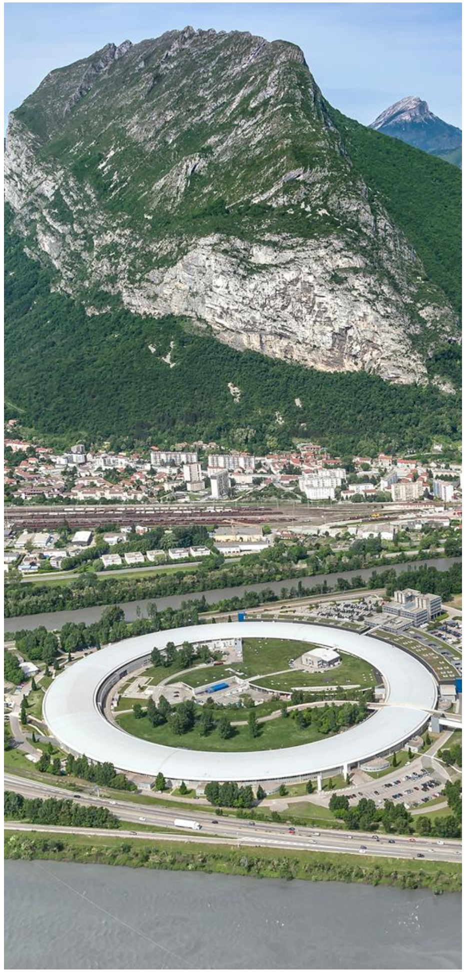

SRI2024
15th International Conference on
Synchrotron Radiation Instrumentation
26-30 August 2024 • Hamburg, Germany

SHADOW4: the popular ray tracing revived for evolving synchrotron sources in 4th-generation storage rings

Manuel Sánchez del Río*,
Juan Reyes-Herrera, Xianbo Shi and Luca Rebufi

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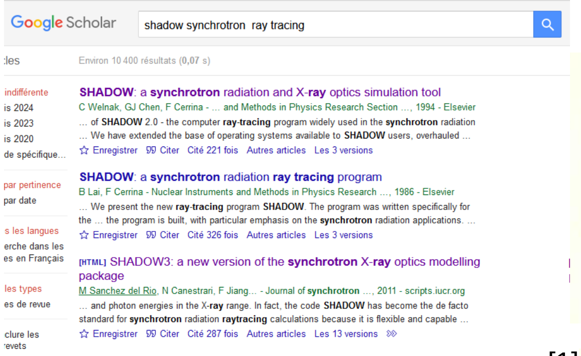
Advanced Analysis & Precision Unit, MEG/ISDD, ESRF

Mikrosymposium MS 1/1: Beamline Optics and Diagnostics: 13:00 Tuesday 27 August, 2024

40 YEARS OF SHADOW

SHADOW

- Generic ray tracing package for optics
- Specialized in SR (storage ring sources, grazing optics…)
- Helped to most 2-4th generation SR facilities
- Open source



Google Scholar

shadow synchrotron ray tracing

:les

Environ 10 400 résultats (0,07 s)

indifférente
is 2024
is 2023
is 2020
de spécifique...

par pertinence
par date

s les langues
erche dans les
es en Français

les types
es de revue

clure les
evets

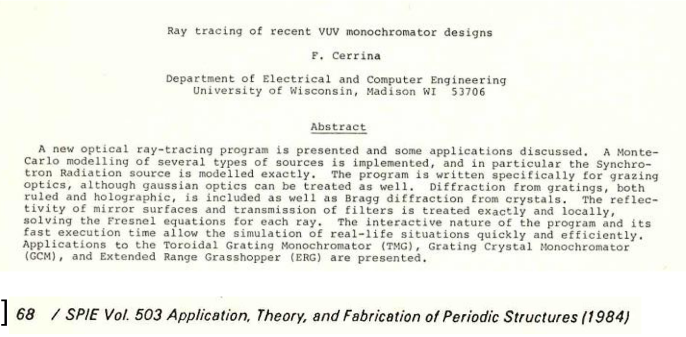
SHADOW: a **synchrotron** radiation and X-**ray** optics simulation tool
C Welnak, GJ Chen, F Cerrina - … and Methods in Physics Research Section …, 1994 - Elsevier
… of **SHADOW** 2.0 - the computer **ray-tracing** program widely used in the **synchrotron** radiation … We have extended the base of operating systems available to **SHADOW** users, overhauled …
☆ Enregistrer 99 Citer Cité 221 fois Autres articles Les 3 versions

SHADOW: a **synchrotron** radiation **ray tracing** program
B Lai, F Cerrina - Nuclear Instruments and Methods in Physics Research …, 1986 - Elsevier
… We present the new **ray-tracing** program **SHADOW**. The program was written specifically for the … the program is built, with particular emphasis on the **synchrotron** radiation applications. …
☆ Enregistrer 99 Citer Cité 326 fois Autres articles Les 3 versions

[HTML] SHADOW3: a new version of the **synchrotron** X-**ray** optics modelling package
M Sanchez del Rio, N Canestrari, F Jiang… - Journal of **synchrotron** …, 2011 - scripts.iucr.org
… and photon energies in the X-**ray** range. In fact, the code **SHADOW** has become the de facto standard for **synchrotron** radiation **raytracing** calculations because it is flexible and capable …
☆ Enregistrer 99 Citer Cité 287 fois Autres articles Les 13 versions »

SHADOW 1[1] & 2

Franco Cerrina (✝2010)



Ray tracing of recent VUV monochromator designs

F. Cerrina

Department of Electrical and Computer Engineering
University of Wisconsin, Madison WI 53706

Abstract

A new optical ray-tracing program is presented and some applications discussed. A Monte-Carlo modelling of several types of sources is implemented, and in particular the Synchrotron Radiation source is modelled exactly. The program is written specifically for grazing optics, although gaussian optics can be treated as well. Diffraction from gratings, both ruled and holographic, is included as well as Bragg diffraction from crystals. The reflectivity of mirror surfaces and transmission of filters is treated exactly and locally, solving the Fresnel equations for each ray. The interactive nature of the program and its fast execution time allow the simulation of real-life situations quickly and efficiently. Applications to the Toroidal Grating Monochromator (TMG), Grating Crystal Monochromator (GCM), and Extended Range Grasshopper (ERG) are presented.

[1] 68 / SPIE Vol. 503 Application, Theory, and Fabrication of Periodic Structures (1984)

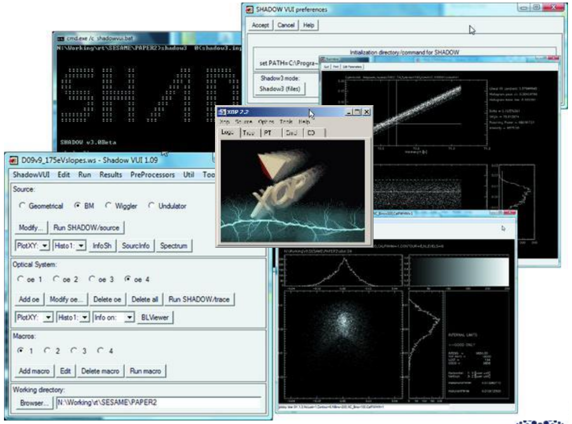
SHADOW3

M. Sanchez del Rio, et al.J. Synchr. Rad. ***18****, (2011)*
http://dx.doi.org/10.1107/S0909049511026306

Kernel (Fortran9x)

Python API

XOP/ShadowVUI



cmd.exe /c shadowvui.bat

```
N:\Working\rt\SESAME\PAPER2>shadow3  0<shadow3.inp
SHADOW v3.0Beta
```

SHADOW VUI preferences

Initialization directory/command for SHADOW: set PATH=C:\Progra~

Shadow3 mode: Shadow3 (files)

D09v9_175eVslopes.ws - Shadow VUI 1.09

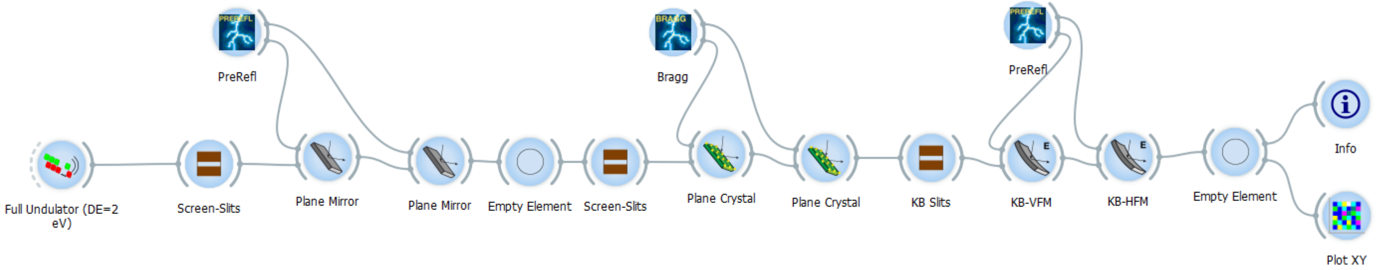
Source: ○ Geometrical ● BM ○ Wiggler ○ Undulator

Optical System: ○ oe 1 ○ oe 2 ○ oe 3 ● oe 4

Macros: ● 1 ○ 2 ○ 3 ○ 4

Working directory: N:\Working\rt\SESAME\PAPER2

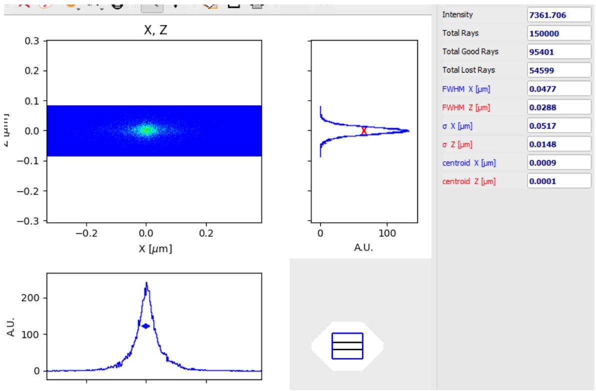
In 2014: ShadowOUI[1]= SHADOW3 + ORANGE[2]



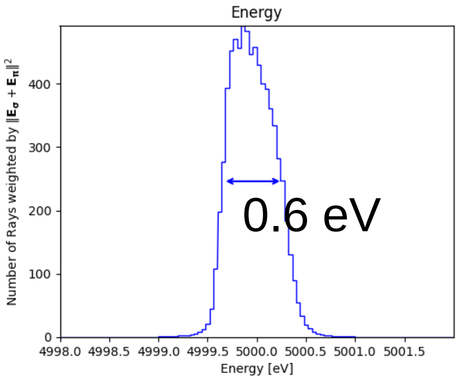
SIZE

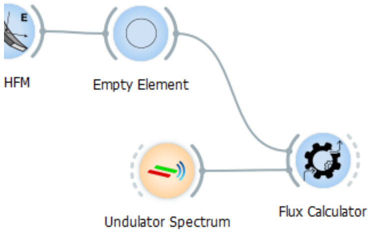
RESOLUTION

FLUX



Intensity	7361.706
Total Rays	150000
Total Good Rays	95401
Total Lost Rays	54599
FWHM X [μm]	0.0477
FWHM Z [μm]	0.0288
σ X [μm]	0.0517
σ Z [μm]	0.0148
centroid X [μm]	0.0009
centroid Z [μm]	0.0001





---> Integrated Flux : 1.25321e+13 ph/s

[1] L Rebuffi and M Sanchez del Rio J Synchr. Rad. **23** 1357-1367 (2016) https://doi.org/10.1107/S1600577516013837
[2] https://orangedatamining.com/

ShadowOUI: not only SHADOW3

- Corrections for coherent optics (HYBRID[1])

Hybrid Screen

- Surface error databases DABAM, DABAM2D (see poster 1.181)

DABAM Prepare Profile

DABAM Height Profile

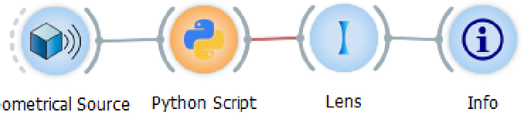
- Preprocessors (surfaces, VLS, diaboloids[2], reflectivity)

Height Profile

VLS PGM Coefficients

Diaboloid

- Python Scripting / Capturing beam



- Compound Elements: CRL, TF

Compound Refractive

Transfocator

- New elements: Benders, etc.

Bendable Ellipsoid

Double-Rod Bendable Ellipsoid Mirror

- Loops

Loop Point

Scanning Variable Loop Point

Scanning File Loop Point

- Heat load loops[3]

Power Density Loop

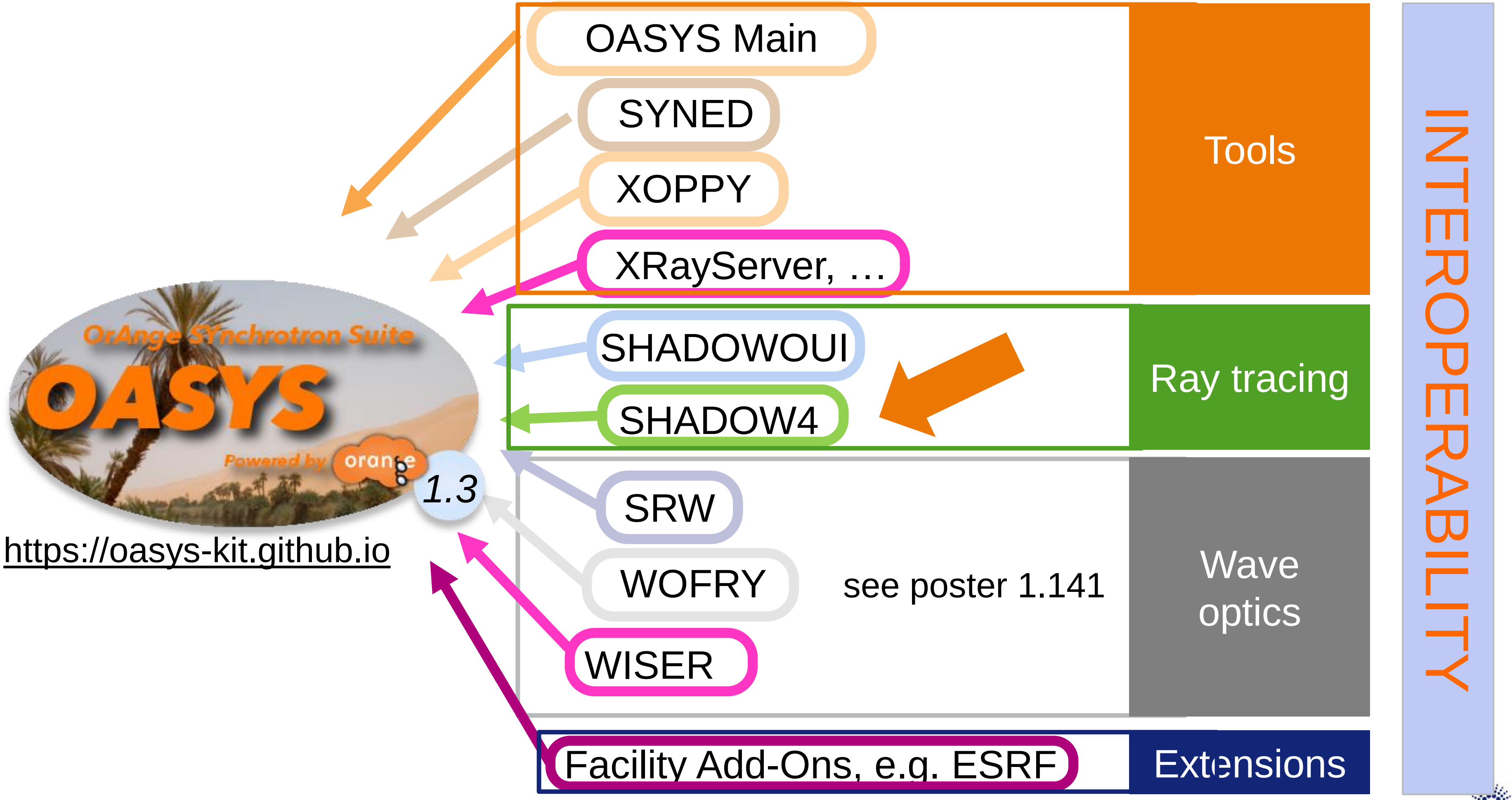
Power Plot XY - Undulator

- High d-spacing crystals[4]

Bragg

[1] Shi et al. 2014 https://doi.org/10.1107/S160057751400650X
[2] Sanchez del Rio et al. 2021 https://doi.org/10.1107/S160057752100401X
[3] Rebuffi et al. 2020 https://doi.org/10.1107/S160057752000778X
[4] Yu et al. 2022 https://doi.org/10.1107/S160057752200707X

OASYS add-ons



https://oasys-kit.github.io

OASYS Main

SYNED

XOPPY

XRayServer, …

Tools

SHADOWOUI

SHADOW4

Ray tracing

SRW

WOFRY

see poster 1.141

WISER

Wave optics

Facility Add-Ons, e.g. ESRF

Extensions

INTEROPERABILITY

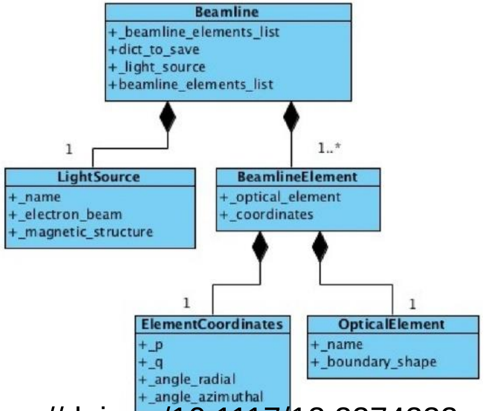
SHADOW4

SHADOW3 problems:

- Fortran compilation / python API / python packaging
- Maintenance and development of poorly structure fortran code
- Obsolete technology, using spaghetti code and old libraries
- File-oriented structure with extensive use of preprocessors

SHADOW4 is a new Kernel,

- Fully developed in Python
- OO programming
- OASYS experience and ad-hoc developments
- Extended the SYNED[1] concept
- Fast enough
- https://github.com/oasys-kit/shadow4



Beamline
+_beamline_elements_list
+dict_to_save
+_light_source
+beamline_elements_list

1

1..*

LightSource
+_name
+_electron_beam
+_magnetic_structure

BeamlineElement
+_optical_element
+_coordinates

1

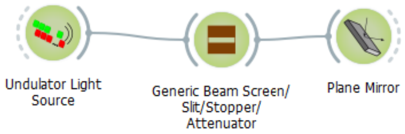
1

ElementCoordinates
+_p
+_q
+_angle_radial
+_angle_azimuthal

OpticalElement
+_name
+_boundary_shape

and a new interface,

- SHADOW is an interactive tool adapted for common laptops
- Just called SHADOW4
- Simplified interface (less widgets, generic mirros, crystals, etc.)
- Optimized (better communication)
- Automatic scripting
- Easier calculations of flux and power



for new generations of sources

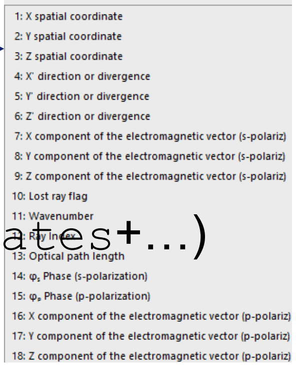
Preparing 5th generation

- Facilitate interoperability with other tools (e.g. for partial coherence)
- Focus on Visualization and User Interfaces
- Create synthetic data and AI integration
- Run simulations in Digital Twins
- Adapt to new generation of users and developers
- Easy transition from laptop-based prototyping to High-Performance Computing (HPC) and Cloud Computing
- Open Source and Collaborative Development
- Contribute to create educational tools by interactive leaning

[1] https://doi.org/10.1117/12.2274232

Shadow4 Kernel: User interface

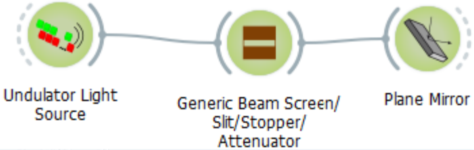
- S4Beam: traditional beam data `(nrays, 18)`

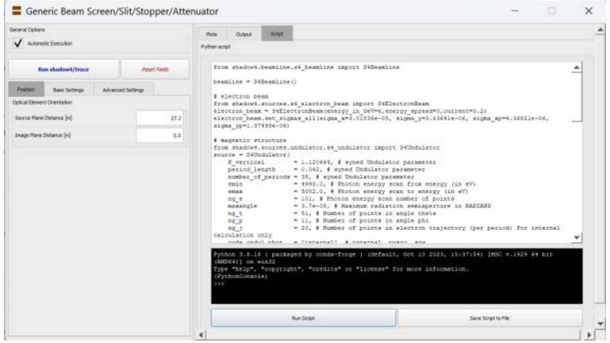


1: X spatial coordinate
2: Y spatial coordinate
3: Z spatial coordinate
4: X' direction or divergence
5: Y' direction or divergence
6: Z' direction or divergence
7: X component of the electromagnetic vector (s-polariz)
8: Y component of the electromagnetic vector (s-polariz)
9: Z component of the electromagnetic vector (s-polariz)
10: Lost ray flag
11: Wavenumber
12: Ray Index
13: Optical path length
14: φ_s Phase (s-polarization)
15: φ_p Phase (p-polarization)
16: X component of the electromagnetic vector (p-polariz)
17: Y component of the electromagnetic vector (p-polariz)
18: Z component of the electromagnetic vector (p-polariz)

- User interface:
  - `S4LightSource` (`S4ElectronBeam`+`S4MagneticStructure`)
  - `S4BeamlineElement`(`S4OpticalElement`+`ElementCoordinates`+...)
  - ...
  - `S4Beamline` = `S4LightSource`+`S4BeamlineElement`

- Automated scripts with OASYS





☑ Automatic Execution

Optical Element Orientation

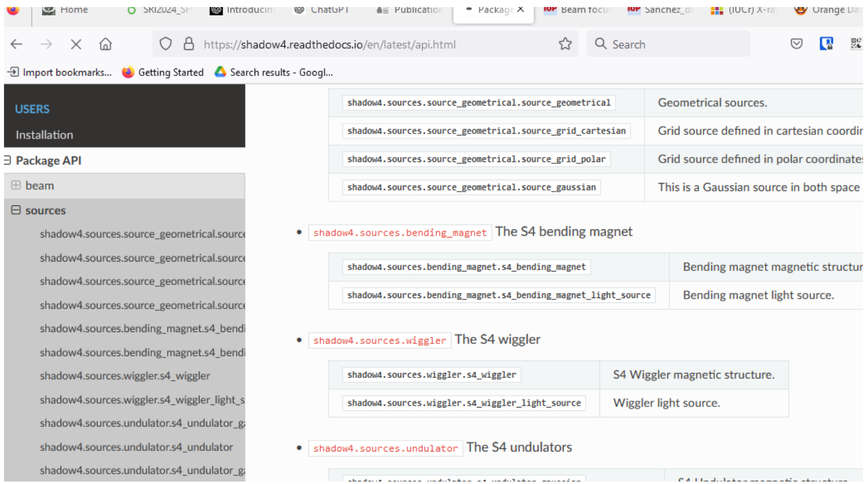
Source Plane Distance [m] 27.2

Image Plane Distance [m] 0.0

```
from shadow4.beamline.s4_beamline import S4Beamline

beamline = S4Beamline()

# electron beam
from shadow4.sources.s4_electron_beam import S4ElectronBeam
electron_beam = S4ElectronBeam(energy_in_GeV=6,energy_spread=0,current=0.2)
electron_beam.set_sigmas_all(sigma_x=3.01836e-05, sigma_y=3.63641e-06, sigma_xp=4.36821e-06,
sigma_yp=1.37498e-06)

# magnetic structure
from shadow4.sources.undulator.s4_undulator import S4Undulator
source = S4Undulator(
    K_vertical        = 1.120664, # syned Undulator parameter
    period_length     = 0.042, # syned Undulator parameter
    number_of_periods = 38, # syned Undulator parameter
    emin              = 4998.0, # Photon energy scan from energy (in eV)
    emax              = 5002.0, # Photon energy scan to energy (in eV)
    ng_e              = 101, # Photon energy scan number of points
    maxangle          = 3.7e-05, # Maximum radiation semiaperture in RADIANS
    ng_t              = 51, # Number of points in angle theta
    ng_p              = 11, # Number of points in angle phi
    ng_j              = 20, # Number of points in electron trajectory (per period) for internal
calculation only
    code_undul_phot   = 'internal', # internal, pysru, srw
```

```
Python 3.8.18 | packaged by conda-forge | (default, Oct 10 2023, 15:37:54) [MSC v.1929 64 bit
(AMD64)] on win32
Type "help", "copyright", "credits" or "license" for more information.
(PythonConsole)
>>>
```

- Documentation: https://shadow4.readthedocs.io



https://shadow4.readthedocs.io/en/latest/api.html

USERS

Installation

Package API

- beam
- sources
  - shadow4.sources.source_geometrical.source
  - shadow4.sources.source_geometrical.source
  - shadow4.sources.source_geometrical.source
  - shadow4.sources.source_geometrical.source
  - shadow4.sources.bending_magnet.s4_bendi
  - shadow4.sources.bending_magnet.s4_bendi
  - shadow4.sources.wiggler.s4_wiggler
  - shadow4.sources.wiggler.s4_wiggler_light_s
  - shadow4.sources.undulator.s4_undulator_ga
  - shadow4.sources.undulator.s4_undulator
  - shadow4.sources.undulator.s4_undulator_ga

`shadow4.sources.source_geometrical.source_geometrical`	Geometrical sources.
`shadow4.sources.source_geometrical.source_grid_cartesian`	Grid source defined in cartesian coordir
`shadow4.sources.source_geometrical.source_grid_polar`	Grid source defined in polar coordinate:
`shadow4.sources.source_geometrical.source_gaussian`	This is a Gaussian source in both space

- `shadow4.sources.bending_magnet` The S4 bending magnet

`shadow4.sources.bending_magnet.s4_bending_magnet`	Bending magnet magnetic structur
`shadow4.sources.bending_magnet.s4_bending_magnet_light_source`	Bending magnet light source.

- `shadow4.sources.wiggler` The S4 wiggler

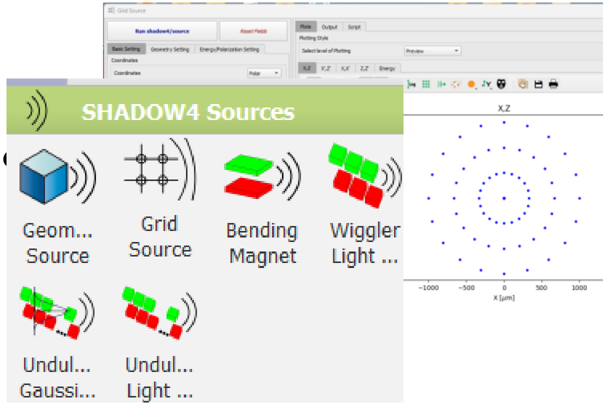
`shadow4.sources.wiggler.s4_wiggler`	S4 Wiggler magnetic structure.
`shadow4.sources.wiggler.s4_wiggler_light_source`	Wiggler light source.

- `shadow4.sources.undulator` The S4 undulators

`shadow4.sources.undulator.s4_undulator_gaussian`	S4 Undulator magnetic structure

Shadow4 Kernel: beamline components

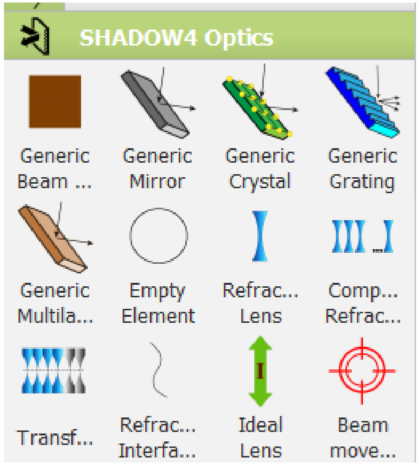
- Sources
  - SourceGeometrical, SourceGridCartesian, **SourceGri**
  - S4BendingMagnet (**upgraded** methods[1])
  - S4Wiggler (included short IDs)
  - S4GaussianUndulator, S4Undulator (**upgraded**: see talk S1/2 of Juan Reyes-Herrera 18:15)



Coordinates: Polar

Select level of Plotting: Preview

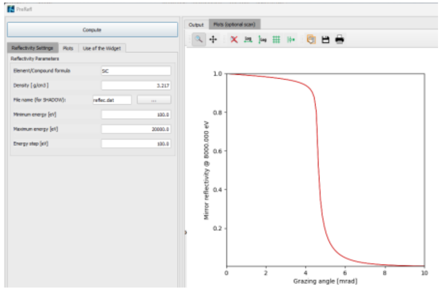
- Beamline elements
  - S4Screen (screens, slits, stops, absorbers)
  - S4IdealLens, S4Empty,… (ideal elements)
  - S4PlaneMirror, S4SphereMirror, S4EllipsoidalMirror, …, **S4AdditionalNumeracalMeshMirror**
  - S4PlaneGrating, S4ToroidGrating, … (including VLS)
  - S4PlaneCrystal, S4ToroidCrystal, … (undistorted perfect crystals in reflection)
  - **S4PlaneMultilayer**, S4SphereMultilayer, … (also graded, in depth or laterally)
  - S4Interface, S4Lens, S4CRL, S4Transfocator (refractors)



[1] https://arxiv.org/abs/2406.16446

Shadow4 Kernel: models and algorithms

- Geometrical model
  - `S4OpticalSurface` (`S4Conic`[1], `S4Toroid`, `S4Mesh`)
  - Include methods for reflection, refraction, scattering (grating)
- Physical models [may avoid preprocessor files]
  - `PreRefl`: Absorption/refraction for attenuators, mirrors, lenses
  - crystalpy[2]: external library for Crystals
  - `MLayer`
  - Optical constants (scattering factors, refraction indices, crystal structures)
    - xraylib[3]
    - DABAX[4]
    - preprocesor data file (can be created with other tools)



Reflectivity Parameters

Element/Compound formula: SiC

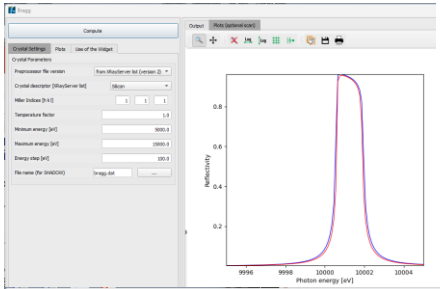
Density [g/cm3]: 3.217

File name (for SHADOW): reflec.dat

Minimum energy [eV]: 100.0

Maximum energy [eV]: 20000.0

Energy step [eV]: 100.0



Crystal Parameters

Preprocessor file version: from XRayServer list (version 2)

Crystal descriptor [XRayServer list]: Silicon

Miller Indices [h k l]: 1 1 1

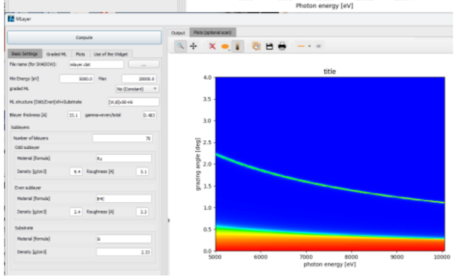
Temperature factor: 1.0

Minimum energy [eV]: 5000.0

Maximum energy [eV]: 15000.0

Energy step [eV]: 100.0

File name (for SHADOW): bragg.dat



File name (for SHADOW): mlayer.dat

Min Energy [eV]: 5000.0 Max: 20000.0

graded ML: No (Constant)

ML structure [Odd,Even]xN+Substrate: [W,B]x50+Si

Bilayer thickness [A]: 33.1 gamma=even/total: 0.483

Sublayers

Number of bilayers: 70

Odd sublayer

Material [formula]: Ru

Density [g/cm3]: 9.4 Roughness [A]: 3.1

Even sublayer

Material [formula]: B4C

Density [g/cm3]: 2.4 Roughness [A]: 3.3

Substrate

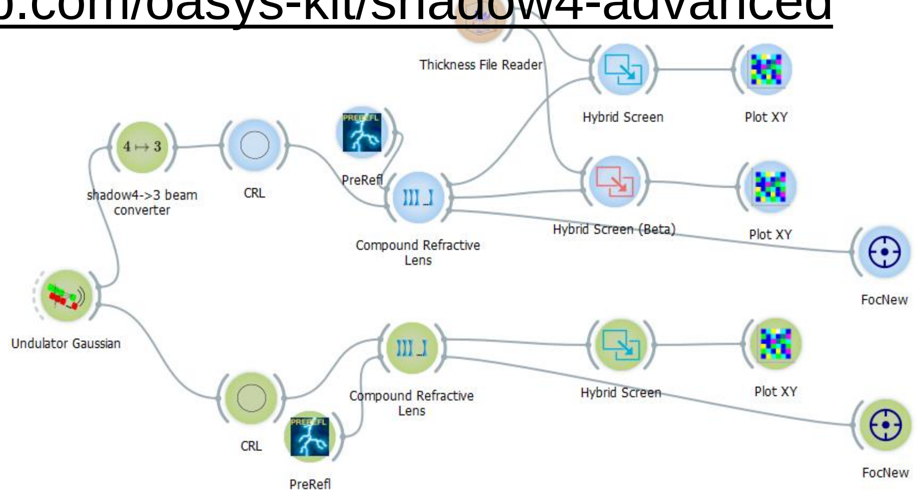
Material [formula]: Si

Density [g/cm3]: 2.33

[1] https://arxiv.org/abs/2406.04079
[2] https://arxiv.org/abs/2406.16960
[3] https://github.com/tschoonj/xraylib
[4] https://github.com/oasys-kit/dabax

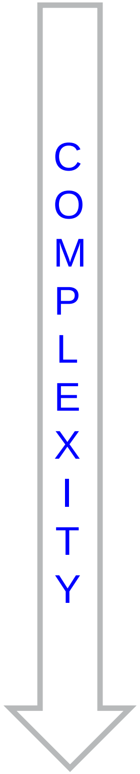
Shadow4: advanced tools – Hybrid[1] method

- corrects ray tracing considering scattering and diffraction when the beam has a high coherence
- Includes scattering by slits, o.e. dimensions (mirrors, gratings, lenses)
- Manages the surface error (delegated from o.e.)
- Fully rewritten methods
- Scriptable
- https://github.com/oasys-kit/shadow4-advanced



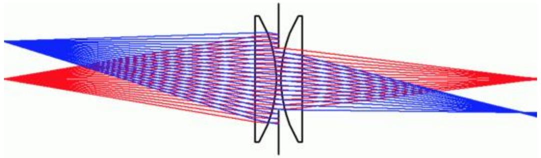
[1] Shi *et al.* 2014 https://doi.org/10.1107/S160057751400650X

HIERARCHICAL[1] BEAMLINE SIMULATIONS WITH OASYS


COMPLEXITY

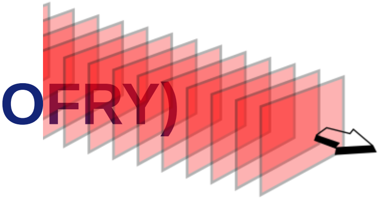
Analytical model (by hand)

Ray tracing (Shadow4)



Hybrid model (Shadow4)

wave optics & partial coherence 1D (WOFRY)



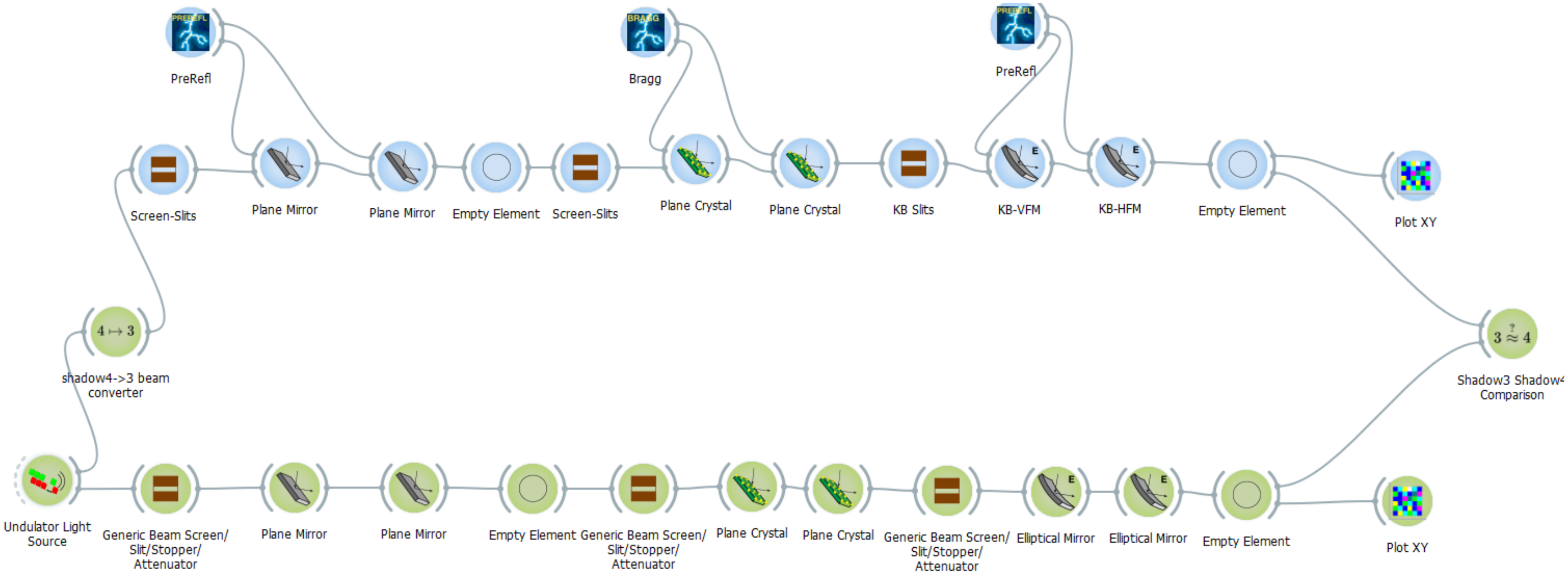
wave optics partial coherence 2D:

Monte Carlo (multi e^-) (SRW)

Coherent Mode Decomposition (COMSYL)

[1] M. Sanchez del Rio *et al.* 2019 https://doi.org/10.1107/S160057751901213X

Shadow4: beta testers welcomed!



Send issues in github https://github.com/oasys-kit/shadow4/issues

Shadow4: summary

- SHADOW4 is announced
  - New Kernel fully in python, modern OO programming
  - New interface in Oasys, including Hybrid
  - Preparting the future SR generations

- Available in OASYS [beta]
  - HERCULES Tutorial updated [1]
  - Library of workspaces (tests against Shadow3) [2]
  - Programmer documentation [3]

- Left for next version: crystals: mosaic, transmission, deformed

- Great software infrastructure to support new ideas and developments

[1] https://github.com/oasys-esrf-kit/oasys_hercules_2024
[2] https://github.com/oasys-kit/shadow4workspaces
[3] https://shadow4.readthedocs.io/

Shadow4: benefits

Thank you

Download slides:

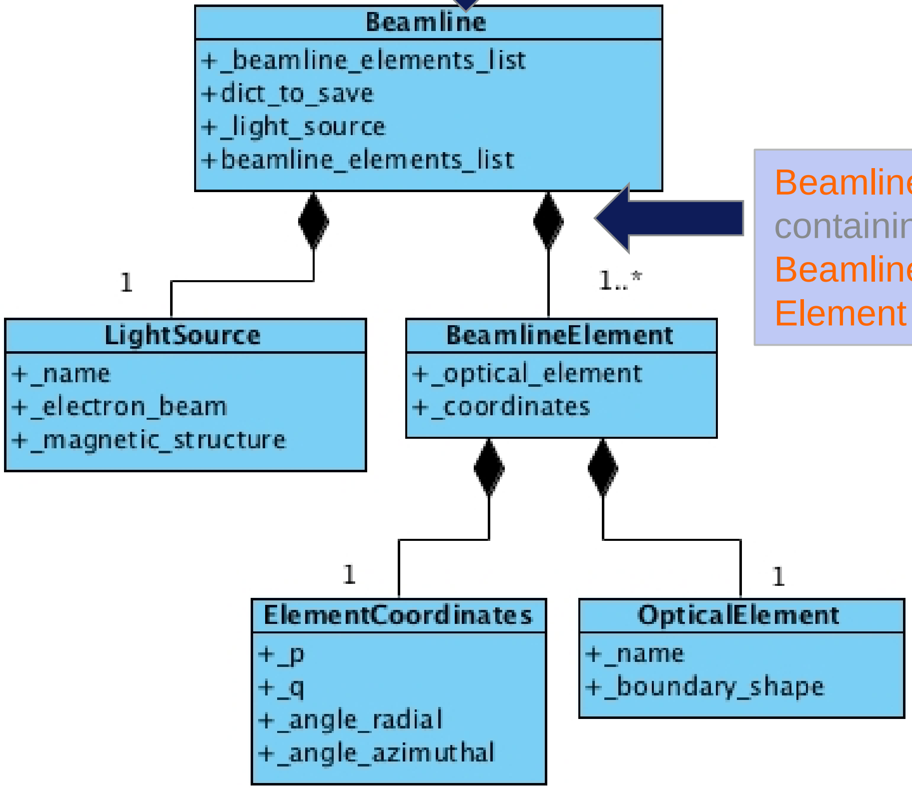
BACKUP SLIDES

Outline

SHADOW4

- History
  - S1-S3
  - Why S4
  - Photon flux
  - Examples
- What we need, what we want, what we do
  - Needed
  - Wanted
  - Done
- Final remarks

The Beamline is the main entity, the container of all the relevant information



Beamline
+_beamline_elements_list
+dict_to_save
+_light_source
+beamline_elements_list

1

LightSource
+_name
+_electron_beam
+_magnetic_structure

1..*

BeamlineElement
+_optical_element
+_coordinates

1

ElementCoordinates
+_p
+_q
+_angle_radial
+_angle_azimuthal

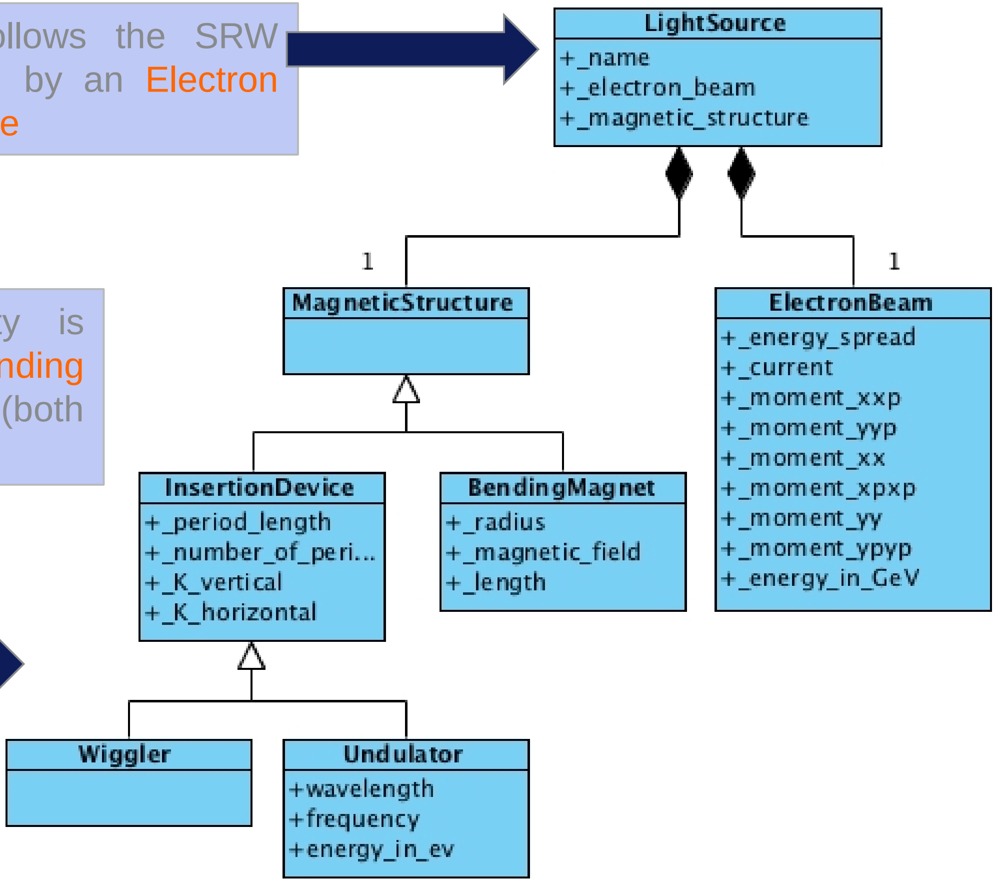
1

OpticalElement
+_name
+_boundary_shape

Beamline is modeled as an aggregate entity containing a Light Source and a collection of Beamline Element entities, defined by an Optical Element and its Element Coordinates

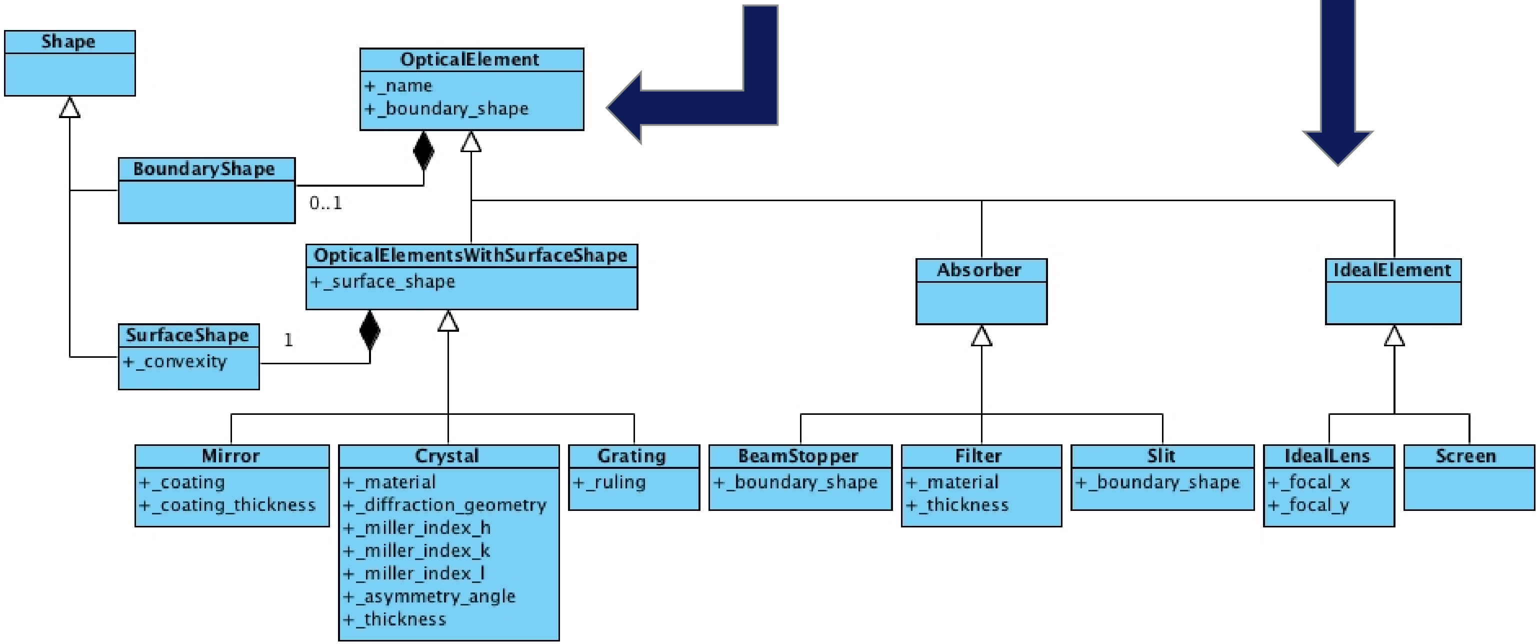
The Light Source definition follows the SRW objects layout, being composed by an Electron Beam and by a Magnetic Structure

The Magnetic Structure entity is specialized by subclasses: Bending Magnet, Undulator and Wiggler (both Insertion Devices)

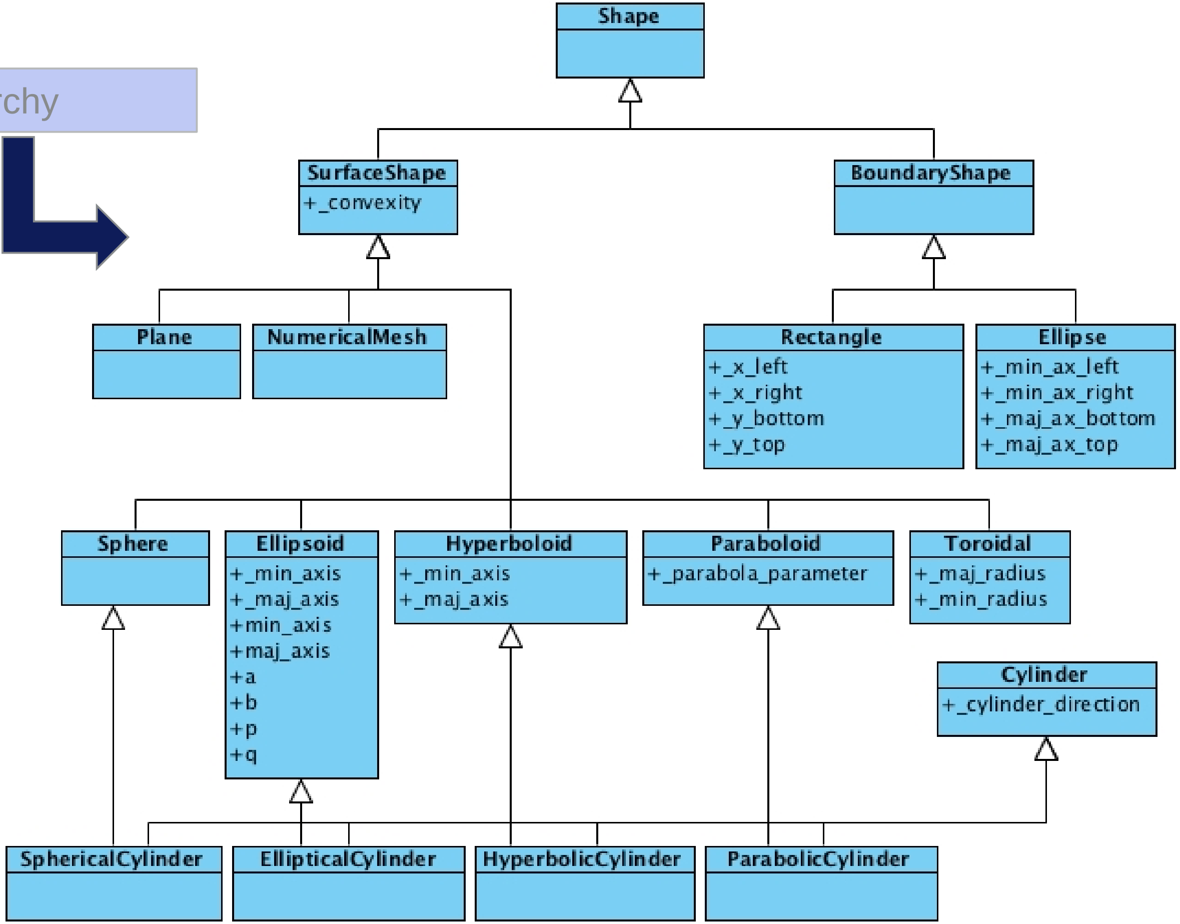


Optical elements are described according to their intrinsic nature

All Optical Elements contain the attribute Boundary Shape (the shape of their contour), while a specialized group of objects contains the attribute Surface Shape



Shape class hierarchy



Shape

SurfaceShape
+_convexity

BoundaryShape

Plane

NumericalMesh

Rectangle
+_x_left
+_x_right
+_y_bottom
+_y_top

Ellipse
+_min_ax_left
+_min_ax_right
+_maj_ax_bottom
+_maj_ax_top

Sphere

Ellipsoid
+_min_axis
+_maj_axis
+min_axis
+maj_axis
+a
+b
+p
+q

Hyperboloid
+_min_axis
+_maj_axis

Paraboloid
+_parabola_parameter

Toroidal
+_maj_radius
+_min_radius

Cylinder
+_cylinder_direction

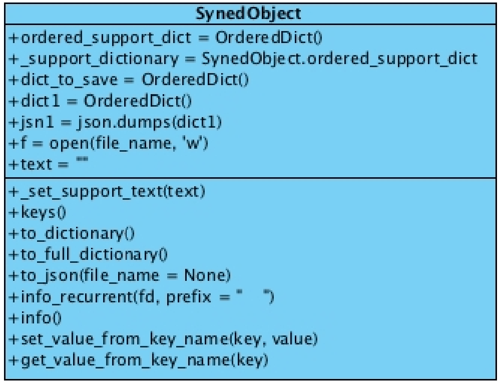
SphericalCylinder

EllipticalCylinder

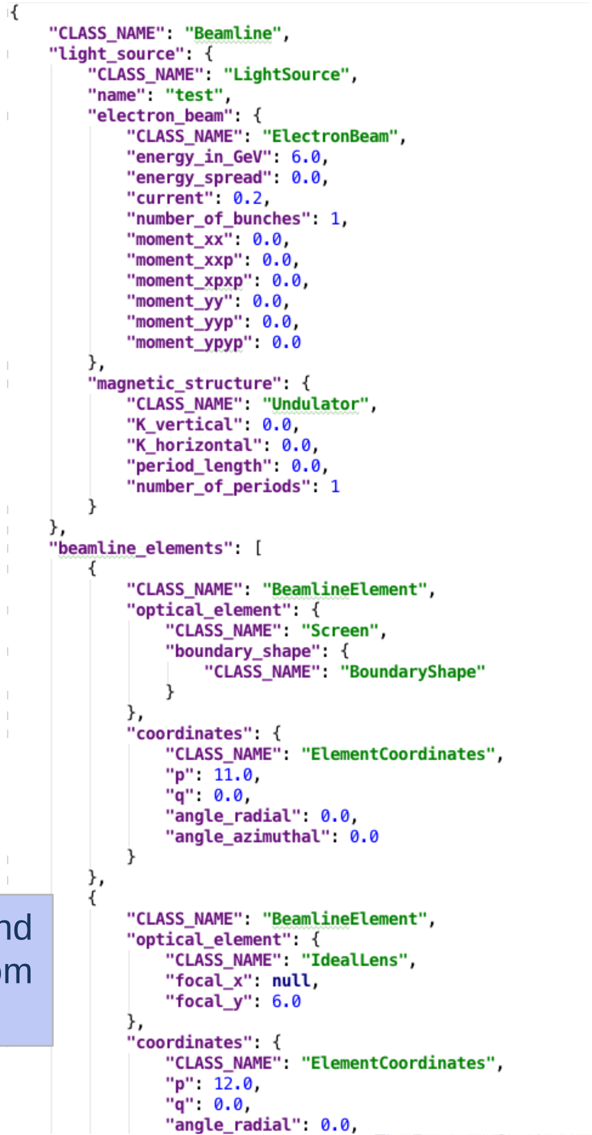
HyperbolicCylinder

ParabolicCylinder

All the main entities in SYNED derive their nature from a common abstract object called SynedObject


SynedObject
+ordered_support_dict = OrderedDict()
+_support_dictionary = SynedObject.ordered_support_dict
+dict_to_save = OrderedDict()
+dict1 = OrderedDict()
+jsn1 = json.dumps(dict1)
+f = open(file_name, 'w')
+text = ""
+_set_support_text(text)
+keys()
+to_dictionary()
+to_full_dictionary()
+to_json(file_name = None)
+info_recurrent(fd, prefix = "   ")
+info()
+set_value_from_key_name(key, value)
+get_value_from_key_name(key)

This kernel entity is the main common data type, and contains the features to import/export information to/from SYNED object and text files by using the **JSON** format



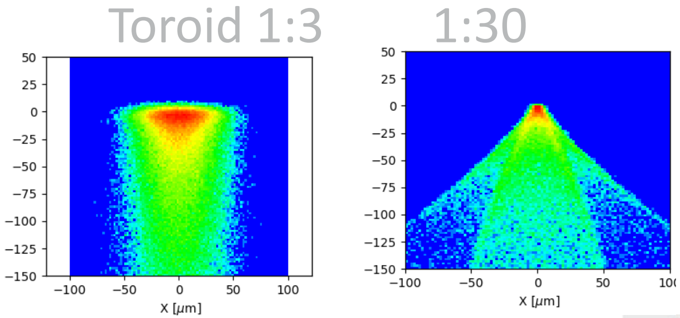
```
{
    "CLASS_NAME": "Beamline",
    "light_source": {
        "CLASS_NAME": "LightSource",
        "name": "test",
        "electron_beam": {
            "CLASS_NAME": "ElectronBeam",
            "energy_in_GeV": 6.0,
            "energy_spread": 0.0,
            "current": 0.2,
            "number_of_bunches": 1,
            "moment_xx": 0.0,
            "moment_xxp": 0.0,
            "moment_xpxp": 0.0,
            "moment_yy": 0.0,
            "moment_yyp": 0.0,
            "moment_ypyp": 0.0
        },
        "magnetic_structure": {
            "CLASS_NAME": "Undulator",
            "K_vertical": 0.0,
            "K_horizontal": 0.0,
            "period_length": 0.0,
            "number_of_periods": 1
        }
    },
    "beamline_elements": [
        {
            "CLASS_NAME": "BeamlineElement",
            "optical_element": {
                "CLASS_NAME": "Screen",
                "boundary_shape": {
                    "CLASS_NAME": "BoundaryShape"
                }
            },
            "coordinates": {
                "CLASS_NAME": "ElementCoordinates",
                "p": 11.0,
                "q": 0.0,
                "angle_radial": 0.0,
                "angle_azimuthal": 0.0
            }
        },
        {
            "CLASS_NAME": "BeamlineElement",
            "optical_element": {
                "CLASS_NAME": "IdealLens",
                "focal_x": null,
                "focal_y": 6.0
            },
            "coordinates": {
                "CLASS_NAME": "ElementCoordinates",
                "p": 12.0,
                "q": 0.0,
                "angle_radial": 0.0,
```

RAY TRACING CALCULATIONS WITH OASYS/SHADOWOUI

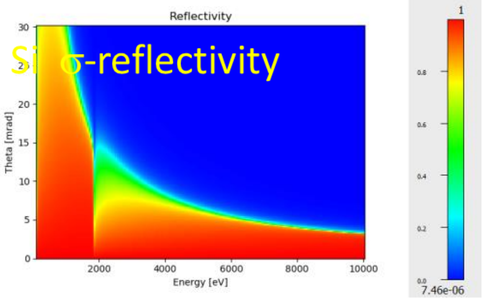
Evolved from SHADOW

Accurate values of

Beam sizes including cropping, and aberrations



Flux including o.e. physical models (reflectivity transmittivity)

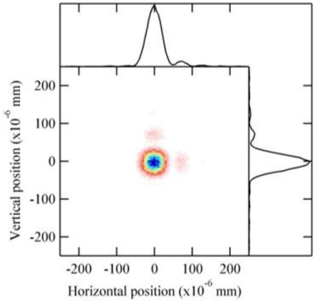


Monochromators/Analysers

Incoherent addition of rays (no interference/diffraction)

New features

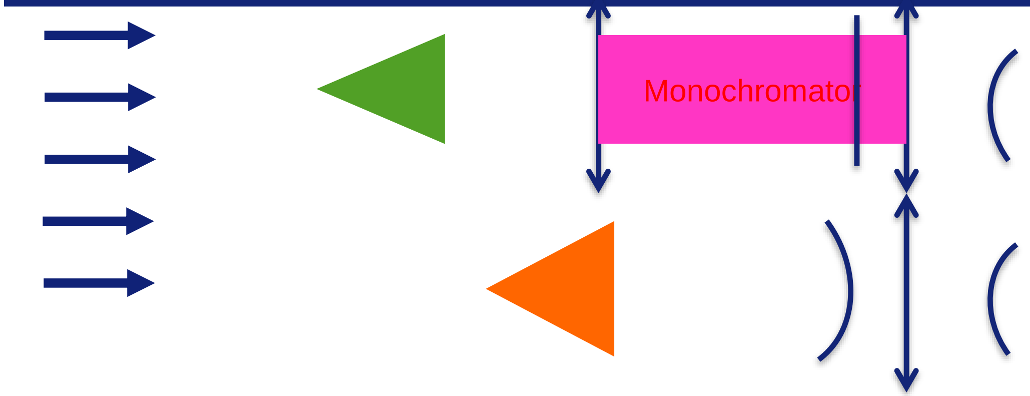
Interoperability

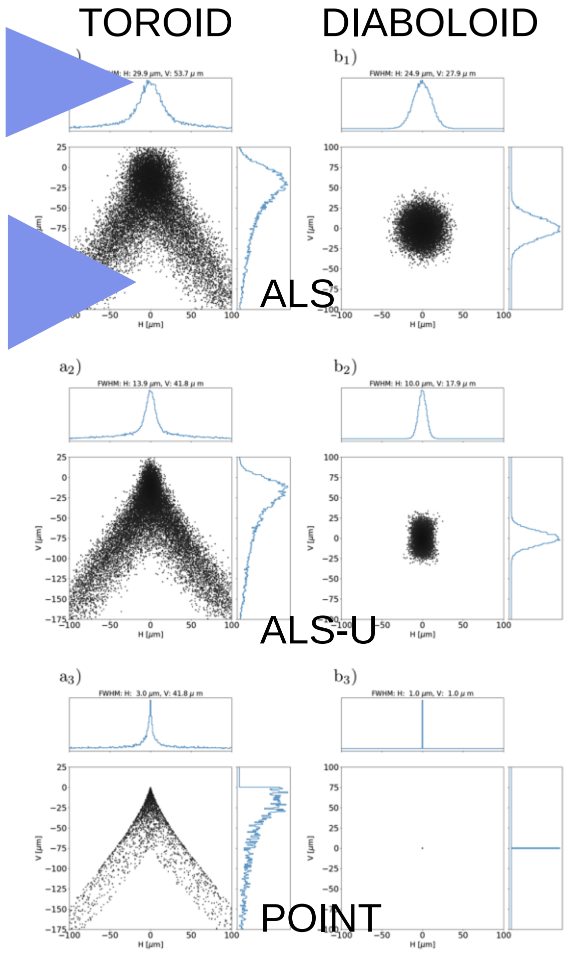


Optical element deformation database DABAM (Sanchez del Rio *et al.* http://dx.doi.org/10.1107/S1600577516005014)

Corrections for coherence with Hybrid (Shi *et al.* http://dx.doi.org/10.1107/S160057751400650X)

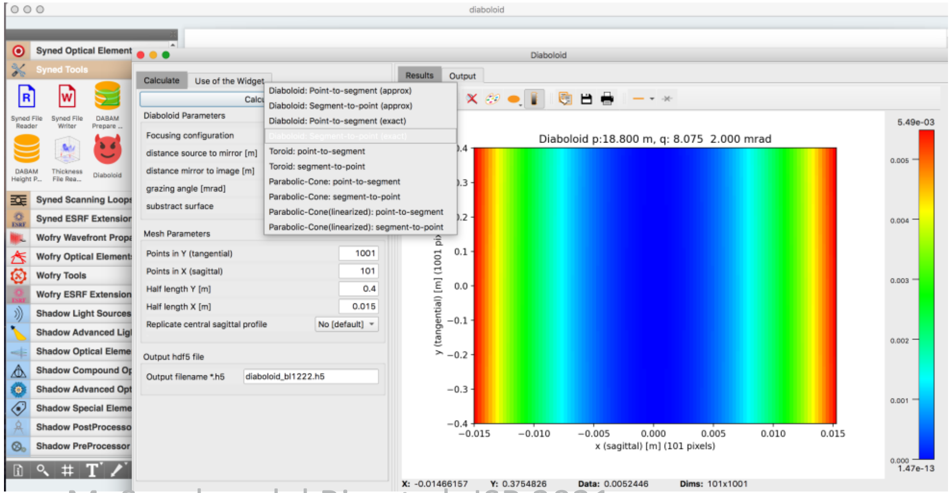
EXAMPLE OF RAY TRACING: DIABOLOID





Approximated surface: Toroid (aberrations, good for 3rd SR, not for 4th)

Exact surface: Diaboloid (converts a wavefront from cylindrical to spherical)



Diaboloid Parameters

Focusing configuration

distance source to mirror [m]

distance mirror to image [m]

grazing angle [mrad]

substract surface

Mesh Parameters

Points in Y (tangential)	1001
Points in X (sagittal)	101
Half length Y [m]	0.4
Half length X [m]	0.015
Replicate central sagittal profile	No [default]

Output hdf5 file

Output filename *.h5: diaboloid_bl1222.h5

X: -0.01466157 Y: 0.3754826 Data: 0.0052446 Dims: 101x1001

M. Sanchez del Rio et al, JSR 2021 https://doi.org/10.1107/S160057752100401X

V. Yashchuk et al. JSR 2021 https://doi.org/10.1107/S1600577521004860