ESRF | The European Synchrotron

Beamline Simulation
Introduction to OASYS

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OASYS AND PHYSICS

Outline:

- What is OASYS?
  - Brief history and context
  - Its structure
- OASYS as a tool for synchrotron beamline instruments design:
  - XOPPY: Source spectra simulation, power density, etc.
  - ShadowOui: Ray tracing
- Final Remarks

In order to design and optimize synchrotron (and FEL) radiation beamlines, it is necessary to computer simulate light sources and optical components.

There are diverse codes for numerical simulations, which implements different physical approaches.

RAY-TRACING
Geometrical Optics

- Shadow
- McXtrace
- XRT
- ART
- RAY

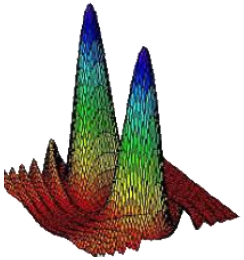
WAVEFRONT PROPAGATION

- SRW
- WISE
- PHASE

SRW

Synchrotron Radiation Workshop

1998 – Oleg Chubar & Pascal Elleaume



The code computes the synchrotron radiation from relativistic electrons with high precision and efficiency in the near and far field range. Provides a collection of computational tools for synchrotron radiation, e.g., source spectrum, flux. But also to propagate the beam trough various optical components [1].

https://github.com/ochubar/SRW

[1] O. Chubar, P. Elleaume, "Accurate And Efficient Computation Of Synchrotron Radiation In The Near Field Region", proc. of the EPAC98 Conference, 22-26 June 1998, p.1177-1179.

INTRODUCTION TO OASYS: XOP

XOP

X-ray OPtics utilities

1997 – Manuel Sanchez del Rio & Roger J. Dejus

This code is a graphical user interface that performs calculations of radiation characteristics of X-ray sources and their interaction with matter, such as: insertion devices (undulator or wiggler) spectra and angular distributions, mirror and multilayer reflectivities, and crystal diffraction profiles [1].

XOP + python = XOPPY

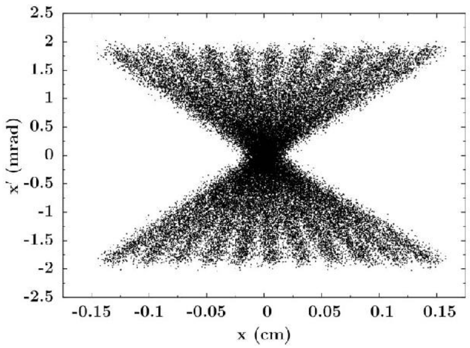
[1] Manuel Sanchez del Rio and Roger J. Dejus "XOP: a multiplatform graphical user interface for synchrotron radiation spectral and optics calculations", Proc. SPIE 3152, Materials, Manufacturing, and Measurement for Synchrotron Radiation Mirrors, (1 November 1997); https://doi.org/10.1117/12.295554.

SHADOW

A synchrotron radiation ray-tracing program

1986 – Barry P. Lai & Franco Cerrina

A simulation code that is flexible, fast and easy that performs ray-tracing; which accurate models synchrotron radiation sources, and optical components present in radiation beamlines [1].



SHADOW3: a new version of the synchrotron X-ray optics modelling package

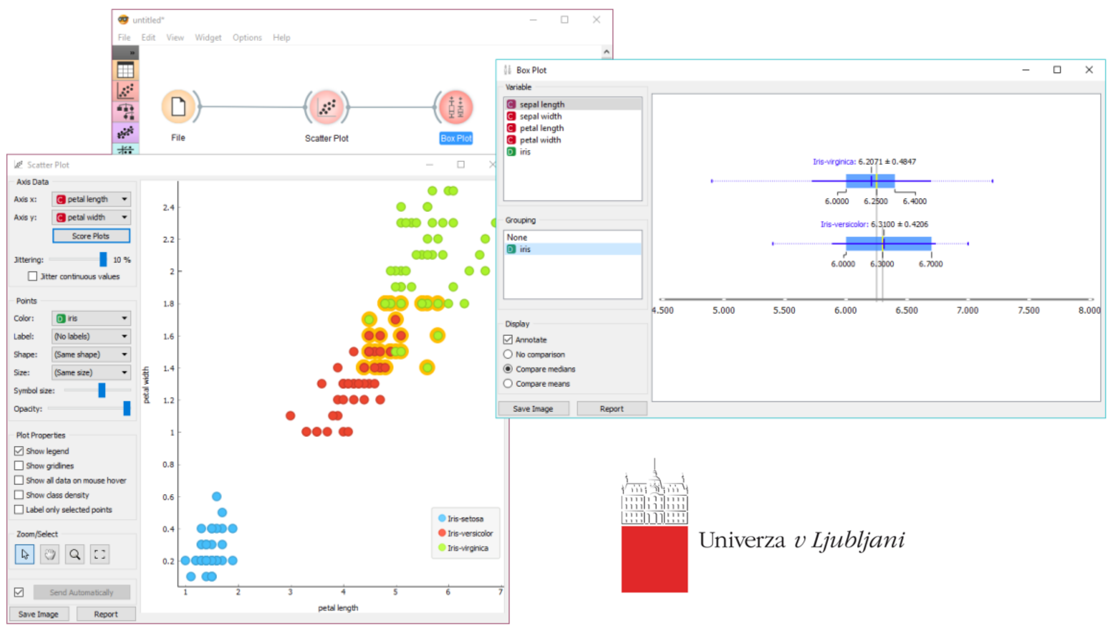
2011 – Manuel Sánchez del Río, Niccolo Canestrari, Fan Jiang & Franco Cerrina.

New code structure prepared to challenging new methods and new algorithms that will deal with polarizing optics, coherence and partial coherence, sample simulation, and full and simplified implementation of new devices [2].

https://github.com/srio/shadow3

[1] B. Lai & F. Cerrina "Shadow: A synchrotron radiation ray tracing program" Nuclear Instruments and Methods Research A246 (1986) 337-341. https://doi.org/10.1016/0168-9002(86)90101-4.
[2] Manuel Sanchez del Rio, Niccolo Canestrari, Fan Jiang, Franco Cerrina "SHADOW3: a new version of the synchrotron X-ray optics modelling package" J. Synchrotron Radiat. 2011 Sep 1; 18(Pt 5): 708–716. DOI: 10.1107/S0909049511026306.

Orange is a component-based visual programming software package for data visualization, machine learning, data mining, and data analysis. [1].



Univerza v Ljubljani

[1] Demšar, J., Curk, T., and Erjavec, A. "Orange: Data Mining Toolbox in Python," Journal of Machine Learning Research 14, 2349−2353 (2013). https://orange.biolab.si

SRW

WOFRY

XOPPY

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

SHADOWOUI

SYNED

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

COMSYL

https://github.com/mark-glass/comsyl

Orange

Utilities

OASYS = OrAnge SYncrotron Suite

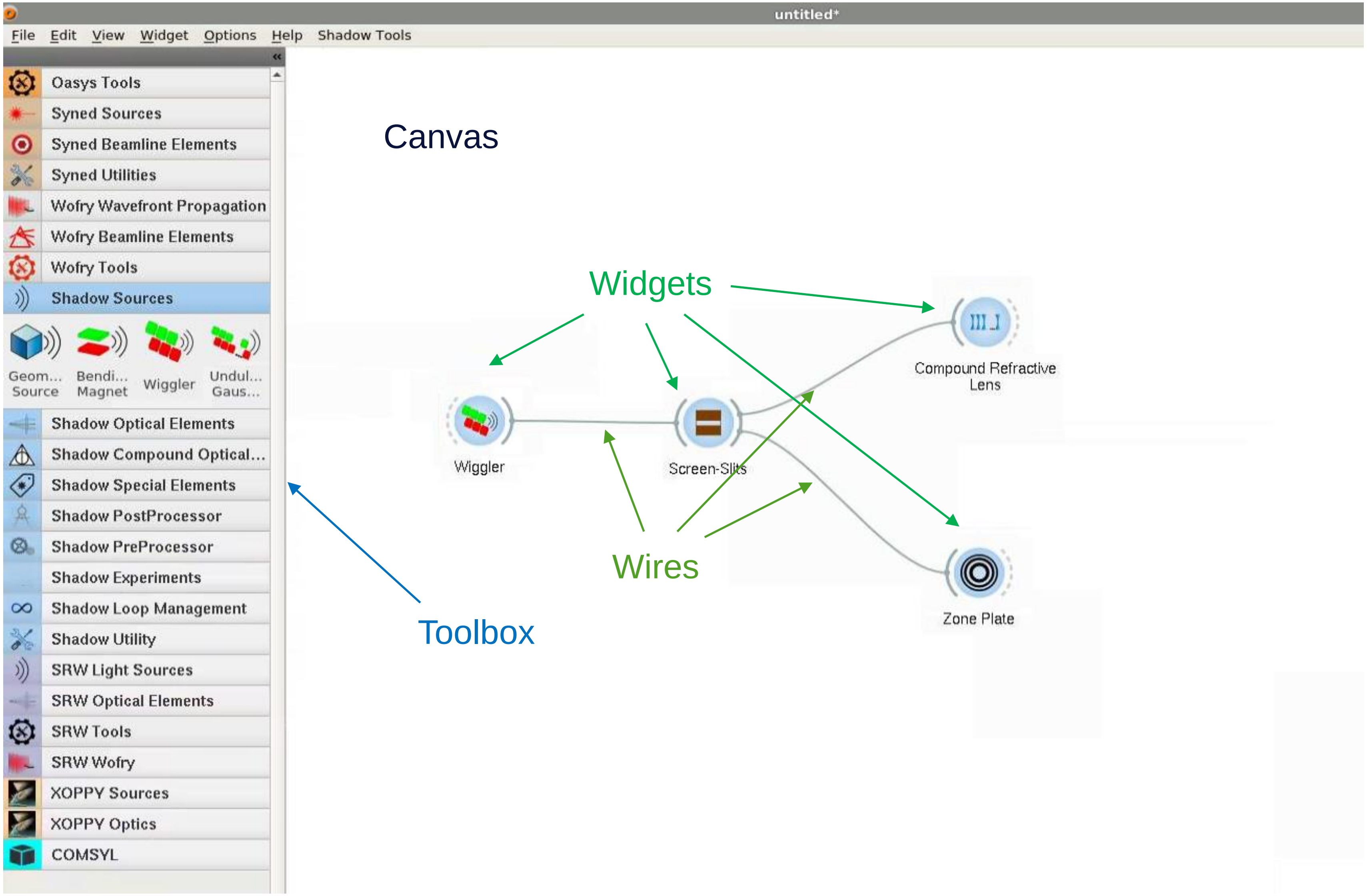
Luca Rebuffi (ANL) & Manuel Sánchez del Río (ESRF) [1].

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

https://github.com/oasys-kit

[1] 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.

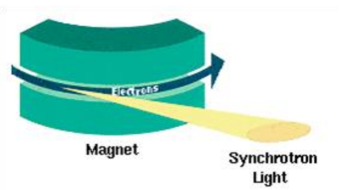
INTRODUCTION TO OASYS

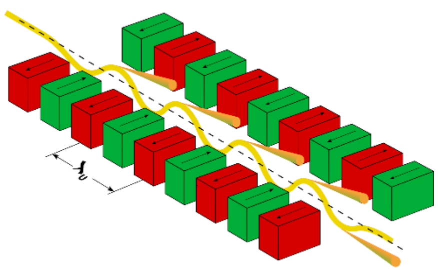


EXAMPLES OF WIDGETS (TOOLS)

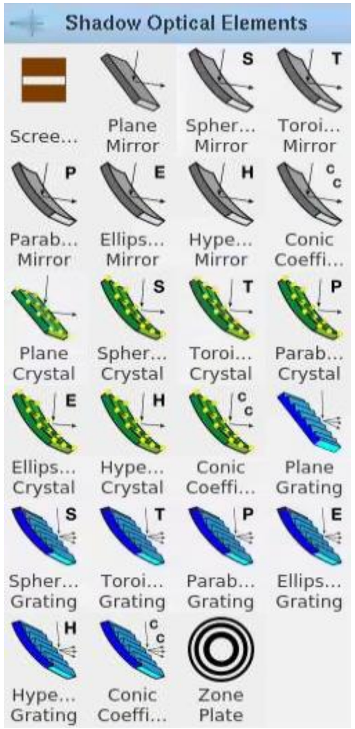
Mirrors, crystals, gratings and lenses

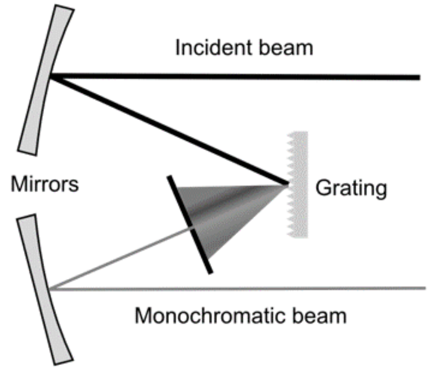
XOPPY

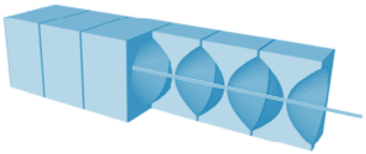




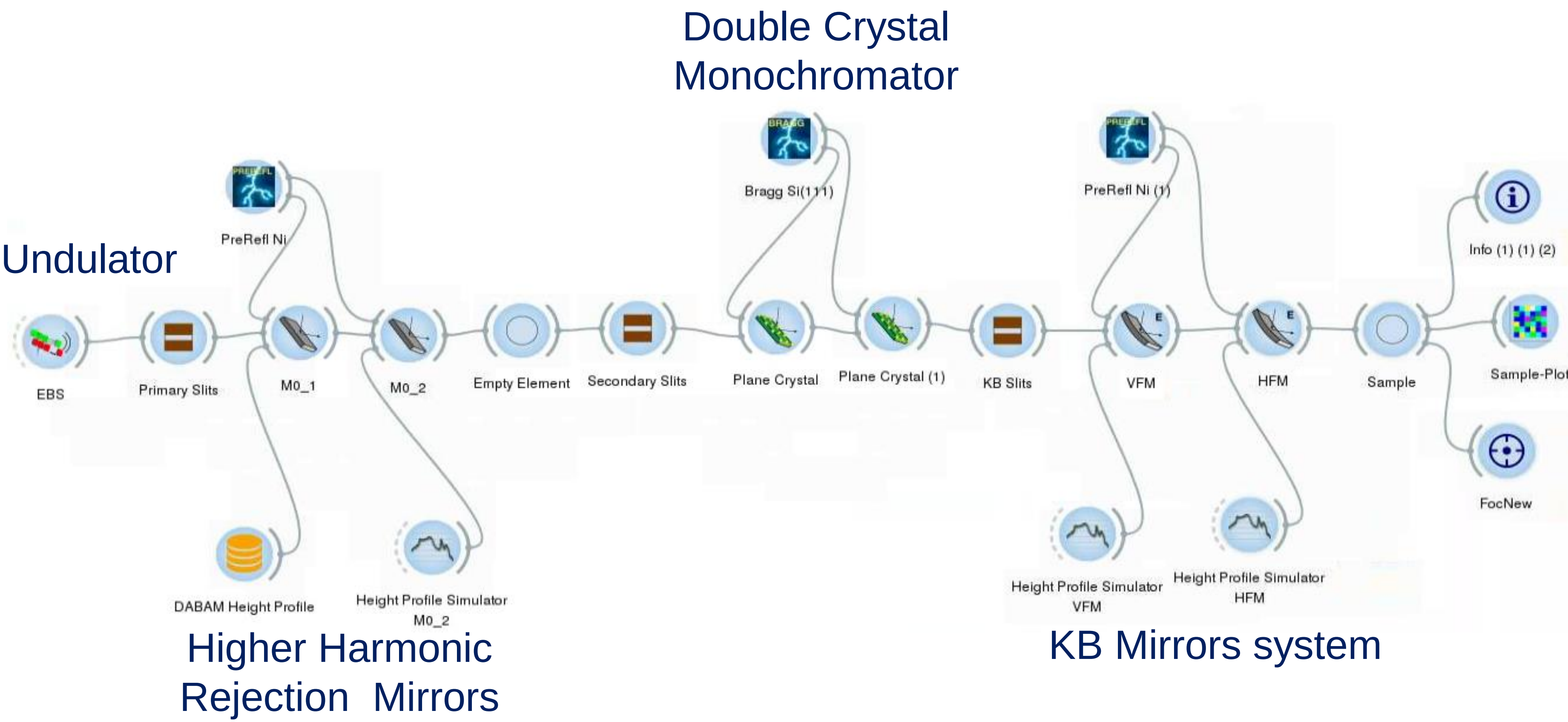
SHADOWOUI



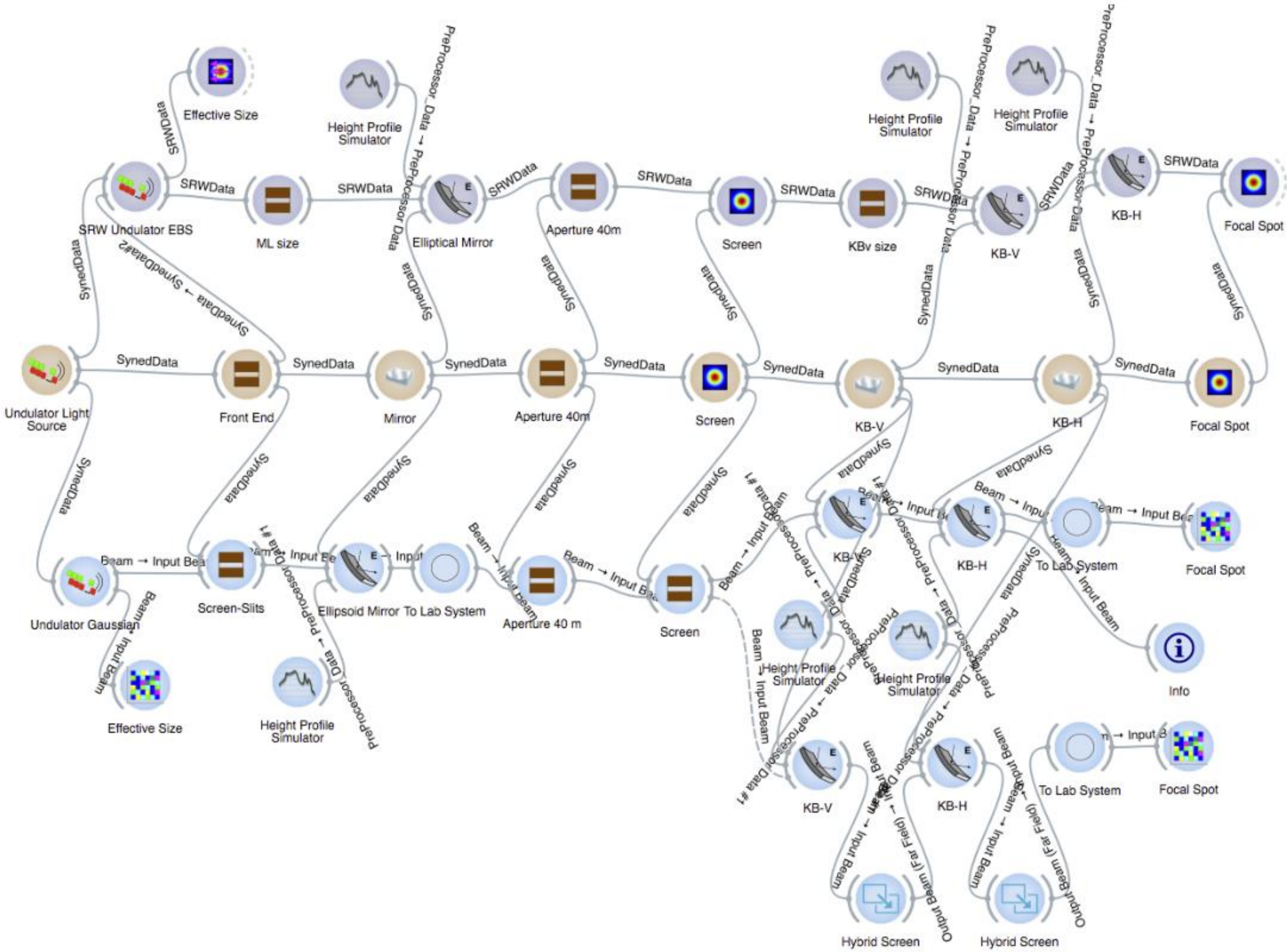




ESRF-ID21


Double Crystal
Monochromator
Undulator
PreRefl Ni
Bragg Si(111)
PreRefl Ni (1)
Info (1) (1) (2)
EBS
Primary Slits
M0_1
M0_2
Empty Element
Secondary Slits
Plane Crystal
Plane Crystal (1)
KB Slits
VFM
HFM
Sample
Sample-Plot
FocNew
DABAM Height Profile
Height Profile Simulator
M0_2
Height Profile Simulator
VFM
Height Profile Simulator
HFM
Higher Harmonic
Rejection Mirrors
KB Mirrors system

INTRODUCTION TO OASYS: INTEROPERABILITY



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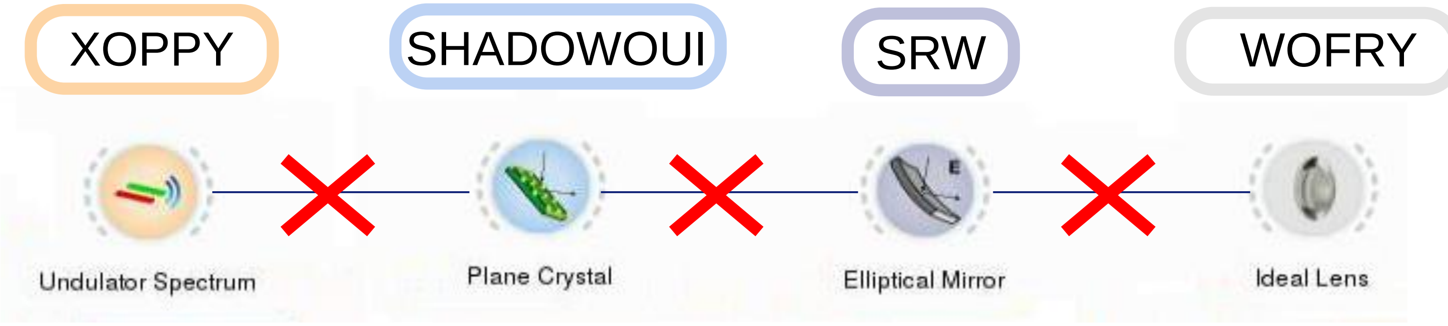
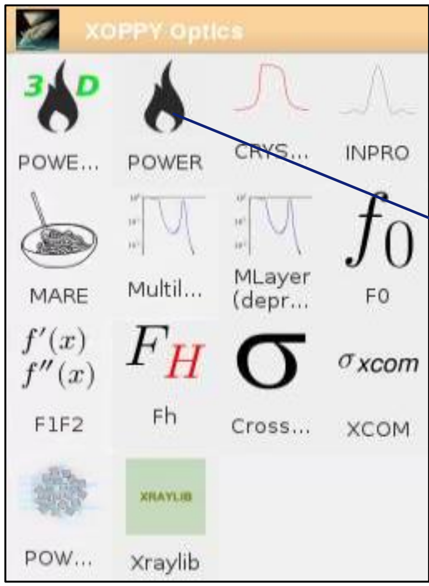
INTRODUCTION TO OASYS: DIFFERENT FRAMEWORKS

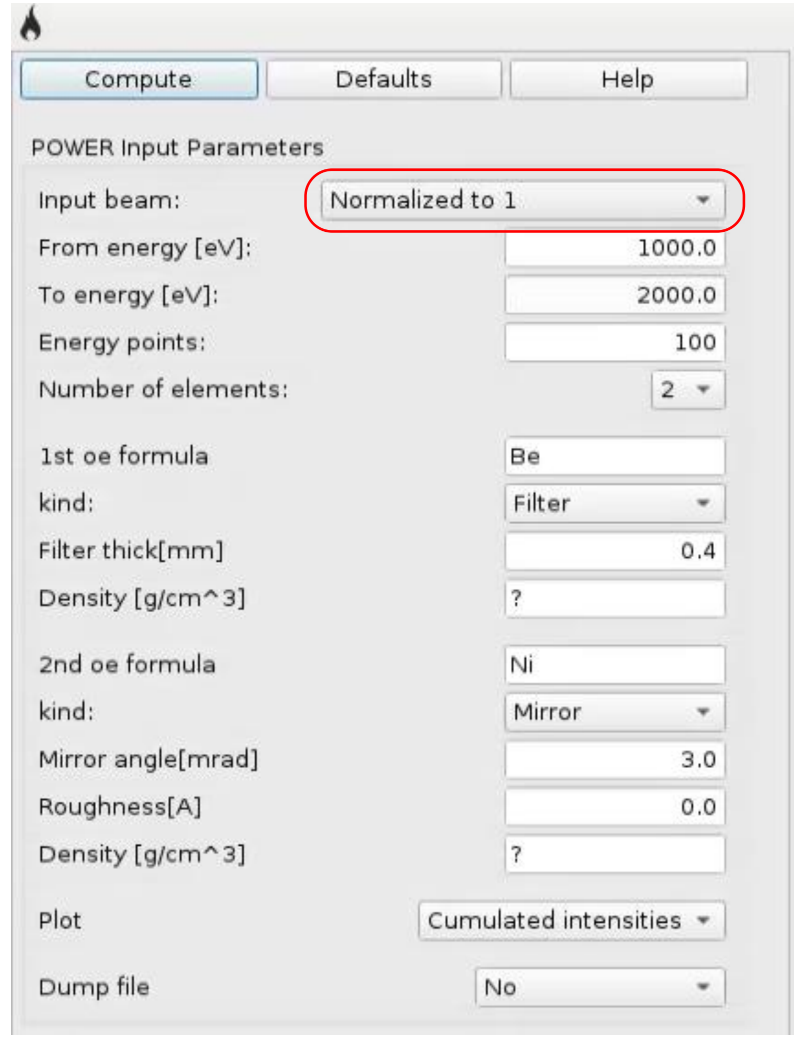


Hint: always keep an eye on the color code

XOPPY

Interaction of radiation with matter

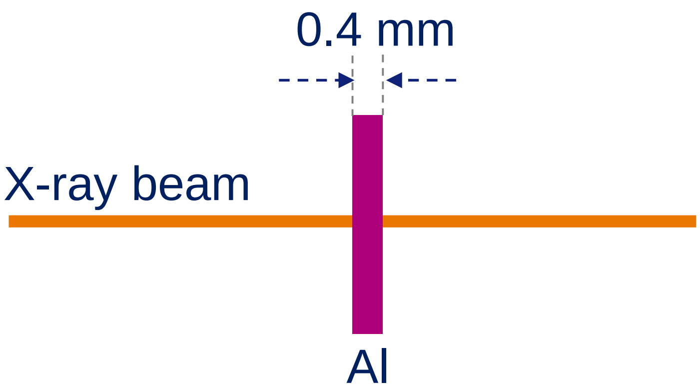


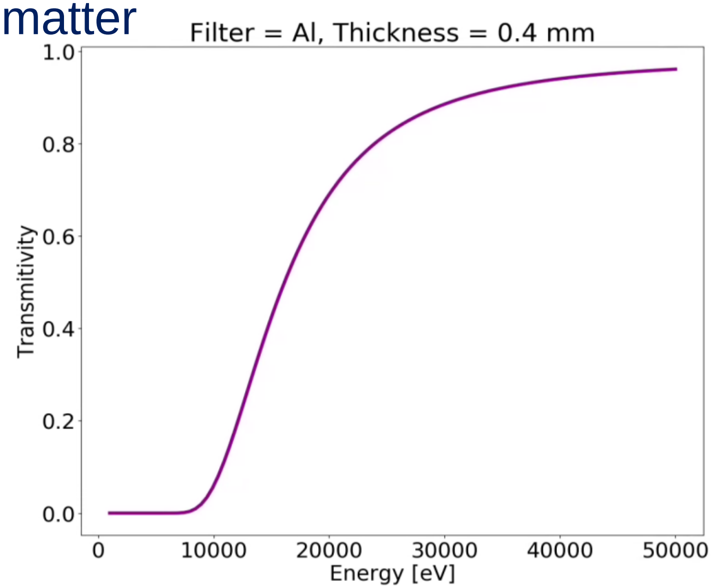


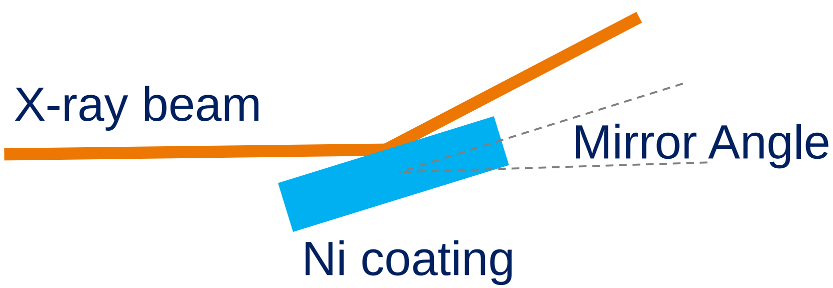
XOPPY

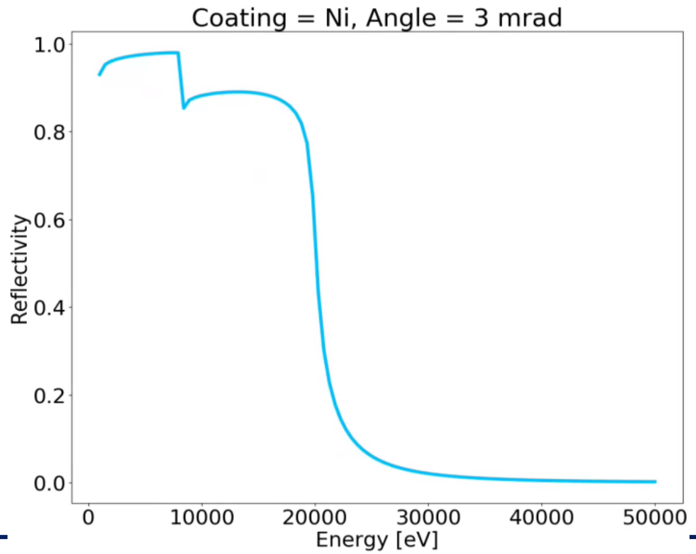
POWER

Interaction of radiation with matter



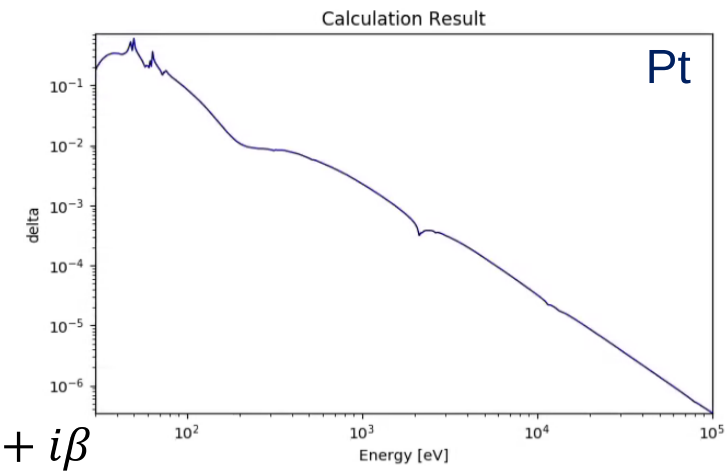






XOPPY

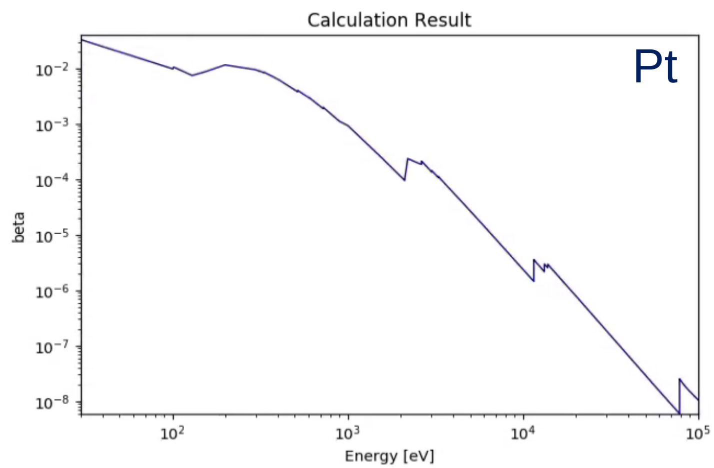
Interaction of radiation with matter



$$n = 1 - \delta + i\beta$$

0 Fluorescence line energy
1 Absorption edge energy
2 Atomic weight
3 Elemental density
4 Total absorption cross section
5 Photoionization cross section
6 Partial photoionization cross section
7 Rayleigh scattering cross section
8 Compton scattering cross section
9 Klein-Nishina cross section
10 Mass energy-absorption cross section

.
.
.
and more.



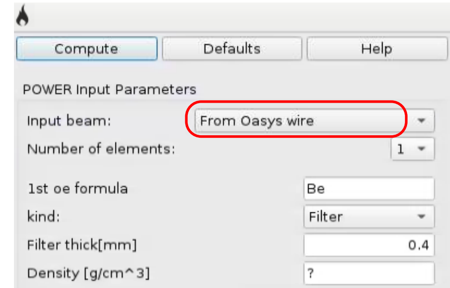

```
Inside xoppy_calc_xraylib with FUNCTION = 1 Absorption edge energy.
K_SHELL  4.966400   keV
L1_SHELL  0.563700   keV
L2_SHELL  0.461500   keV
L3_SHELL  0.455500   keV
M1_SHELL  0.060300   keV
M2_SHELL  0.034600   keV
M3_SHELL  0.034600   keV
M4_SHELL  0.003700   keV
M5_SHELL  0.003700   keV
No result
```

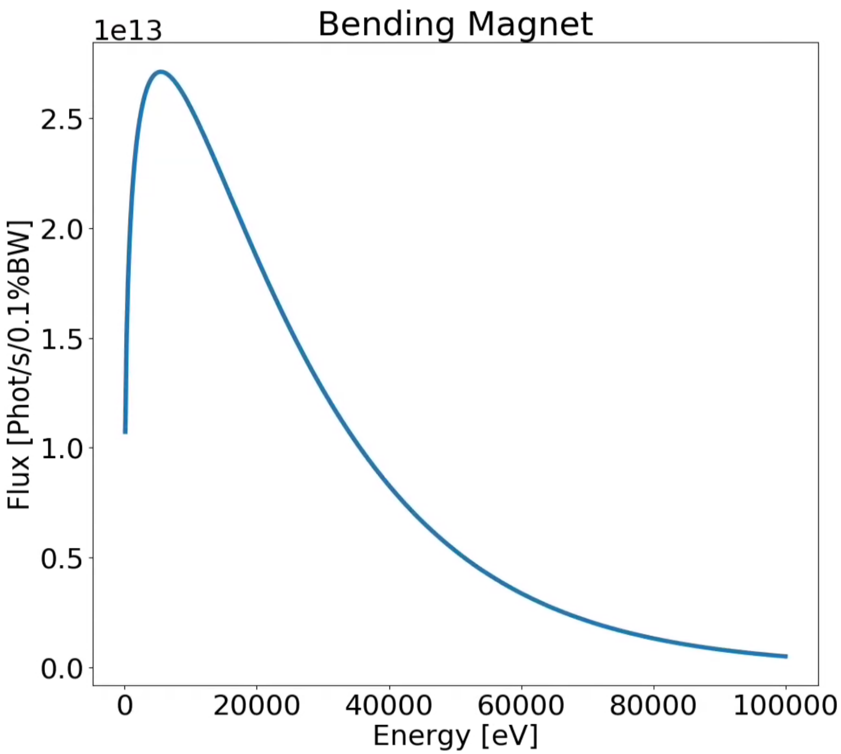
Ti –absorption edges

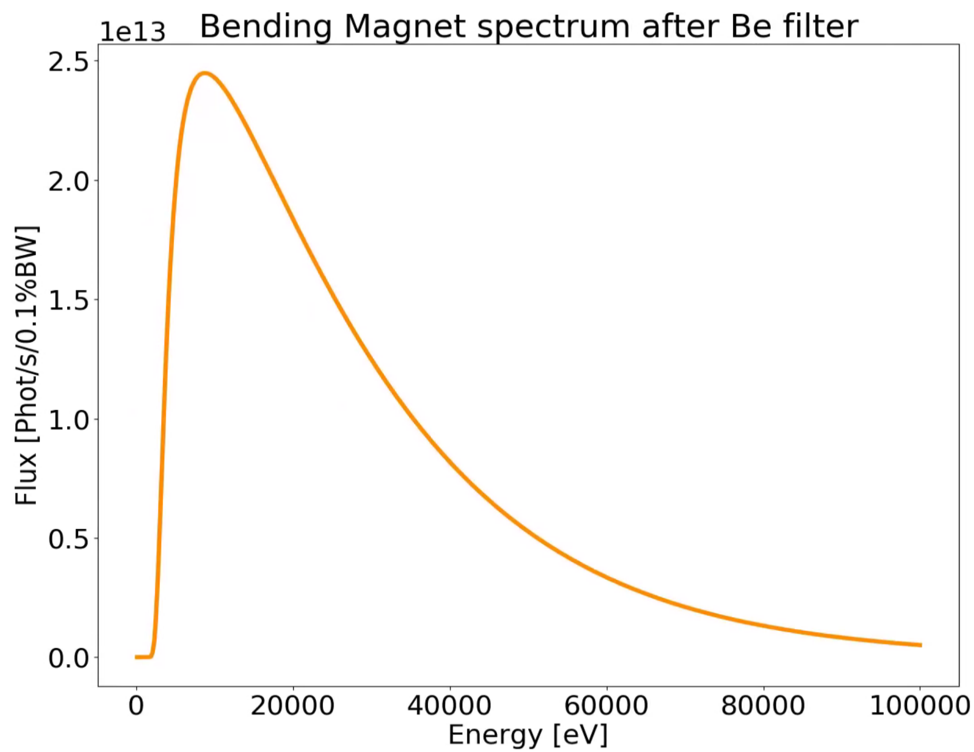
OASYS: XOPPY

XOPPY

White beam Calculations

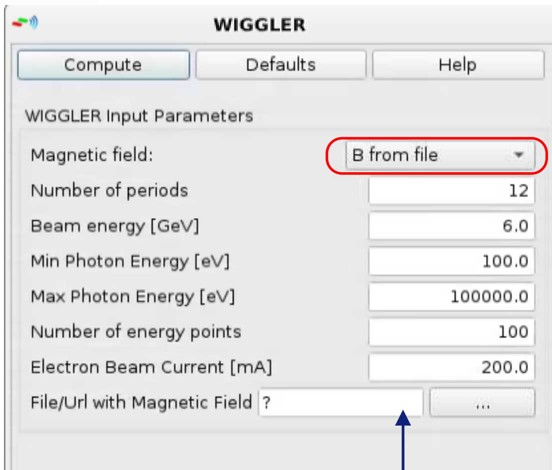


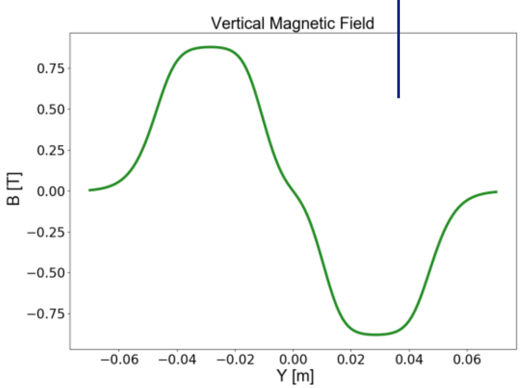


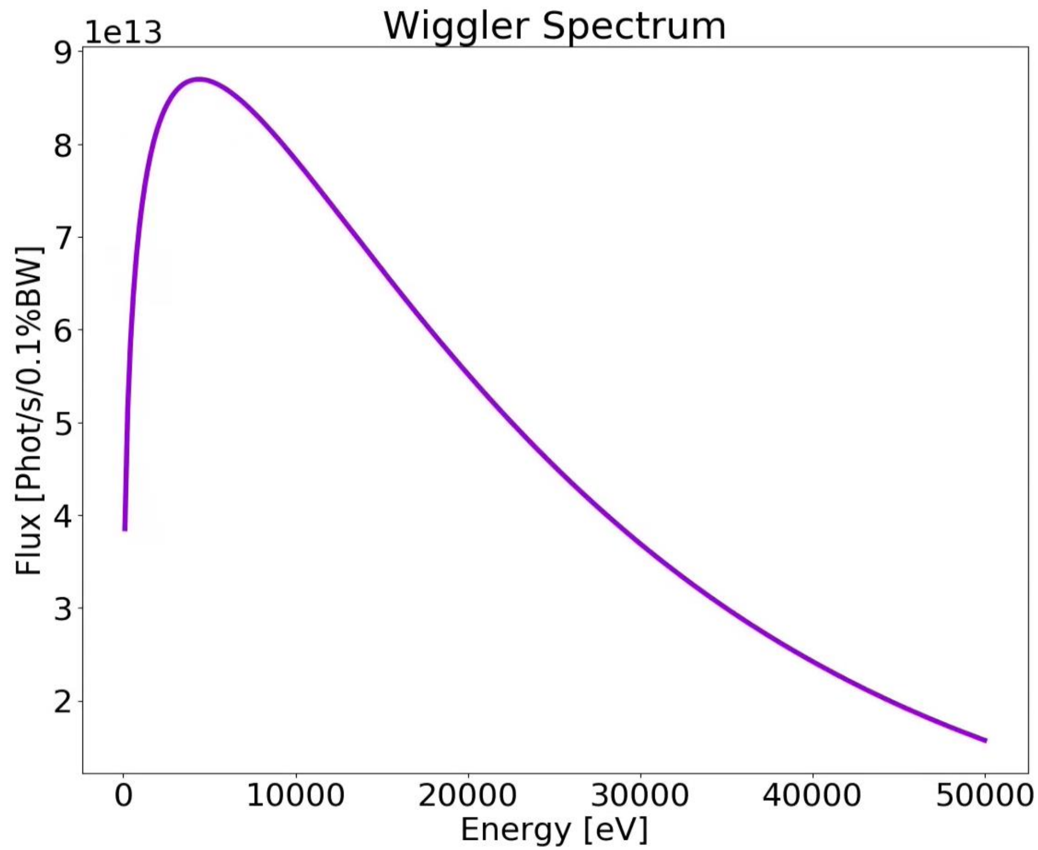


XOPPY

White beam Calculations

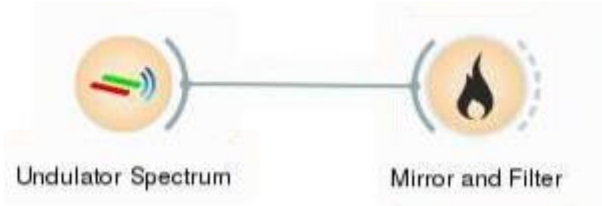


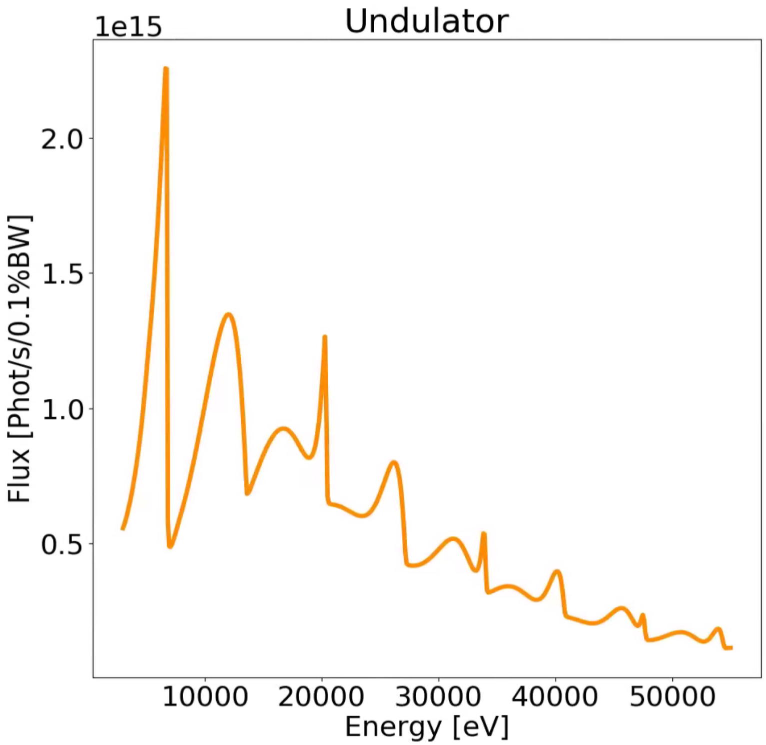


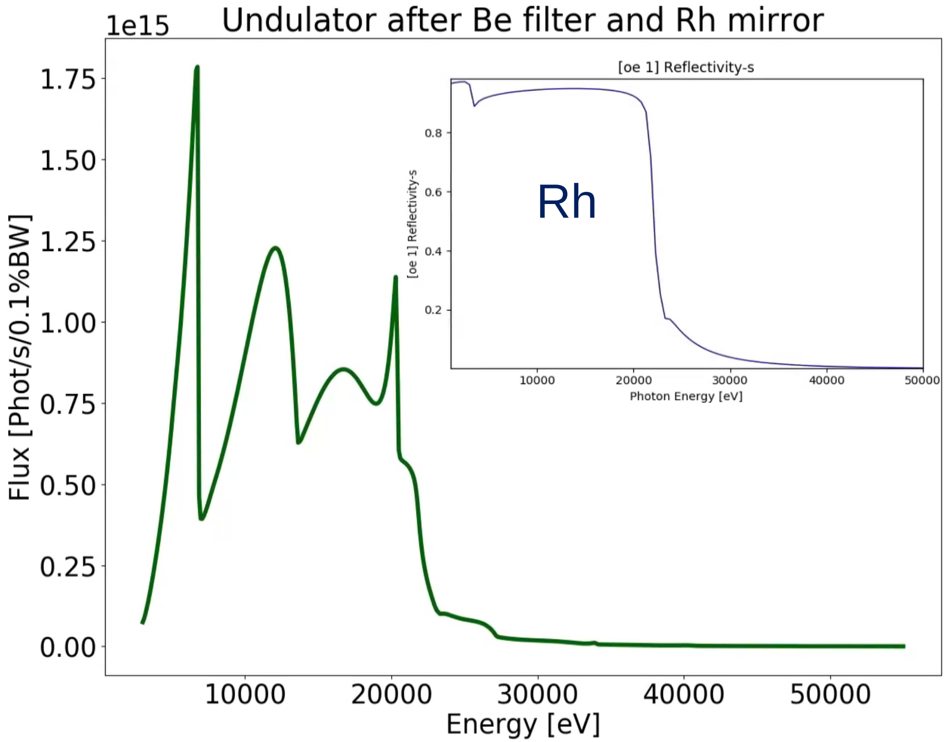


XOPPY

White beam Calculations

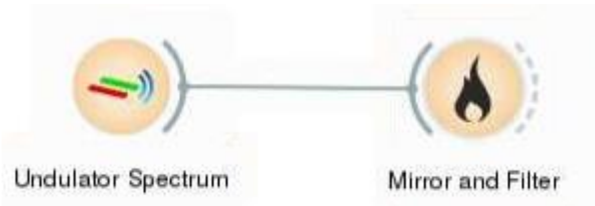




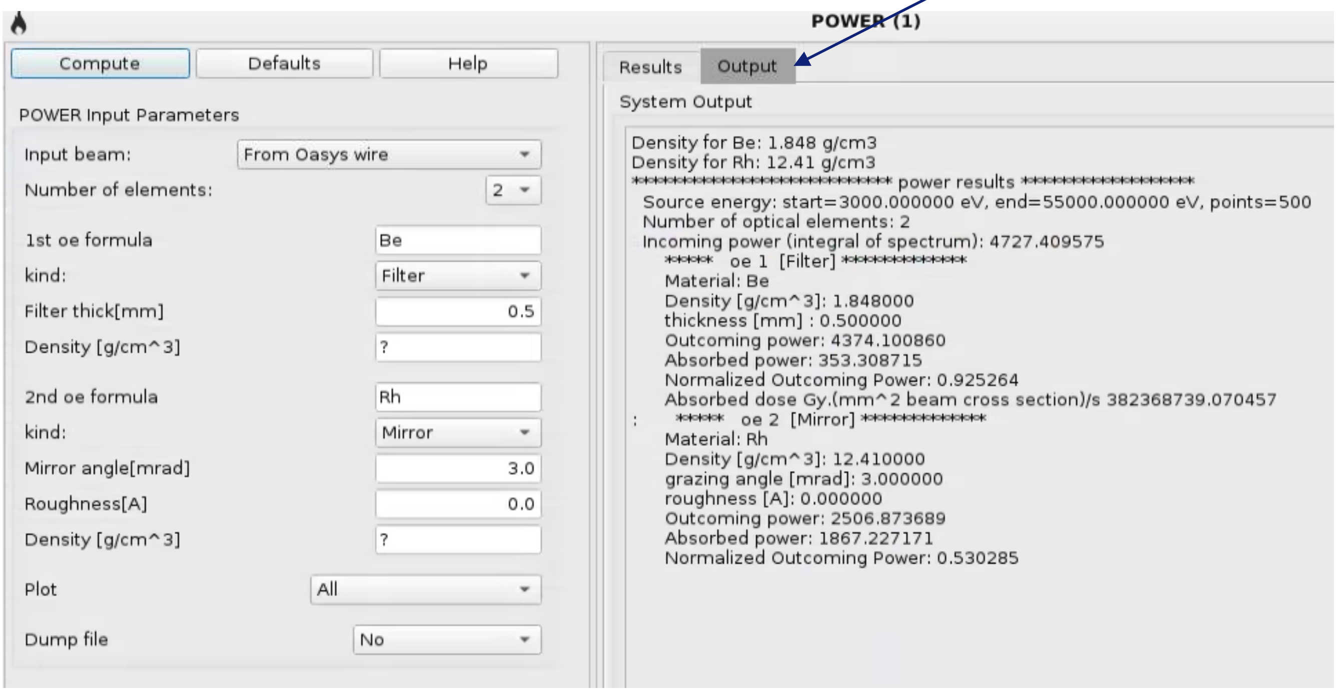


XOPPY

White beam Calculations



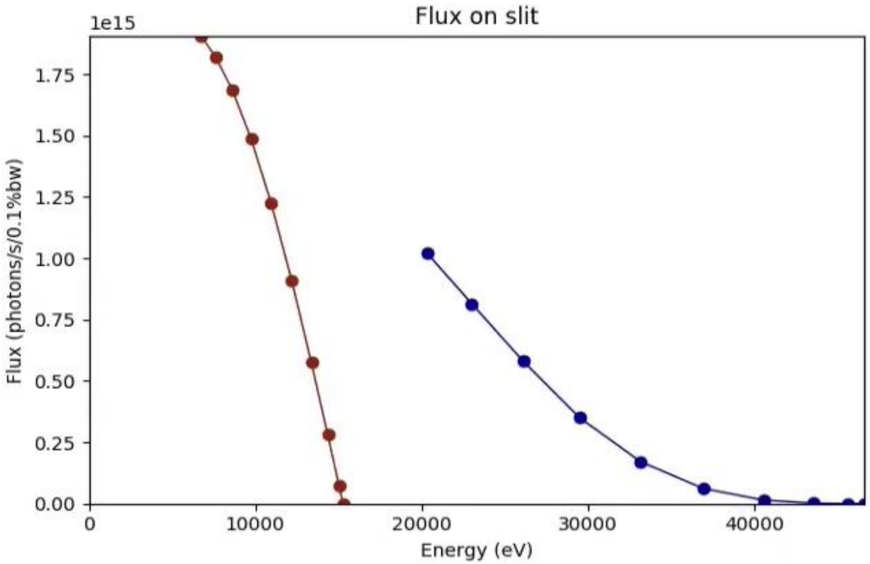
Power load calculations:
- Power from the Undulator
-Absorbed power by the Filter and the Mirror

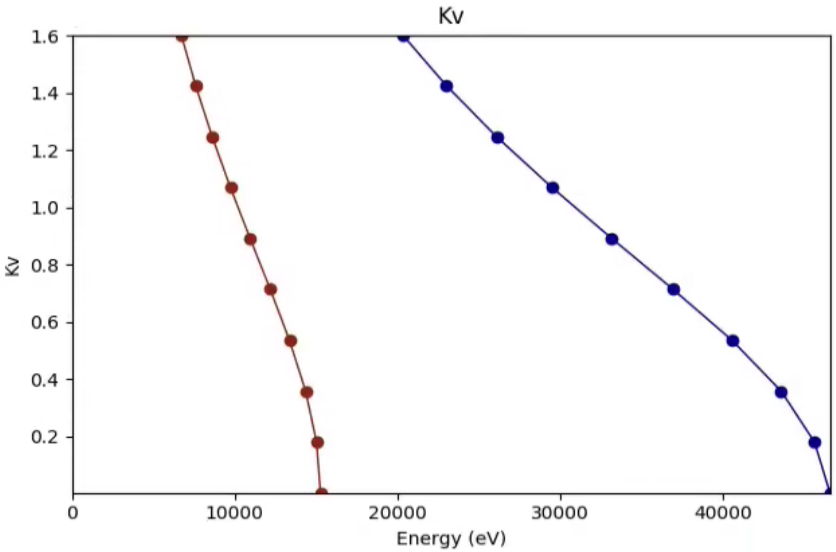


XOPPY

White beam Calculations

Undulator deflection parameter

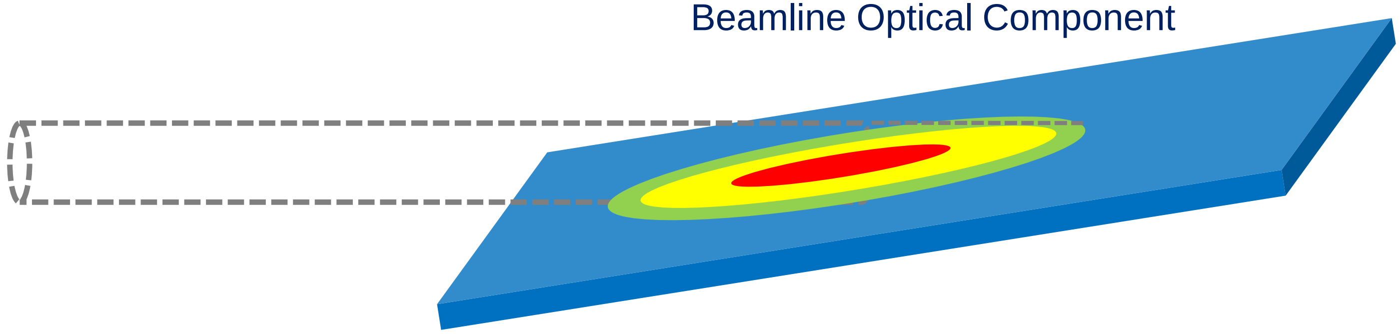


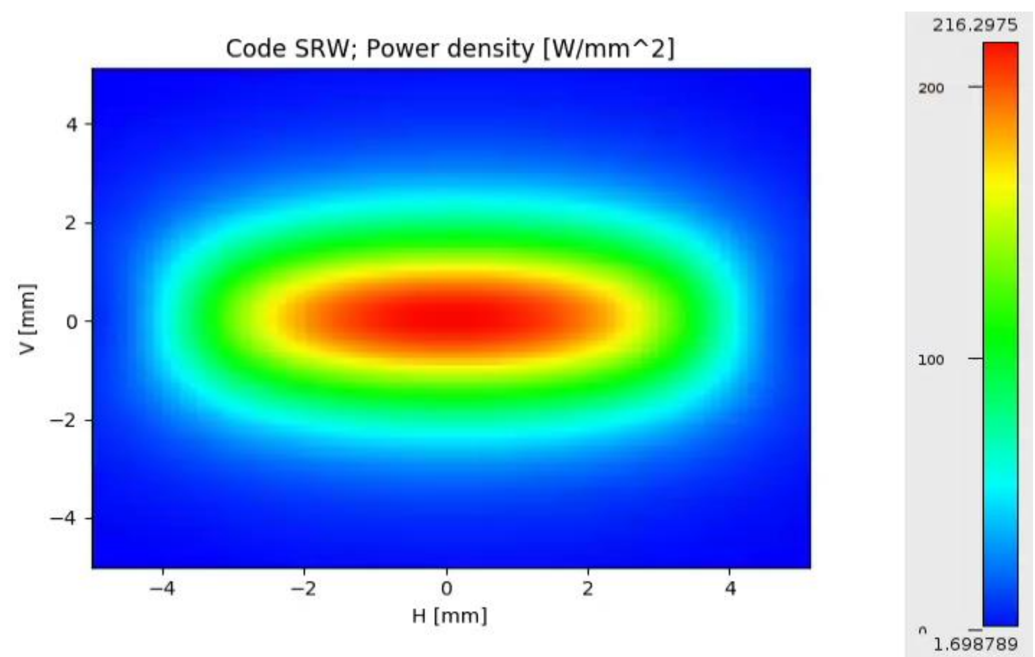


XOPPY

White beam Calculations

Heat load Distribution on a Beamline Optical Component

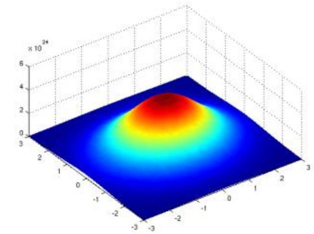




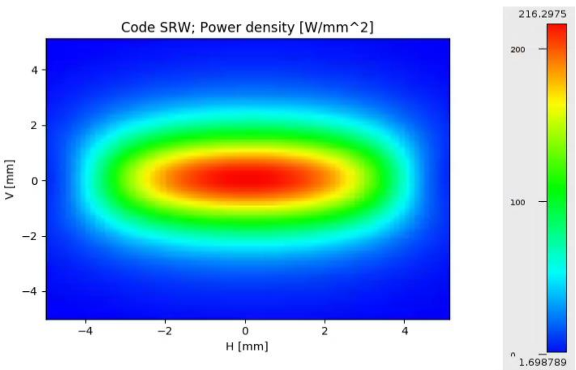
XOPPY White beam Calculations

Undulator Power Density

2D Gaussian fitting



Heat load Distribution on a Beamline Optical Component



Undulator Power Density

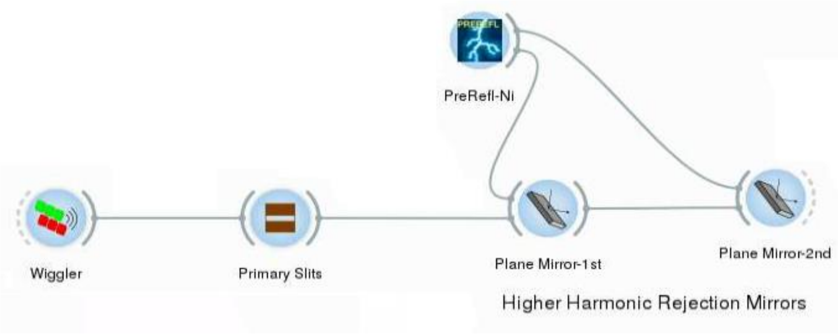
Results | Output | Script

System Output

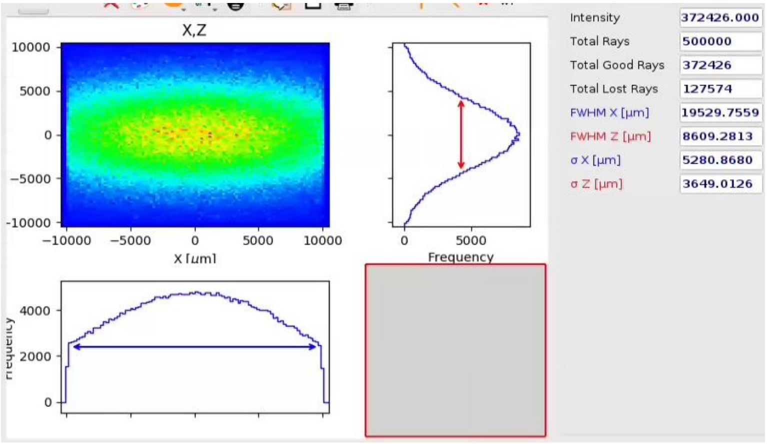
```
Inside xoppy_calc_undulator_power_density.
Undulator power_density calculation using SRW. Please wait...
Inside calc2d_srw
Running SRW (SRWLIB Python)
Performing Power Density calculation (from field) ...
Done Performing Power Density calculation (from field).
File written to disk: /mntdirect/_users/reyesher/Oasys_test/undulator_power_density.spec
Power density peak SRW: [W/mm2]: 216.29754638671875
Total power SRW [W]: 5272.3511678967625
Done

Total power radiated by the undulator with fully opened slits [W]: 5490.74

==================== power density ======================
 Power density peak: 216.297546 W/mm2
 Total power: 5272.351168 W
=======================================================

============= Fitting power density to a 2D Gaussian. ==============

Please use these results with care: check if the original data looks like a Gaussian.

Fit 2D Gaussian function:

 offset + A * exp( - (1/2)*((x-x0)/sigmax)**2 - (1/2)*((y-y0)/sigmay)**2 )
  Height A: 221.980907
  center x0:     0.000251
  center y0:     -0.000012
  sigmax: 2.568957
  sigmay: 1.409114
  offset: 4.595320

 Total power in the fitted data [W]:  5272.351292823832
=======================================================


Result arrays (shapes):  (81,) (81,) (81, 81)
```

SHADOWOUI

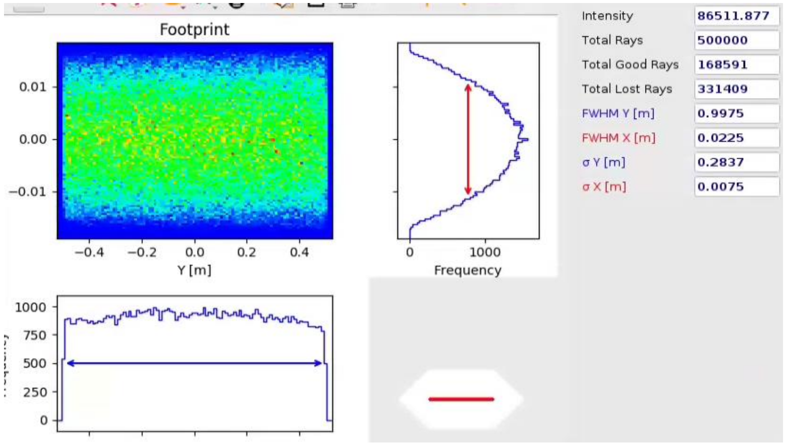
Study the beam propagation thought the different components



Primary slits @ 10 m, 20 cm x 20 cm aperture

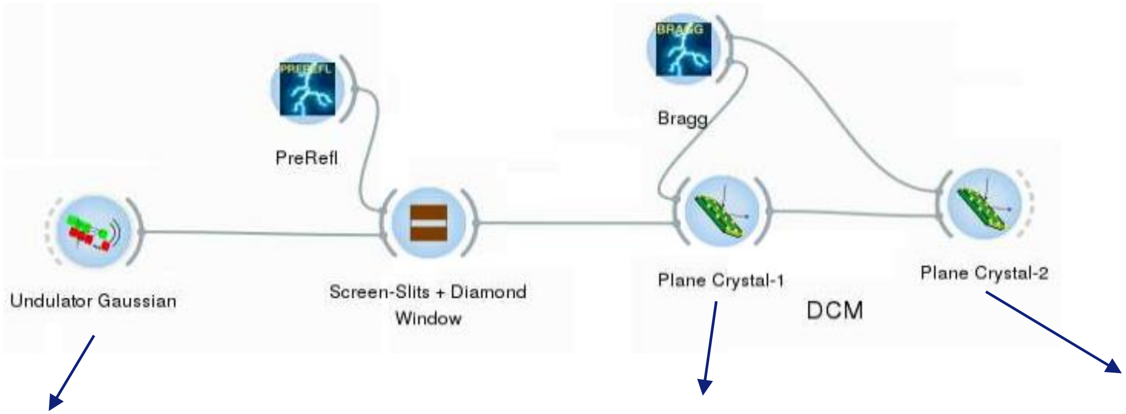


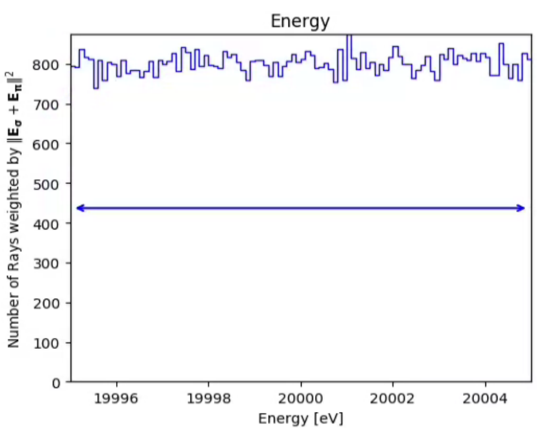
Footprint on mirror @ 20 m, 5 mrad



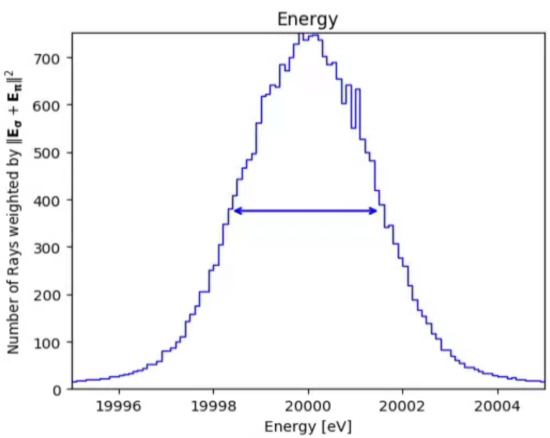
SHADOWOUI

Study the beam propagation thought the different components

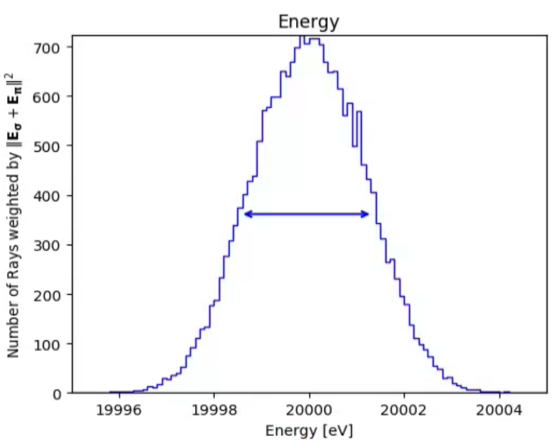




$\Delta E = 10$ eV



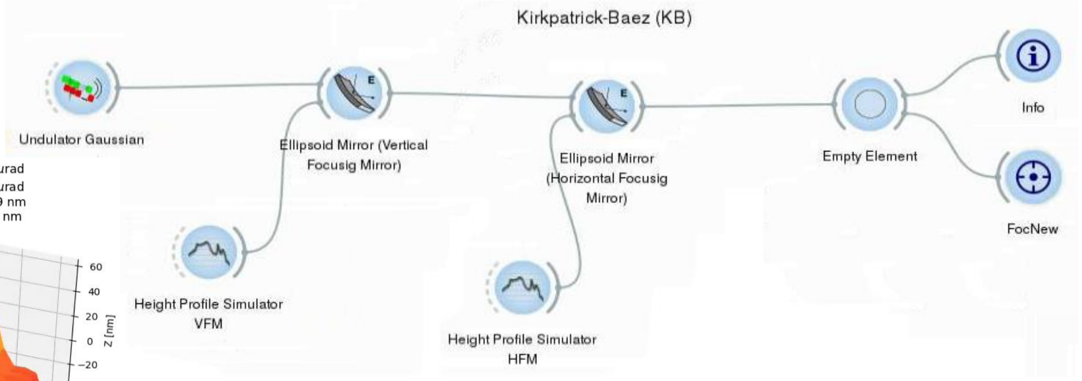
$\Delta E = 3.2$ eV

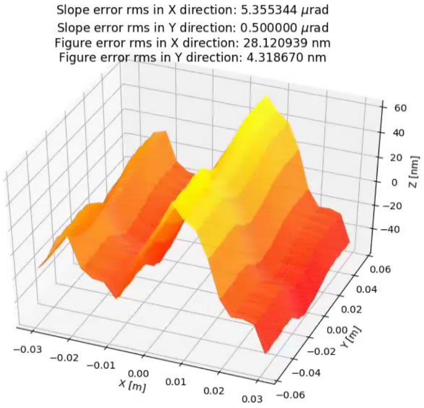


$\Delta E = 2.8$ eV

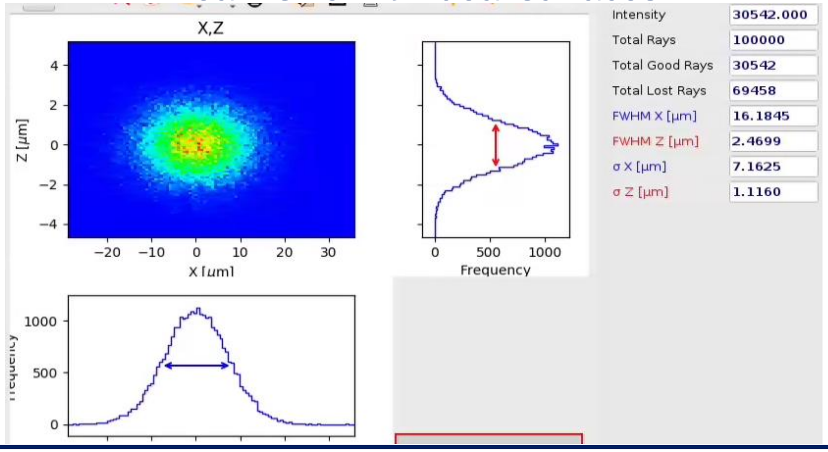
SHADOWOUI

Study the beam propagation thought the different components

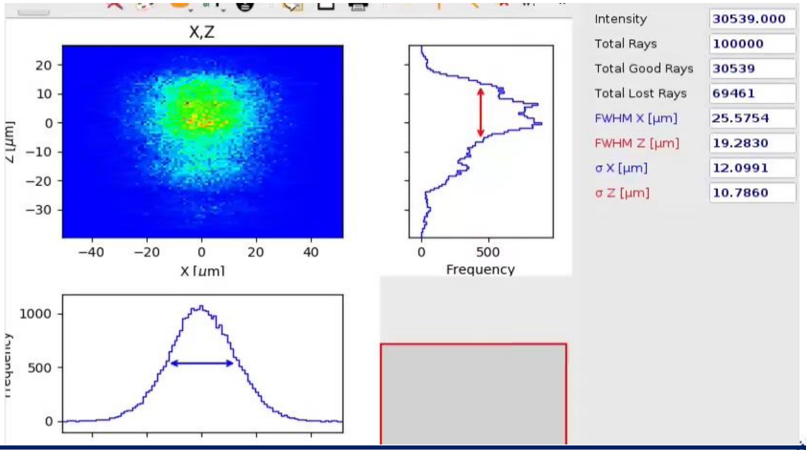




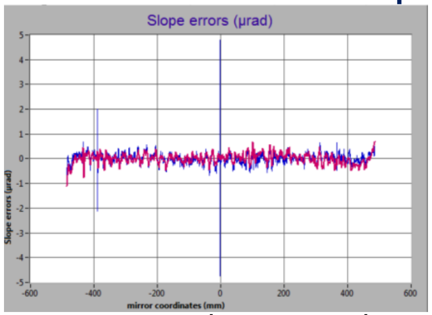
Beam size with ideal surfaces



Beam size with slope errors

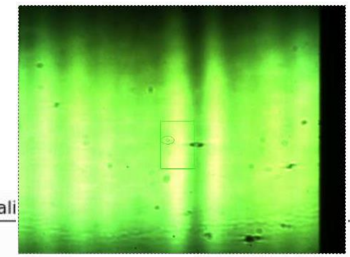


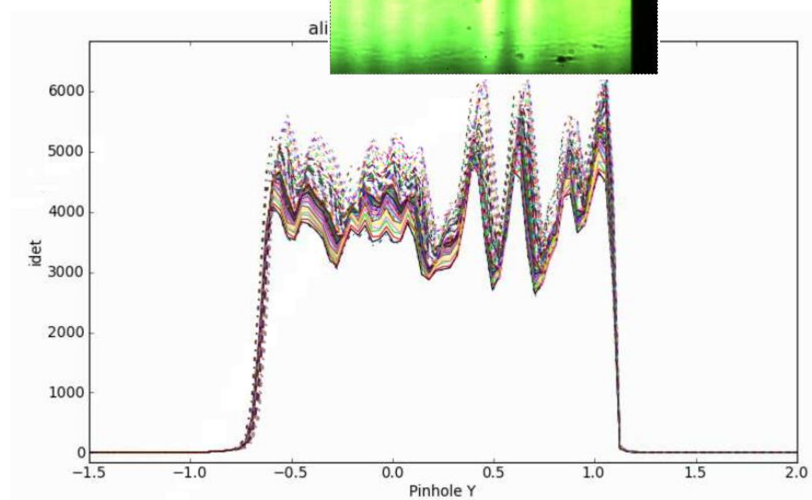
Measurements of Mirror Slope Errors



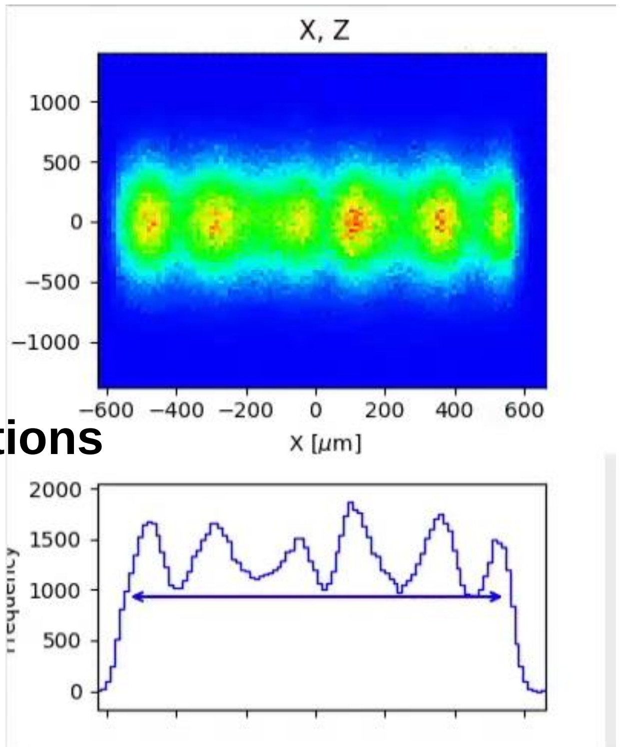
© A.Vivo - F.Perrin

Beam Profile at the Beamline

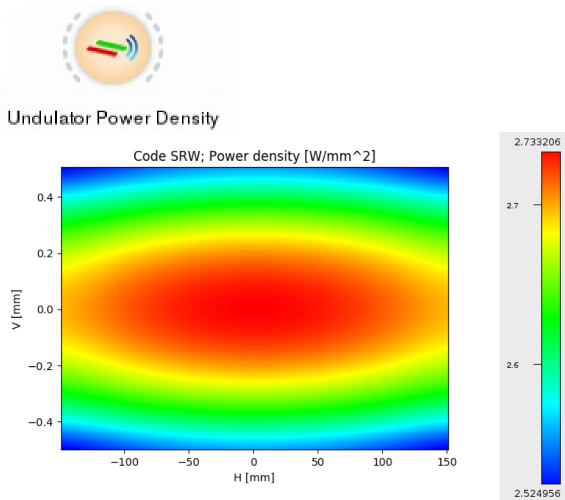


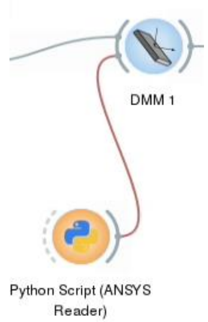


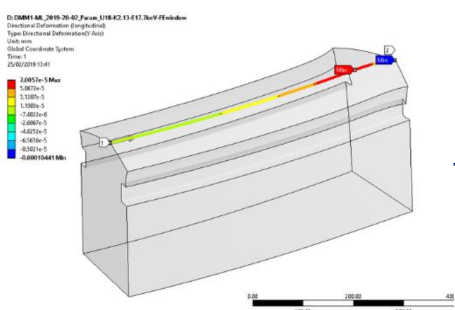
Simulations



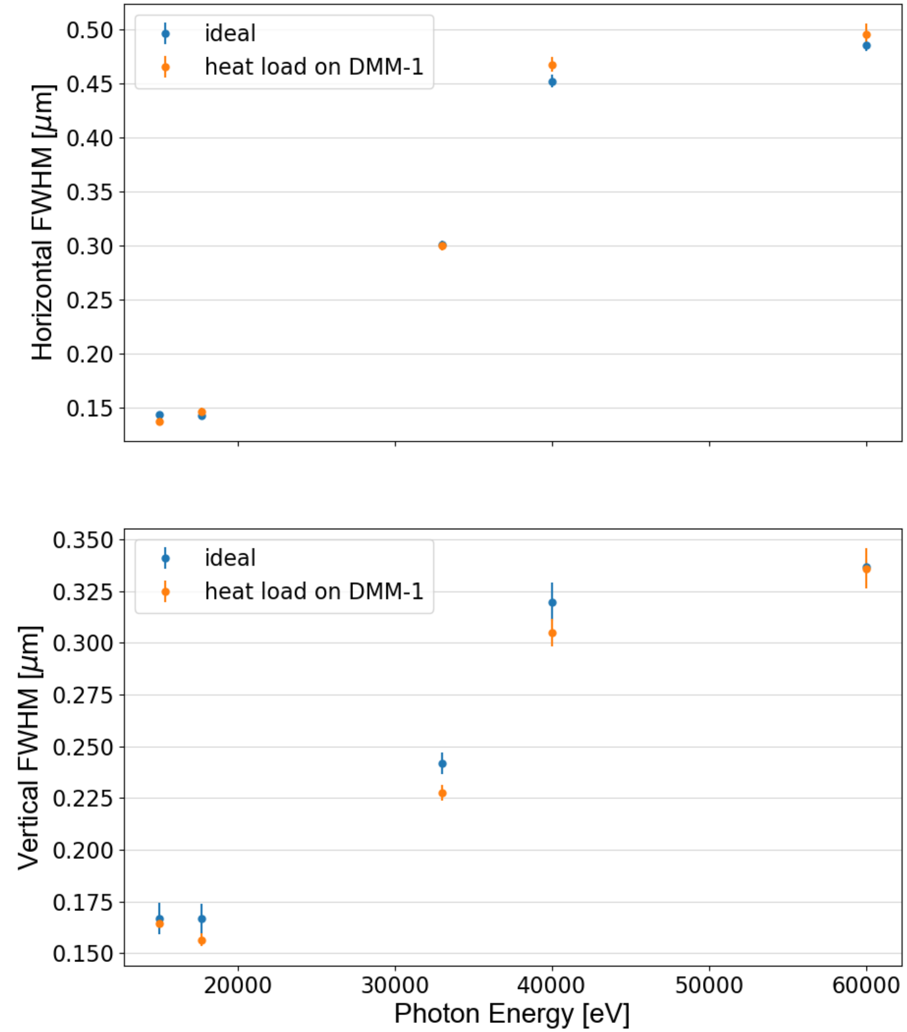
OASYS: HEAT LOAD EFFECT ON MIRROR



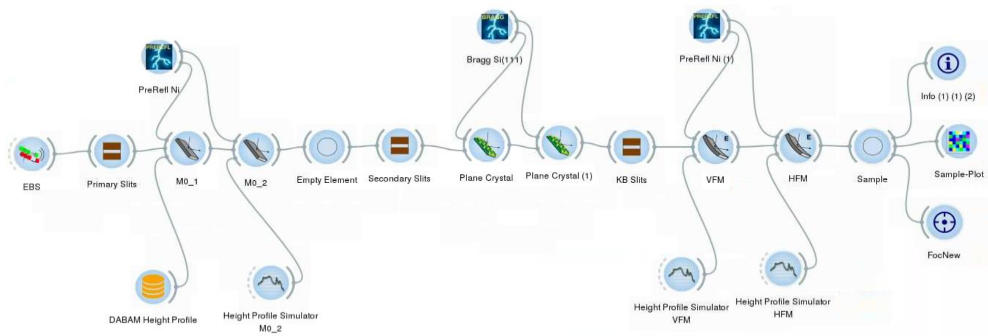




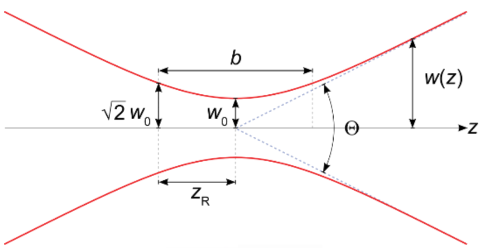
Finite Element Analysis
© Philipp Brumund



OASYS: DOF

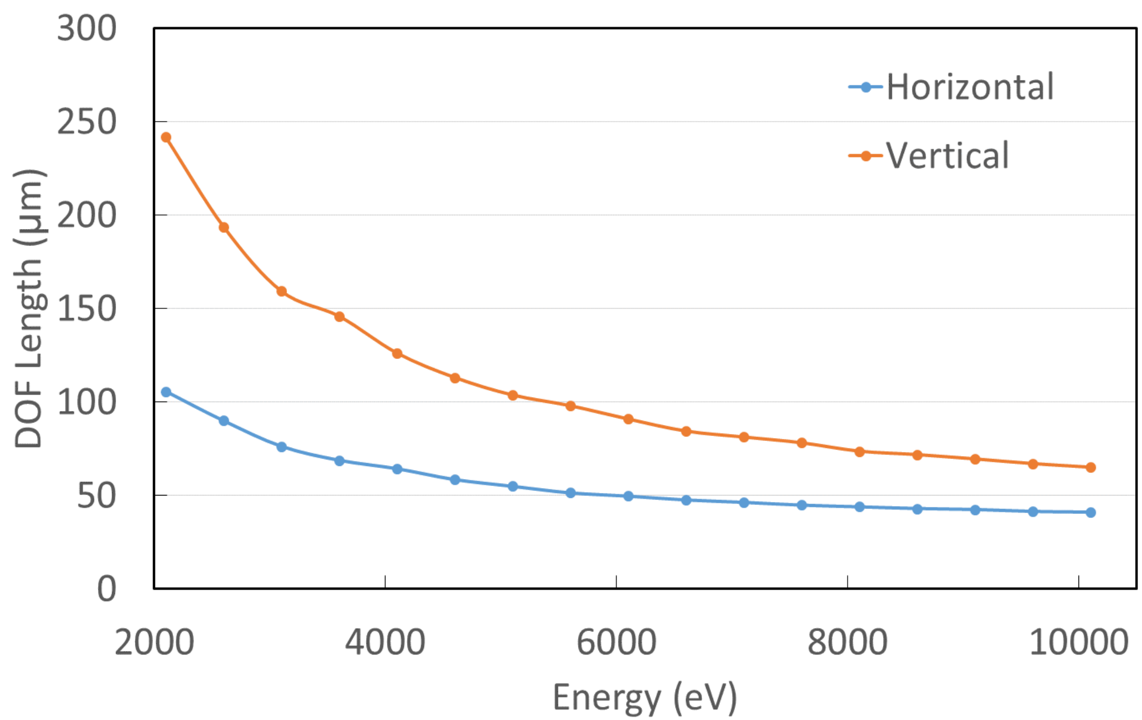


PreRefl Ni
Bragg Si(111)
PreRefl Ni (1)
Info (1) (1) (2)
EBS
Primary Slits
M0_1
M0_2
Empty Element
Secondary Slits
Plane Crystal
Plane Crystal (1)
KB Slits
VFM
HFM
Sample
Sample-Plot
FocNew
DABAM Height Profile
Height Profile Simulator M0_2
Height Profile Simulator VFM
Height Profile Simulator HFM



b
w(z)
√2 w0
w0
Θ
z
zR

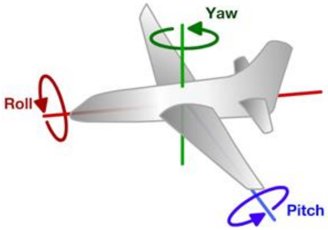
FocNew

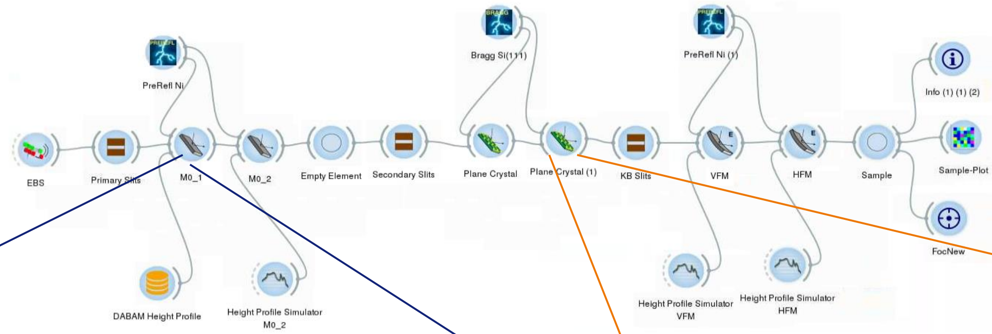


Horizontal
Vertical
DOF Length (μm)
Energy (eV)
0
50
100
150
200
250
300
2000
4000
6000
8000
10000

FINAL REMARKS

- OASYS is graphical interface software that provides an useful collection of tools to simulate the synchrotron radiation and its propagation through optical elements.
- Heat load calculations can be performed fast and in a fairly straightforward way (visual programing).
- This computational code allows to have, in the same place, many tools to improve the design and the optimization of beamlines.


Yaw
Roll
Pitch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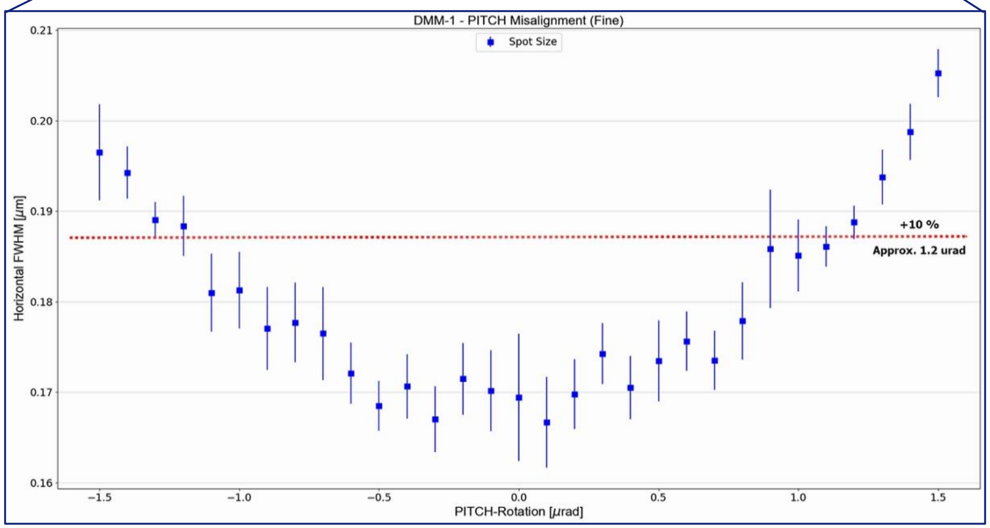
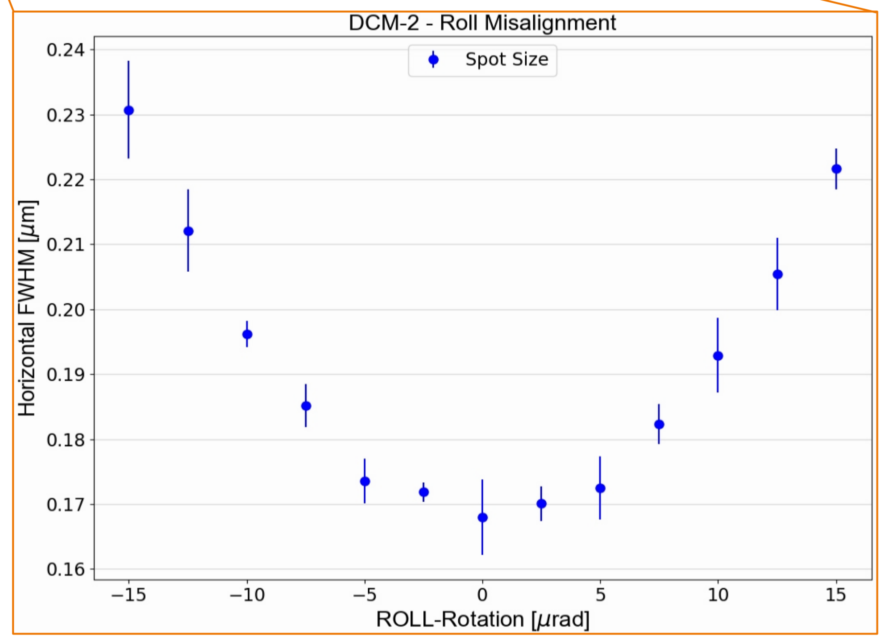
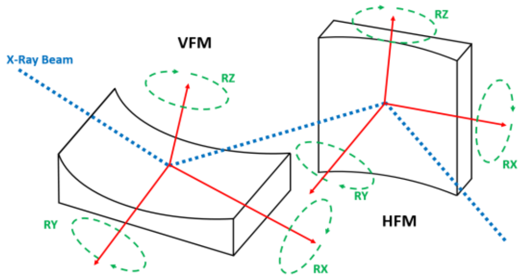
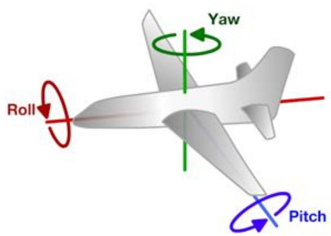

DMM-1 - PITCH Misalignment (Fine)
Spot Size
+10 %
Approx. 1.2 urad
Horizontal FWHM [μm]
PITCH-Rotation [μrad]

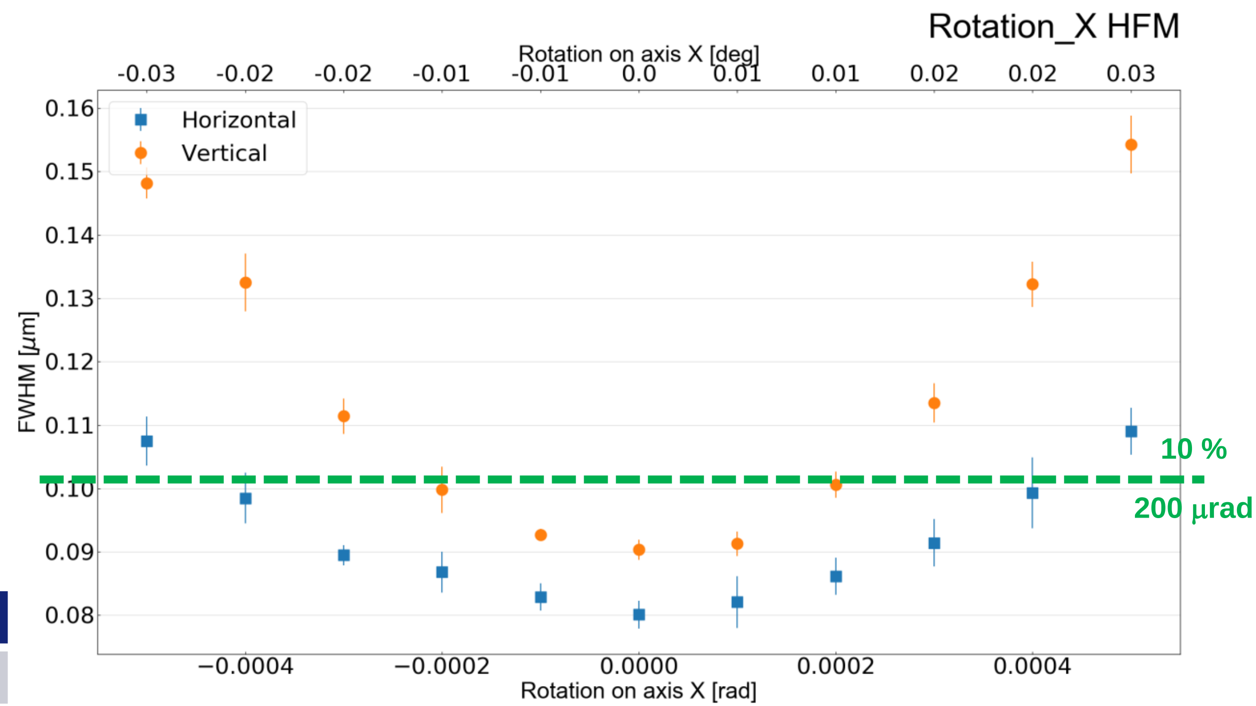

DCM-2 - Roll Misalignment
Spot Size
Horizontal FWHM [μm]
ROLL-Rotation [μrad]

OASYS: MISALIGNMENTS





Rotation	VFM	HFM
YAW	RZ	RY
ROLL	RX	RX



Undulator strength parameter **K**

$$K = \delta\gamma = \frac{e\lambda_o B_o}{2\pi mc} = 0.934\ B_o\,\lambda_o$$

where $\gamma = E/mc^2 = 1957\ E$

E is the electron energy in GeV

δ is the maximum deflection angle of the electron path

B is the magnetic field amplitude in Tesla

λ_o is the length of one undulator period in centimeter

e is the electronic charge

m is the rest mass of the electron

c is the speed of light in vacuum