

Monte Carlo simulations of x-ray grating interferometry based imaging systems

S. Tessarini^{a,b}

M. Fix^c, W. Volken^c, M. Stampanoni^{a,b}

^aInstitute for Biomedical Engineering, University and ETH Zürich, 8092 Zürich, Switzerland

^bSwiss Light Source, Paul Scherrer Institut, 5232 Villigen, Switzerland

^cDivision of Medical Radiation Physics and Department of Radiation Oncology, Inselspital University Hospital Bern and University of Bern, Bern, Switzerland



Goal

- Implementation of a Monte Carlo simulation tool for grating based imaging systems including quantitative dose estimations



Absorption



Phase



Dark field

Basic principle: Phase shift

- Light propagating through media picks up a phase shift
- The refractive index of the material, for x-rays:
$$n = 1 + \delta$$
- Consider 17 keV x-ray beam passing through a μm thick sheet of biological tissue
 - Phase shift of the order of π
 - Absorption of a few percent.
- This is used as a new source of contrast.

Talbot effect and x-ray grating interferometry

- Self image of periodic structures
- Understood by Fresnel diffraction

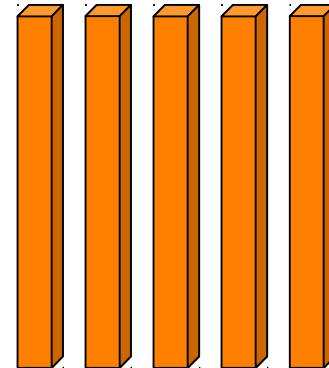
Talbot effect and x-ray grating interferometry

- Self image of periodic structures
- Understood by Fresnel diffraction



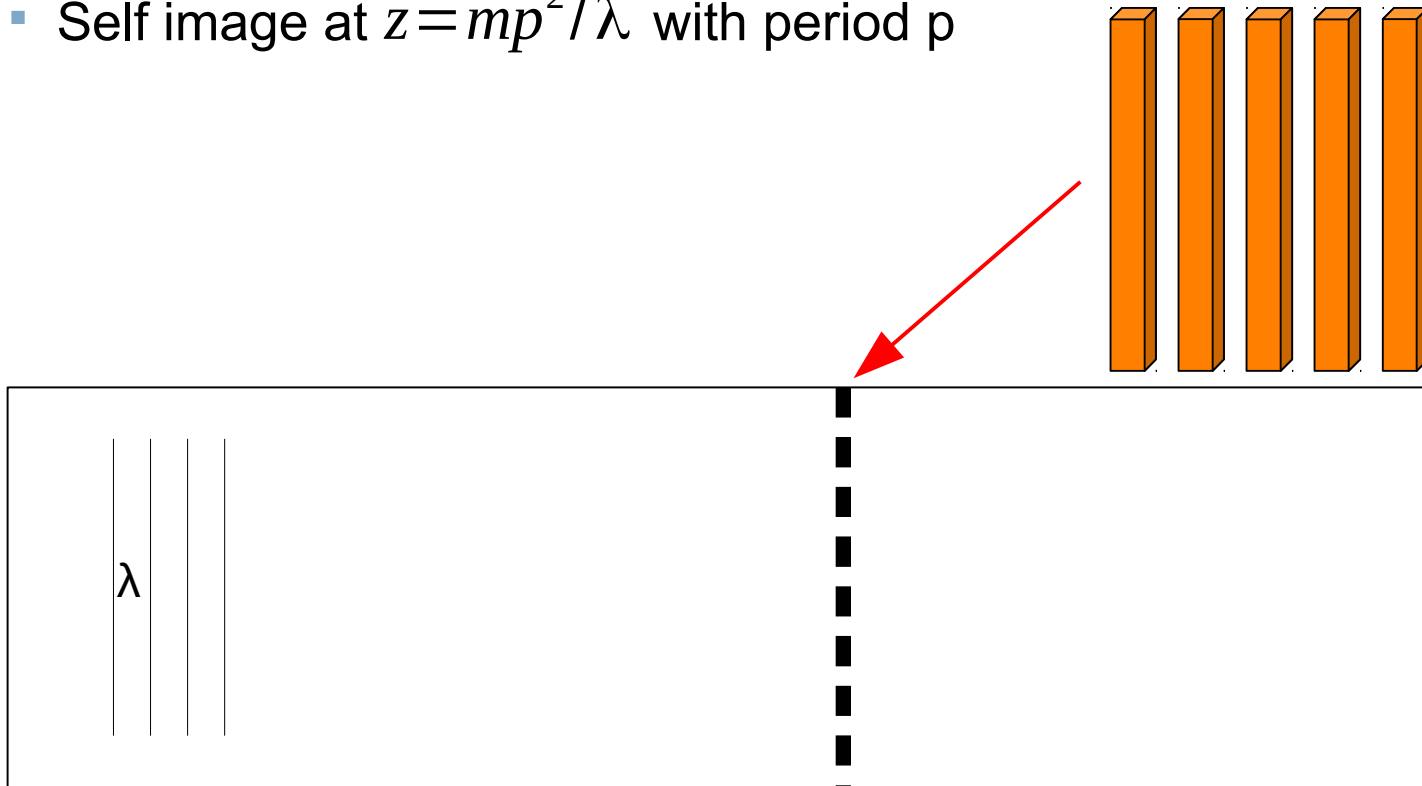
Talbot effect and x-ray grating interferometry

- Self image of periodic structures
- Understood by Fresnel diffraction
- Absorption grating with period p (typically Au):
 - Self image at $z = mp^2/\lambda$ with period p



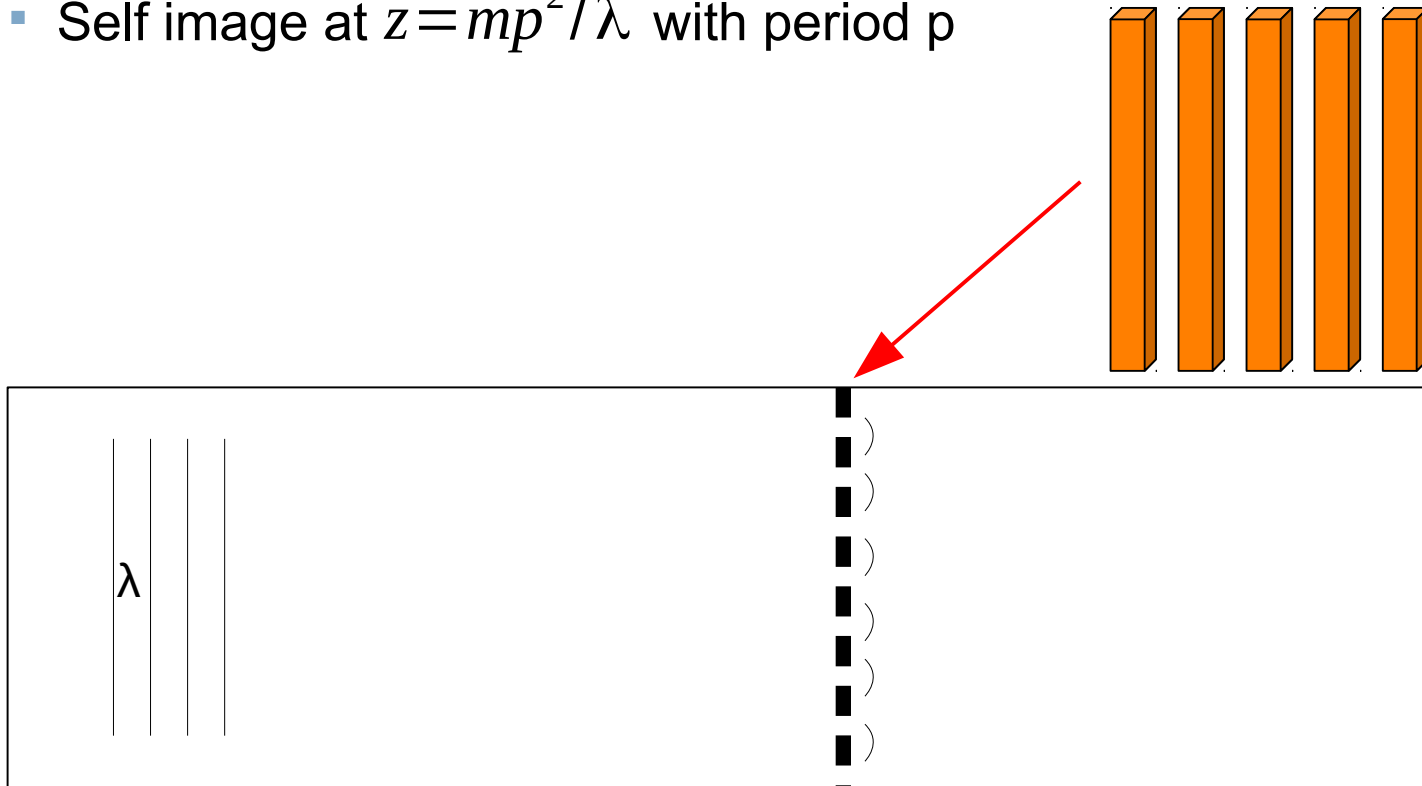
Talbot effect and x-ray grating interferometry

- Self image of periodic structures
- Understood by Fresnel diffraction
- Absorption grating with period p (typically Au):
 - Self image at $z = mp^2 / \lambda$ with period p



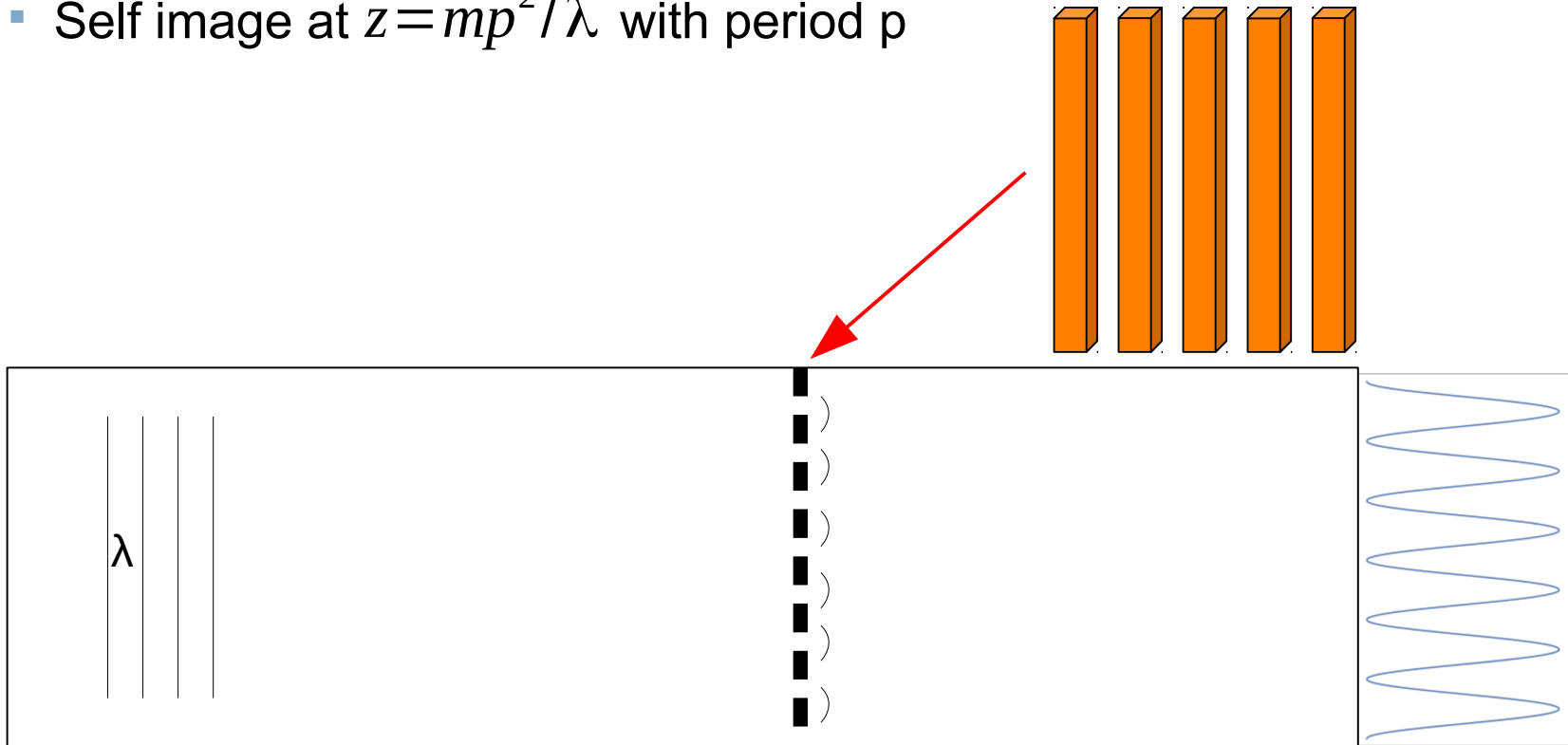
Talbot effect and x-ray grating interferometry

- Self image of periodic structures
- Understood by Fresnel diffraction
- Absorption grating with period p (typically Au):
 - Self image at $z = mp^2/\lambda$ with period p



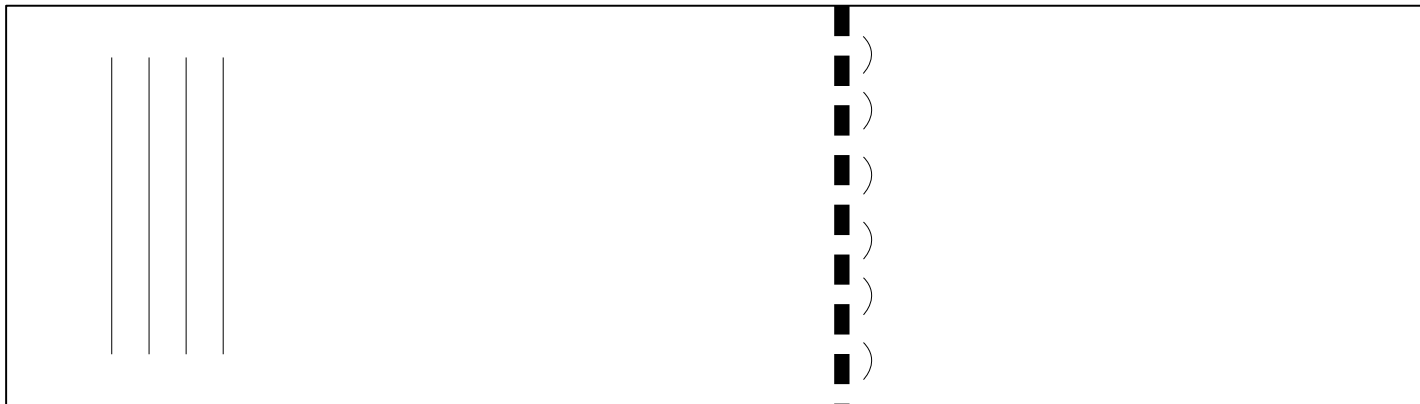
Talbot effect and x-ray grating interferometry

- Self image of periodic structures
- Understood by Fresnel diffraction
- Absorption grating with period p (typically Au):
 - Self image at $z = mp^2 / \lambda$ with period p



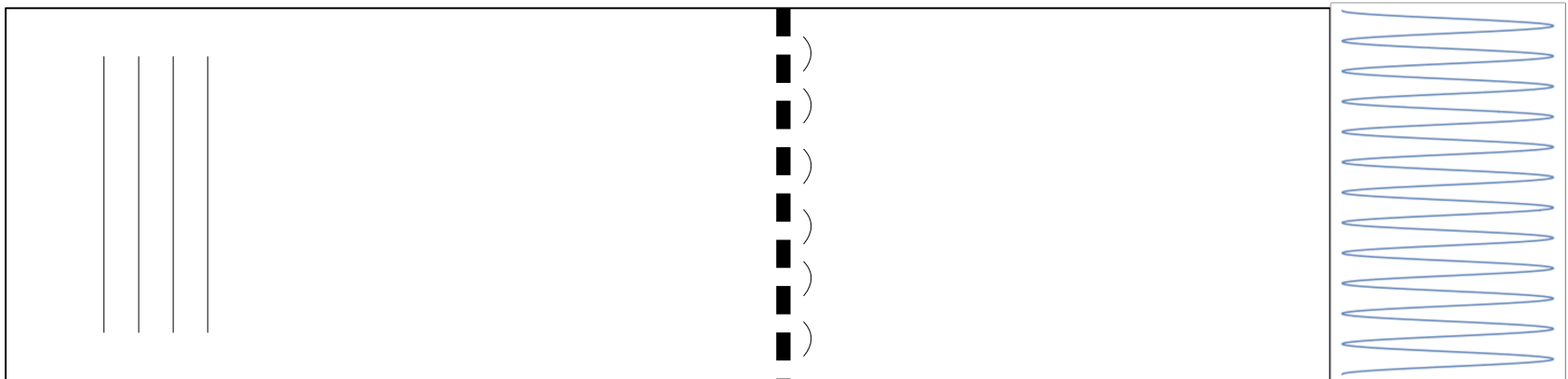
Talbot effect and x-ray grating interferometry

- The self image of periodic structures.
- Understood by Fresnel diffraction
- Absorption grating with period p (typically Au):
 - Self image at $z = mp^2/\lambda$ with period p
- π -Phase grating with period p (typically Si):
 - Self image at $z = (m + 0.5) p^2/\lambda$ with period $p/2$



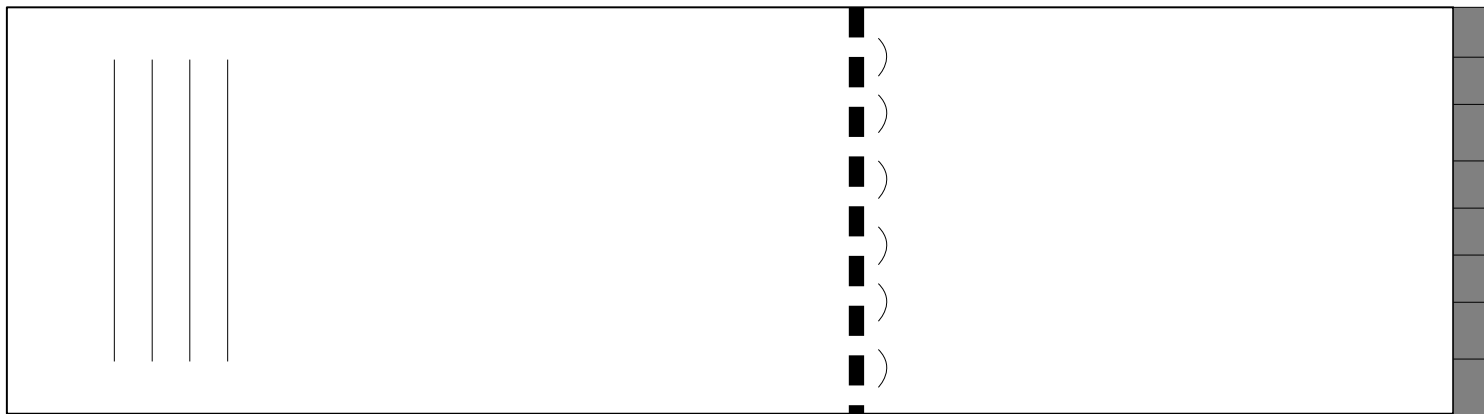
Talbot effect and x-ray grating interferometry

- The self image of periodic structures.
- Understood by Fresnel diffraction
- Absorption grating with period p (typically Au):
 - Self image at $z = mp^2/\lambda$ with period p
- π -Phase grating with period p (typically Si):
 - Self image at $z = (m + 0.5) p^2/\lambda$ with period $p/2$



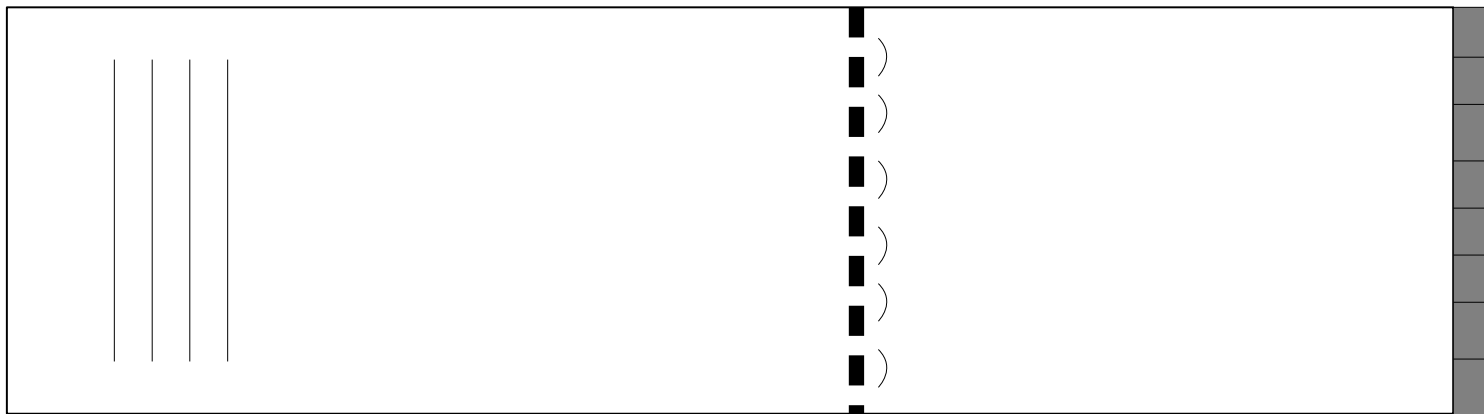
Measurement of the phase signal

- Typical period of the phase grating: $4\ \mu\text{m}$



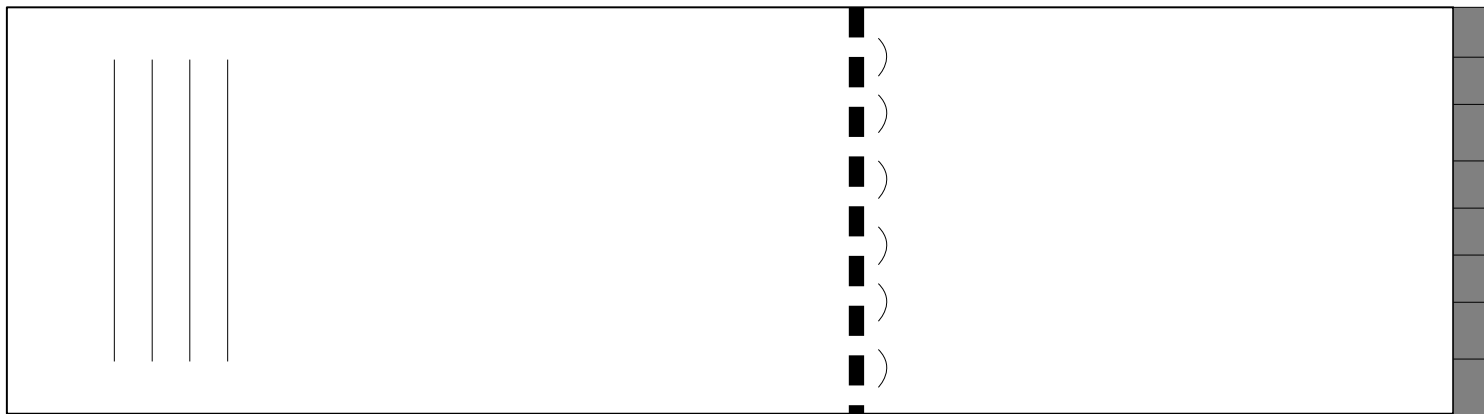
Measurement of the phase signal

- Typical period of the phase grating: $4\ \mu\text{m}$
- Period of the intensity pattern: $2\ \mu\text{m}$



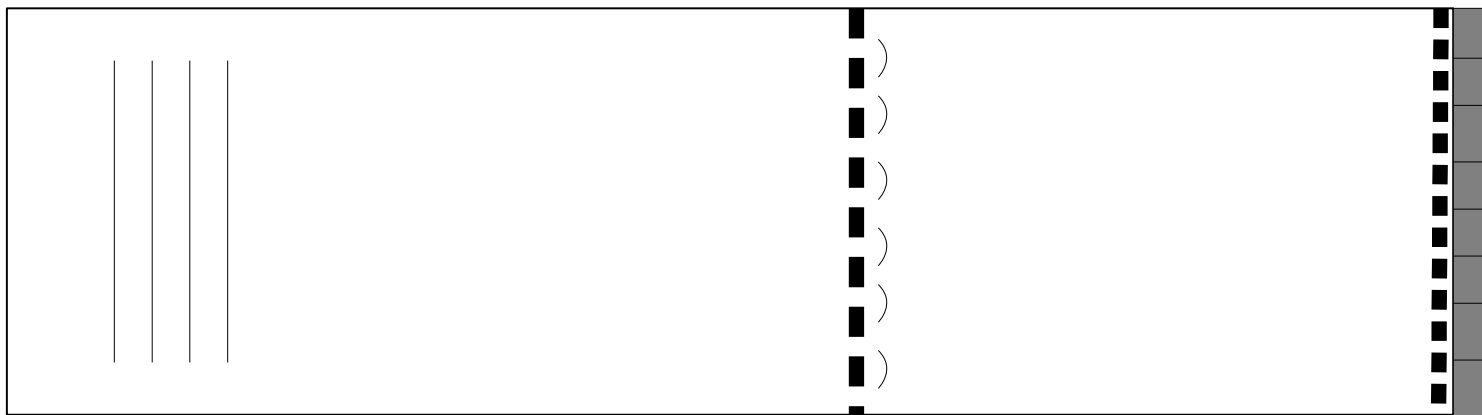
Measurement of the phase signal

- Typical period of the phase grating: $4\ \mu\text{m}$
- Period of the intensity pattern: $2\ \mu\text{m}$
- Typically this is smaller then the pixel size



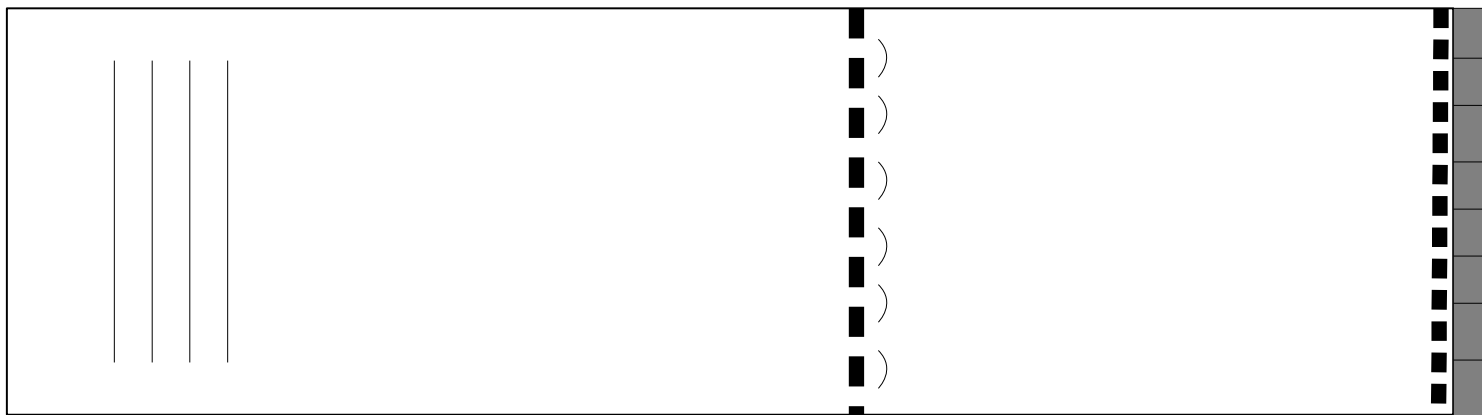
Measurement of the phase signal

- Typical period of the phase grating: $4\text{ }\mu\text{m}$
- Period of the intensity pattern: $2\text{ }\mu\text{m}$
- Typically this is smaller than the pixel size
- Introduce absorbing grating at detector



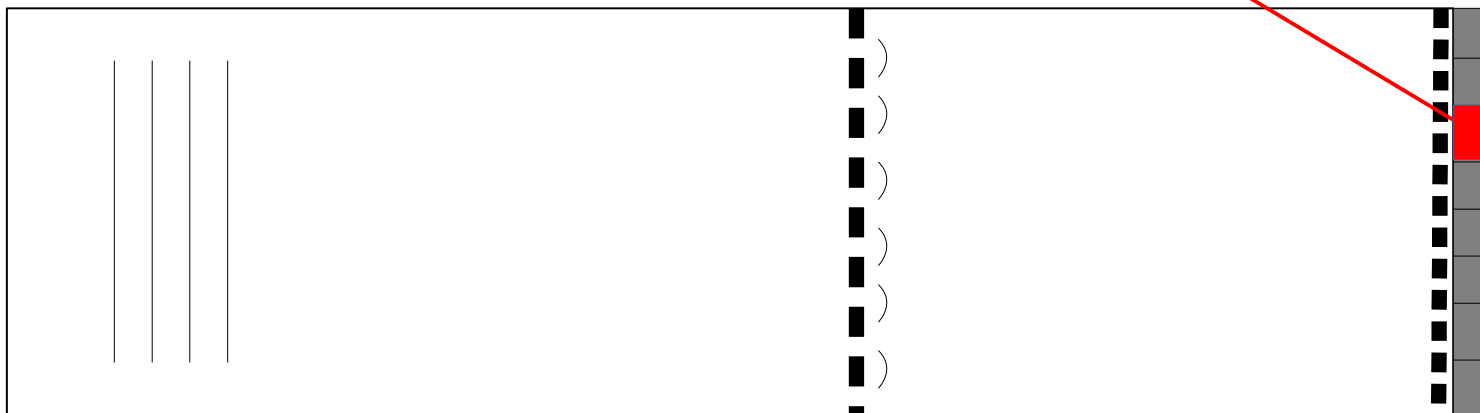
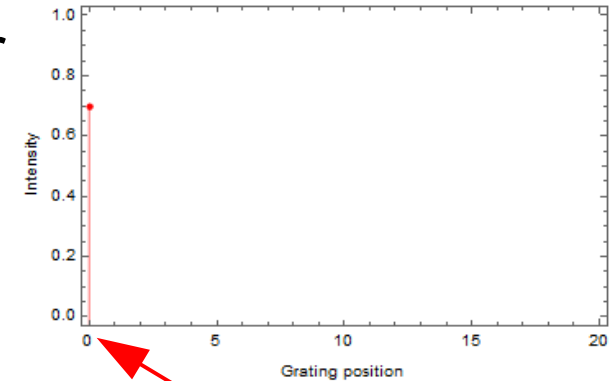
Measurement of the phase signal

- Typical period of the phase grating: $4\text{ }\mu\text{m}$
- Period of the intensity pattern: $2\text{ }\mu\text{m}$
- Typically this is smaller then the pixel size
- Introduce absorbing grating at detector
- Perform phase stepping
 - Move the gratings relative to each other
 - Record the signal for different positions



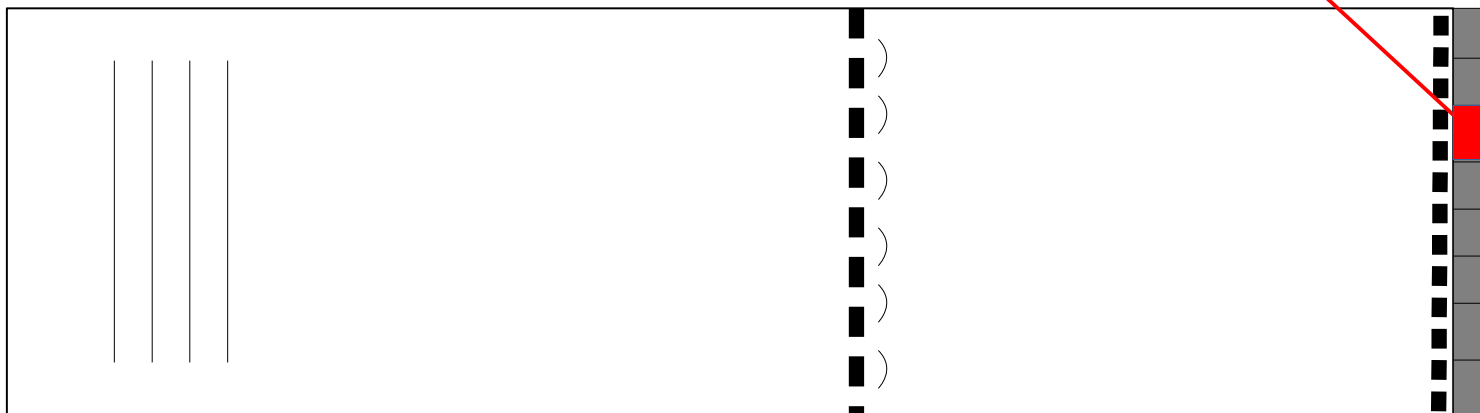
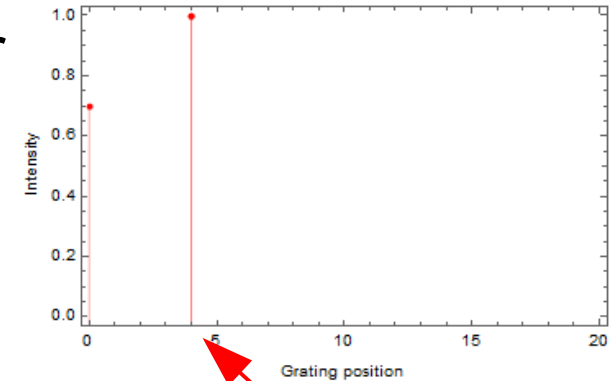
Measurement of the phase signal

- Typical period of the phase grating: $4\ \mu\text{m}$
- Period of the intensity pattern: $2\ \mu\text{m}$
- Typically this is smaller than the pixel size
- Introduce absorbing grating at detector
- Perform phase stepping
 - Move the gratings relative to each other
 - Record the signal for different positions



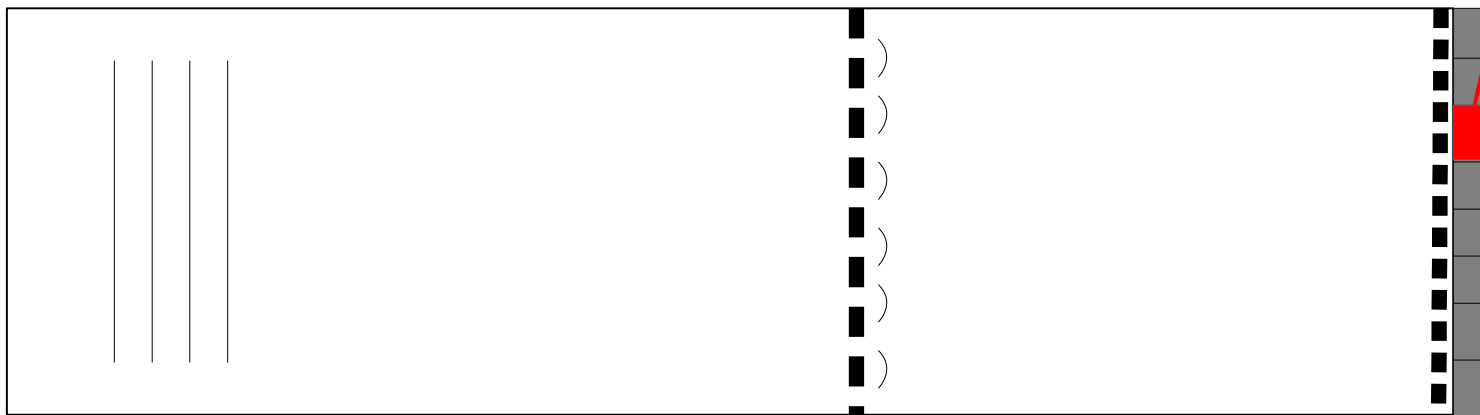
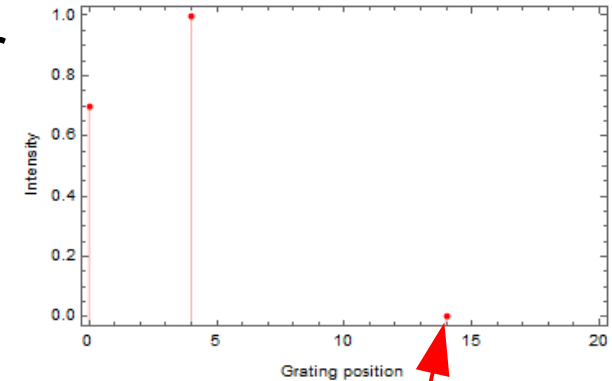
Measurement of the phase signal

- Typical period of the phase grating: $4\text{ }\mu\text{m}$
- Period of the intensity pattern: $2\text{ }\mu\text{m}$
- Typically this is smaller than the pixel size
- Introduce absorbing grating at detector
- Perform phase stepping
 - Move the gratings relative to each other
 - Record the signal for different positions



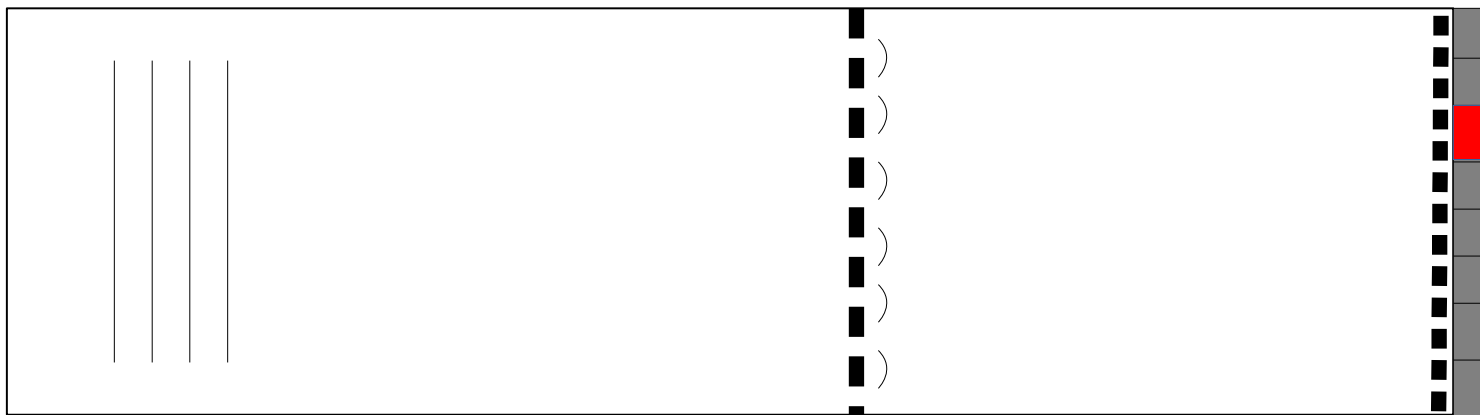
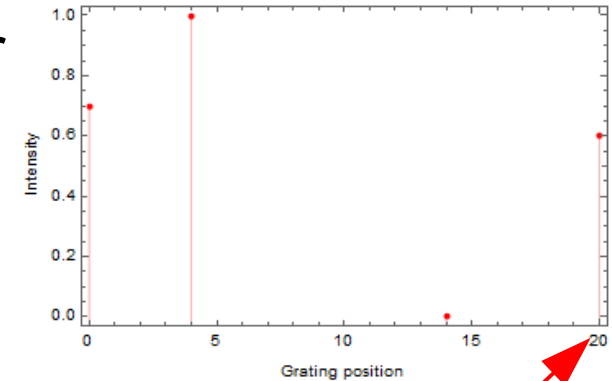
Measurement of the phase signal

- Typical period of the phase grating: $4\text{ }\mu\text{m}$
- Period of the intensity pattern: $2\text{ }\mu\text{m}$
- Typically this is smaller than the pixel size
- Introduce absorbing grating at detector
- Perform phase stepping
 - Move the gratings relative to each other
 - Record the signal for different positions



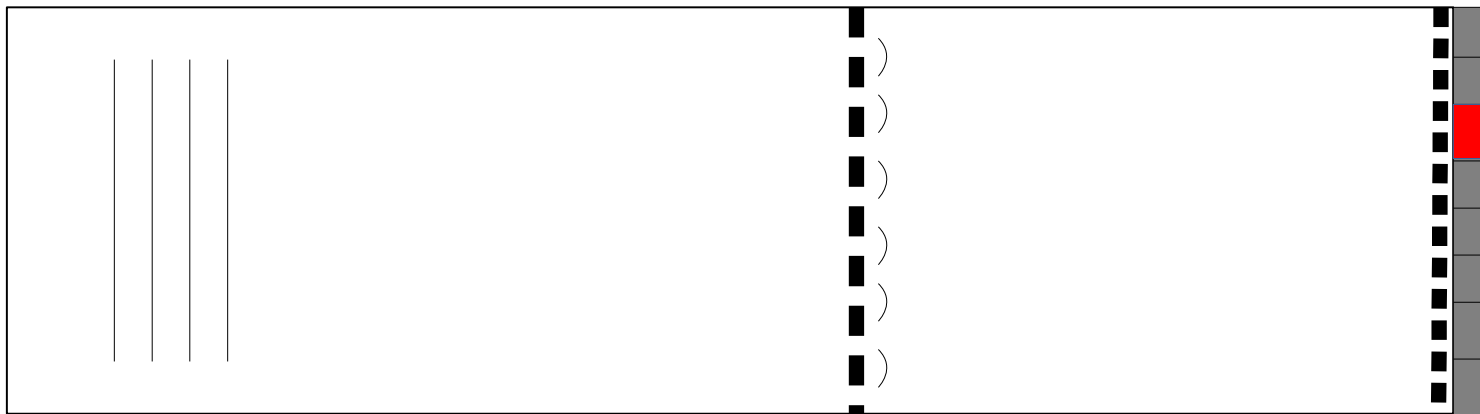
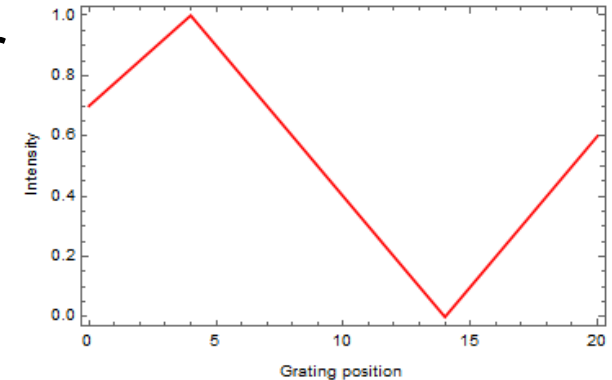
Measurement of the phase signal

- Typical period of the phase grating: $4\text{ }\mu\text{m}$
- Period of the intensity pattern: $2\text{ }\mu\text{m}$
- Typically this is smaller than the pixel size
- Introduce absorbing grating at detector
- Perform phase stepping
 - Move the gratings relative to each other
 - Record the signal for different positions



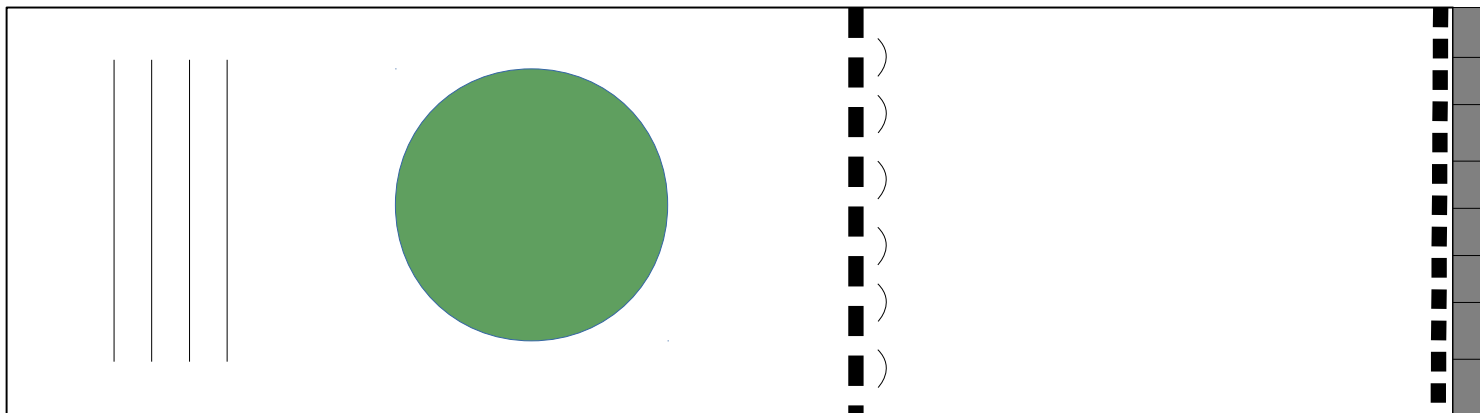
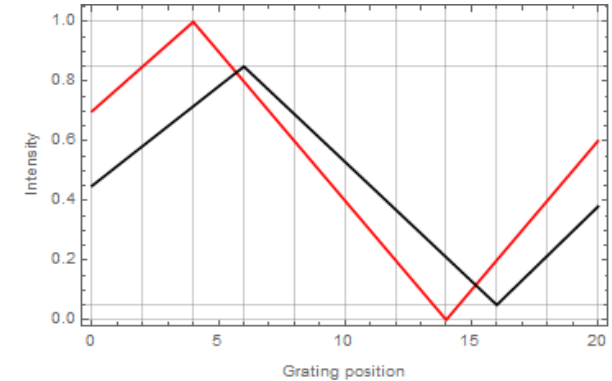
Measurement of the phase signal

- Typical period of the phase grating: $4\text{ }\mu\text{m}$
- Period of the intensity pattern: $2\text{ }\mu\text{m}$
- Typically this is smaller than the pixel size
- Introduce absorbing grating at detector
- Perform phase stepping
 - Move the gratings relative to each other
 - Record the signal for different positions



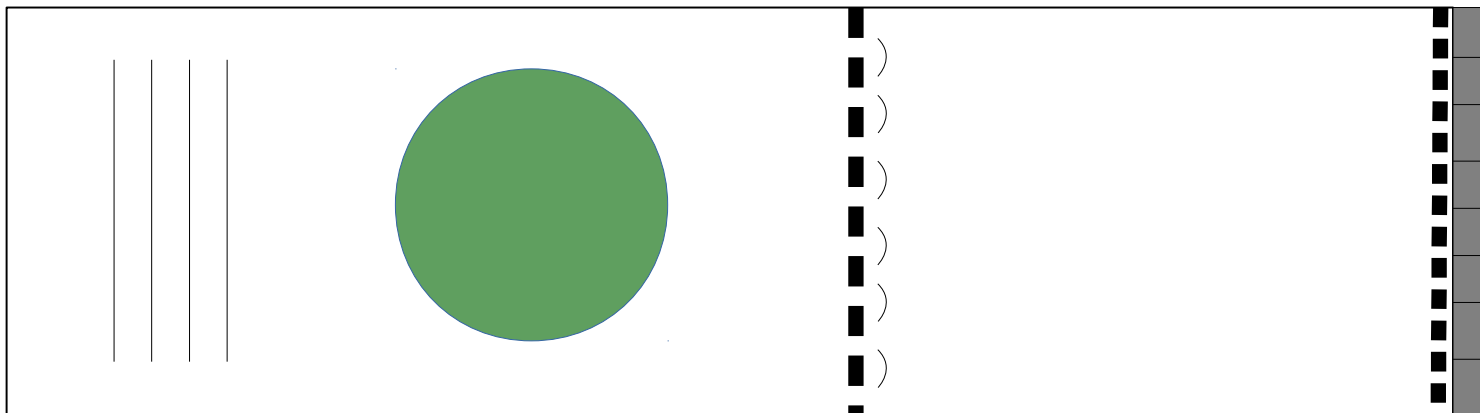
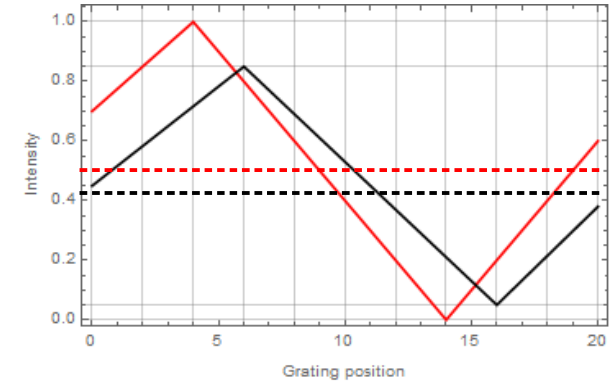
Measurement of the phase signal

- Inserting a sample introduces a phase shift
 - Distortion of the interference pattern



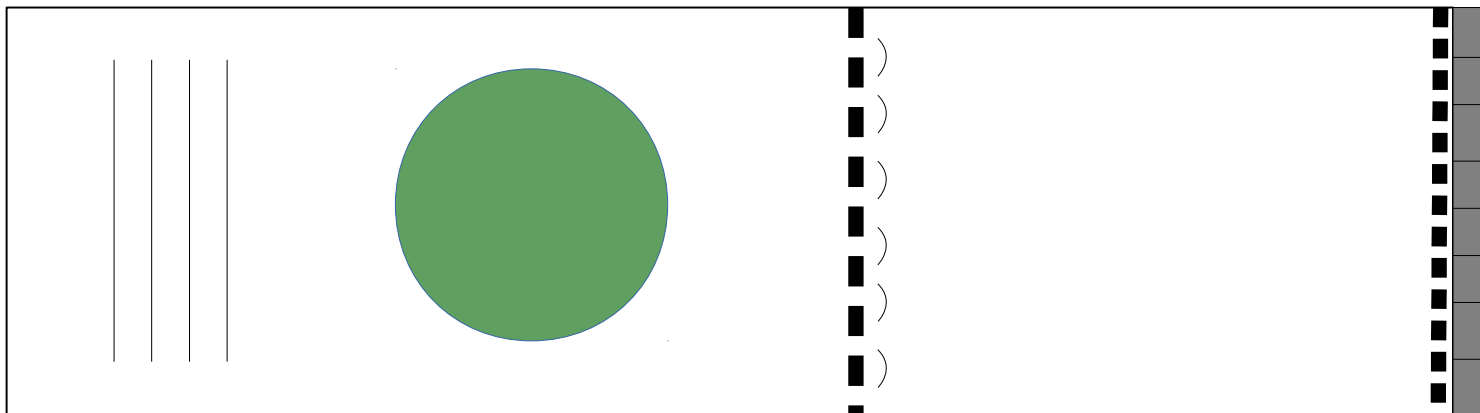
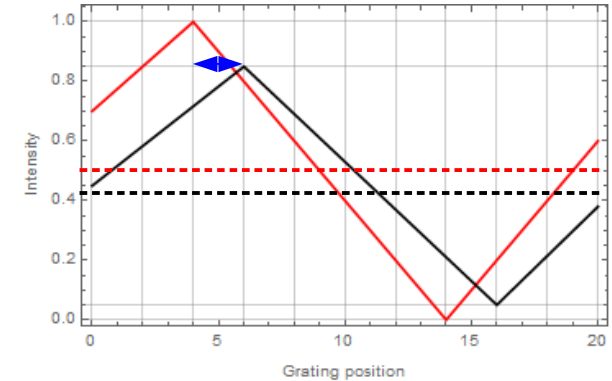
Measurement of the phase signal

- Inserting a sample introduces a phase shift
 - Distortion of the interference pattern
- Reduced mean value of the intensity
 - Absorption signal



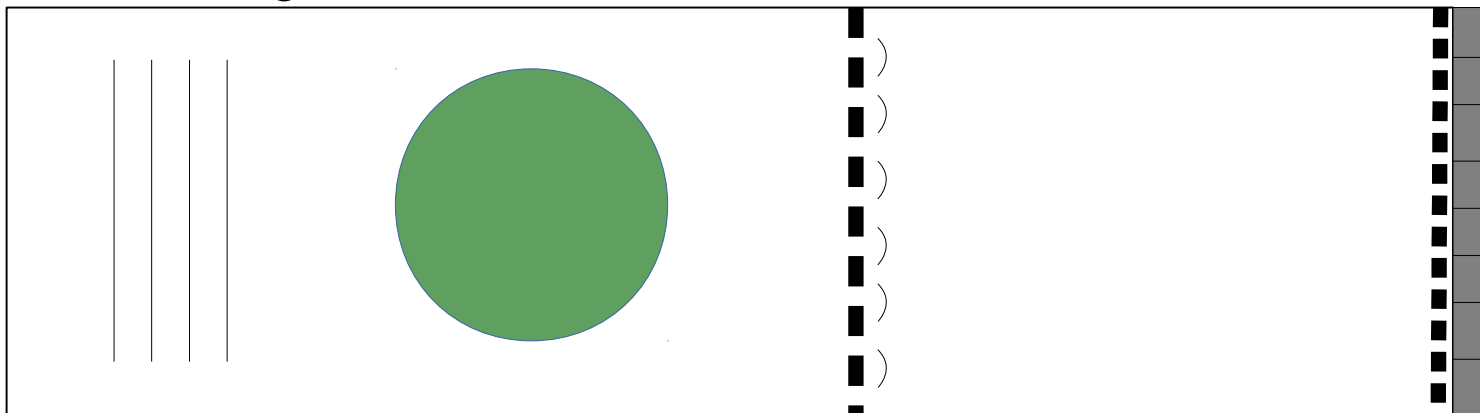
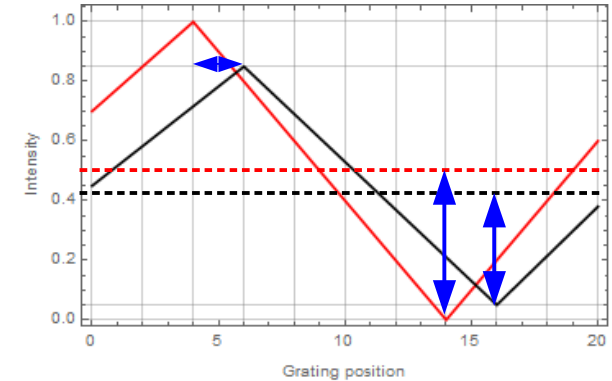
Measurement of the phase signal

- Inserting a sample introduces a phase shift
 - Distortion of the interference pattern
- Reduced mean value of the intensity
 - Absorption signal
- Shift of the intensity curve
 - Phase signal

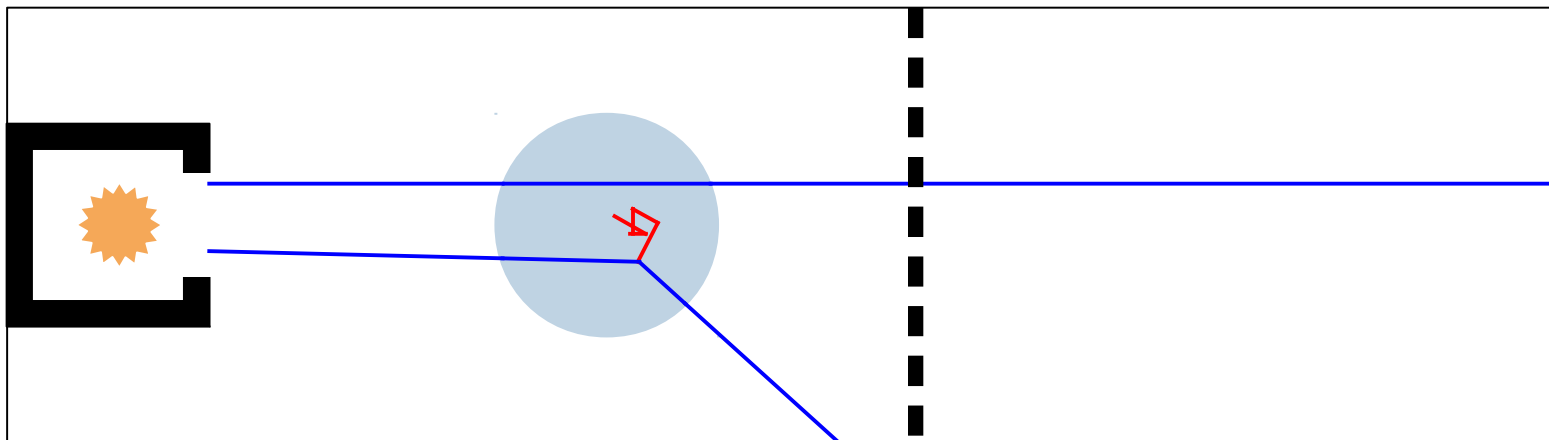


Measurement of the phase signal

- Inserting a sample introduces a phase shift
 - Distortion of the interference pattern
- Reduced mean value of the intensity
 - Absorption signal
- Shift of the intensity curve
 - Phase signal
- Decrease of the amplitude
 - Dark field signal

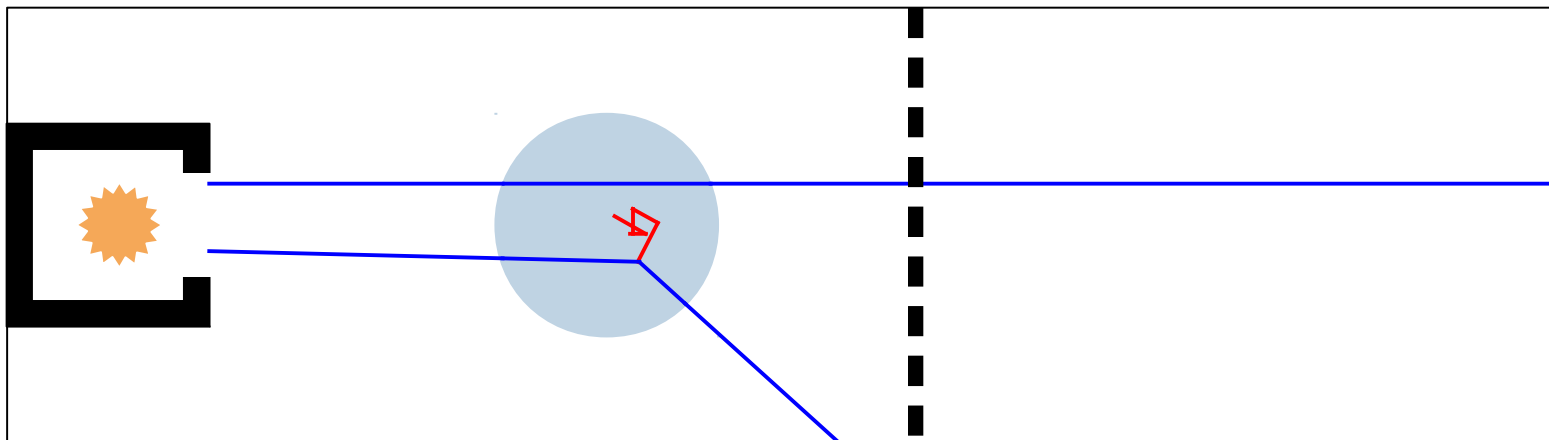


Particle transport in EGSnrc: the missing parts



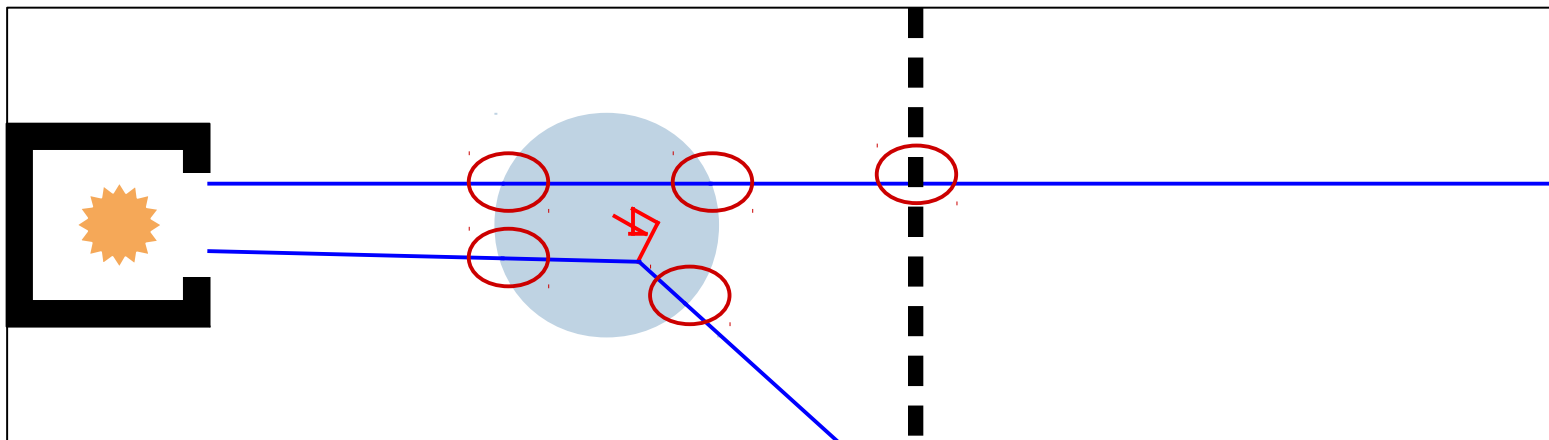
Particle transport in EGSnrc: the missing parts

- Phase shift



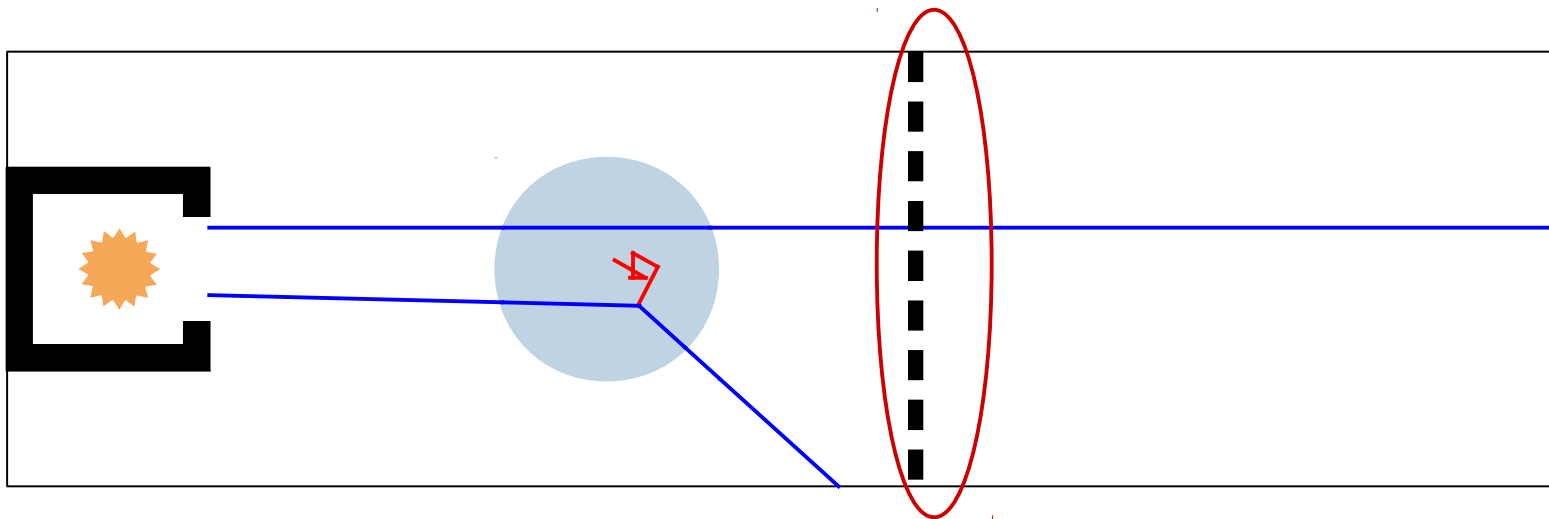
Particle transport in EGSnrc: the missing parts

- Phase shift
- Refraction



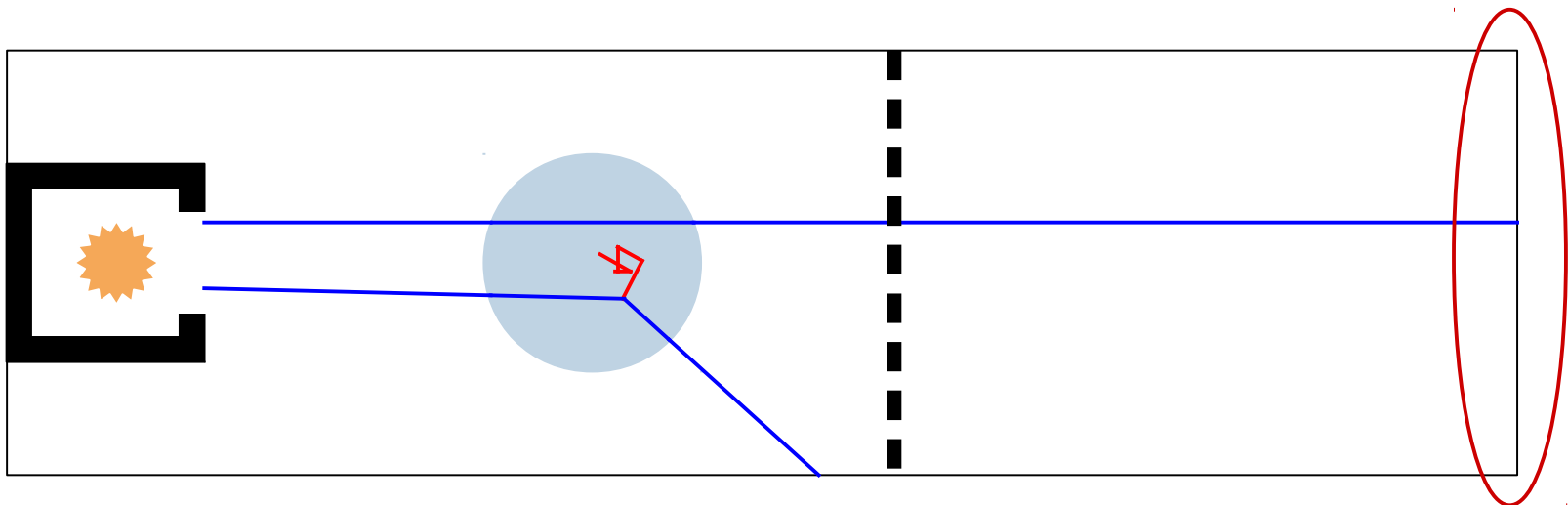
Particle transport in EGSnrc: the missing parts

- Phase shift
- Refraction
- Diffraction



Particle transport in EGSnrc: the missing parts

- Phase shift
- Refraction
- Diffraction
- Detector

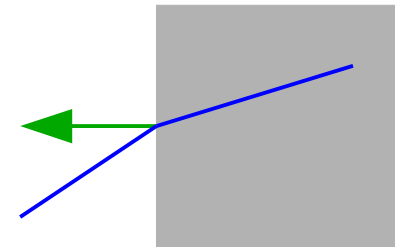


Modeling the missing parts

- Phase shift in media
 - Add a phase variable similar to (E, x, p, w, \dots)
 - Assign real part of refractive index to the media

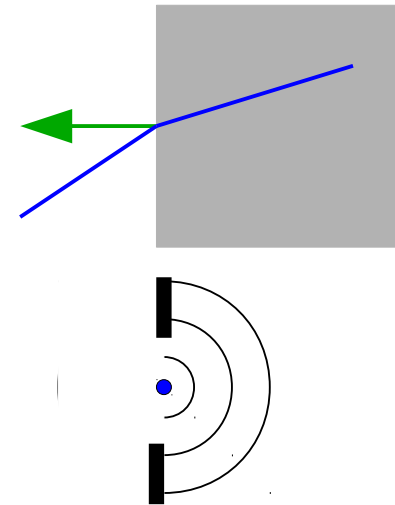
Modeling the missing parts

- Phase shift in media
 - Add a phase variable similar to (E, x, p, w, \dots)
 - Assign real part of refractive index to the media
- Refraction
 - According to Snell's law
 - Refractive index
 - Surface normal vectors



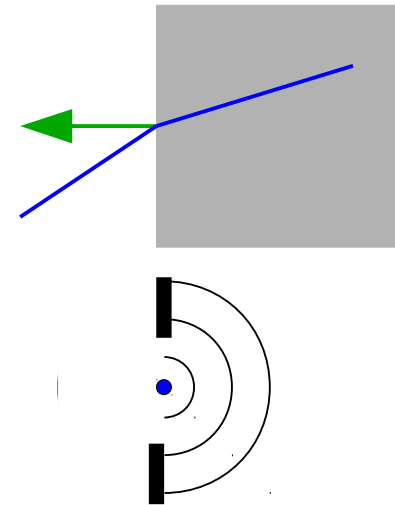
Modeling the missing parts

- Phase shift in media
 - Add a phase variable similar to (E, x, p, w, \dots)
 - Assign real part of refractive index to the media
- Refraction
 - According to Snell's law
 - Refractive index
 - Surface normal vectors
- Diffraction at the grating
 - Splitting algorithm modeling Huygens Principle

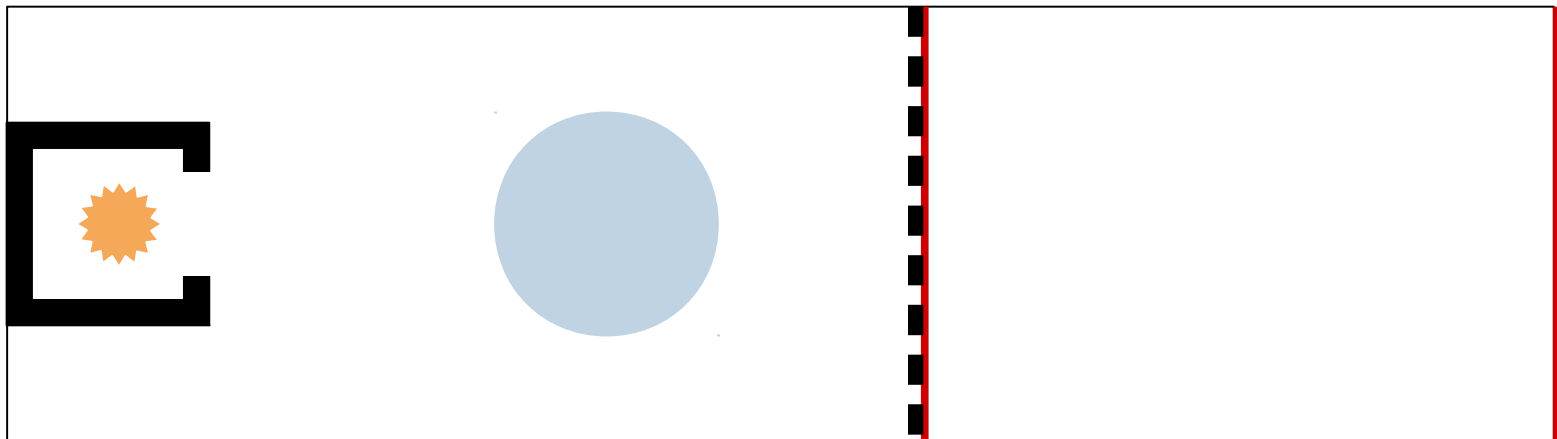


Modeling the missing parts

- Phase shift in media
 - Add a phase variable similar to (E, x, p, w, \dots)
 - Assign real part of refractive index to the media
- Refraction
 - According to Snell's law
 - Refractive index
 - Surface normal vectors
- Diffraction at the grating
 - Splitting algorithm modeling Huygens Principle
- Detector
 - Scoring a complex valued signal at the detector

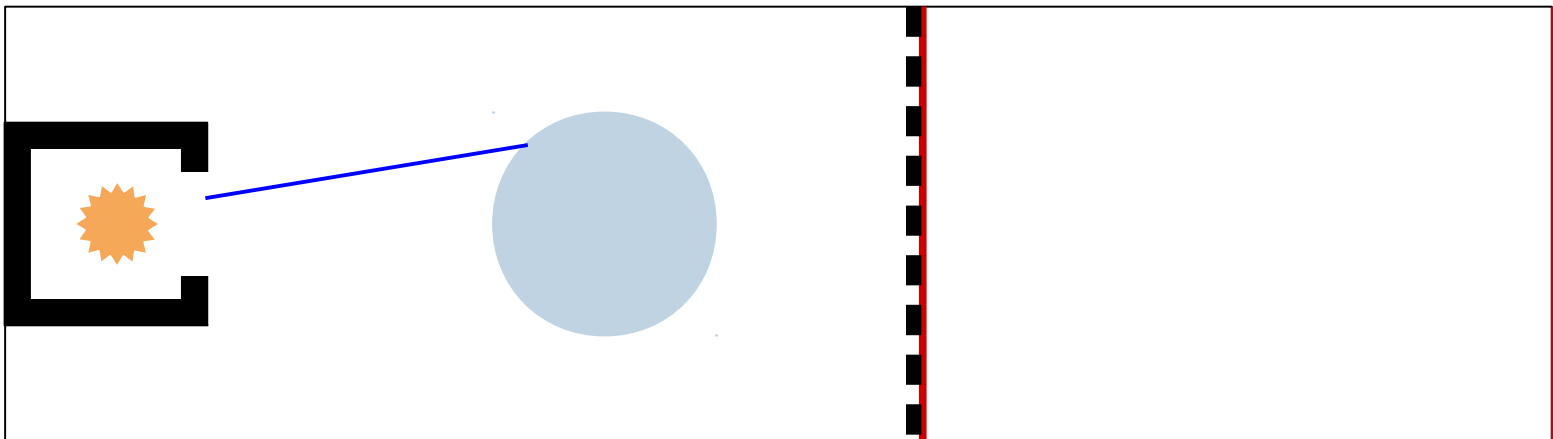


Particle histories in the modified EGSnrc



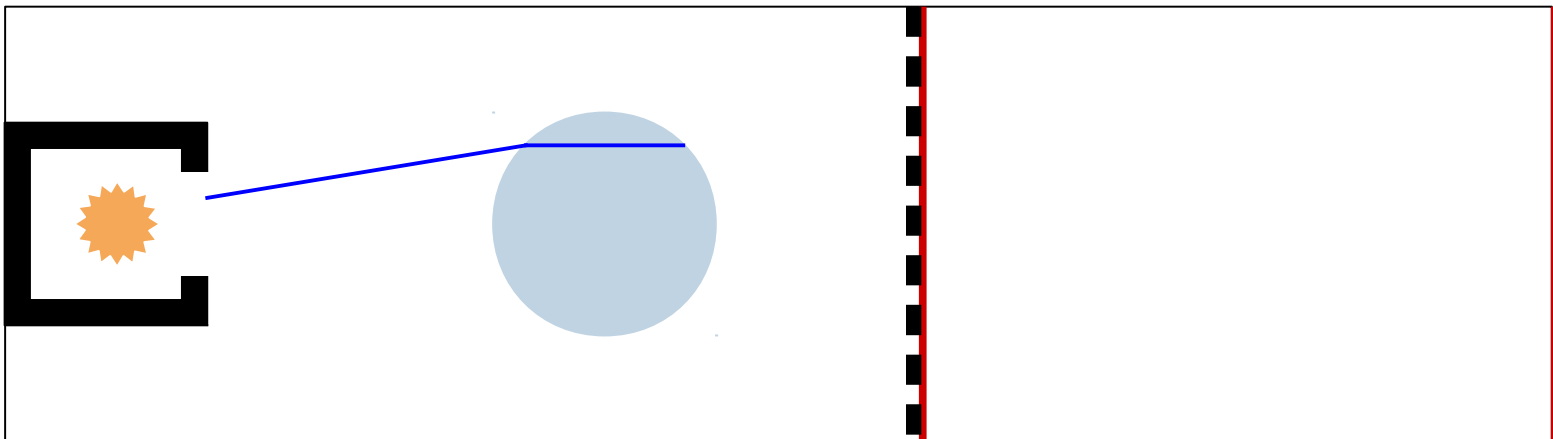
Particle histories in the modified EGSnrc

- Phase shift



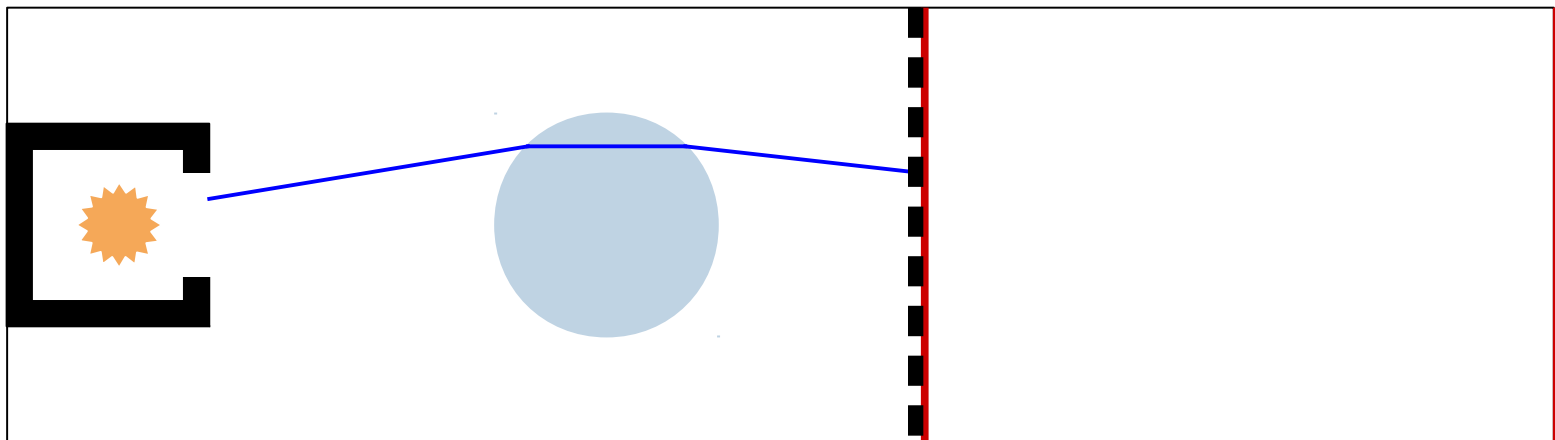
Particle histories in the modified EGSnrc

- Phase shift
- Refraction



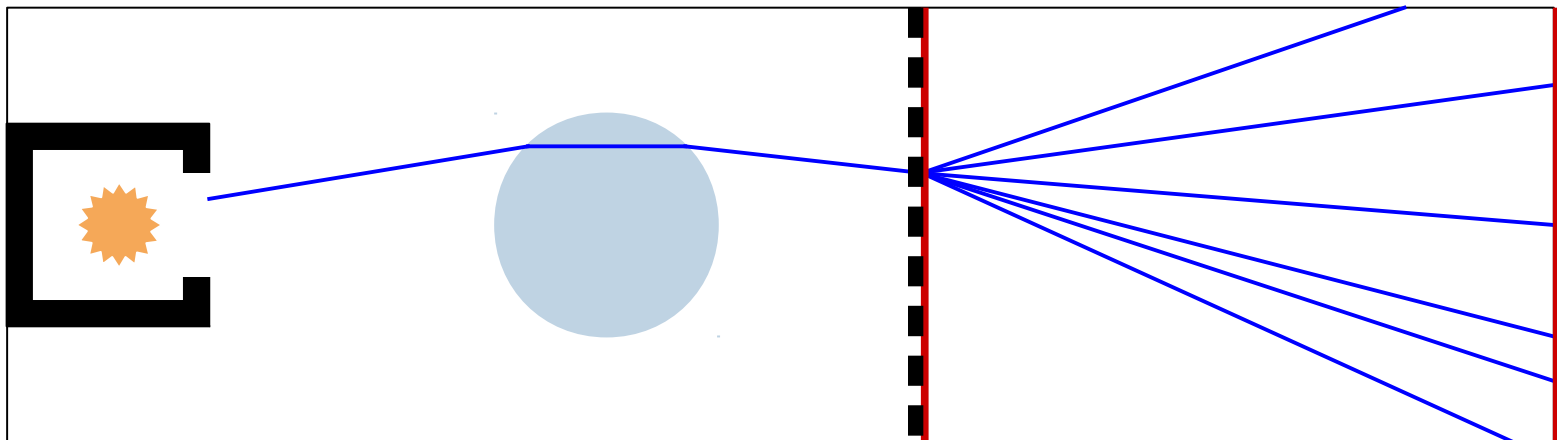
Particle histories in the modified EGSnrc

- Phase shift
- Refraction
- Diffraction



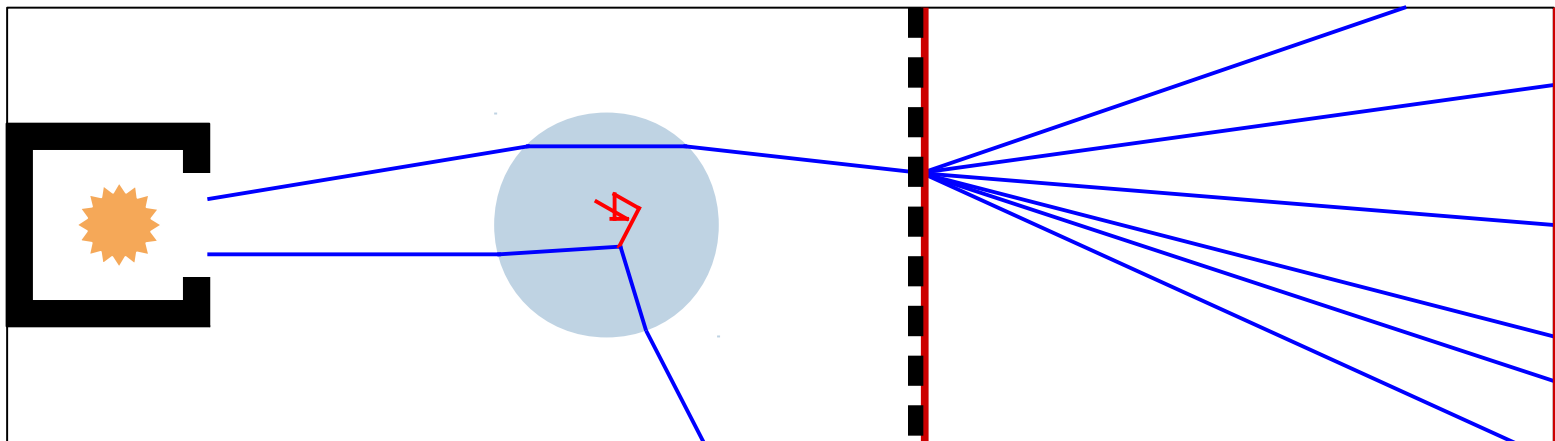
Particle histories in the modified EGSnrc

- Phase shift
- Refraction
- Diffraction



Particle histories in the modified EGSnrc

- Phase shift
- Refraction
- Diffraction
- Interactions (EGSnrc)

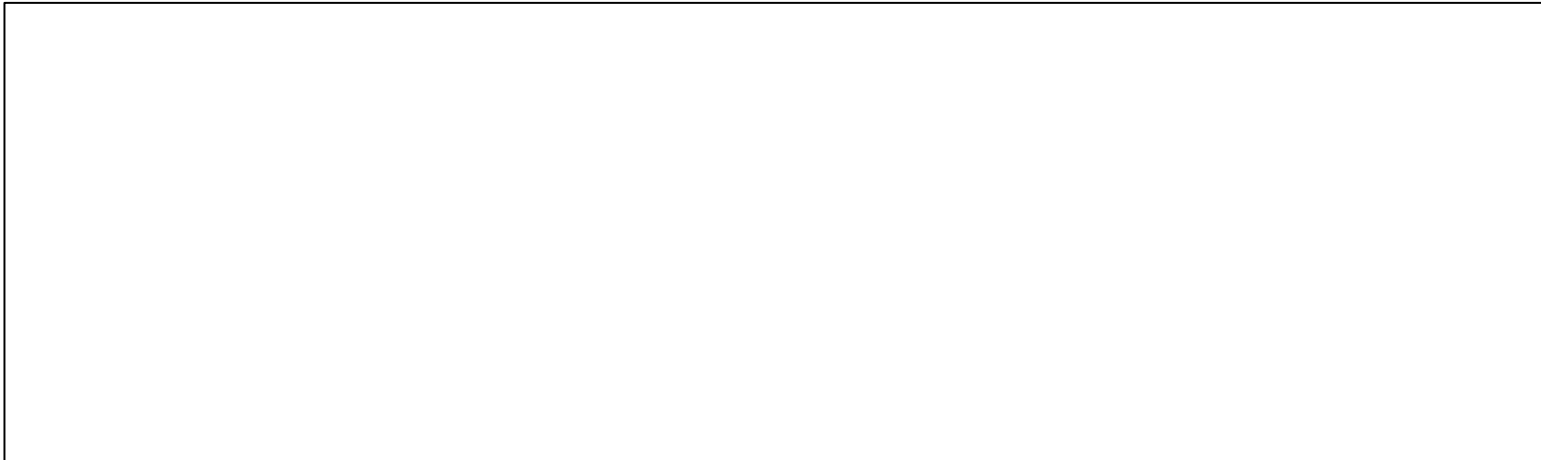


Basic functionality test

- Simulation of a Talbot carpet
- Interference pattern at different grating to detector distances
- Setup:

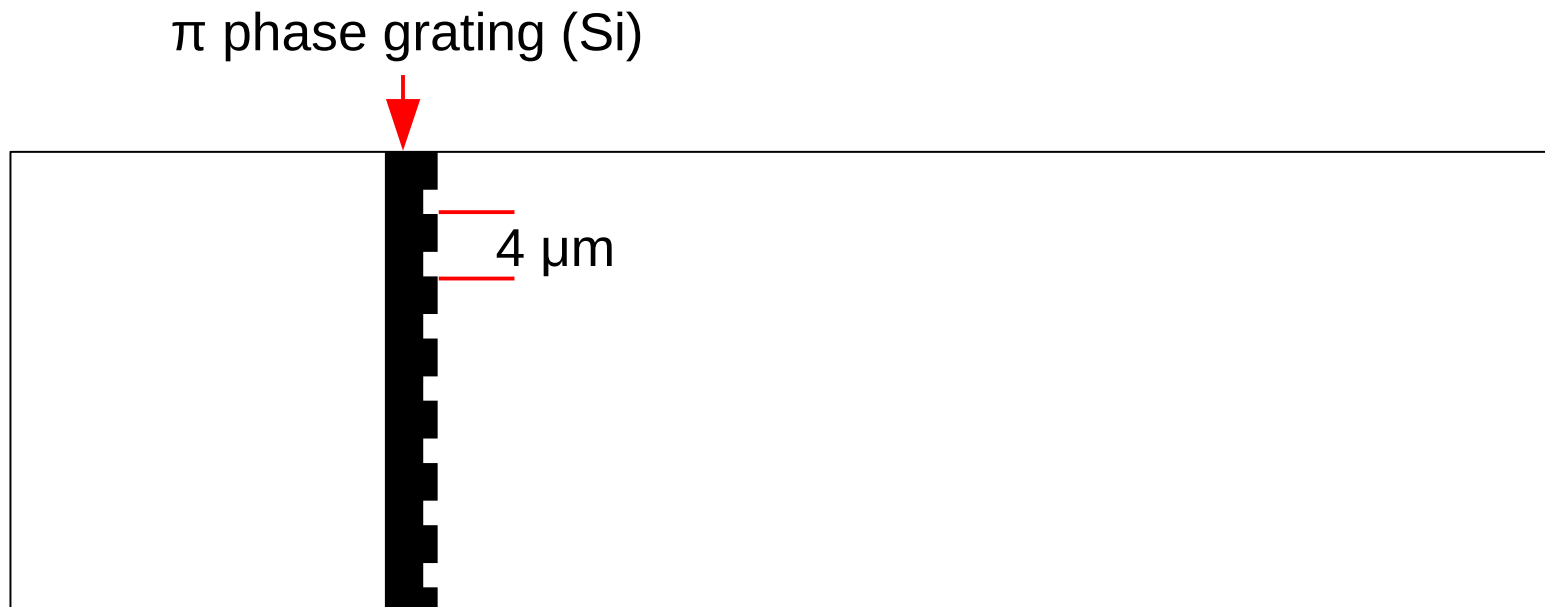
Basic functionality test

- Simulation of a Talbot carpet
- Interference pattern at different grating to detector distances
- Setup:



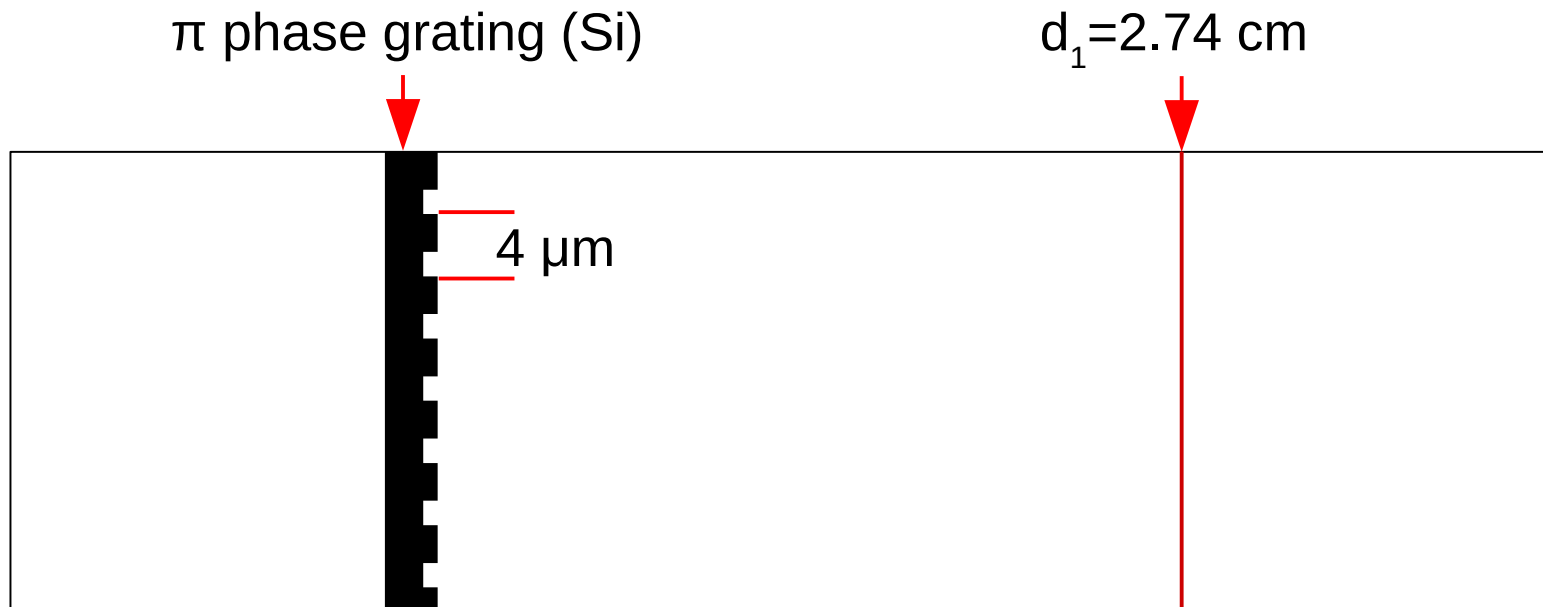
Basic functionality test

- Simulation of a Talbot carpet
- Interference pattern at different grating to detector distances
- Setup:



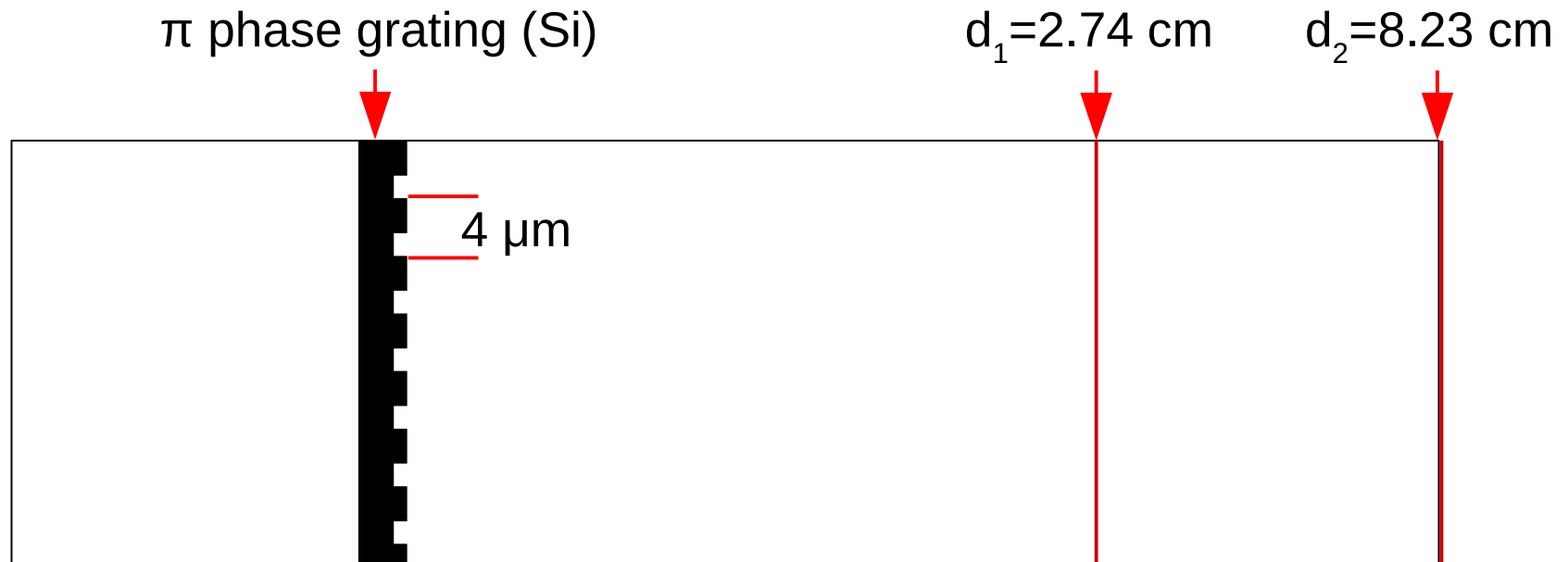
Basic functionality test

- Simulation of a Talbot carpet
- Interference pattern at different grating to detector distances
- Setup:



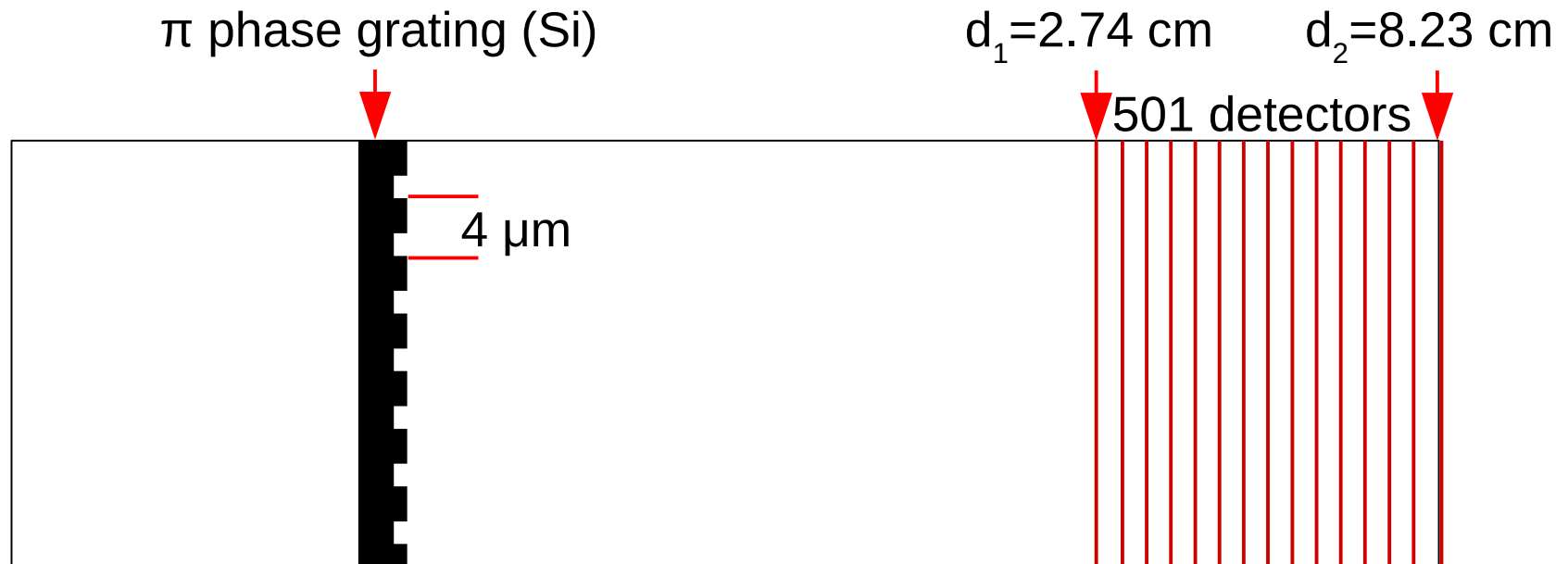
Basic functionality test

- Simulation of a Talbot carpet
- Interference pattern at different grating to detector distances
- Setup:



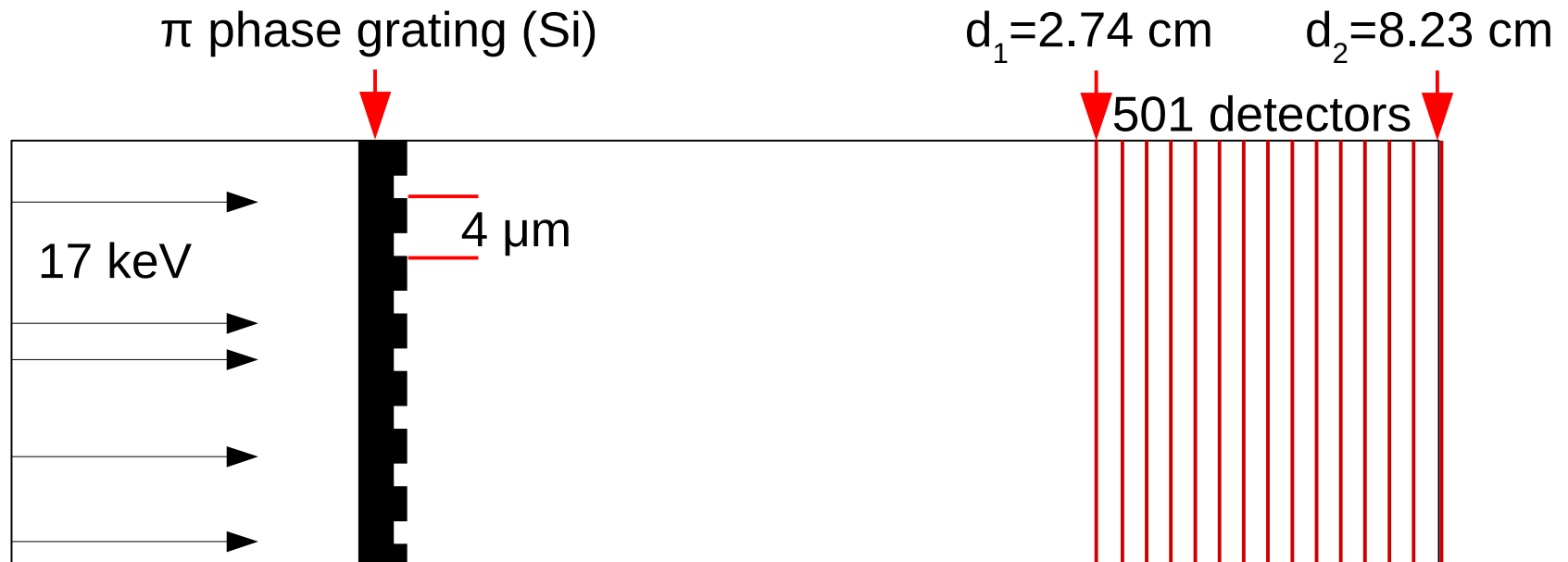
Basic functionality test

- Simulation of a Talbot carpet
- Interference pattern at different grating to detector distances
- Setup:



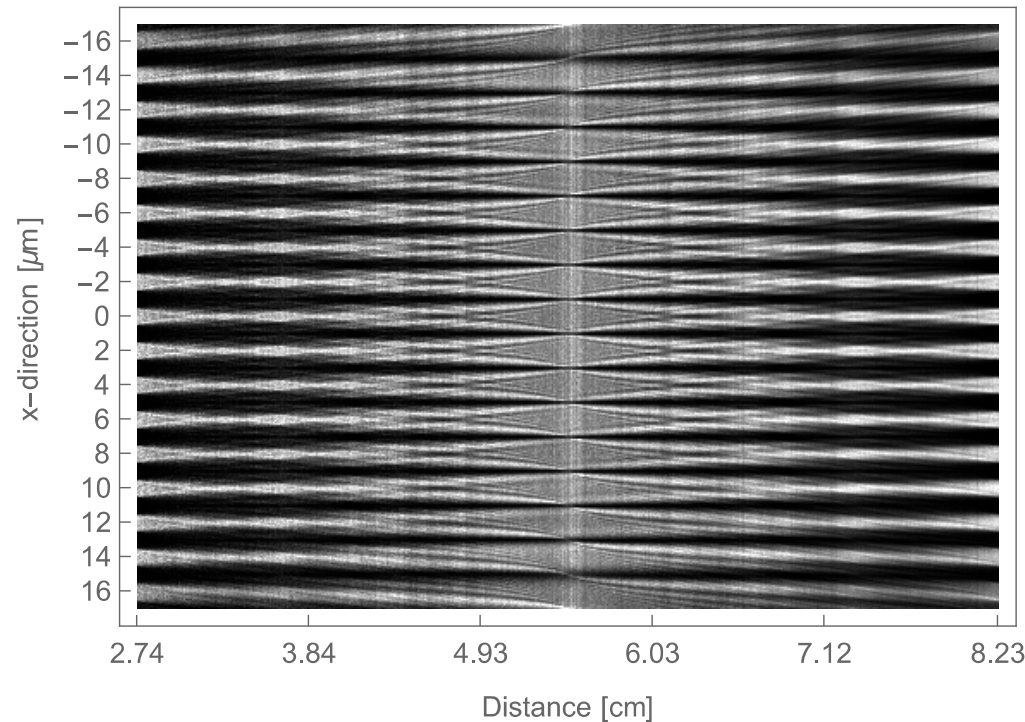
Basic functionality test

- Simulation of a Talbot carpet
- Interference pattern at different grating to detector distances
- Setup:

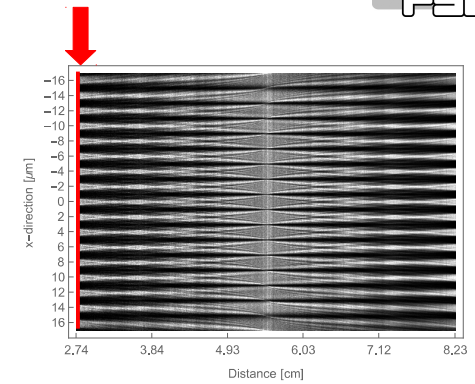


Results and Discussion

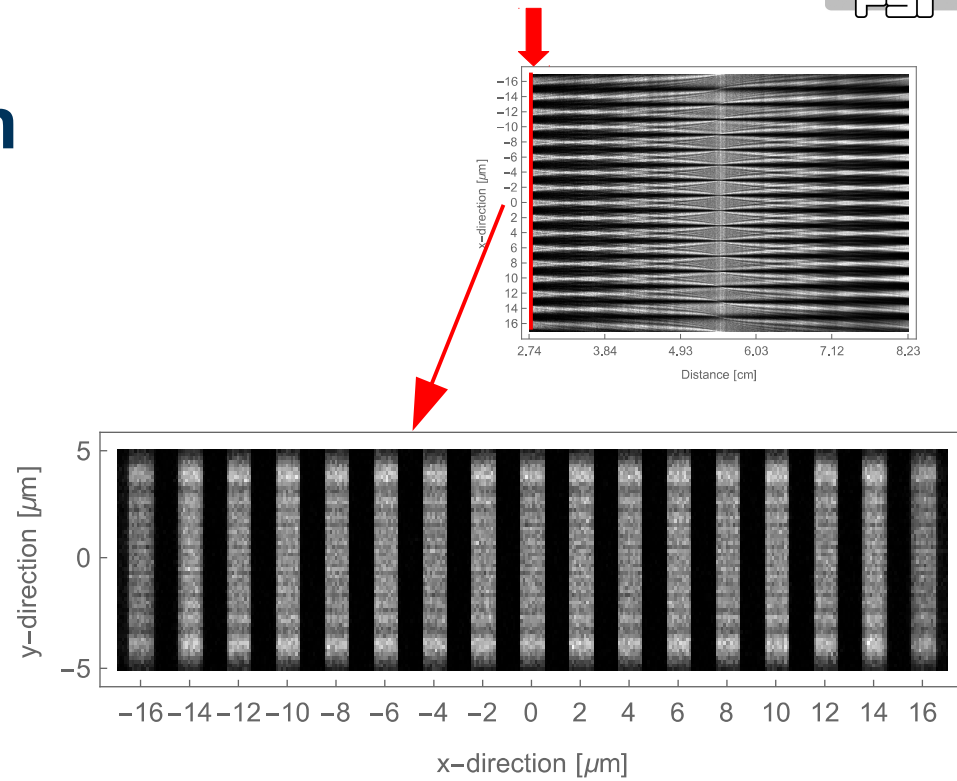
- The resulting Talbot carpet
 - Intensity pattern along middle line of the detectors plotted for each detector
- Observation
 - Self images of the phase grating at d_1 and d_2
 - Periodic patterns except for regions near the boundary
 - Boundary effect
 - Nearly flat signal in the middle of d_1 and d_2



Results and Discussion

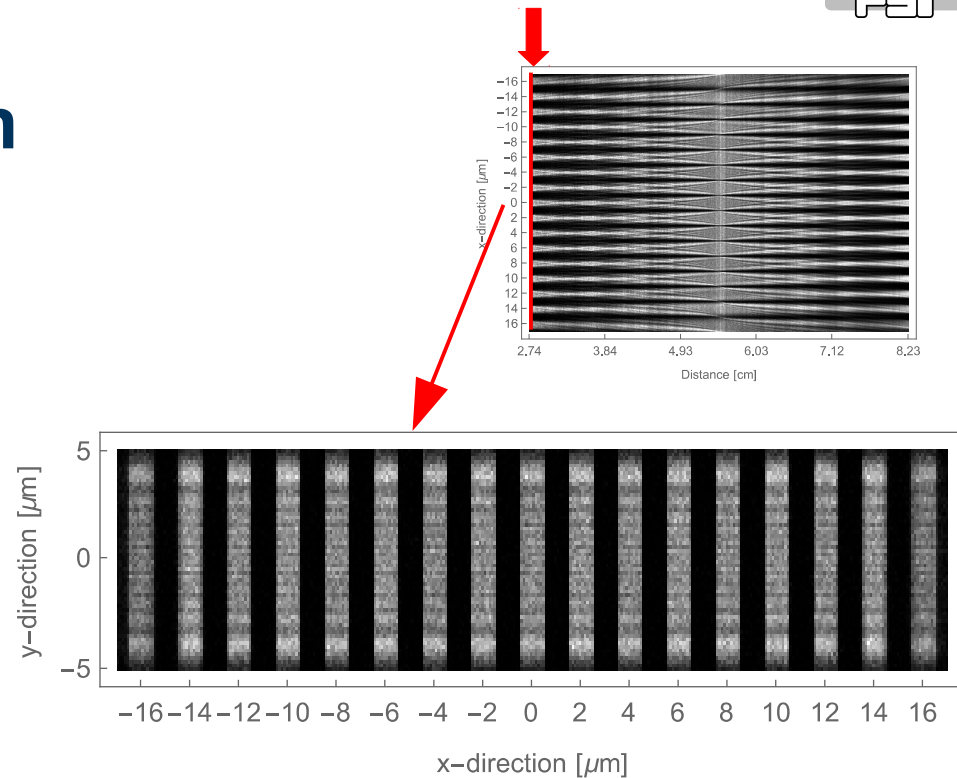


Results and Discussion



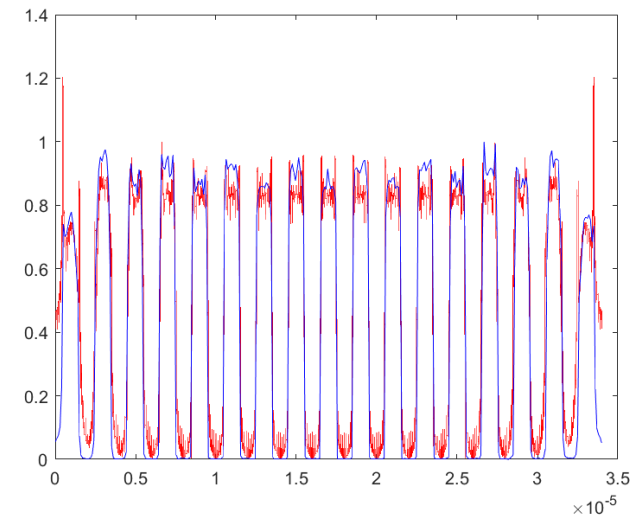
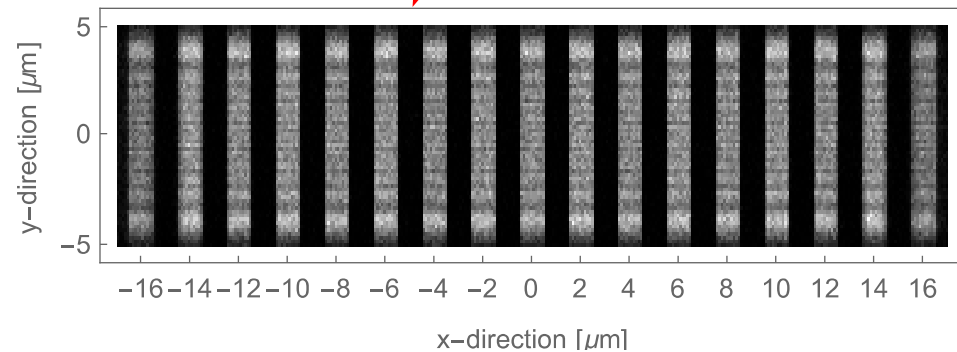
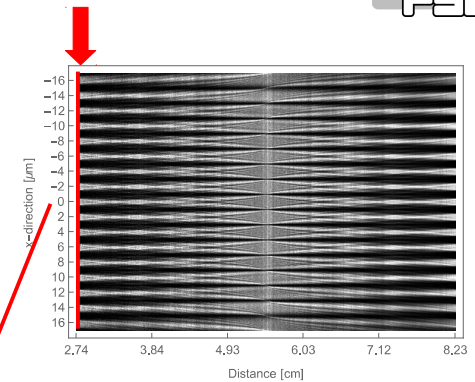
Results and Discussion

- Periodic line pattern in x-direction with 2 μm period
- Slightly faded signal close to the boundaries
 - Boundary effect
- Line pattern in y-direction
 - Boundary effect
 - Small grating dimensions



Results and Discussion

- Periodic line pattern in x-direction with $2\ \mu\text{m}$ period
- Slightly faded signal close to the boundaries
 - Boundary effect
- Line pattern in y-direction
 - Boundary effect
 - Small grating dimensions



Conclusion

- Preliminary results
 - Algorithm feasible to model interference patterns occurring at a phase grating
 - Boundary effects
- Short term developments
 - Extend to finite source sizes and polychromatic sources
 - More efficient splitting algorithms
- Outlook
 - Implement dark field signal
 - Develop realistic source models

Acknowledgments

- Silvia Peter
- Tomcat team
- Carolina Arboleda
- AMS team at Inselspital Bern
- Reto Küng
- Silvan Müller
- Daniel Frei

Computations

- Ubelix linux cluster of university of Bern
 - Nodes: 273
 - CPU: 5828
- Simulation of a single detector
 - Parallelized on 41 nodes
 - Computation time for $20 \cdot 10^6$ histories with 32044 splittings per particle: 1-2 hours
- Talbot Carpet
 - Separate job for each of the 501 detectors
 - $20 \cdot 10^6$ histories per job
 - 32044 splittings per particle on the grating
 - Computation time \sim 2.5 days per job

