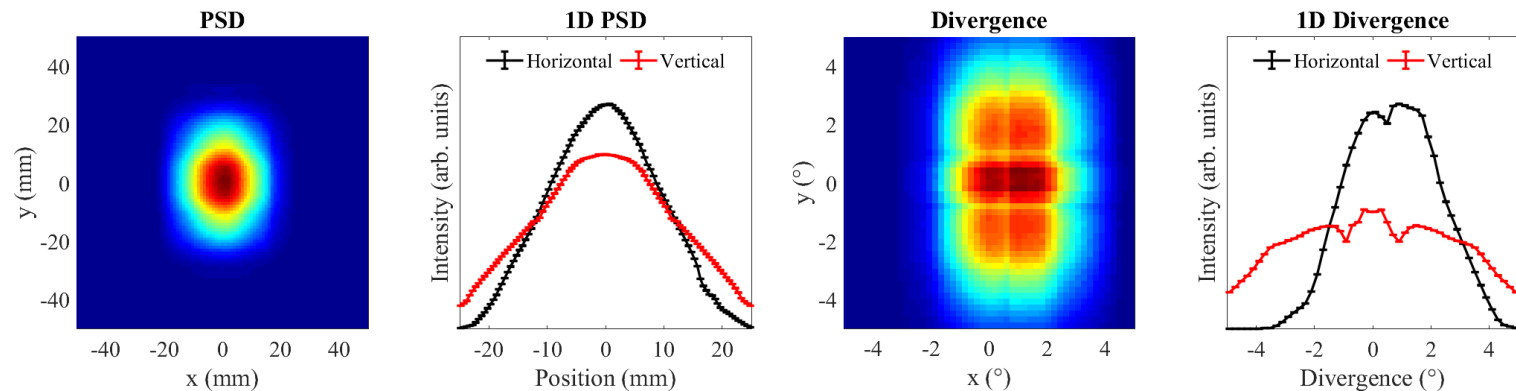
- elliptic sections, $m = 6$
- curved section, $m = 4$

McStas simulation

- gain (geometry only) in intensity of 4.5 for $1 \times 1 \text{ cm}^2$ and 4.0 for $2 \times 3 \text{ cm}^2$ samples

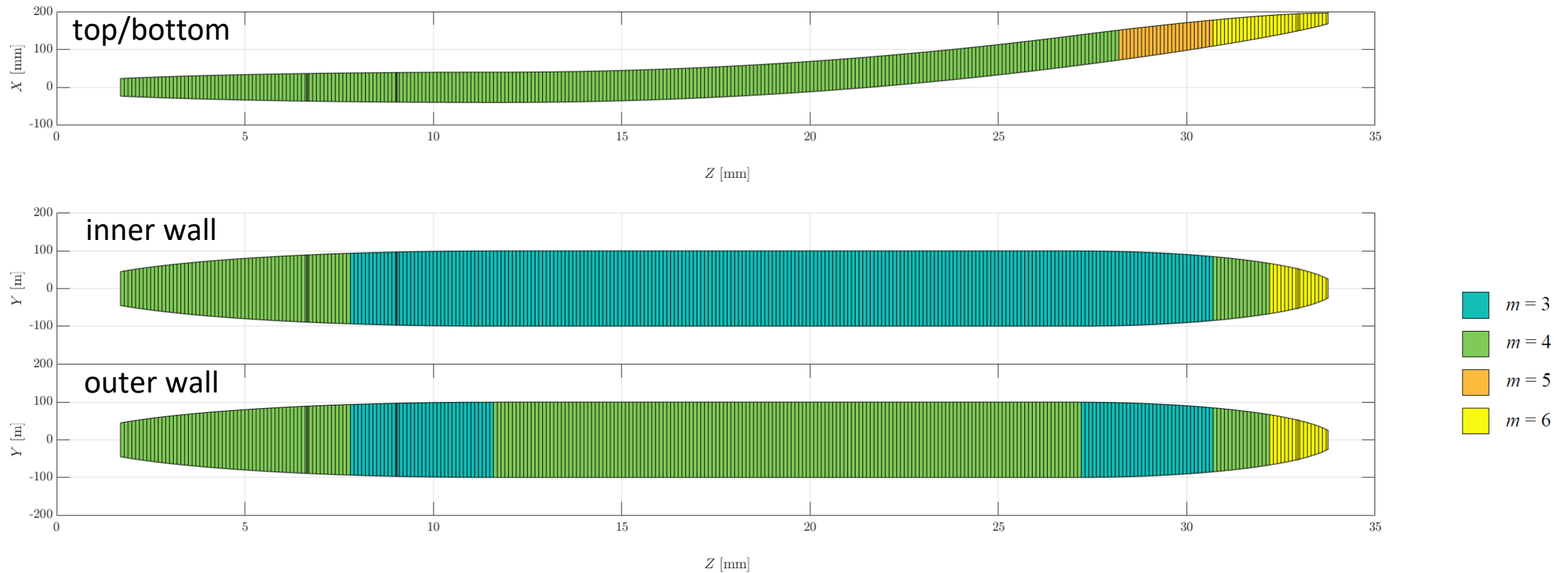


id 737467.6005 4.508(<0.034%) counts / $10 \times 10 \text{ mm}^2$ 4.005(<0.014%) counts / $20 \times 30 \text{ mm}^2$

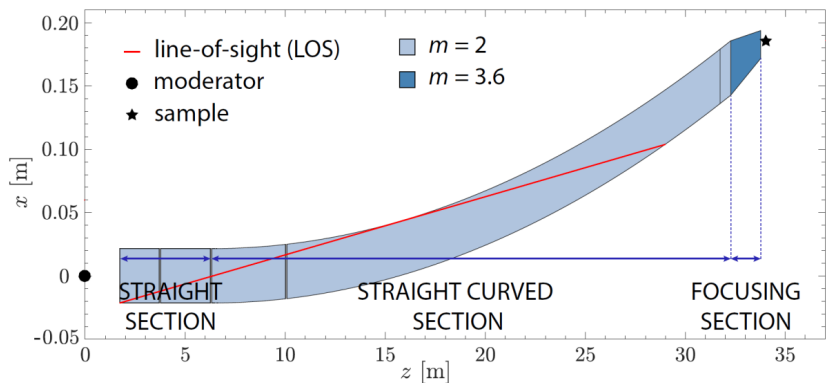


Coating profile

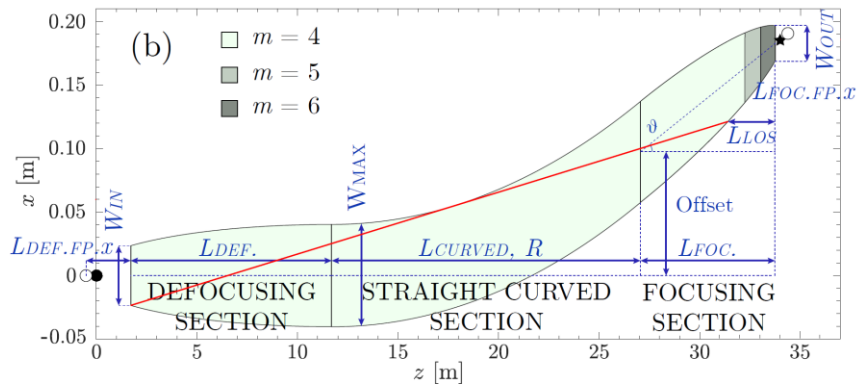
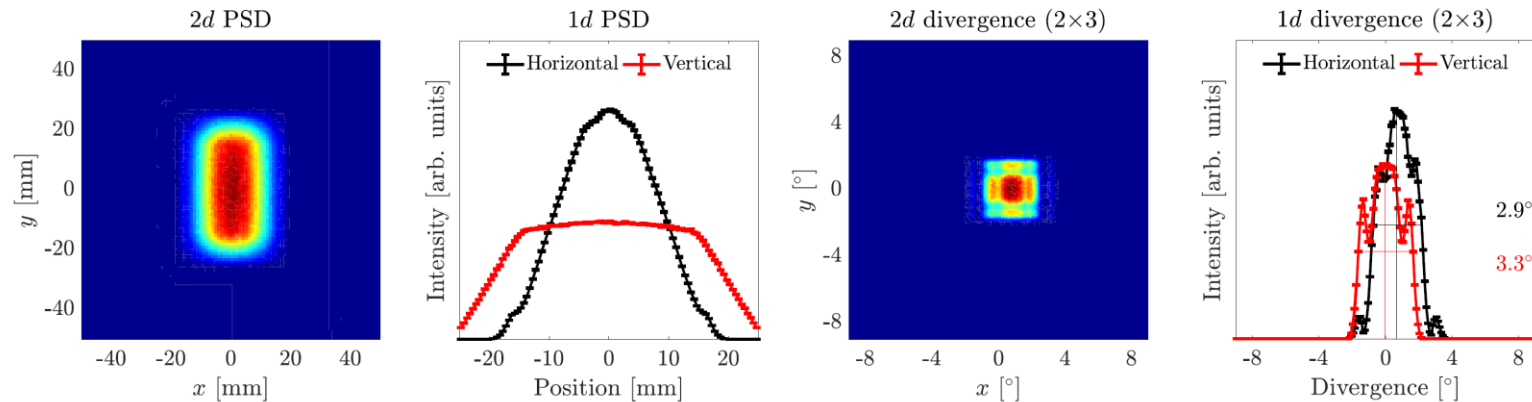
- Optimised for short wavelength neutrons (10–20 meV)
- Updated reflectivity profiles



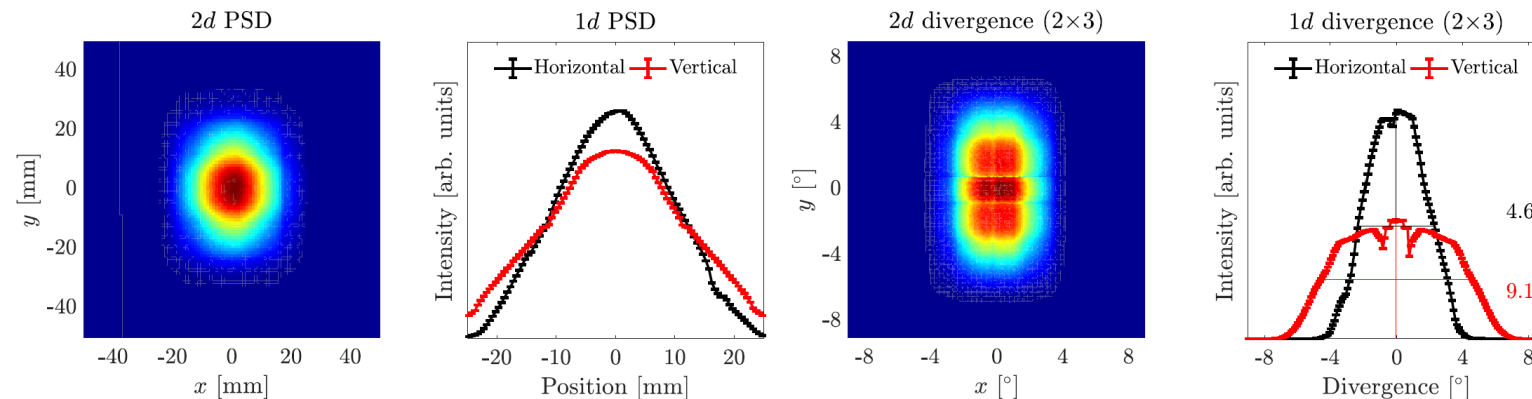
Beam profile



id 737768.6590 413780.467(<0.155 %) counts / 10x10 mm² 2080750.035(<0.070 %) counts / 20x30 mm²

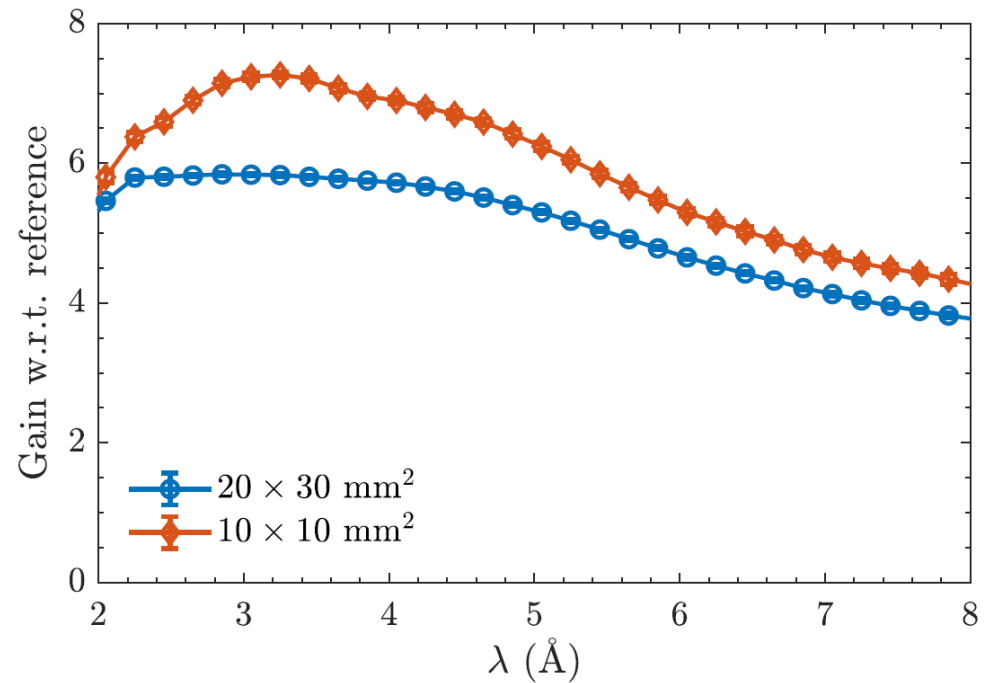
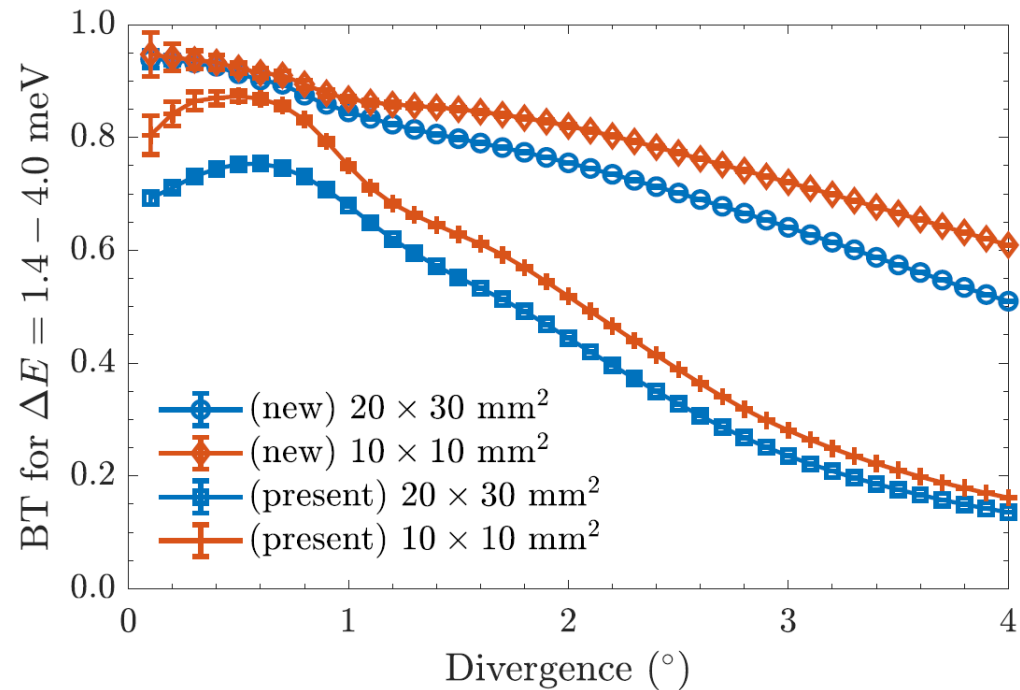


id 737803.6161 5.617(<0.032 %) counts / 10x10 mm² 4.824(<0.016 %) counts / 20x30 mm²



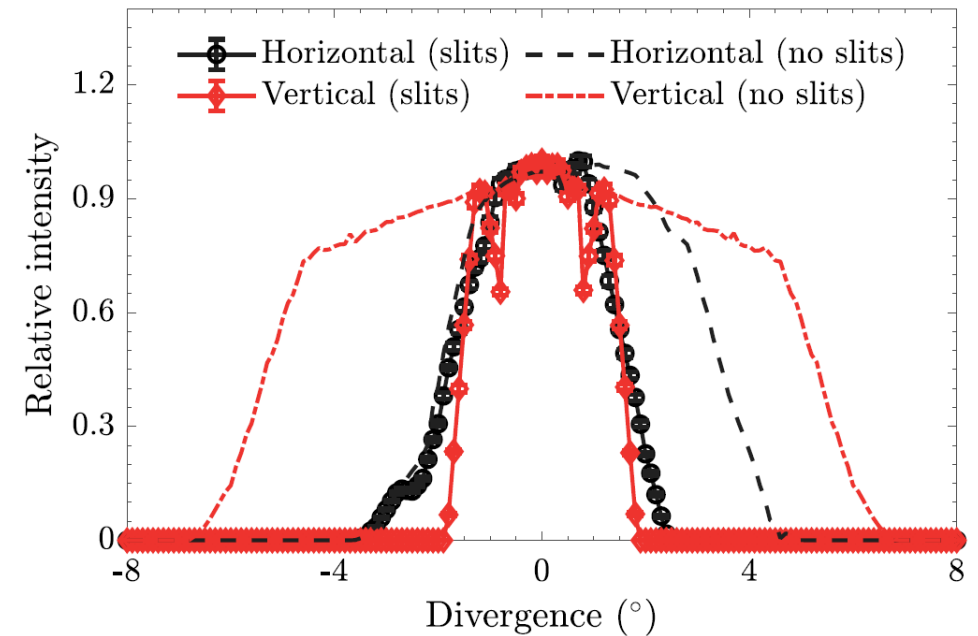
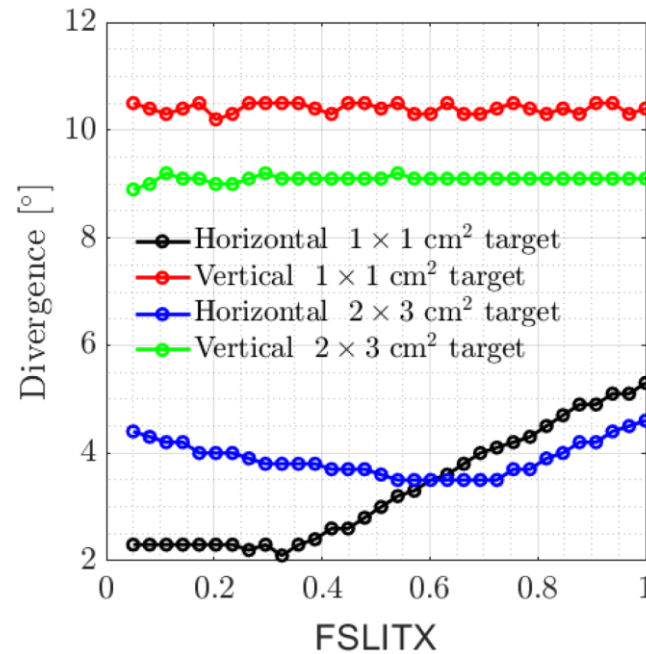
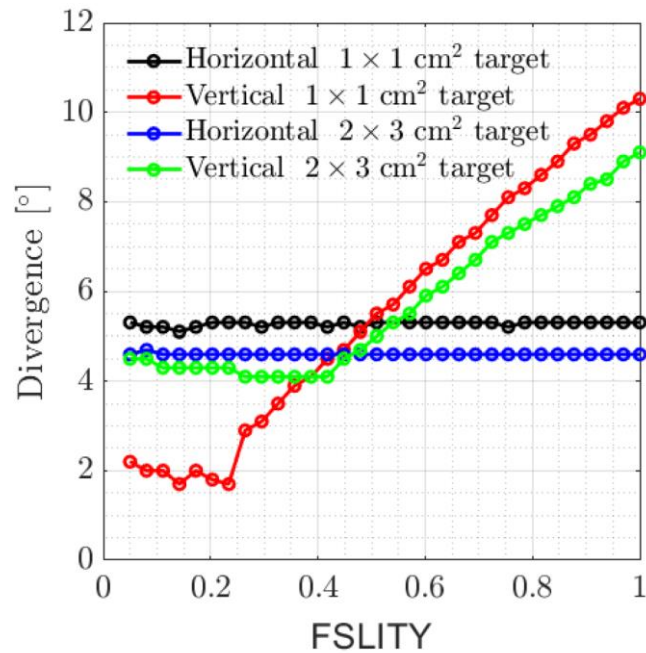
Brilliance transfer & gain factor

- Possibly higher gain since present guide degradation not accounted for
- Additional factor 2 from TS-1 moderator upgrade
- At least 10-fold increase in flux



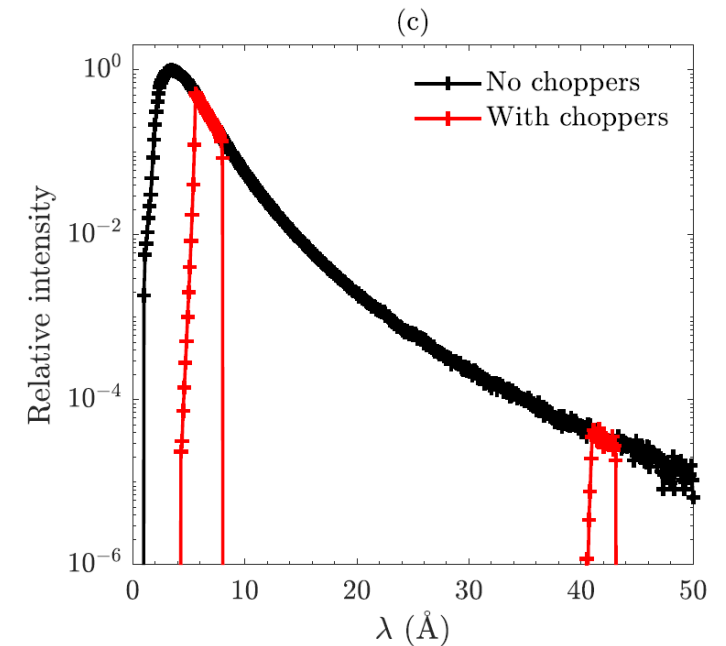
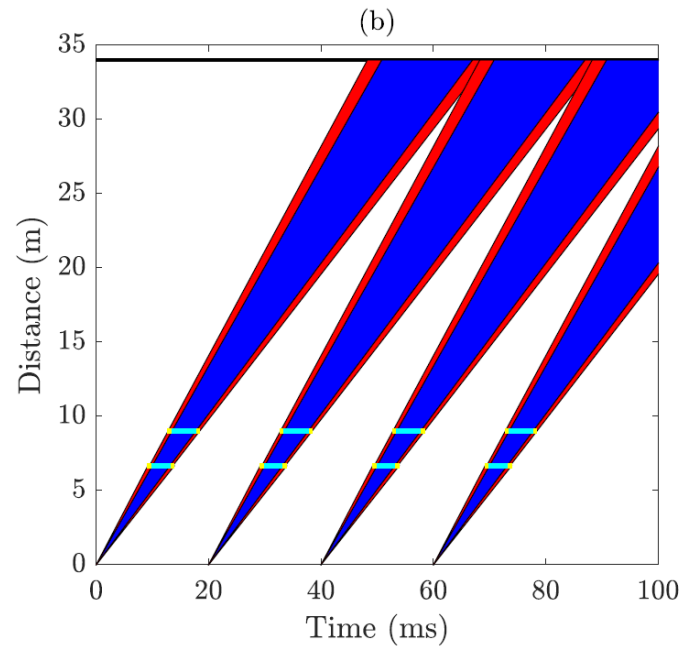
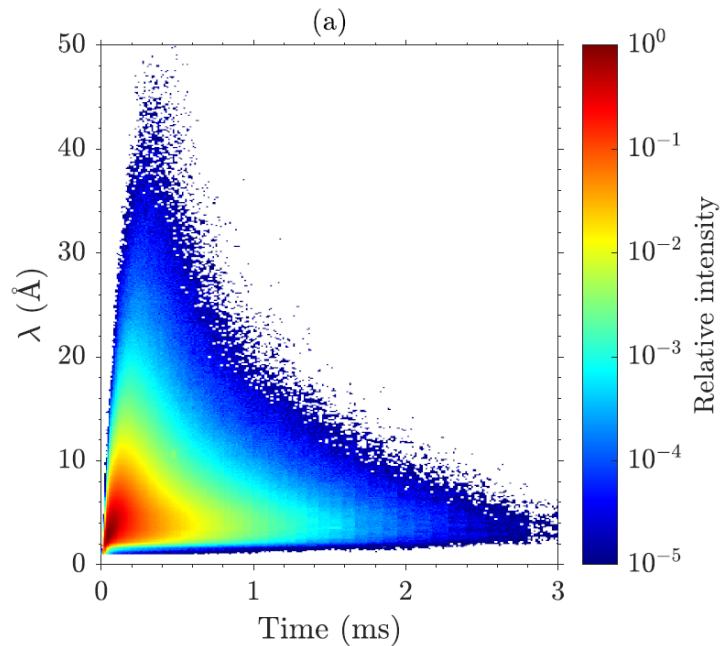
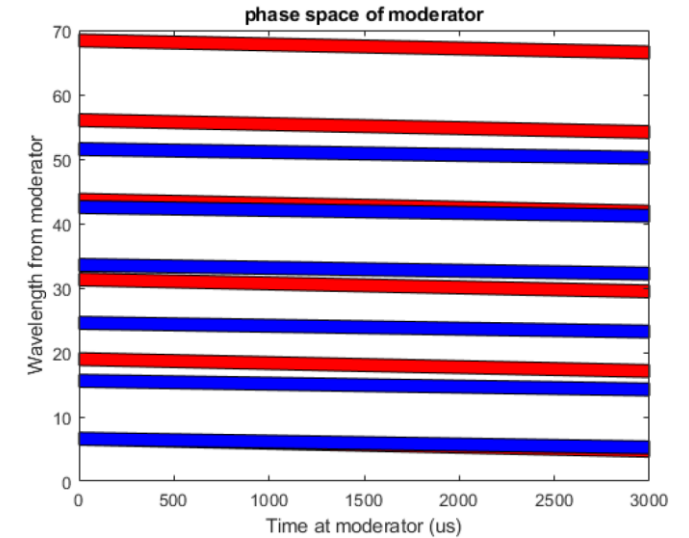
Slit system for single-crystal experiments

- Single slit at guide end, controlled divergence down to 4° for large samples, down to 2.5° for small samples
- Two slits, at guide exit & outside the tank, flexible control of the divergence down to 1° (for diffraction)



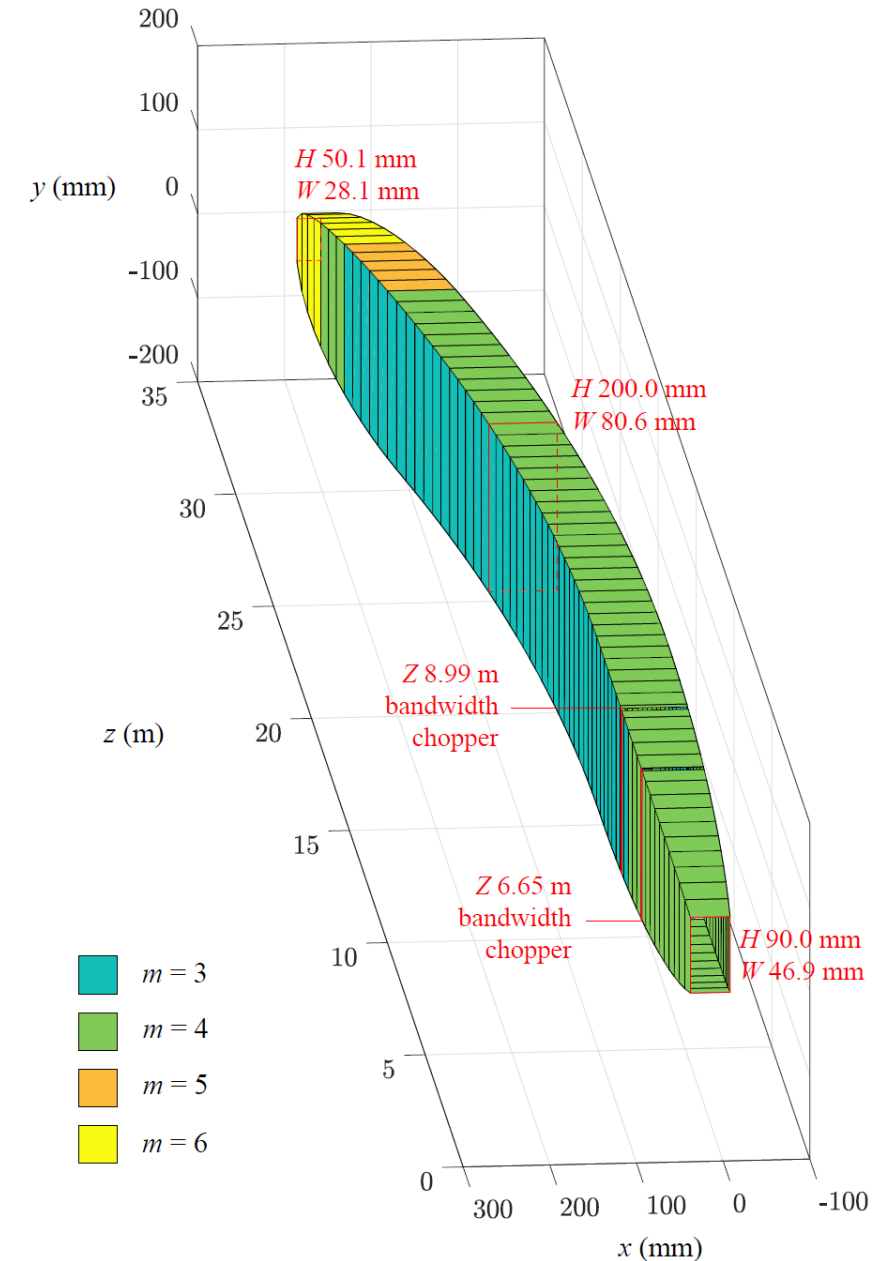
Chopper system

- Bandwidth chopper at 6.4–7.3 m, located at 3 o'clock, cuts height (180 mm)
- Frame overlap chopper at 8.8–15 m, located at 12 o'clock cuts width (81 mm)
- Counter-rotating discs at 6.65 m (\varnothing 810 mm) and 8.99 m (\varnothing 1000 mm)



OSIRIS primary spectrometer upgrade

- Curved guide with elliptically tapered defocusing and focusing sections
- Gain factors of 4.8–5.6 in the PG002/Si111 regime, probably 10+ including moderator upgrade and degradation of current guide
- Smaller beam spot
- Large divergence can be reduced with two-slit system
- Requires large counter-rotating disc choppers



OSIRIS+

Paula Luna Dapica
Franz Demmel

OSIRIS & MoISpec

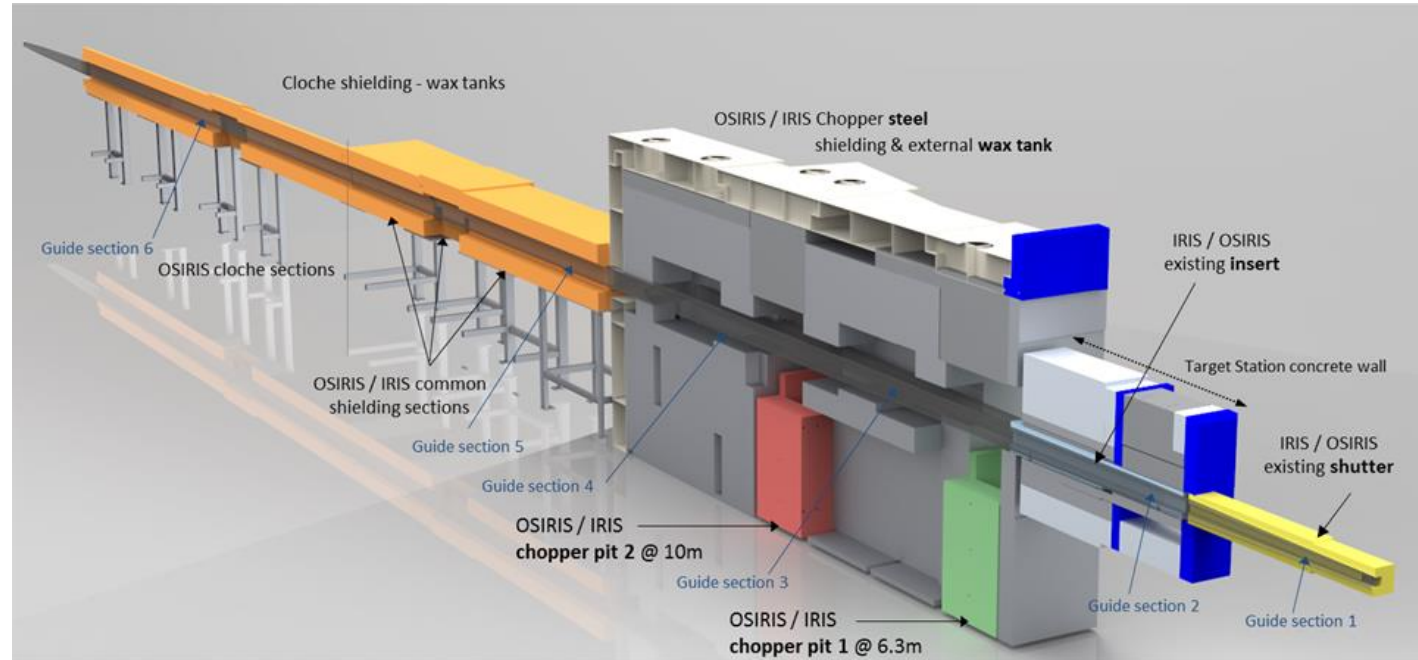
Sanghamitra Mukhopadhyay
Ian Silverwood
Stewart Parker
Victoria García Sakai

Design division

Kevin Jones
Nick Webb
Peter Galsworthy

NMIDG

Rob Bewley



Thank you for your attention!

