ESRF | The European Synchrotron

Modelling synchrotron radiation beamlines with OASYS

NSRL Seminar

Juan Reyes Herrera
juan.reyes-herrera@esrf.fr

Advanced Analysis & Precision Unit, MEG/ISDD, ESRF

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Outline

1. Brief introduction:
   - What is OASYS? What is its structure?
   - What kind of simulations can be performed with it?

2. Power management: OASYS-XOPPY
   - Heat-load on slits, filters/windows and mirrors

3. Photon transport: OASYS-SHADOWOUI
   - Using a mirror surface errors
   - Modelling mirror misalignments

4. Coherence propagation: OASYS-WOFRY1D
   - Few examples on undulator wavefront propagation

Some material for this seminar:
https://github.com/jureyherrera/OASYS_NSRL_seminar

Introduction to OASYS

Computer simulation of light sources and optical components is a mandatory step in the design and optimization of synchrotron and FEL radiation beamlines

different codes for numerical simulations are available, implementing different physical approaches

EMISSION SPECTRA

XOPPY | Spectra

XOPPY has tools to calculate absorbed and transmitted power

RAY-TRACING

Shadow | McXtrace

RAY | XRT | ART

Incoherent X-ray beams

WAVEFRONT PROPAGATION

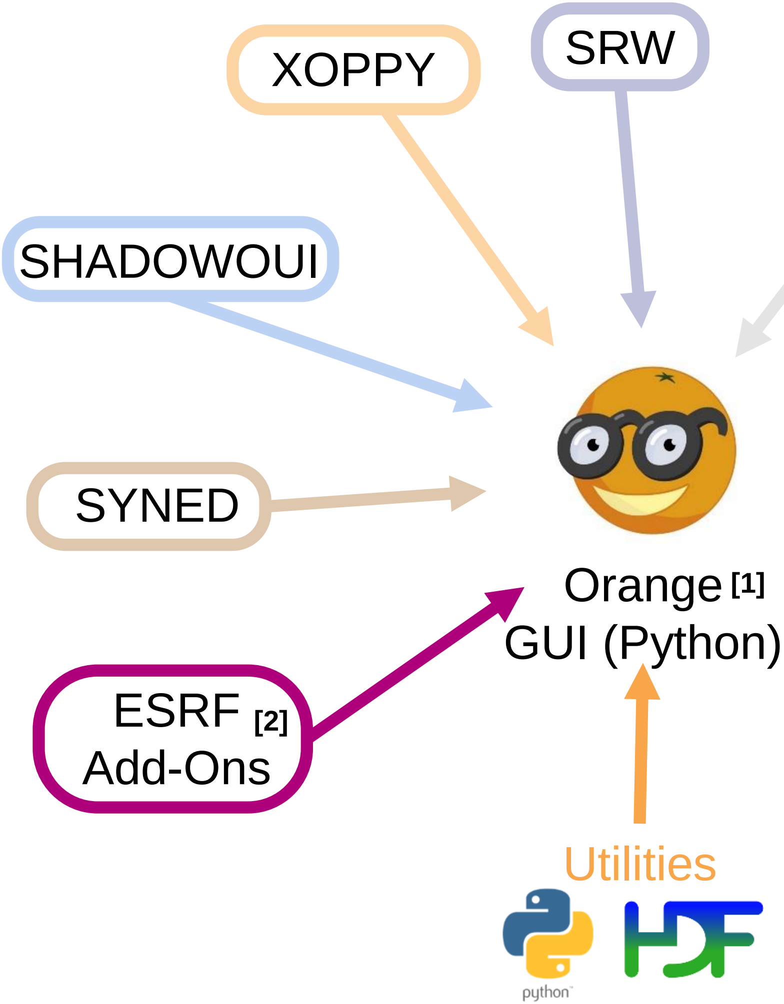
SRW | PHASE | WISE

WOFRY — Fully coherent X-ray beams

WOFRY1D | COMSYL

Partially coherent X-ray beams

Quick note: OASYS



Luca Rebuffi (ANL) & Manuel Sánchez del Río (ESRF)

L. Rebuffi, M. Sanchez del Rio, "**OASYS (OrAnge SYnchrotron Suite): an open-source graphical environment for x-ray virtual experiments**", Proc. SPIE 10388, 103880S (2017). DOI: 10.1117/12.2274263.

[1] Demšar et al. "Orange: Data Mining Toolbox in Python," Journal of Machine Learning Research 14, 2349−2353 (2013). https://orange.biolab.si

[2] ESRF Add-Ons: https://github.com/oasys-esrf-kit/OASYS1-ESRF-Extensions

What is OASYS?

OASYS (Orange Synchrotron Suite) is graphical environment for modelling synchrotron beamlines.

In OASYS, we can perform visual programing: using “boxes and arrows” to recreate a photon beamline

OASYS integrates different simulation strategies via the implementation of adequate simulation tools for X-ray Optics

https://www.aps.anl.gov/Science/Scientific-Software/OASYS

Modelling a beamline with OASYS

Main components of the beamline:

Source

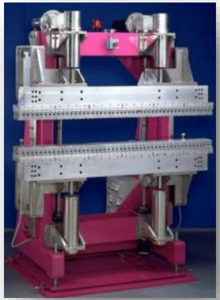
Bending magnet, wiggler or undulator

Optics

Slits, mirrors, crystals, filters, refractive lens, Fresnel lens, multilayers, etc.

Experimental station

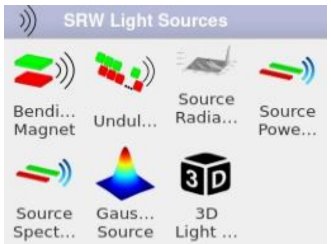
Sample, detectors, etc.

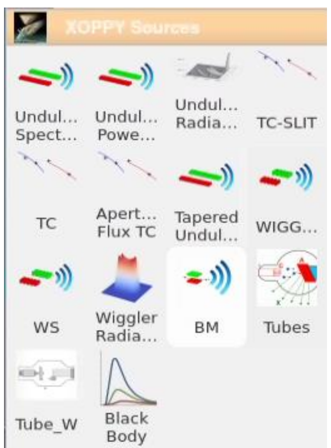


Modelling a beamline with OASYS

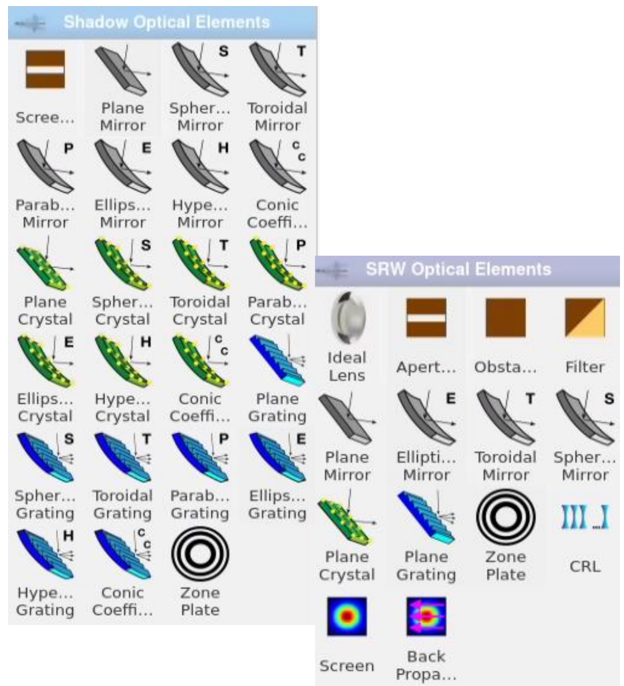
The visual programing boxes, in OASYS, are called ***Widgets*** and they represent optical components, including a wide variability of tools, example:

Sources:





Optics:

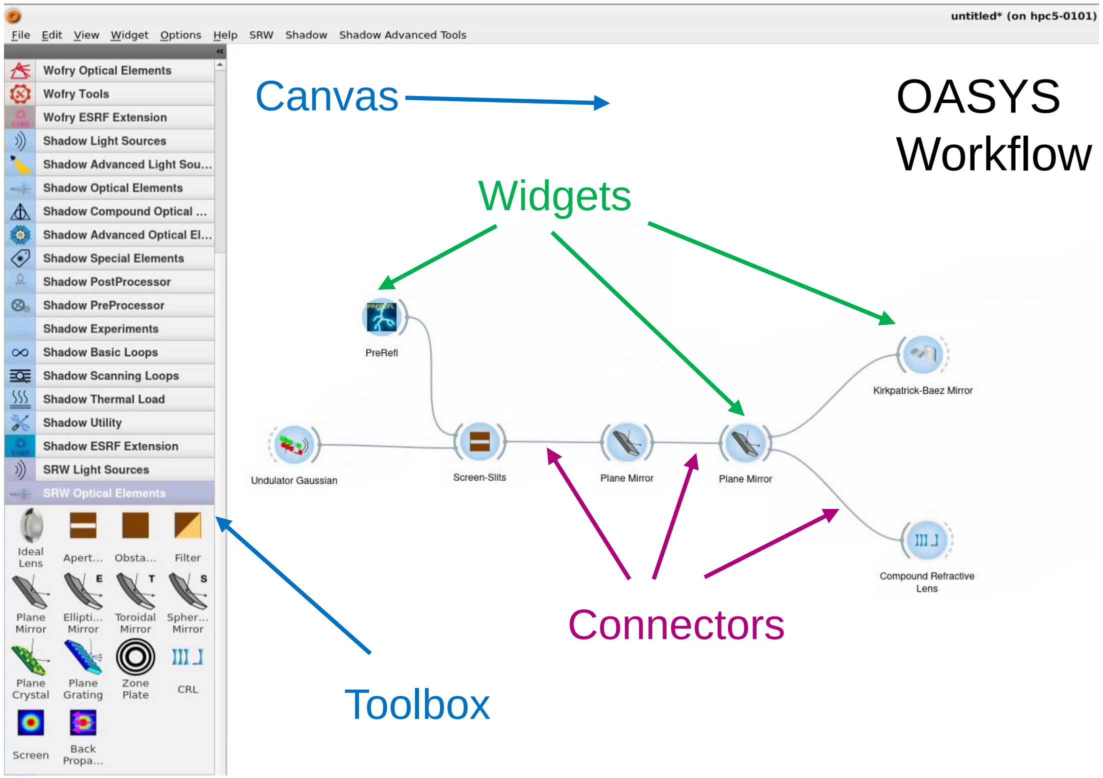


Allowing to get at the Sample:

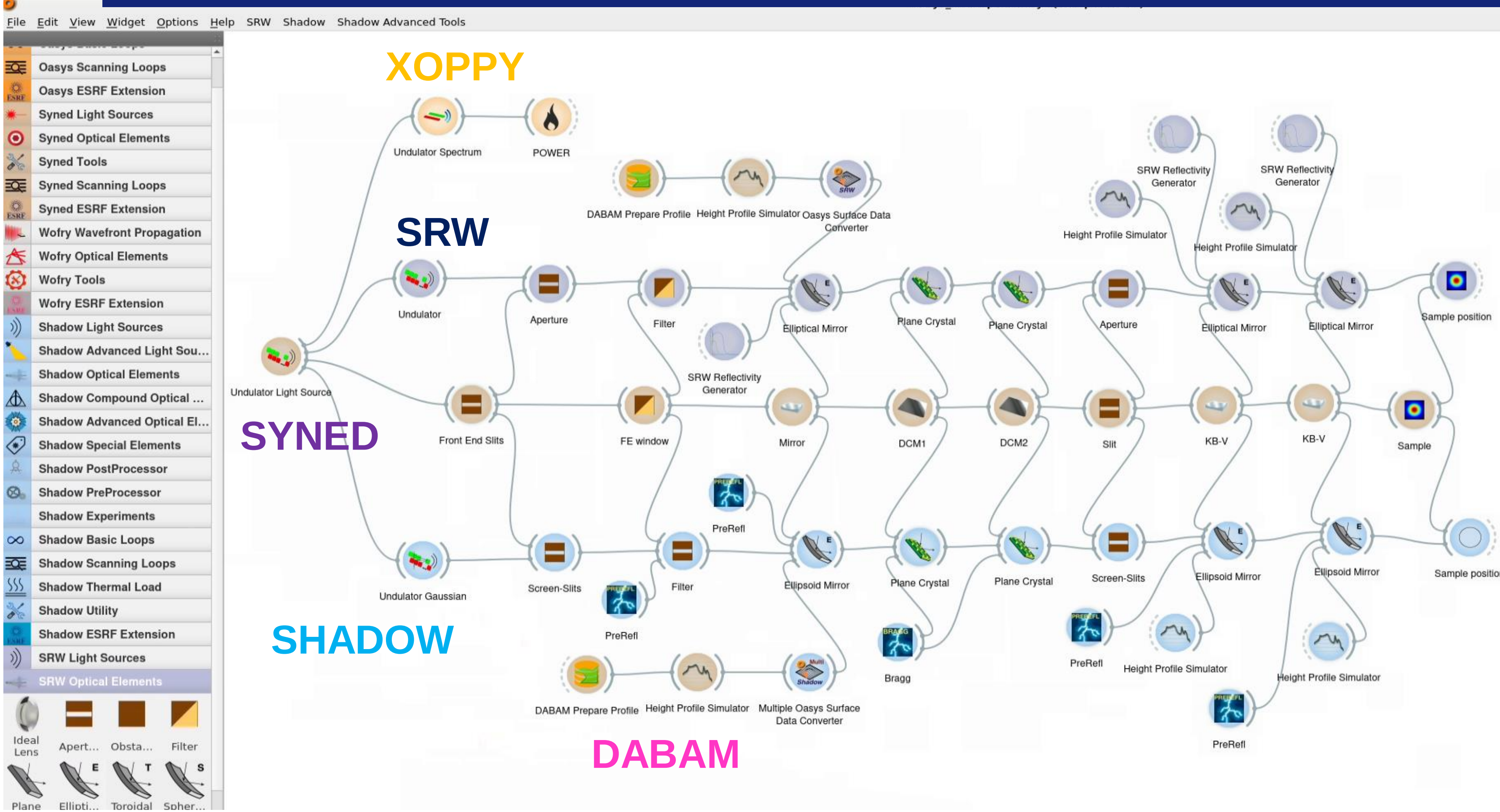
Energy distribution, intensity (photon flux), beam size and divergence, coherence, etc.

Modelling a beamline with OASYS

The ***Widgets*** are connected as a workflow (or dataflow) in the OASYS canvas:

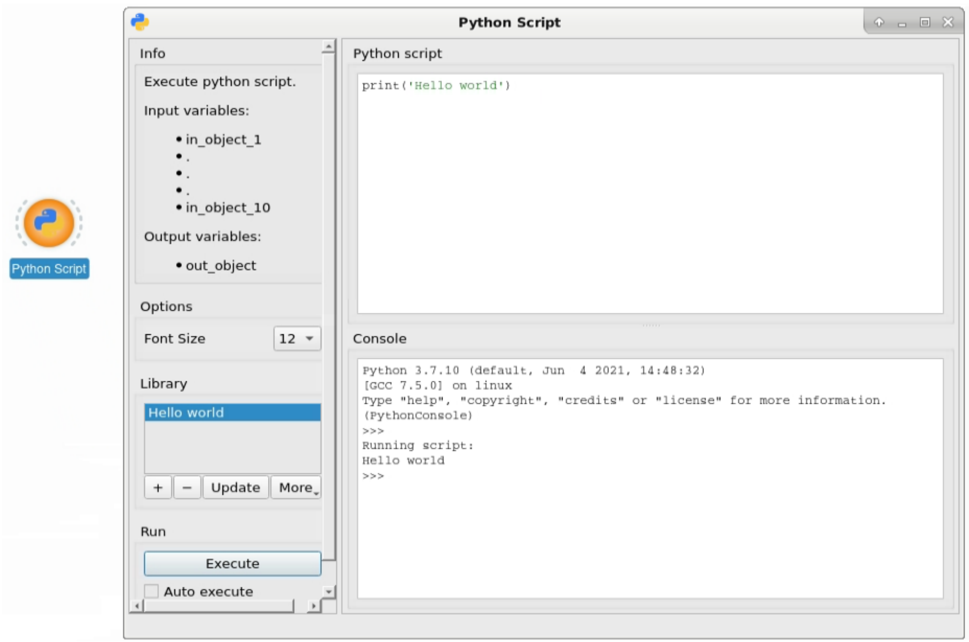


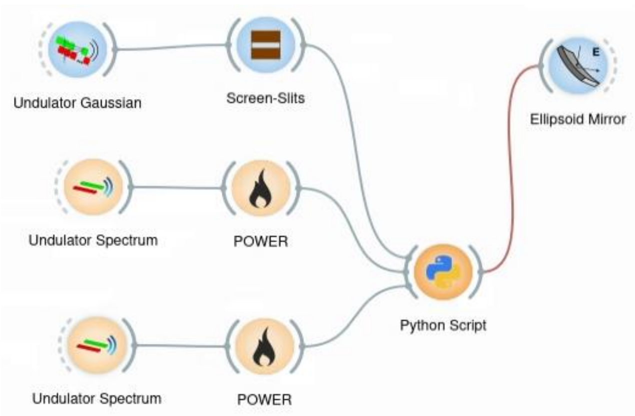
OASYS interoperability



Other OASYS features

- Python has been chosen as the main programming language, and code can be included in the workflow





Other OASYS features

- Open Source, many synchrotron facilities are developing their own customized widgets, Add-ons, for example:

oasys-elettra-kit https://github.com/oasys-elettra-kit

LNLS - Brazilian Synchrotron Light Laboratory https://github.com/oasys-lnls-kit

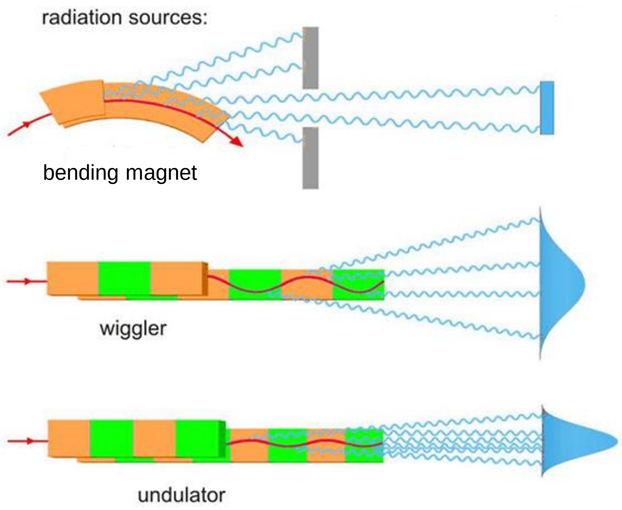
oasys-als-kit https://github.com/oasys-als-kit

oasys-esrf-kit https://github.com/oasys-esrf-kit *

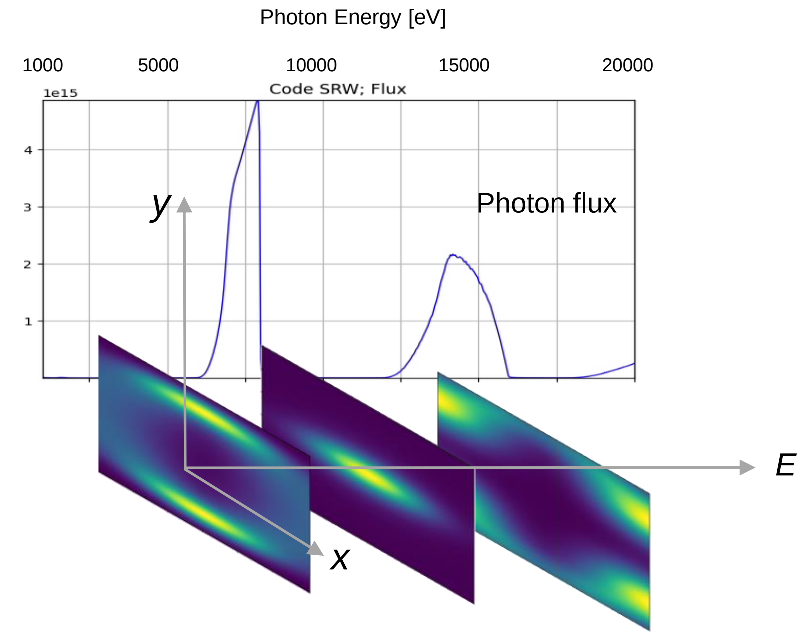
* Add-ons installation example

Reminder: Synchrotron radiation

Synchrotron radiation depends on spatial (*x, y*) and energy (*E*)

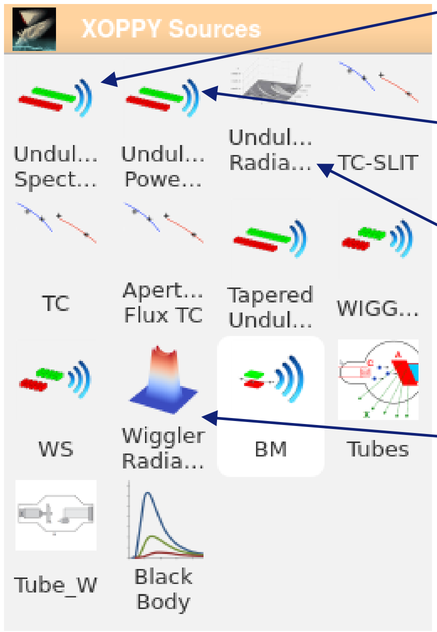


Example: Undulator radiation



Power management with OASYS/XOPPY

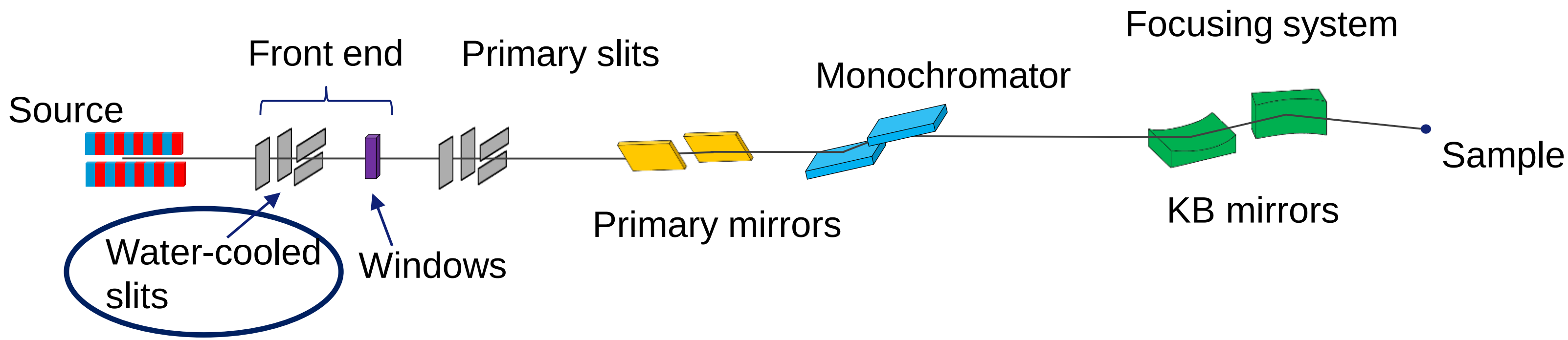
XOPPY (X-ray Optics for Python) is a software package designed for X-ray optics simulations and calculations



- Undulator spectrum (*flux/power* vs *x, y, E*)
- Undulator power density (*power* vs *x, y*)
- Undulator spectral flux density (*flux/power* vs *x, y, E*)
- Wiggler spectral flux density (*flux/power* vs *x, y, E)*

Power transport on a beamline

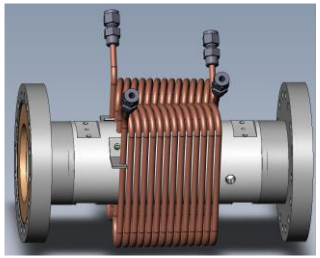
Optical components that could be present in a beamline:



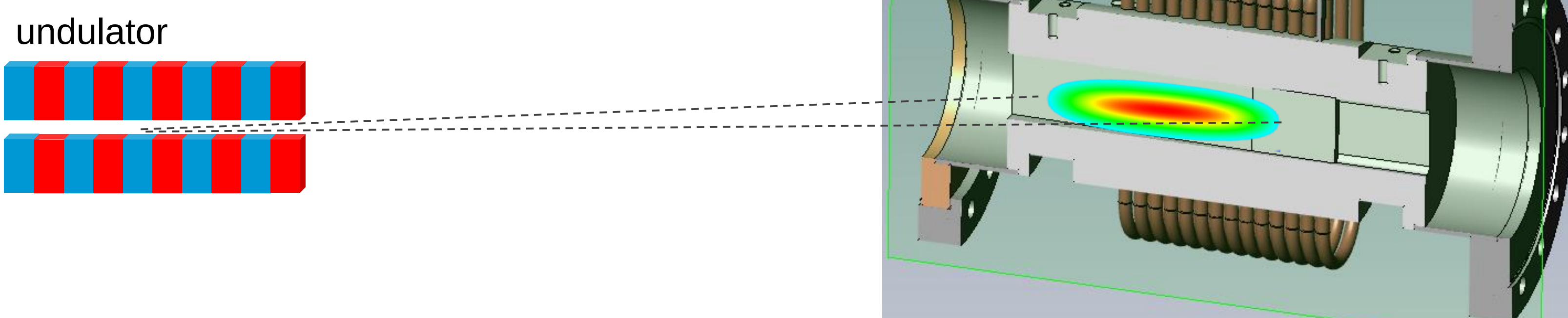
Undulator power density (*Power* vs *x*, *y*)

For example, this tool is very useful to get the heat load on a slit:

Undulator Power Density



Water cooled
beamline slit

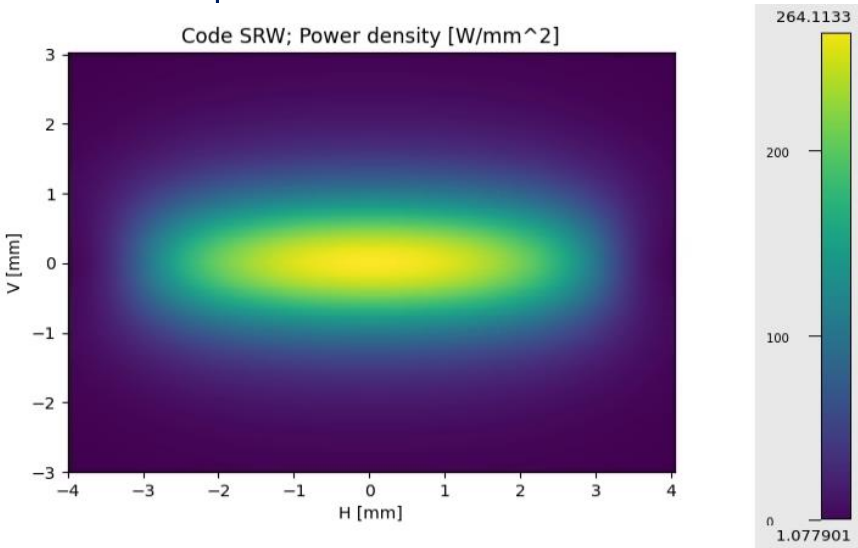


Undulator power density (*Power* vs *x, y*)

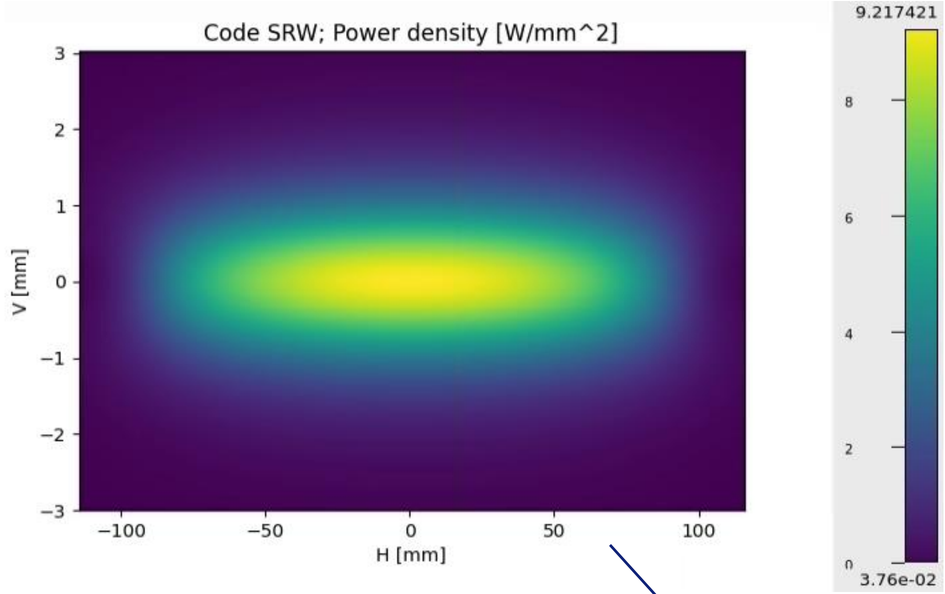
Undulator Power Density

In most of the beamlines at the ESRF the are horizontal slits at 16 m from the source:

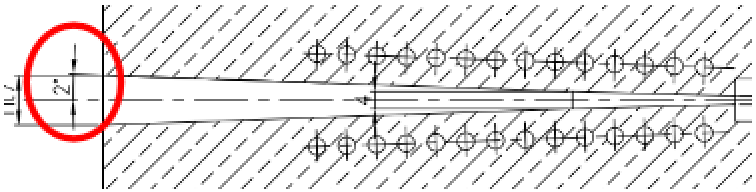
Perpendicular to the beam



Project over the slit surface (2º angle)



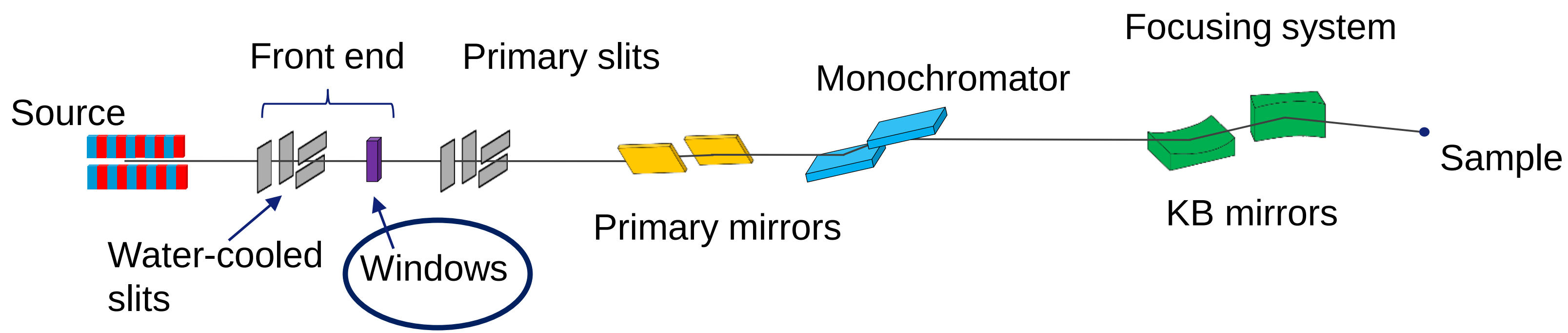
X-ray beam

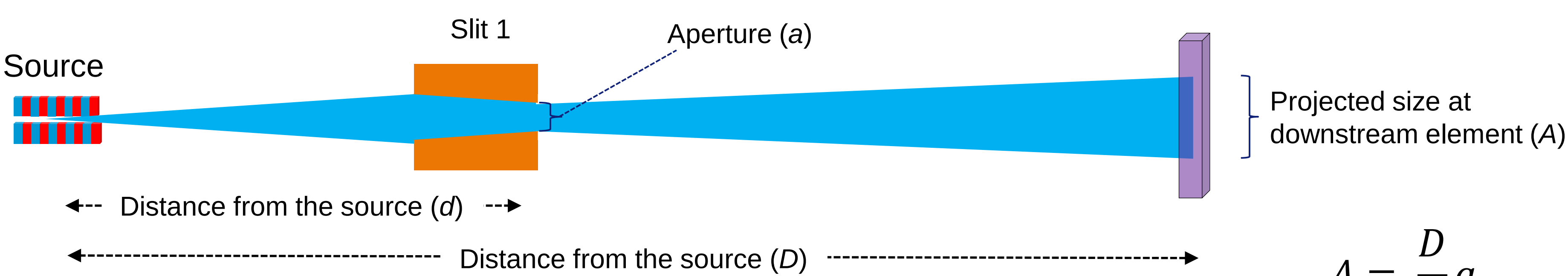


Finite element analysis

Power transport on a beamline

Optical components that could be present in a beamline:





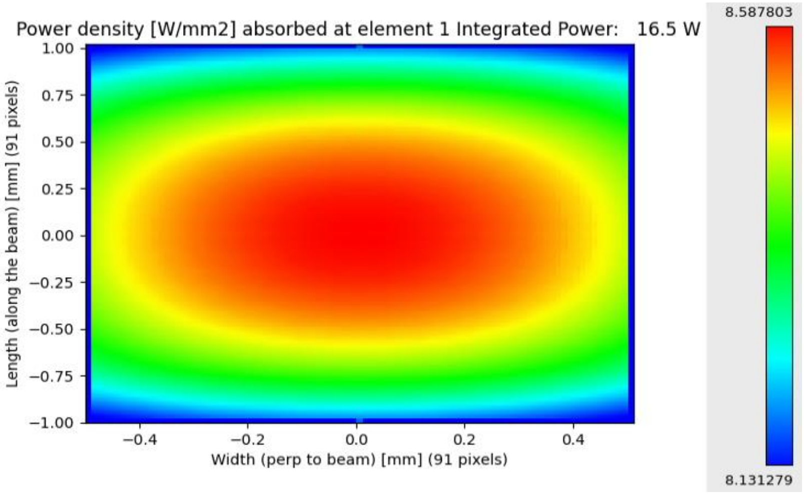
$$A = \frac{D}{d} a$$

Power absorbed by a filter

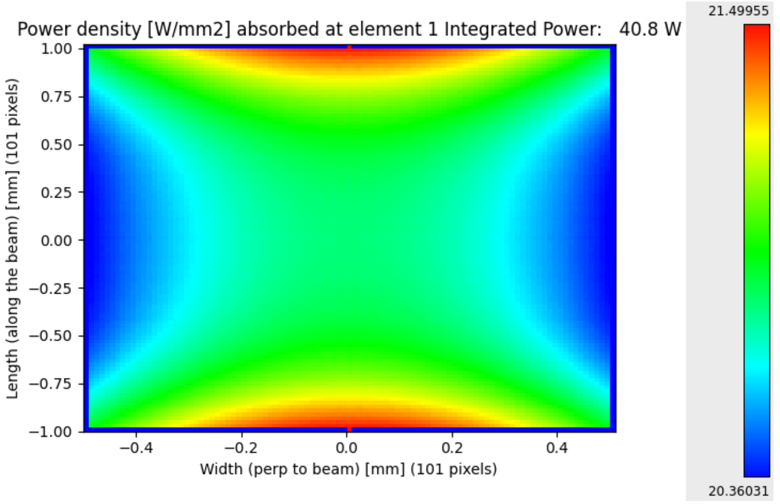
Heat load on filters @ 23 m with a projection of 2 mm x 1 mm:

SRCALC-IDPOWER

Be (300 μm)

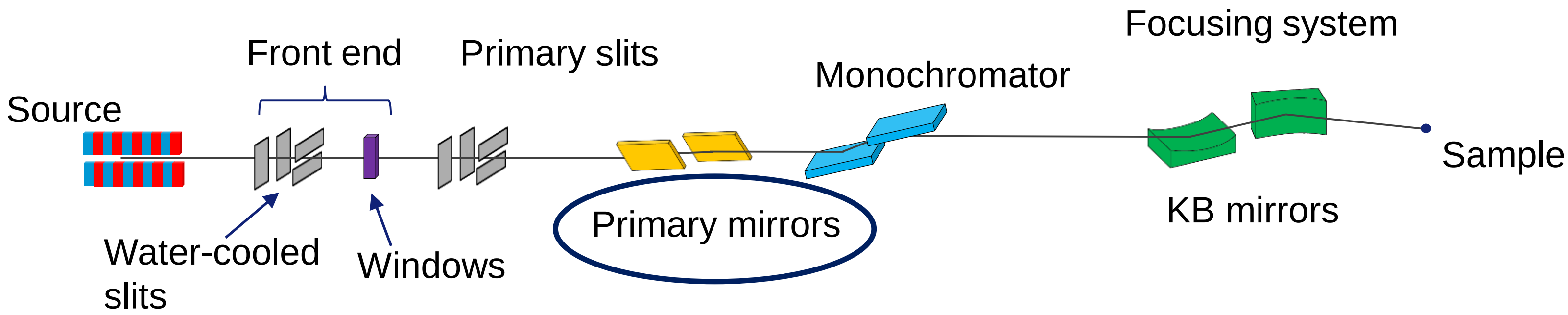


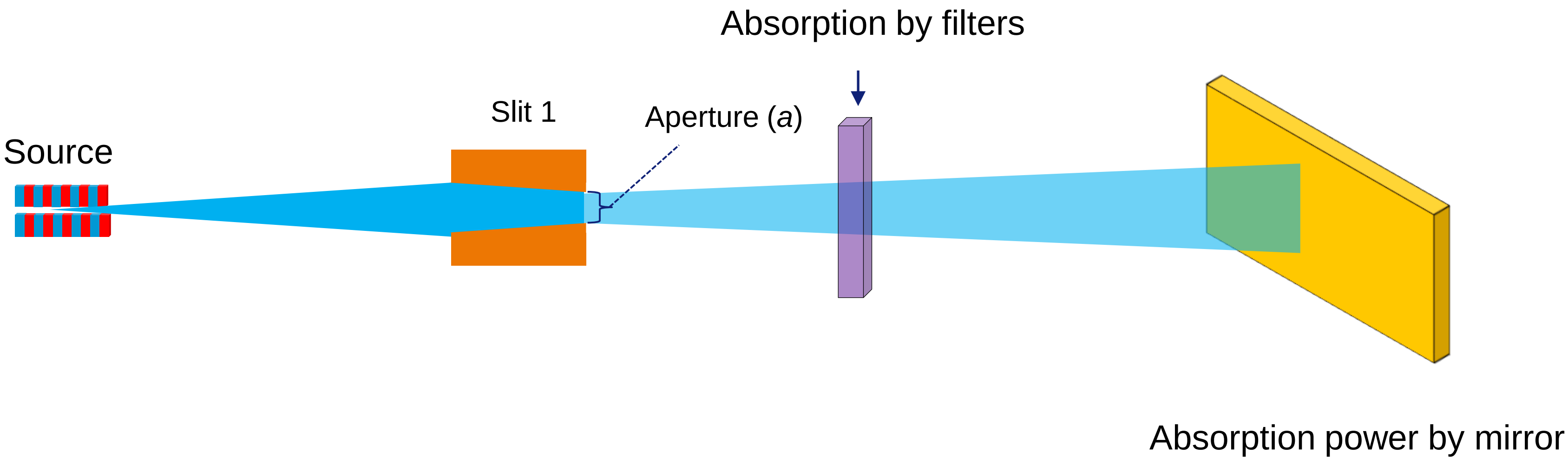
Diamond (300 μm)



Power transport on a beamline

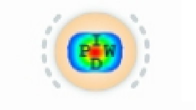
Optical components that could be present in a beamline:





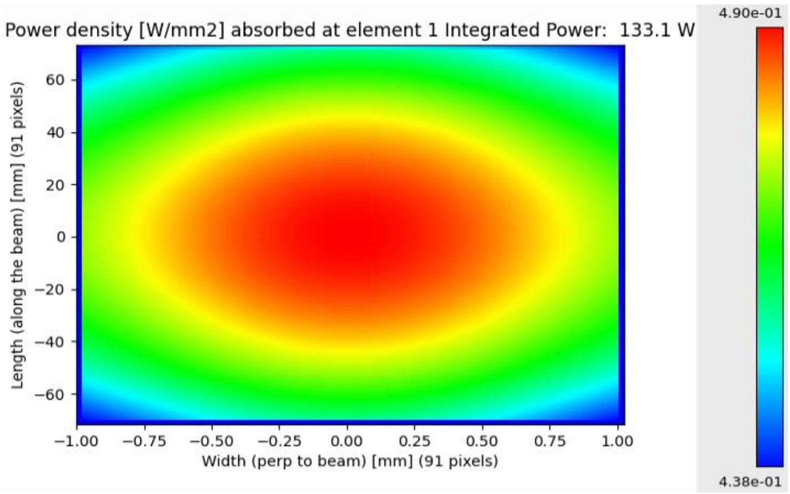
Power absorbed by a mirror

Heat load on mirrors @ 30 m:

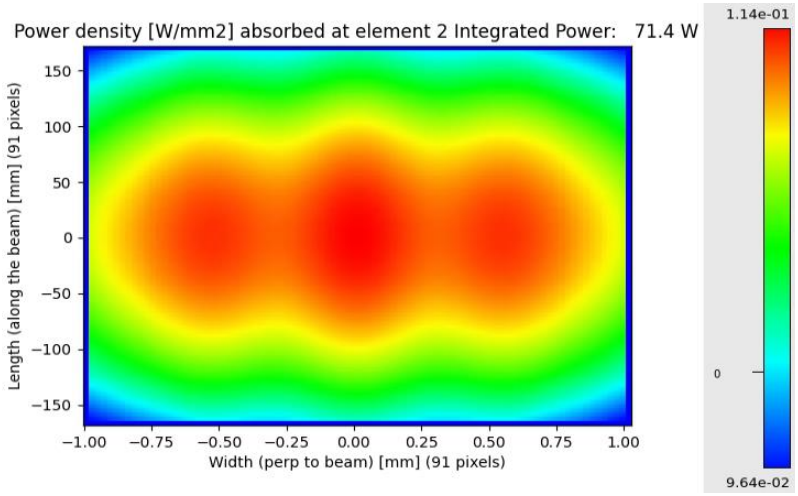


SRCALC-IDPOWER

Si (7 mrad)

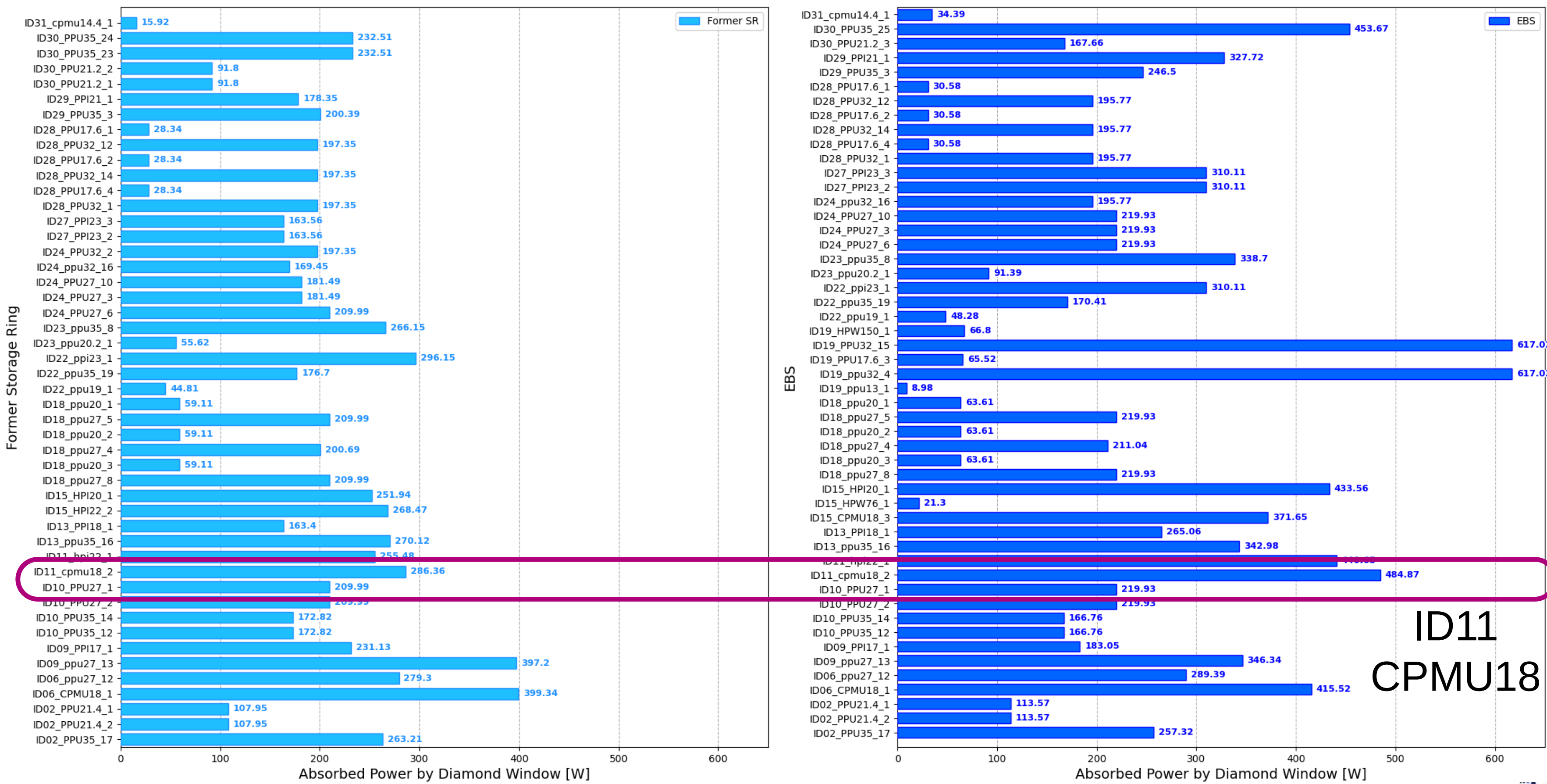


Diamond (100 μm) + Rh (3 mrad)



Power management

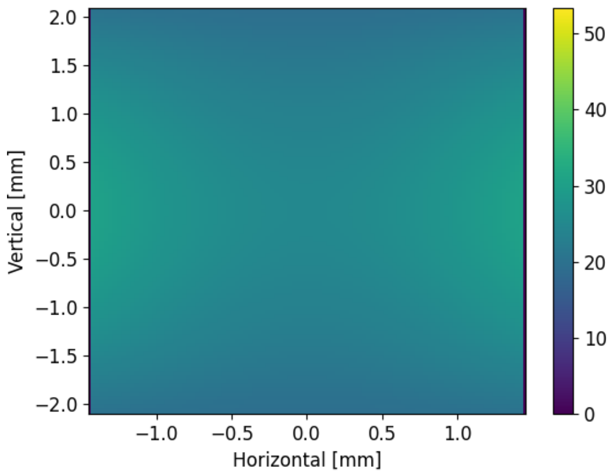
ESRF-I vs EBS: absorbed power by FE diamond window



Power management

Absorbed power
by diamond window

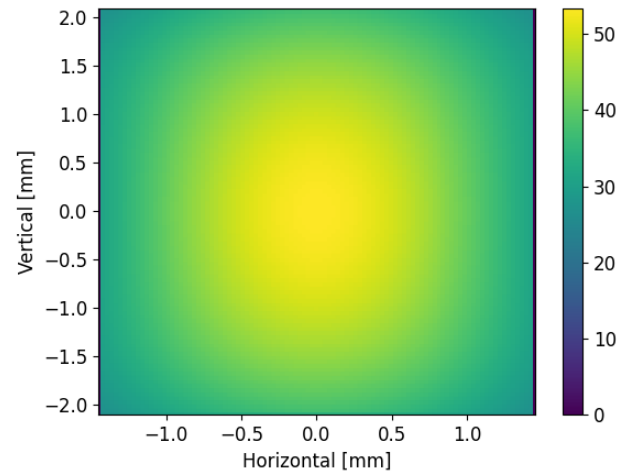
ESRF-I-ID11
CPMU18



Total: 293 W
Max: 30.5 W/mm^2

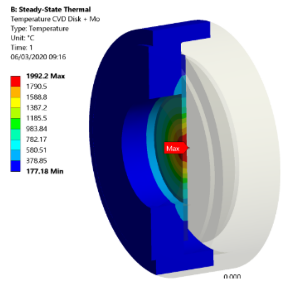
vs

EBS-ID11
CPMU18



Total: 497 W
Max: 53.4 W/mm^2

FEA



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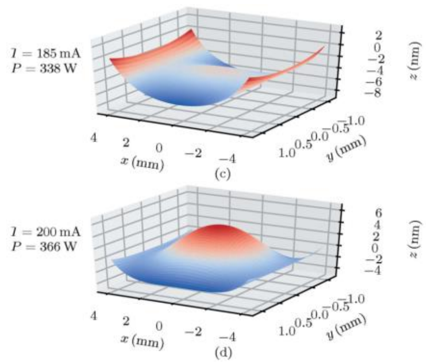
Power management

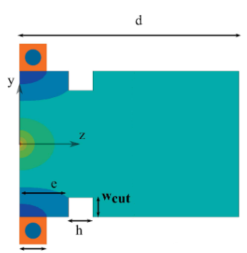
Horizontal deflection optics:

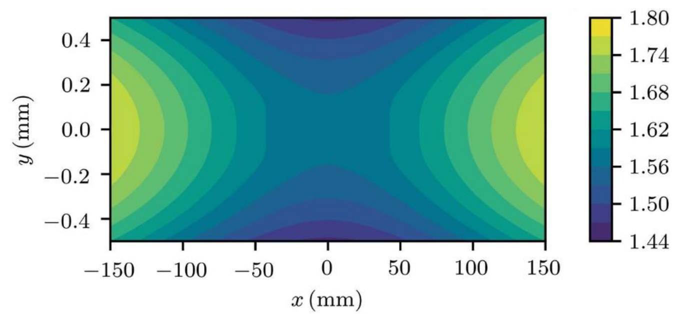
- High heat-load crystal monochromator [1].



Negligible effects on vertical plane due thermal load over the crystal, will be implemented in the refurbish nuclear resonant ID14 beamline.

- Optimization of high heat-load multilayer monochromator for the new hard X-ray microscope at ID03 [2].





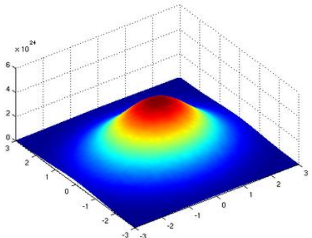
Absorbed power
by a multilayer mirror

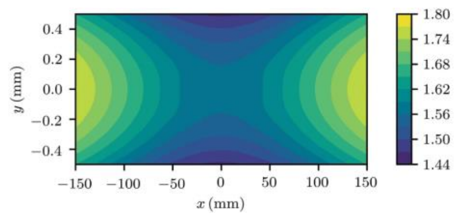
[1] P. Brumund et al., J. Synchrotron Rad. (2021) **28** 91 . https://doi.org/10.1107/S1600577520014009

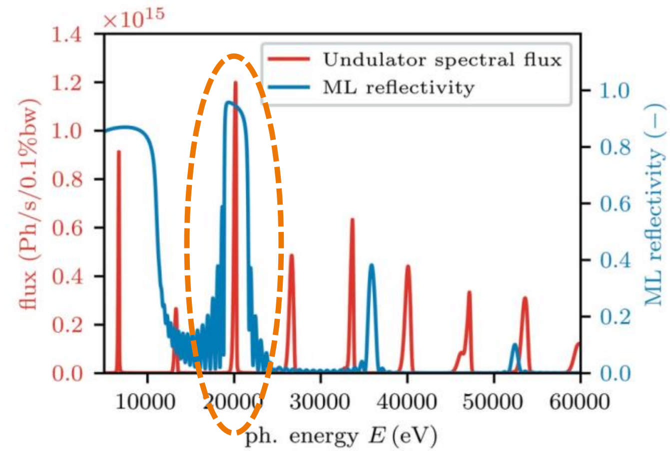
[2] P. Brumund et al., J. Synchrotron Rad. (2021) **28** 1423. https://doi.org/10.1107/S160057752100758X

Power management

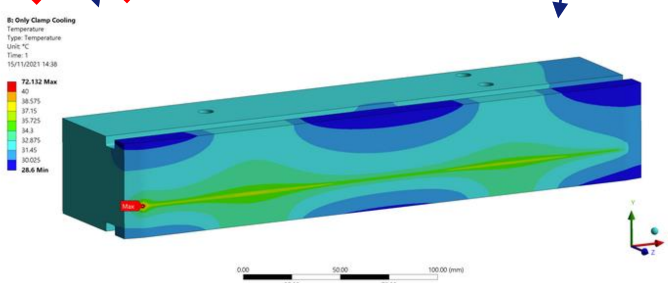
Multilayer X-ray optics: absorbed power



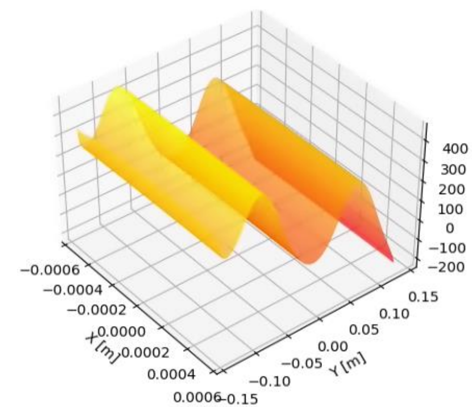




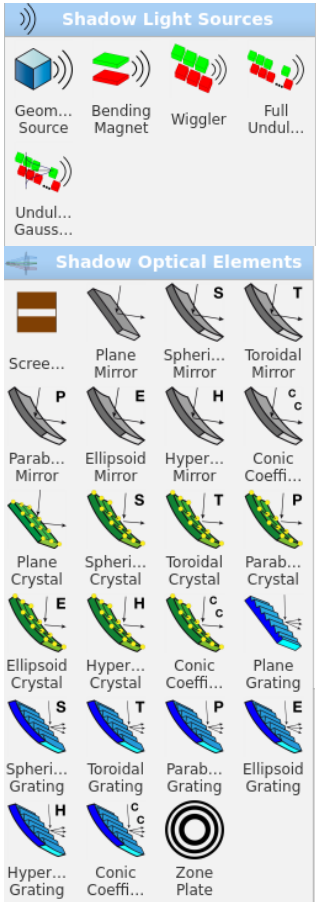
Absorbed power density distribution not Gaussian !

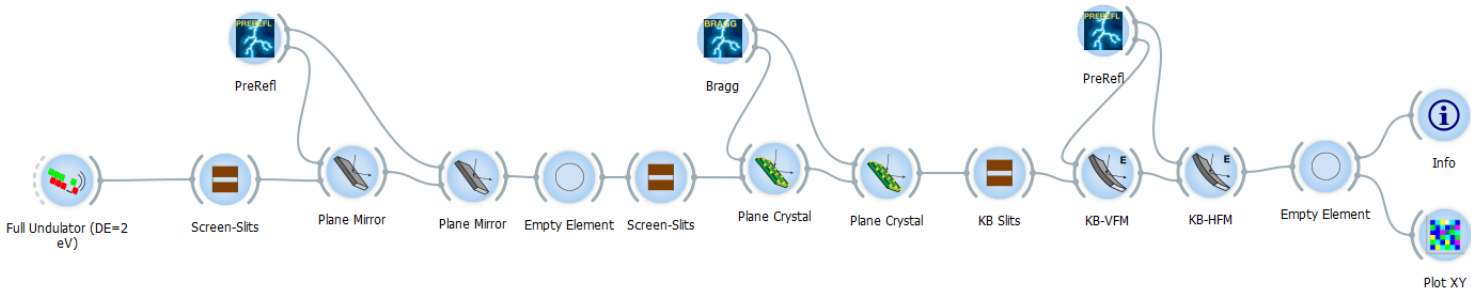


Finite element analysis



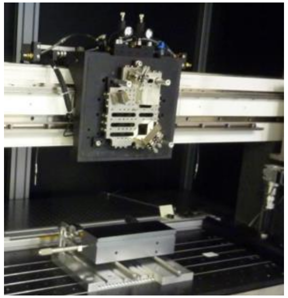
Photon transport





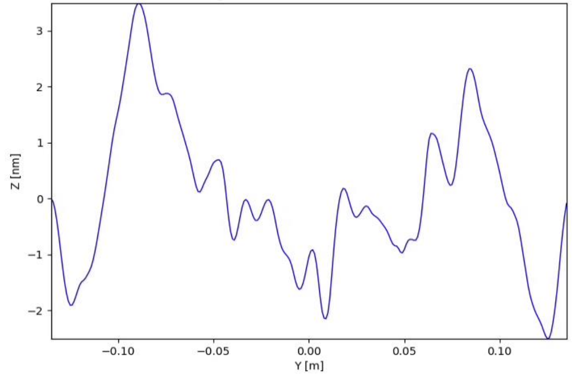
Photon transport

Mirror metrology

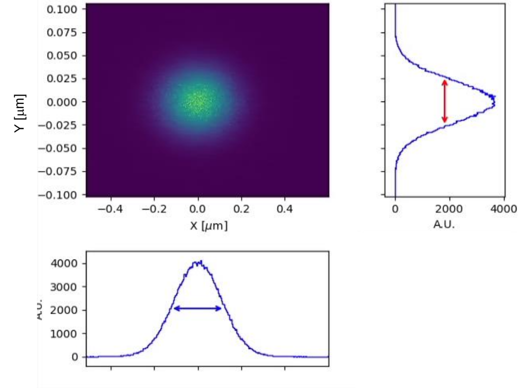


LTP measurements

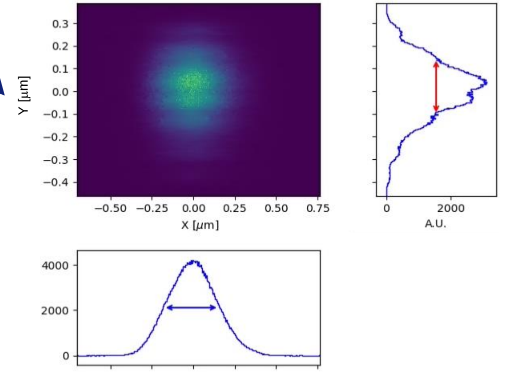
Height profile



Ideal surfaces



Slope errors



Photon transport

Measurements

DABAM Prepare Profile

Profile file:

```
position(m) slope_errors(um)
2.999999999999999889e-01 5.847589565563402481e-01
2.989999999999999880e-01 5.316997267566142549e-01
2.979999999999999871e-01 6.446404969568864107e-01
2.969999999999999862e-01 7.115812671571627446e-01
2.959999999999999853e-01 6.805220373574376591e-01
2.949999999999999845e-01 6.634628075577126971e-01
2.939999999999999836e-01 7.014035777579897823e-01
2.929999999999999827e-01 8.063443479582647067e-01
2.919999999999999818e-01 8.352851181585424500e-01
2.909999999999999809e-01 8.322258883588177225e-01
2.899999999999999800e-01 8.411666585590922285e-01
2.889999999999999791e-01 7.671074287593643293e-01
2.880000000000000338e-01 6.430481989596452674e-01
2.870000000000000329e-01 5.359889691599195594e-01
2.860000000000000320e-01 4.159297393601991688e-01
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```
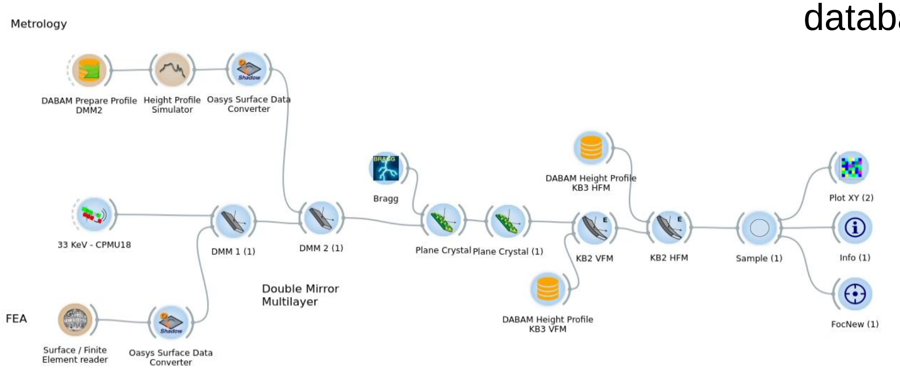



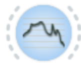
Measurements similar mirrors

DABAM Height Profile

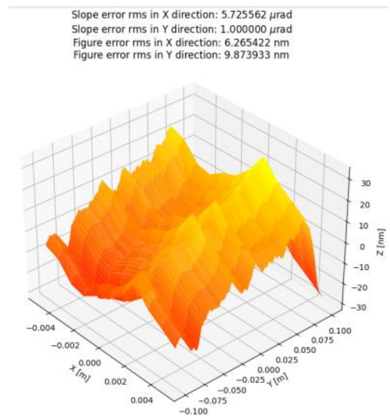
DABAM: Height profiles database

Simulation

Tangential slope error	<1.0 µrad RMS over active length
Sagittal slope error	<5 µrad RMS

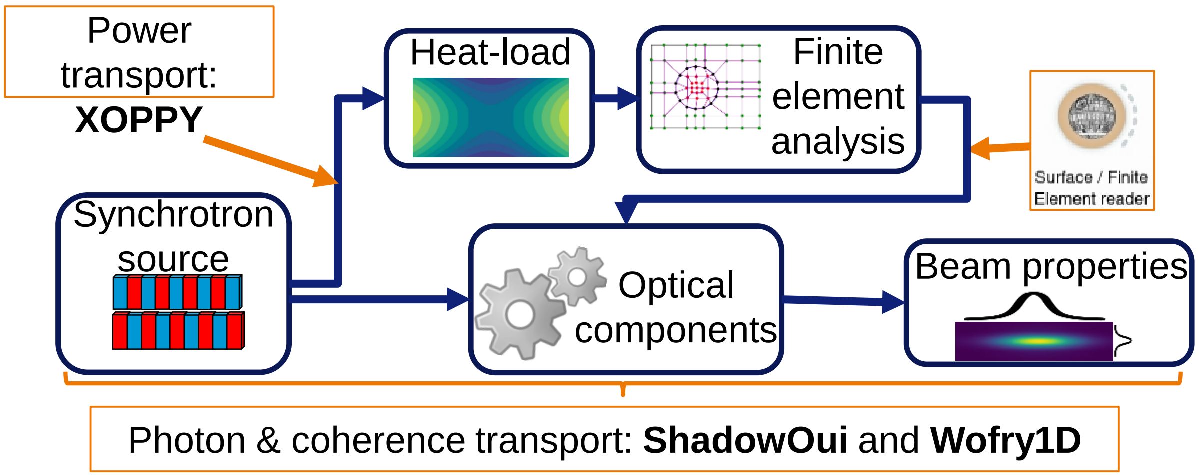


Height Profile Simulator



[1] M. Sanchez del Rio et al. *DABAM: an open-source database of X-ray mirrors metrology* J. Synchrotron Rad. (2016) **23** 665 http://dx.doi.org/10.1107/S1600577516005014

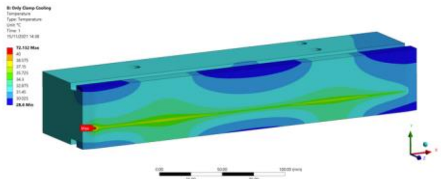
Power management & Photon transport

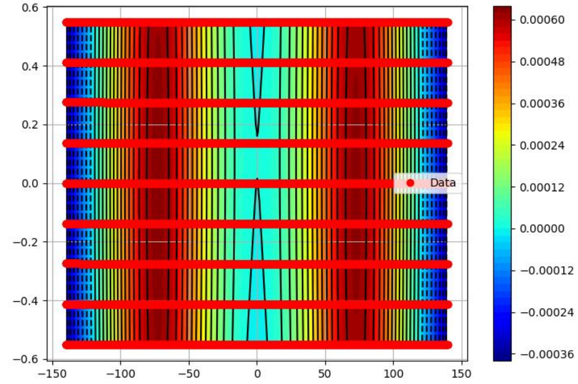


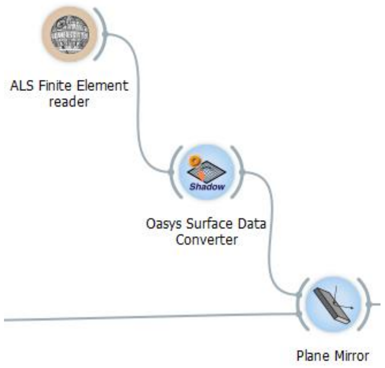
Power management & Photon transport

Surface / Finite Element reader

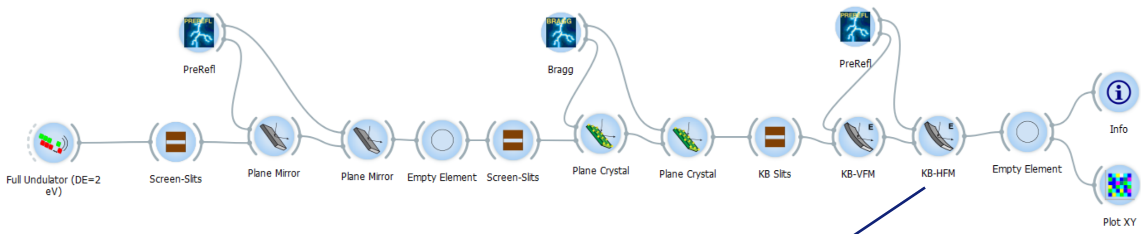
Finite element analysis

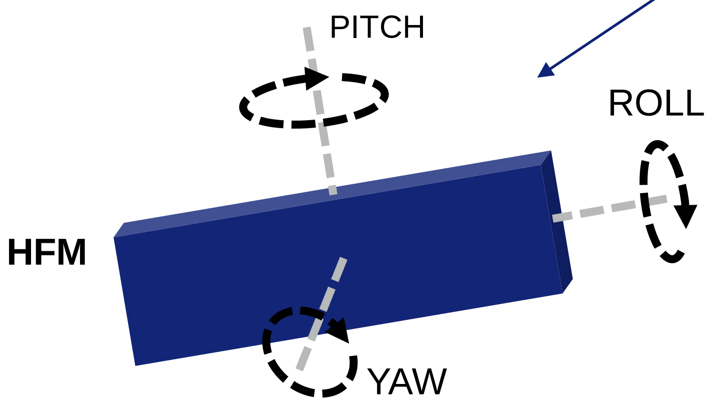


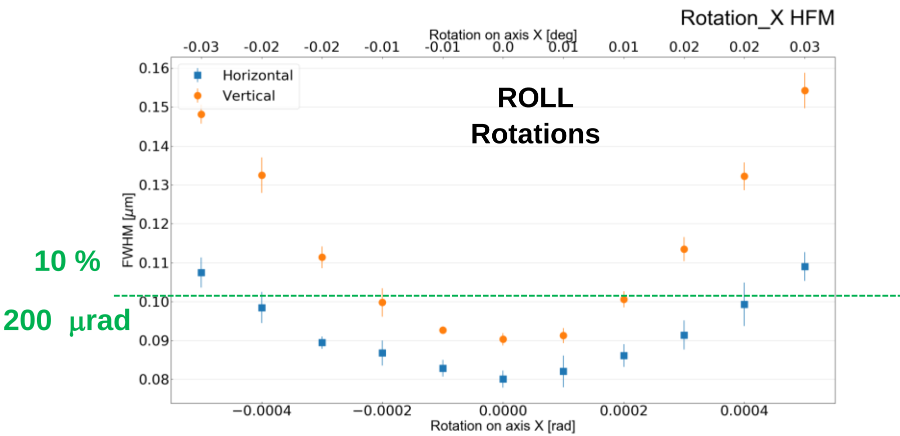




Photon transport: Misalignments

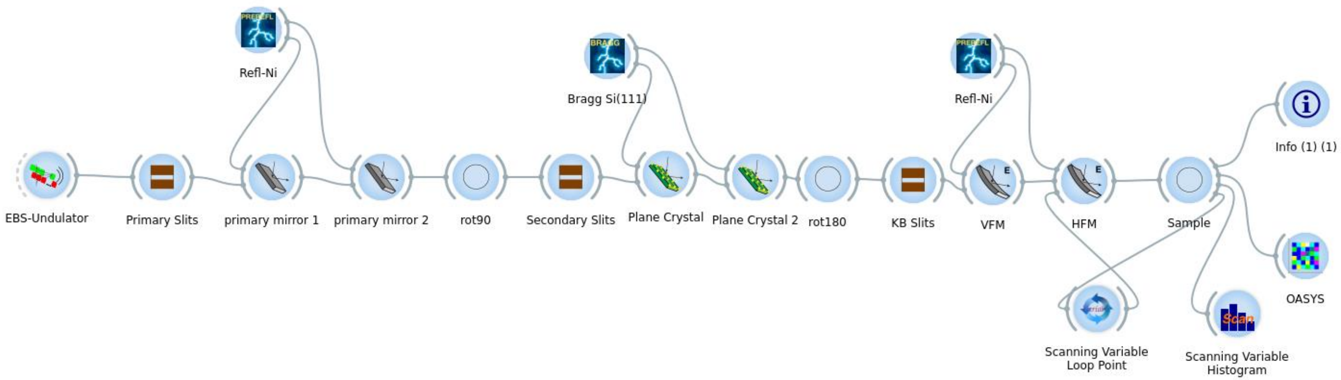


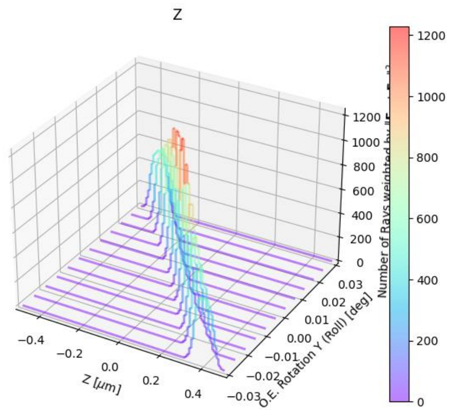


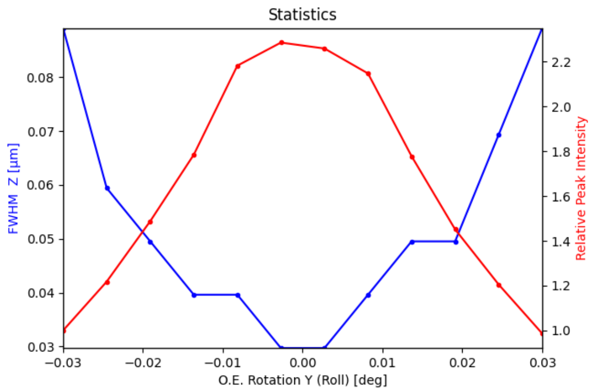


Photon transport: Misalignments

1. Using the GUI

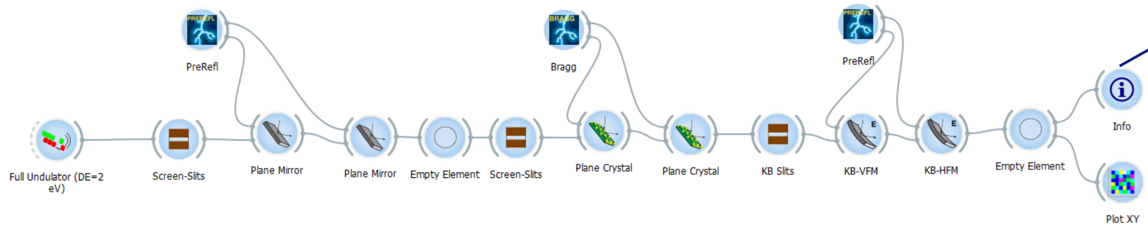


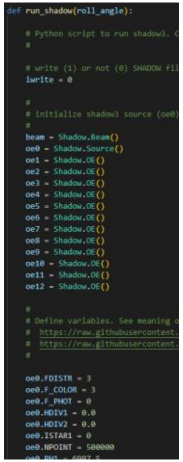




Photon transport: Misalignments

2. Using a Python script

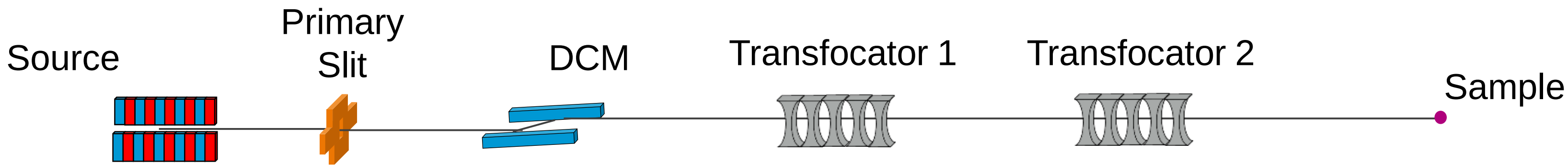


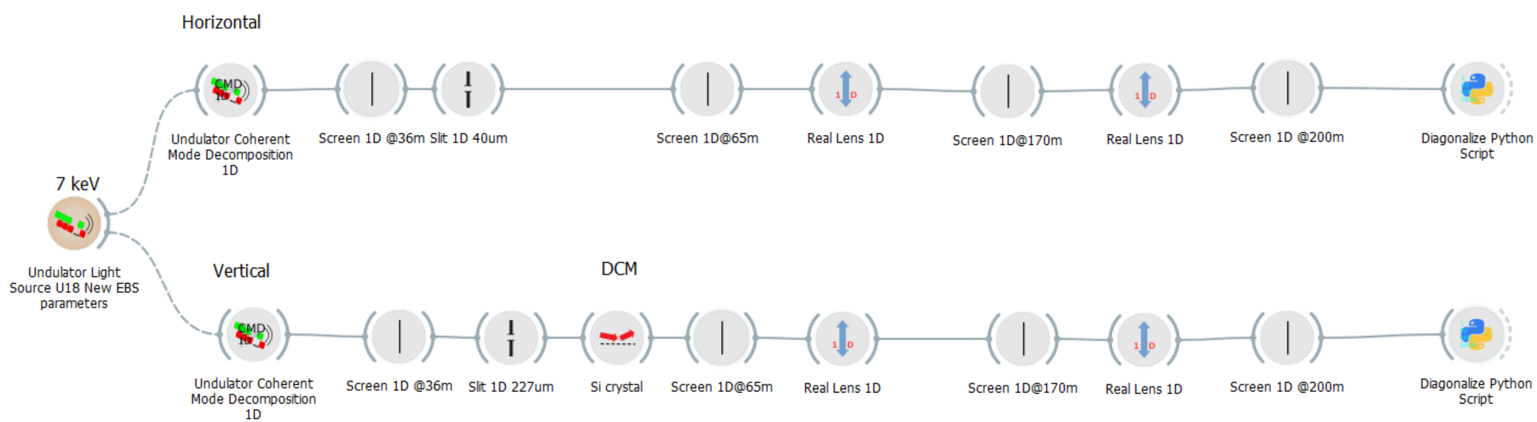


```
def run_shadow(roll_angle):

    # Python script to run shadow3. C
    #

    # write (1) or not (0) SHADOW fil
    iwrite = 0

    #
    # initialize shadow3 source (oe0)
    #
    beam = Shadow.Beam()
    oe0 = Shadow.Source()
    oe1 = Shadow.OE()
    oe2 = Shadow.OE()
    oe3 = Shadow.OE()
    oe4 = Shadow.OE()
    oe5 = Shadow.OE()
    oe6 = Shadow.OE()
    oe7 = Shadow.OE()
    oe8 = Shadow.OE()
    oe9 = Shadow.OE()
    oe10 = Shadow.OE()
    oe11 = Shadow.OE()
    oe12 = Shadow.OE()

    #
    # Define variables. See meaning o
    #  https://raw.githubusercontent.
    #  https://raw.githubusercontent.
    #

    oe0.FDISTR = 3
    oe0.F_COLOR = 3
    oe0.F_PHOT = 0
    oe0.HDIV1 = 0.0
    oe0.HDIV2 = 0.0
    oe0.ISTAR1 = 0
    oe0.NPOINT = 500000
```

Loop changing variables

Coherence propagation

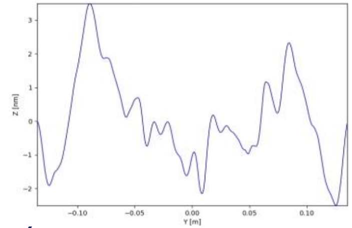


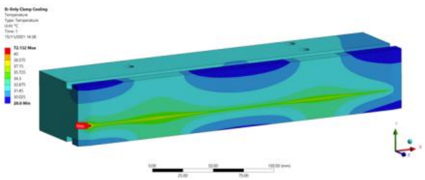


[1] M. Sanchez del Rio et al., *A fast and lightweight tool for partially coherent beamline simulations in fourth-generation storage rings based on coherent mode decomposition*, J. Synchrotron Rad. (2022) **29** 1354
https://doi.org/10.1107/S1600577522008736

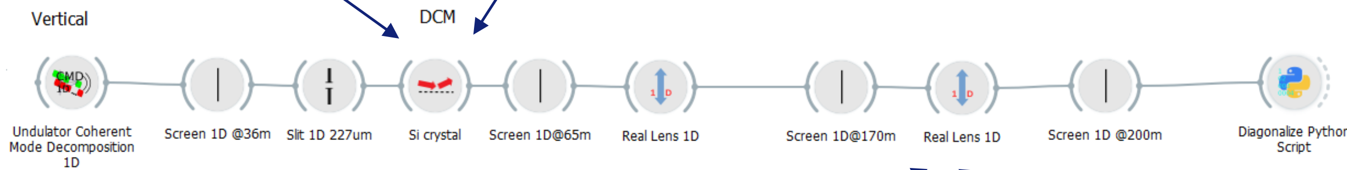
Coherence propagation

Measured height profile



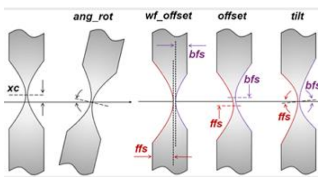


FEA



Lens error profile

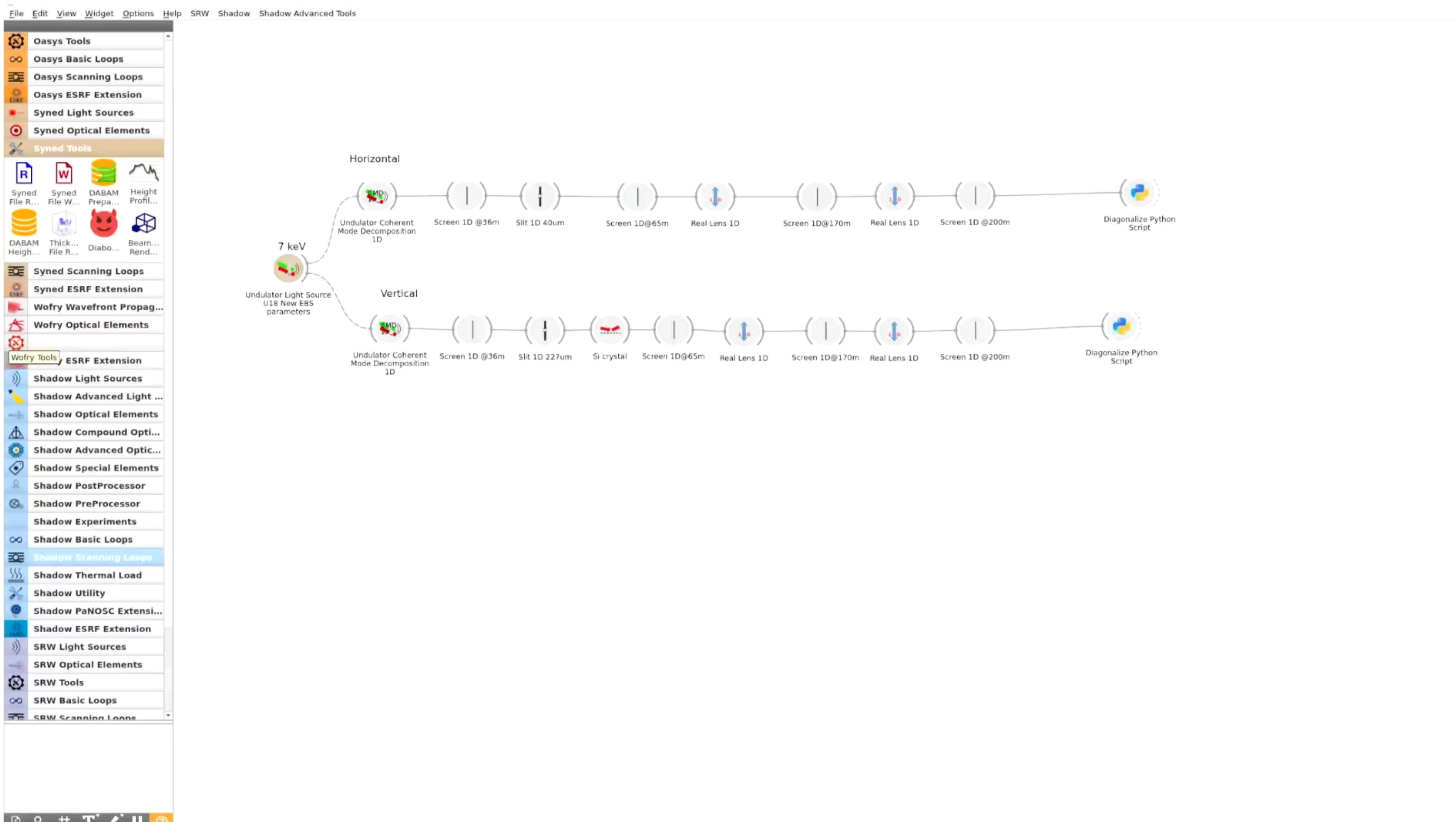
Lens misalignment



Rafael Celestre's barc4ro

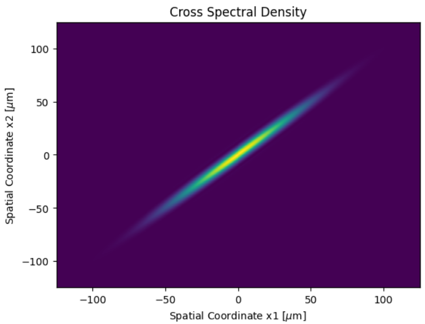
https://github.com/rafaelcelestre/oasys-barc4ro

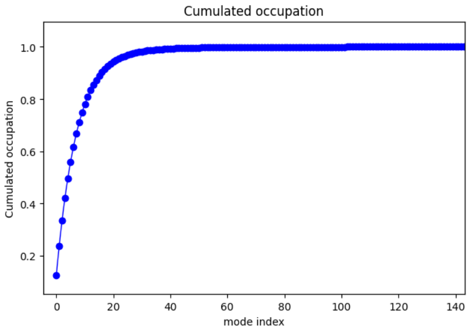
Coherence propagation



Coherence propagation

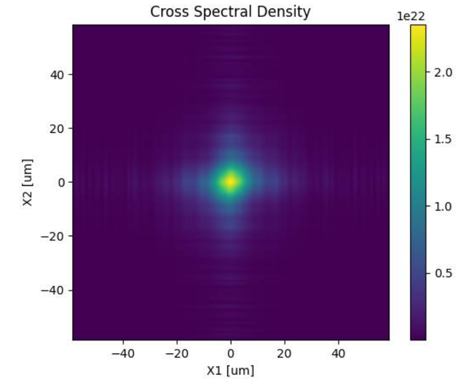
Source CSD

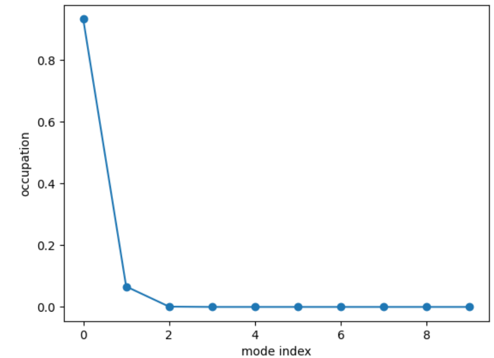




Horizontal
Coherence Fraction = 0.12

Sample position CSD





Horizontal
Coherence Fraction = 0.93

Summarizing

Modelling tools:

Power management

Photon transport

Coherence propagation

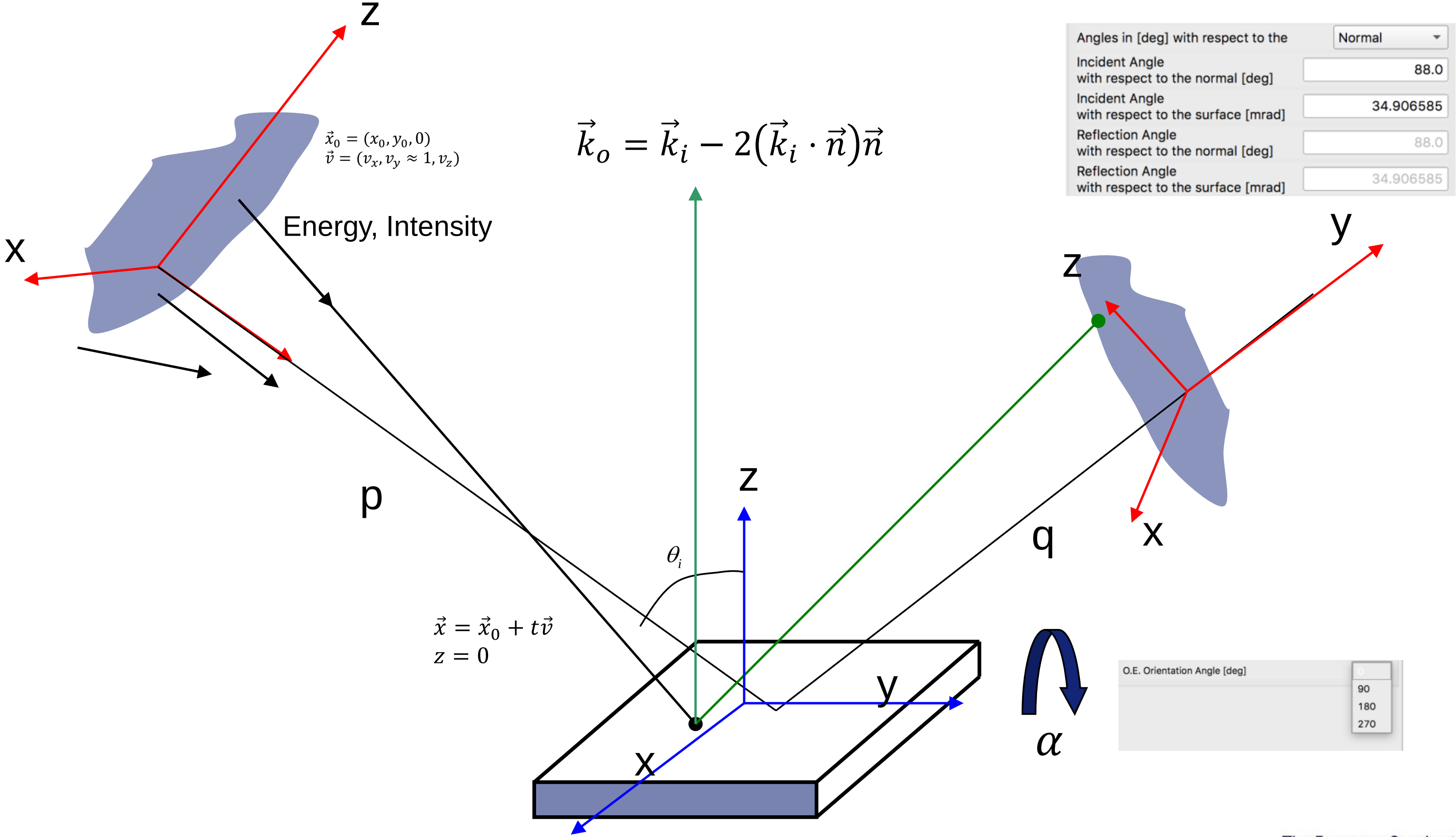
Thank you for your attention

Extra slides

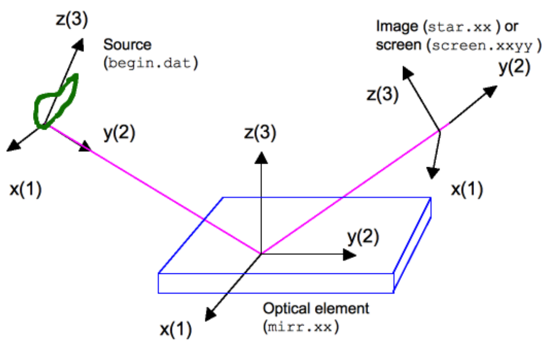
Extra slides

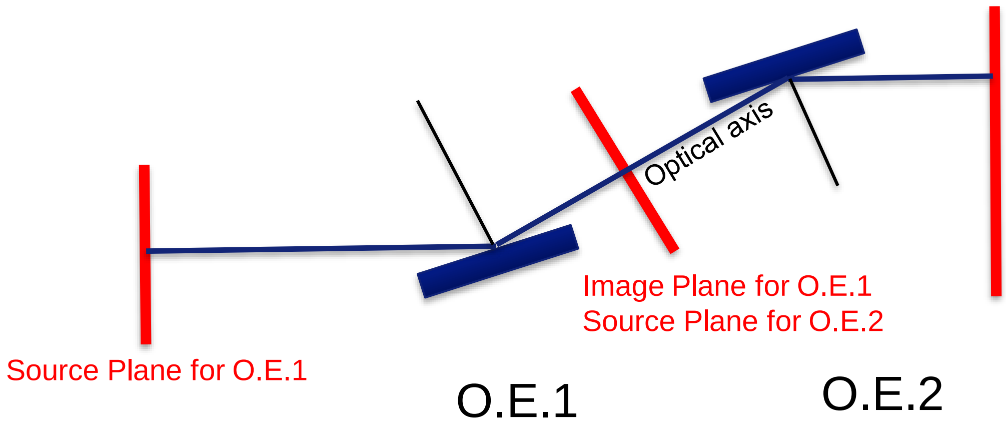
Photon transport with OASYS/SHADOWOUI

Ray tracing (schematic)



References and continuation planes





Note that (VERY IMPORTANT!):

- The y (column 2) coordinate is along the beam direction
- The position (Source Plane Distance), orientation (O.E. Orientation Angle) of any O.E. is always referred to the previous one
- Source Plane and Image Plane for each optical element are the “Continuation Planes”
- The frame is rotated if one O.E. is rotated