HERCULES 2018

Simulating beamline optics by ray-tracing using ShadowOui

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Outline

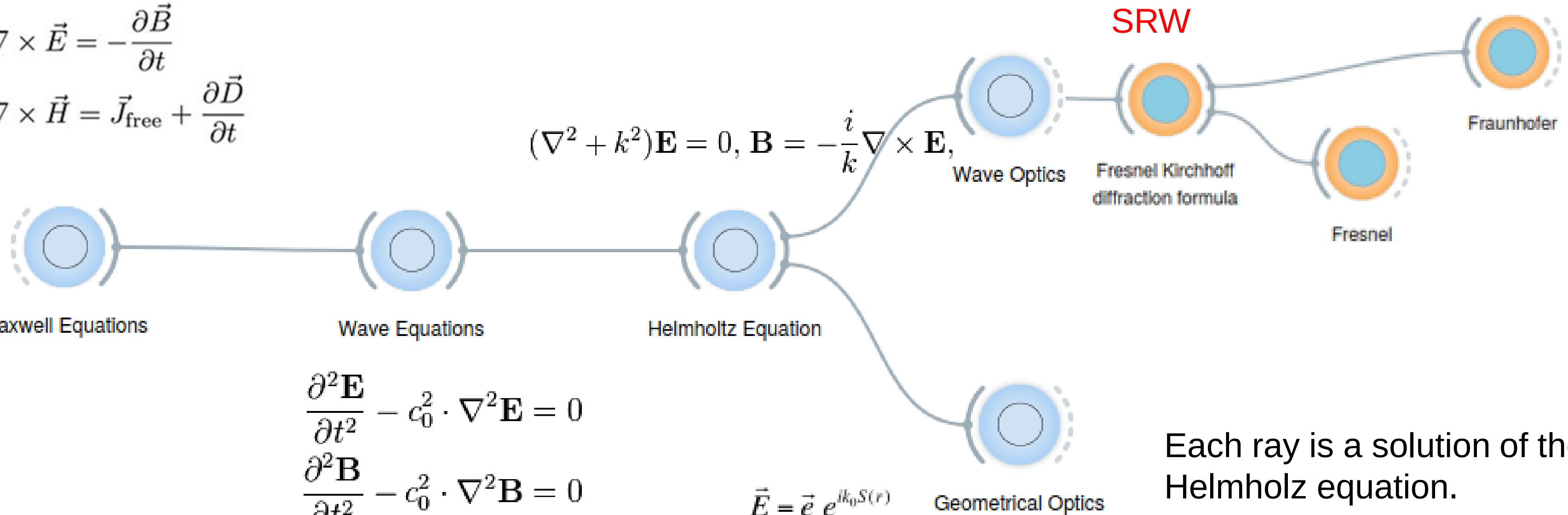
- Software
- Sources (BM, wigglers and undulators)
- Optics
  - Reflective (aberrations, slope errors)
  - Diffractive (dispersion)
  - Refractive (chromatic aberrations)
  - Coherence

Each wavefront is a solution of the Helmholz equation, and it is fully coherent.

Partial coherence require working with many wavefronts. Each individual wavefront is coherent, but incoherent with respect to others
SRW

$$\nabla \cdot \vec{D} = \rho_{\text{free}}$$
$$\nabla \cdot \vec{B} = 0$$
$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$
$$\nabla \times \vec{H} = \vec{J}_{\text{free}} + \frac{\partial \vec{D}}{\partial t}$$

$$(\nabla^2 + k^2)\mathbf{E} = 0, \ \mathbf{B} = -\frac{i}{k}\nabla \times \mathbf{E},$$



$$\frac{\partial^2 \mathbf{E}}{\partial t^2} - c_0^2 \cdot \nabla^2 \mathbf{E} = 0$$
$$\frac{\partial^2 \mathbf{B}}{\partial t^2} - c_0^2 \cdot \nabla^2 \mathbf{B} = 0$$

$$\vec{E} = \vec{e}\ e^{ik_0 S(r)}$$
$$\vec{H} = \vec{h}\ e^{ik_0 S(r)}$$
$$(\nabla S)^2 = n^2$$
$$\nabla S = n\,\vec{s}$$
$$\frac{d}{ds}\left(n \frac{d\vec{r}}{ds}\right) = \nabla n$$
$$\nabla n = 0 \Rightarrow \frac{d\vec{r}}{ds} = 0 \Rightarrow \vec{r} = s\vec{a} + \vec{b}$$

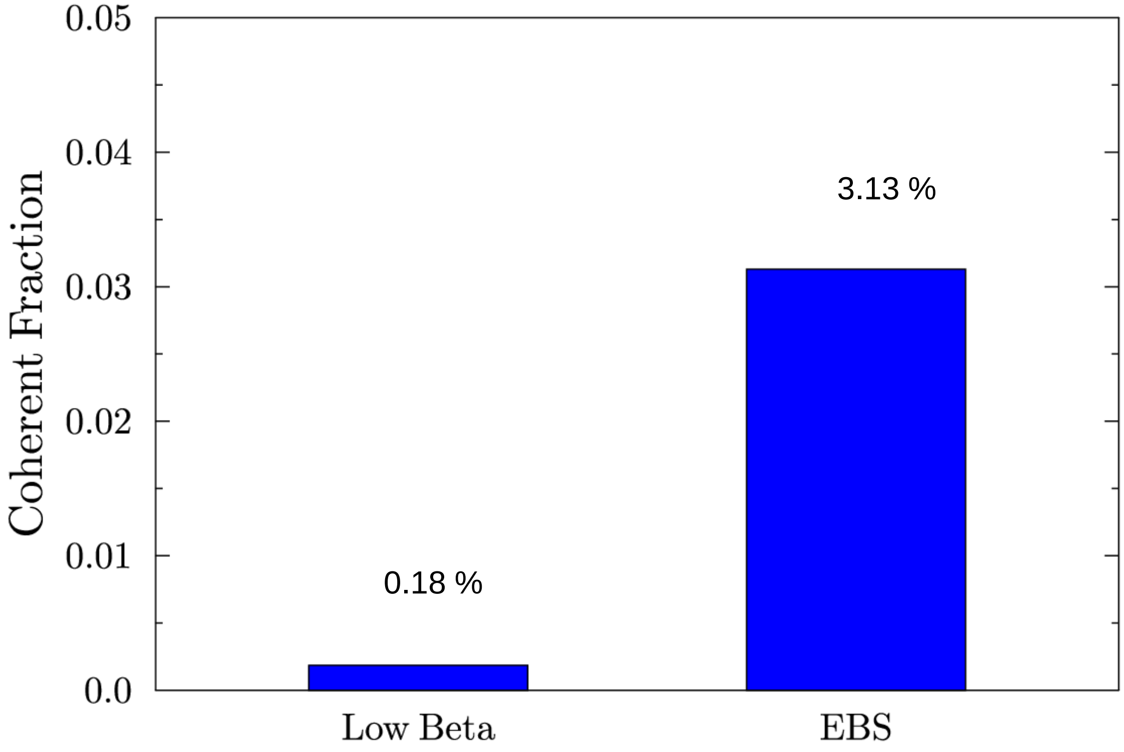
Each ray is a solution of the Helmholz equation.

Many rays represent an incoherent beam. Each individual ray is coherent, but incoherent with respect to others
SHADOW

AT HIGH ENERGIES, WE ARE FAR FROM DIFFRACTION-LIMIT (=FULLY COHERENCE)

U17 2m @ 17 keV (K=0.4842) L=2m Coherent Fraction

THEREFORE, ANY BEAMLINE SIMULATION MUST START WITH RAY TRACING (INCOHERENT BEAMS)



CONTEXT: OASYS TOOLBOX TO SIMULATE VIRTUAL EXPERIMETS

Beamline Experiment Chain

Storage Ring (e$^-$ optics) → Radiation devices (e$^-$ -> γ) → Beamline (γ optics) → Sample (γ –matter interactions)

NEW OASYS-BASED TOOLBOX

ShadowOui

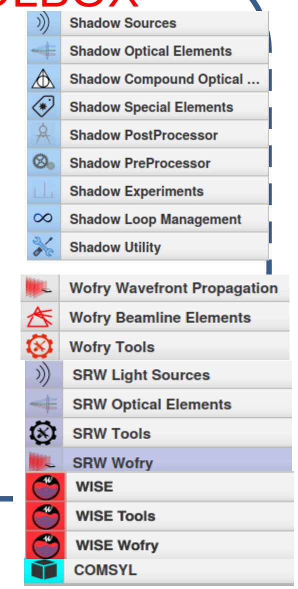
XOPPY

SRW

WOFRY

X-rayserver

wise

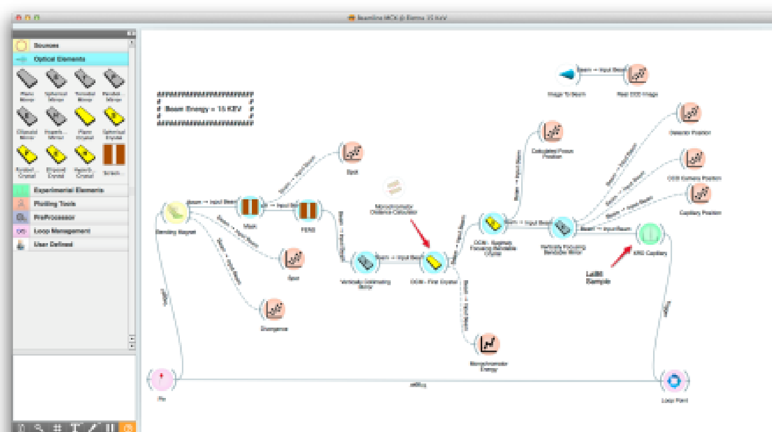


OrAnge SYnchrotron Suite OASYS Powered by orange

http://www.elettra.eu/oasys.html

OASYS: A NEW PLATFORM FOR BEAMLINE SIMULATIONS

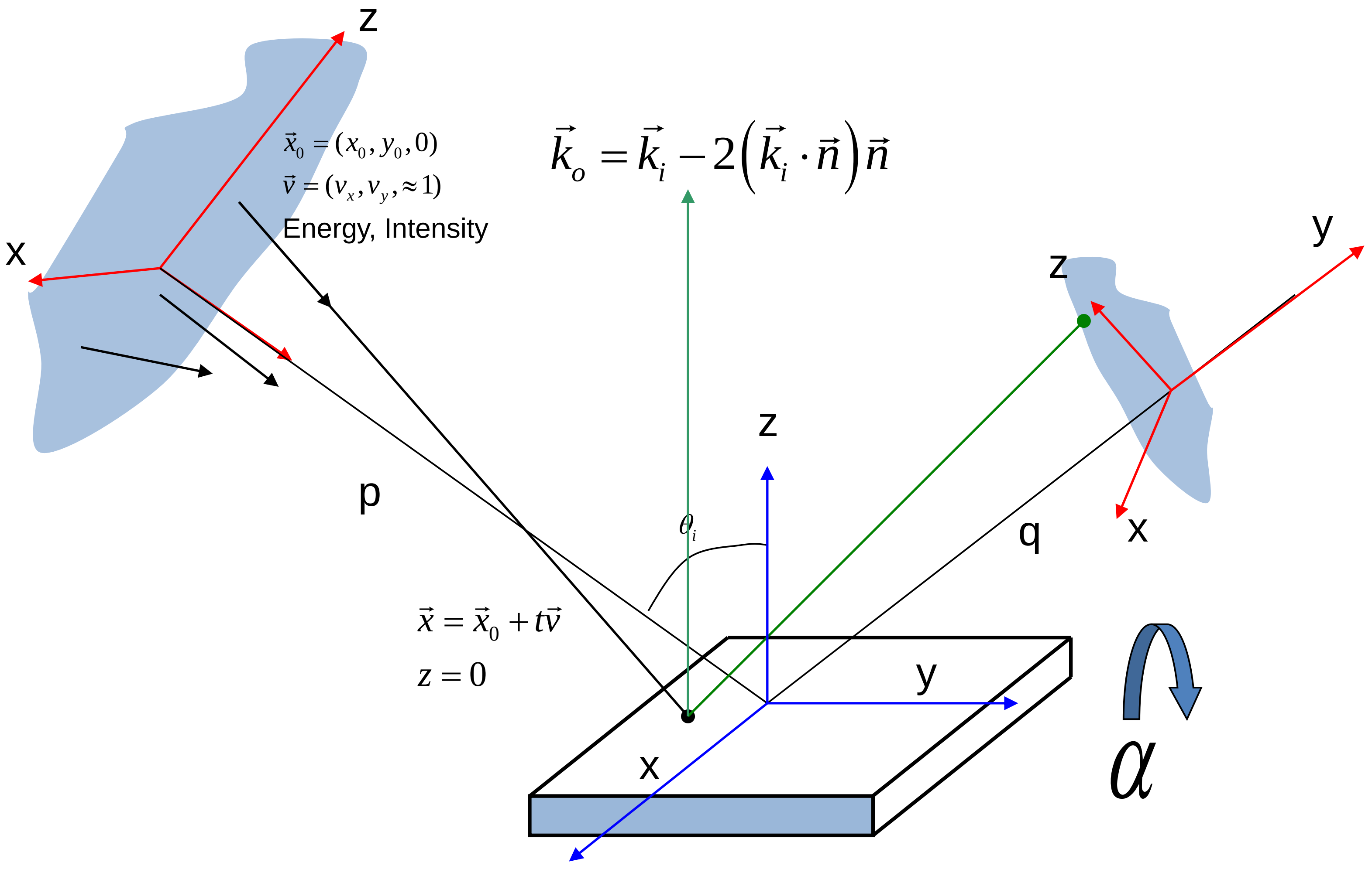
- Oasys is a new software platform for simulating virtual experiments in the synchrotron radiation world
- Oasys is the result of a collaboration among ESRF, Elettra and University of Ljubljana.
- It integrates different state-of-the-art simulation packages for beamline simulation and X-ray optics.



Oasys+ShadowOui

- Install Oasys+ShadowOui:
  - https://github.com/oasys-kit/oasys-installation-scripts/wiki
- Today: Use rnice.
- Download Tutorials:
  - `export all_proxy=http://proxy.esrf.fr:3128/`
  - `git clone` https://github.com/srio/ShadowOui-Tutorial
- Start OASYS:
  - `oarsub -I -l nodes=1/cpu=1/core=8,walltime=10:00:00`
  - `/scisoft/XRayOptics/OASYS1_RNICE8/start_oasys.sh`

Trace (the beamline)



X-ray sources

- X-ray tubes
- Radioactive sources / Excitation by radioactive decay
- Synchrotron Bending Magnets
- Synchrotron insertion devices (wigglers and undulators)
- X-ray lasers
- Others: Inverse Compton, Channeling
- Pulsars/Quasars/Black holes etc.

ShadowOui has tools to simulate synchrotron sources. In addition a “Geometrical Source” can be used to approximate any source.

Compute e$^-$ beam sizes

$$\Sigma = \begin{pmatrix} \langle x^2 \rangle & \langle xx' \rangle \\ \langle xx' \rangle & \langle x'^2 \rangle \end{pmatrix} = \begin{pmatrix} \beta_x \varepsilon_x & -\alpha_x \varepsilon_x \\ -\alpha_x \varepsilon_x & \gamma_x \varepsilon_x \end{pmatrix} + \eta^2 \sigma_\delta{}^2 I_{2x2}$$

With ε the emittance (constant), and Twiss parameters:

$$\alpha = -\frac{1}{2}\frac{d\beta}{ds}; \quad \gamma = \frac{1+\alpha^2}{\beta}$$

At s (any point of the trajectory):

$$\sigma_x = \sqrt{\langle x^2 \rangle} = \sqrt{\beta_x \varepsilon_x}; \quad \sigma_{x'} = \sqrt{\langle x'^2 \rangle} = \sqrt{\gamma_x \varepsilon_x}; \quad \sigma_x \sigma_{x'} = \varepsilon_x \sqrt{1+\alpha_x^2}$$

At waist (zero correlation, $\rho=\alpha=0$, β is minimum):

$$\sigma_x = \sqrt{\langle x^2 \rangle} = \sqrt{\beta_x \varepsilon_x}; \quad \sigma_{x'} = \sqrt{\langle x'^2 \rangle}\Big|_w = \sqrt{\frac{\varepsilon_x}{\beta_x}}; \quad \boxed{\sigma_x \sigma_{x'} = \varepsilon_x}$$

ShadowOui asks for σ and ε at waist (plus distance from waist to center of device) ex13_insertiondevices.ows

Onuki & Elleaume Undulators, Wigglers and their applications, CRC press, 2002

below resonance

on resonance

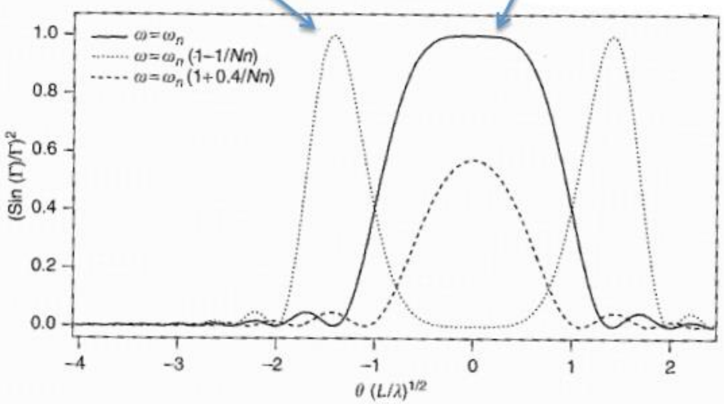


Figure 3.3 Graph of $(\sin(\Gamma)/\Gamma)^2$ as a function of the angle $\theta = \sqrt{\theta_x^2+\theta_z^2}$ for three different frequencies. ω_n is an abbreviation for $n\omega_1\,(0,0)$.

78 *P. Elleaume*

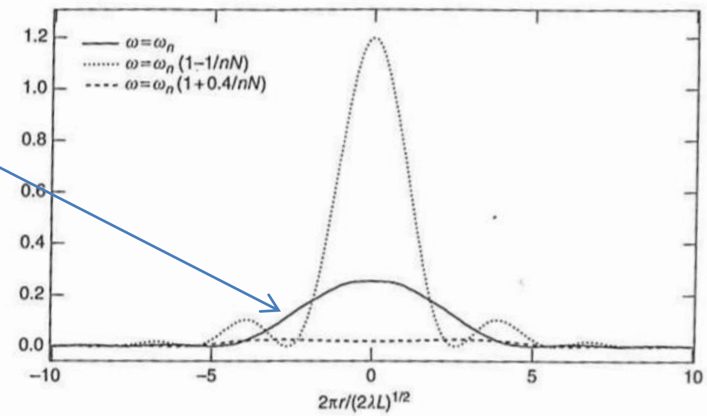


Figure 3.4 Spectral flux per unit surface in the middle of the undulator for three frequencies close to the on-axis resonant frequency $\omega_n = n\omega_1(0,0)$.

Even on resonance, beam is not fully Gaussian
But for resonance, can be reasonably approximated as Gaussian

$$\sigma_r = \frac{2.704}{4\pi}\sqrt{\lambda L} \approx \sqrt{\frac{\lambda L}{2\pi^2}}$$

$$\sigma_{r'} = 0.69\sqrt{\frac{\lambda}{L}} \approx \sqrt{\frac{\lambda}{2L}}$$

$$\sigma_r \sigma_{r'} = \frac{1.89\lambda}{4\pi} \approx \frac{\lambda}{2\pi}$$

- Undulator beams have not Gaussian profiles (even at resonances)
- BY NOW, WE APPROXIMATE UNDULATORS BY GEOMETRIC SOURCES WITH GAUSSIAN SIZES AND DIVERGENCES

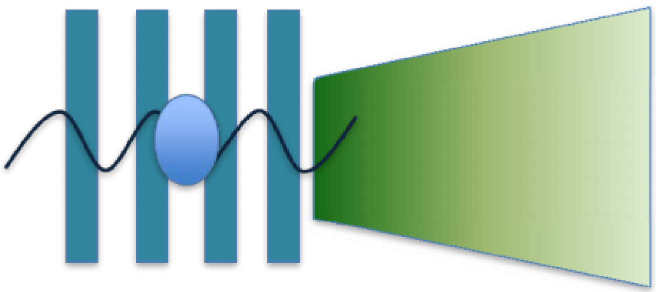
Photon beam size and divergence is determined by a combination of electron beam and single electron emission

$$\Sigma_x^2 = \sigma^2_{x,elec} + \sigma^2_{x,photon}$$

$$\Sigma_{x'}^2 = \sigma^2_{x',elec} + \sigma^2_{x',photon}$$

$$\Sigma_z^2 = \sigma^2_{z,elec} + \sigma^2_{z,photon}$$

$$\Sigma_{z'}^2 = \sigma^2_{z',elec} + \sigma^2_{z',photon}$$



Courtesy: Boaz Nash

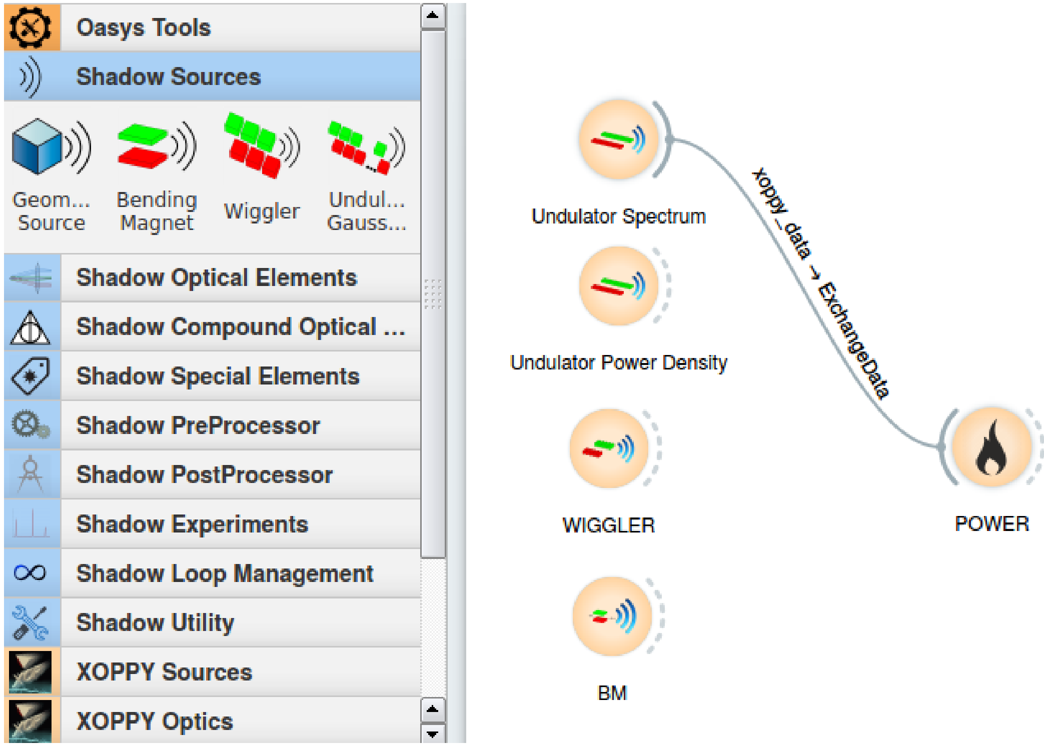
These are at source. A distance D away, beam size become: $\Sigma^2_{x,0} + \Sigma^2_{x',0} D^2$

(FOR UNDULATORS, THESE FORMULAS ARE VALID AT THE WAIST, AT THE UNDULATOR RESONANCE, AND SUPOSSING GAUSSIAN EMISSION OF PHOTONS)

ShadowOui performs “numeric convolution” by Monte Carlo sampling of the electron beam [Gaussian] and photon emission [non Gaussian]

Source characteristics (XOPPY)

- Undulator spectrum – power
- Undulator power density
- Wiggler spectrum
- BM



Optical elements

For each optics element SHADOW includes:

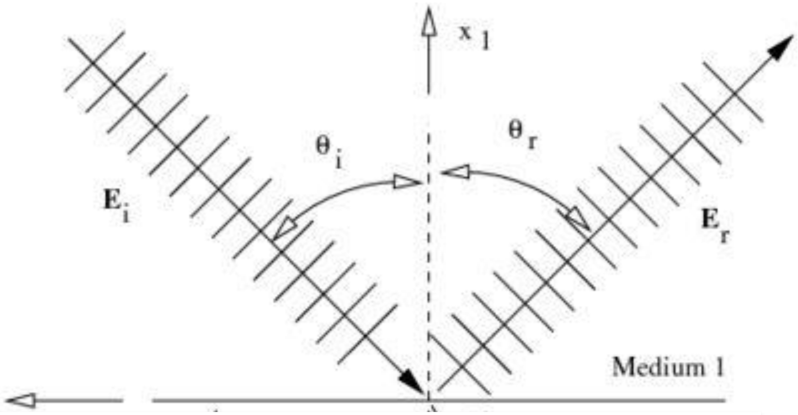
- Geometrical model: how the direction of the rays are changed (reflected, refracted or diffracted)
- Physical model: how the ray intensity (in fact electric fields) decreases because of the interaction

•Structures along the surface =>playing with the direction

•Structures in depth => playing with the reflectivity ex15_aberration.ows

Mirrors

Geometrical model

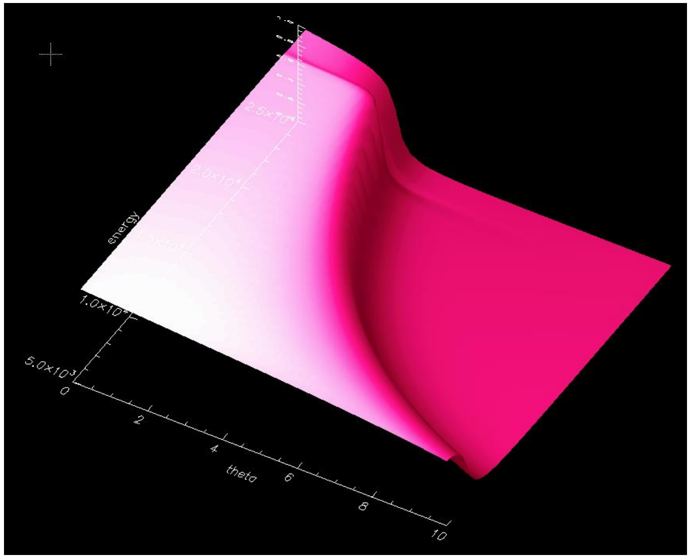


$$\hat{\mathrm{d}}_s = 2\left(\hat{\mathrm{d}}_n \cdot \hat{\mathrm{d}}_i\right)\hat{\mathrm{d}}_n - \hat{\mathrm{d}}_i,$$

Physical model

Fresnel equations give the reflectivity as a function of angle and photon energy. As a consequence, one gets the critical angle:

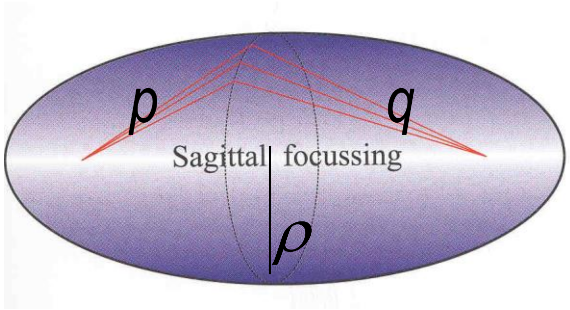
$$1 = \left(\frac{n_1}{n_2}\right)^2 \cos^2\theta_c \quad \Leftrightarrow \quad \sin\theta_c = \sqrt{2\delta - \delta^2} \approx \sqrt{2\delta}$$



ex15_aberration.ows

Mirror shape

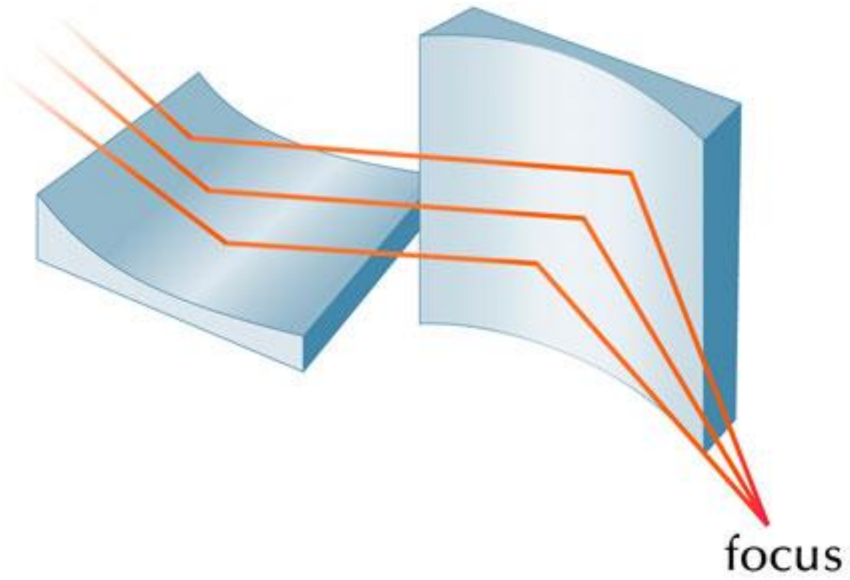
- Point to point focusing (ellipsoid)
- Collimating (paraboloid)
- Focalization in two planes
  - Tangential or Meridional (ellipse or parabola)
  - Sagittal (circle)
- Demagnification: M=p/q
- Easier manufactiring:
  - 2D: Ellipsoid => Toroid
  - Only one plane: cylinder Ellipsoid (ellipse)=> cylinder (circle)
  - Sagittal radius: non-linear (ellipsoid) => constant (cylinder) or linear (cone),
- Aberrations



$$\frac{1}{p}+\frac{1}{q}=\frac{2}{R\sin\theta}$$

$$\frac{1}{p}+\frac{1}{q}=\frac{2\sin\theta}{\rho}$$

Kirkpatrick-Baez



ex16_kb.ows

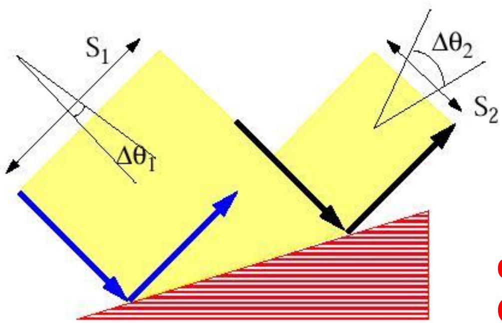
Crystals

Geometrical model

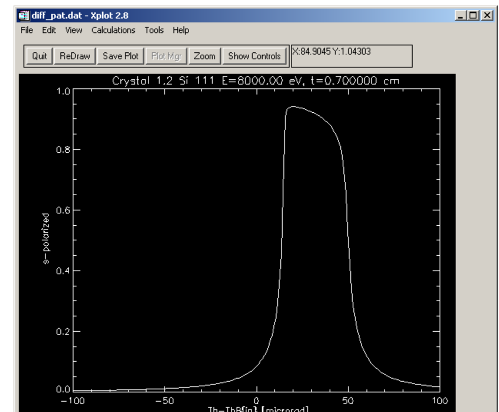
like a grating originated by the truncation of the Bragg planes with the crystal surface. Crystals are dispersive elements, except for the most used case of Bragg-Symmetric reflection.

Physical model

(crystal reflectivity) is given by the Dynamical Theory of Diffraction and gives the "Darwin width"



BRAGG or reflection



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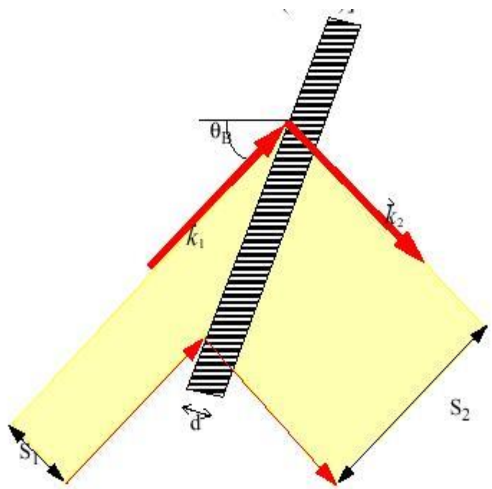
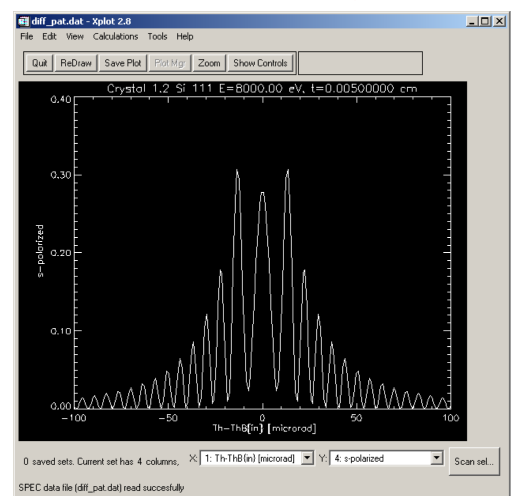


LAUE or transmission

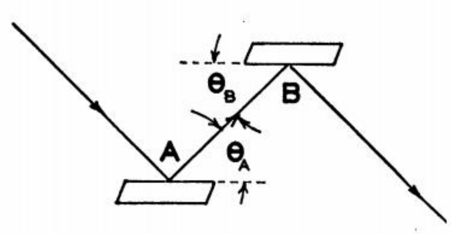
(ex23_crystal_laue.ows)

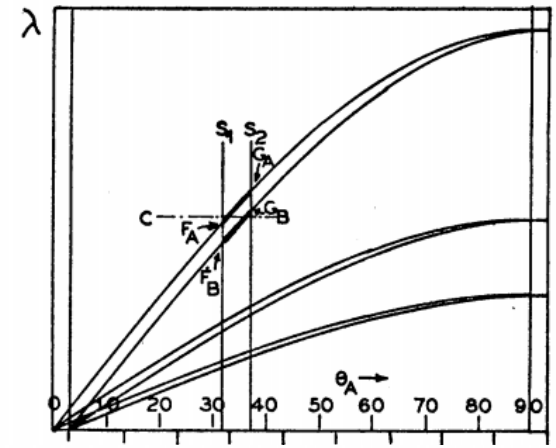


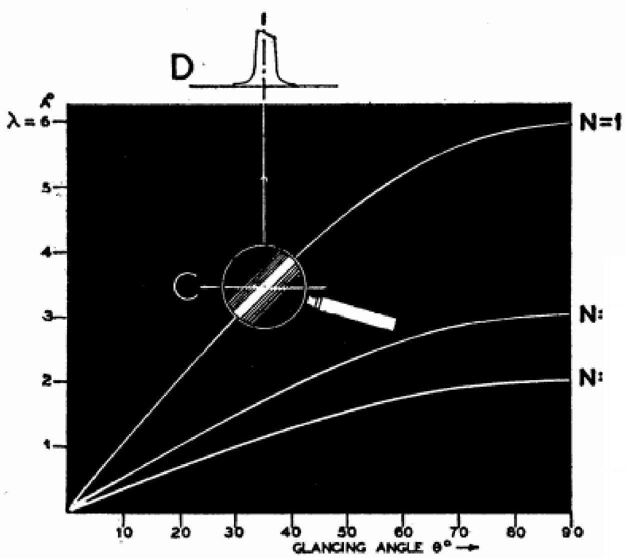
Theory of the Use of More Than Two Successive X-Ray Crystal Reflections to Obtain Increased Resolving Power

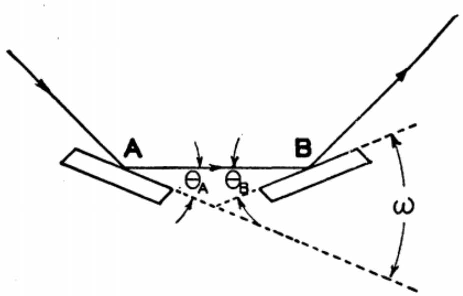
J W. M. DuMond Phys. Rev. **52**, 872 – (1937)

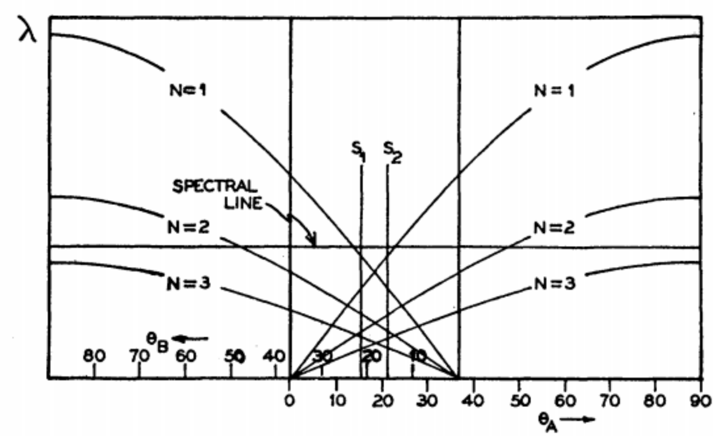
http://dx.doi.org/10.1103/PhysRev.52.872



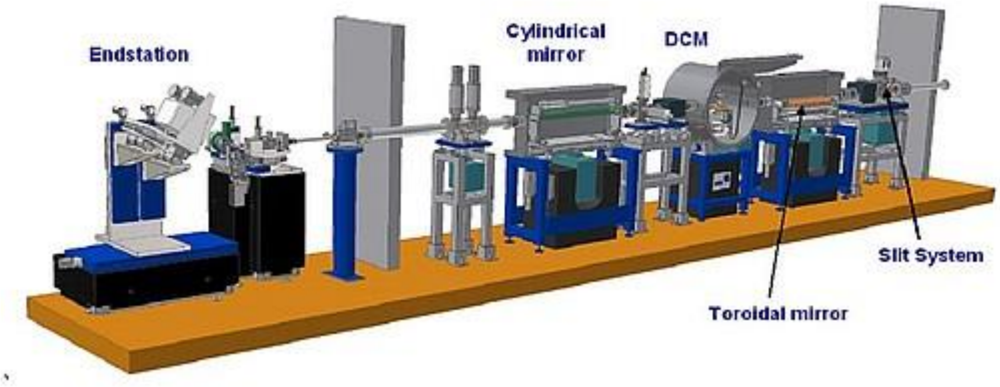








Other



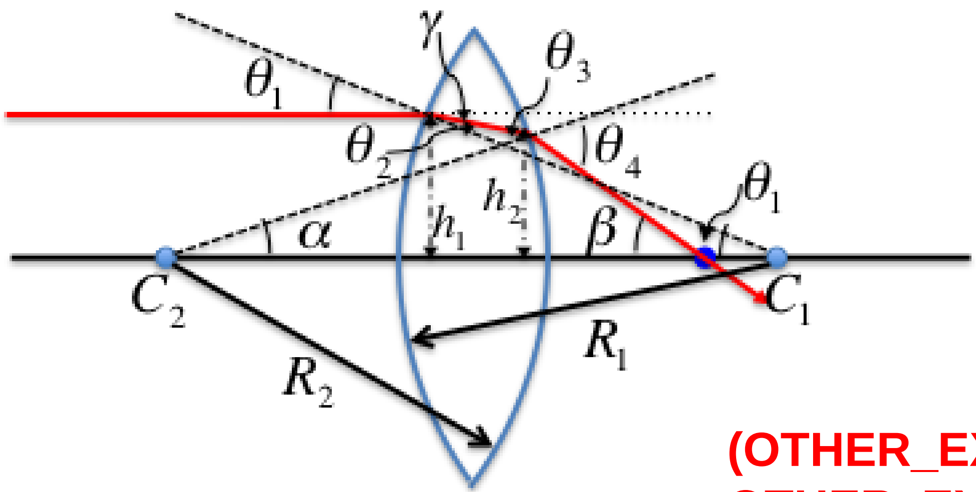
ex19_beamline.ows

LENSE = TWO INTERFACES

Geometrical model

Law of Refraction (Snell's Law)

$$n_1 \sin\theta_1 = n_2 \sin\theta_2$$



Physical model

absorption in media

$I/I_0 = \exp(-\mu\ t)$

(OTHER_EXAMPLES/lens_elliptical.ows)
OTHER_EXAMPLES/CRL_Snigirev_1996.ows
ex24_transfocator.ows

CRL = *n* identical Lenses

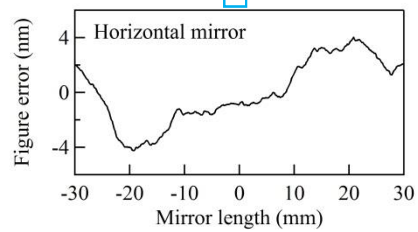
TRANSFOCATOR = *m* different CRLs

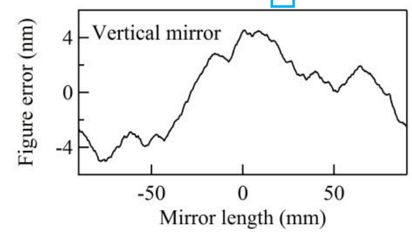
HYBRID METHOD IN SHADOW (X. Shi *et al.*)

Combining ray tracing and wavefront propagation

$$\text{Plane wave} \times \exp\left[-ik\left(\frac{x^2}{2f_x}+\frac{z^2}{2f_z}\right)\right] \times \exp[-i2k\sin\theta_x \cdot \text{Height}(x)] \times \exp[-i2k\sin\theta_z \cdot \text{Height}(z)]$$

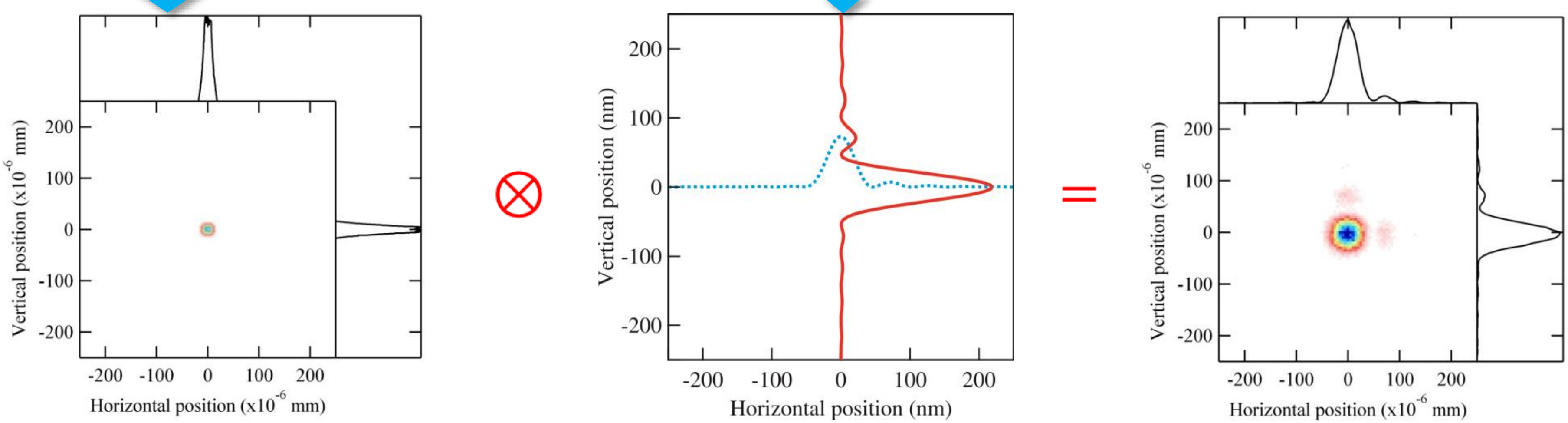
Ideal lens with focal lengths of f_x and f_z





$$E(x,z) \rightarrow \boxed{\text{FFT}} \xrightarrow{\mathcal{F}(u,v)} \boxed{\times \exp\left[-\frac{i2\pi^2}{k}(u^2+v^2)y\right]} \xrightarrow{\mathcal{F}'(u,v)} \boxed{\text{Inverse FFT}} \rightarrow E(x',z')$$

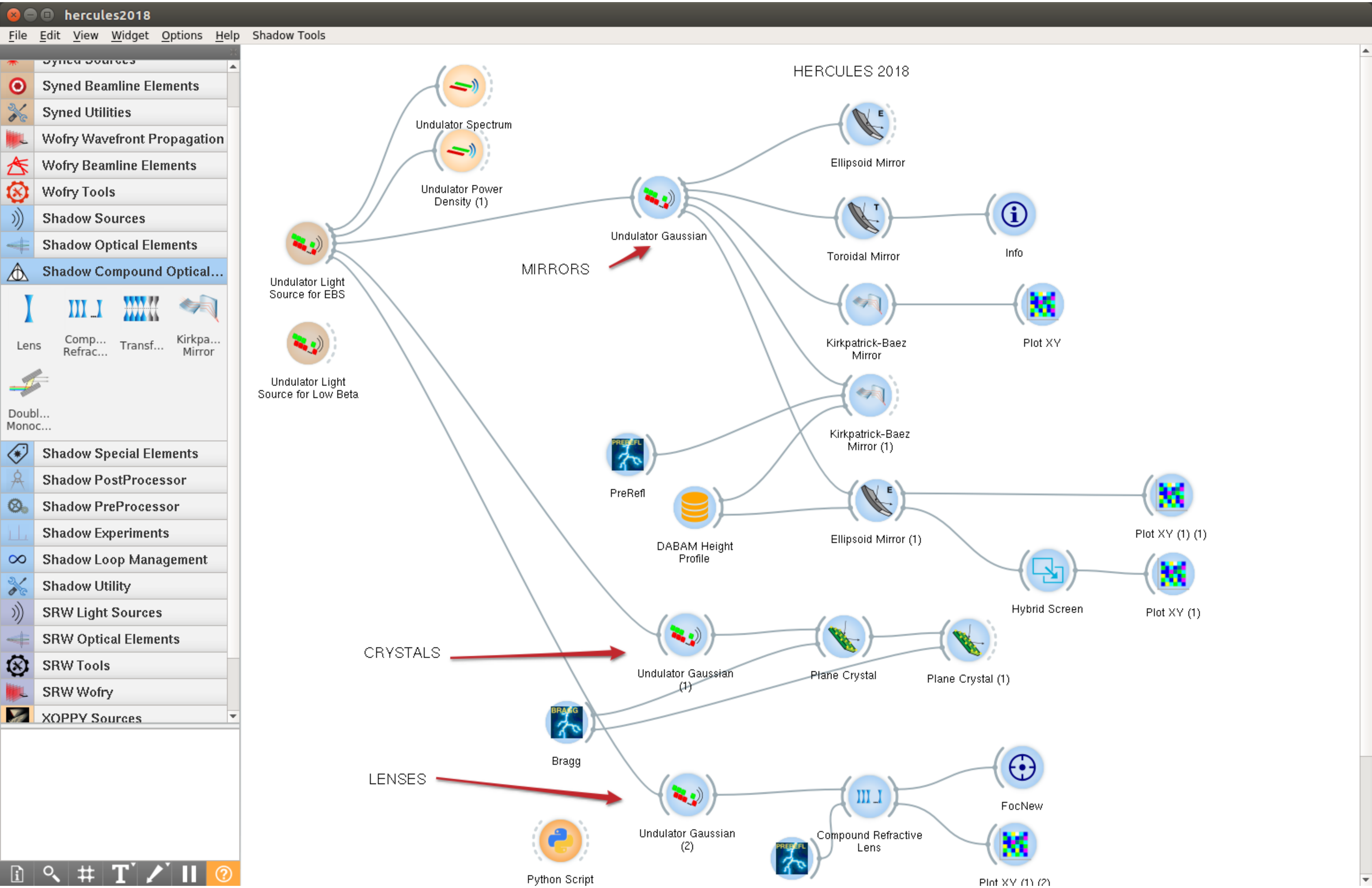
Ray tracing of the beamline



X. Shi, R. Reininger, M. Sanchez del Rio, L. Assoufid " J. Synchrotron Rad. (2014) 21, doi:10.1107/S160057751400650X

X. Shi, M. Sanchez del Rio and Ruben Reininger Proc. SPIE 9209, 920911 (2014); doi:10.1117/12.2061984

X. Shi, R. Reininger, M. Sánchez del Río, J. Qian and L. Assoufid Proc. SPIE 9209, 920909 (2014); doi:10.1117/12.2061950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Transf...
Kirkpa... Mirror
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Shadow Special Elements
Shadow PostProcessor
Shadow PreProcessor
Shadow Experiments
Shadow Loop Management
Shadow Utility
SRW Light Sources
SRW Optical Elements
SRW Tools
SRW Wofry
XOPPY Sources
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Undulator Power Density (1)
Undulator Light Source for EBS
Undulator Light Source for Low Beta
Undulator Gaussian
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Kirkpatrick-Baez Mirror (1)
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DABAM Height Profile
Ellipsoid Mirror (1)
Plot XY (1) (1)
Hybrid Screen
Plot XY (1)
CRYSTALS
Undulator Gaussian (1)
Plane Crystal
Plane Crystal (1)
Bragg
LENSES
Undulator Gaussian (2)
Compound Refractive Lens
FocNew
Python Script