



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

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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, crystals...)
- Helped to most 2-4th generations of SR facilities
- Used/cited in a huge number of papers

SHADOW 1 & 2



Franco Cerrina (†2010)

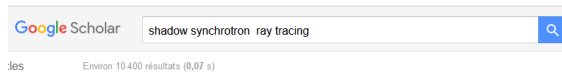
SHADOW3

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

Kernel (Fortran9x)

Python API

XOP/ShadowVUI



SHADOW: a synchrotron radiation and X-ray optics simulation tool
C. Welhak, G.J. 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 ...
is 2024
is 2023
is 2020
de spécifique...

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 ...
par pertinence
par date

SHADOW3: a new version of the synchrotron X-ray optics modelling package
M. Sanchez del Rio, N. Canestrini, 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 ...
les types
es de revue

SHADOW: a synchrotron radiation and X-ray optics simulation tool
C. Welhak, G.J. 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 90 Citer Cité 221 fois Autres articles Les 3 versions

Ray tracing of recent VUV monochromator designs

F. Cerrina

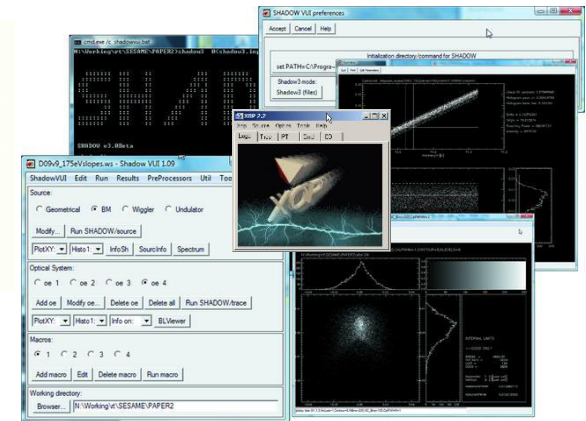
Department of Electrical and Computer Engineering
University of Wisconsin, Madison WI 53706

Abstract

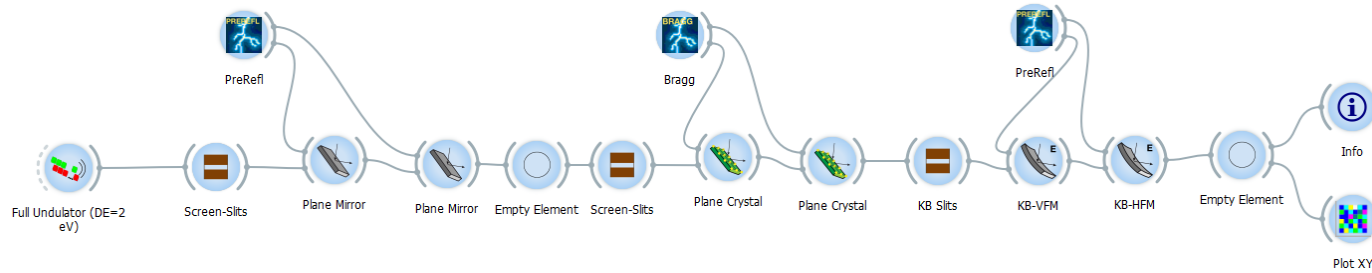
A new optical ray-tracing program is presented and some applications discussed. A Monte-Carlo modelling of several types of sources is implemented, and in particular the Synchrotron Radiation source is modelled exactly. The program is written specifically for grazing optics, although gaussian optics 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 (TGM), Grating Crystal Monochromator (GCM), and Extended Range Grasshopper (ERG) are presented.

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

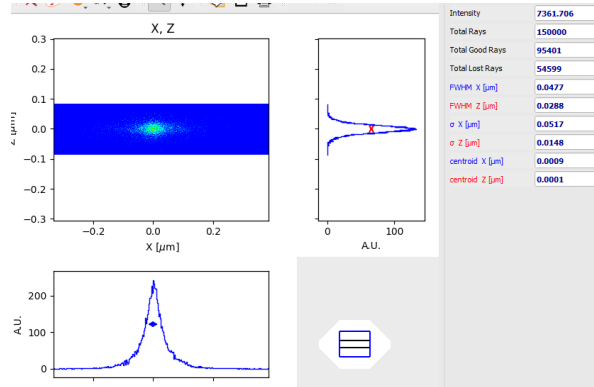
SHADOW1 1984-1990 VAX-VMS mainframes
SHADOW2 1990-2010 Unix workstations+Windows



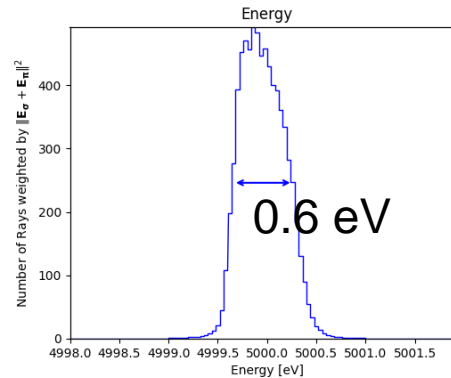
2014: ShadowOUI¹= SHADOW3 + ORANGE²



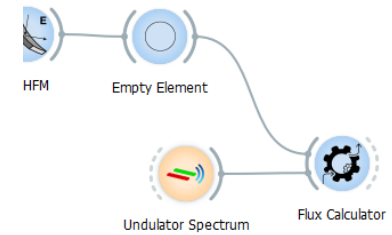
SIZE



RESOLUTION



FLUX



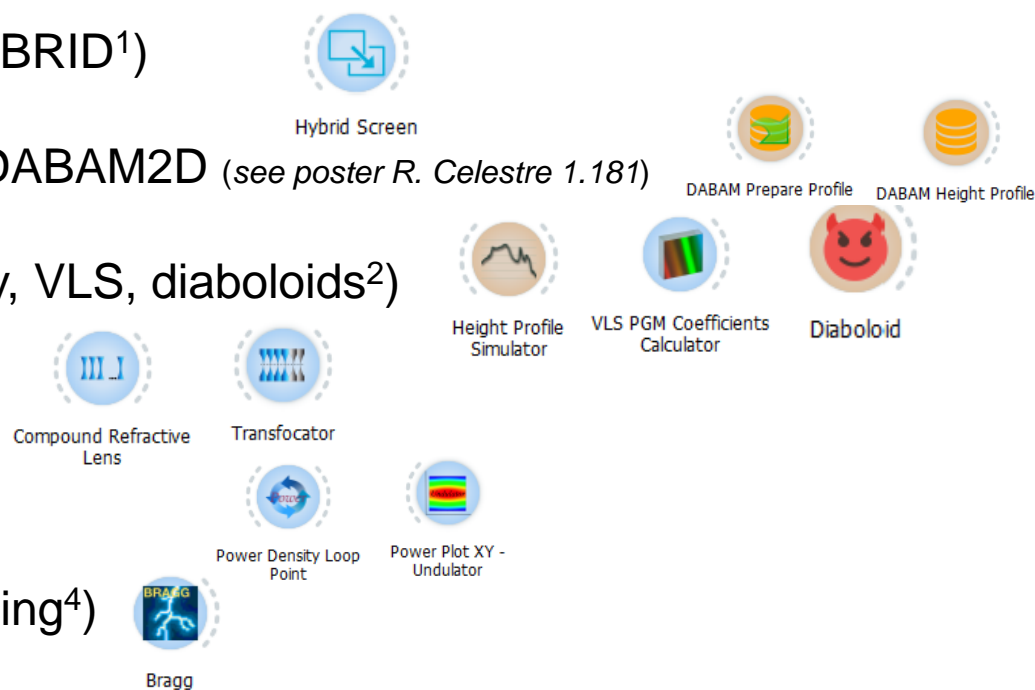
---> Integrated Flux : 1.25321e+13 ph/s

[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 (HYBRID¹)
- Surface error databases DABAM, DABAM2D (*see poster R. Celestre 1.181*)
- Preprocessors (surfaces, reflectivity, VLS, diaboloids²)
- Elements: CRL, TF, Benders, etc.
- Loops & Heat load loops³
- New crystal structures (high d-spacing⁴)



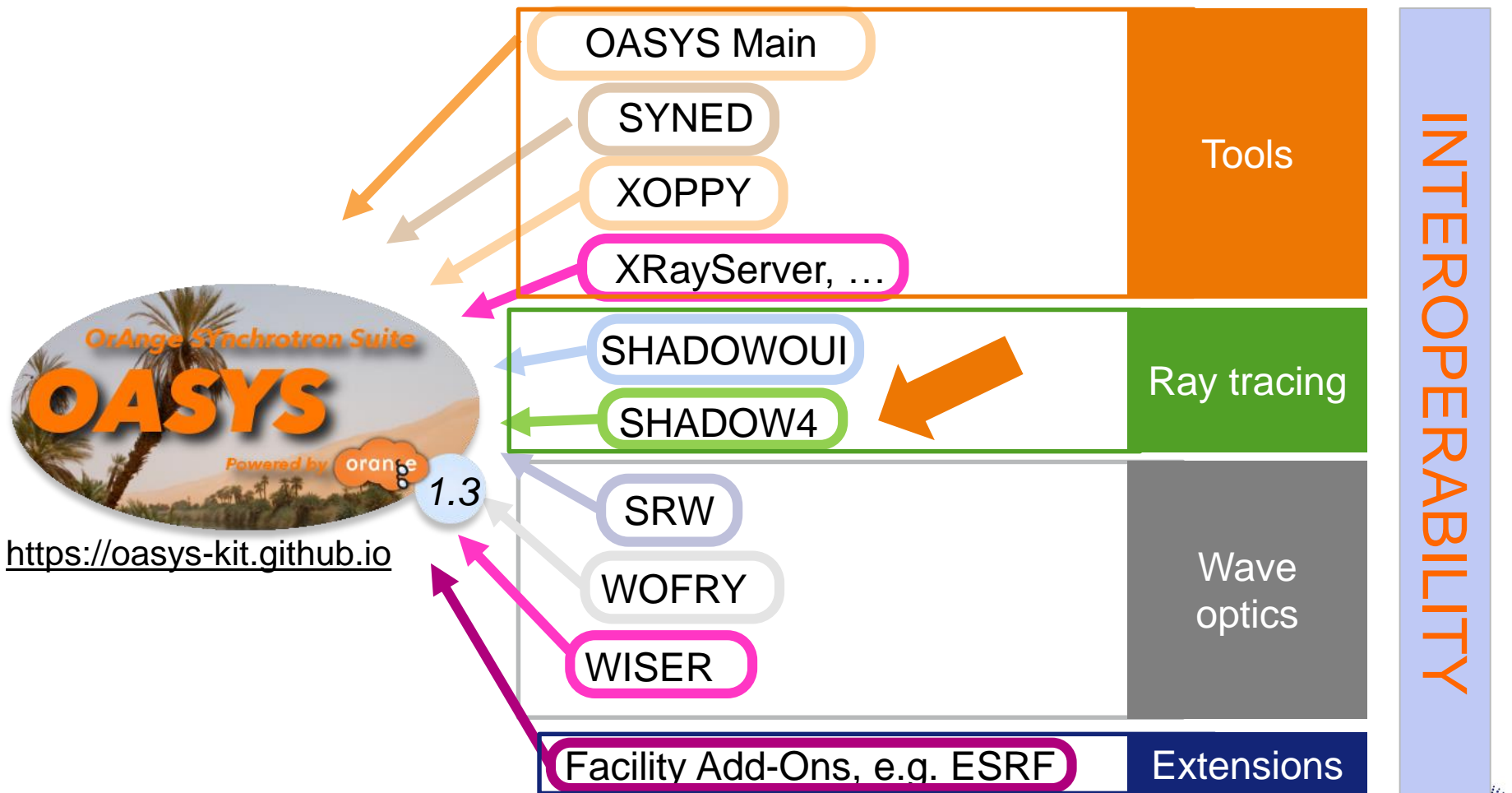
[1] Shi et al. 2014 <https://doi.org/10.1107/S160057751400650X>

[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



SHADOW3 problems:

- Fortran: compilation: obsolete technology, poorly structured code
- Python API maintenance and extension
- Python packaging (wheels)

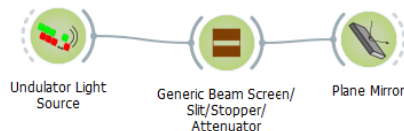
SHADOW4 is a new Kernel, and a new interface, for new generations of sources

- Fully developed in Python
- OO programming
- OASYS experience and ad-hoc developments
- Fast enough

- SHADOW is an interactive tool adapted for common laptops
- Just called SHADOW4
- Simplified interface (less widgets, generic mirrors, crystals, etc.)
- Optimized (better communication)
- Automatic scripting

Preparing 5th generation

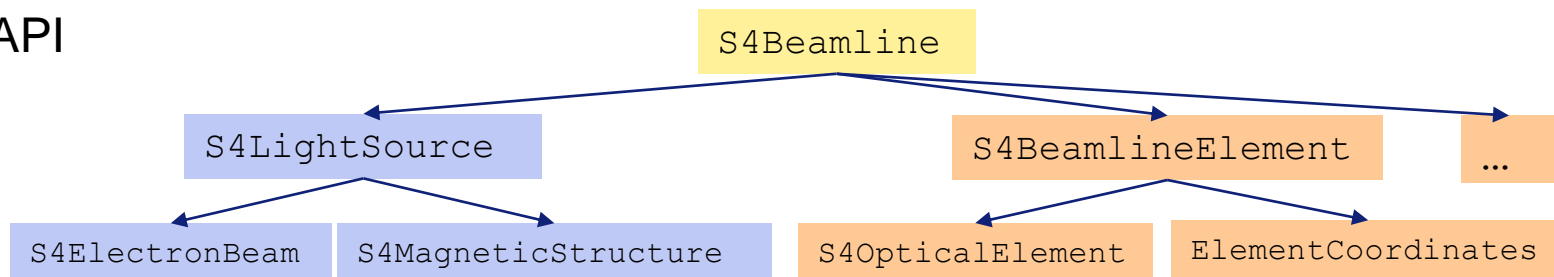
- Facilitate interoperability with other tools (e.g. for partial coherence)
- Adapted for AI integration and Digital Twins (*see L Rebuffi's talk 3/3 Fri 14:00*)
- Easy transition from laptop prototyping to High-Performance Computing (HPC) and Cloud Computing
- Open Source and Collaborative Development
- Educational material for interactive learning



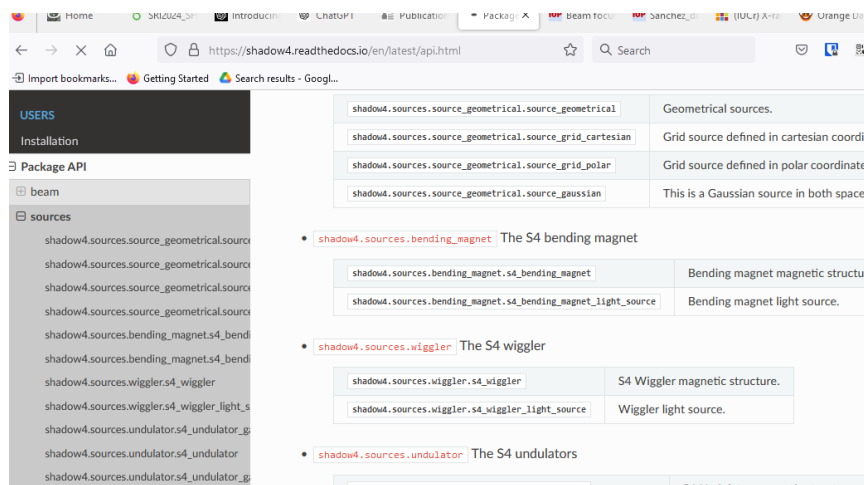
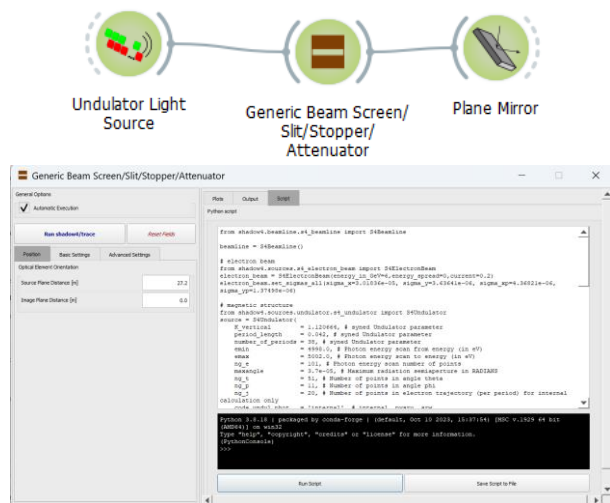
Shadow4 Kernel: Application User Interface

- S4Beam: traditional beam data (nrays, 18)

- API

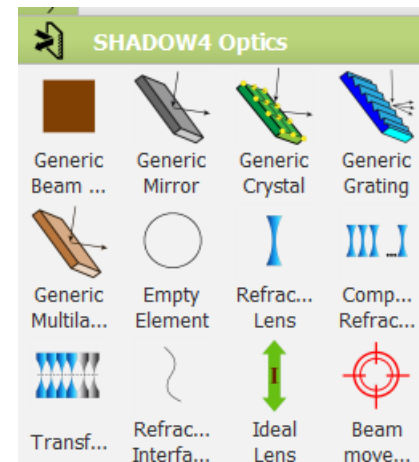
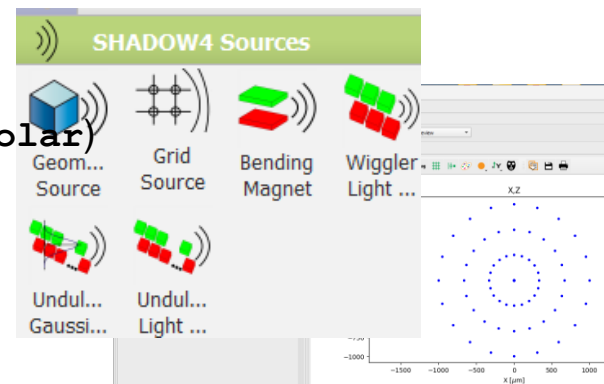


- Automated scripts with OASYS
- Documentation: <https://shadow4.readthedocs.io>



Shadow4 Kernel: beamline components

- Sources/Magnetic structures
 - SourceGeometrical, **SourceGridCartesian**, **SourceGridPolar**)
 - S4BendingMagnet (**upgraded methods¹**)
 - S4Wiggler (included short IDs)
 - S4GaussianUndulator, S4Undulator (**upgraded**: see talk 1/2 of Juan Reyes-Herrera Today 18:15)
- Optical elements
 - S4Screen (screens, slits, stops, absorbers)
 - S4IdealLens, S4Empty,... (ideal elements)
 - S4PlaneMirror, S4SphereMirror, S4EllipsoidalMirror, ..., S4AdditionalNumericalMeshMirror
 - S4PlaneGrating, ... (including VLS)
 - S4PlaneCrystal, ... (undistorted perfect crystals in reflection)
 - **S4PlaneMultilayer**, ... (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 (S4Conic¹, S4Toroid, S4Mesh)
- Include methods for reflection, refraction, grating scattering

Physical model (reflectivities)

Optical constants (scattering factors, refraction indices, crystal structures)

- preprocessor data file
- direct link
 - xraylib³
 - DABAX⁴

preprocessors



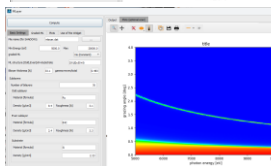
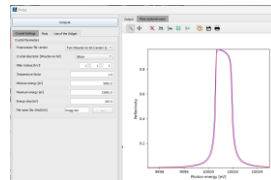
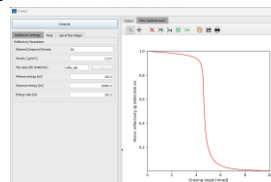
PreRefl



Bragg



MLayer



code

- PreRefl:
Absorption/refraction for attenuators, mirrors, lenses
- crystalpy²: external library for Crystals
- MLayer

[1] <https://arxiv.org/abs/2406.04079>

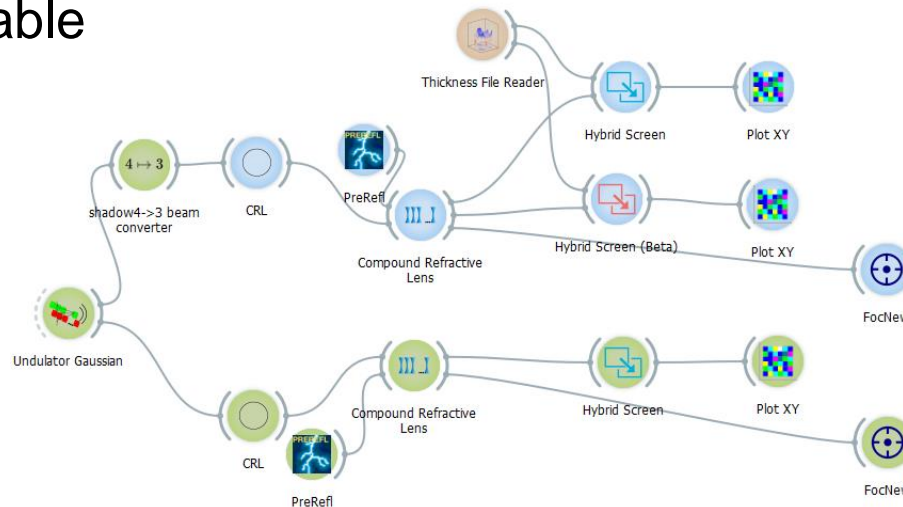
[2] <https://arxiv.org/abs/2406.16960> <https://github.com/oasys-kit/crystalpy>

[3] <https://github.com/tschoonj/xraylib>

[4] <https://github.com/oasys-kit/dabax>

Shadow4: advanced tools – Hybrid¹ method

- Corrects ray tracing considering scattering and diffraction when the beam has a high coherence
- Includes scattering by o.e.'s boundaries (slits, mirrors, gratings, lenses)
- Manages the surface error (delegated from o.e.)
- Fully rewritten code²
- Scriptable

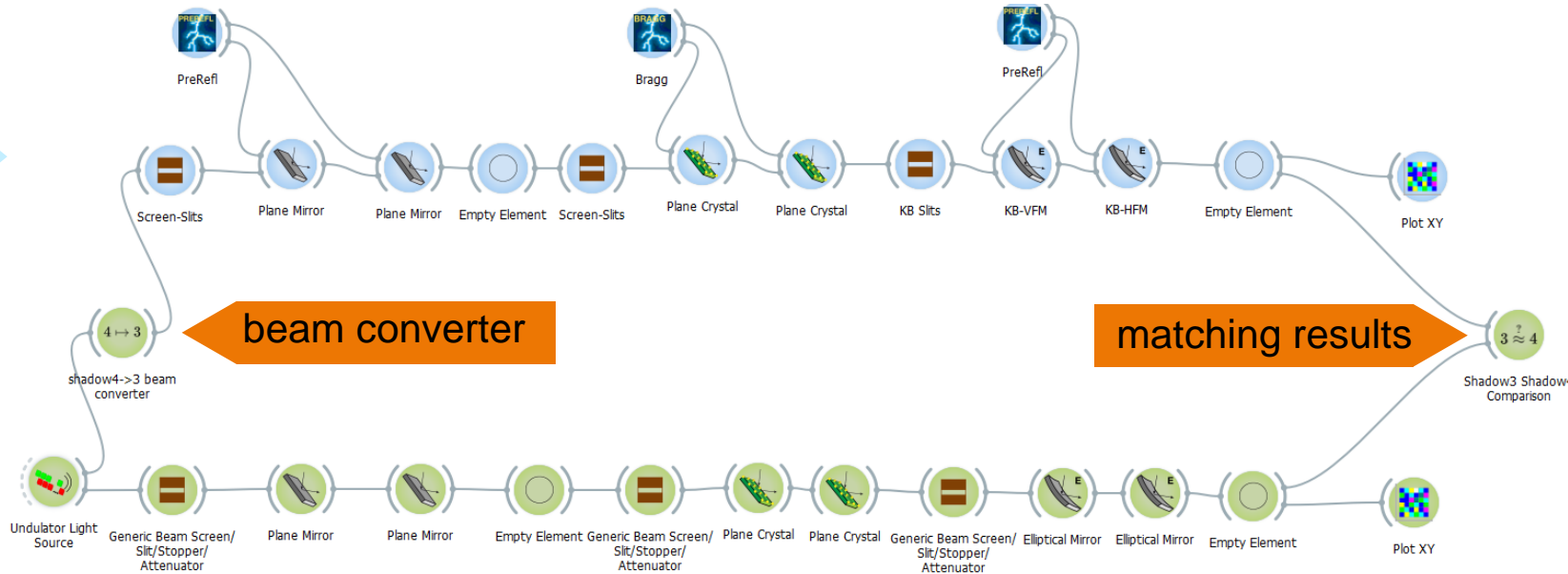


[1] Shi *et al.* 2014 <https://doi.org/10.1107/S160057751400650X>

[2] <https://github.com/oasys-kit/shadow4-advanced>

Shadow4: beta testers are welcomed!

Shadow3



Send issues in <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
 - Preparing the future SR generations
- Already available in OASYS [beta]
- Didactical material^{1,2} available.
- Future OASYS schools (done at ESRF^{3,4}, APS³, ALS⁵)



[1] https://github.com/oasys-esrf-kit/oasys_hercules_2024

[2] <https://github.com/oasys-kit/shadow4workspaces>

[3] https://github.com/oasys-kit/oasys_school

[4] <https://doi.org/10.1080/08940886.2019.1654832>

[5] <https://doi.org/10.1080/08940886.2023.2274746>

Thank you

Download slides:

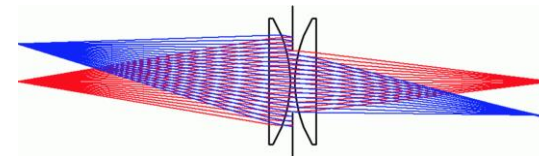


Analytical model (by hand)

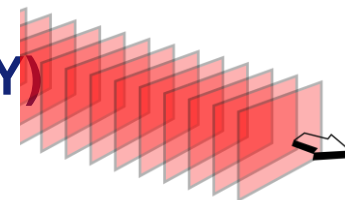


Ray tracing (Shadow4)

Hybrid model (Shadow4)



wave optics & partial coherence 1D (WOFRY)
(see poster 1.141)



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>