EUROPEAN
SPALLATION
SOURCE

Introducing Effects of Surface Physics in McStas Union

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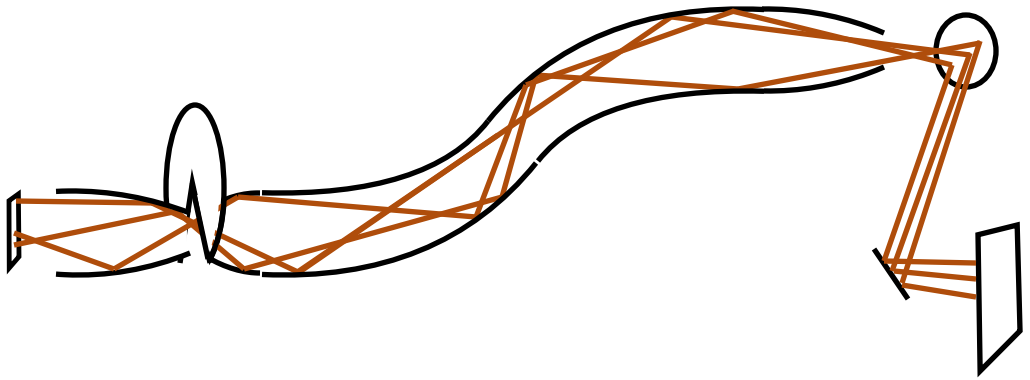
Introduction

McStas instrument structure



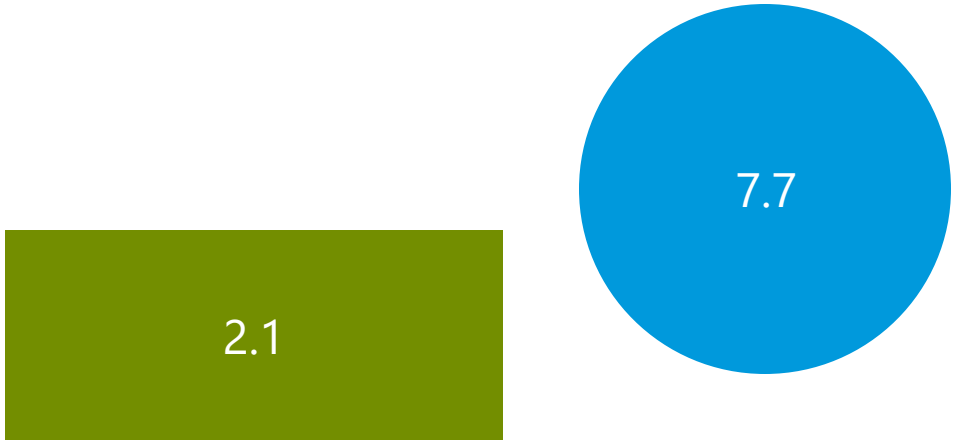
Component sequence

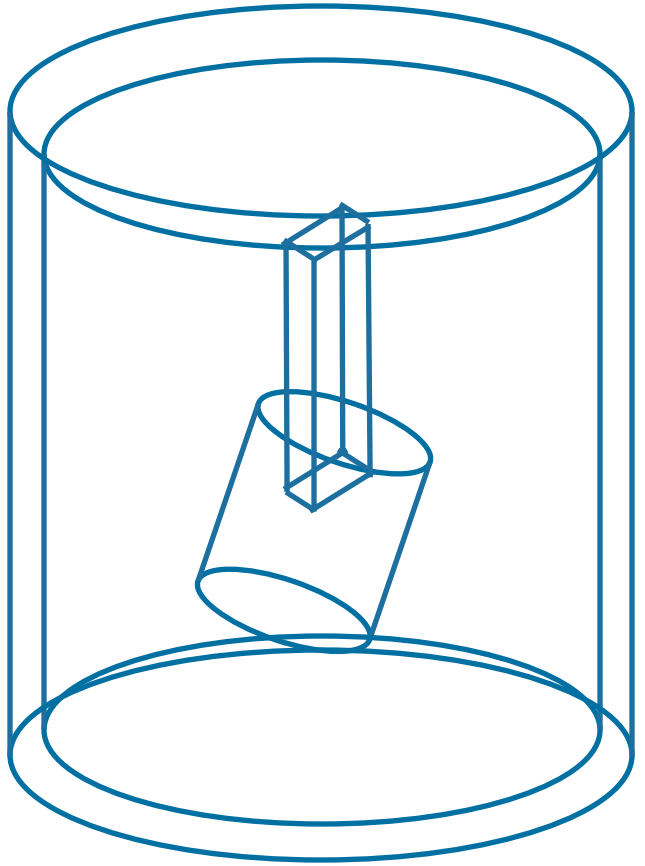
- Source
- Guide_bunker
- Chopper
- Guide_1
- Guide_2
- Guide_3
- Sample
- Analyzer
- Detector

Union components

Geometry

- Geometry constructed from simple shapes
- Each assigned a material
- All shapes given a priority value
- Can overlap
- In overlap, largest priority value decides material



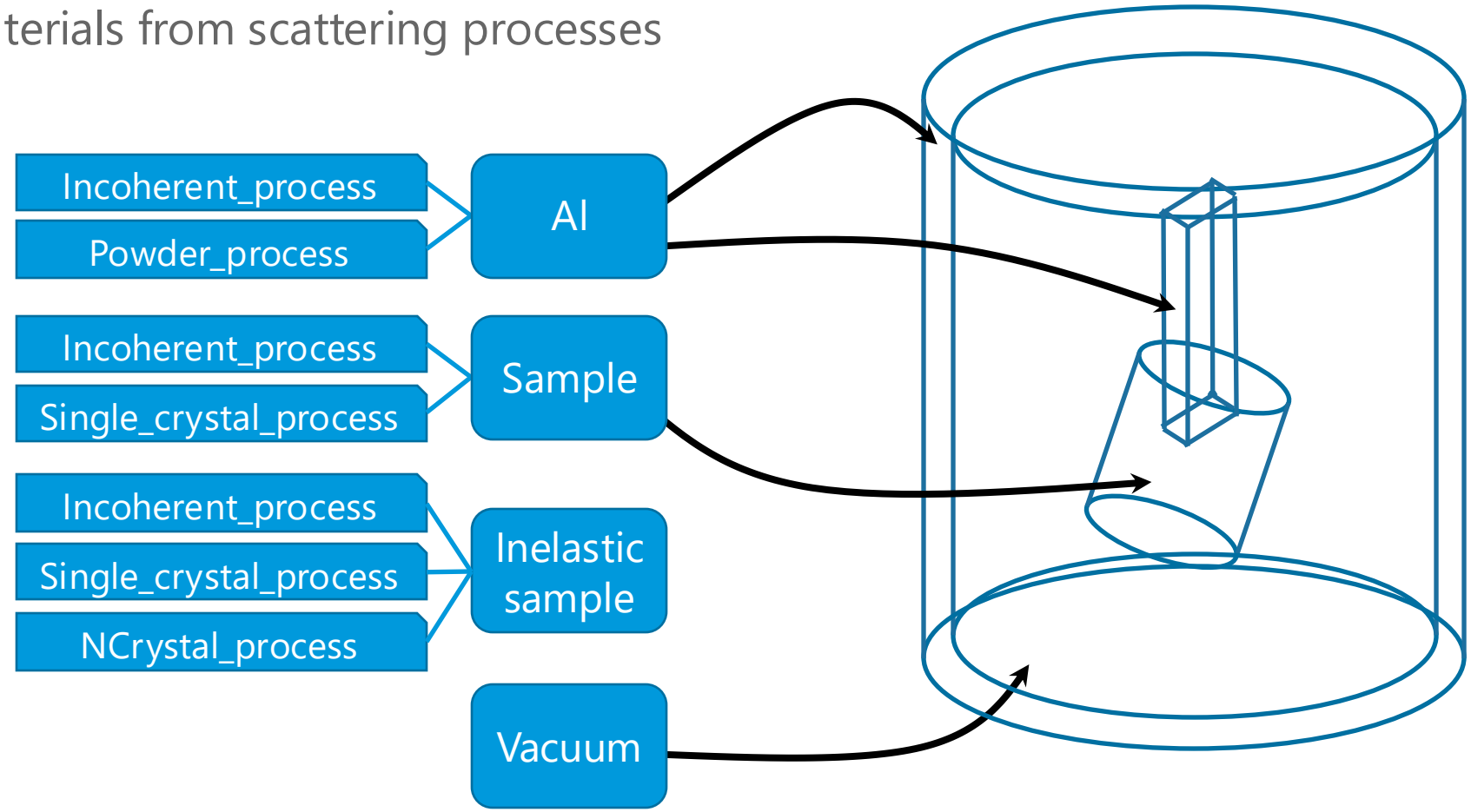


Boxes, cylinders, cones, spheres

Union components

Geometry

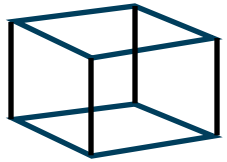
- Assemble materials from scattering processes



Union components

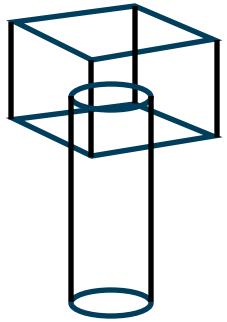
Using the Union components

Typical sample component



Single_crystal.comp
- Geometry
- Raytracing
- Absorption
- Scattering
  - Incoherent
  - Single crystal Bragg
- Multiple scattering loop

Union components



Union_cylinder.comp

Union_init.comp

Incoherent_process.comp
- Incoherent scattering

Single_crystal_process.comp
- Single crystal scattering

Union_make_material.comp

Union_box.comp

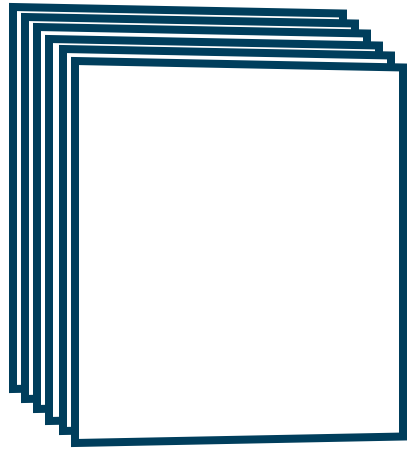
Union_master.comp
- Raytracing
- Absorption
- Sampling scattering physics
- Multiple scattering

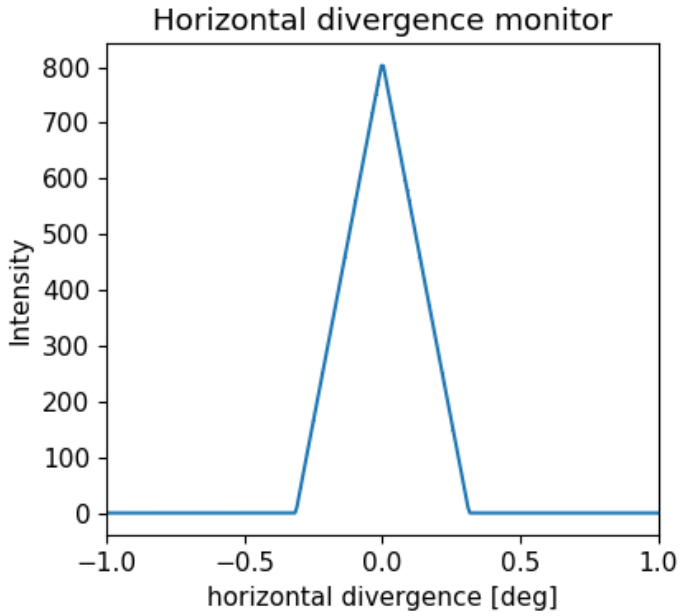
Union_stop.comp

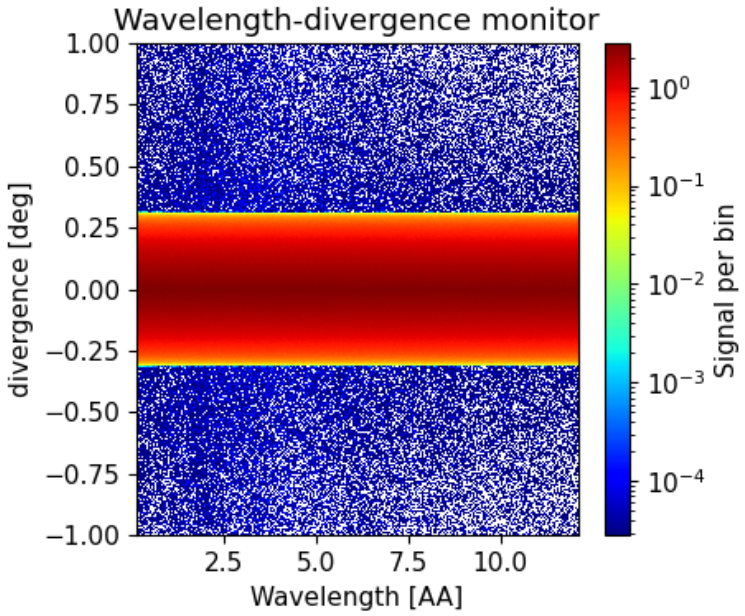
Union components

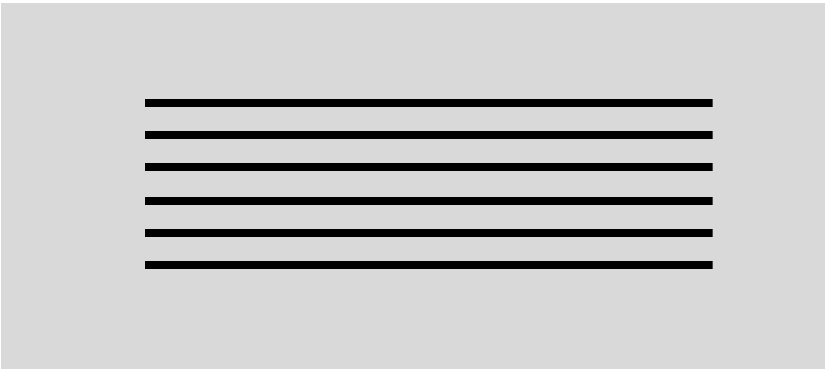
Simple example - colimator

- Lets make a colimator
- Absorbing blades limit divergence







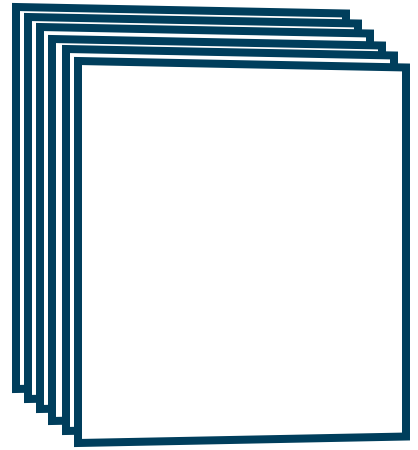


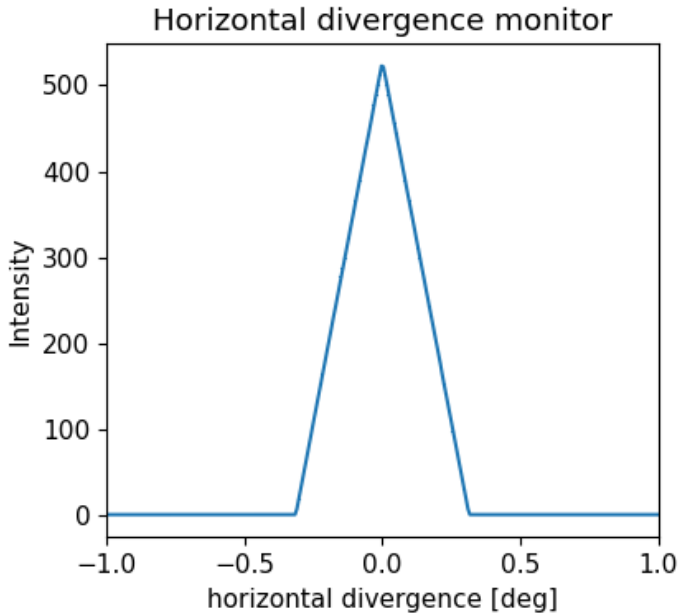
Cd Air

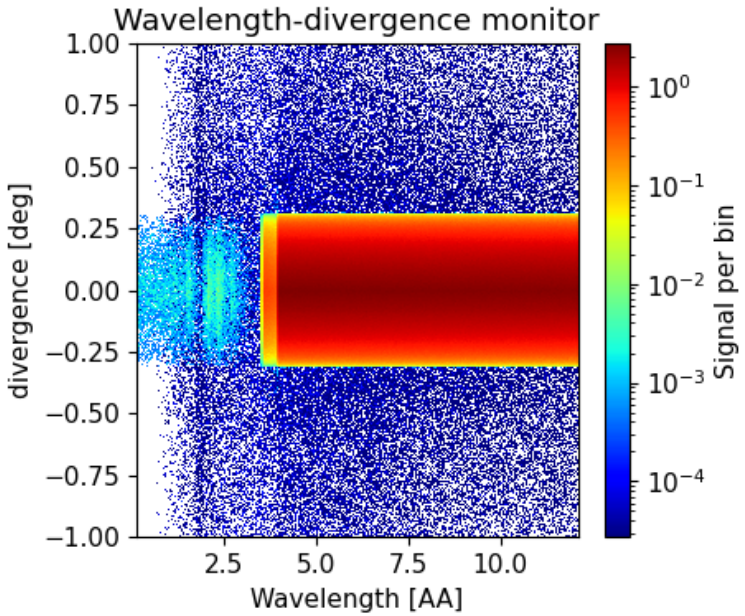
Union components

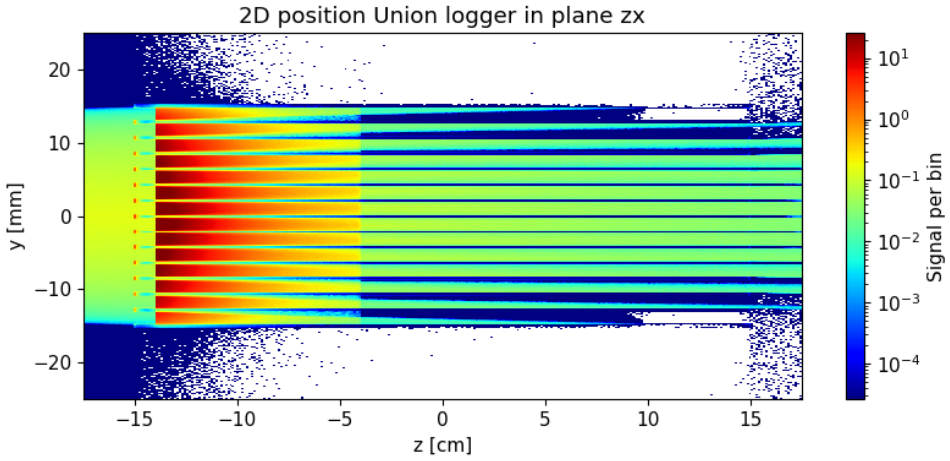
Simple example - filter

- Lets make a colimator
- Absorbing blades limit divergence
- Add a Be block, now its a filter





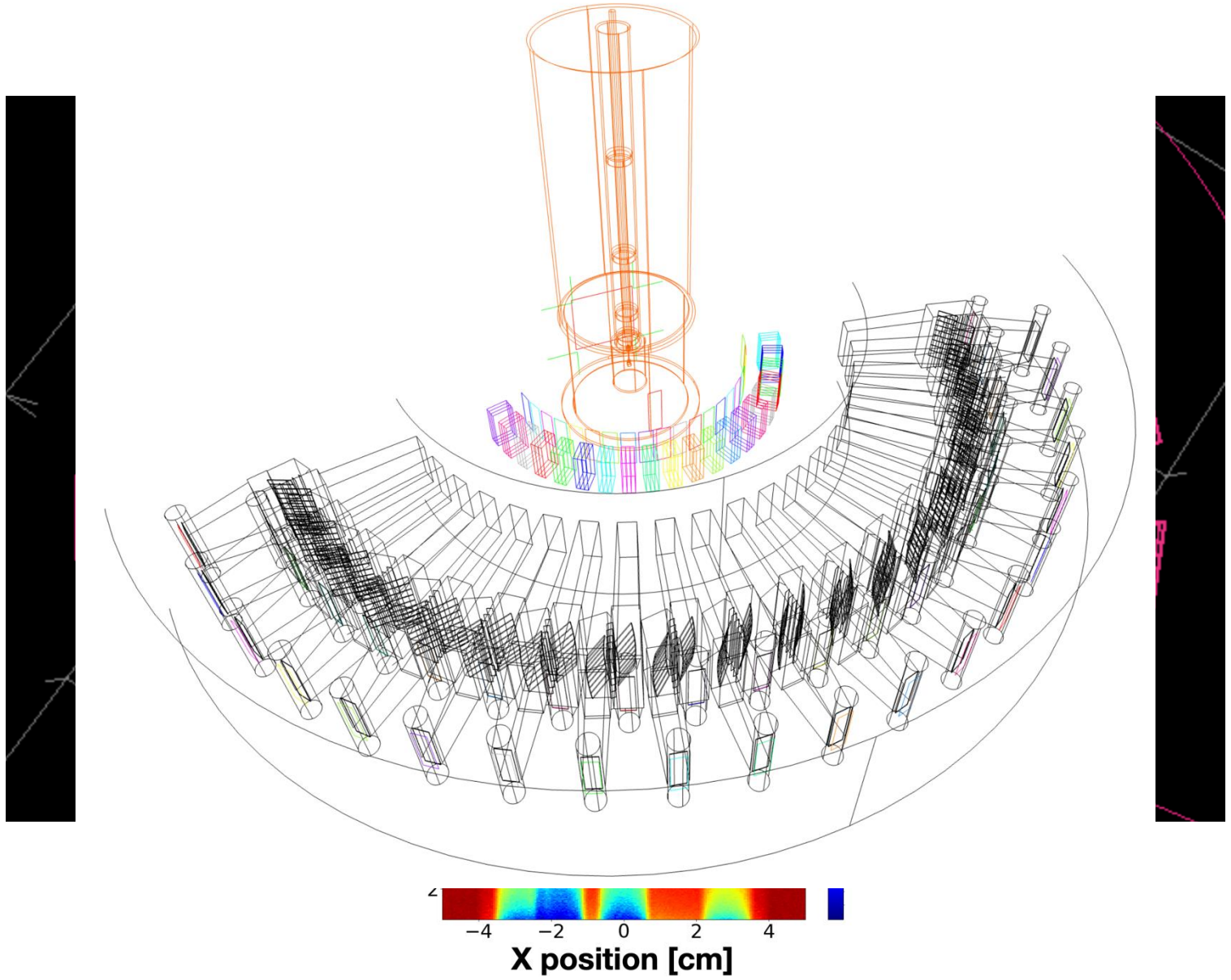




Cd | Air | Be

Use cases

- Samples
- Sample holder
- Air
- Sample environment
- Colimators
- Filters
- Beam monitors
- Monochromators
- Detectors
- Instrument backends



Union components

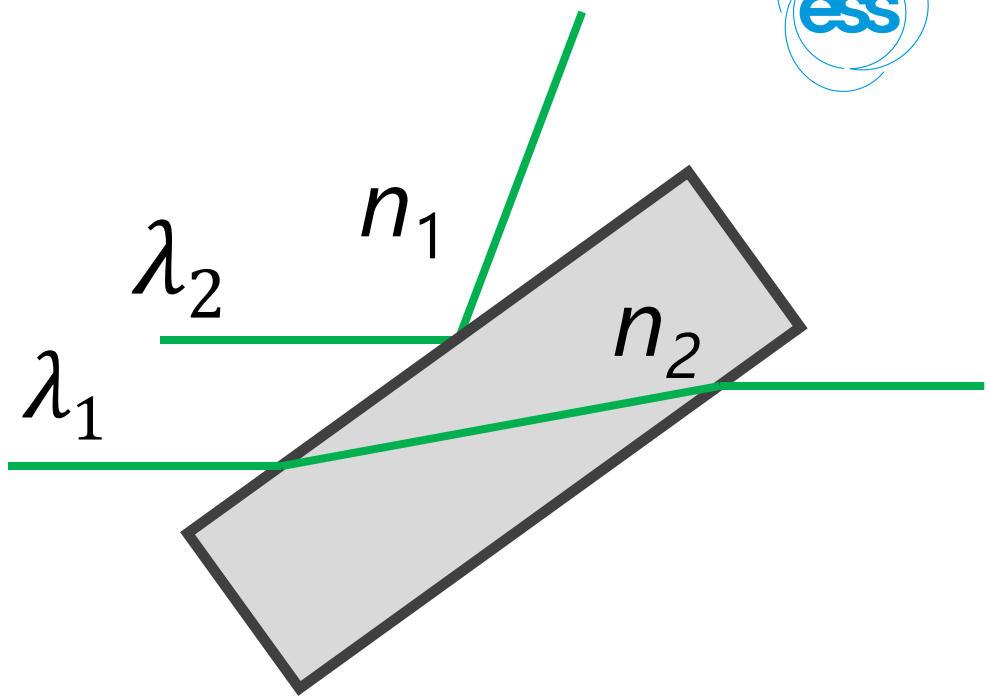
Assumptions

- Bulk scattering, scattering properties independent of position in material
- Gravity not simulated
- Polarization not supported
- No physics when rays cross an interface

Interface physics update

Refraction

- Code from Refractor.comp by E. Farhi, B. Cubitt
- Scattering length density provided with material definitions
- Refraction calculation require SLD for both materials
- Snells law with fall of



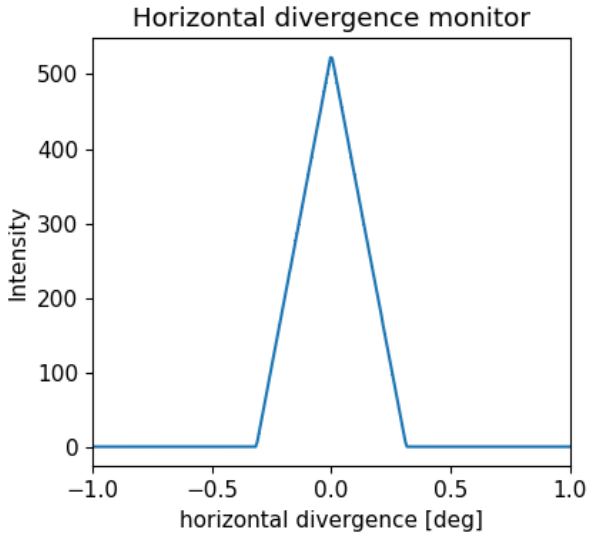
n = sqrt(1.0-(lambda*lambda*SLD/PI))

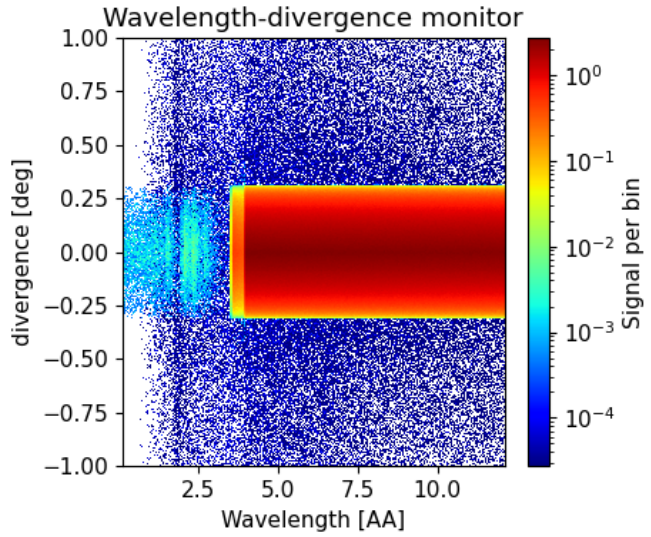
n1 sin(theta1) = n2 sin(theta2)

Interface physics update

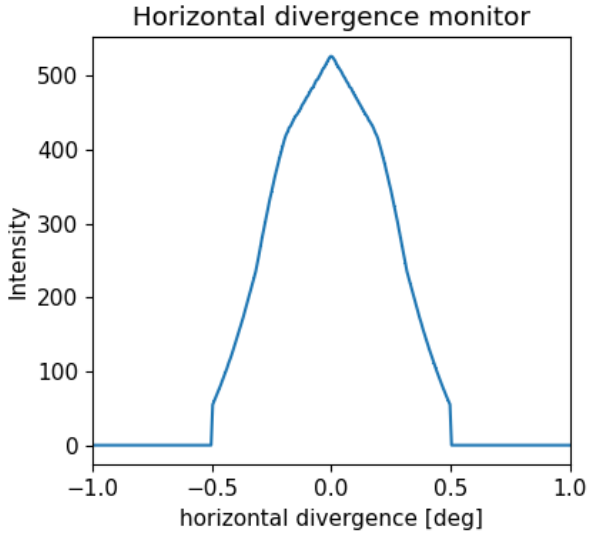
Simple example - filter

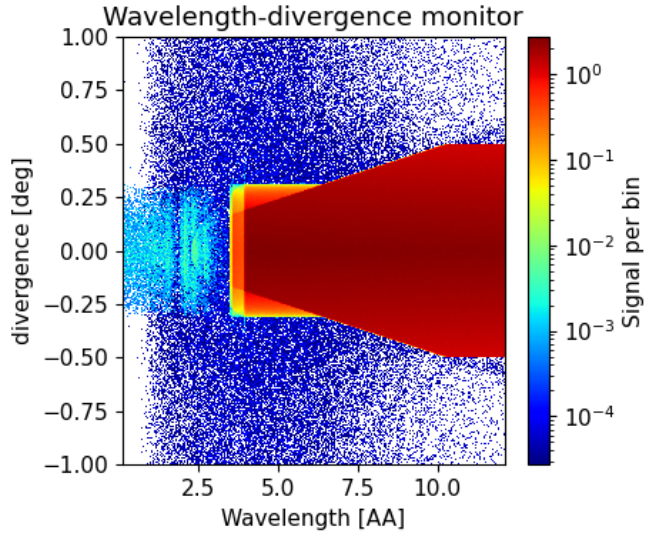
No refraction

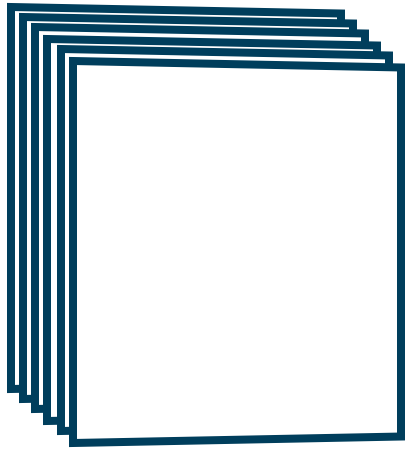


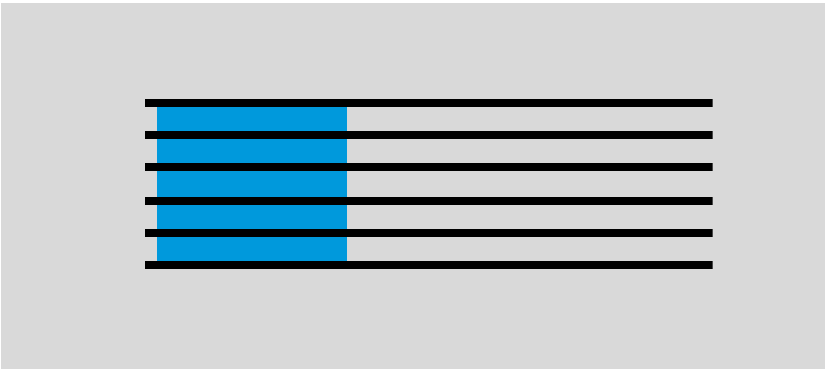


Refraction





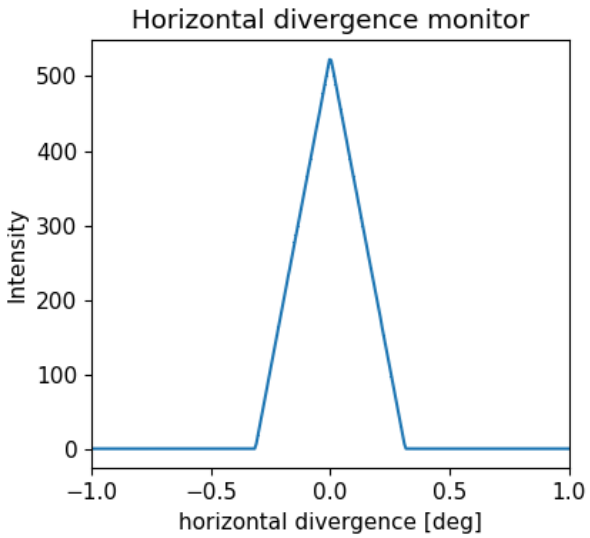


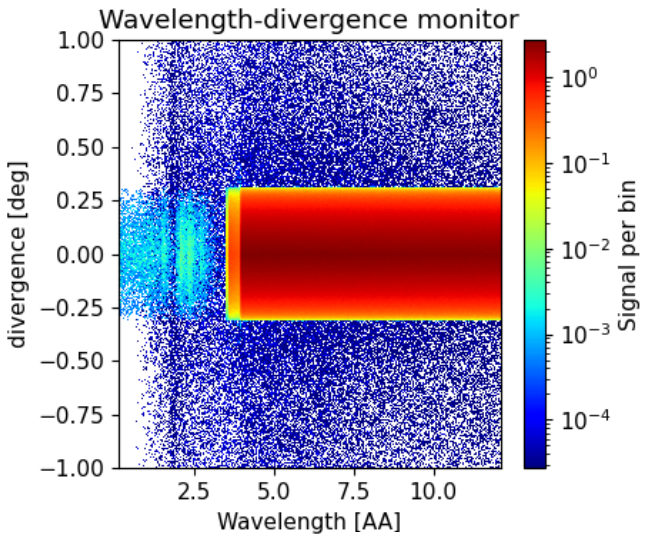


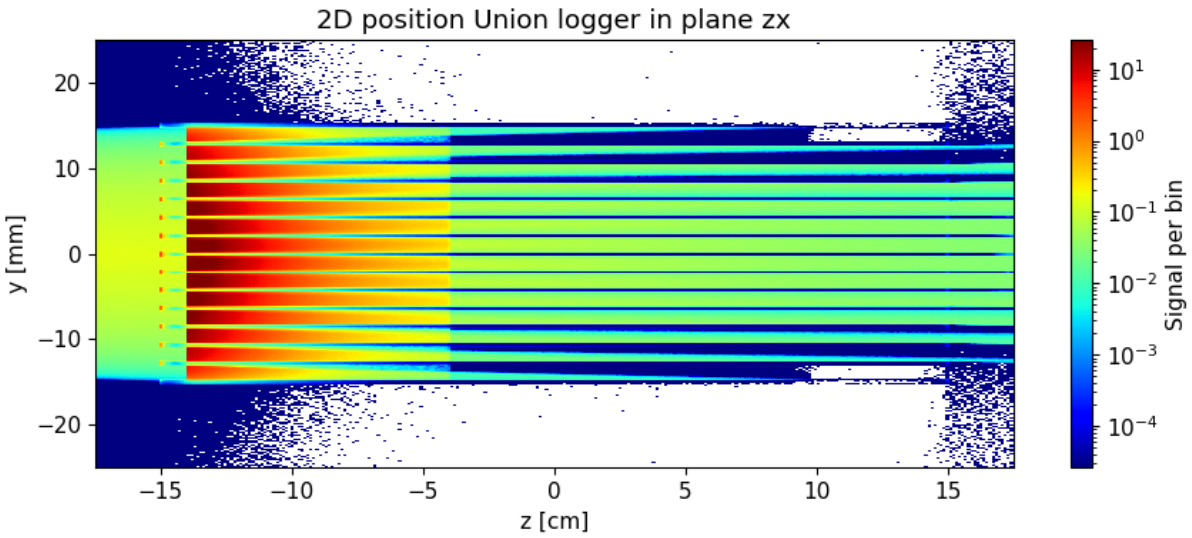
Cd | Air | Be

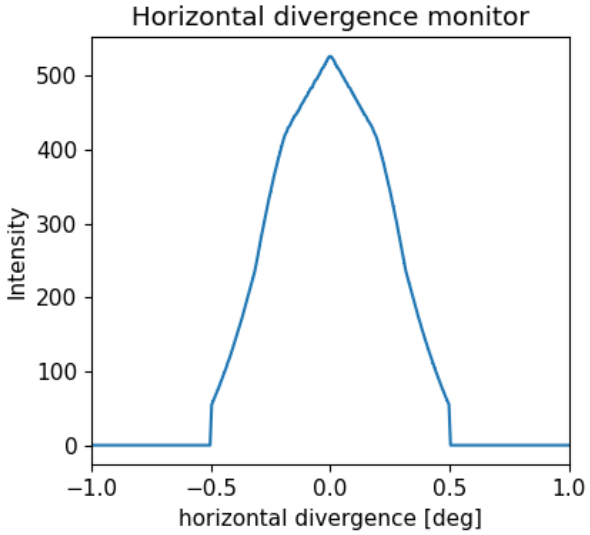
Interface physics update

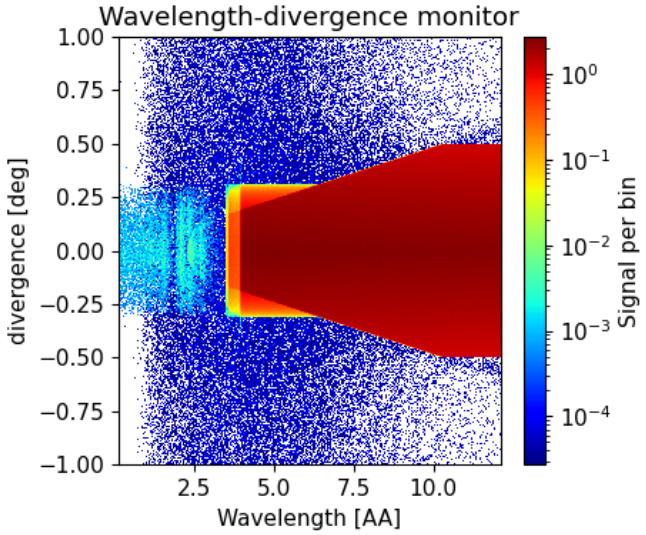
Simple example - filter

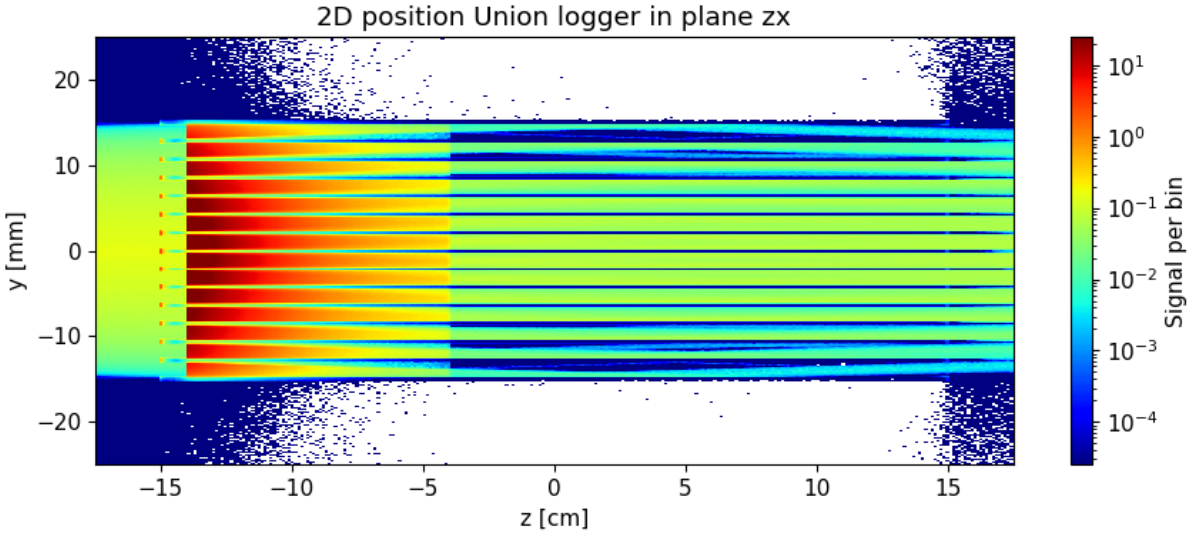








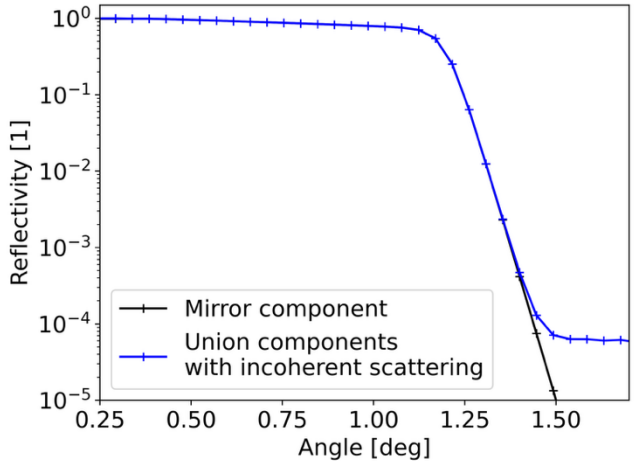


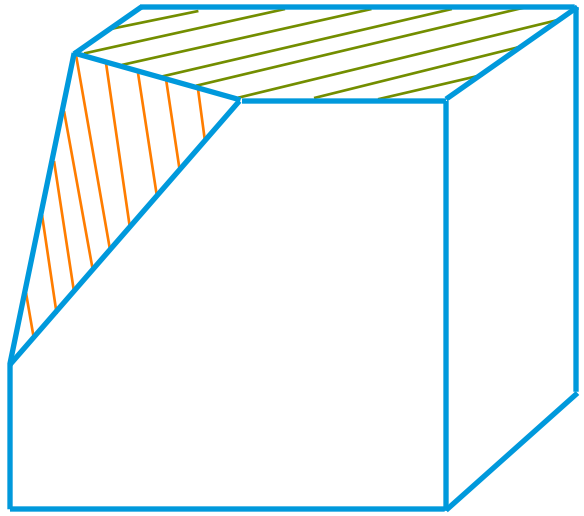


Interface physics update

Surface processes

- Surface process components
  - Gets normal vector, initial wavevector and weight
  - Returns final wavevector and weight
- Allows
  - Reflectivity curve
  - Thin absorbing paints
  - …
- Can be attached to geometry faces
  - Each outside face
  - … and one for all cuts in inside of material





Interface physics update

Surface stacks

- Surface process components
  - Gets normal vector, initial wavevector and weight
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- Allows
  - Reflectivity curve
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- Can be attached to geometry faces
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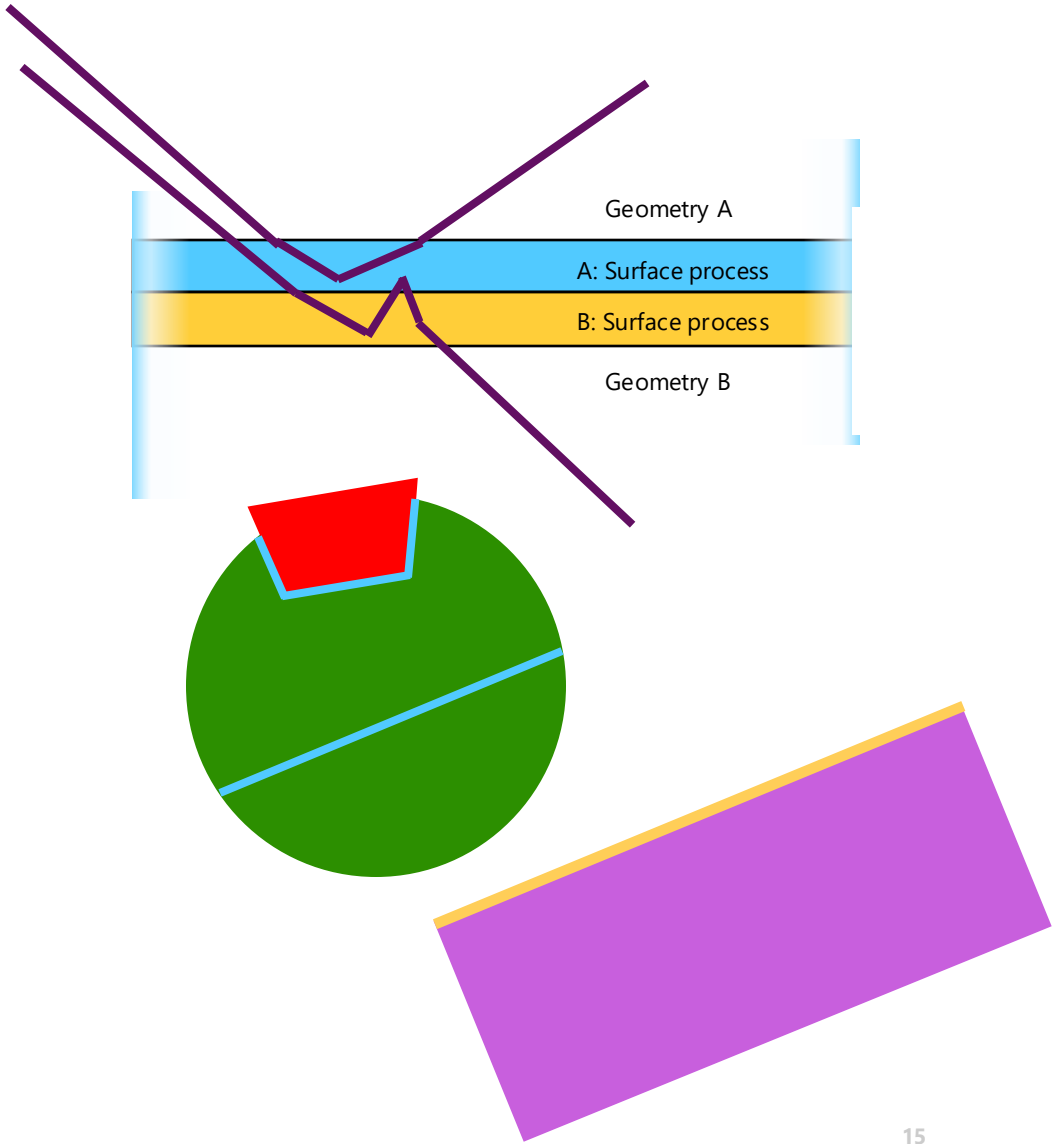
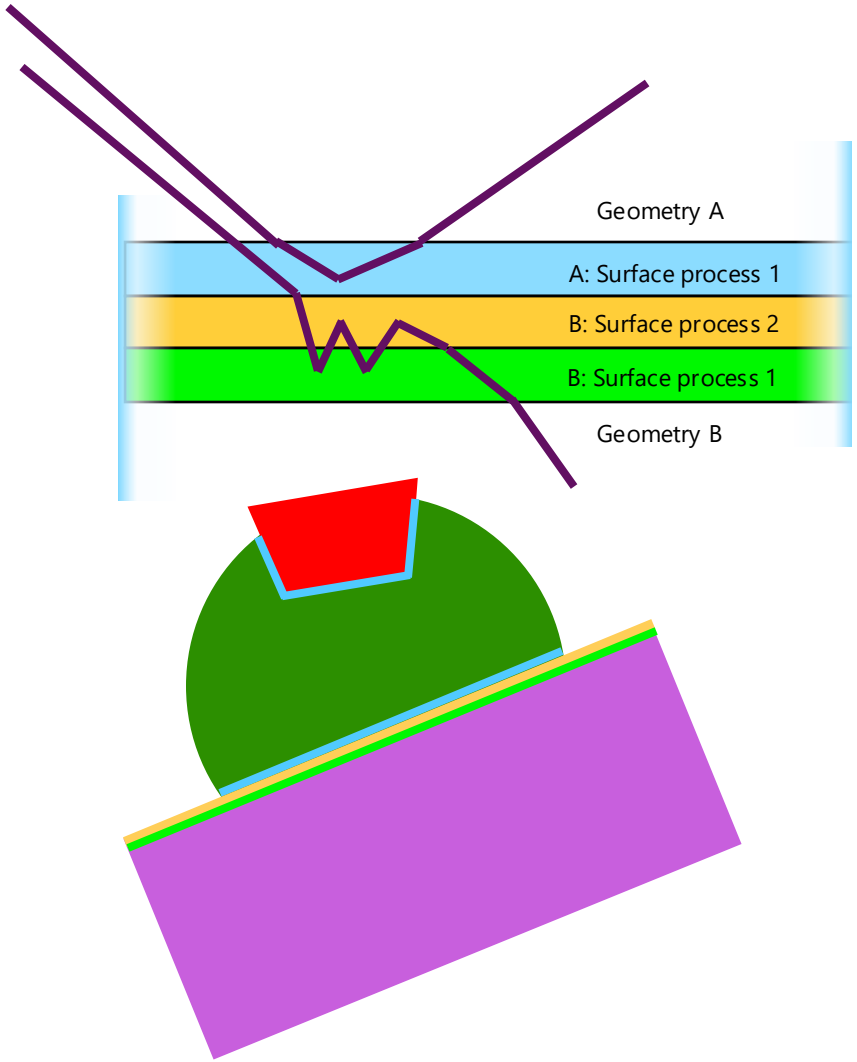


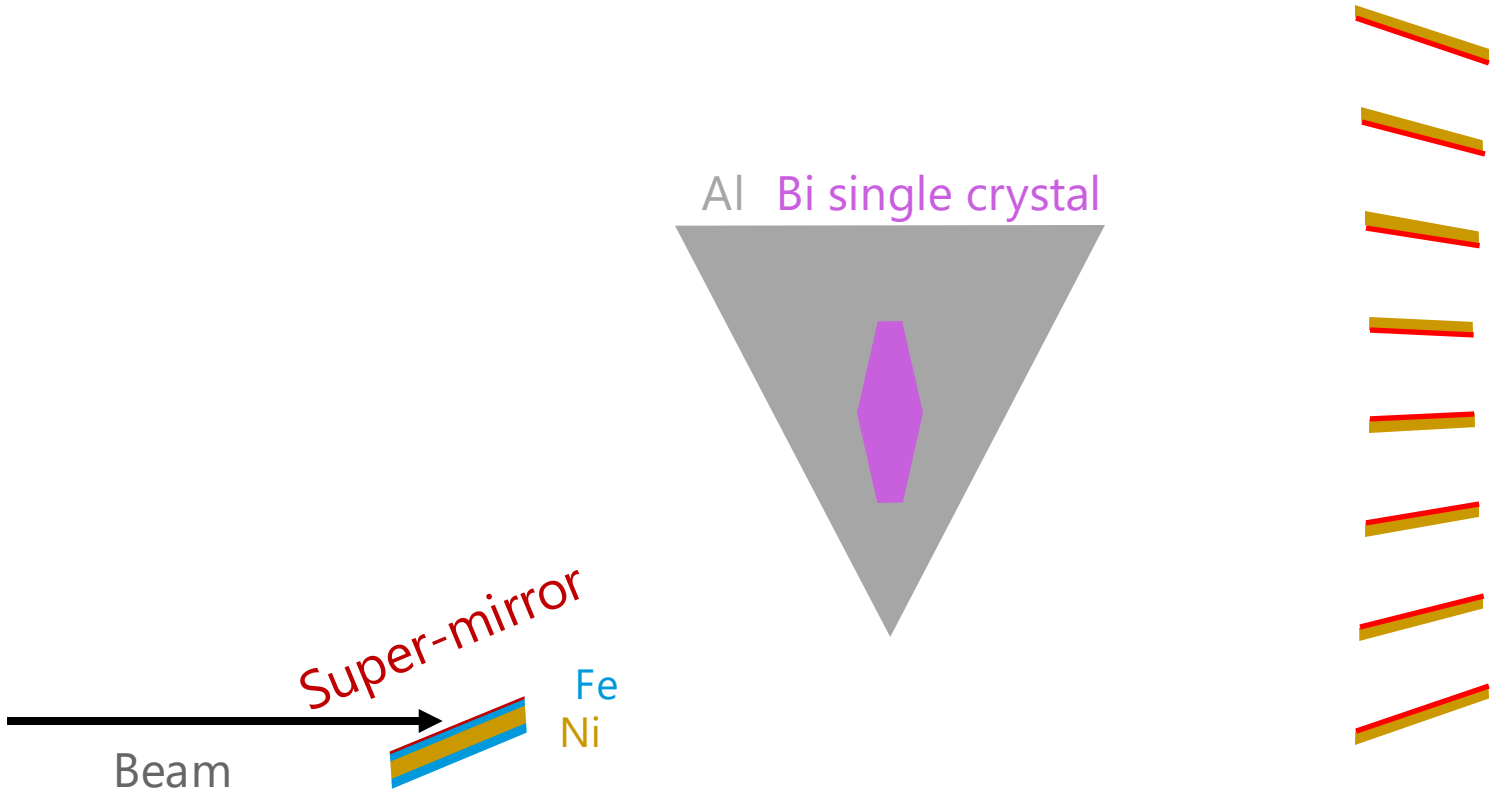
Interface physics update

Surface stacks

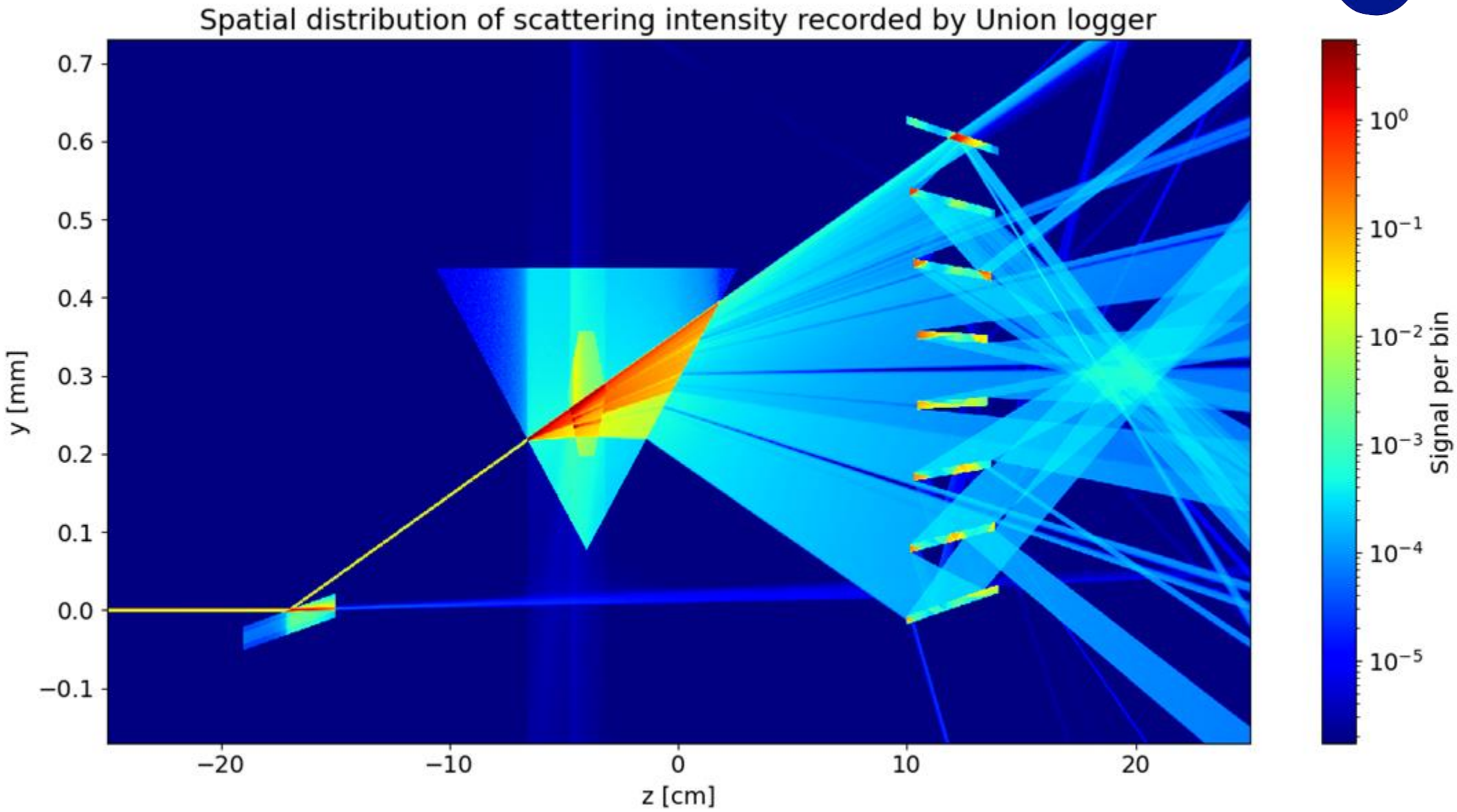
- Surface process components
  - Gets normal vector, initial wavevector and weight
  - Returns final wavevector and weight
- Allows
  - Reflectivity curve
  - Thin absorbing paints
  - …
- Can be attached to geometry faces
  - Each outside face
  - … and one for all cuts in inside of material
  - Several processes can be combined into a stack



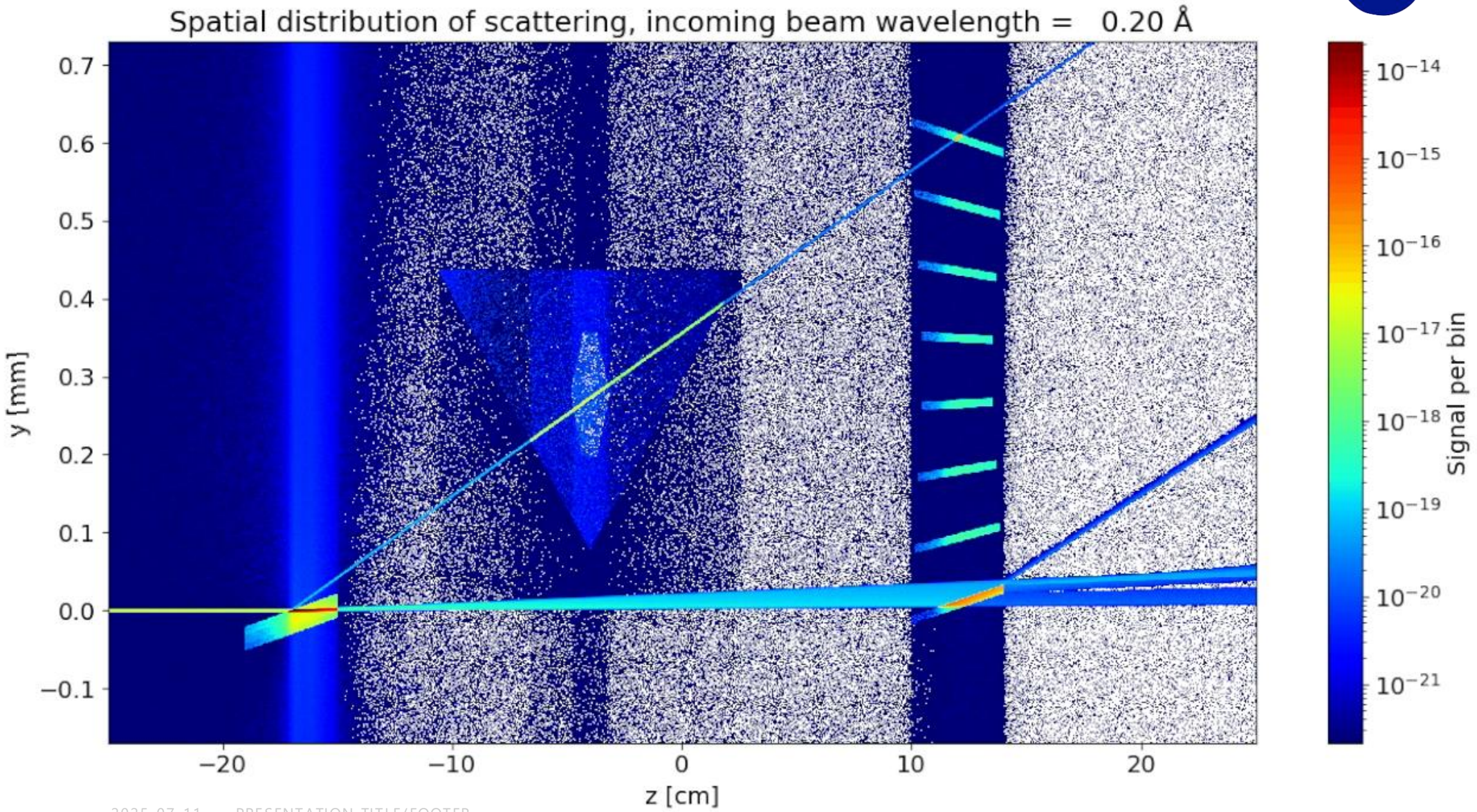
Interface physics demo



Interface physics demo



Interface physics demo



Interface physics use-case

Surface physics relevant for

- Optics
  - *Guides*
  - *Focusing optics*
  - *Refractive optics*
  - *.. in sample environments*
- Reflectometry
  - Sample
  - Substrate

Conclusion

- Union components constitutes a powerful tool in McStas to simulate complex systems
- Newly added interface physics expands their use case to optics, reflectometry and more
- Remaining limitations:
  - No simulation of gravity
  - Lack support for polarization

Thanks for your attention!