



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...)
- Helped to most 2-4th generation SR facilities
- Open source

SHADOW 1¹ & 2



Franco Cerrina (†2010)

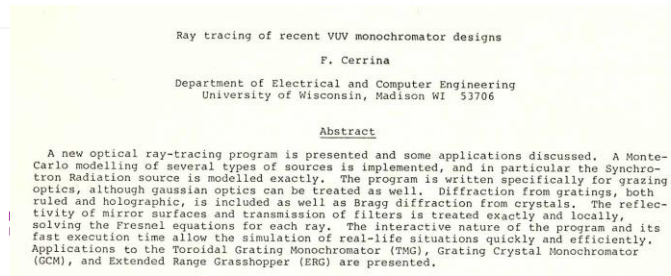
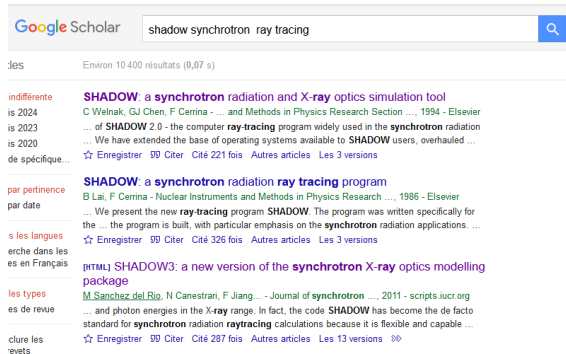
SHADOW3

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

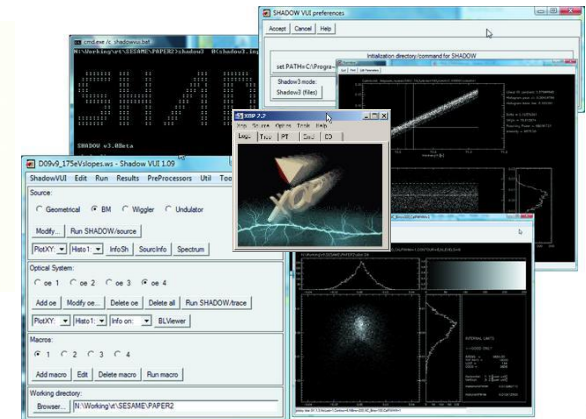
Kernel (Fortran9x)

Python API

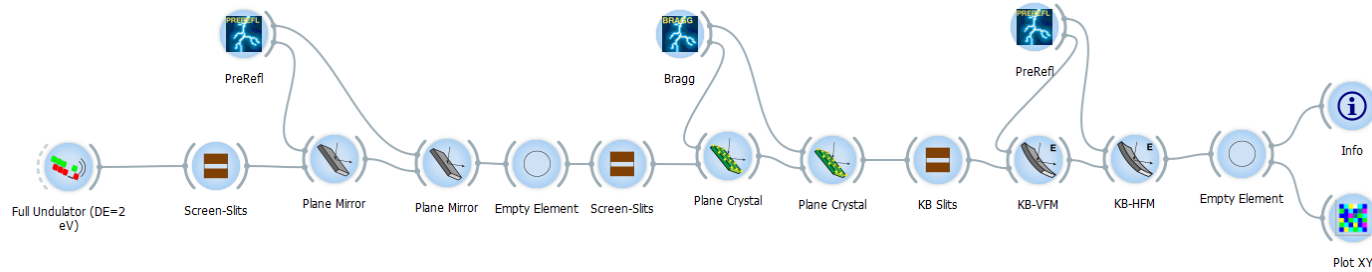
XOP/ShadowVUI



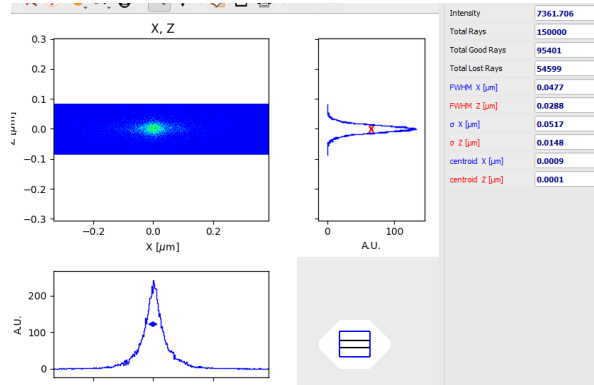
[1] 68 / SPIE Vol. 503 Application, Theory, and Fabrication of Periodic Structures (1984)



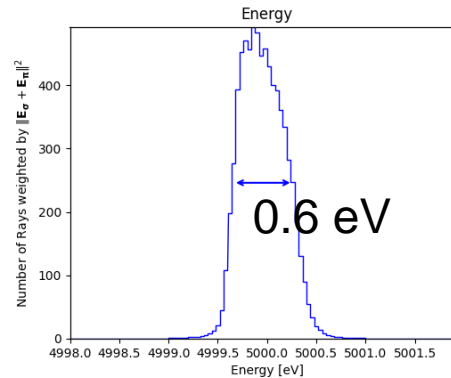
In 2014: ShadowOUI¹= SHADOW3 + ORANGE²



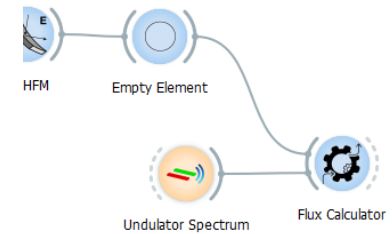
SIZE



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 1.181)
- Preprocessors (surfaces, VLS, diaboloids², reflectivity)
- Python Scripting / Capturing beam
- Compound Elements: CRL, TF
- New elements: Benders, etc.
- Loops
- Heat load loops³
- High d-spacing crystals⁴



Hybrid Screen



DABAM Prepare Profile



DABAM Height Profile



Height Profile



VLS PGM Coefficients



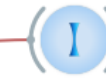
Diaboloid



Geometrical Source



Python Script



Lens



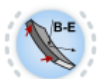
Info



Compound Refractive



Transfocator



Bendable Ellipsoid



Double-Rod Bendable Ellipsoid Mirror



Loop Point



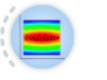
Scanning Variable Loop Point



Scanning File Loop Point



Power Density Loop



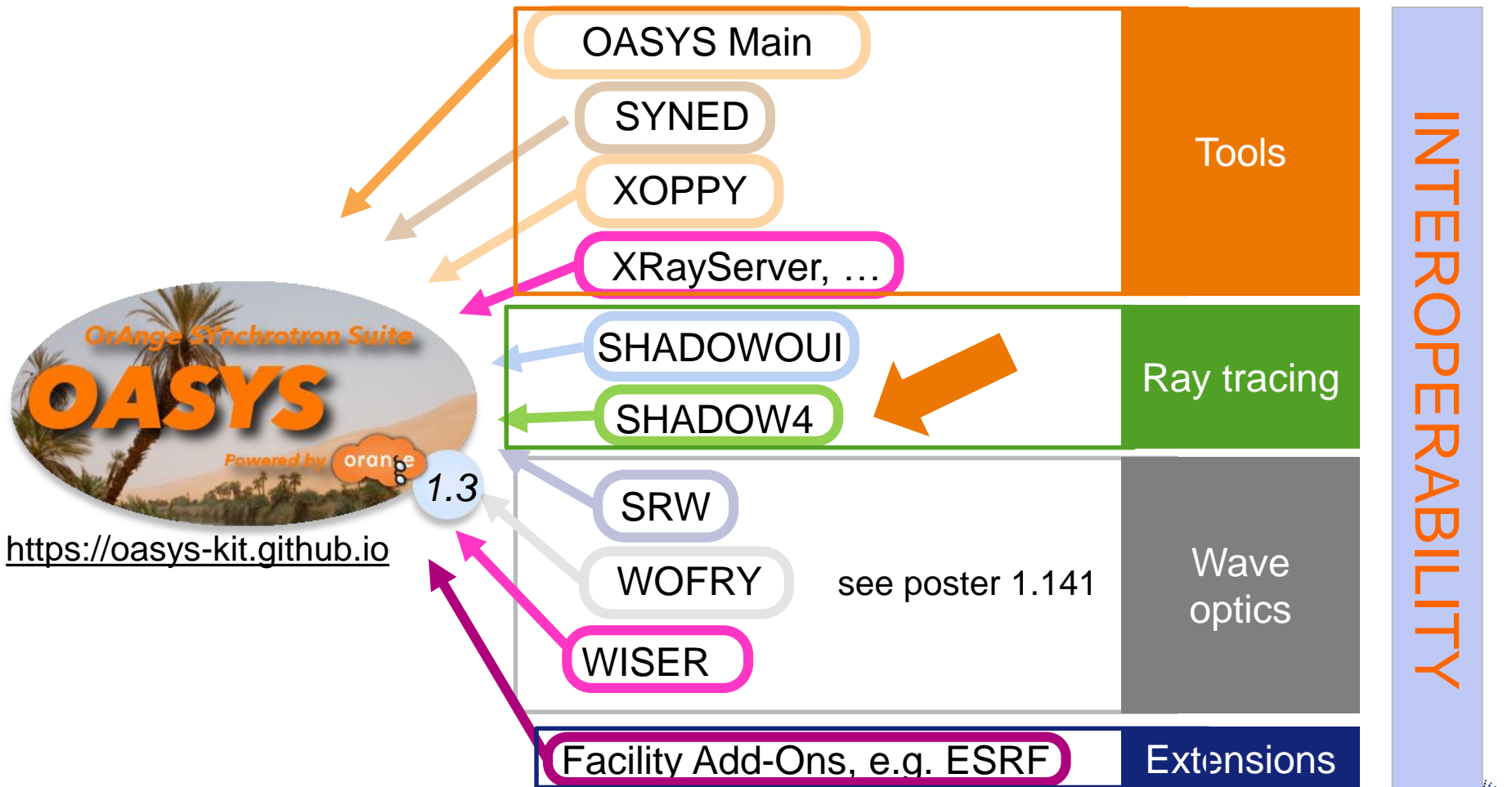
Power Plot XY - Undulator



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



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

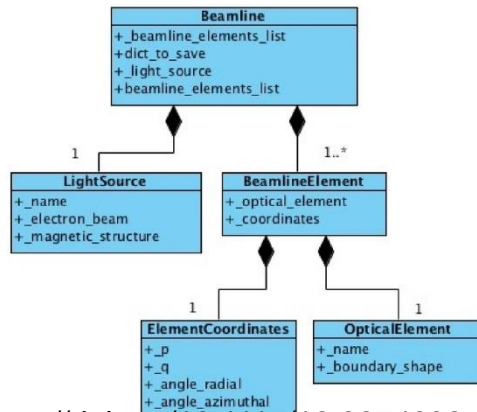
SHADOW4 is a new Kernel, and a new interface, for new generations of sources

- Fully developed in Python
- OO programming
- OASYS experience and ad-hoc developments
- Extended the SYNED¹ concept
- Fast enough
- <https://github.com/oasys-kit/shadow4>

- 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

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

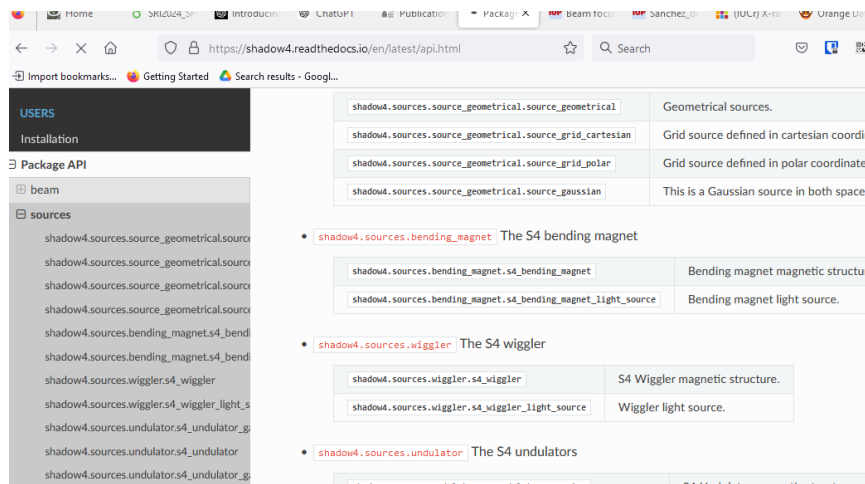
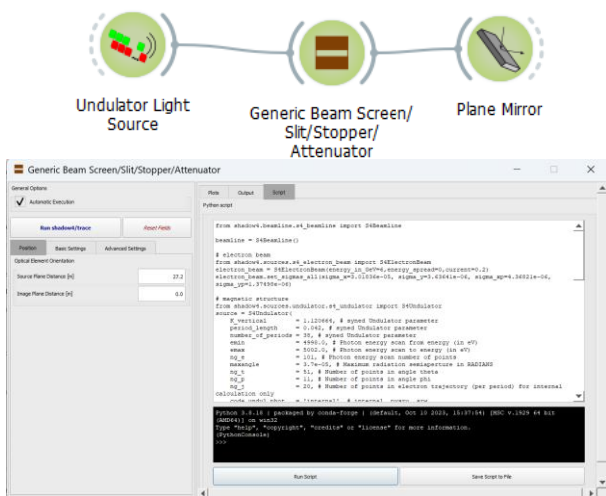


[1] <https://doi.org/10.1117/12.2274232>

Shadow4 Kernel: User interface

- S4Beam: traditional beam data (nrays, 18) →
- User interface:
 - S4LightSource (S4ElectronBeam+S4MagneticStructure)
 - S4BeamlineElement(S4OpticalElement+ElementCoordinates+...)
 - ...
 - S4Beamline = S4LightSource+S4BeamlineElement
- Automated scripts with OASYS • Documentation: <https://shadow4.readthedocs.io>

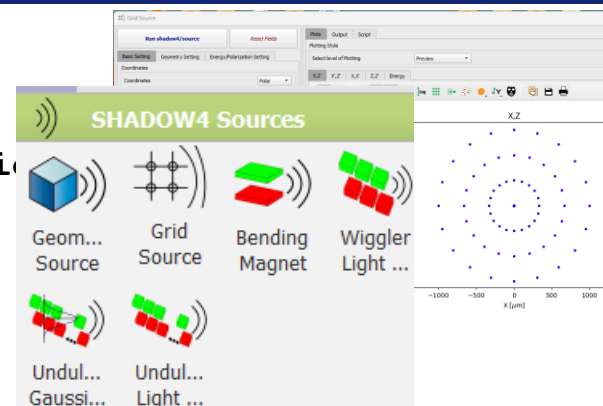
1: X spatial coordinate
 2: Y spatial coordinate
 3: Z spatial coordinate
 4: X' direction or divergence
 5: Y' direction or divergence
 6: Z' direction or divergence
 7: X component of the electromagnetic vector (s-polariz)
 8: Y component of the electromagnetic vector (s-polariz)
 9: Z component of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



Shadow4 Kernel: beamline components

- Sources

- SourceGeometrical, SourceGridCartesian, **SourceGrid**
- S4BendingMagnet (**upgraded methods¹**)
- S4Wiggler (included short IDs)
- S4GaussianUndulator, S4Undulator (**upgraded**: see talk S1/2 of Juan Reyes-Herrera 18:15)



- Beamline elements

- S4Screen (screens, slits, stops, absorbers)
- S4IdealLens, S4Empty,... (ideal elements)
- S4PlaneMirror, S4SphereMirror, S4EllipsoidalMirror, ..., **S4AdditionalNumericalMeshMirror**
- 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

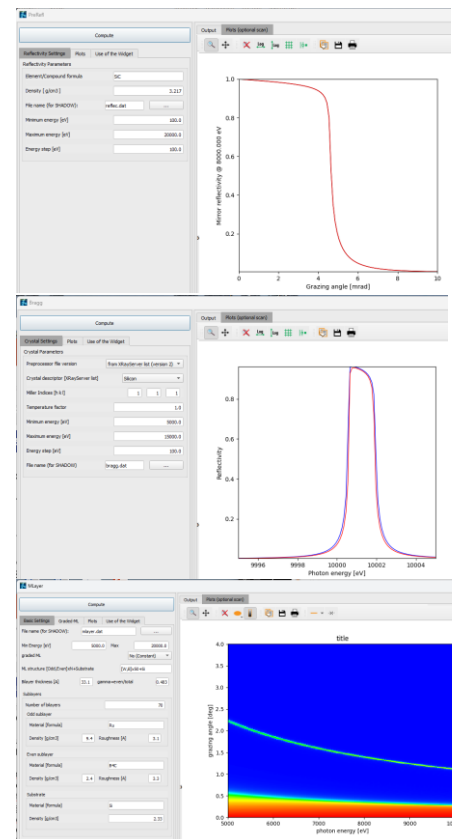
- Geometrical model
 - S4OpticalSurface (S4Conic¹, S4Toroid, S4Mesh)
 - Include methods for reflection, refraction, scattering (grating)
- Physical models [may avoid preprocessor files]
 - PreRefl: Absorption/refraction for attenuators, mirrors, lenses
 - crystalpy²: external library for Crystals
 - MLayer
 - Optical constants (scattering factors, refraction indices, crystal structures)
 - xraylib³
 - DABAX⁴
 - preprocessor data file (can be created with other tools)

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

[2] <https://arxiv.org/abs/2406.16960>

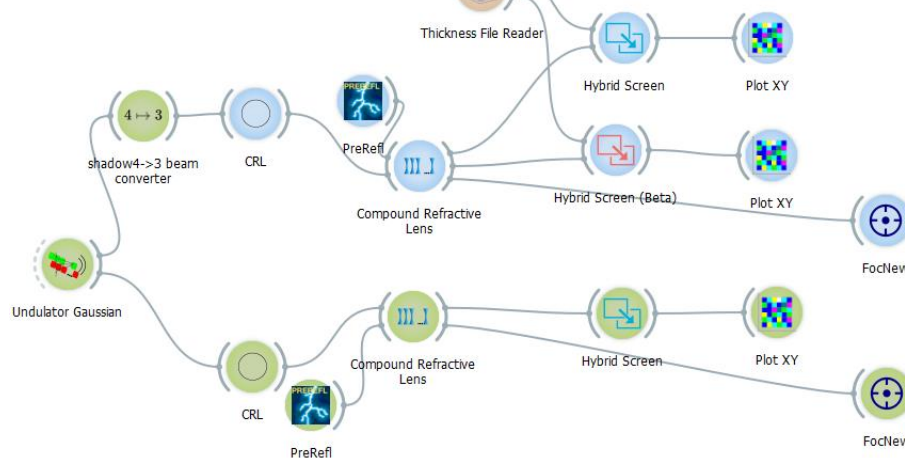
[3] <https://github.com/tschoonj/xraylib>

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



Shadow4: advanced tools – Hybrid¹ 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>

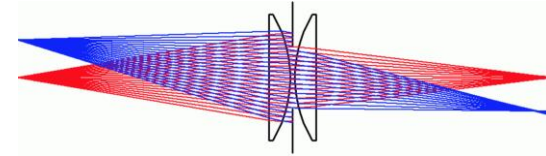


[1] Shi *et al.* 2014 <https://doi.org/10.1107/S160057751400650X>

Analytical model (by hand)

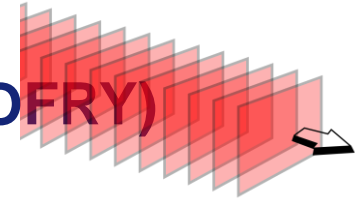


Ray tracing (Shadow4)



Hybrid model (Shadow4)

wave optics & partial coherence 1D (WOFRY)



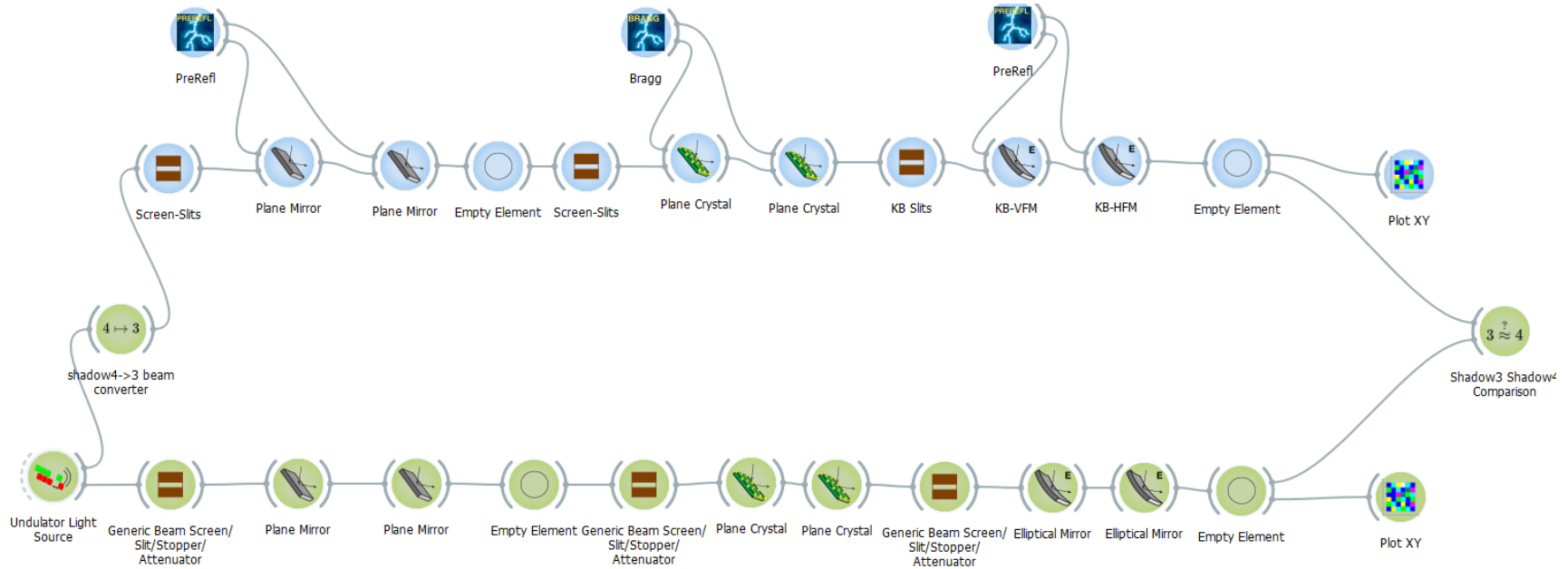
wave optics partial coherence 2D:

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
 - Preparing 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/>

Thank you

Download slides:

