Introduction to SHADOW and ShadowOui

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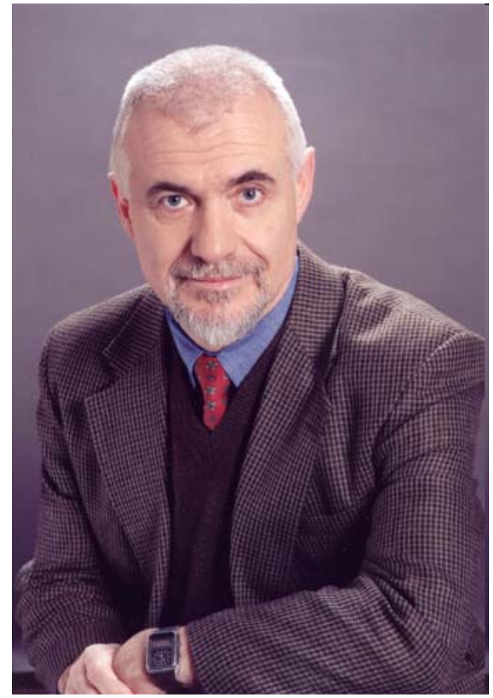
Outlook

- History
- What you must know of SHADOW and ShadowOui does not do it for you
- Exercises
  - Sources: Geometrical, Undulator Gaussian, Undulator Full
  - Mirror systems and aberrations
  - Crystal monochromators
  - Lenses
  - Complete Beamline ISN

Birth of SHADOW (~1980)

- Scientific motivation:
  Grating monochromator design, TGM, ERG, toridal, spherical mirrors.
- Monte Carlo ray tracing program ***designed*** to simulate X-ray optical systems
- Requirements
  - Accuracy and reliability
  - Easy to use
  - Flexibility
  - Economy of computer resources
  - VAX-11 Computers
- Efficient MC approach
  - Reduced number of rays
  - Exact simulation os SR sources
  - Vector calculus
  - Modular
  - User-interface
  - Available to users
- Two years development
- Fortran 77+VAX/VMS extensions



Ray tracing of recent VUV monochromator designs

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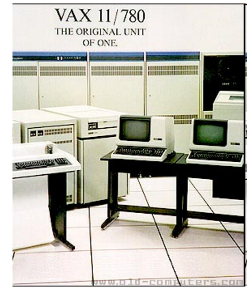
Abstract

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.

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

Shadow 1

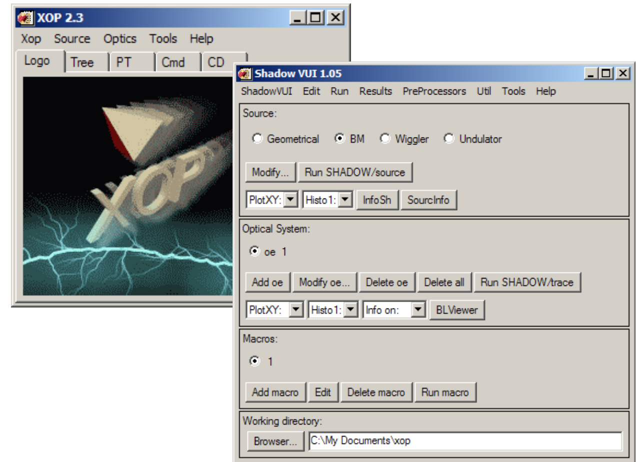
VAX-VMS 1980-1990



Shadow 2

1990 Unix workstations

XOP interface



Shadow 3

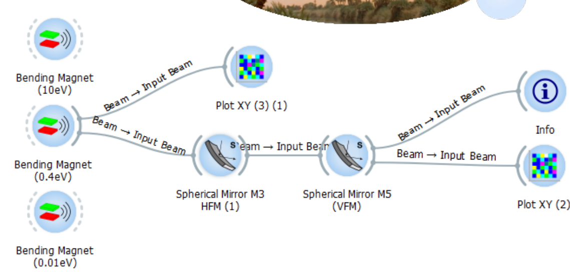
2010 F90+Python binding

2014 Orange interface: Oasys

Shadow 4

2020? Full python version

Exploit Oasys framework



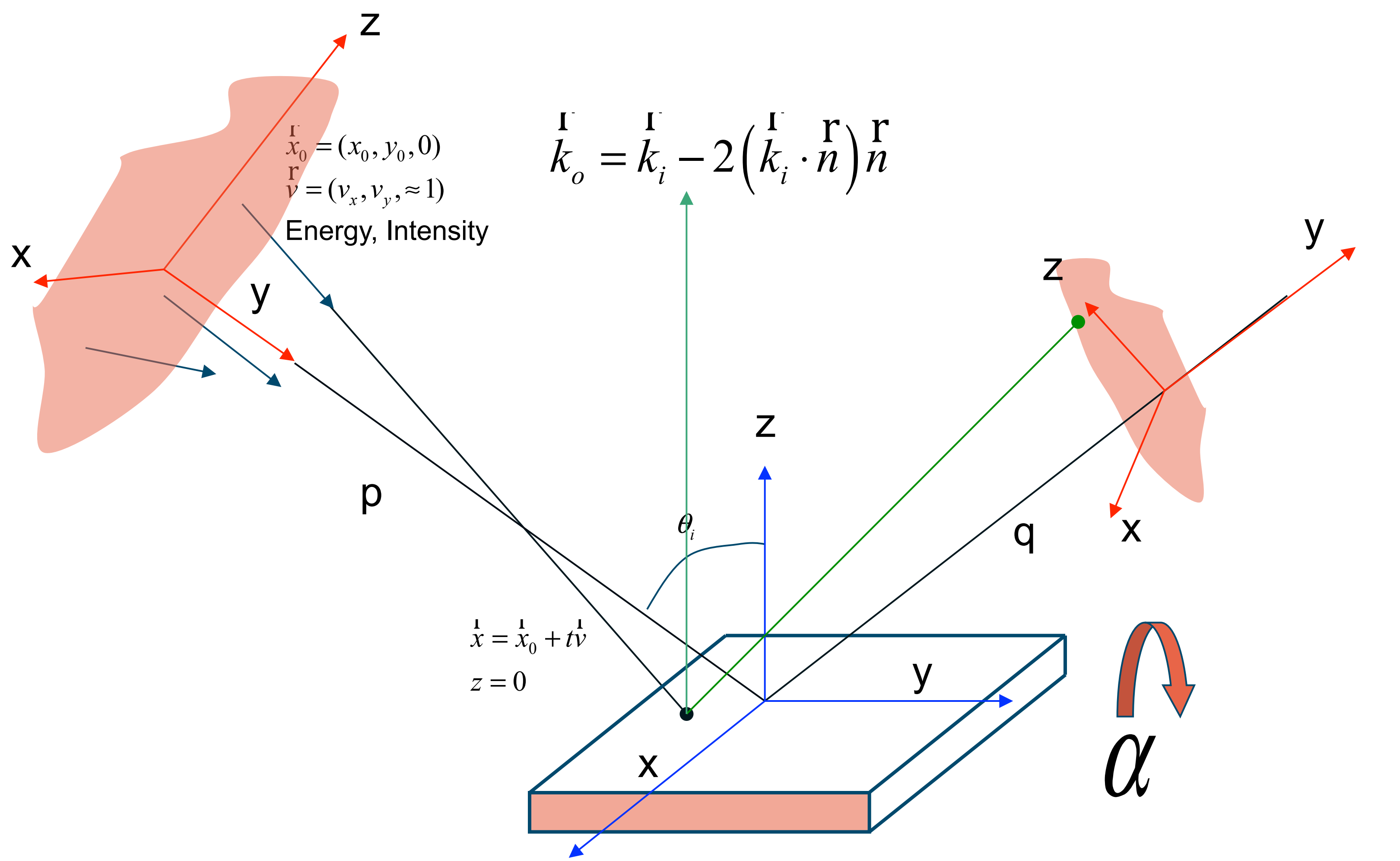
OrAnge SYnchrotron Suite (OASYS)

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

ShadowOui	XOPpy	SRW	WOFRY	COMSYL
shadow3	xraylib	srwlib	wofry	comsyl

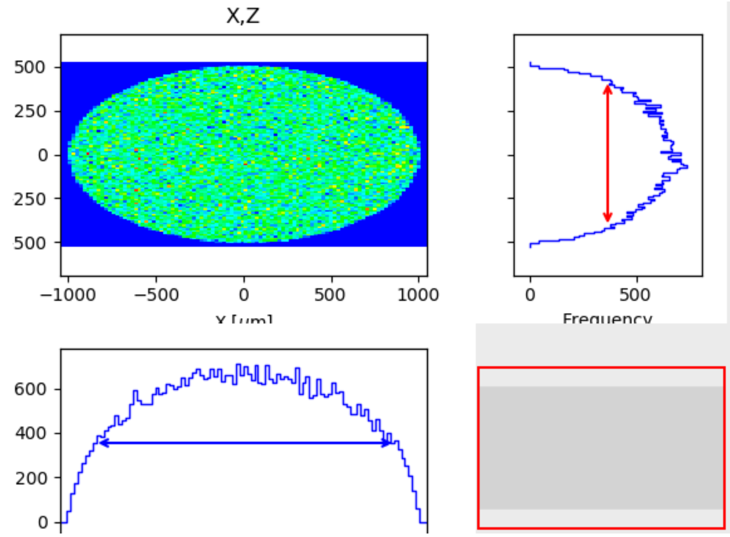
Ray tracing

Trace (the beamline)

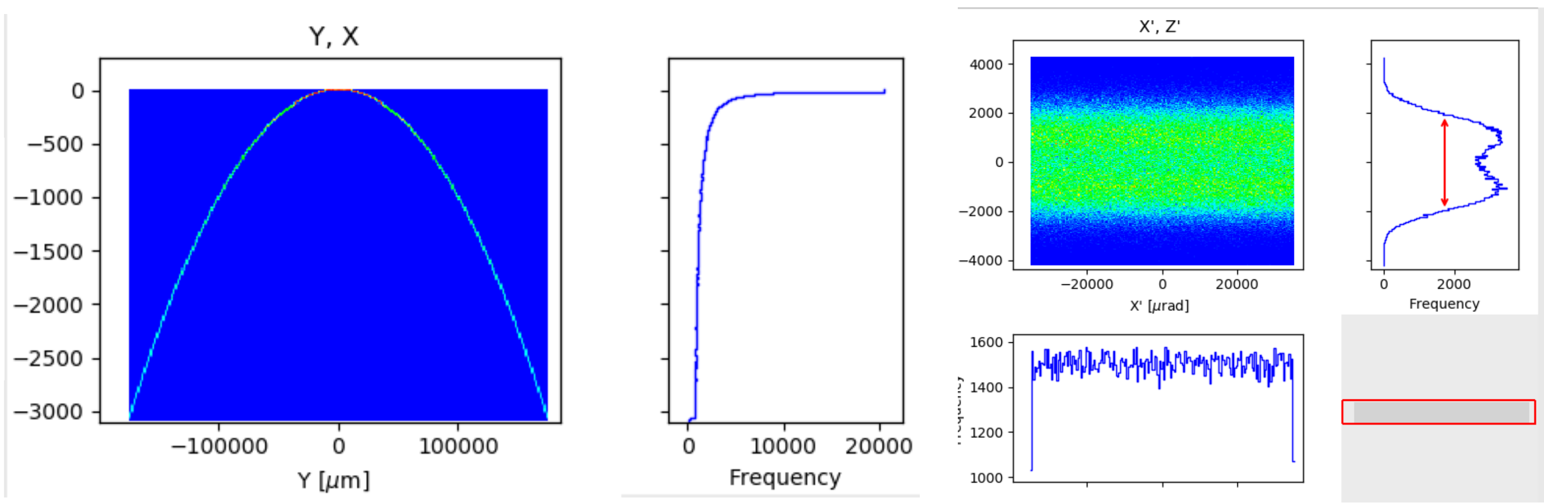


ShadowOUI Sources I

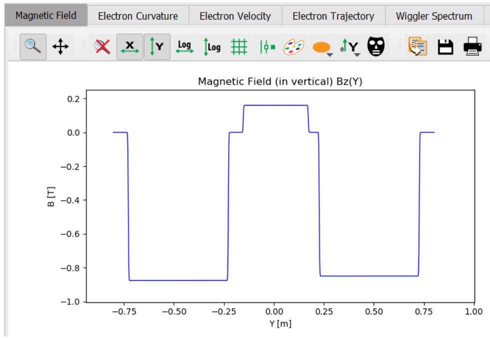
Geometrical Source



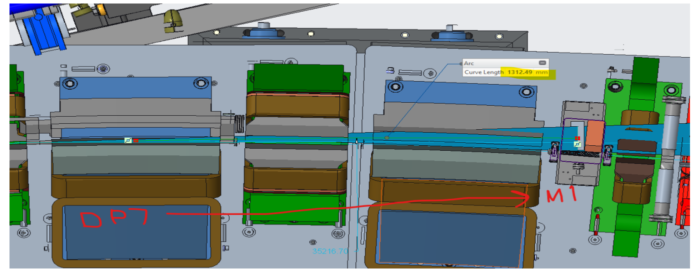
Bending Magnet

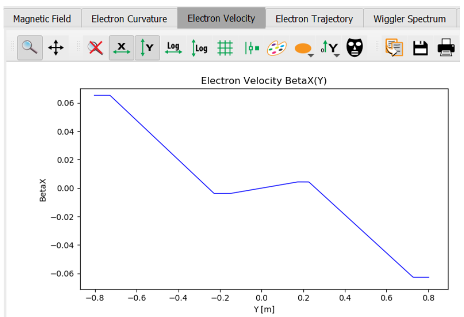


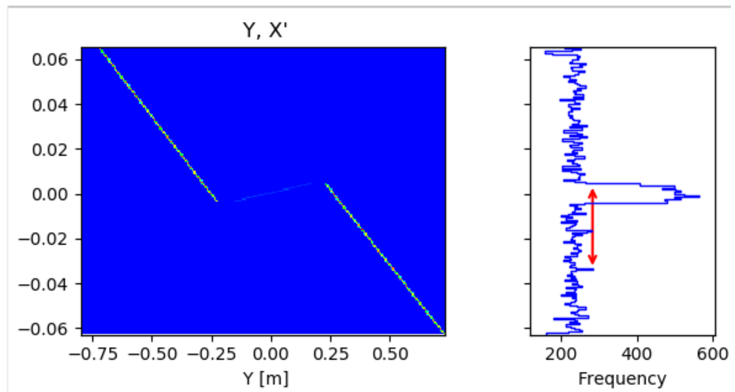
Sources II (Wiggler)

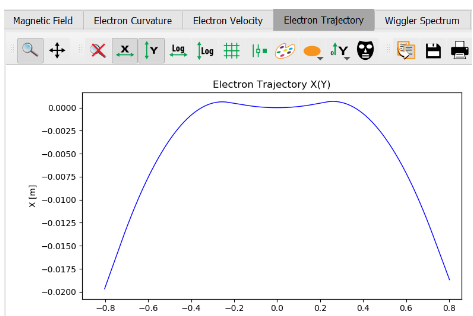


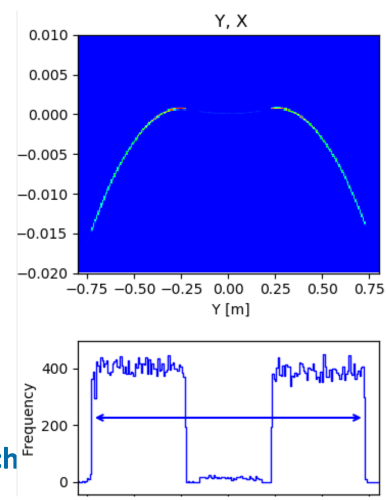
Wiggler











Sources III (Undulator)

Fake Geometrical Source (Gaussian spatial + Gaussian divergency)

Undulator Gaussian

Single e$^-$

Divergence:

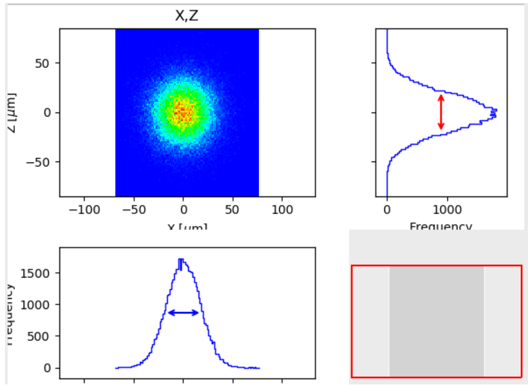
$$\sigma_{r'} = 0.69\sqrt{\frac{\lambda}{L}} \approx \sqrt{\frac{\lambda}{2L}}$$

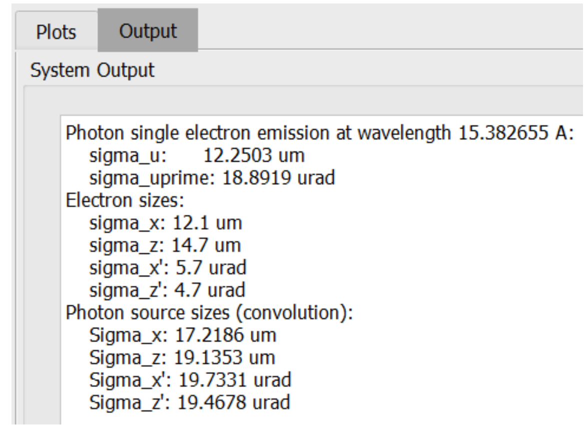
Size:

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

Photon source:

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



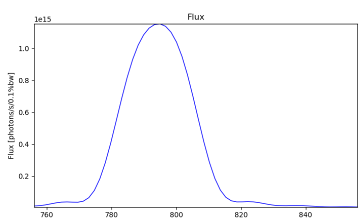

Plots | Output

System Output

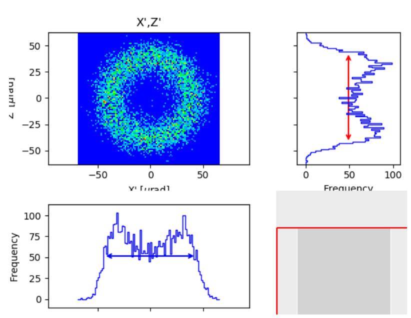
Photon single electron emission at wavelength 15.382655 A:
sigma_u: 12.2503 um
sigma_uprime: 18.8919 urad
Electron sizes:
sigma_x: 12.1 um
sigma_z: 14.7 um
sigma_x': 5.7 urad
sigma_z': 4.7 urad
Photon source sizes (convolution):
Sigma_x: 17.2186 um
Sigma_z: 19.1353 um
Sigma_x': 19.7331 urad
Sigma_z': 19.4678 urad

Full Undulator

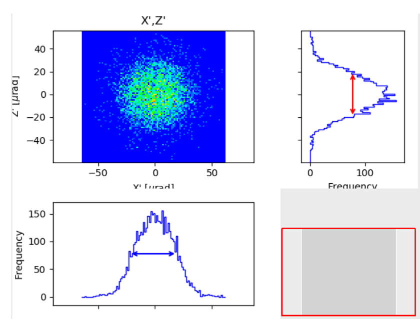
Full Undulator



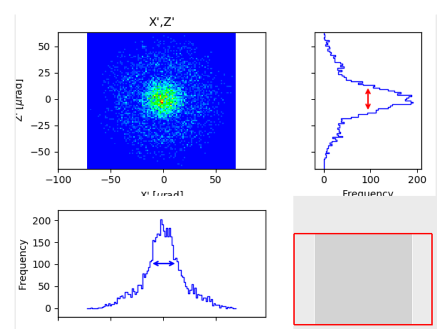
789.938eV



806.060eV

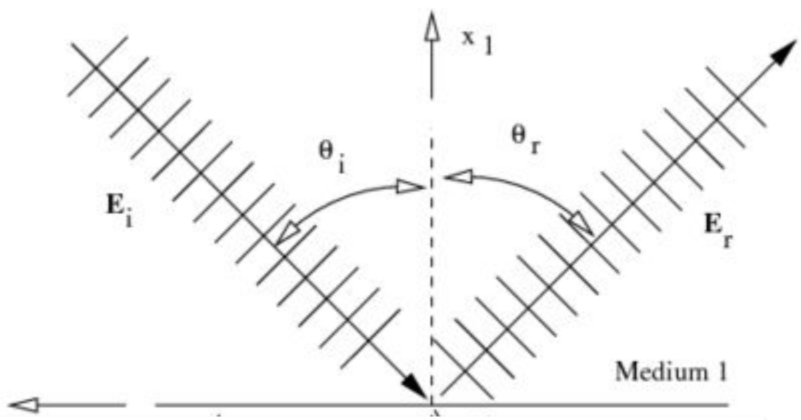


814.121eV



Optical Elements (mirrors)

Geometrical model

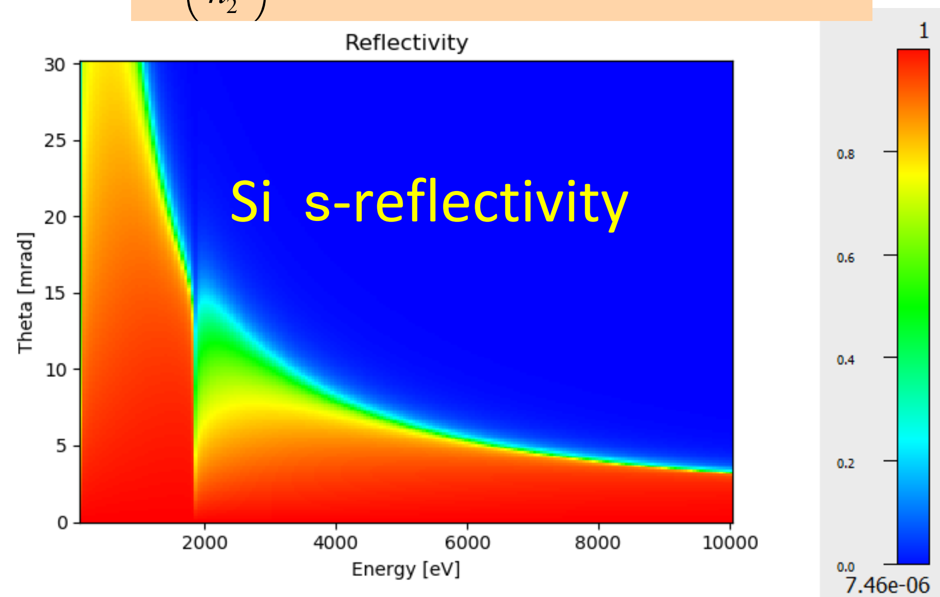


$$\hat{\mathbf{d}}_s = 2\left(\hat{\mathbf{d}}_n \cdot \hat{\mathbf{d}}_i\right)\hat{\mathbf{d}}_n - \hat{\mathbf{d}}_i,$$

Physical model

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

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



Optical Elements (gratings)

Geometrical model

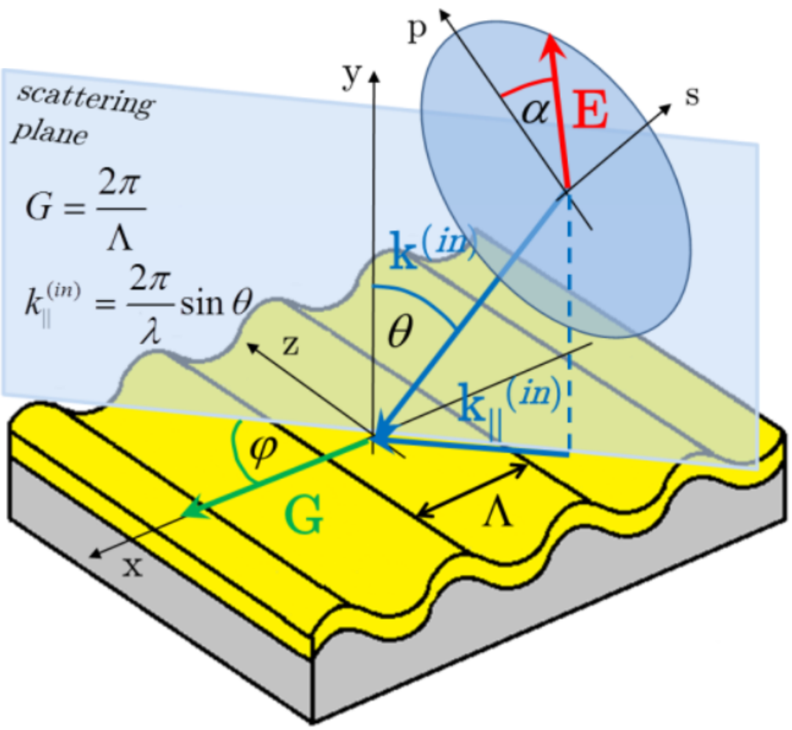


Figure from doi.org/10.5772/51044

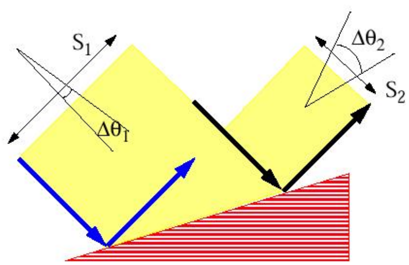
Physical model

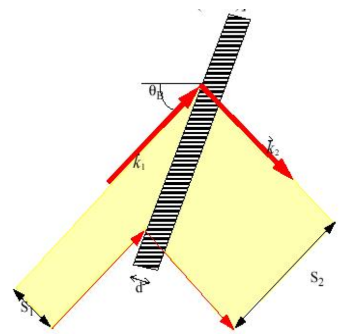
No model (yet) in SHADOW for grating efficiency

SHADOW uses Fresnel equations like for mirrors

Optical Elements (crystals)

Geometrical model



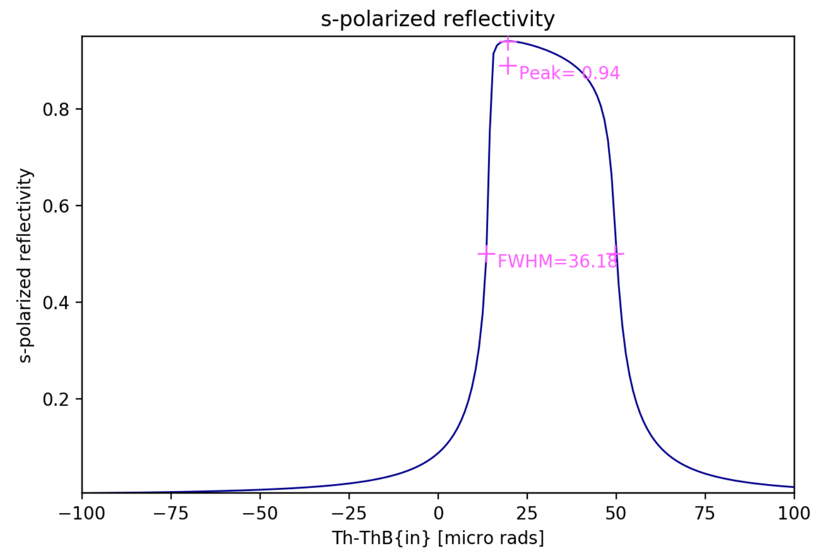


$$|\vec{k}_1| = |\vec{k}_2|$$

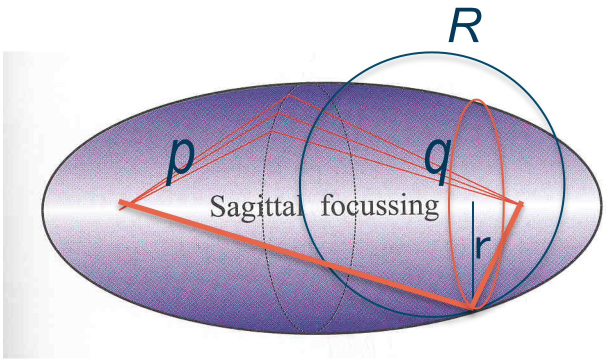
$$\vec{k}_{2,||} = \vec{k}_{1,||} + \vec{G}_{||}$$

Physical model

$$r^{\mathrm{Bragg}}(\alpha_Z) \equiv \frac{1}{|b|}\frac{I^H}{I^0} = \frac{1}{|b|}\left|\frac{x_1 x_2 (c_1 - c_2)}{c_2 x_2 - c_1 x_1}\right|^2$$



Mirrors and aberrations



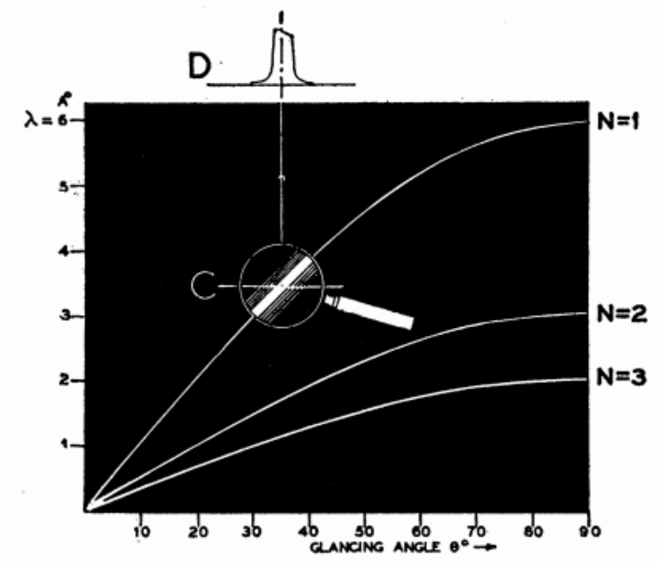
- Ellipsoid: Point to point focusing
- Paraboloid: Collimating
- Focalization in two planes
  - Tangential or Meridional (ellipse or parabola)
  - Sagittal (circle)
- Demagnification: M=p/q
- Easier manufacturing:
  - 2D: Ellipsoid => Toroid
  - Only one plane: cylinder Ellipsoid (ellipse)=> cylinder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

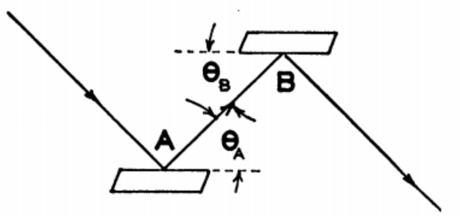
$$\frac{1}{p}+\frac{1}{q}=\frac{2}{R\sin\theta}$$

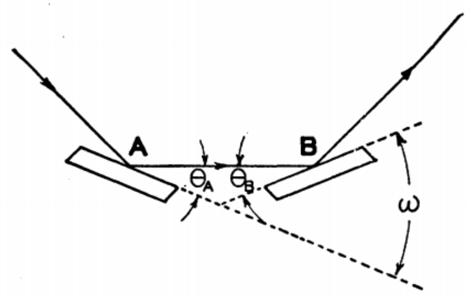
$$\frac{1}{p}+\frac{1}{q}=\frac{2\sin\theta}{\rho}$$

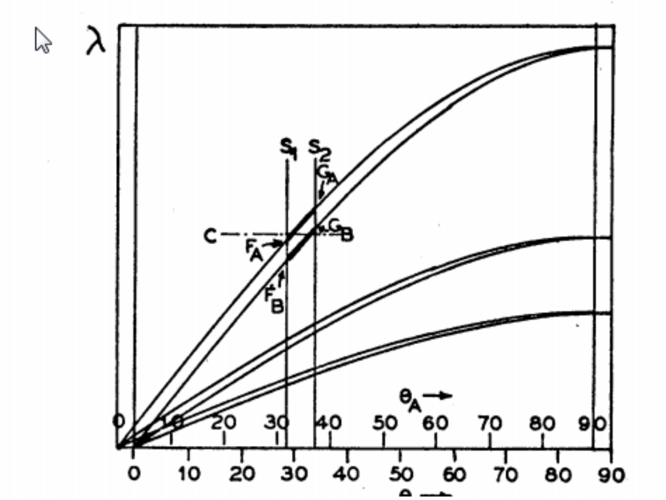
Crystal monochromators ex17_crystalmono.ows

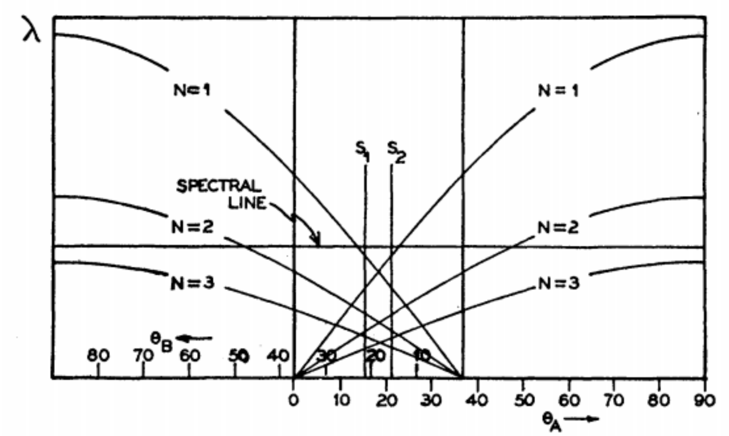
Theory of the Use of More Than Two Successive X-Ray Crystal Reflections to Obtain Increased Resolving Power
J W. M. DuMond Phys. Rev. 52, 872 – (1937)
http://dx.doi.org/10.1103/PhysRev.52.872











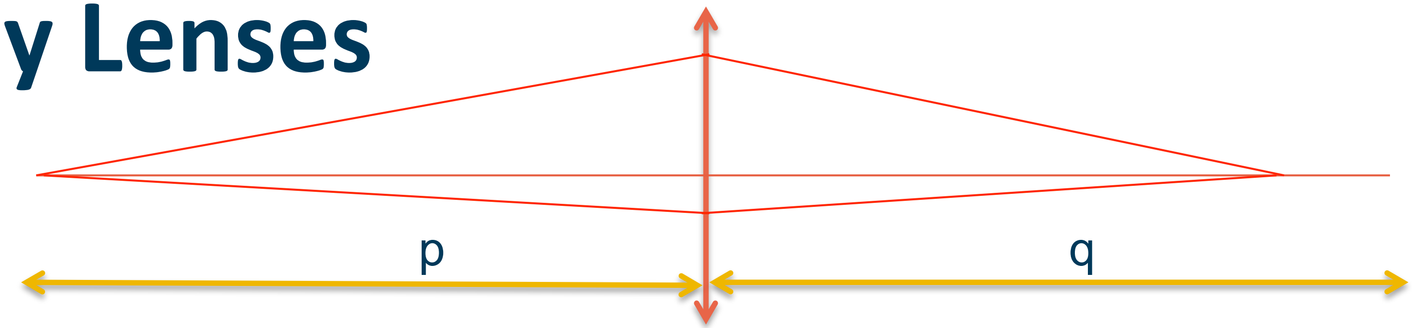
Crystal curvature and spectral resolution

$$\frac{\Delta\lambda}{\lambda_0} = \frac{\Delta E}{E_0} = (\Delta_{src} + \omega_D)\cot\theta_0$$

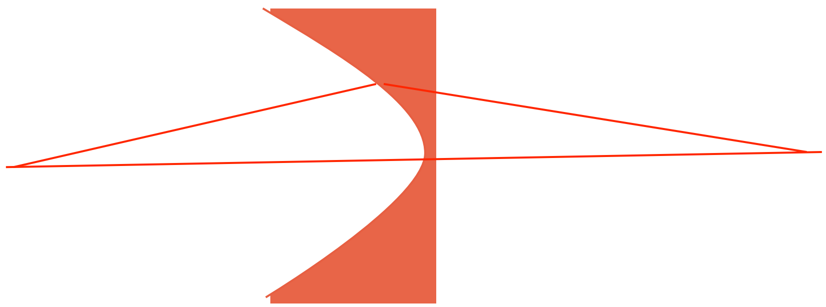
$$\frac{\Delta\lambda}{\lambda_0} = \frac{\Delta E}{E_0} \approx \sqrt{\omega_D^2 + (\Delta_{geom} + \Delta_{ss})^2}\cot\theta_0 = \sqrt{\omega_D^2 + \left[\boxed{\left(\frac{p}{R\sin\theta_1} - 1\right)\Delta_{src}} + \frac{s_1}{p}\right]^2}\cot\theta_0.$$

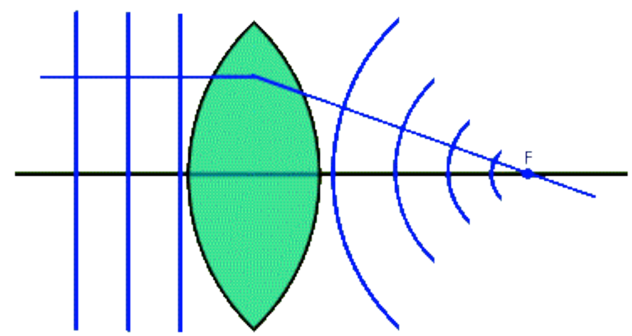
Zero for Rowland mounting:
p = R sin(q) that for Bragg
symmetric reflection means
1:1 magnification

X-ray Lenses



$$\frac{1}{F} = \frac{1}{p} + \frac{1}{q}$$





$$\sin\theta_1 = (1-\delta)\sin\theta_2$$

$$\frac{1}{F} = (n-1)\left(\frac{1}{R_1} - \frac{1}{R_2} + \frac{(n-1)d}{nR_1R_2}\right) \approx \frac{\delta}{R_1}$$

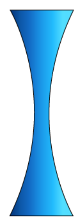
$$E = E_0 e^{i\frac{kr^2}{2f}}$$

CRL (COMPOUND REFRACTIVE LENSES) = replicate N lenses

Single interface

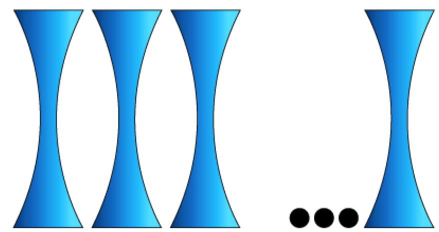
$$F = \frac{R}{\delta}$$

Lens



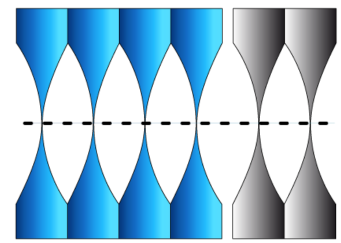
$$F = \frac{R}{2\delta}$$

Compound Refractive Lens (CRL)



$$F = \frac{R}{2N\delta}$$

Transfocator



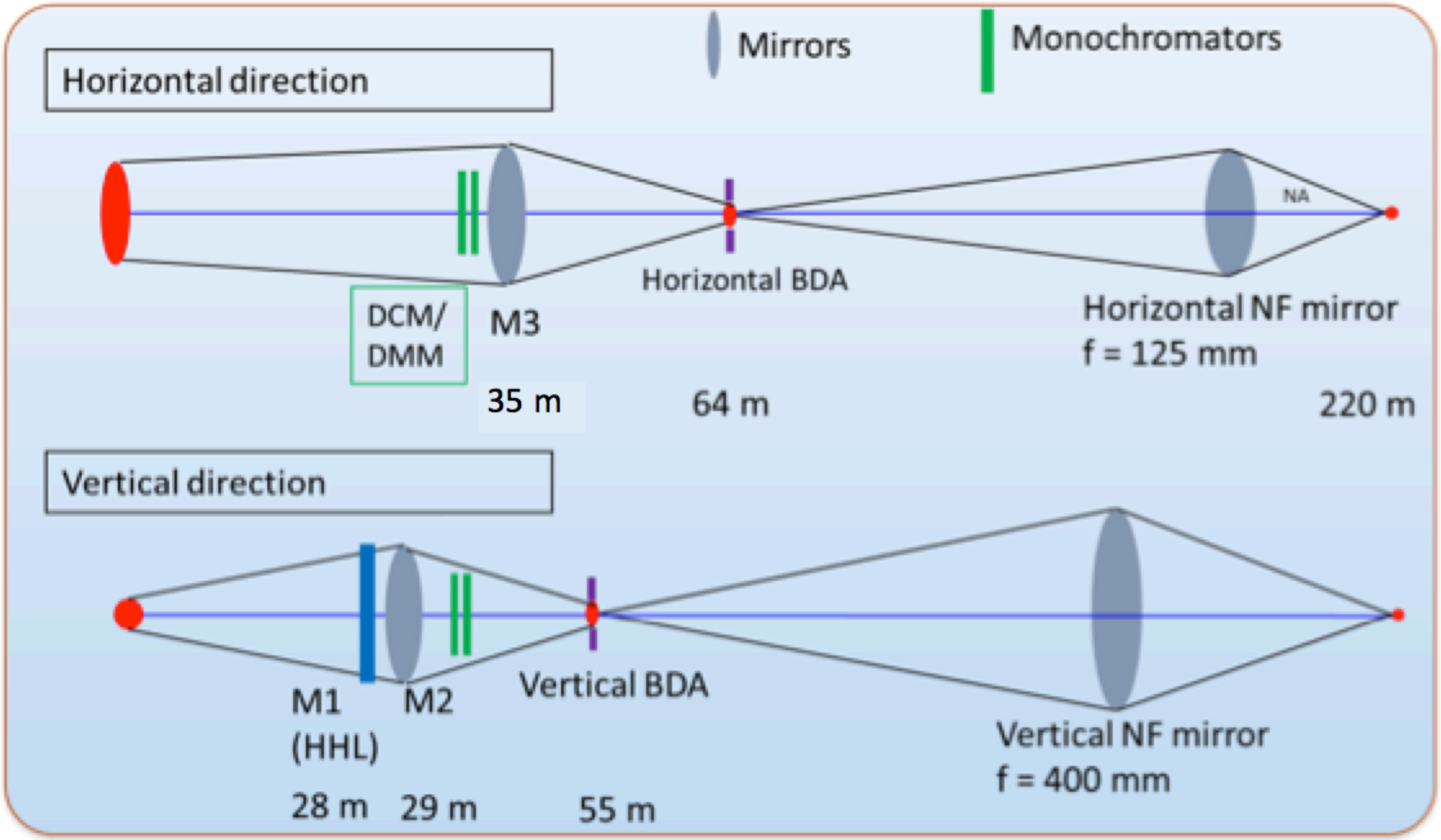
$$\frac{1}{F} = \frac{1}{F_1} + \frac{1}{F_2} + \ldots$$

1996 Experimental demonstration of CRL

- A. Snigirev *et al* Nature 384 (1996) 49

2011 Transfocator

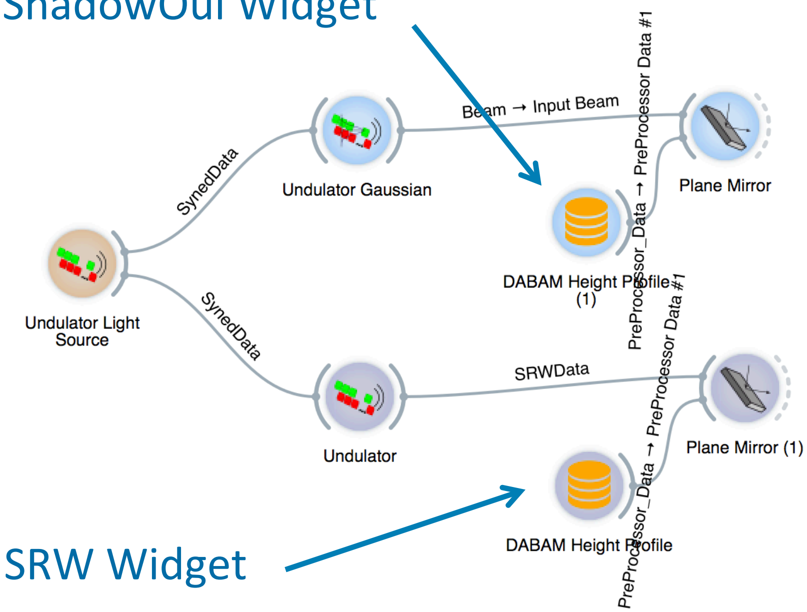
Beamline ISN



Surface Errors: DABAM

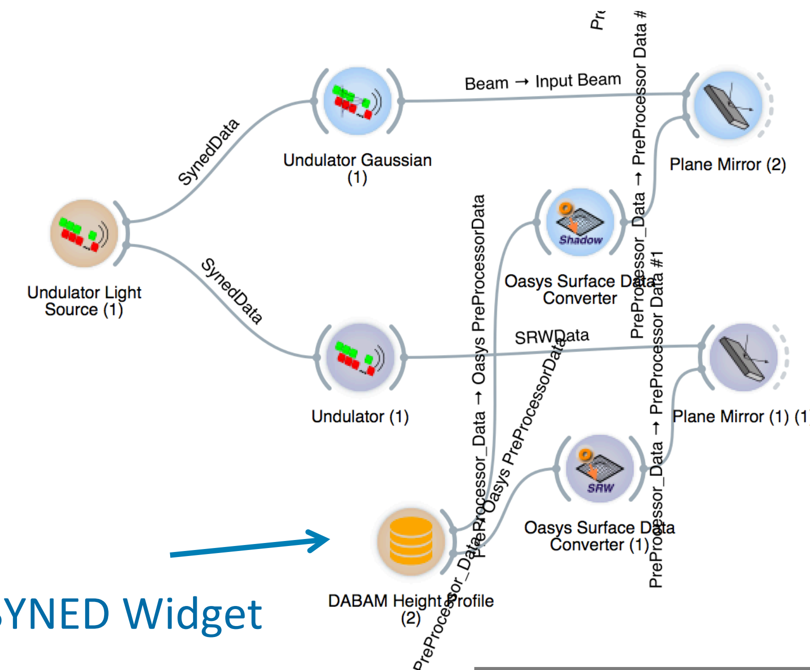
Direct link

ShadowOui Widget

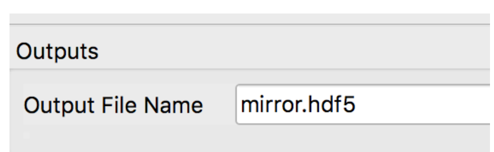


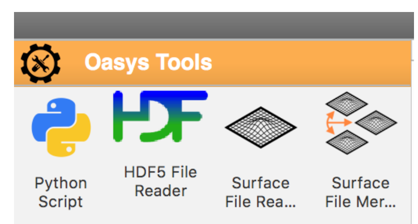
SRW Widget

Common format



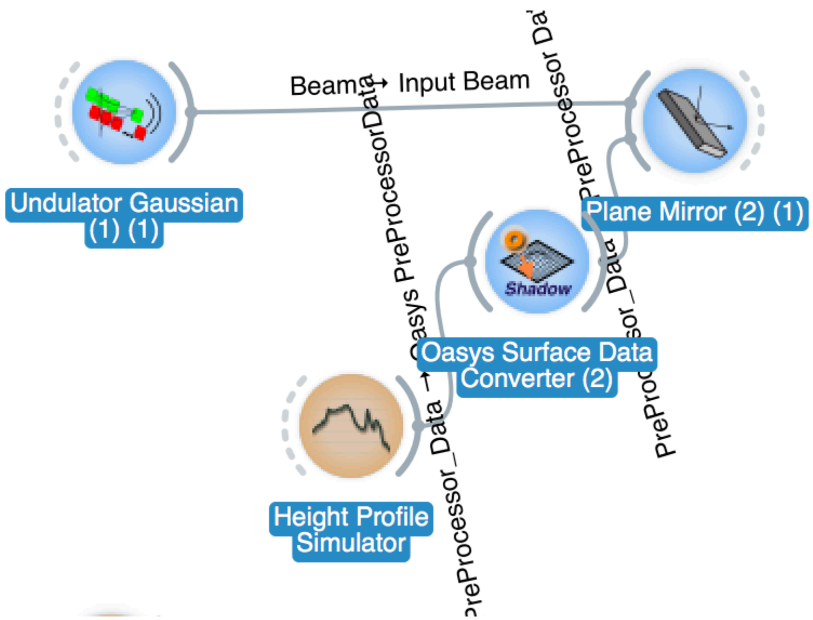
SYNED Widget





Surface Errors

Height Profile Simulator



Pre-DABAM