Principles of X-ray and Neutron Scattering

Lecture 12: Neutron Instrument Development

15. 02. '24

Lectures by: Prof. Philip Willmott, Prof. Johan Chang and **Dr. Artur Glavic**

Course Outline

Monday	Tuesday	Wednesday	Thursday	Friday
Lecture 1 10-10h45 Philip	**Lecture 4** 10-10h45 Philip	**Lecture 7** 10-10h45 Artur	**Lecture 10** 10-10h45 Artur	**Lecture 13** 10-10h45 Johan
Lecture 2 11-11h45 Philip	**Lecture 5** 11-11h45 Philip	**Lecture 8** 11-11h45 Artur	**Lecture 11** 11-11h45 Artur	**Lecture 14** 11-11h45 Johan
Lunch - Mensa	**Lunch - Mensa**	**Lunch - Mensa**	**Lunch - Mensa**	**Lunch - Mensa**
Lecture 3 13h00-13h45 Philip	**Lecture 6** 13h00-13h45 Philip	**Lecture 9** 13h00-13h45 Artur	**Lecture 12** 13h00-13h45 Artur	**Lecture 15** 13h00-13h45 Johan
		Exercise Class 14h30-16		Exercise Class 14h30-16

X-ray scattering

Neutron Scattering

Resonant x-ray scattering

Neutron Lectures:

7: Neutrons & Scattering to Determine Structure
8: Inelastic Neutron Scattering to Investigate Dynamics
9: Magnetic Scattering
10: Neutron Polarization Analysis
11: Studying quantum matter for nanoscale applications
12: Neutron Instrument Development

Lecture 12: Neutron Instrument Development

Theoretical Background

- Fundamental limits, trade-off between resolution and intensity
- Instrument simulations and neutron optics

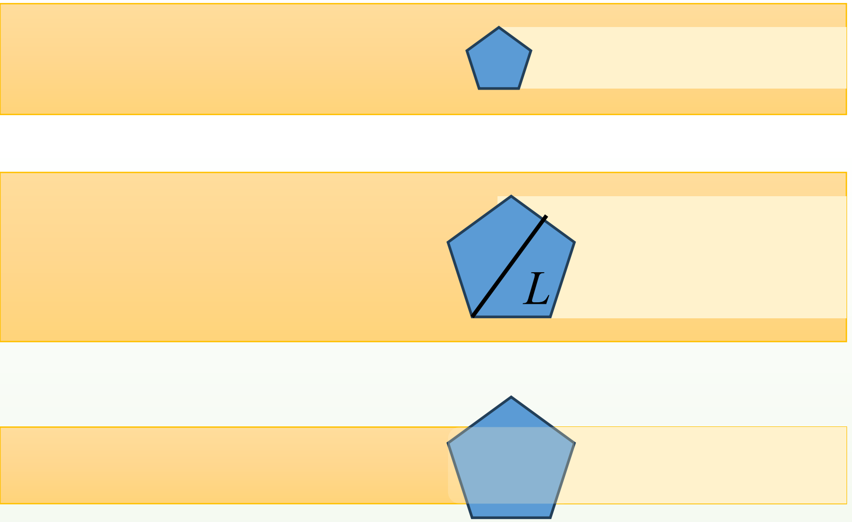
Practical Implementation

- Modeling guides and spurious scattering
- Neutron guides and focusing optics

Example Application

- Specialized optical devices
- Focusing reflectometry for small samples (Estia @ ESS)

Intensity in a (Neutron) Scattering Experiment

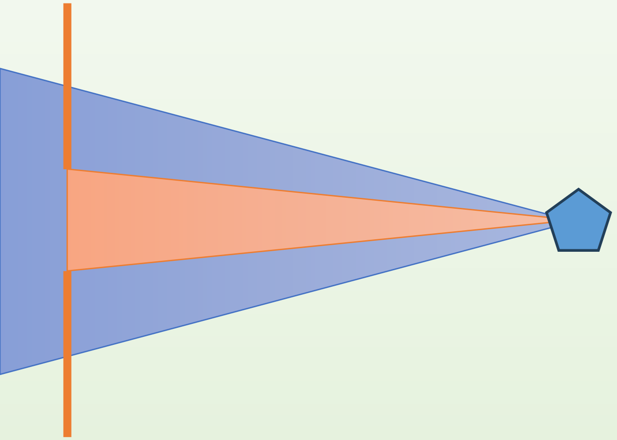


- The scattering signal scales with the number of atoms and thus the sample volume within the beam

➔ Sample diameter L³ determines signal

- In first approximation the beam intensity scales linearly with wavelength and angular resolution

➔ Total intensity scales as:

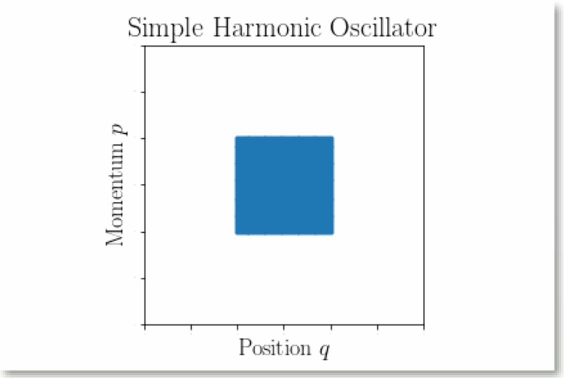


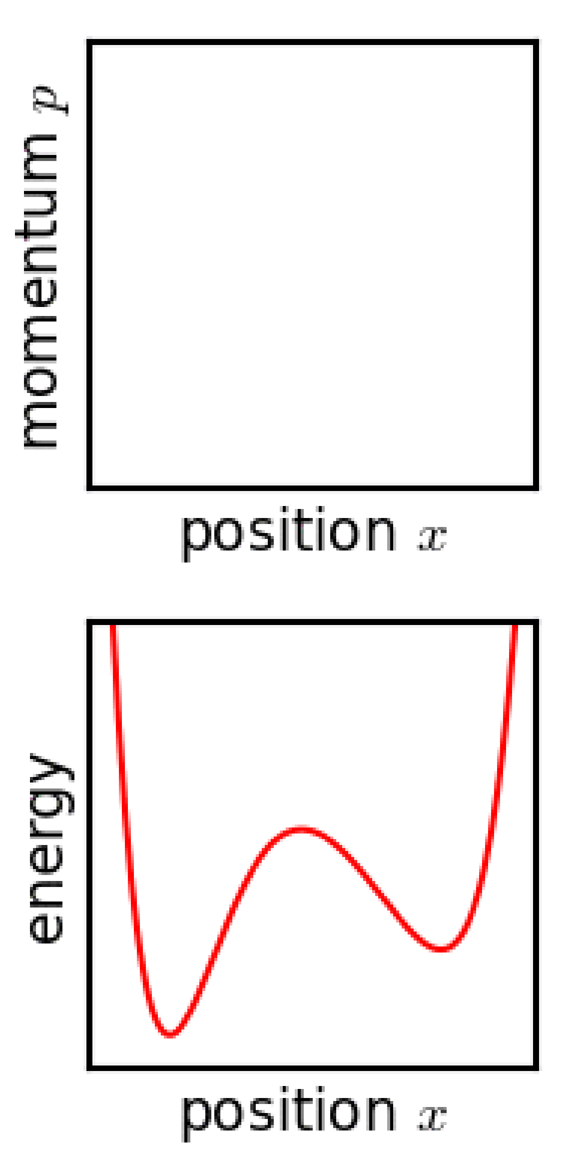
$$I \propto \frac{L^3}{\Delta\Theta_x \Delta\Theta_y \Delta\lambda}$$

Liouville's theorem

The phase-space volume of a closed system is constant

$$\Delta p_i \Delta q_i = \mathrm{const}$$





➔The brilliance (neutrons/(time · area · solid angle)) can never be increased (but decreased by losses as e.g. absorption)

To increase instrument performance you can only do 3 things:

1. Generate more neutrons (source itself)
2. Relax resolution (where not necessary)
3. Improve efficiency
   (usable neutrons detected / neutrons generated)

Optimizing Neutron Instruments

Relax resolution (where not necessary)

$$I \propto \frac{L^3}{\Delta\Theta_x \Delta\Theta_y \Delta\lambda}$$

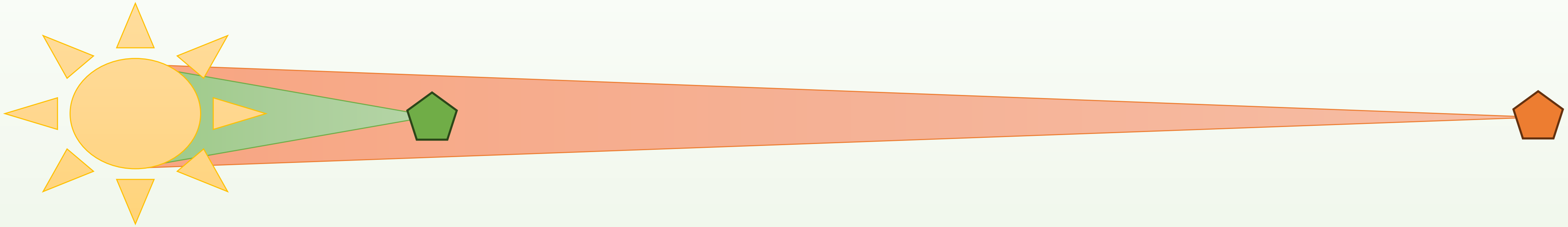
Neutron instruments are optimized for particular experiments to be able to relax resolution where ever possible!

Experiment	Signal	Vertical Res.	Horizontal Res.	Wavelength Res.	Detector Area
Single crystal diffraction	high	medium	medium	medium-heigh	small
Powder diffraction (1D-det.)	medium	low	high	high	medium
Powder diffraction + texture	medium	medium	high	high	large
3-axes spectroscopy	low	low	medium	high	small
ToF spectroscopy	low	low	medium	medium	large
SANS	medium	high	high	low	medium
Reflectometry	low	low	high	low-medium	small
Spin-echo	low	low	low	very-high*	small
Back-scattering spec.	low	low	low	very-high	large

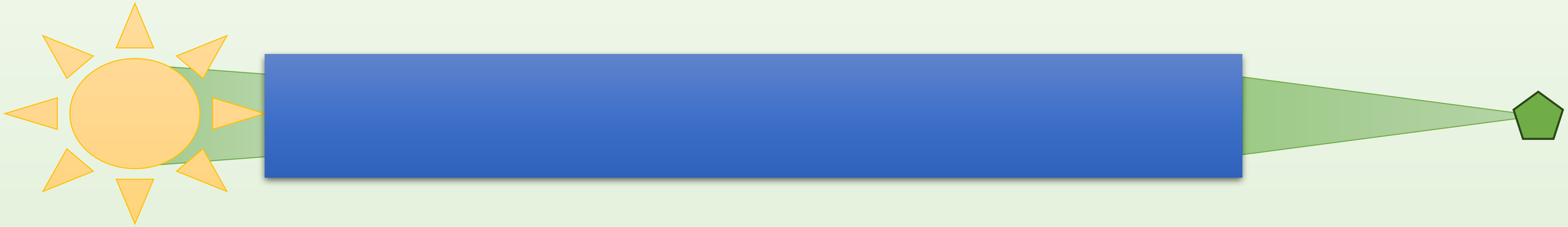
Optimizing Neutron Instruments

How to get the divergence you want?

The size of the neutron source is limited, thus a divergent beam is not possible with a direct view alone.

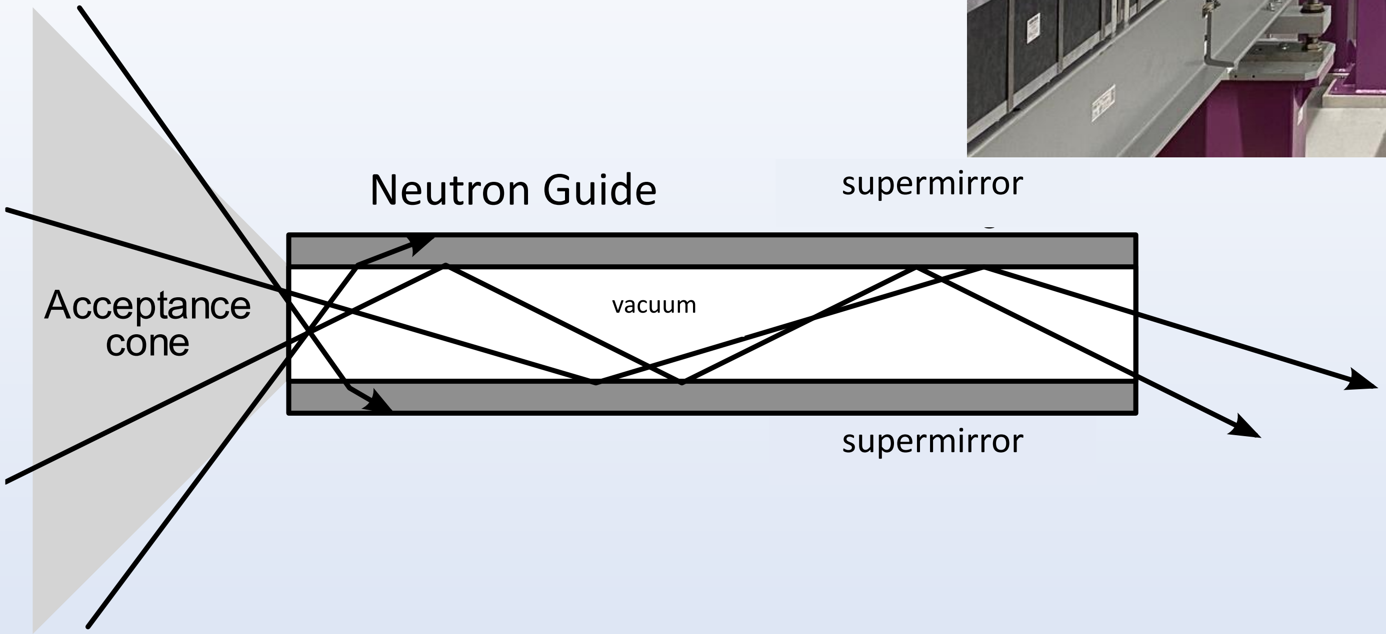


Neutron guides to the rescue…



How Neutron Guides Work

Neutron guides use reflective surfaces to transport beams over long distances (10-150 m)



Neutron Supermirrors

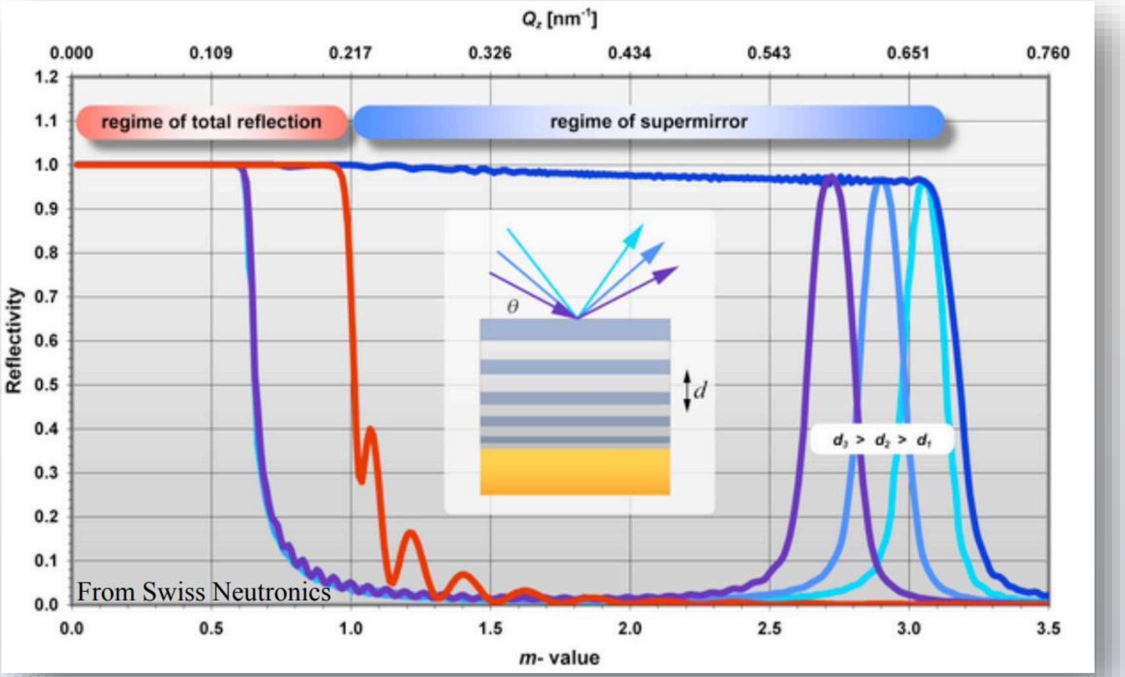
- Alternating layers with large (magnetic) contrast
    - Ni (ρ=9.4 Å^{-6})/Ti (ρ=-1.9 Å^{-6})
    - Fe (ρ=8.0±6.3 Å^{-6})/Si(ρ=2.1 Å^{-6})

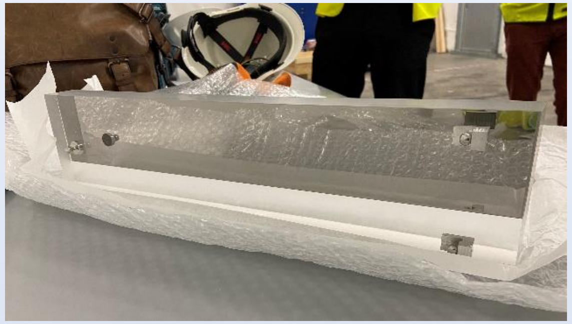
      ➔ $\Delta\rho_{\uparrow}$= 12.2 Å^{-6} / $\Delta\rho_{\downarrow}$= -0.4 Å^{-6}

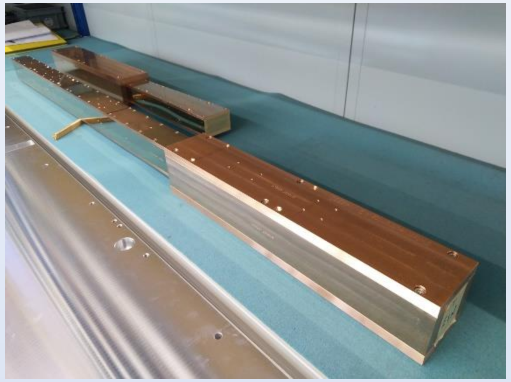
- Increase bi-layer thickness from substrate to surface

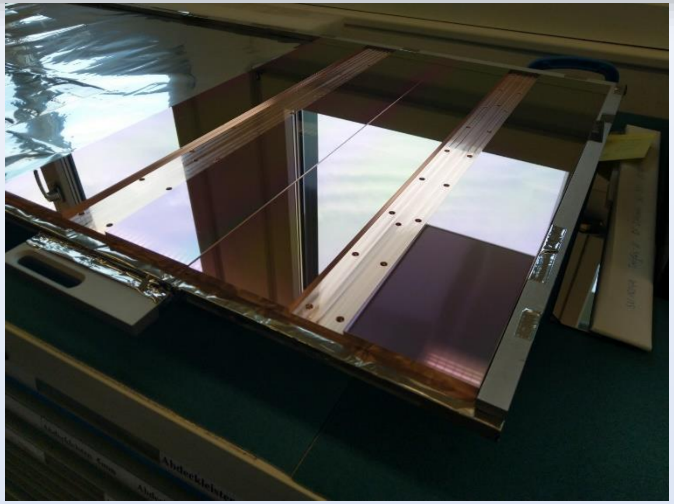
➔ Extent angle of (almost) total reflection multiple times

- m-value defined as relative angle compared to critical angle from natural nickel







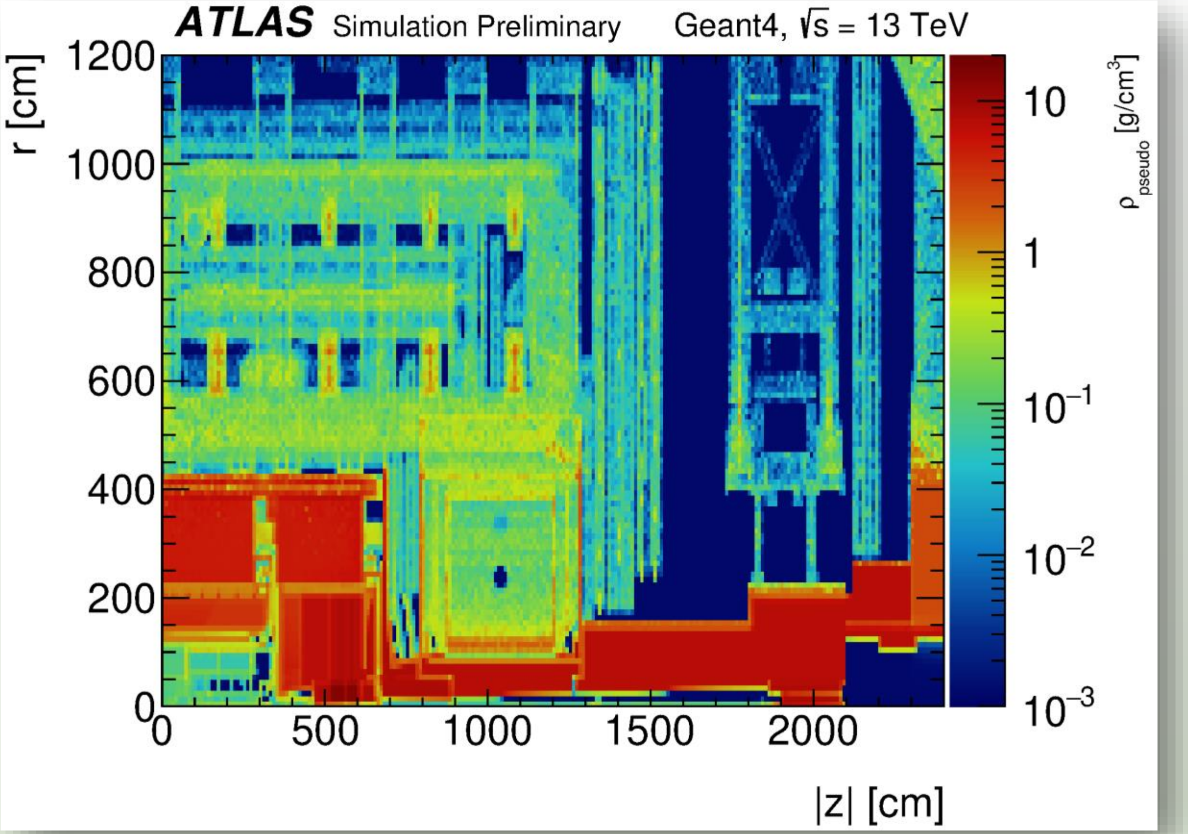


Modeling Neutron Instruments - Why Ray-Tracing?

Improve efficiency

Problem:

- How does radiation pass through a complex real-world geometry



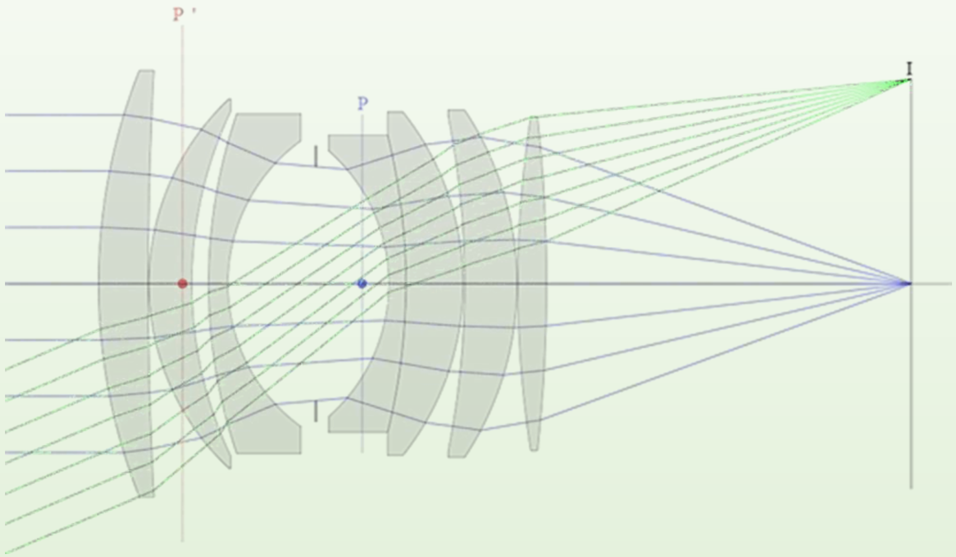
Modeling Neutron Instruments - Why Ray-Tracing?

Problem:

- How does radiation pass through a complex real-world geometry

Known prerequisites:

- Wavelength much smaller than features of the geometry
- All relevant interactions between the radiation and material
- Material parameters and extension in space



Modeling Neutron Instruments - Why Ray-Tracing?

Problem:

- How does radiation pass through a complex real-world geometry

Known prerequisites:

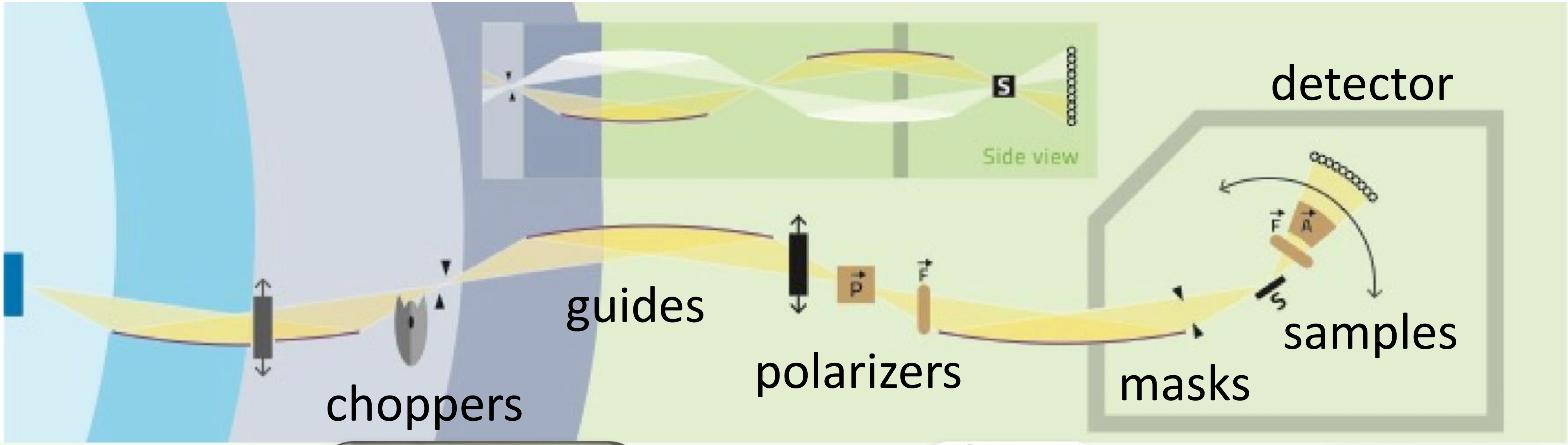
- Wavelength much smaller than features of the geometry
- All relevant interactions between the radiation and material
- Material parameters and extension in space

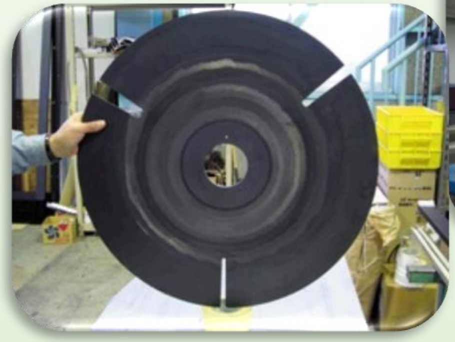
MC RT approach:

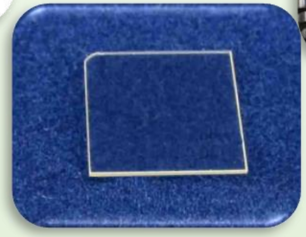
- Describe by particle rays
- Trace ray until interaction point, interact, repeat
- Approach to infinite rays is solution of the problem (multi dimensional integral)

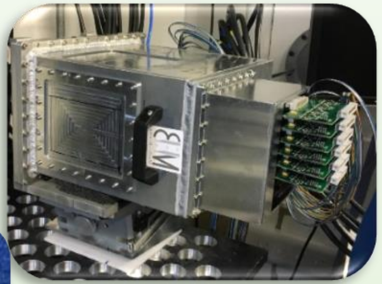
Modeling Neutron Instruments

MC ray-tracing simulations (e.g. McStas) describe full instrument & sample

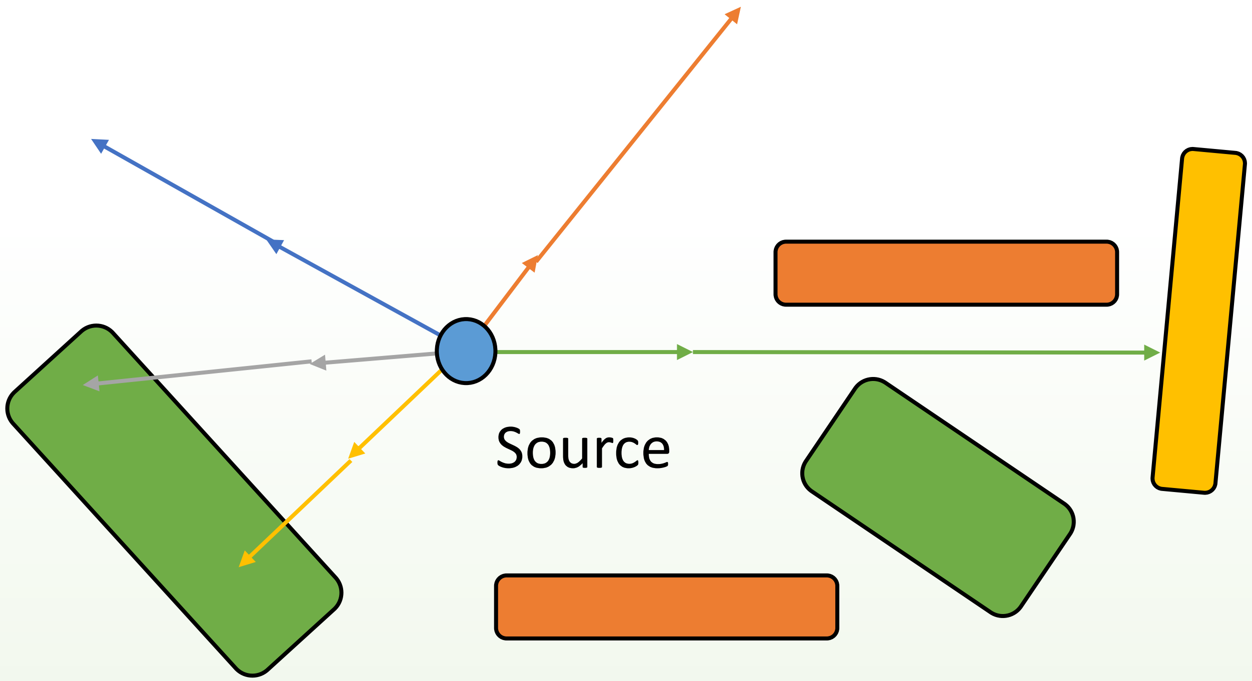








Ray-Tracing in Practice

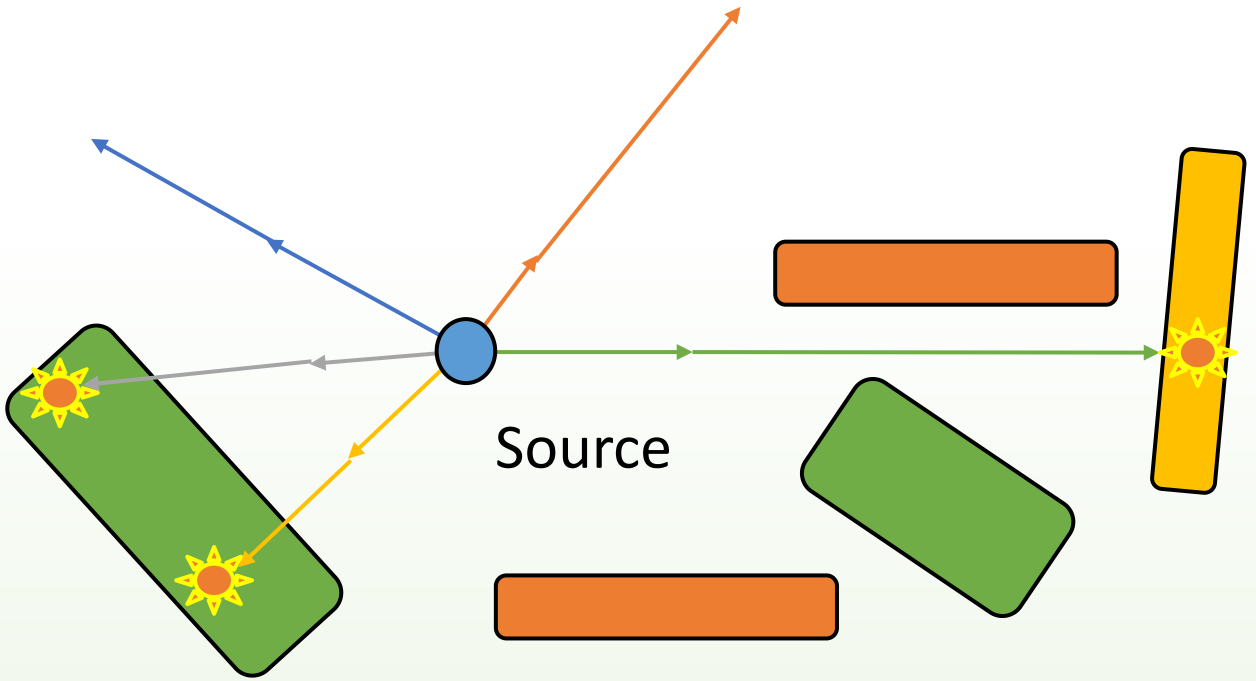


→ Particle ray with all relevant physical parameters:

- direction (x,y,z)
- energy
- polarization (px, py, pz)
- ....

1. Choose random direction and energy (from distribution)
2. Trace trajectory until next point of interaction

Ray-Tracing in Practice



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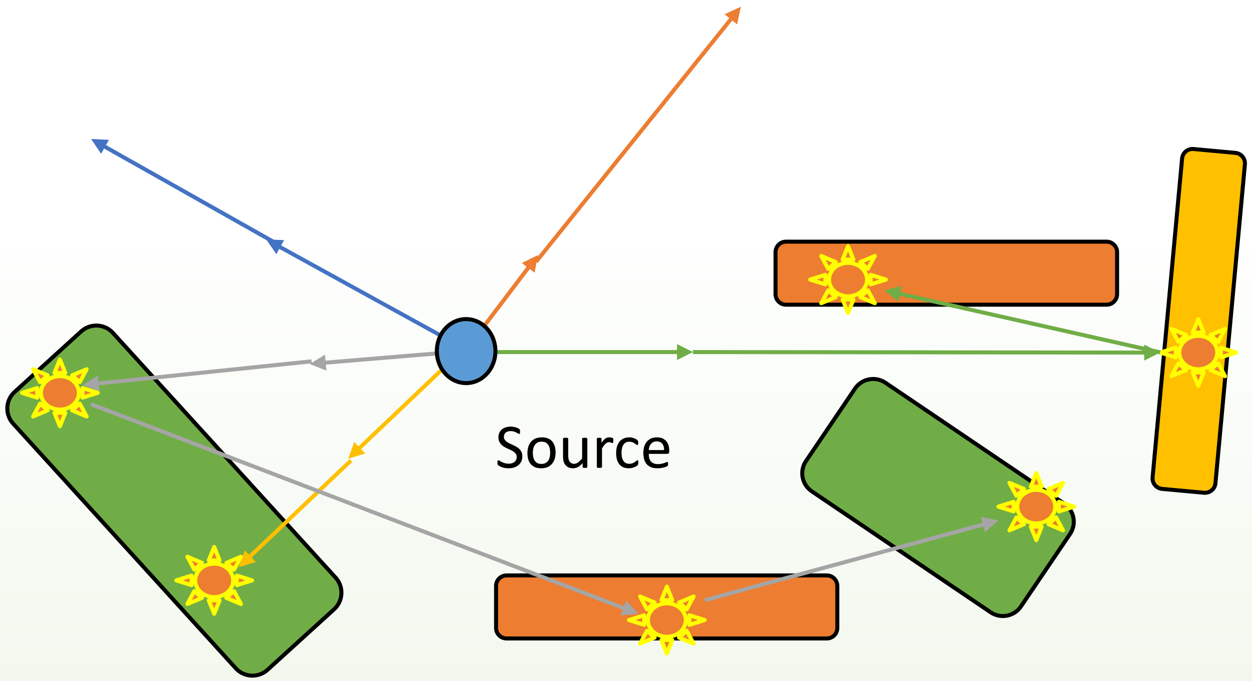
3. Choose random possible interaction and/or outcome energy/direction

Ray-Tracing in Practice

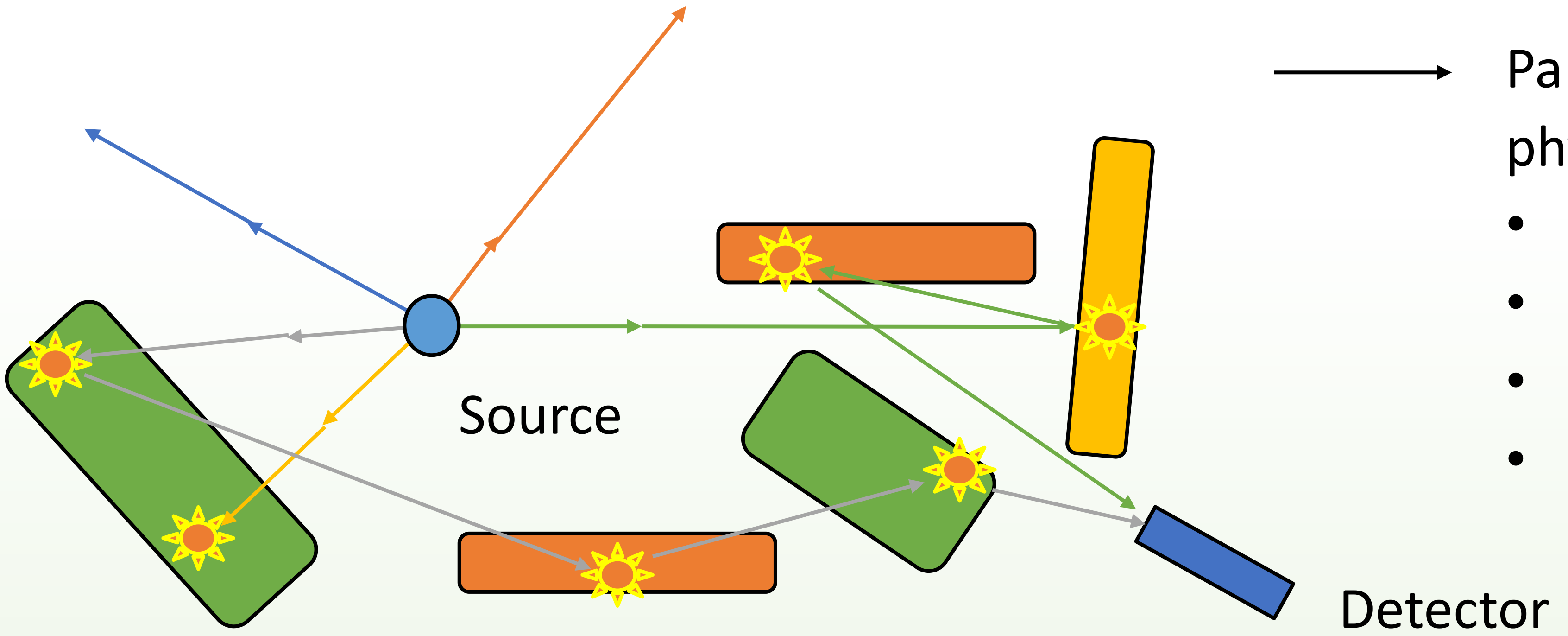


→ Particle ray with all relevant physical parameters:

- direction (x,y,z)
- energy
- polarization (px, py, pz)
- ….

1. Choose random direction and energy (from distribution)
2. Trace trajectory until next point of interaction
3. Choose random possible interaction and/or outcome energy/direction
4. Trajectory ends or continues with 2.

Ray-Tracing in Practice



Particle ray with all relevant physical parameters:

- direction (x,y,z)
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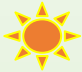
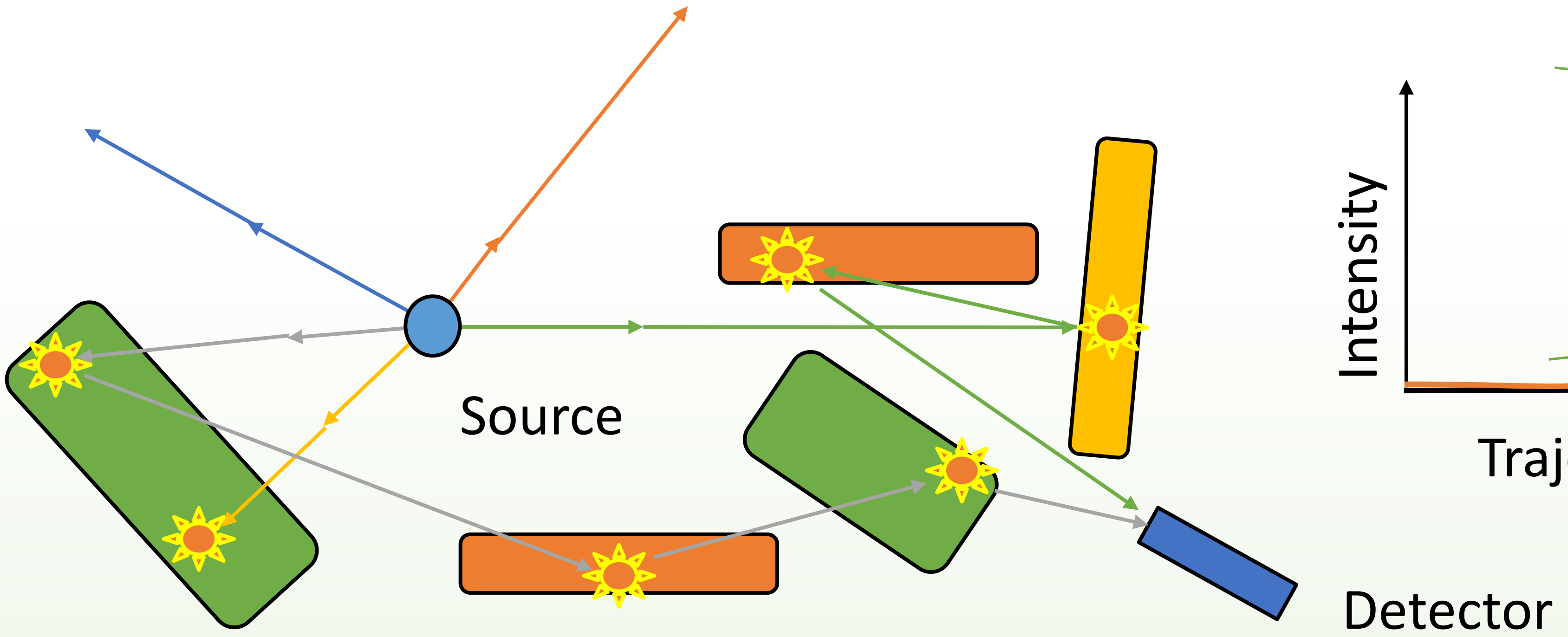
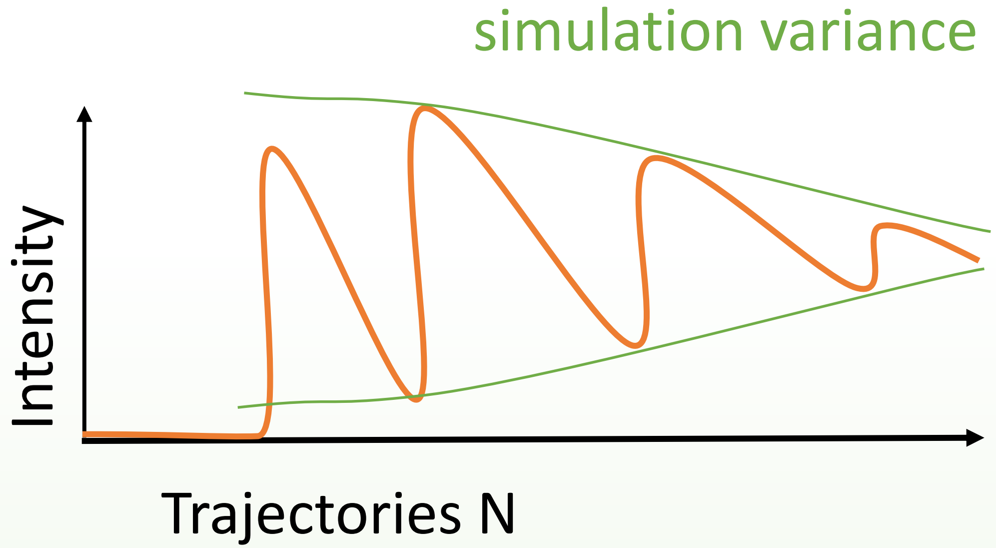
3. Choose random possible interaction and/or outcome energy/direction 
4. Trajectory ends or continues with 2.
5. Record all trajectories at location (detector/tally) of interest

Variance Problem



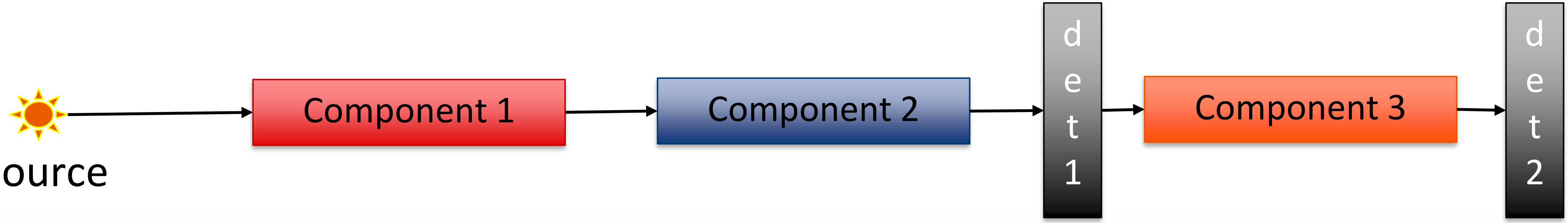


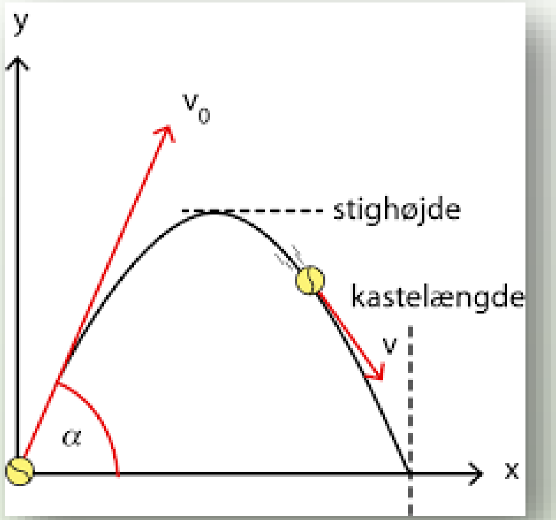
- 3D space is large, detector covers very small region
- Many possible reactions, any absorbed trajectory is lost
- Some problems; reactions that are important have low likelihood

➔ Probability to record trajectory can be very low (1:10^{20} source particles)

Computation can be impossible or very expensive to collect sufficient trajectories

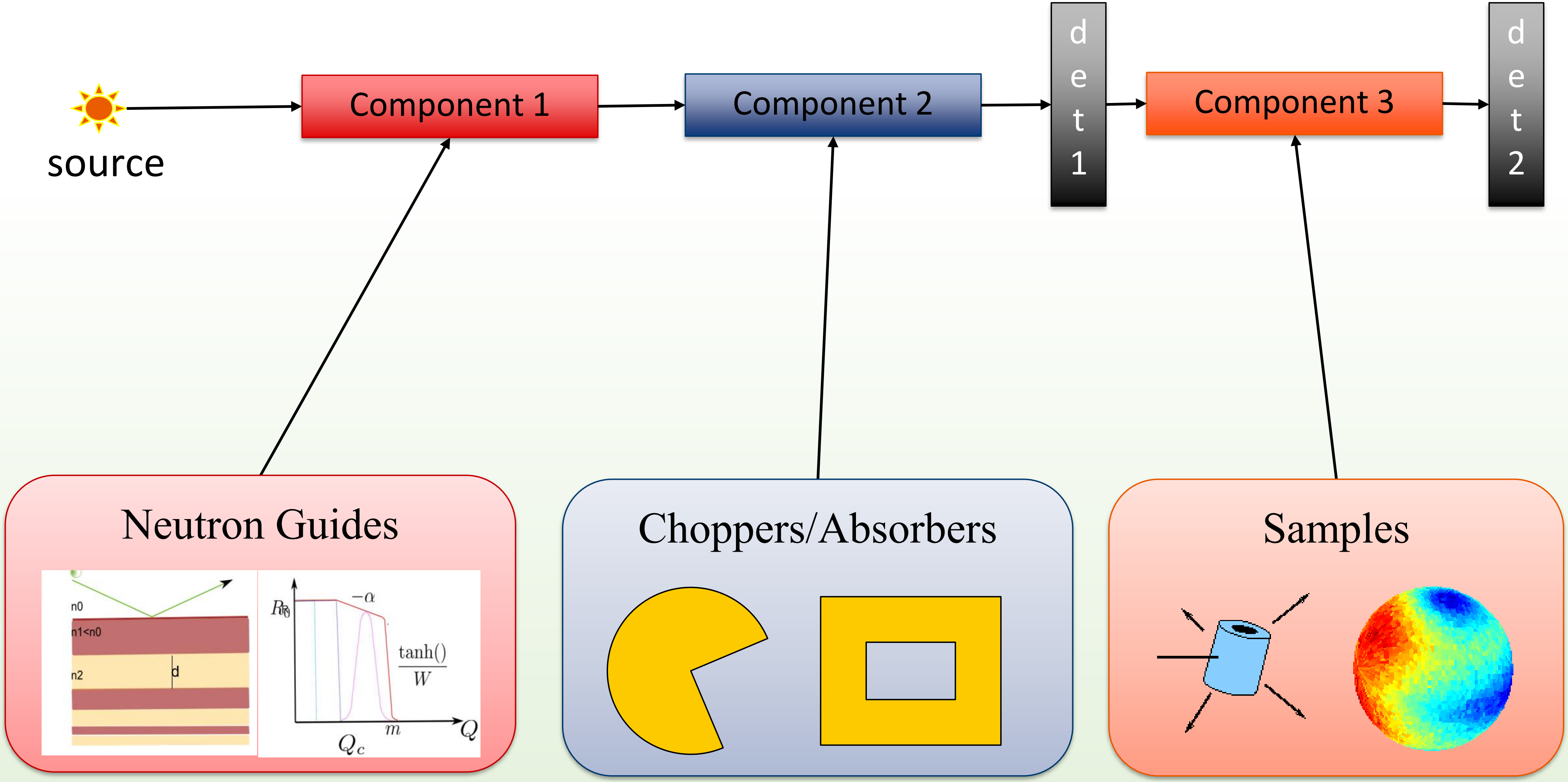
Neutronics Calculations: McStas



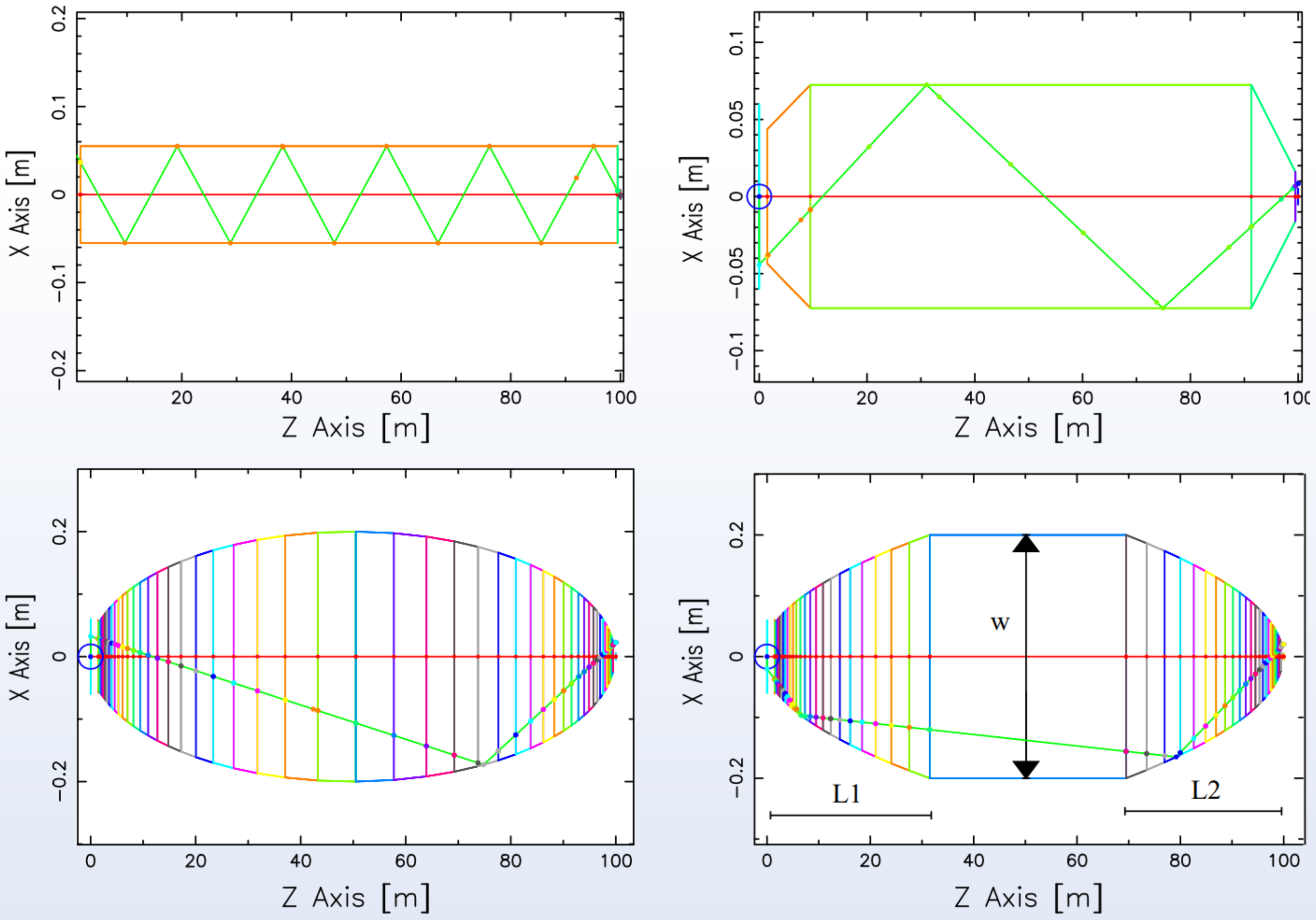


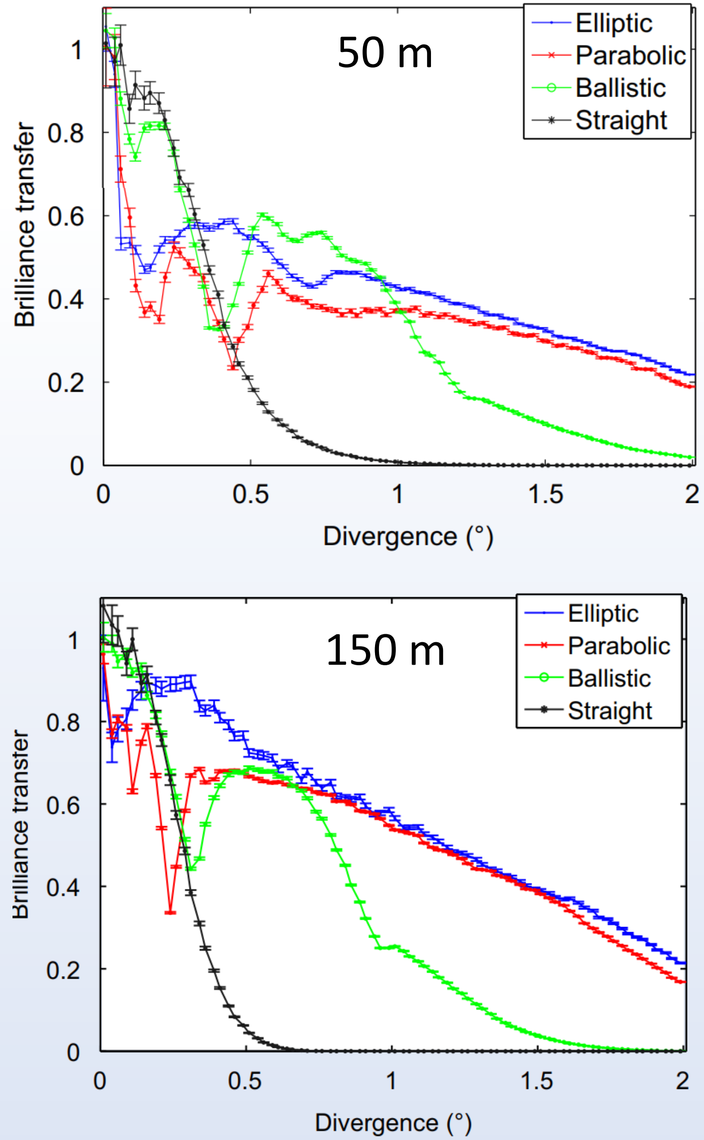
- Limit source particles to desired wavelength range and tight directionality (what would hit the first guide)
- Linear sequence of components connected
  - Large reduction in possible interaction pathways
  - Each component defines its own “physics”
  - No cross-talk (can be problematic in some cases)
- For cold neutrons, non-straight trajectories (gravity) has to be taken into account

Neutronics Calculations: McStas



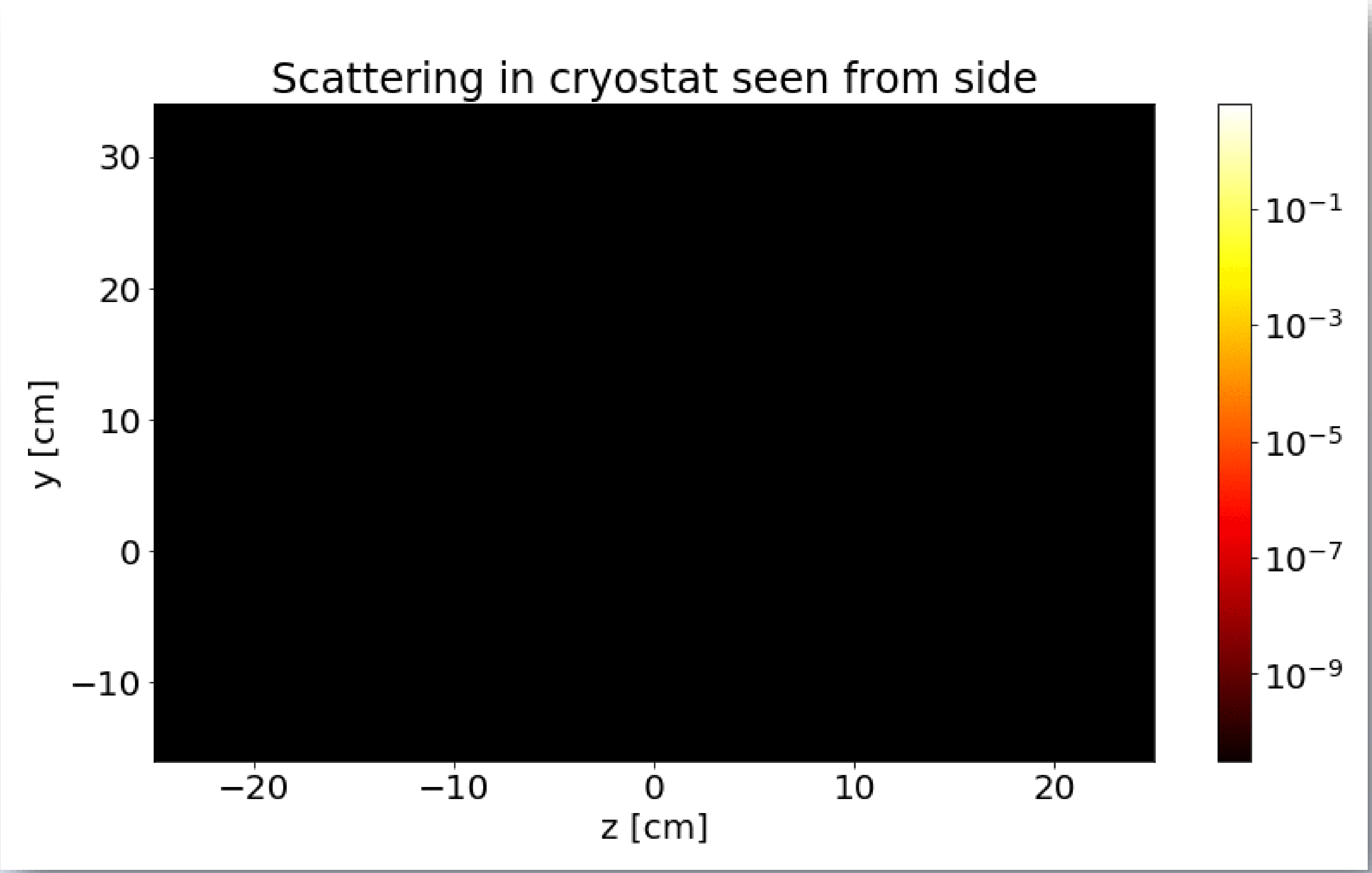
McStas to Simulate Neutron Guide Geometry





K. H. Klenø, *et al.*, Nuc. Inst. Meth. A, **696** 75-84 (2012)

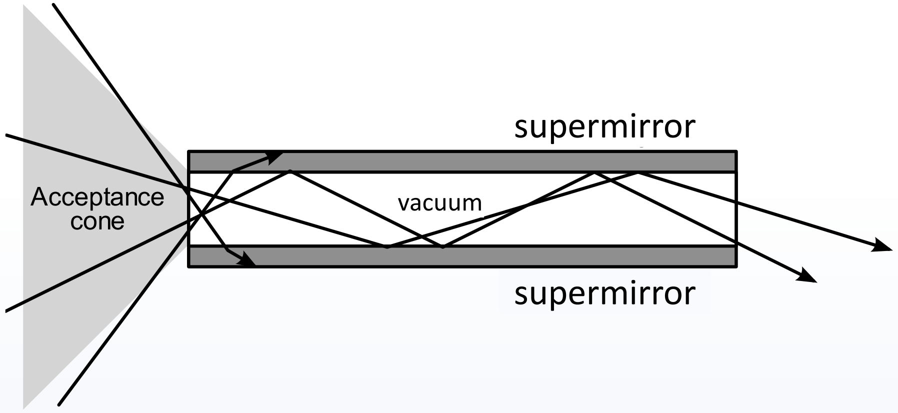
McStas to Simulate Spurions



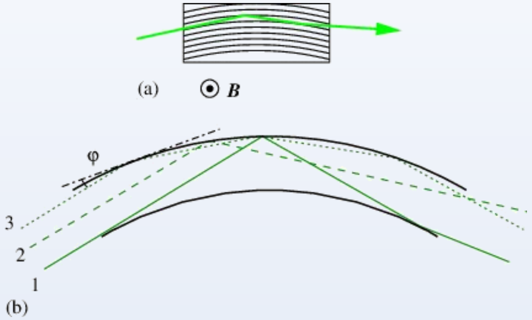
cryomagnet

Neutron Optical Elements

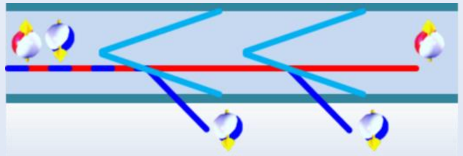
Neutron Guide



(polarizing) bender

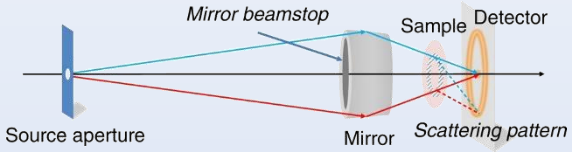


transmission polarizer V-cavity

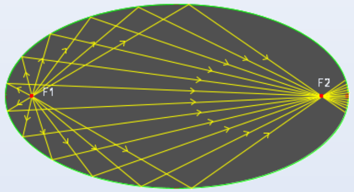


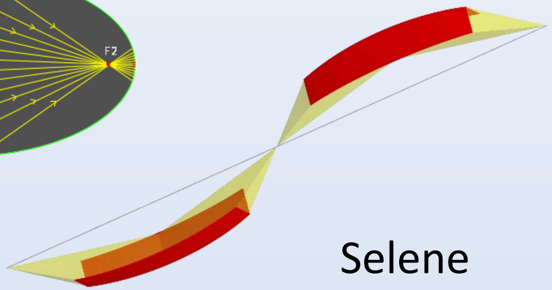
focusing optics

Wolter-optic



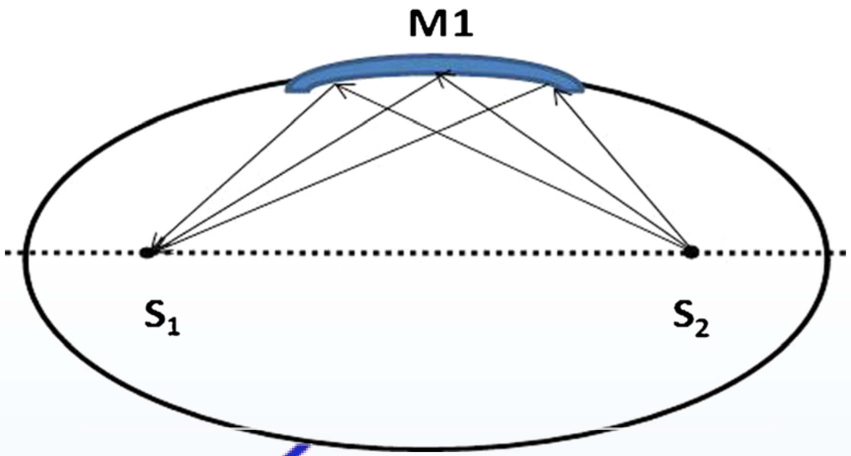
Ellipse

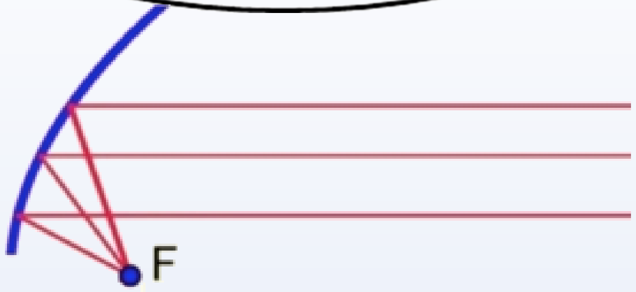




Selene

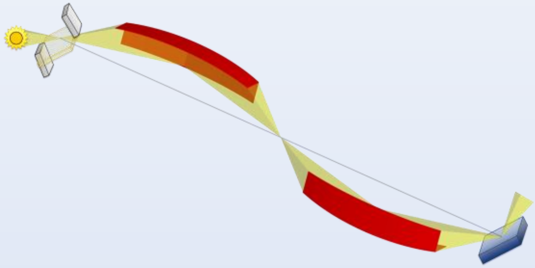
Neutron Focusing Elements



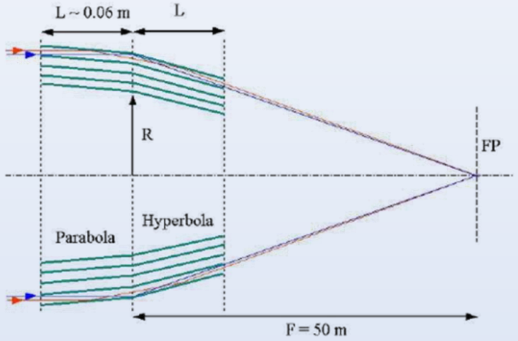


Ellipse:
All beams from focus S_1 are reflected to focus S_2

Parabola:
All beams from focus F are parallel



2xellipse (Selene)

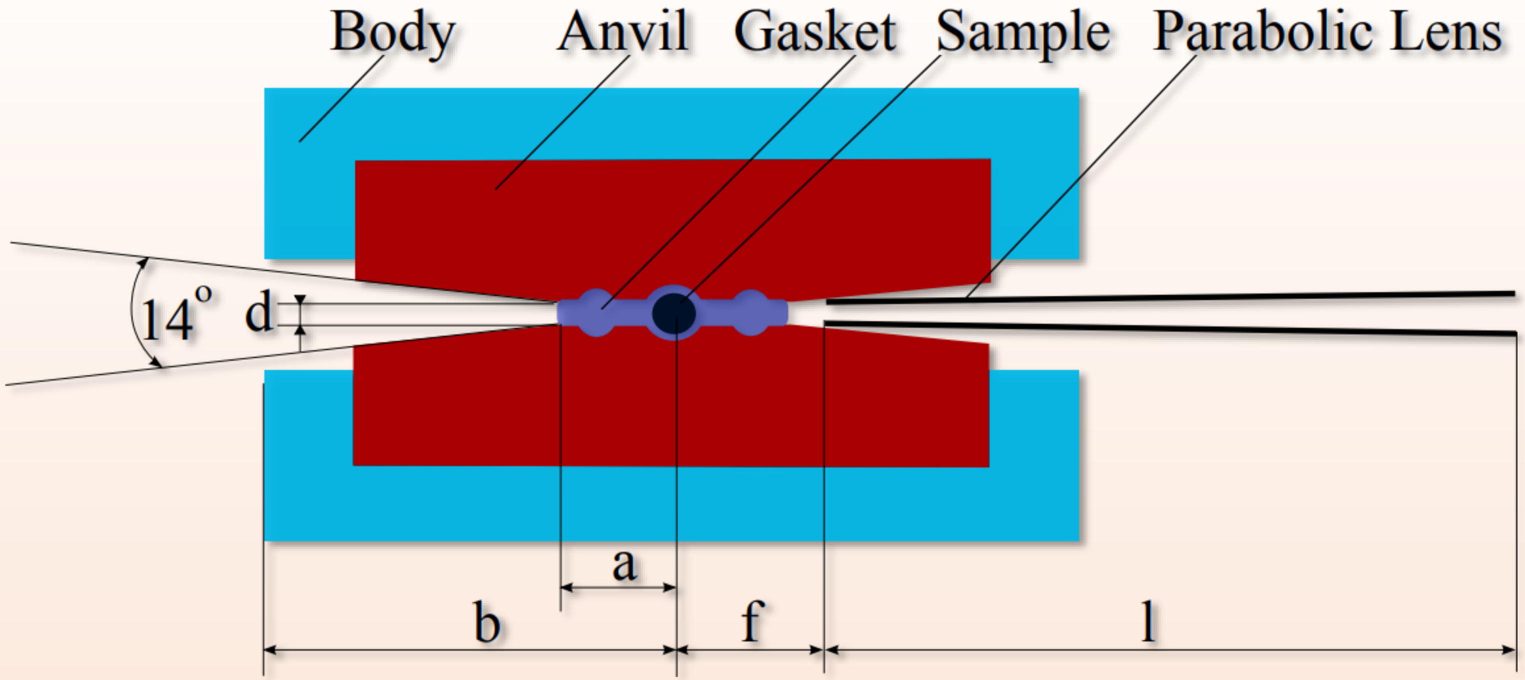


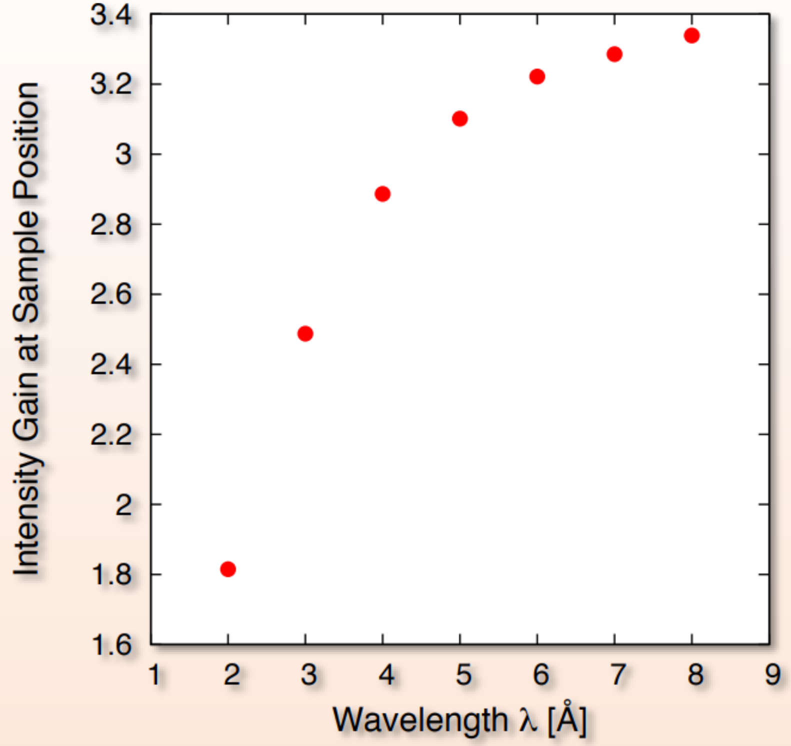
nested (Wolter) optics

Aberration correcting optics:
Focus extended beam spot onto similar image (can be increased/decreased in size)

Neutron Focusing within Sample Environment

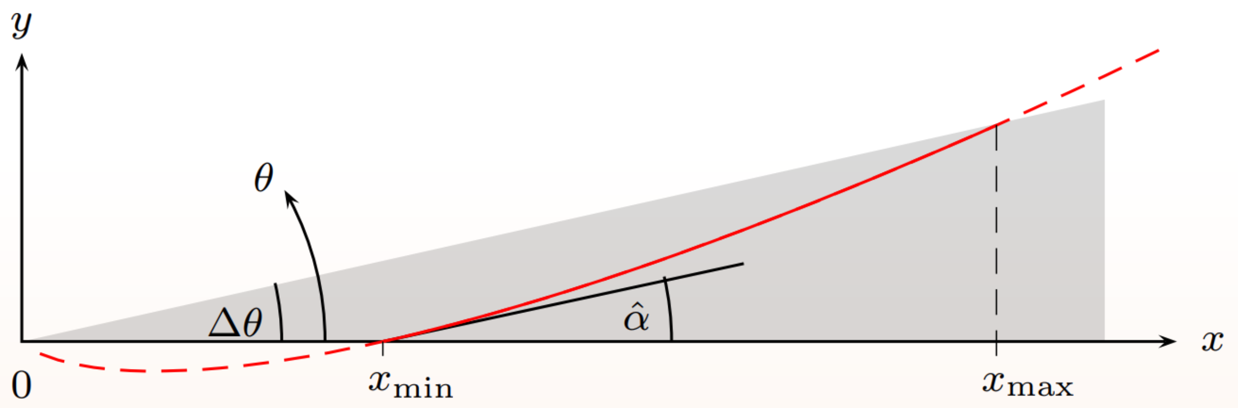
Measure sample under high pressure requires small samples and large pressure cells that can be hit by the neutron beam. Integrating a parabolic focusing optics into the sample environment increases signal on the sample while decreasing background from the cell.



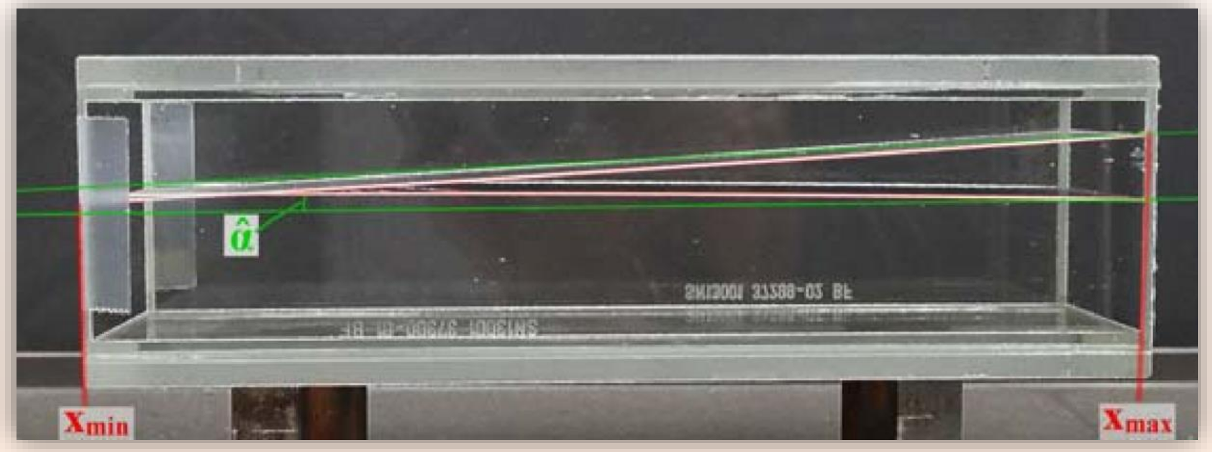


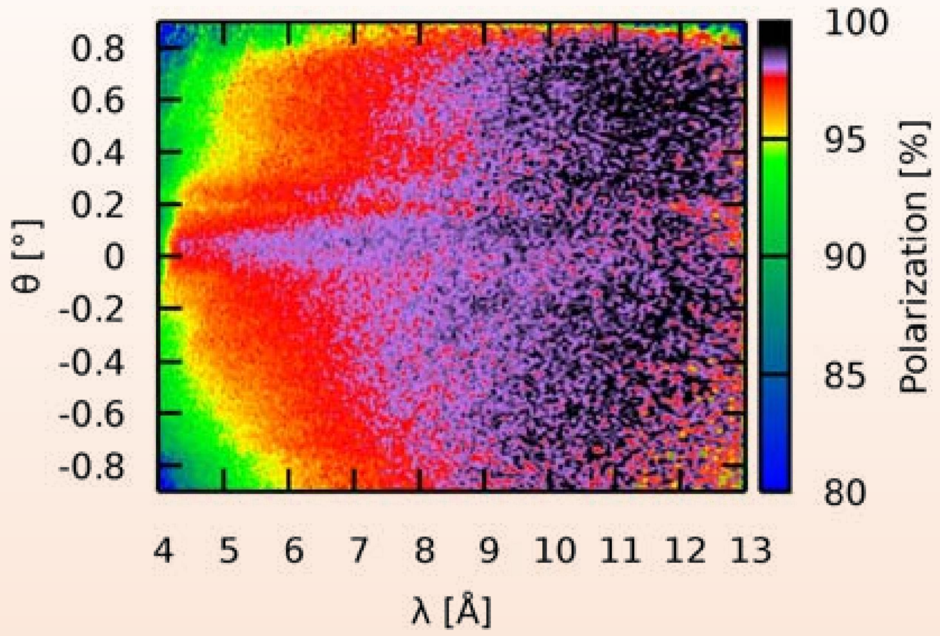
M. Bartkowiak, *et al.*, J. Phys. Conf. **340**, 012021 (2012)

Polarizing Focused Beams



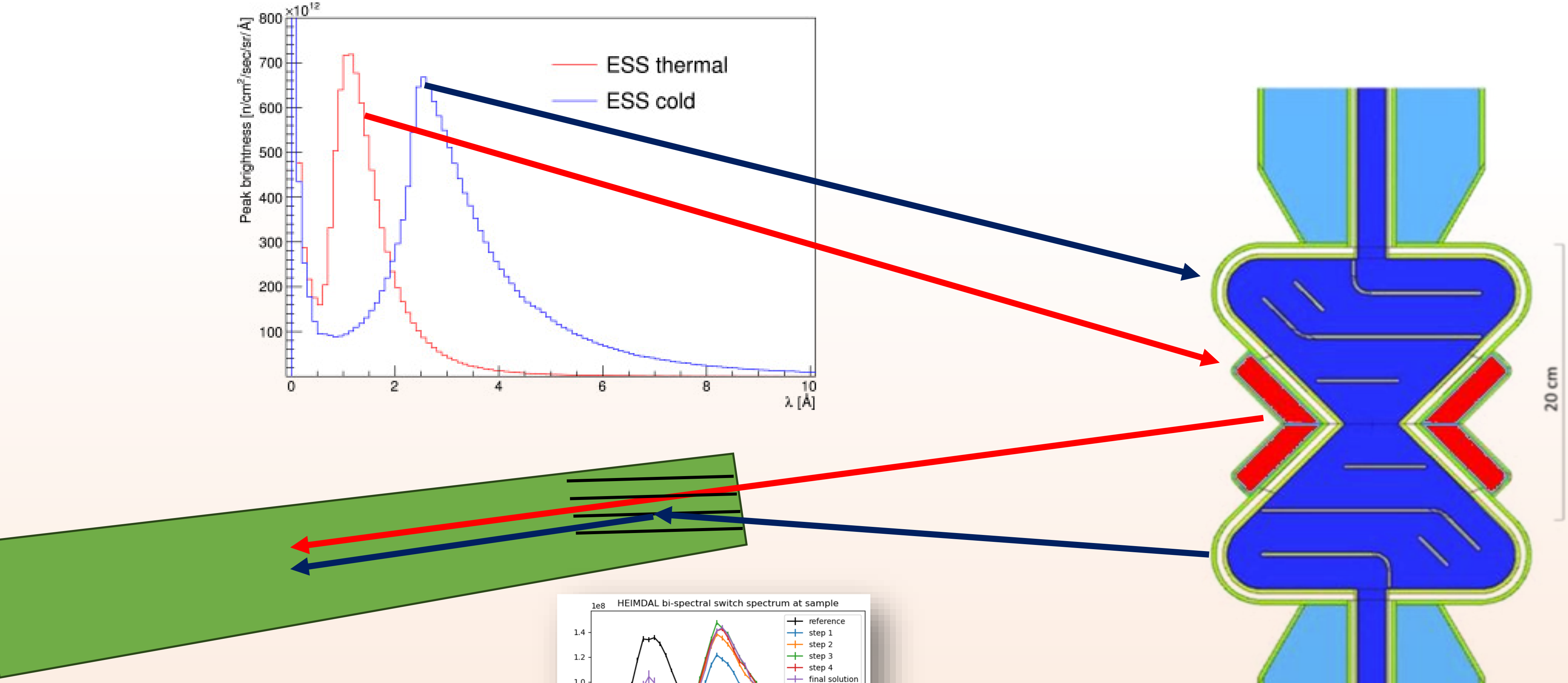
A beam with small focus and large divergence is harder to polarize as the angle on the mirror changes the q-value. A shape of a logarithmic spiral keep the angle the same for all directions.



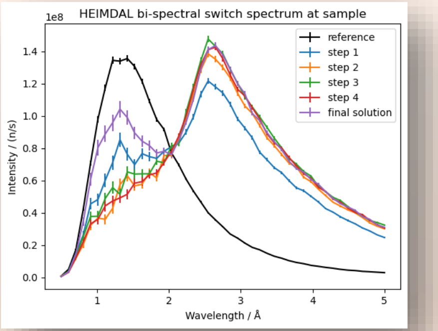


J. Stahn & A. Glavic, J. Phys.: Conf. Ser. **862** 012007 (2017)

Improving Bandwidth – Bi-spectral Switches

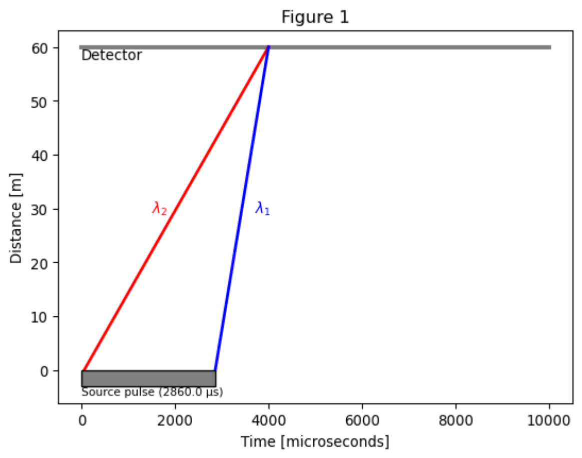


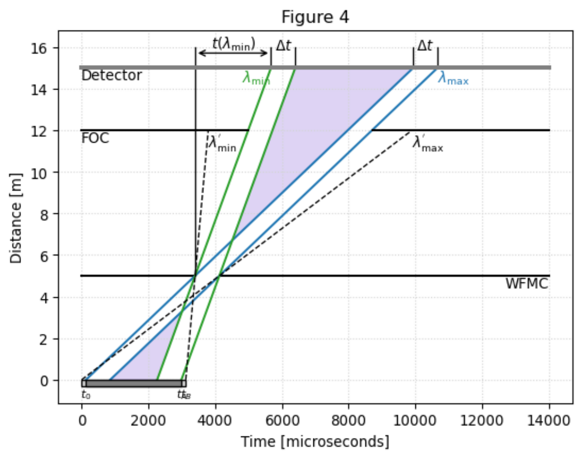
Example HEIMDAL:

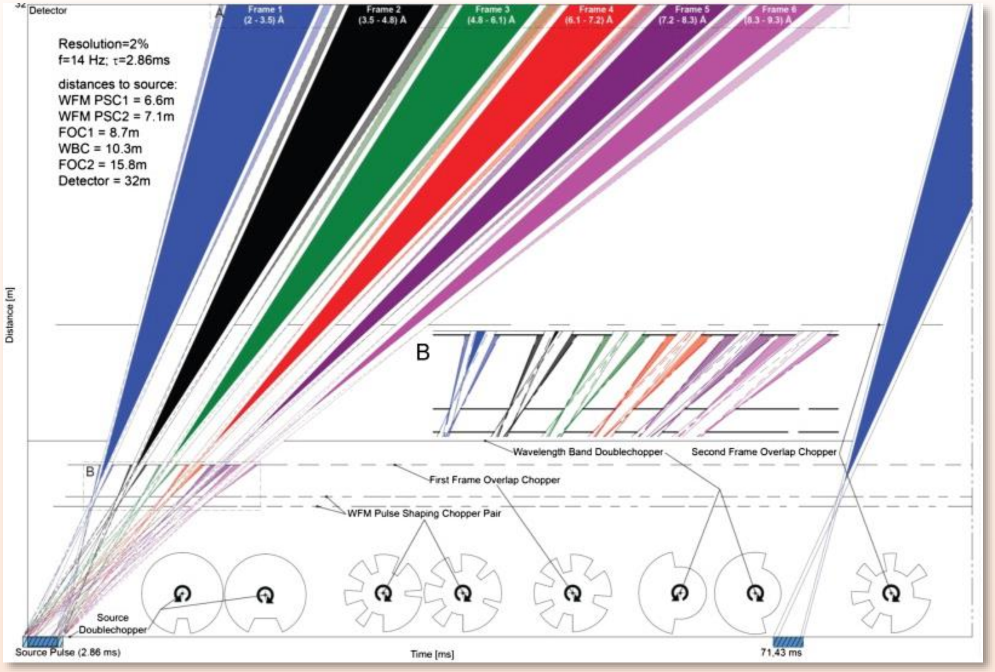


Wavelength Frame Multiplication

- If the time resolution of a pulsed source is not good enough for a given instrument length it is possible to use a chopper to shorten the pulse.
- As the chopper has to have a minimum distance to the source the resulting wavelength band does not cover the full time between two source pulses.
- Using multiple, well designed pulses one can select several “frames” allowing to fill the unused time gap and increase efficiency.
- The WFM technique requires multiple, sophisticated choppers to work together in a concerted fashion.







Traditional NR Experiments

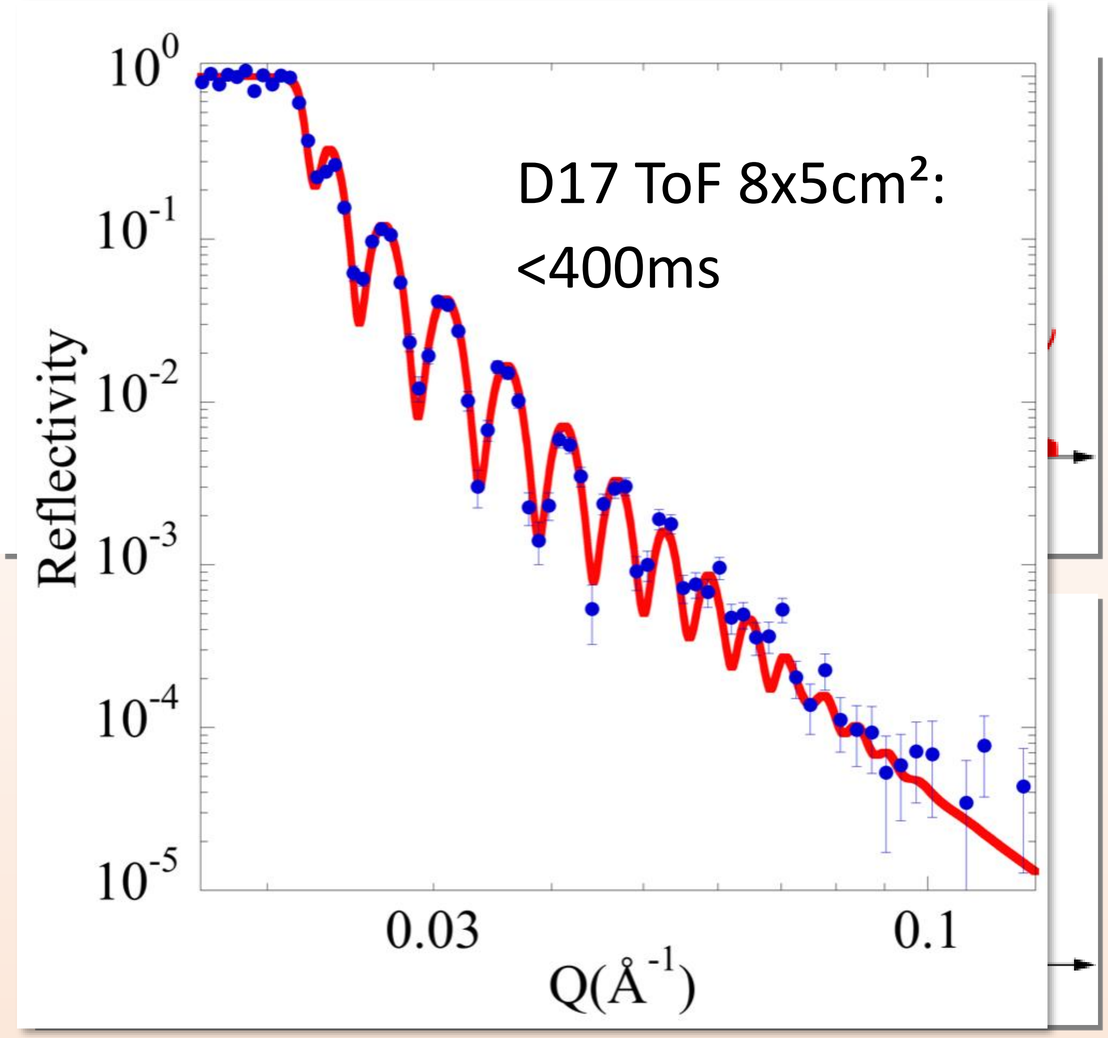
$$q_z = \frac{2\pi}{\lambda}\left(\sin\alpha_i + \sin\alpha_f\right) = \frac{4\pi}{\lambda}\sin\alpha_i$$

Angle-dispersive set-up:

- variation of ω with fixed λ
- detection under 2ω

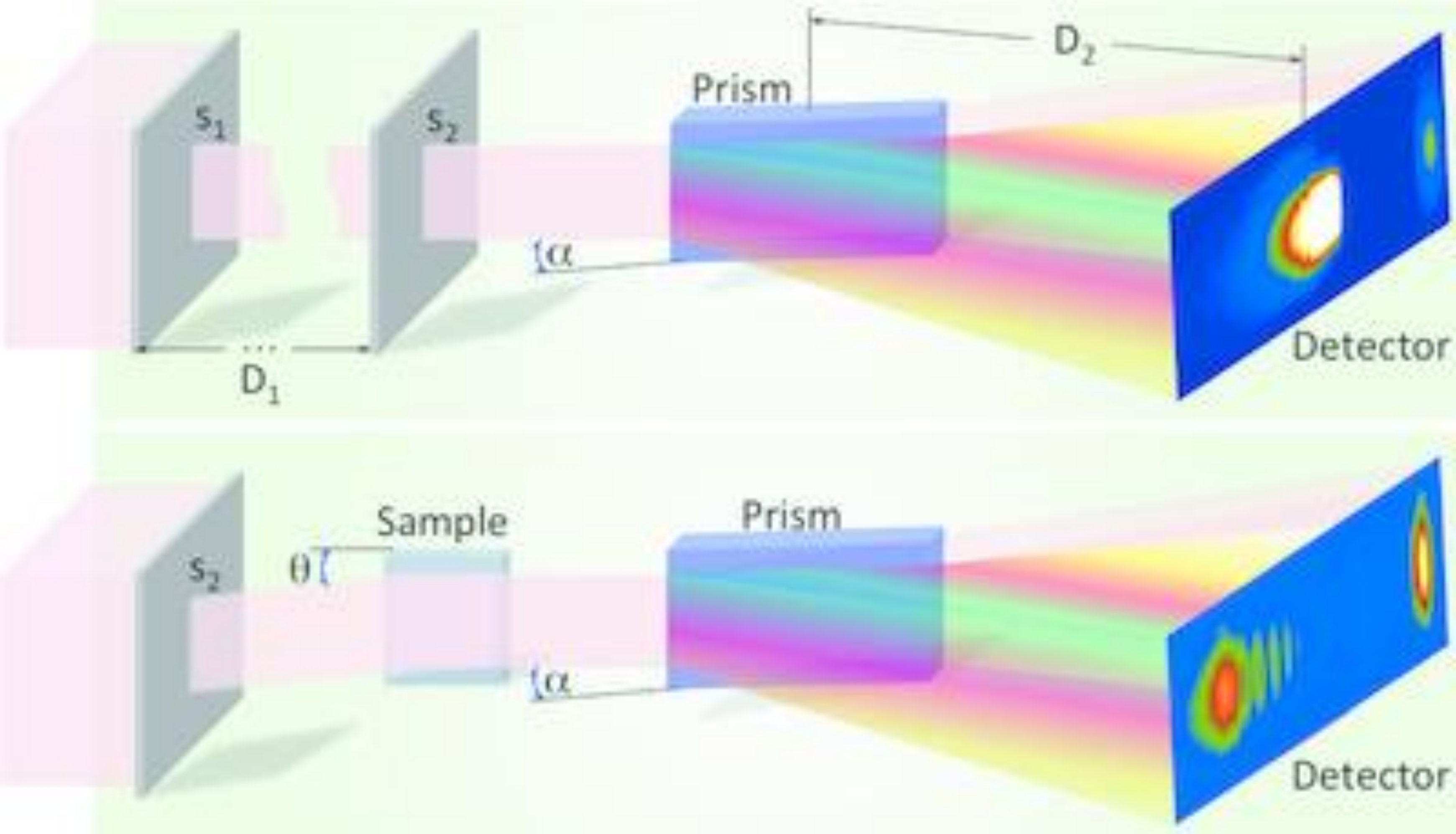
Energy-dispersive set-up:

- variation of λ with fixed ω
- detection via time-of-flight



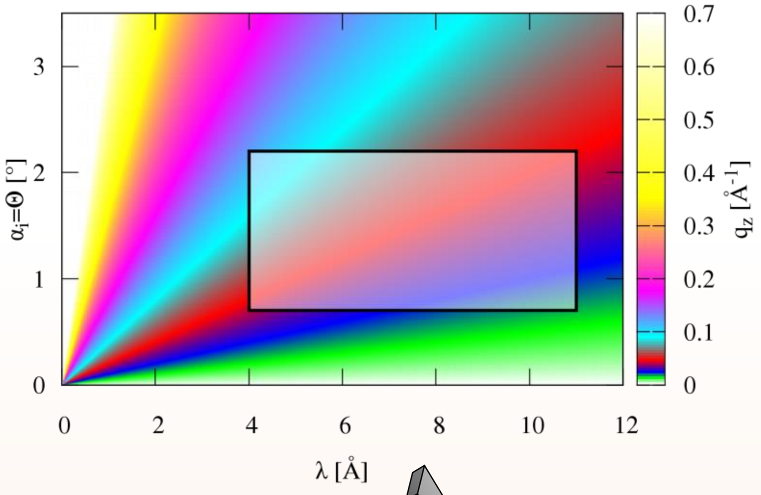
Reflectometry with a White Beam

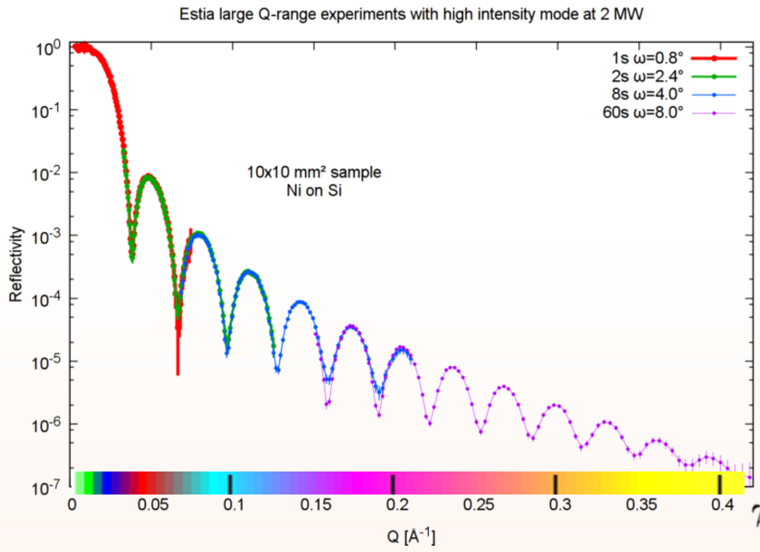
RAINBOWS concept



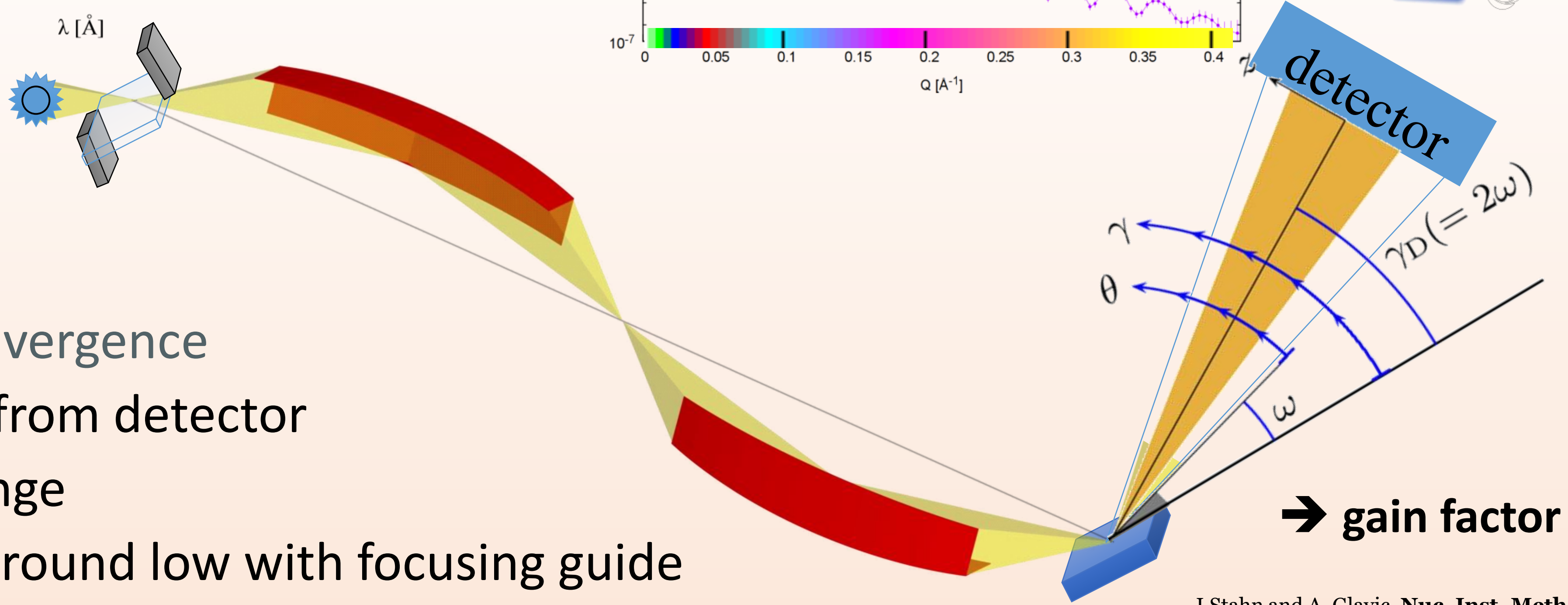
R. Cubitt, *et al.*, J. Appl. Crys. **51** 2/257 (2018)

Relax Resolution - Divergent Beam PNR





Small Sample Polarized Reflectometer Estia Instrument



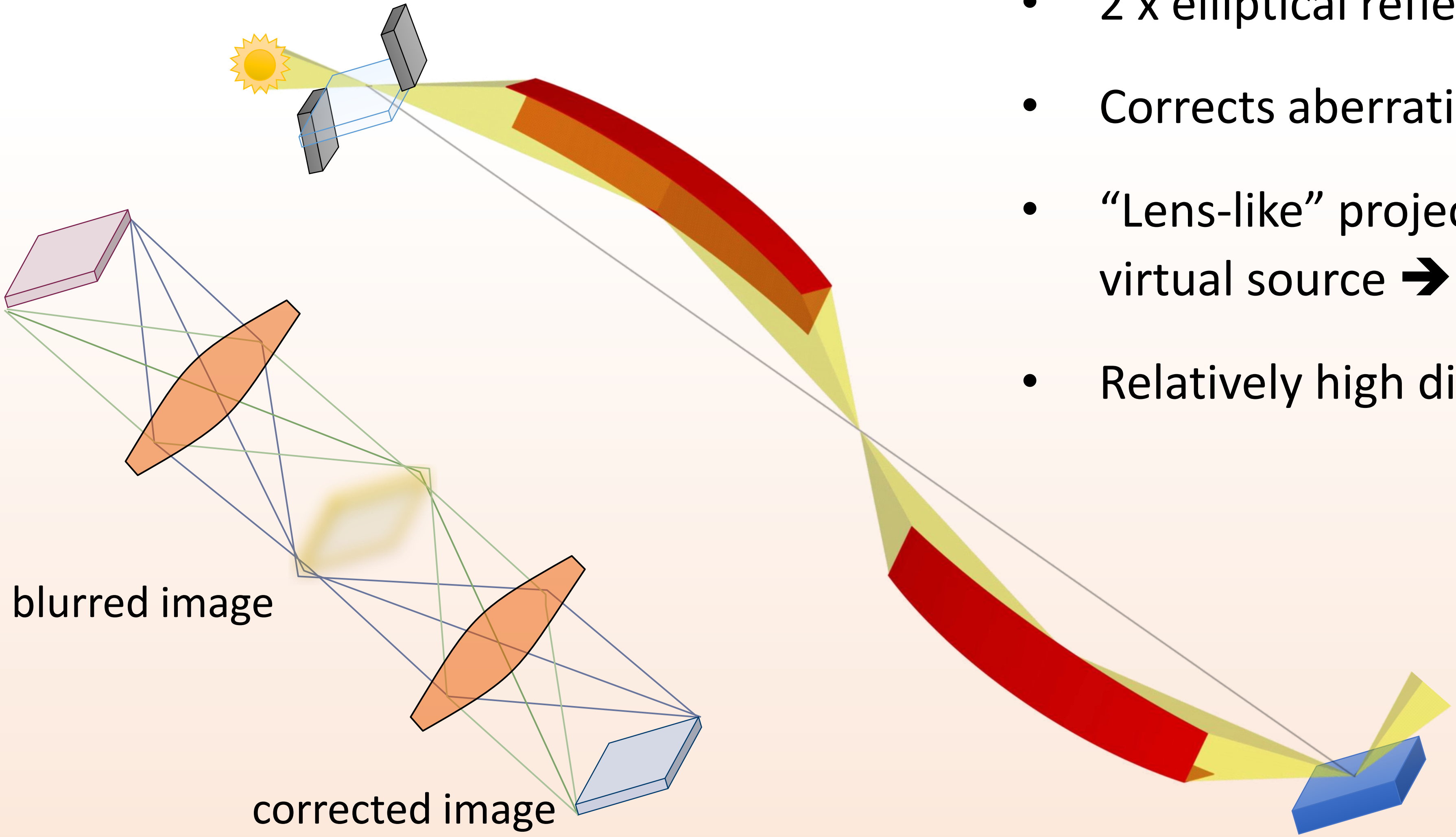
ToF + large divergence

- resolution from detector
- larger q-range
- keep background low with focusing guide

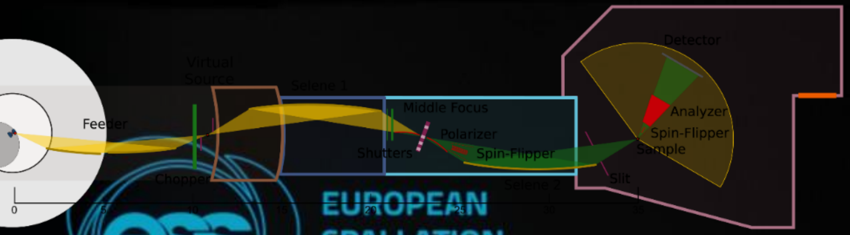
➔ **gain factor ≈ 10-30**

J.Stahn and A. Glavic, **Nuc. Inst. Metho. A 821**, 44-54 (2016)

Selene (Montel) Optics



- 2 x elliptical reflector
- Corrects aberrations
- "Lens-like" projection
  virtual source ➔ sample
- Relatively high divergence



EUROPEAN SPALLATION SOURCE

Small Sample Polarized Reflectometer

PAUL SCHERRER INSTITUT

ESS Instrument Project:

Beam Port: E2

User Operation: 2024

Class: Large-Scale Structures

In-Kind Partner: PSI

Parameters:

Band: 3.75Å-10.7Å

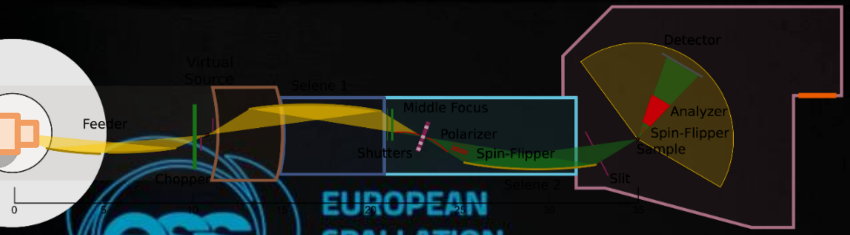
Resolution: <7%

Q-max: 3.15/Å

Length: 39m

Neutron Wavelength

4Å 6Å 8Å 10Å 11Å



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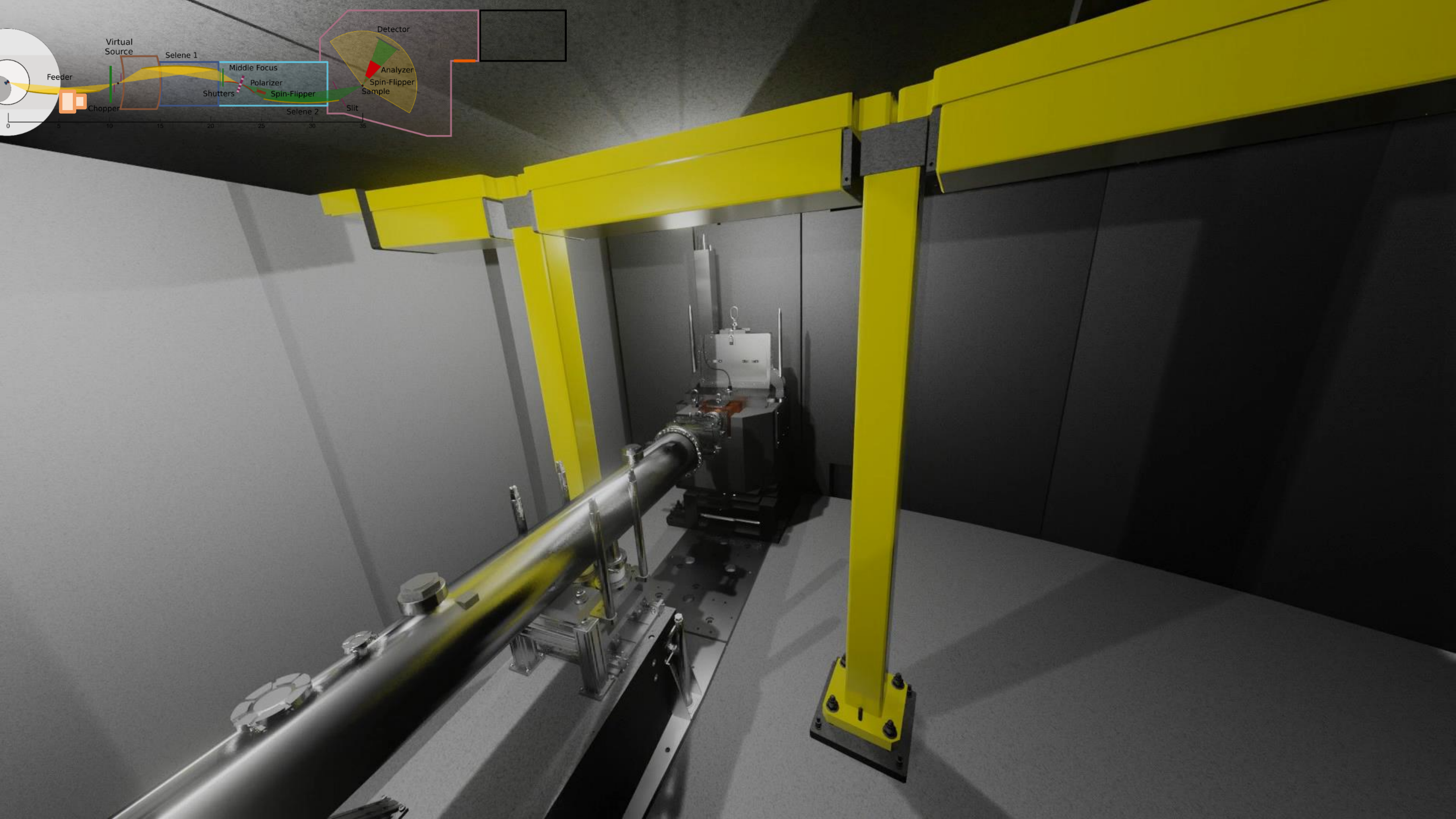
Neutron Wavelength

4Å 6Å 8Å 10Å 11Å

Neutron feeder:

- Moderator ➔ virtual source
- Elliptic guides
- Two beams
- Two sections
  - Cu upstream
  - Al downstream


Detector
Virtual Source
Selene 1
Feeder
Middle Focus
Analyzer
Polarizer
Spin-Flipper
Shutters
Spin-Flipper
Sample
Chopper
Slit
Selene 2
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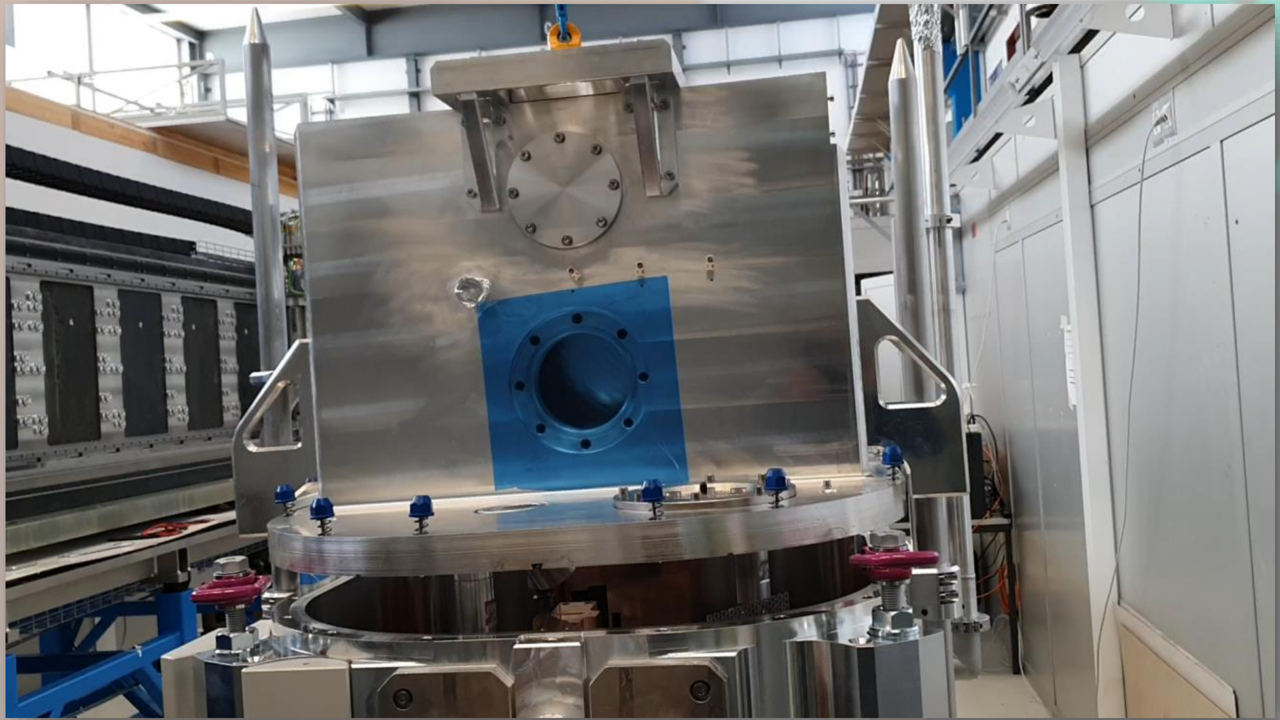

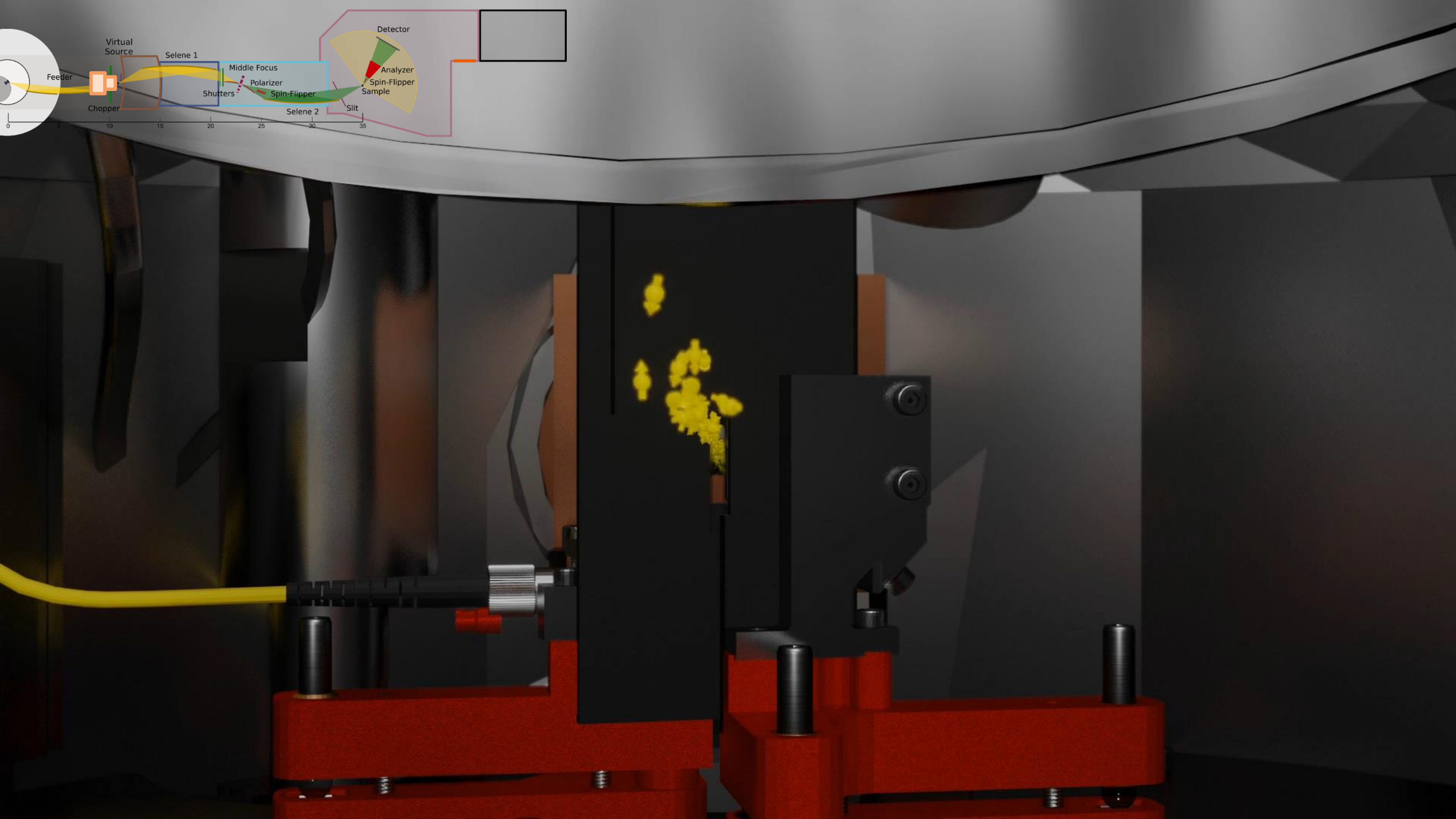
Virtual Source
Selene 1
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Polarizer
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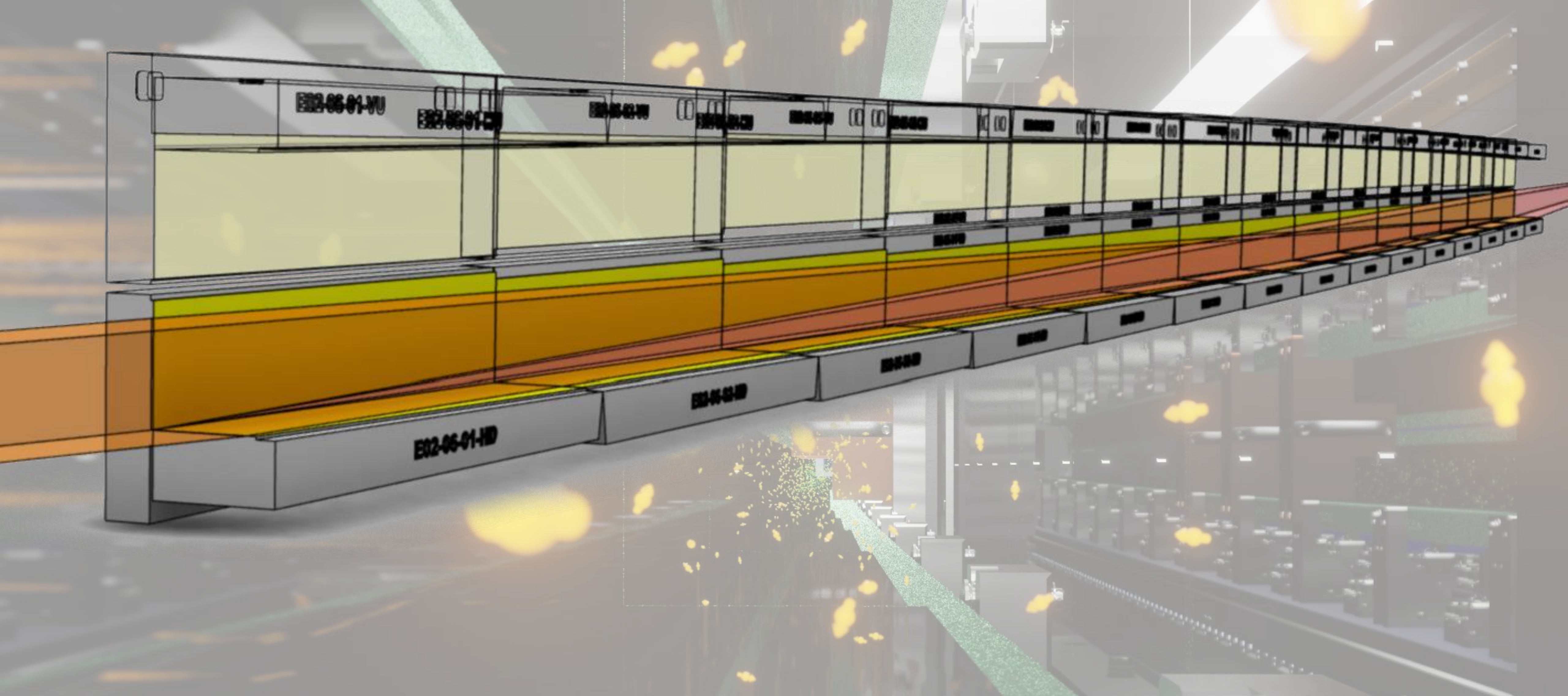
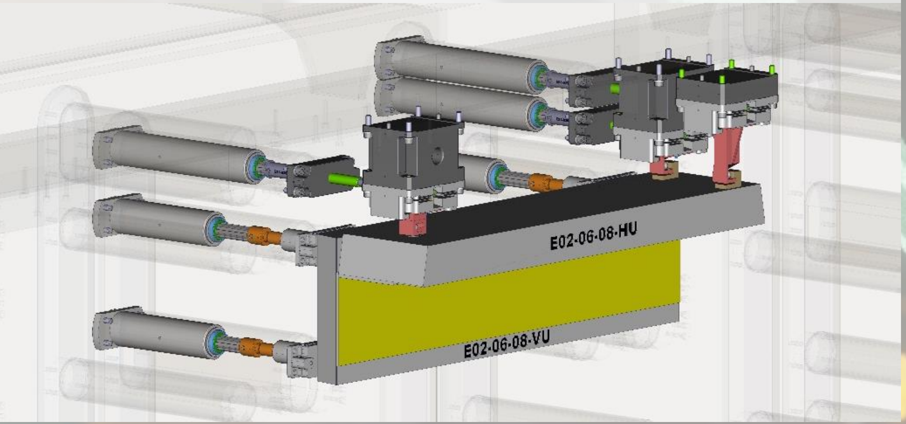
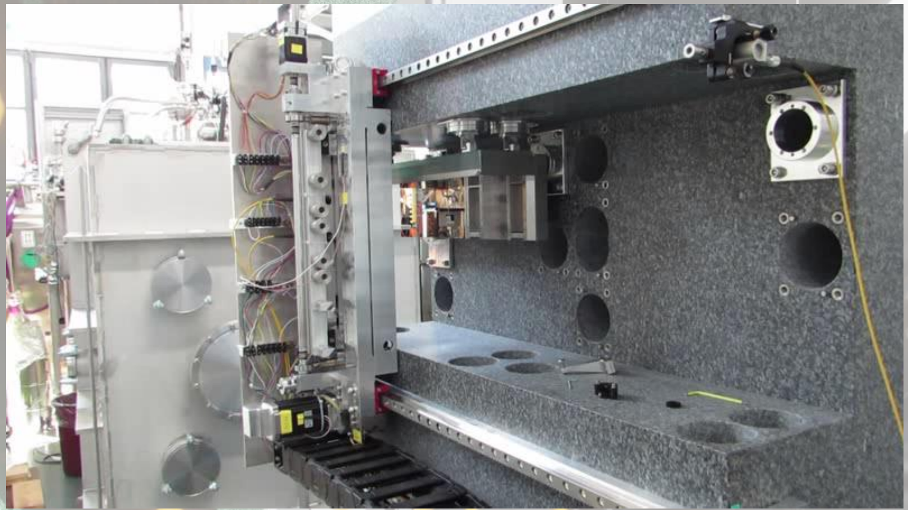


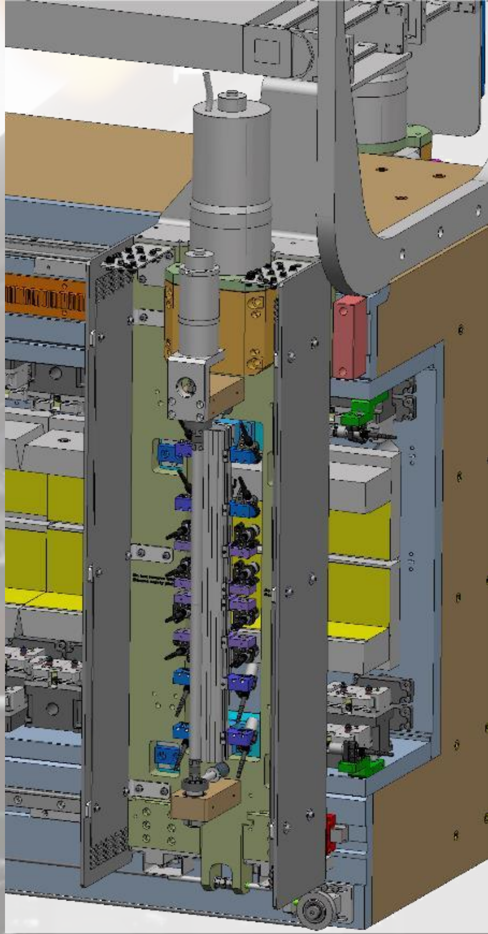
Necessary precision:

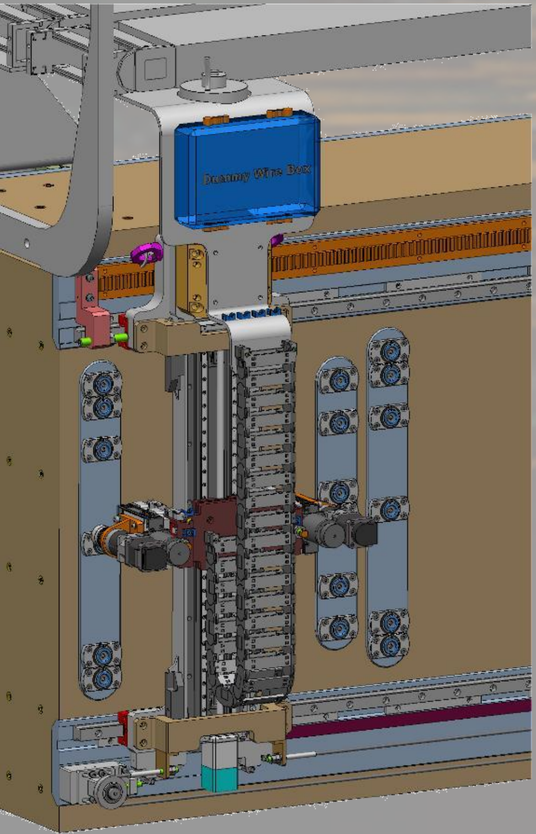
60µm/24m -> 2.5e-6 rad

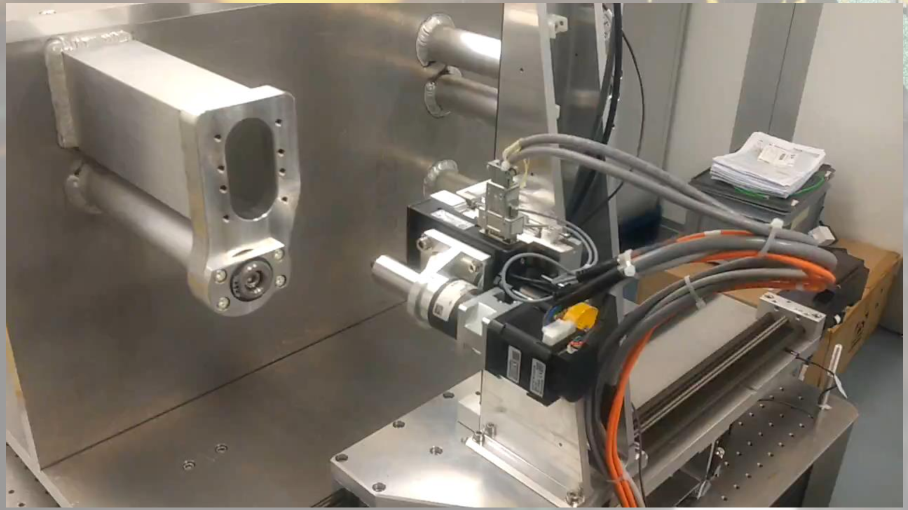
Adjustment of reflector



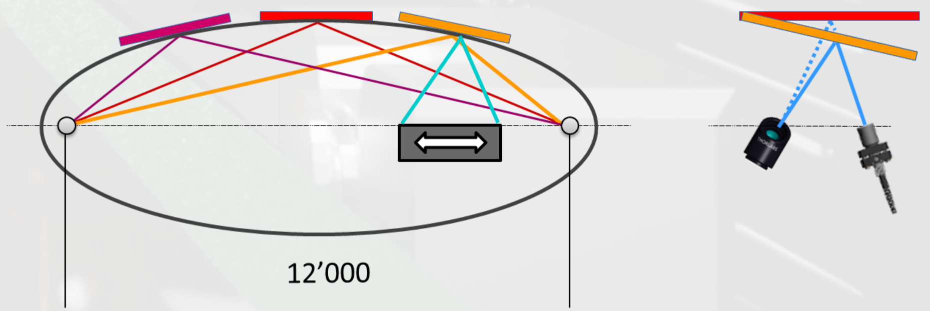


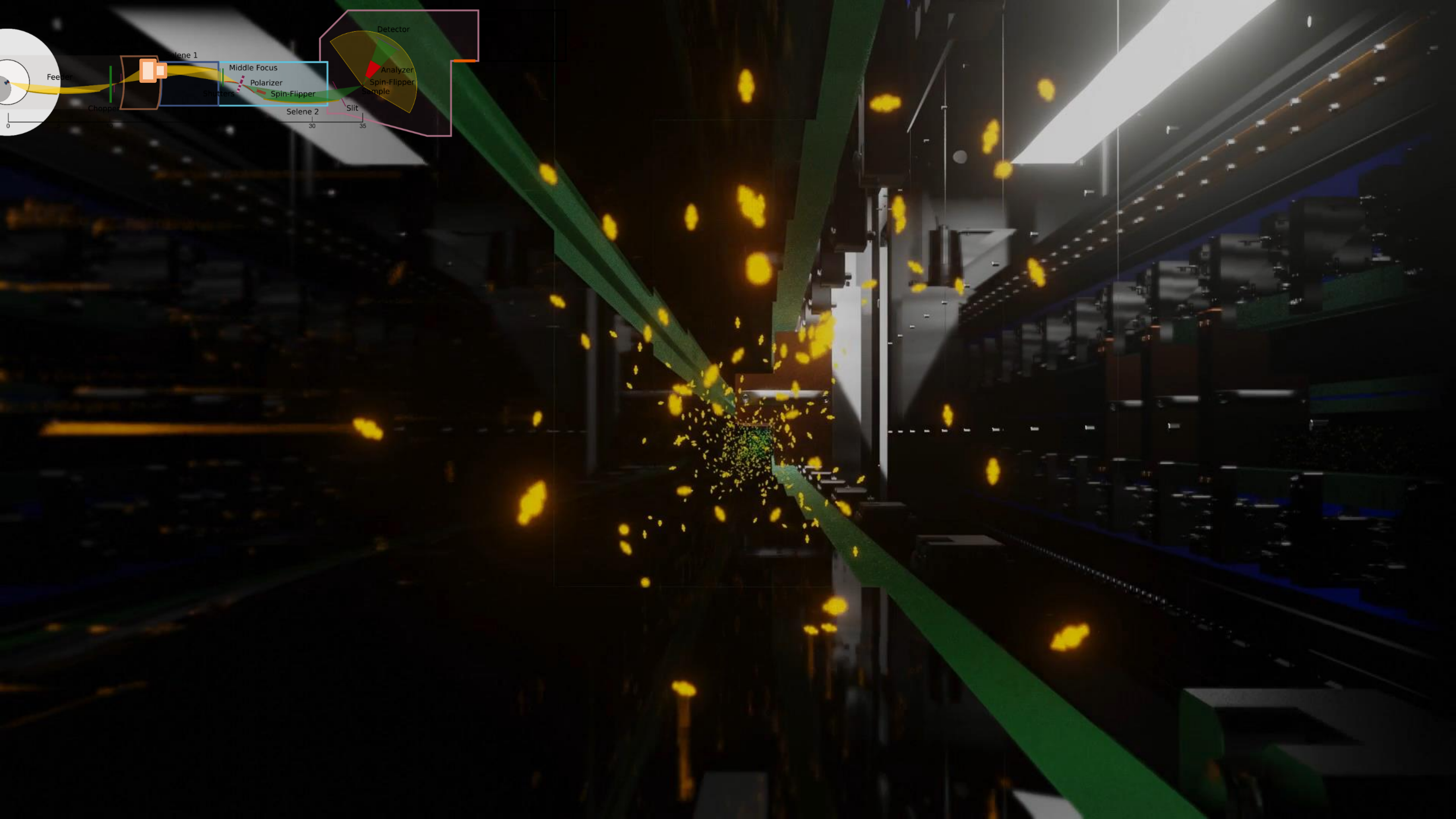






Measurement of reflector position




Detector
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Spin-Flipper
Shutters
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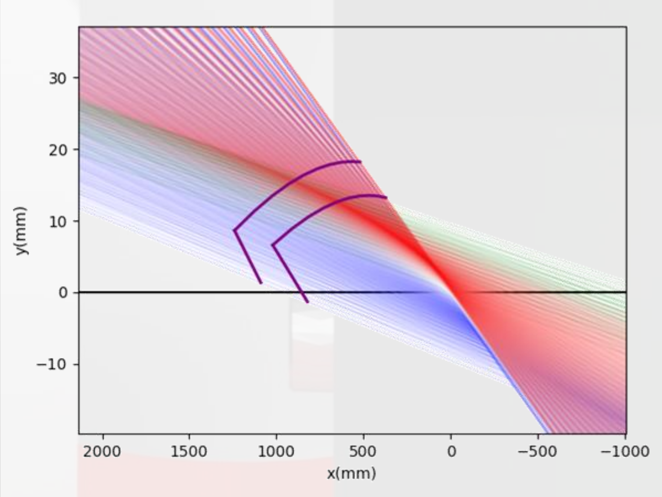
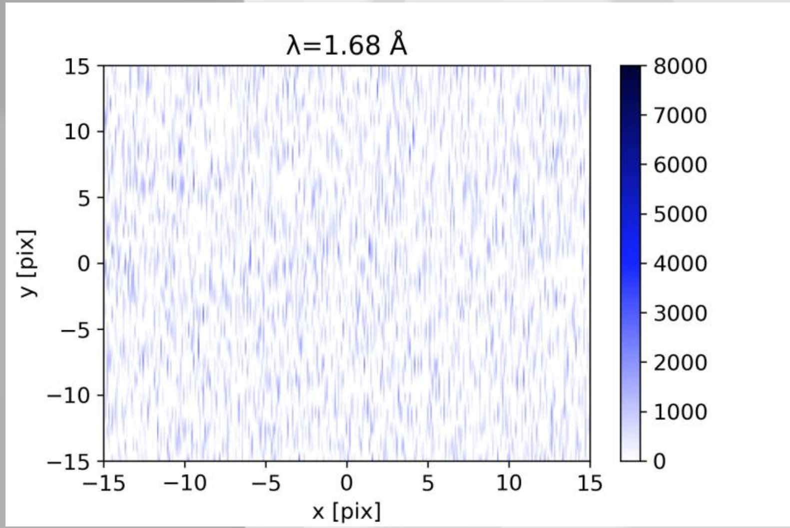
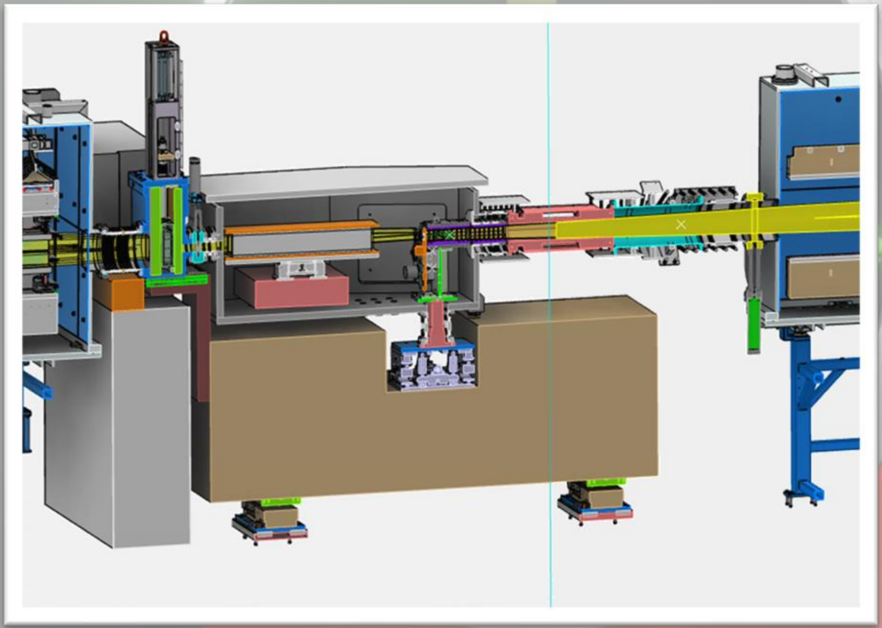
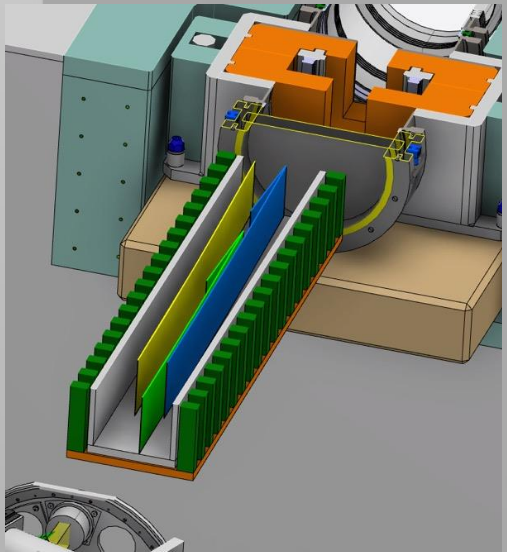


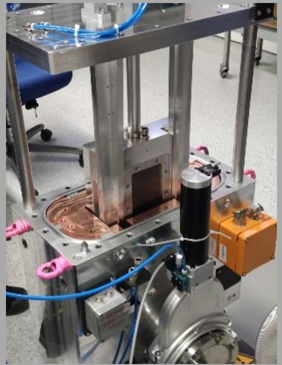


Transmission polarizers:

- Transmission supermirrors
- Two logarithmic spirals
- Polarization >98% full band

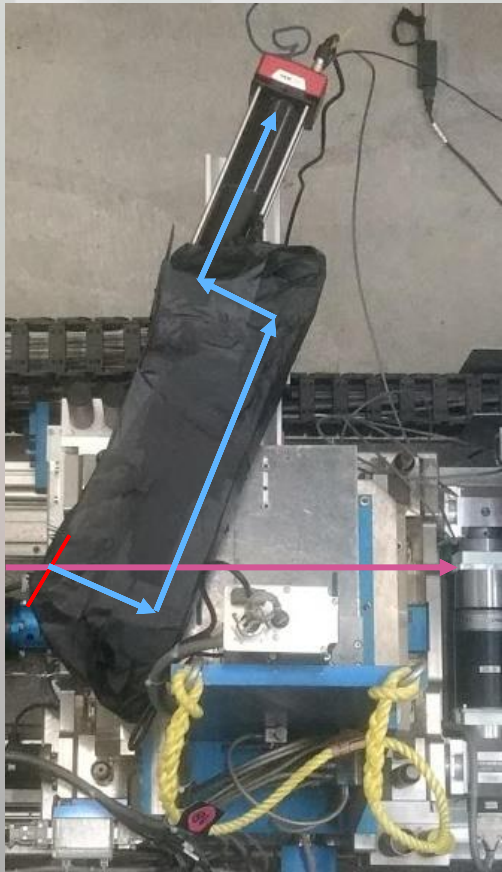


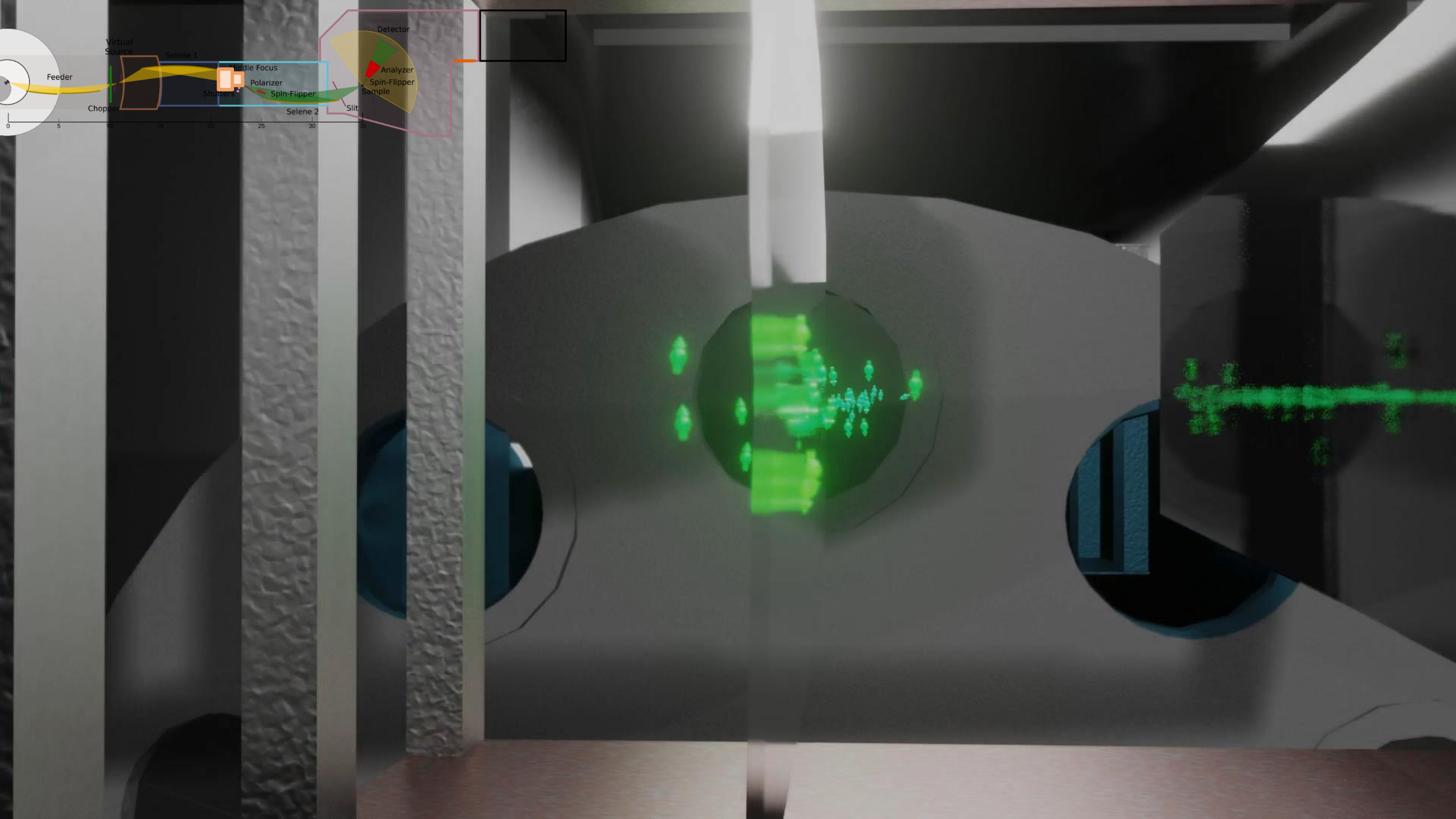




Filters and monitor:

- Monitor beam shape
- Attenuate beam
- Reduce background





Feeder
Virtual Source
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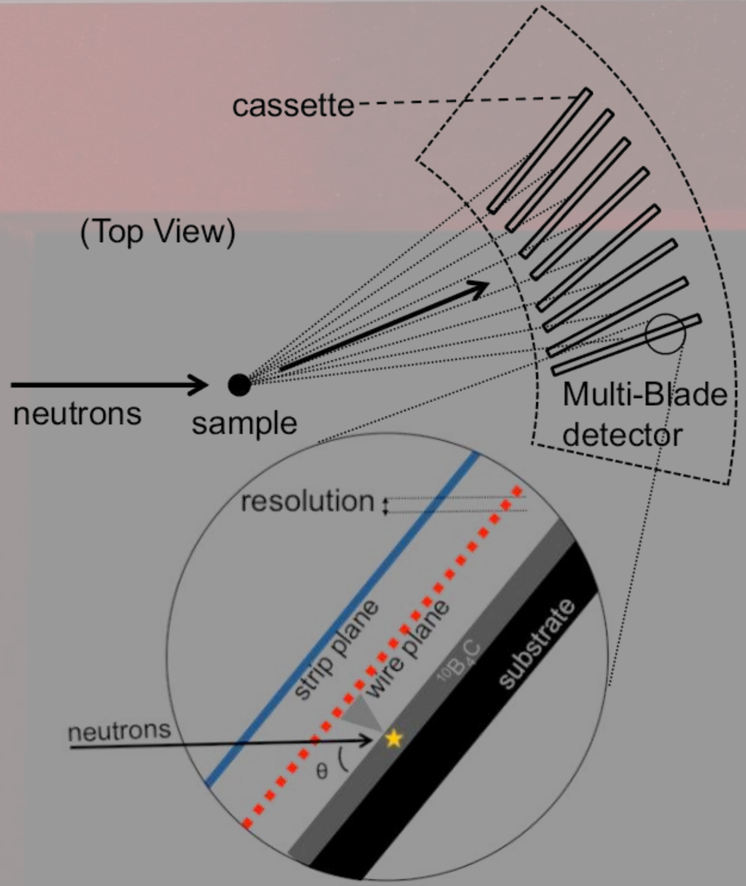
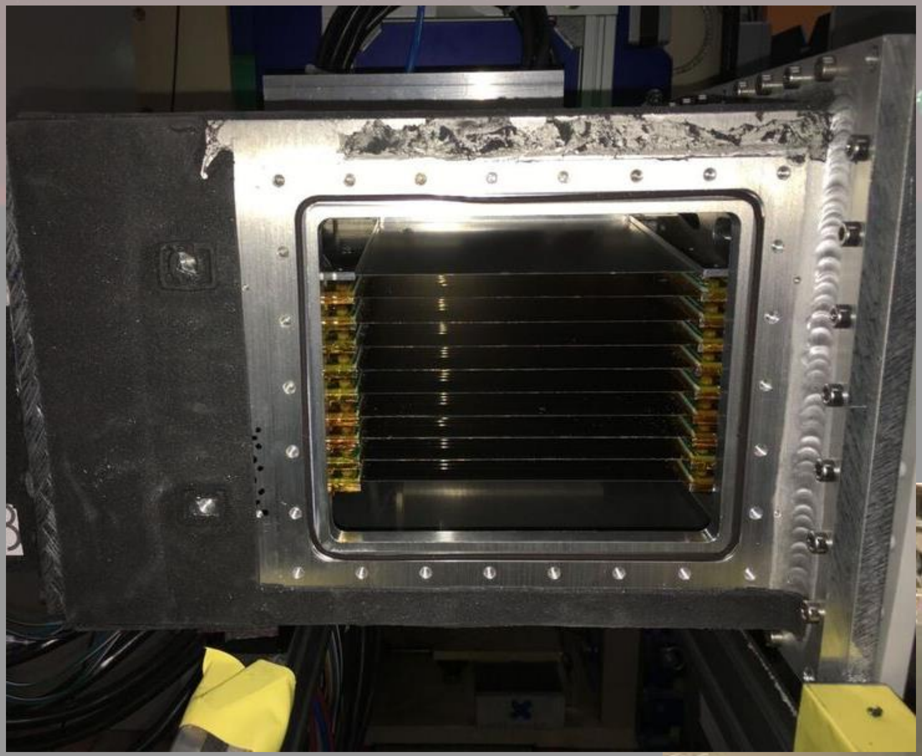
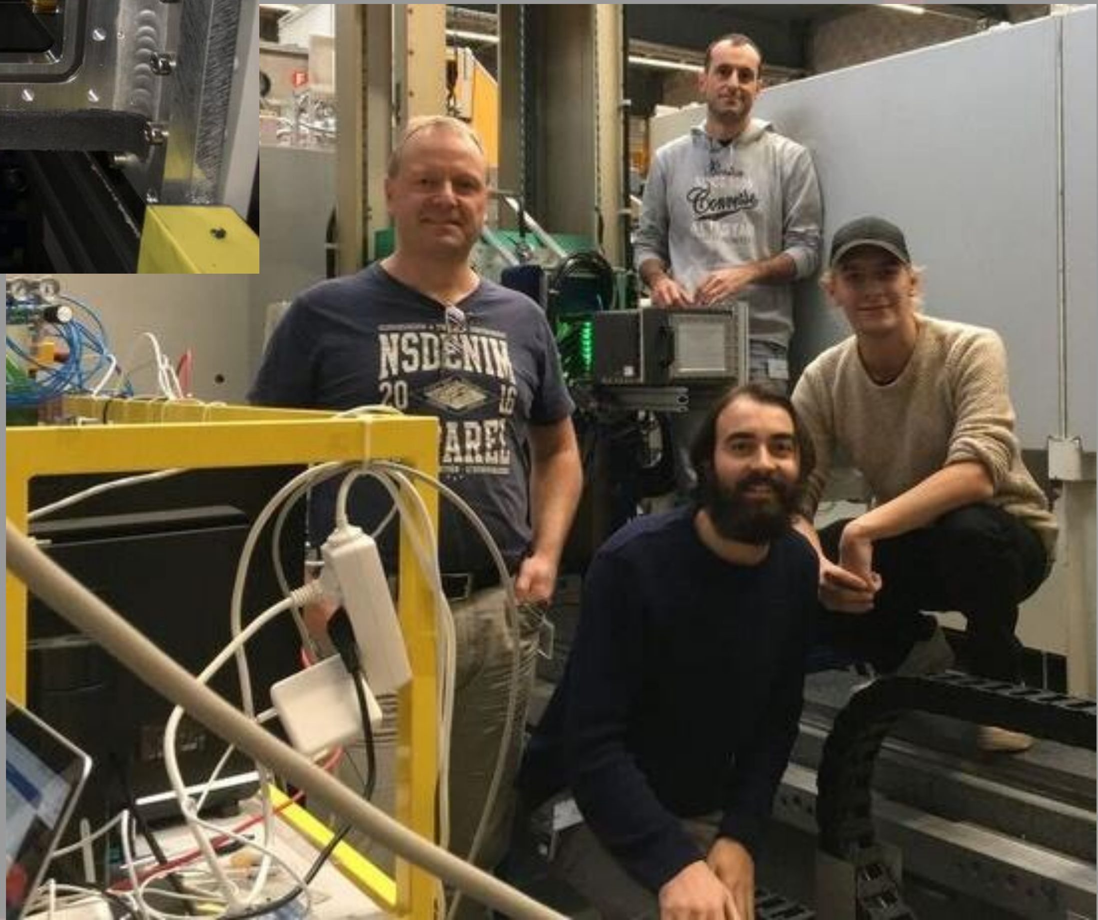
F. Piscitelli et al.,
Journal of Instrumentation **13**, 05 (2018).







Multiblade Detector:

- ^{10}B coated plates under small angle
- High resolution 0.5x4 mm²
- Very high count rate (~100kHz/mm²)
- Thin entrance window

Thank you for your attention!

2023