NMX Key
Technical
Choices Meeting
Requirements

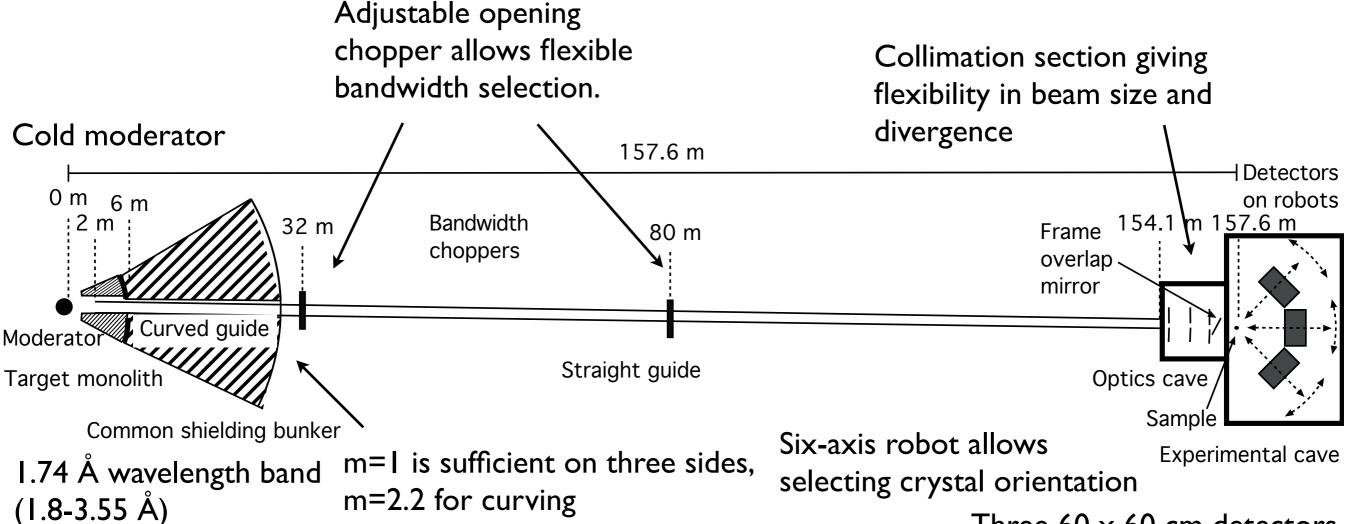


Esko Oksanen Instrument Scientist, Macromolecular Crystallography

NMX Tollgate 2 Review 2014–12–11



NMX - A quasi-Laue time-of-flight diffractometer with high q-resolution



- Match beam size to sample size (max 5 x 5 mm)
- Match beam divergence to sample mosaicity (max. ±0.2°)
- Maximize (useful) flux at sample!

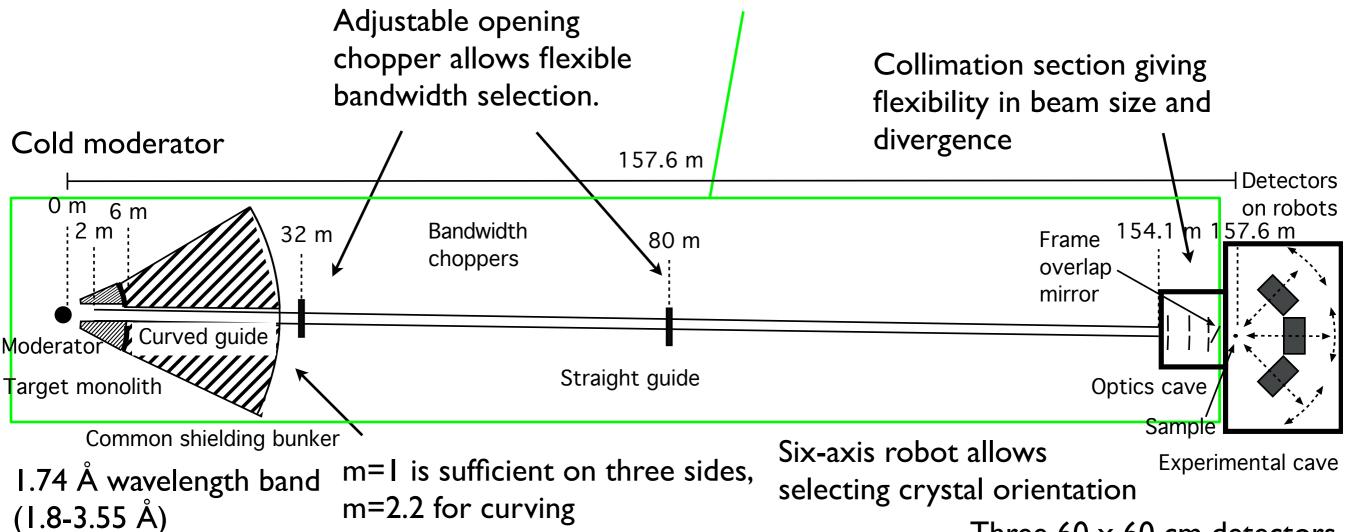
Three 60 x 60 cm detectors with 0.2 mm spatial resolution Variable sample-detector distance (0.2-1.0 m)

Variable 2 θ angle (0-110°)



NMX - A quasi-Laue time-of-flight diffractometer with high q-resolution

Existing technology



- Match beam size to sample size (max 5 x 5 mm)
- Match beam divergence to sample mosaicity (max. $\pm 0.2^{\circ}$)
- Maximize (useful) flux at sample!

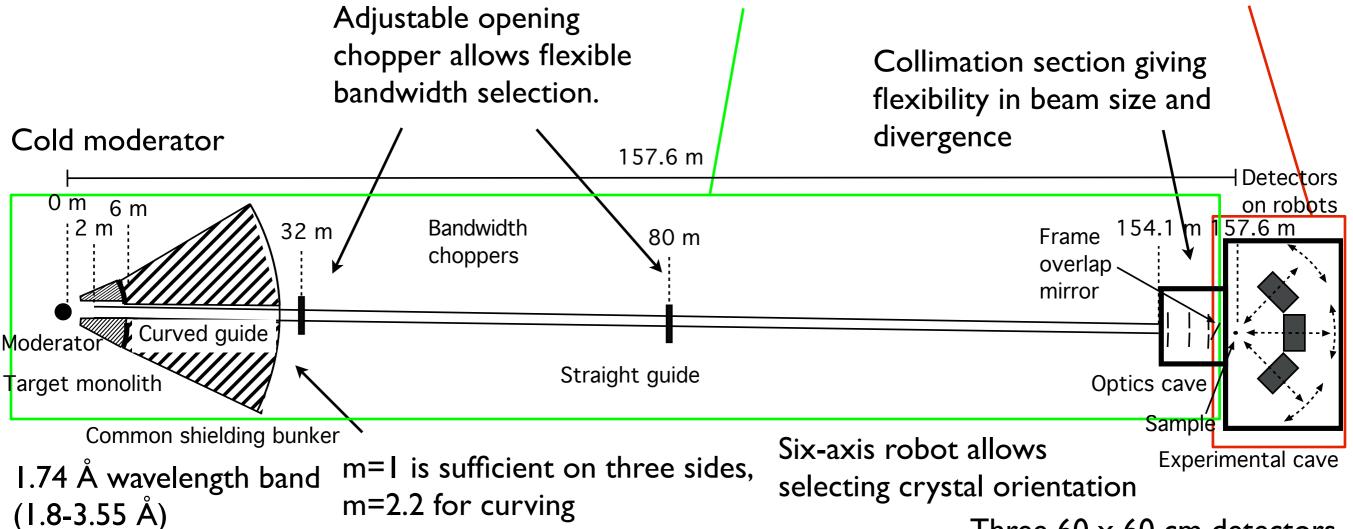
Three 60 x 60 cm detectors with 0.2 mm spatial resolution Variable sample-detector distance (0.2-1.0 m)

Variable 2 θ angle (0-110°)



NMX - A quasi-Laue time-of-flight diffractometer with high q-resolution

Existing technology Needs R&D



- Match beam size to sample size (max 5 x 5 mm)
- Match beam divergence to sample mosaicity (max. $\pm 0.2^{\circ}$)
- Maximize (useful) flux at sample!

Three 60 x 60 cm detectors with 0.2 mm spatial resolution Variable sample-detector distance (0.2-1.0 m)

Variable 20 angle (0-110°)



Functional requirements

1. Wavelength resolution

- 1.1. The BTS shall transport from the moderator a beam of neutrons to the sample at a distance that leads to a maximal wavelength uncertainty of 5% ($\Delta\lambda/\lambda$) for the detected neutrons using the full ESS pulse
- 1.2. Rationale: A moderate wavelength resolution allows the full pulse to be used while conserving the advantage of TOF for the S/B (see 13.6.4 (5))
- 1.3. Verification: Measurement of the pulse length at sample

Beam size

- 2.1. The BTS shall transport from the moderator to the sample a beam of neutrons with maximum size (full width half maximum) of 5 ± 0.1 mm and minimum size of 0.2 ± 0.02 mm.
- 2.2. Rationale: Matching the beam size to the sample size maximises the S/B (see 13.6.4 (3,5-6))
- 2.3. Verification: Measurement of the beam intensity profile at sample



Functional requirements

1. Wavelength resolution

- 1.1. The BTS shall transport from the moderator a beam of neutrons to the sample at a distance that leads to a maximal wavelength uncertainty of 5% ($\Delta\lambda/\lambda$) for the detected neutrons using the full ESS pulse
- ~150 m flight path
- 1.2. Rationale: A moderate wavelength resolution allows the full pulse to be used while conserving the advantage of TOF for the S/B (see 13.6.4 (5))
- 1.3. Verification: Measurement of the pulse length at sample

Beam size

- 2.1. The BTS shall transport from the moderator to the sample a beam of neutrons with maximum size (full width half maximum) of 5 ± 0.1 mm and minimum size of 0.2 ± 0.02 mm.
- 2.2. Rationale: Matching the beam size to the sample size maximises the S/B (see 13.6.4 (3,5-6))
- 2.3. Verification: Measurement of the beam intensity profile at sample



Functional requirements

1. Wavelength resolution

- 1.1. The BTS shall transport from the moderator a beam of neutrons to the sample at a distance that leads to a maximal wavelength uncertainty of 5% ($\Delta\lambda/\lambda$) for the detected neutrons using the full ESS pulse
- → ~150 m flight path
- 1.2. Rationale: A moderate wavelength resolution allows the full pulse to be used while conserving the advantage of TOF for the S/B (see 13.6.4 (5))
- 1.3. Verification: Measurement of the pulse length at sample

2. Beam size

- 2.1. The BTS shall transport from the moderator to the sample a beam of neutrons with maximum size (full width half maximum) of 5 ± 0.1 mm and minimum size of 0.2 ± 0.02 mm.
- → ~3 cm guide
- 2.2. Rationale: Matching the beam size to the sample size maximises the S/B (see 13.6.4 (3,5-6))
- 2.3. Verification: Measurement of the beam intensity profile at sample



Functional requirements

1. Wavelength resolution

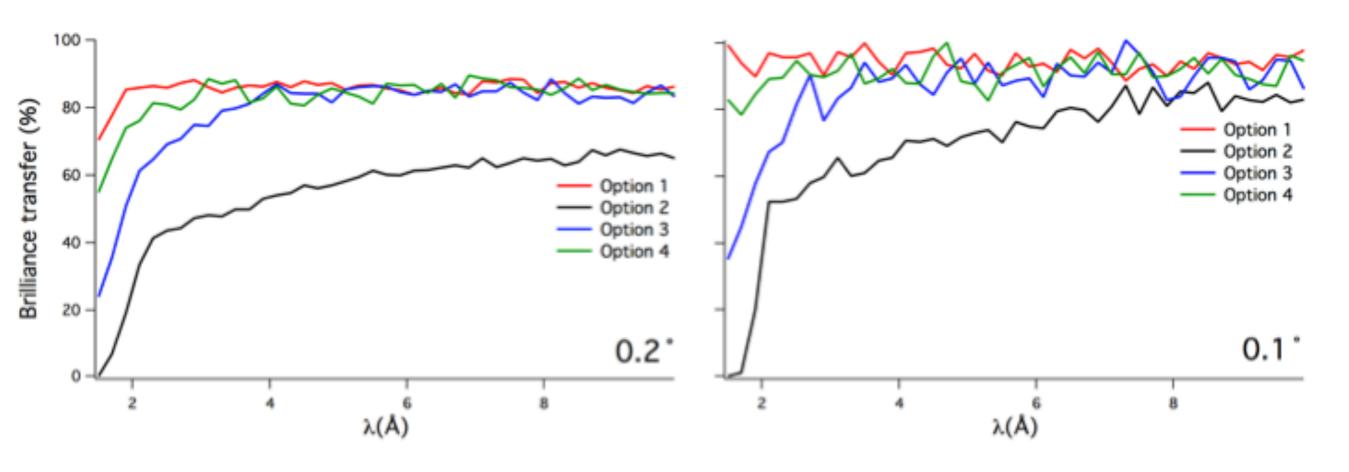
- 1.1. The BTS shall transport from the moderator a beam of neutrons to the sample at a distance that leads to a maximal wavelength uncertainty of 5% ($\Delta\lambda/\lambda$) for the detected neutrons using the full ESS pulse
- → ~150 m flight path
- 1.2. Rationale: A moderate wavelength resolution allows the full pulse to be used while conserving the advantage of TOF for the S/B (see 13.6.4 (5))
- 1.3. Verification: Measurement of the pulse length at sample

2. Beam size

- 2.1. The BTS shall transport from the moderator to the sample a beam of neutrons with maximum size (full width half maximum) of 5 ± 0.1 mm and minimum size of 0.2 ± 0.02 mm.
- → ~ 3 cm guide
- 2.2. Rationale: Matching the beam size to the sample size maximises the S/B (see 13.6.4 (3,5-6))
- ±0.1 K → temperature stability
- 2.3. Verification: Measurement of the beam intensity profile at sample

Optics options – performance

Damian Martin Rodriguez



Option 1: Curved in all the guide length

Option 2: Double Bounce mirror

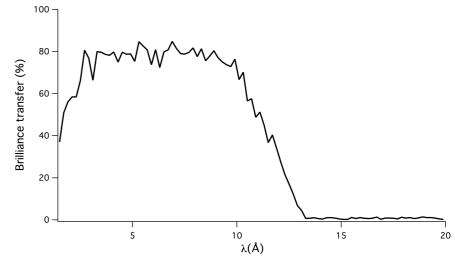
Option 3: Curved inside the bunker

Option 4: Curved inside bunker, optimised for maximum brilliance transfer at 2Å



Optics overview

Curved inside bunker, optimised for maximum brilliance transfer at 2Å



- Monolith insert horizontally straight, vertically tapers from 31 mm to 46 mm, m = 2 horizontal, m = 1 vertical
- 1.2 km curvature radius within bunker
- m = 2.2 on the curve, otherwise m = 1
- Line of sight lost at 31.5 m from the moderator
- Straight guide up to 154.1 m from the moderator, m = 1
- Frame overlap mirror for $\lambda > 10 \text{ Å}$



Optics concept choice – pros

Option 4: Curved inside bunker, optimised for maximum brilliance transfer at 2Å

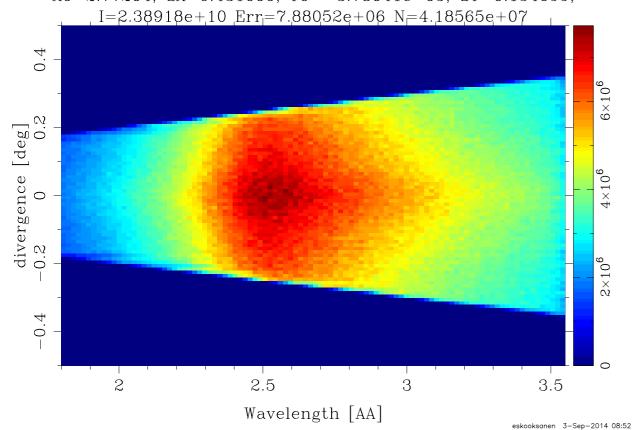
- Acceptable performance for ±0.2° divergence at <
 2 Å
- Good performance all round for ±0.1° divergence this range is more typical for experiments
- Loss of line-of-sight almost within bunker lower shielding cost & easier component maintenance
- Deflects the beam far enough from the sector centreline to allow two beams to be extracted from the same beamport



Chosen concept – verification

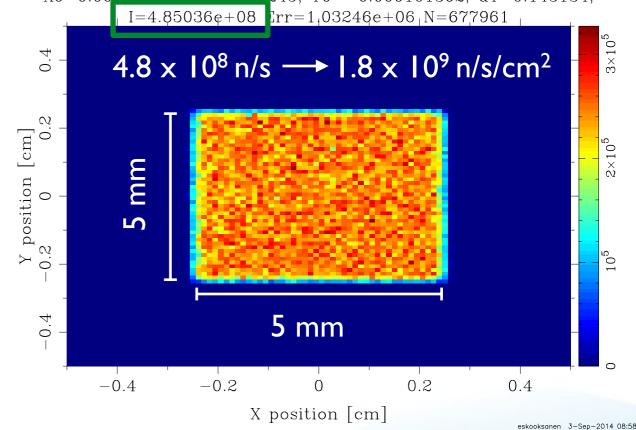
Divergence vs. wavelength at the end of the guide

3 [/Users/eskooksanen/Simulations/140819_test_2/PostStraightGuide2_X0=2.77264; dX=0.431066; Y0=-3.78641e-05; dY=0.154699;



Beam profile at sample

Sample [/Users/eskooksanen/Simulations/140819_test_2/Sample_psd.s X0=0.000665833: dX=0.14245; Y0=-0.000101362; dY=0.143134;





Design drivers

- Choppers are for wavelength selection
- Width and position of wavelength band have to be adjustable
- Transmission has priority
- Frame overlap should be suppressed
- Penumbra should be minimized
- Avoid choppers in bunker



Design drivers

- Choppers are for wavelength selection
- Width and position of wavelength band have to be adjustable
- Transmission has priority
- Frame overlap should be suppressed
- Penumbra should be minimized
- Avoid choppers in bunker

Always 14Hz



Design drivers

- Choppers are for wavelength selection
- Width and position of wavelength band have to be adjustable
- Transmission has priority
- Frame overlap should be suppressed
- Penumbra should be minimized
- Avoid choppers in bunker

Always 14Hz

Change of phase and variable openings



Design drivers

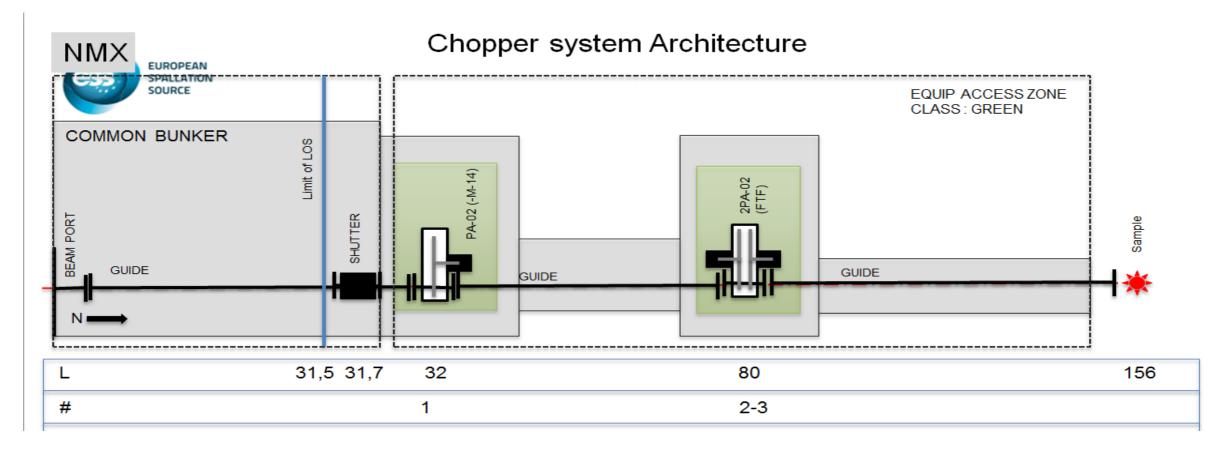
- Choppers are for wavelength selection
- Width and position of wavelength band have to be adjustable
- Transmission has priority
- Frame overlap should be suppressed
- Penumbra should be minimized
- Avoid choppers in bunker

Always 14Hz

Change of phase and variable openings

Chopper or mirror

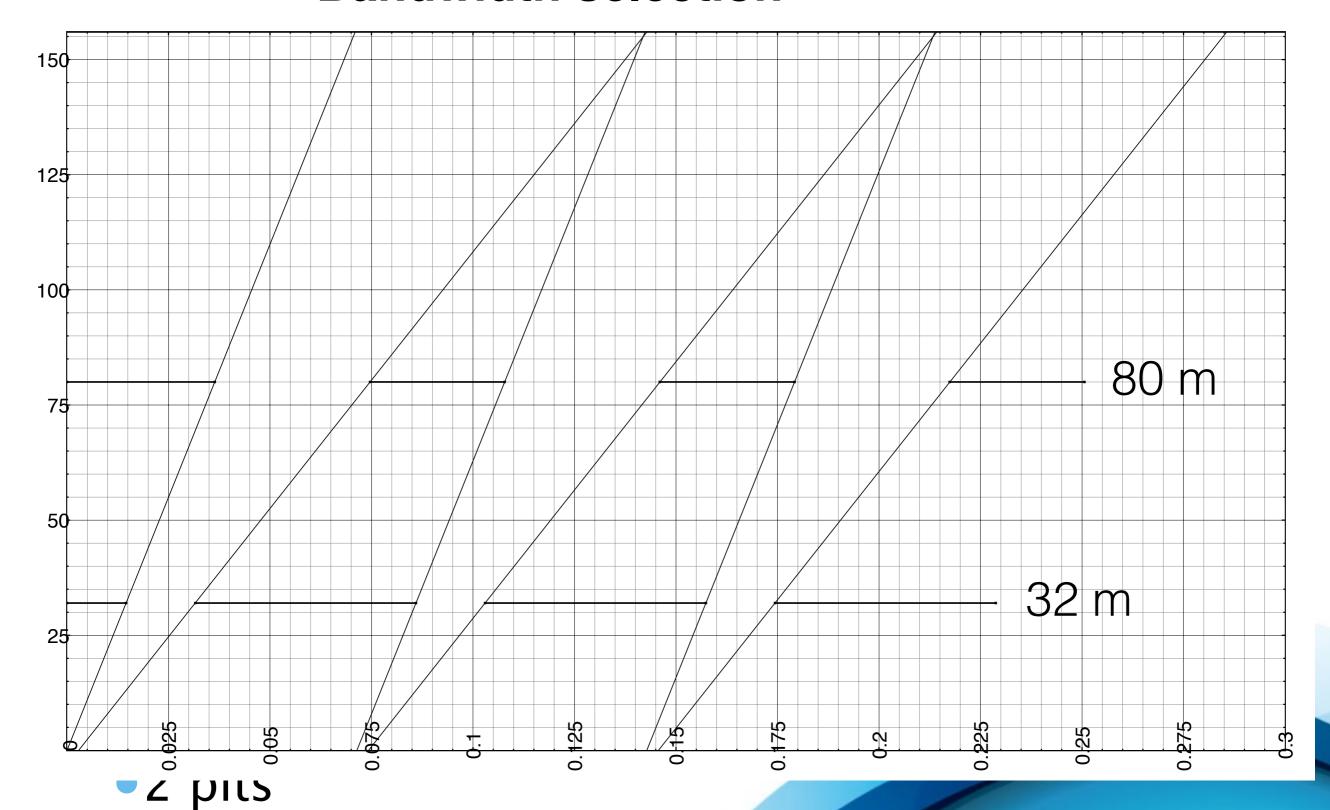




- 3 chopper axis (2 assemblies)
- 1 single chopper axis
- •1 co-rotating double disc chopper
- 2 pits



Bandwidth selection



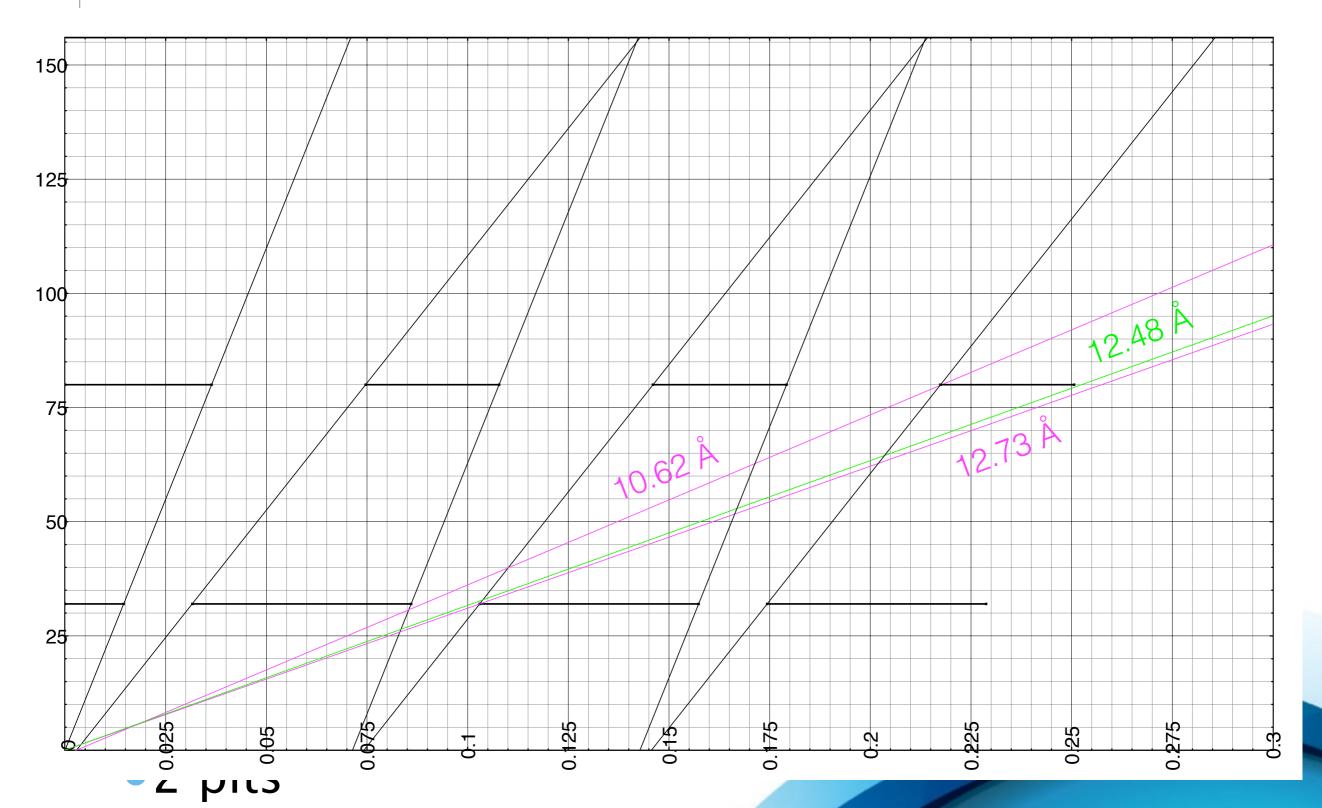


Choppers Frame overlap suppression



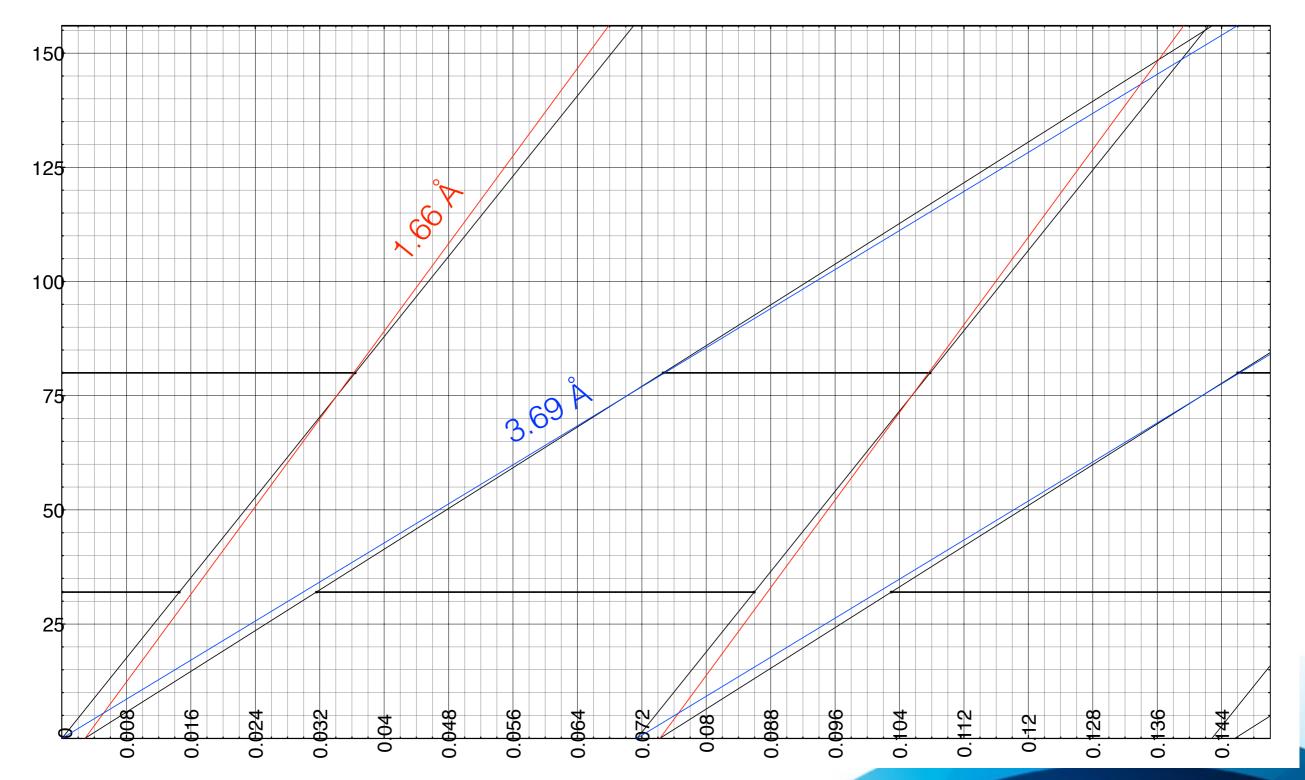


ChoppersFrame overlap suppression





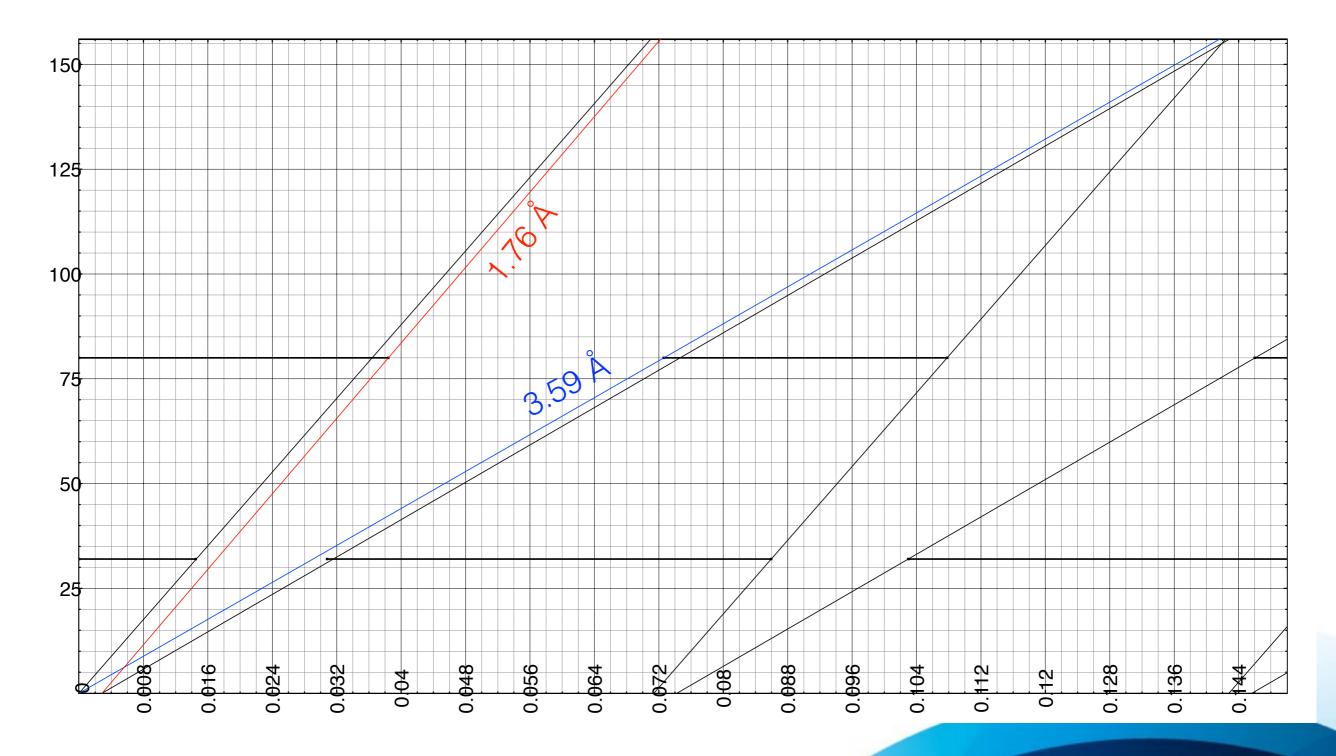
Choppers - Penumbra



1.8-3.55 Å nominal bandpass



Choppers – Penumbra



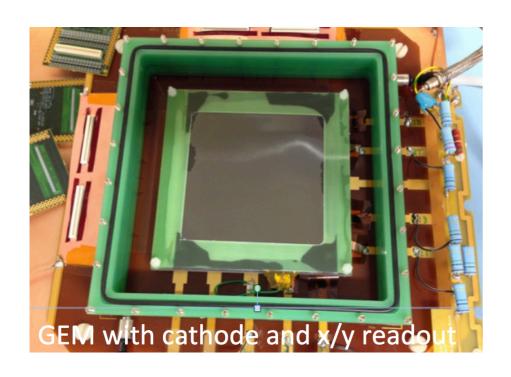
1.9-3.45 Å nominal bandpass

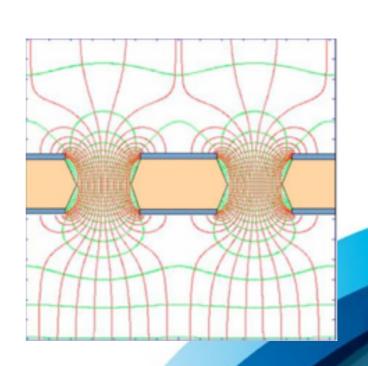


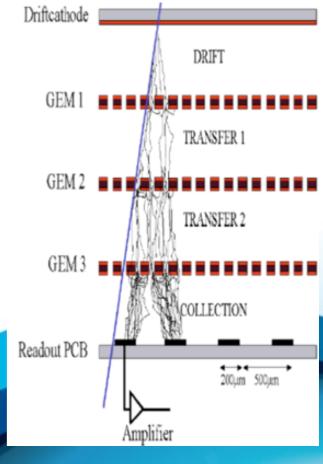
Detectors – technological risk and mitigation strategy

- R&D required to reach 0.2 mm spatial resolution with reasonable area and efficiency
- Gd coated micropattern (GEM) detectors promising prototypes developed at CERN
- GEM detectors widely used in particle physics

Large areas readily available



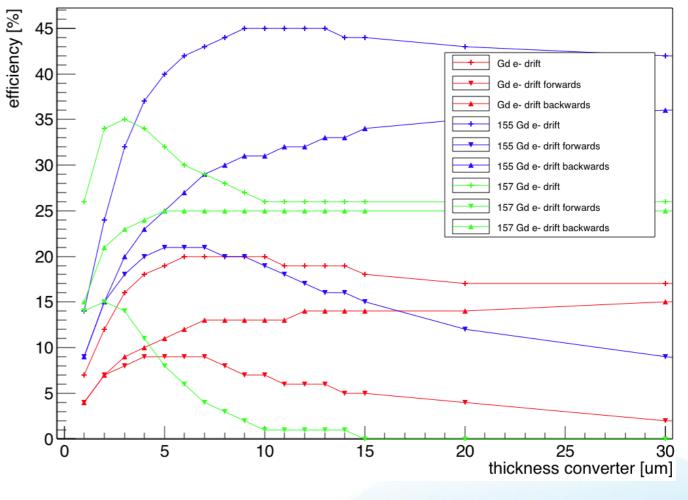






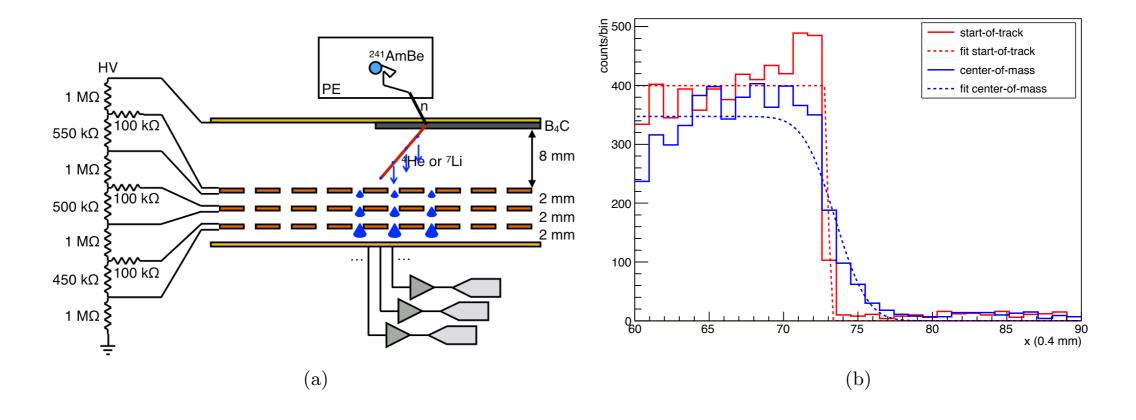
How detect neutrons with a GEM?

- Neutron converter on cathode
- ¹⁰B has been demonstrated to 45 deliver spatial resolution, but 40 low efficiency
- Gd has much higher absorption cross section, but conversion electrons are more difficult to detect
- Enriched ¹⁵⁵Gd would improve efficiency significantly





Spatial resolution – µTPC



- \bullet Spatial resolution of $<100~\mu m$ was achieved with a $^{10}B\text{-}GEM$
- Based on the µTPC concept (algoritms from CERN)



Backup options

- 10B-GEM has been demonstrated, but efficiency is low
- Anger cameras not affordable
- ³He filled MSGCs could be a last resort with reduced area and compromised resolution



Sample positioner



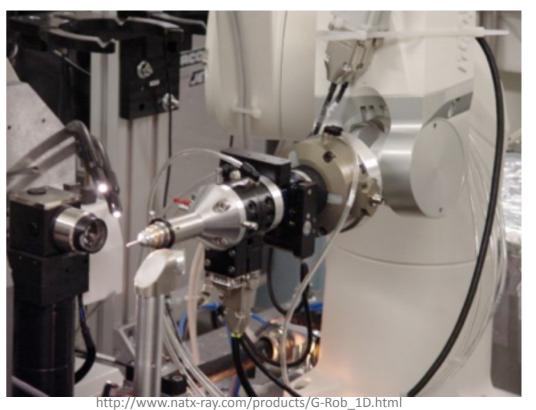
Robotic goniometer

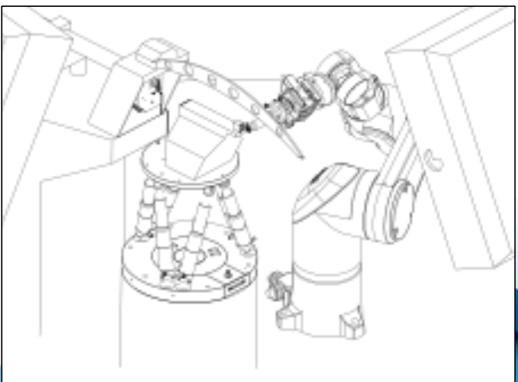
- Six axis industrial robotic arm
- Slim profile
- Tool change.
- Stereoscopic cameras
- Sphere of confusion R< 0.03 mm
- Following error < 6 mdeg

Benefits

- Three clicks sample centering.
- Neutron beam imaging at sample.
- Multiple sample interfaces on tool changer.

Robotic goniometer allows choice of sample rotation axis direction



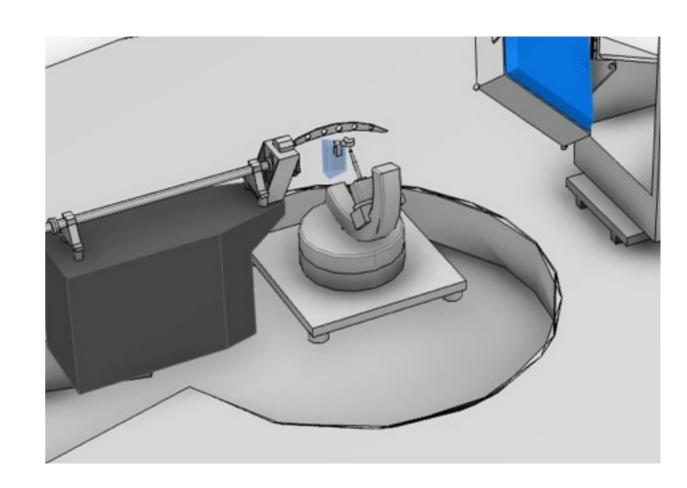




Sample positioner – backup

Conventional goniometer

- Custom solution could be built in-house
- Bulky with limited access to upper hemisphere
- Small cost difference to robotic option – more integration required

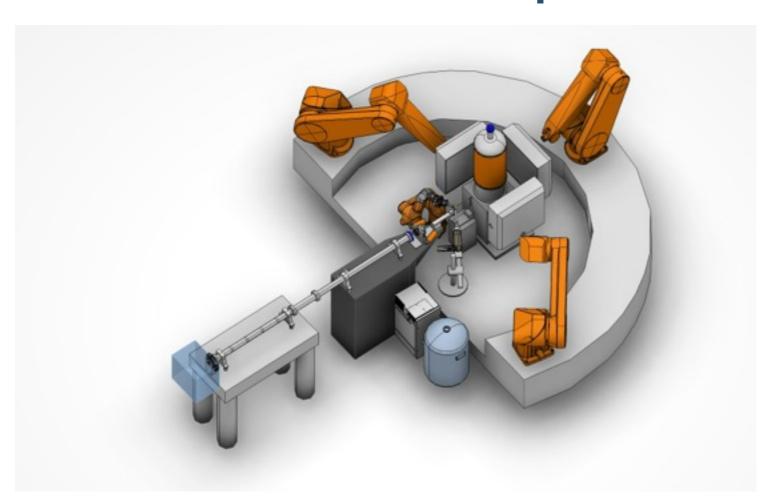






Detector positioners - robotic option



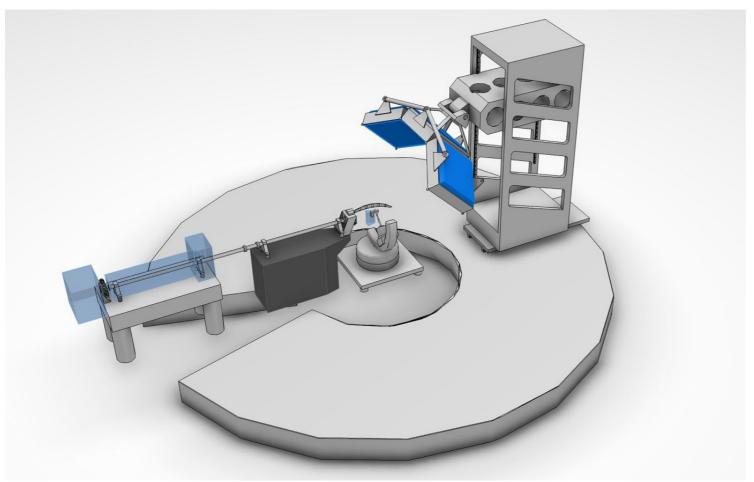


Three 60 x 60 cm detectors with 0.2 mm spatial resolution Sample-detector distance (0.2-1.0 m) and 2θ angle (0-110°) variable

- Solid angle coverage can be traded for unit cell size
- Allows an alternative sample position for bulky sample environments



Detector positioners – linear mechanics option



Three 60 x 60 cm detectors with 0.2 mm spatial resolution Sample-detector distance (0.2-1.0 m) and 2θ angle (0-110°) variable

- Could be implemented in-house
- < 20% cost difference to robotic option</p>
- Limited flexibility with bulky sample environments



Questions?