

HERCULES 2021 - TUTORIAL

Modelling SR beamlines using OASYS

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2021 March 3rd 14:00

Outline

- Introduction to OASYS
- XOPPY toolbox: Source emission and characteristics of optical elements. Power transport
- ShadowOUI: Ray tracing SR beamlines
 - Mirror aberrations
 - Crystal systems
 - Lenses
- WOFRY and SRW: coherent beam transport:
 - Simple examples with WOFRY
 - Introduction to Partial coherence

Outcome

Calculate main characteristics of synchrotron sources (dipoles and IDs)

Simulating beamline optics by ray-tracing to obtain main parameters of beam size, energy resolution and flux

Understand basic principles of x-ray optics: Reflective (aberrations, slope errors), Diffractive (dispersion) and Refractive (chromatic aberrations)

A few concepts about coherence

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The OASYS Project

<https://oasys-kit.github.io/>



Argonne
NATIONAL LABORATORY



Elettra Sincrotrone Trieste



Luca Rebuffi

Manuel Sanchez del Rio

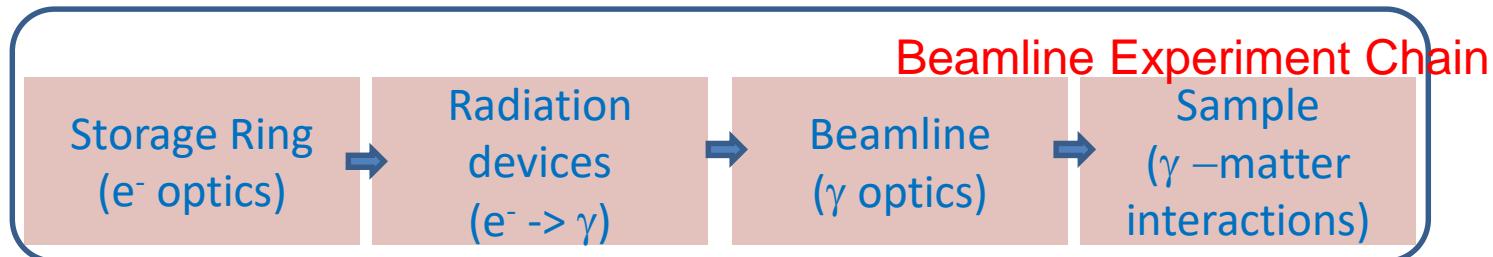
- ✓ OASYS = OrAnge SYnchrotron Suite
- ✓ A common platform to build synchrotron-oriented User Interfaces ***that communicate***
- ✓ The upper layer of the application presented to the user
- ✓ Open Source & Python technology

Luca Rebuffi, Manuel Sanchez del Rio (2017)

OASYS (OrAnge SYnchrotron Suite) : an open-source graphical environment for x-ray virtual experiments

Proc. SPIE 10388: 10388-10388. <http://dx.doi.org/10.1117/12.2274263>

Synchrotron Virtual Experiments



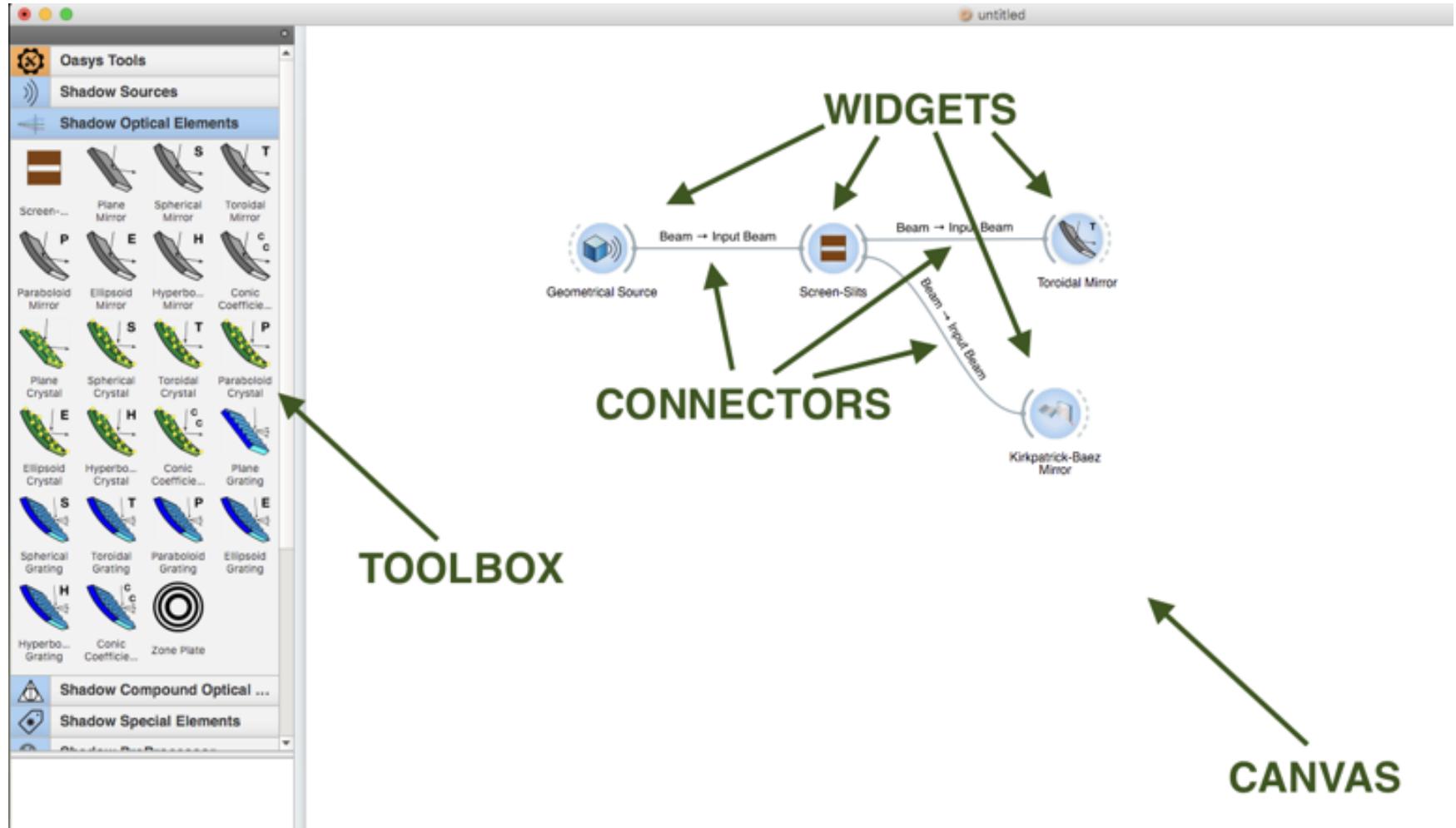
Upper layer based
on ORANGE (U Ljubljana)



Suite of Add-ons



The OASYS language



Multiple tools in the same environment



L. Rebuffi & M. Sanchez del Rio, Proc. SPIE 10388, 103880S (2017)

X. Shi et al., J. Synchrotron Rad. 21, 669 (2014)

L. Rebuffi & M. Sanchez del Rio, J. Synchrotron Rad. 23, 1357 (2016)

M. Sanchez del Rio et al., J. Synchrotron Rad. 23, 665 (2016)

References

Official Web Page

<https://www.aps.anl.gov/Science/Scientific-Software/OASYS>
or <https://oasys-kit.github.io/>

OASYS Publications

- M. Sanchez del Rio, L. Rebuffi, J. Demšar, N. Canestrari and O. Chubar, *A proposal for an open source graphical environment for simulating X-ray optics*, Proc. SPIE 9209, 92090X (2014)
- X. Shi, R. Reininger, M. Sanchez del Rio, L. Assoufid, *A hybrid method for X-ray optics simulation: combining geometric ray-tracing and wavefront propagation*, J. Synchrotron Rad. 21, 669 (2014)
- X. Shi, R. Reininger, M. Sanchez del Rio, J. Qian, L. Assoufid, *X-ray optics simulation and beamline design using a hybrid method: diffraction-limited focusing mirrors*, Proc. SPIE, 9209, 920909 (2014)
- M. Sanchez del Rio, D. Bianchi, D. Cocco, M. Glass, M. Idir, J. Metz, L. Raimondi, L. Rebuffi, R. Reininger, X. Shi, F. Siewert, S. Spielmann-Jaeggi, P. Takacs, M. Tomasset, T. Tonnessen, A. Vivo and V. Yashchuk, *DABAM: an open-source database of X-ray mirrors metrology*, J. Synchrotron Rad. 23 (2016).
- L. Rebuffi, M. Sanchez del Rio, *ShadowOui: A new visual environment for X-ray optics and synchrotron beamline simulations*, J. Synchrotron Rad. 23 (2016)
- L. Rebuffi, M. Sanchez del Rio, *Interoperability and complementarity of simulation tools for beamline design in the OASYS environment*, Proc. SPIE 10388, 1038808 (2017).
- L. Rebuffi, M. Sanchez del Rio, *OASYS (OrAnge SYnchrotron Suite): an open-source graphical environment for x-ray virtual experiments*, Proc. SPIE 10388, 103880S (2017).

Three sessions

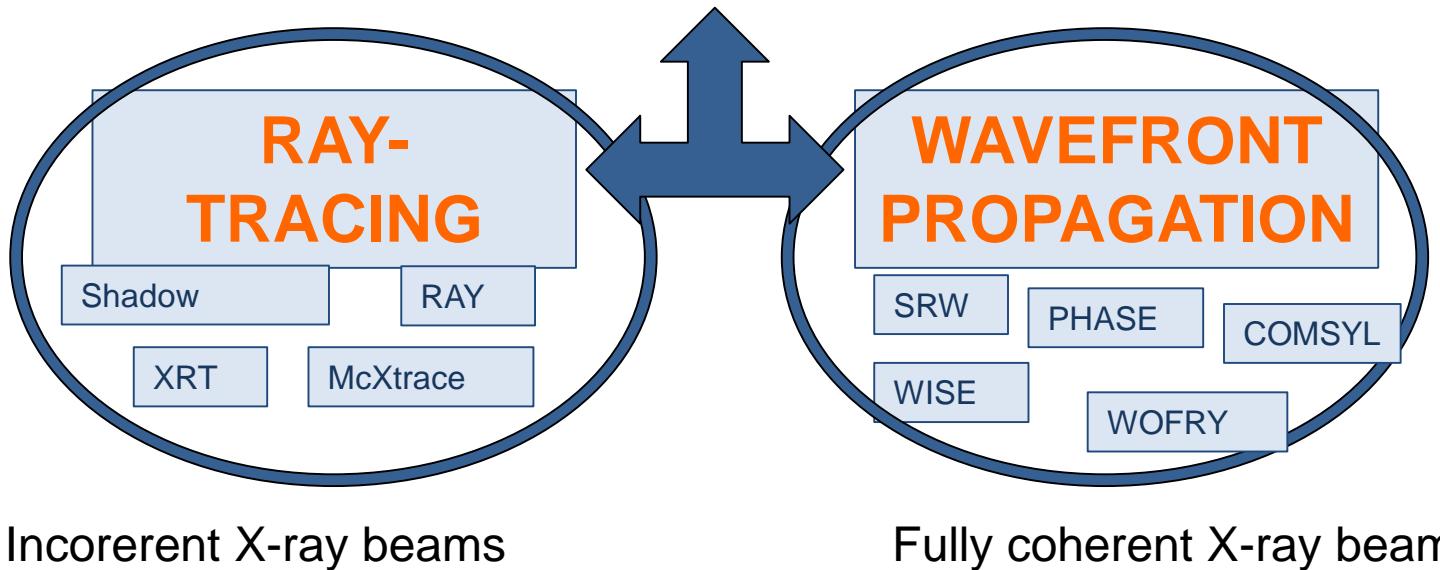
- XOPPY (tools) hercules_xoppy.ows
- ShadowOUI (ray tracing) hercules_shadowoui.ows
- WOFRY (wave optics) hercules_wofry.ows

X-ray optics for synchrotron and XFEL beamlines

Computer simulation of light sources and optical components is a mandatory step in the design and optimization of synchrotron and FEL radiation beamlines



different codes for numerical simulations are available, implementing different physical approaches



Propagation of one wavefront.
One wavefront is coherent by nature.

$$\nabla \cdot \vec{D} = \rho_{\text{free}}$$

$$\nabla \cdot \vec{B} = 0$$

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$$\nabla \times \vec{H} = \vec{J}_{\text{free}} + \frac{\partial \vec{D}}{\partial t}$$



Maxwell Equations



Wave Equations



Helmholtz Equation

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

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

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

$$\vec{E} = \vec{e} e^{ik_0 S(r)} \quad \text{Geometrical Optics}$$

$$\vec{H} = \vec{h} e^{ik_0 S(r)}$$

$$(\nabla S)^2 = n^2$$

$$\nabla S = n \vec{s}$$

$$\frac{d}{ds} \left(n \frac{d\vec{r}}{ds} \right) = \nabla n$$

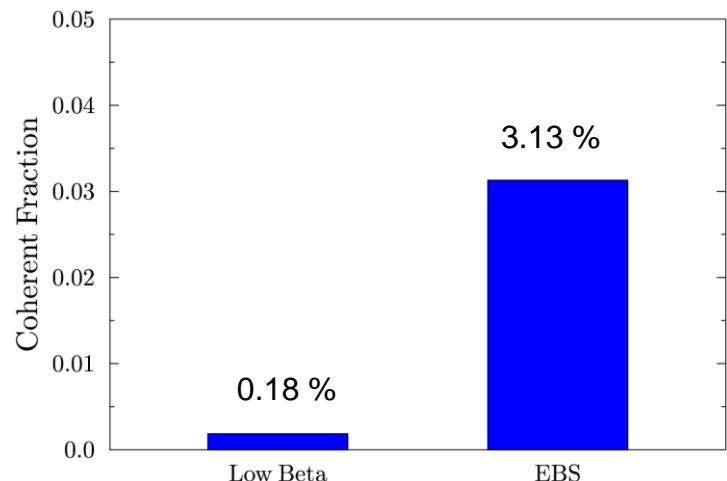
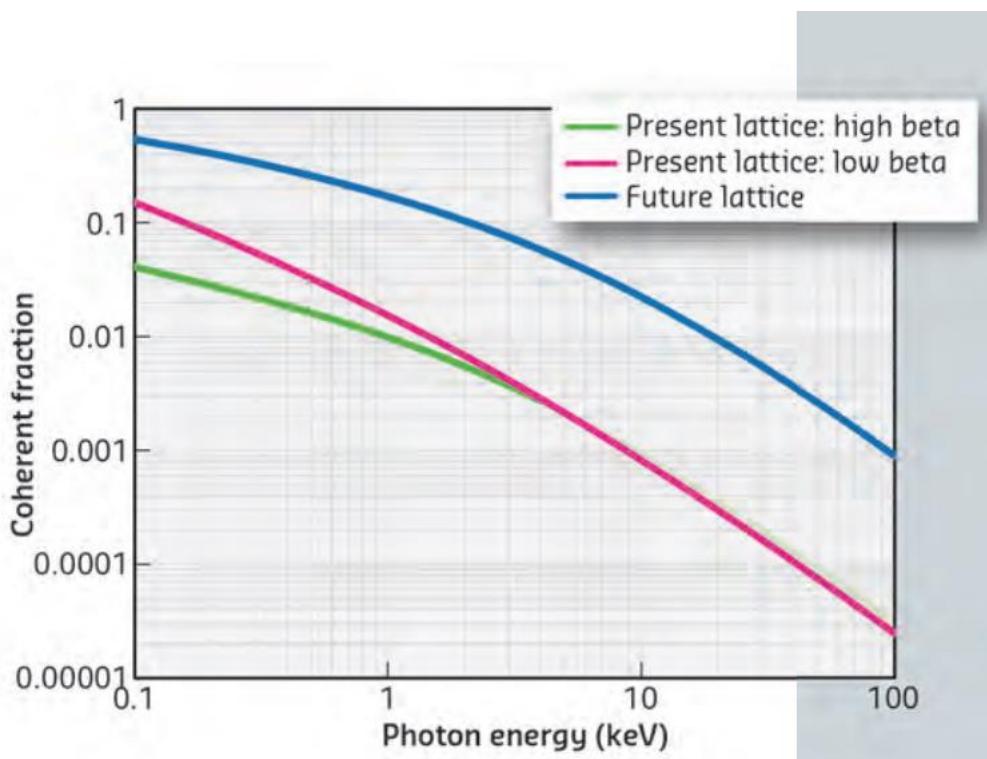
$$\nabla n = 0 \Rightarrow \frac{d\vec{r}}{ds} = 0 \Rightarrow \vec{r} = s\vec{a} + \vec{b}$$



A wavefront is approximated by a ray. Many rays are summed up to form a beam, that is incoherent.

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

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

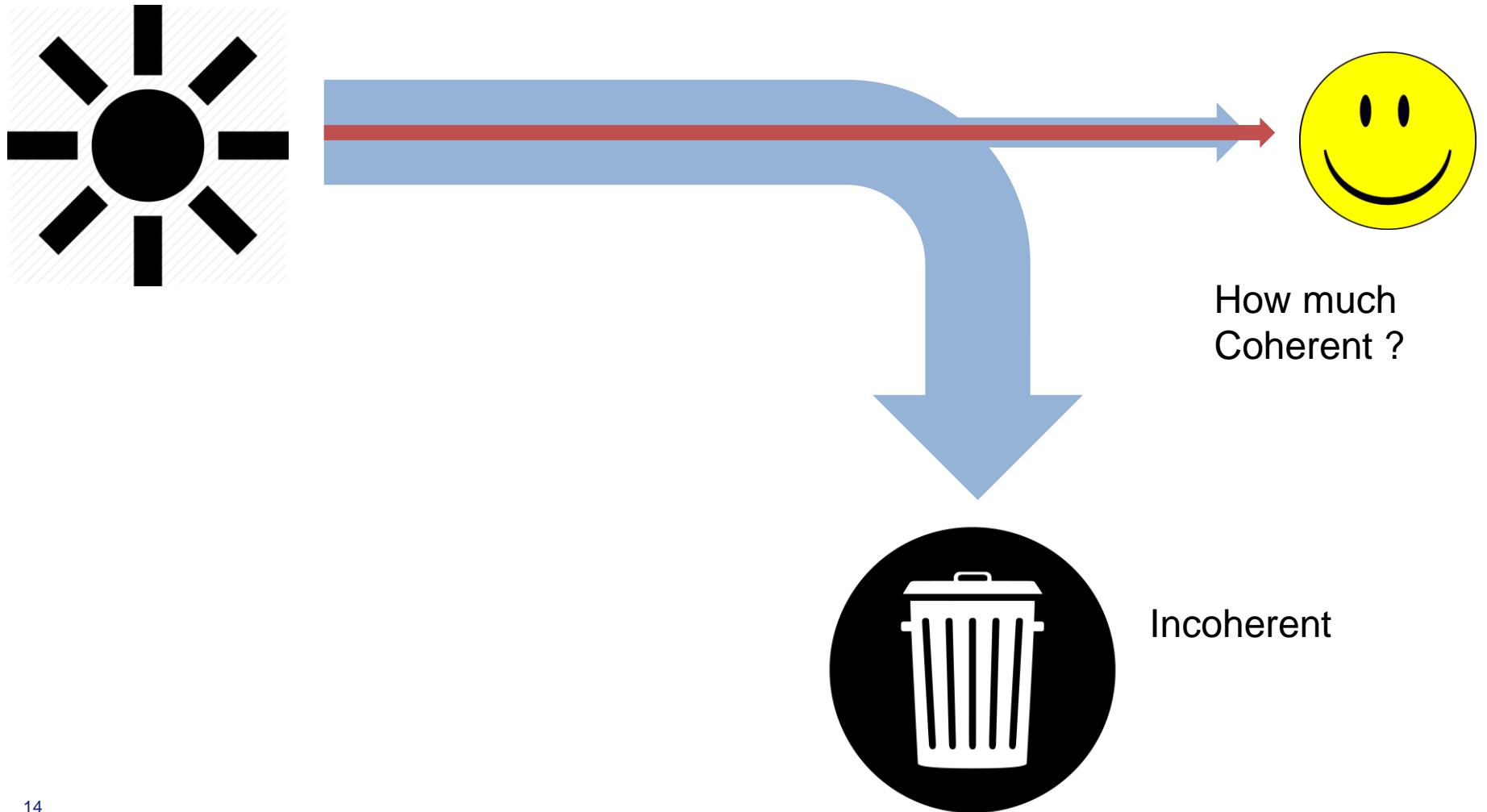


COMSYL calculation
U17 2m @ 17 keV ($K=0.4842$) $L=2\text{m}$

Source: ESRF Orange book

Typical coherence beamline

Partial coherence optics



Hierarchical approach to study beamline optics

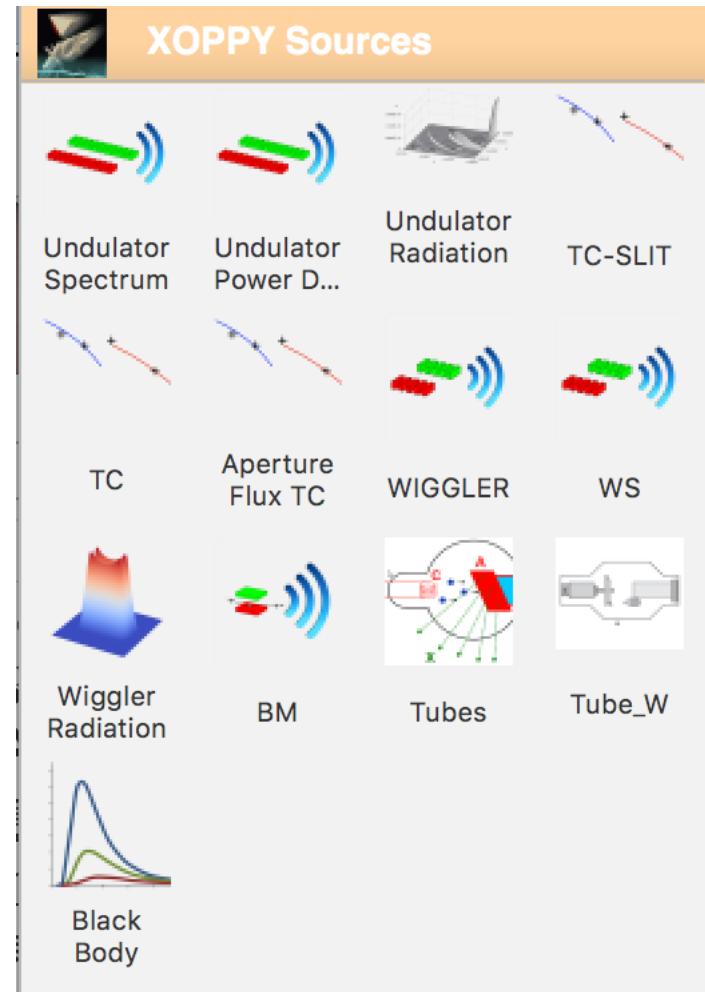
- Hand calculations (sizes divergences and distances define magnification, optical element reflectivities)
- Ray tracing (starting from point sources, monochromatic beams, ideal optics, etc. then integrate finite sizes, polychromicity, real optics with surface errors)
- If coherence is important, apply wave optics
 - Hybrid method: corrections to ray tracing
 - 1D prototyping (fast)
 - 2D full simulation
 - Partial coherence (multielectron, coherent mode decomposition)

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Source emission (XOPPY)

- Undulator spectrum (flux or power versus E)
- Undulator power density (power versus X,Y)
- Undulator Spectrum (flux/power vs X,Y,E)
- Undulator tuning curves
- Wiggler spectrum Spectrum (flux/power vs X,Y,E)
- BM Spectrum (flux/power vs E, angle)
- Others



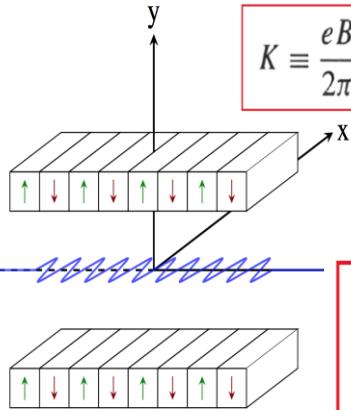
Optical elements (XOPPY)

- Attenuators
- Mirrors
- Multilayers
- Crystals

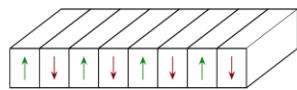


Undulator Memorandum

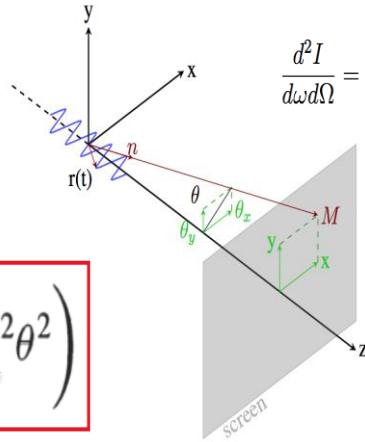
Undulator emission, after classical electrodynamics (e.g., Jackson, etc)



$$K \equiv \frac{eB_0\lambda_u}{2\pi mc} = 0.9337B_0(T)\lambda_u(\text{cm})$$



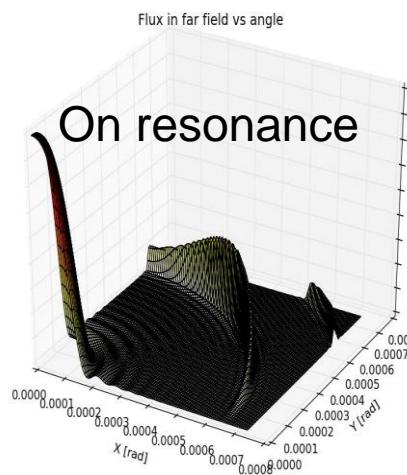
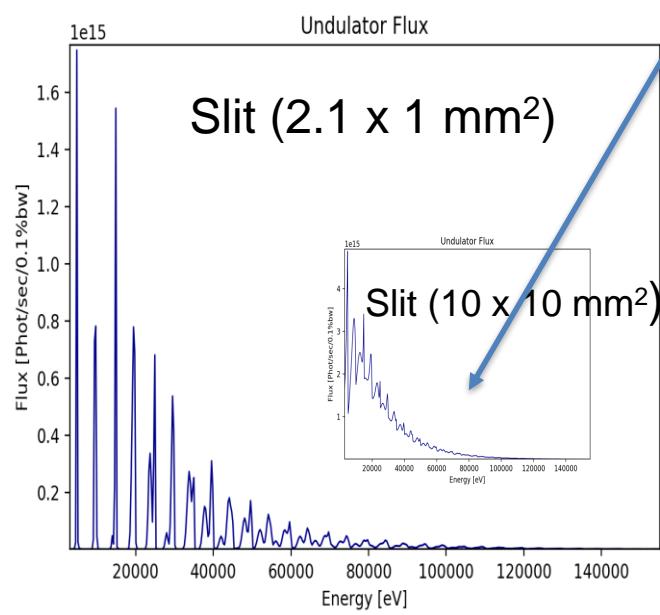
$$\lambda = \frac{\lambda_u}{2\gamma^2} \left(1 + \frac{K^2}{2} + \gamma^2 \theta^2 \right)$$



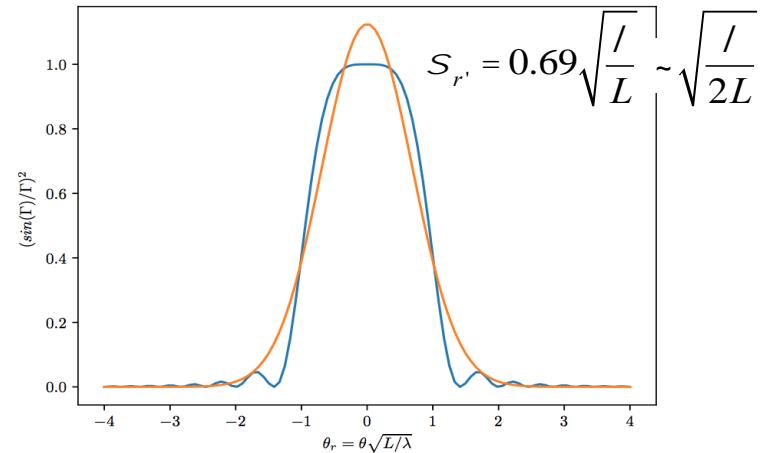
$$\frac{d^2I}{d\omega d\Omega} = \frac{eI}{8\pi^2 c \epsilon_0 h} 10^{-9} \left| \int_{-\infty}^{\infty} \left[\frac{n \times [(n - \beta) \times \dot{\beta}]}{(1 - \beta \cdot n)^2} + \frac{c}{\gamma^2 R} \frac{(n - \beta)}{(1 - \beta \cdot n)^2} \right] e^{i\omega(t' + R(t')/c) dt'} \right|^2$$

$$E = \gamma m_e c^2$$

$$m_e c^2 = 0.51 \text{ MeV}$$



On resonance approximation



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

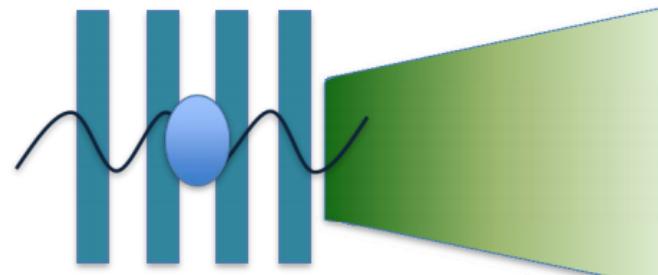
Photon beam size and divergence is determined by a combination of electron beam and single electron emission

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

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

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

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



Courtesy: Boaz Nash

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

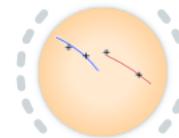
(FOR UNDULATORS, THESE FORMULAS ARE VALID AT THE WAIST, AT THE UNDULATOR RESONANCE, AND SUPPOSING GAUSSIAN EMISSION OF PHOTONS)

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

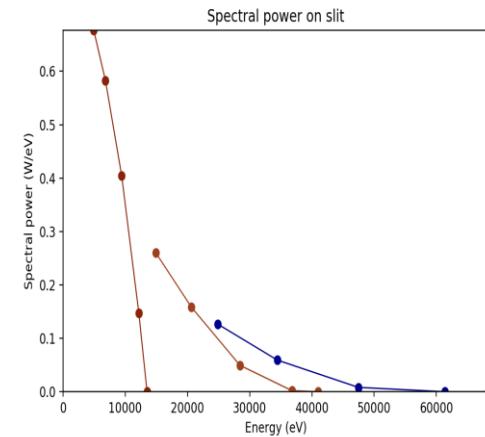
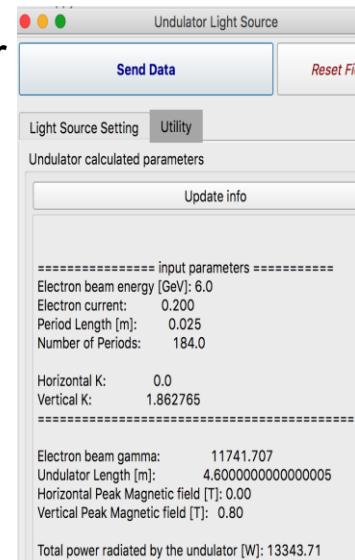
Undulators: Power and spectral calculations

$$Power[kW] \approx 0.633 \cdot B^2 [T] \cdot E^2 [GeV] \cdot I[A] \cdot L[m]$$

$$\frac{Power}{Solid\ Angle} [W/mrad^2] \approx 10.84 \cdot B [T] \cdot E^4 [GeV] \cdot I[A] \cdot L[m] \cdot N \cdot G(K)$$



TC-SLIT

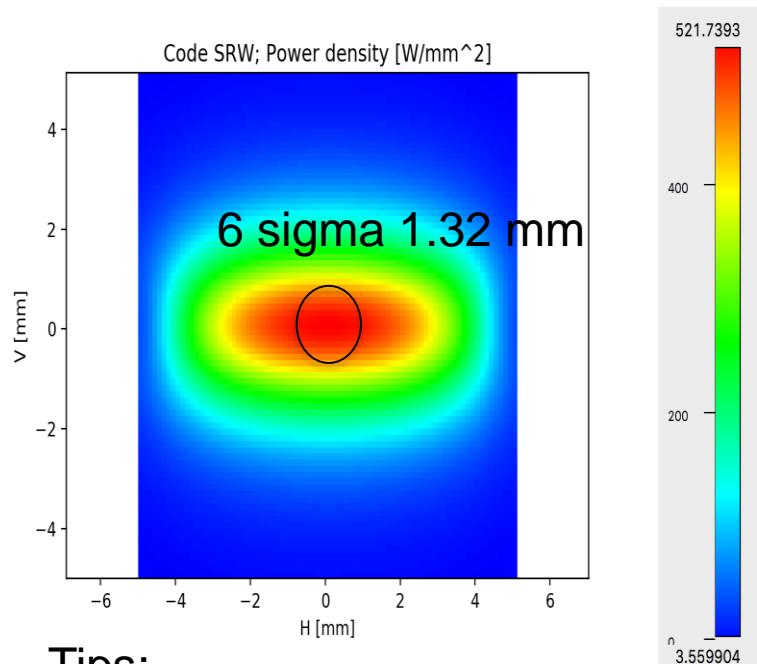


- Maximum power is obtained at highest K (or B) corresponding to the minimum photon energy
- The spectral range covered by undulator is shown by the Tuning Curves.

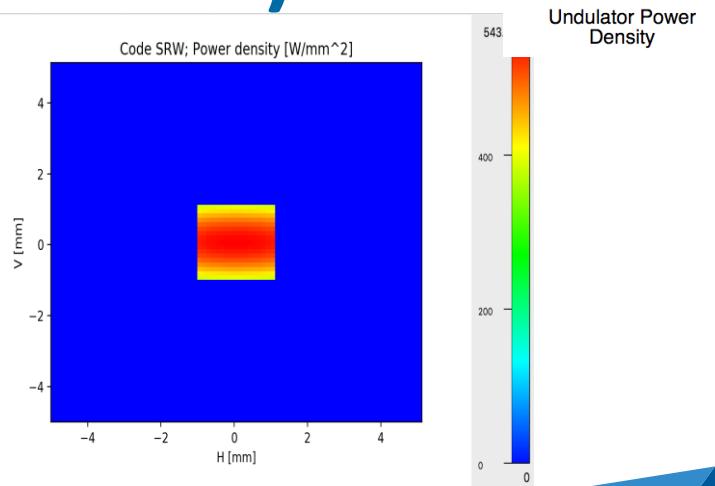
Power density (Power vs X and Y)



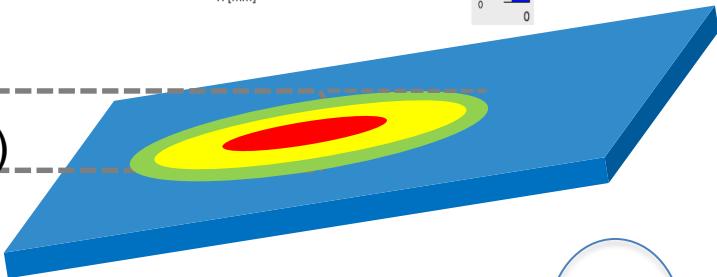
Undulator Power Density



Mask
2x2 mm @
25.4,=m
Or
2.1x2.1 @
28m

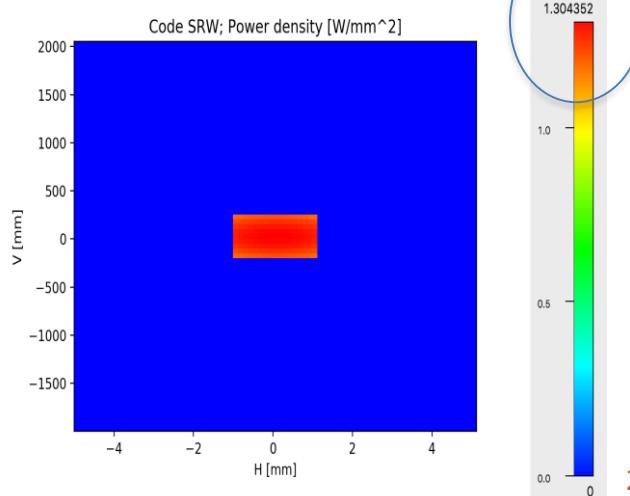


Mirror:
400mm
2.1mm (mask)



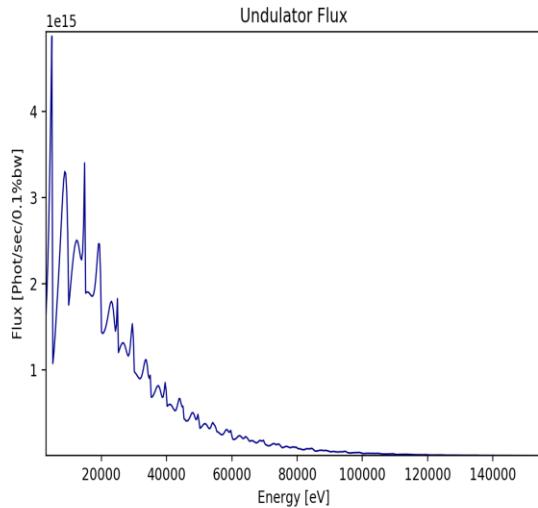
Tips:

- Calculate on aperture large enough to accept all the radiation
- Select “modify slit” to calculate power on smaller slit and to calculate power density on mirror surface

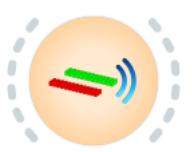
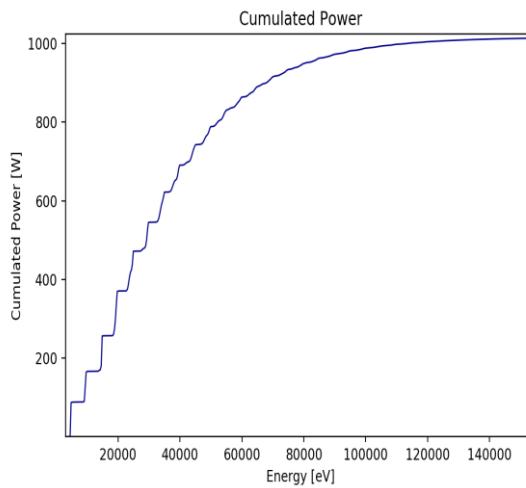
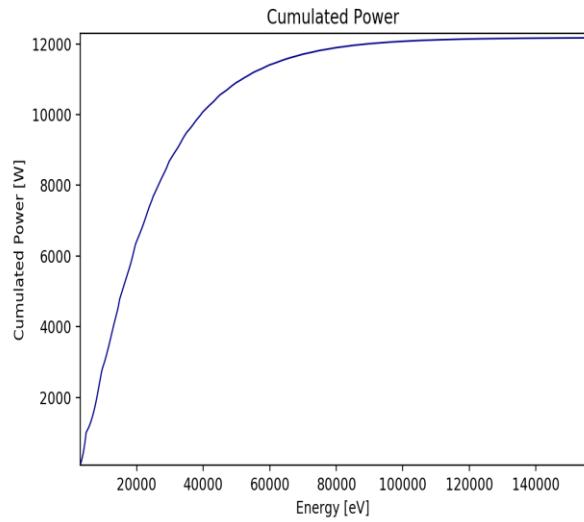
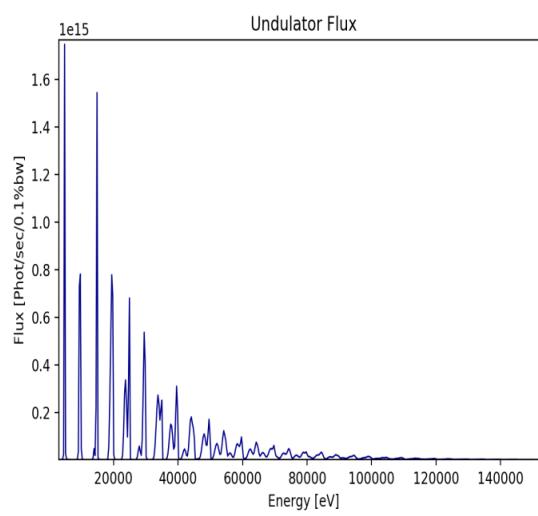


Flux and Spectral Power

Open Slit ($10 \times 10 \text{ mm}^2$)

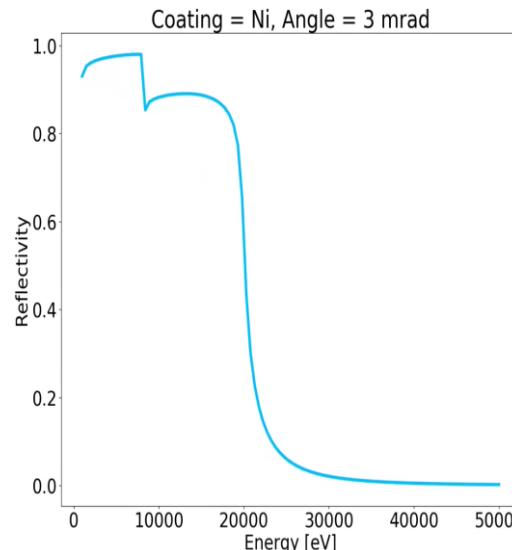
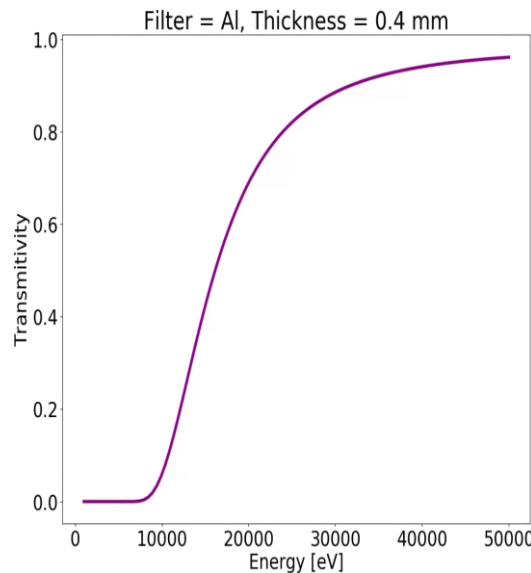
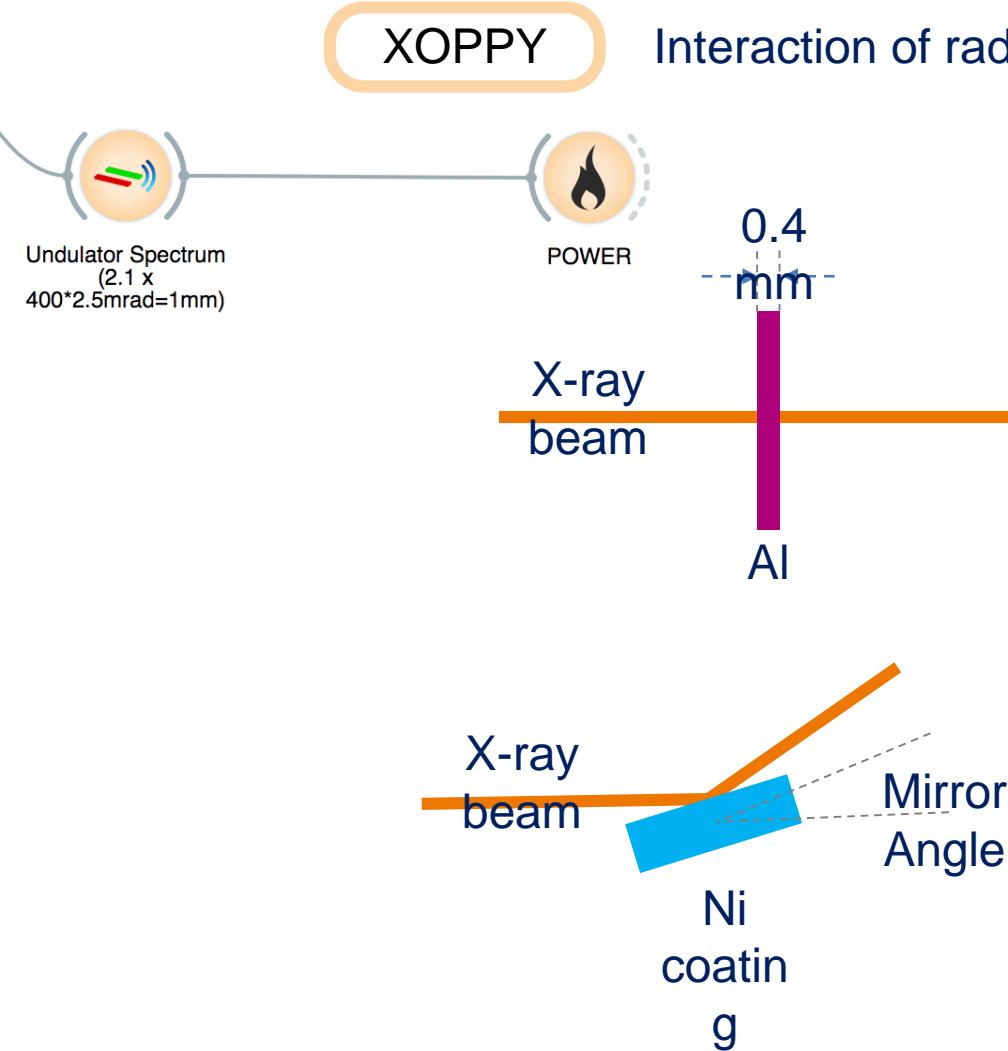


Slit ($2.1 \times 1 \text{ mm}^2$)

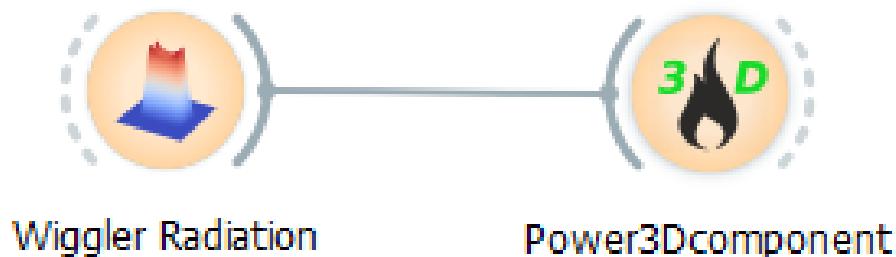
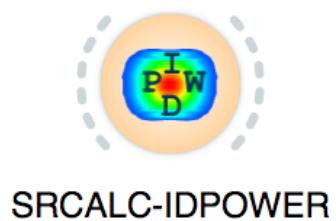


Undulator Spectrum

Spectral response of mirrors and attenuators (filters)



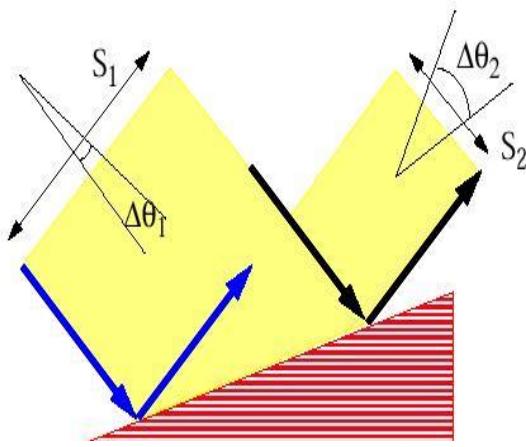
Combined (X,Y,E) effect of optical elements



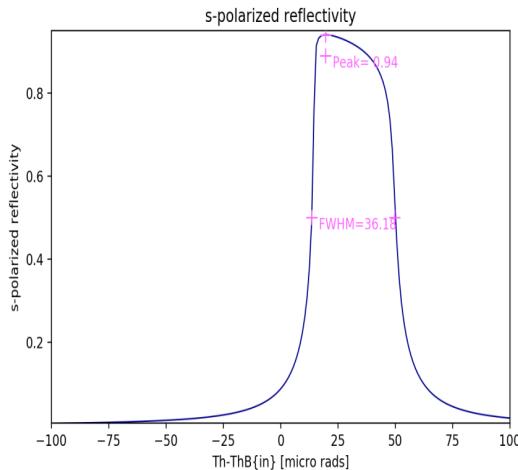


Crystals: Zachariasen treatment for plane crystals

CRYSTAL



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



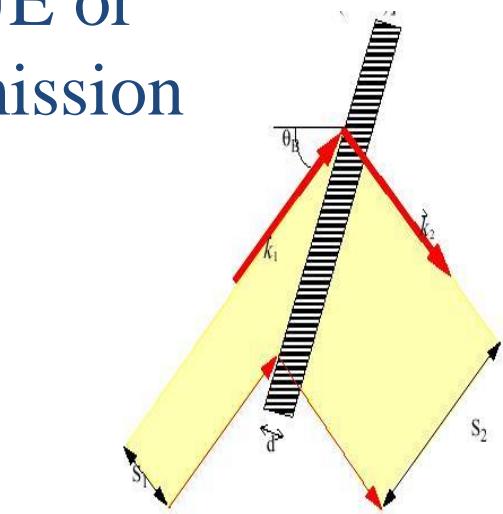
$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \frac{-z \pm (qP^2 + z^2)^{1/2}}{P\Psi_H}$$

$$c_1 = \exp(-i\varphi_1 T), \quad c_2 = \exp(-i\varphi_2 T),$$

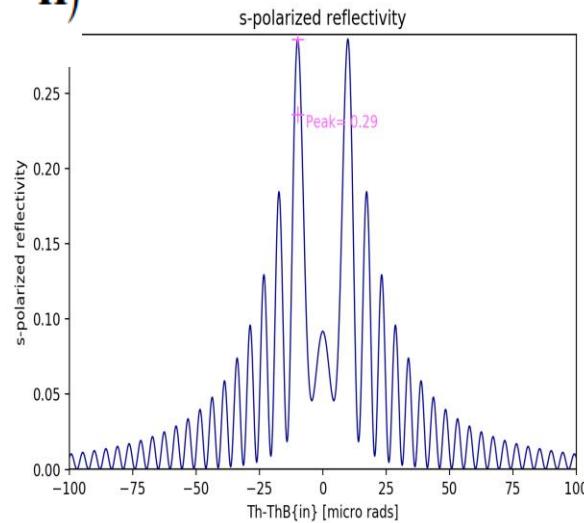
$$\varphi_1 = -\frac{2\pi k^0 \delta'_0}{\omega}, \quad \omega = -\frac{2\pi k^0 \delta''_0}{\omega},$$

$$\begin{pmatrix} \delta'_0 \\ \delta''_0 \end{pmatrix} = \frac{1}{2} [\Psi_0 - z \pm (qP^2 + z^2)^{1/2}]$$

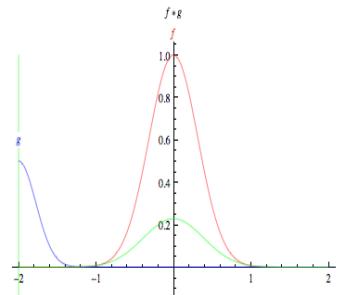
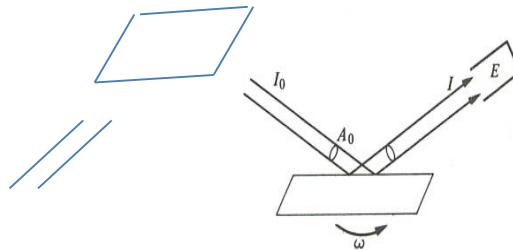
$$\alpha_Z = \frac{1}{|\mathbf{k}^0|^2} (|\mathbf{H}|^2 + 2\mathbf{k}^0 \cdot \mathbf{H})$$



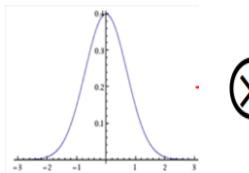
$$r^{\text{Laue}}(\alpha_Z) \equiv \frac{1}{|b|} \frac{I^H}{I^0} = \frac{1}{|b|} \left| \frac{x_1 x_2 (c_1 - c_2)}{x_2 - x_1} \right|^2$$



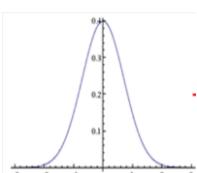
Crystals: Rocking curves



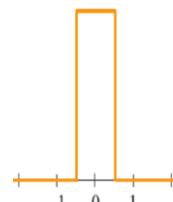
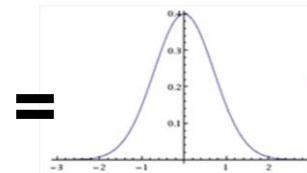
The rocking curve is the **CONVOLUTION** of the two diffraction profiles.



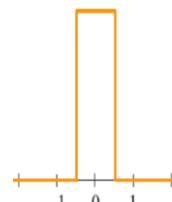
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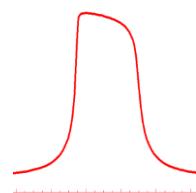
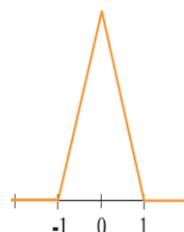
$$\text{FWHM}_R = 1.4 \text{ FWHM}_1$$



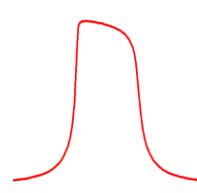
⊗



$$\text{FWHM}_R = 1 \text{ FWHM}_1$$



⊗

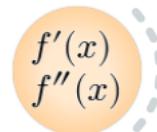


$$\text{FWHM}_R \sim 1.5 \text{ FWHM}_1$$

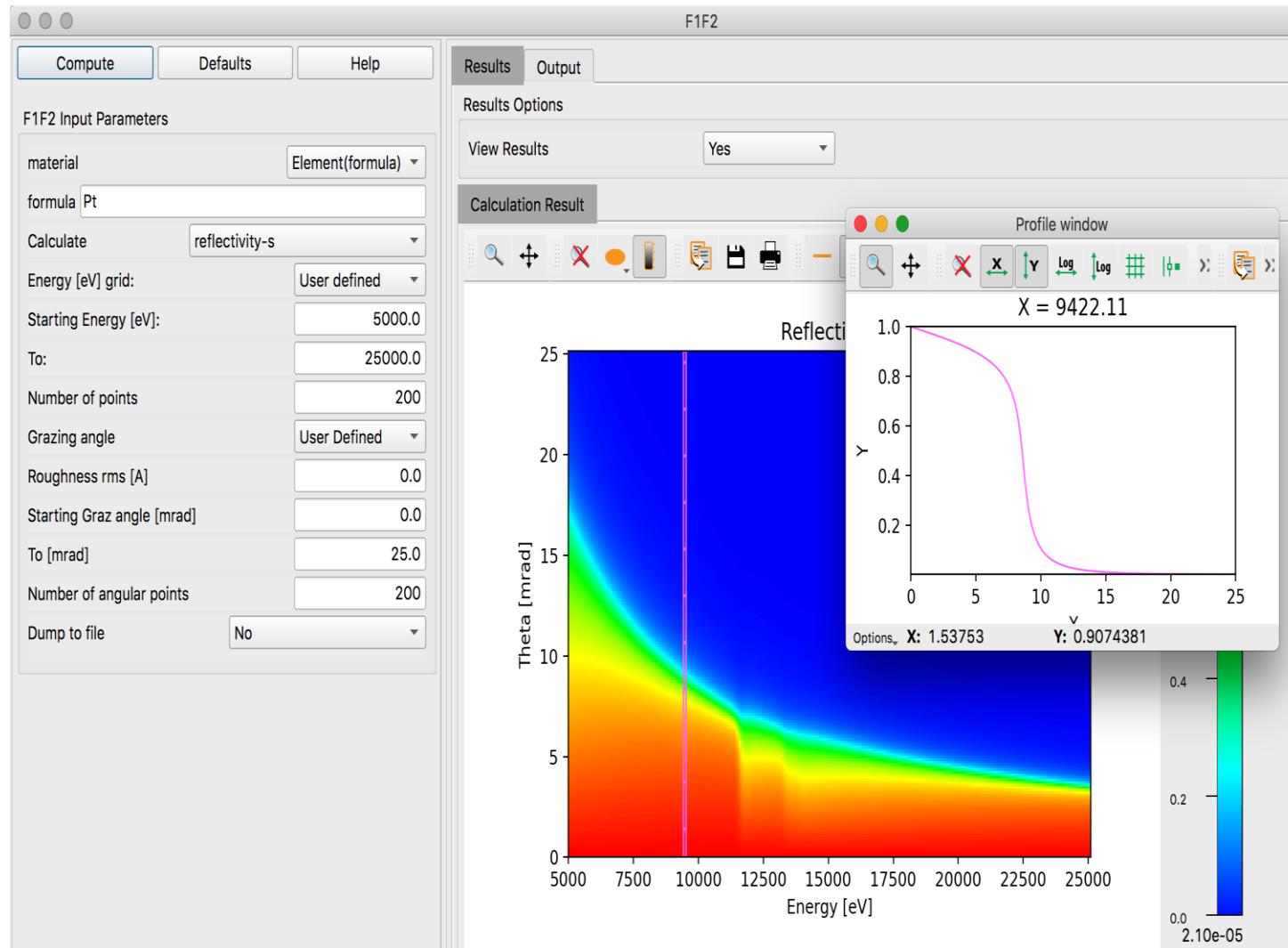
Si111 8 keV

For a full discussion about rocking curves see: Masiello *et al.* J. Appl. Crystall. 47, 1304-1314 (2014)

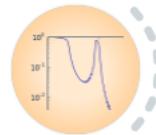
Mirror reflectivity F1F2



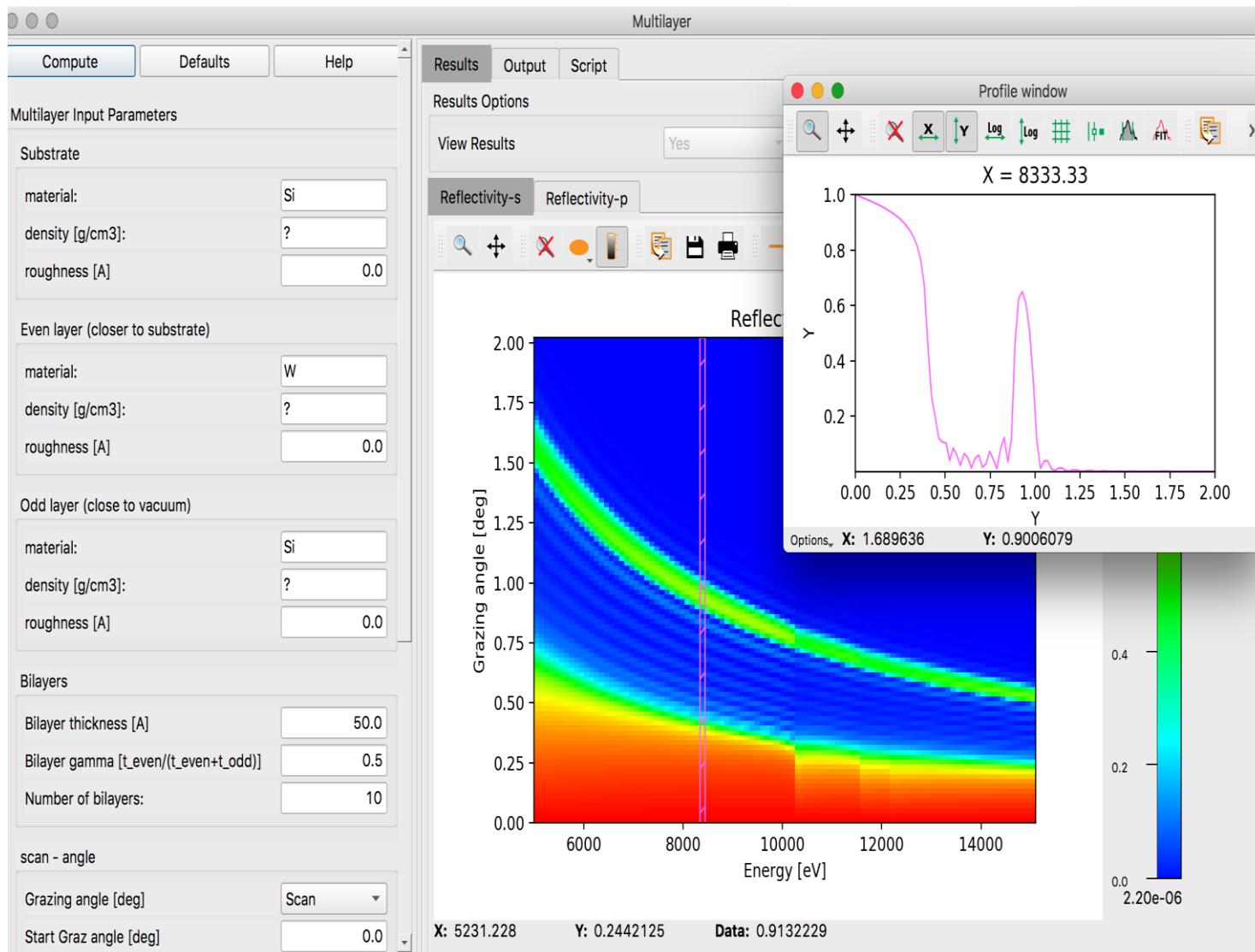
F1F2



Multilayer reflectivity



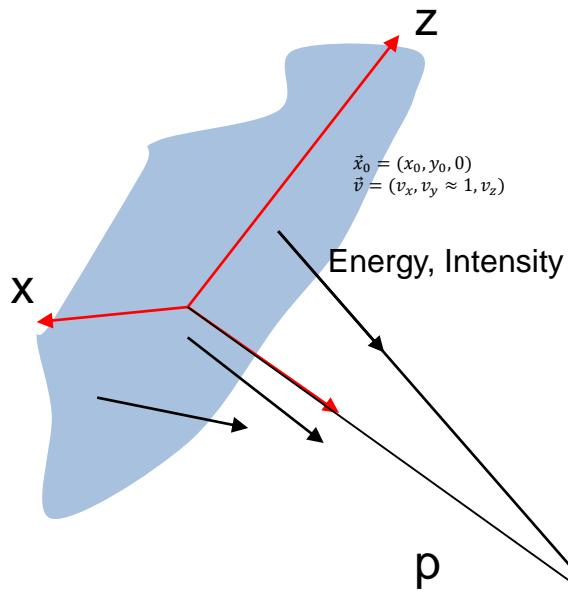
Multilayer



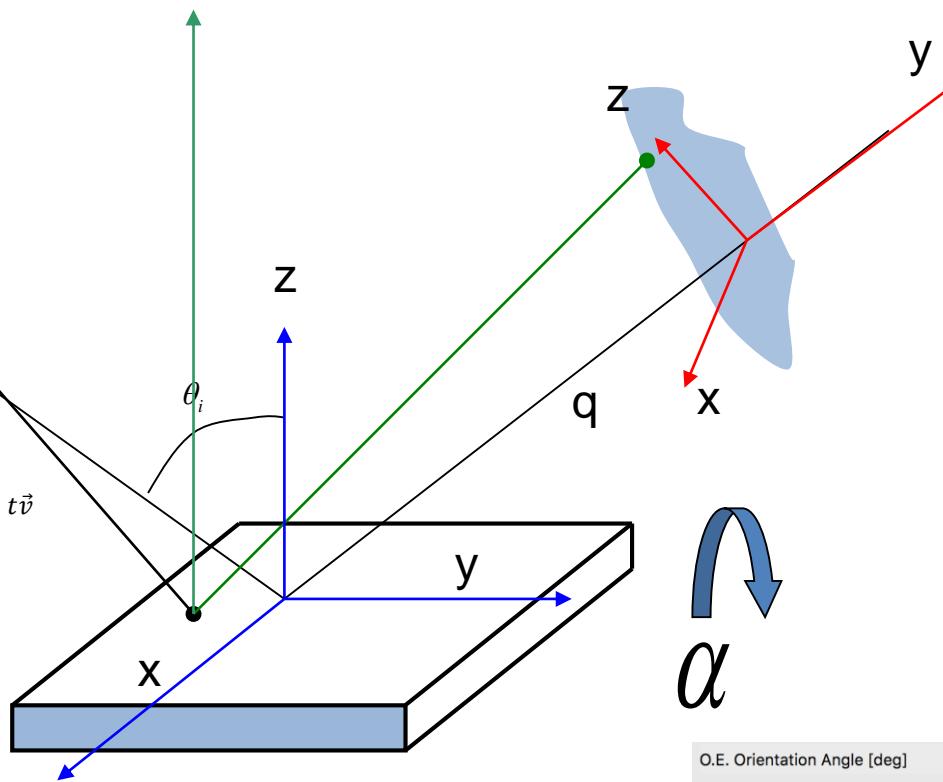
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Trace (the beamline)



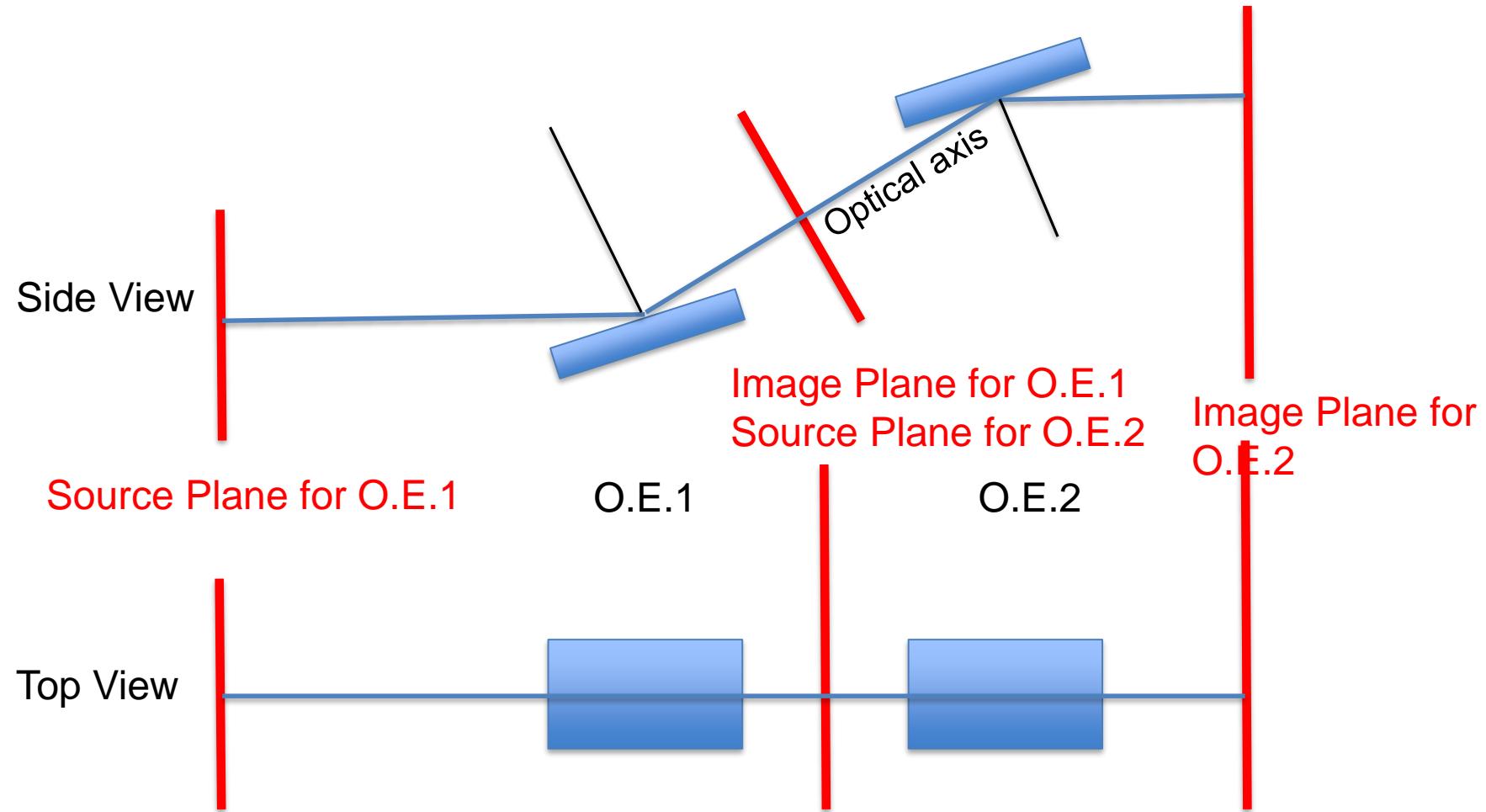
$$\vec{k}_o = \vec{k}_i - 2(\vec{k}_i \cdot \vec{n})\vec{n}$$

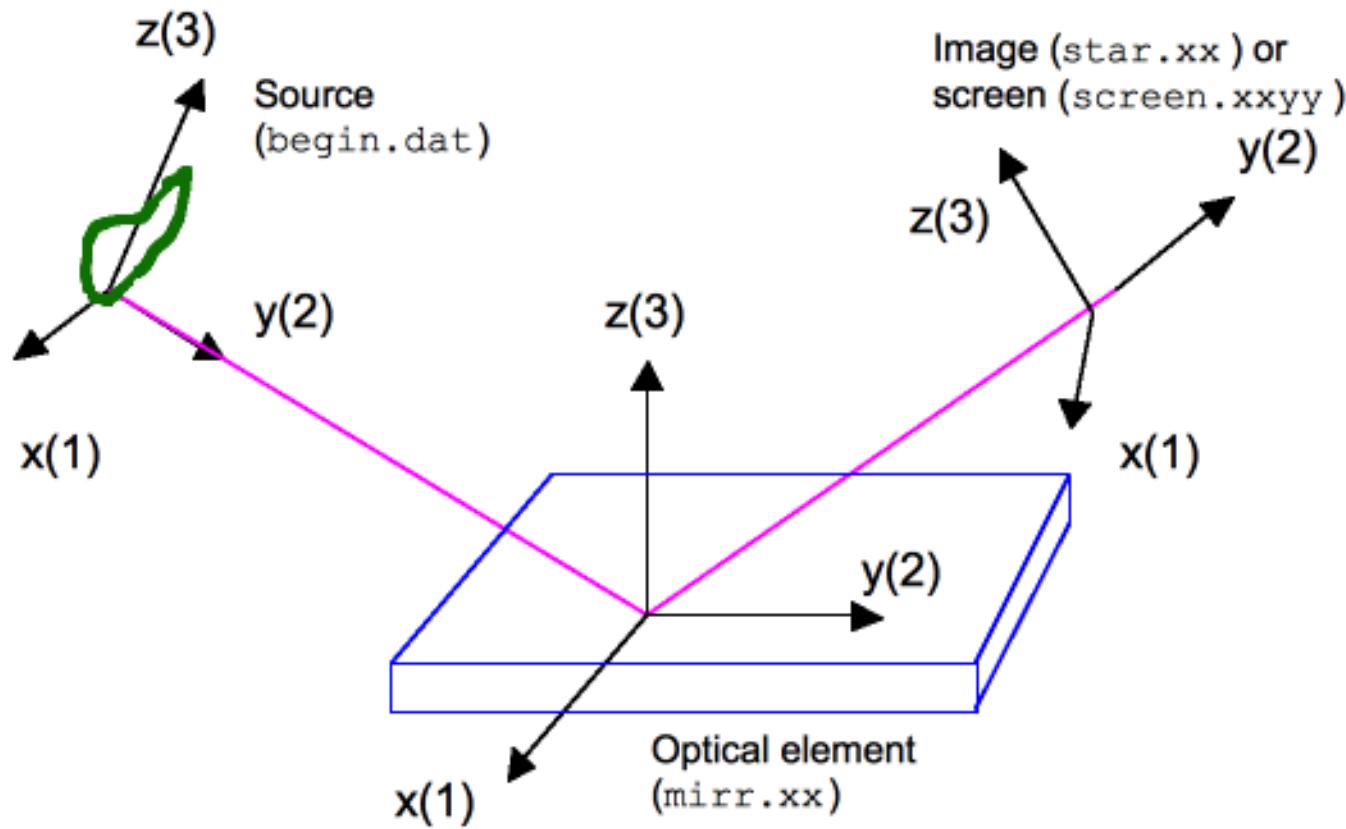


Angles in [deg] with respect to the	Normal
Incident Angle with respect to the normal [deg]	88.0
Incident Angle with respect to the surface [mrad]	34.906585
Reflection Angle with respect to the normal [deg]	88.0
Reflection Angle with respect to the surface [mrad]	34.906585

O.E. Orientation Angle [deg]
0 90 180 270

Continuation planes





Note that (**VERY IMPORTANT!**):

- The y(2) coordinate is along the beam direction
- The position (Source Plane Distance), orientation (O.E. Orientation Angle) of any o.e. is always referred to the previous one
- Source Plane and Image Plane for each optical element are the “Continuation Planes”
- The frame is rotated if one o.e. is rotated

SHADOW ray's variables (*columns*)

Stored:

1: X
2: Y
3: Z
4: X' *
5: Y'
6: Z'
7: E σ X
8: E σ Y
9: E σ Z
10: Ray Flag
11: Energy **
12: Ray Index
13: Optical Path
14: Phase σ
15: Phase π
16: E π X
17: E π Y
18: E π Z

Computed:

19: Wavelength
20: R = $\sqrt{X^2 + Y^2 + Z^2}$
21: Theta (angle from Y axis)
22: Magnitude = |E σ | + |E π |
23: Total Intensity = |E σ |² + |E π |²
24: Σ Intensity = |E σ |²
25: Π Intensity = |E π |²
26: |K|
27: K X
28: K Y
29: K Z
30: S0-stokes = |E π |² + |E σ |²
31: S1-stokes = |E π |² - |E σ |²
32: S2-stokes = 2|E σ ||E π |cos(Phase σ -Phase π)
33: S3-stokes = 2|E σ ||E π |sin(Phase σ -Phase π)
34: Power = Intensity * Energy

* X',Y',Z' is the direction vector (unitary), for small angles (always in SR) Y'<~1, and X' and Z' can be considered “divergences”

** Column 11 is energy in eV. Internally SHADOW stores the wavenumber $2\pi / \lambda$ in cm⁻¹

Optical elements

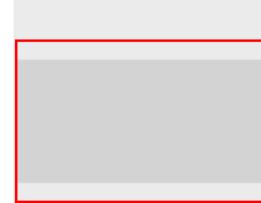
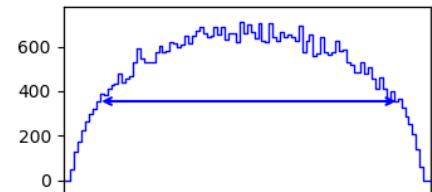
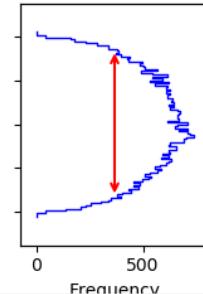
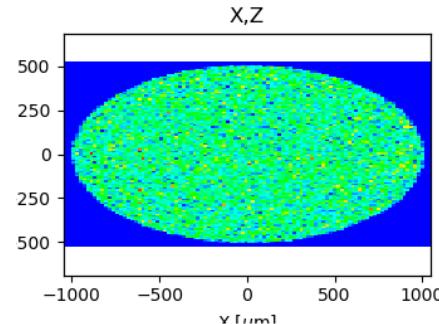
For each optics element SHADOW includes:

- 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

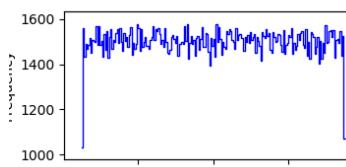
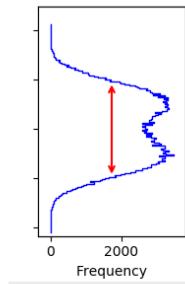
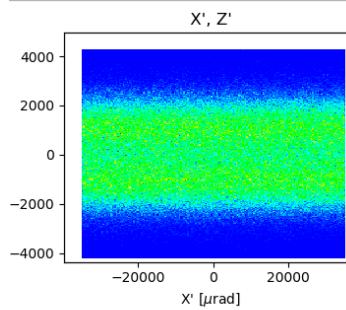
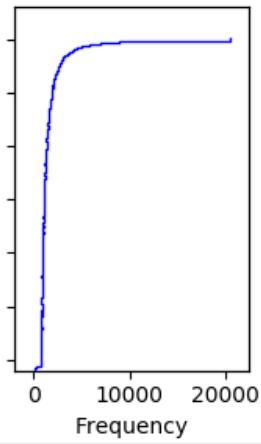
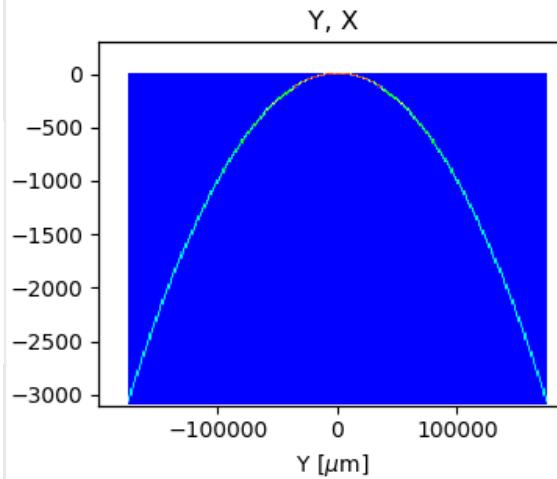
ShadowOUI Sources I



Geometrical Source



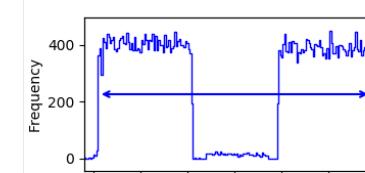
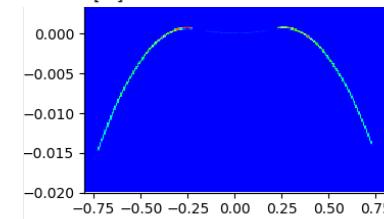
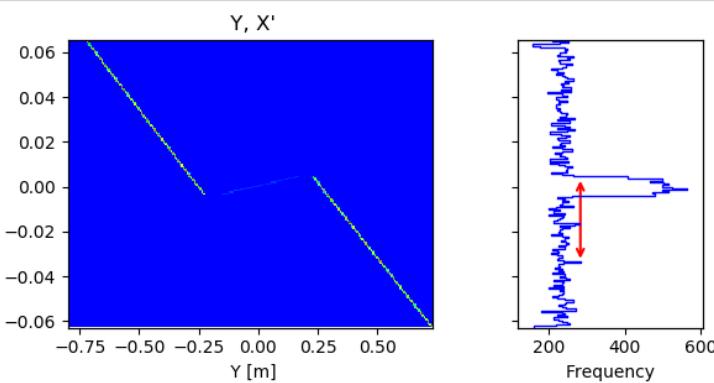
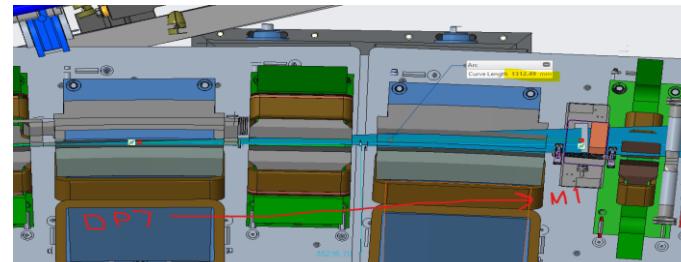
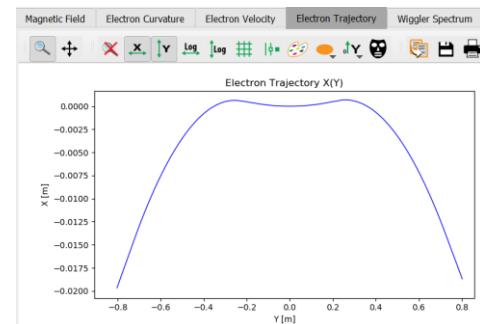
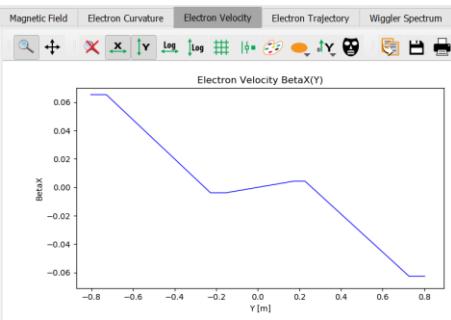
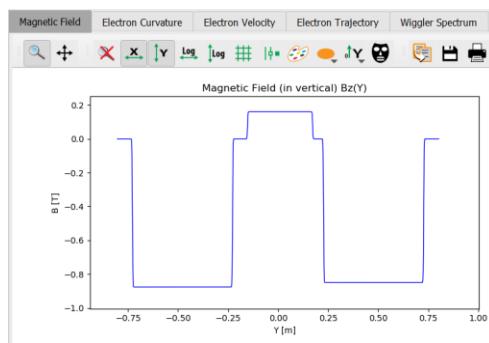
Bending Magnet



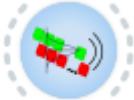
Sources II (Wiggler and also multiple BMs and Short IDs)



Wiggler



Sources III (Undulator)



Undulator Gaussian

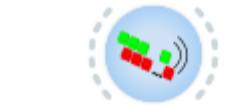
Single e⁻

Divergence:

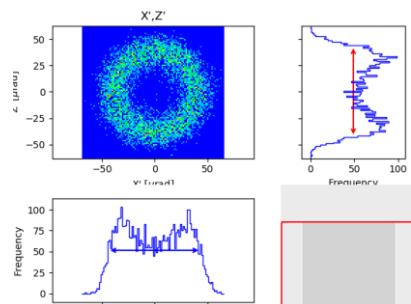
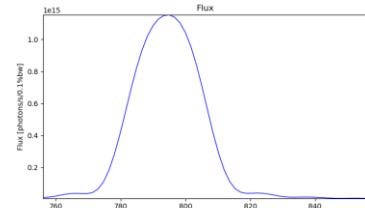
$$\sigma_r = 0.69 \sqrt{\frac{\lambda}{L}} \approx \sqrt{\frac{\lambda}{2L}}$$

Size:

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



Full Undulator

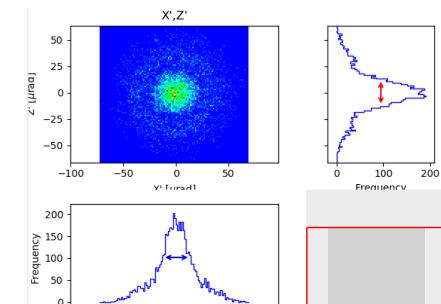
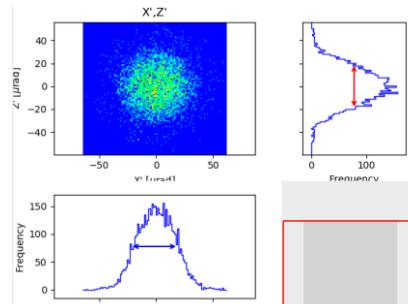
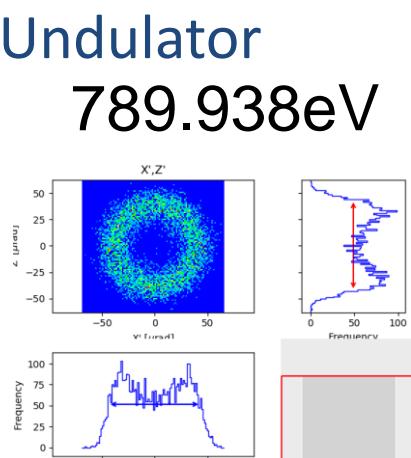
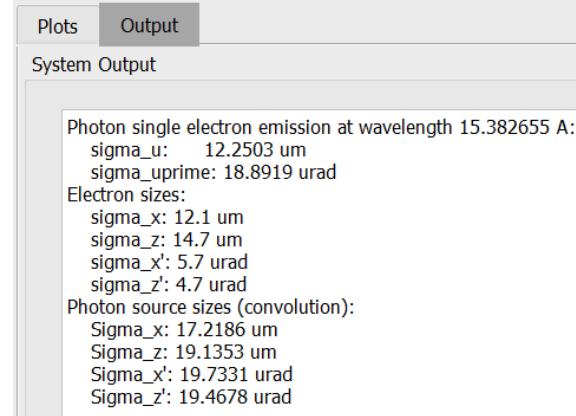
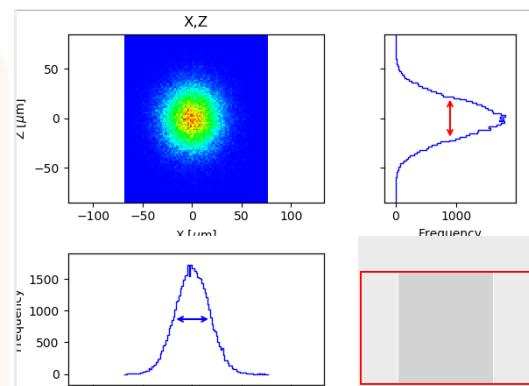


789.938eV

806.060eV

814.121eV

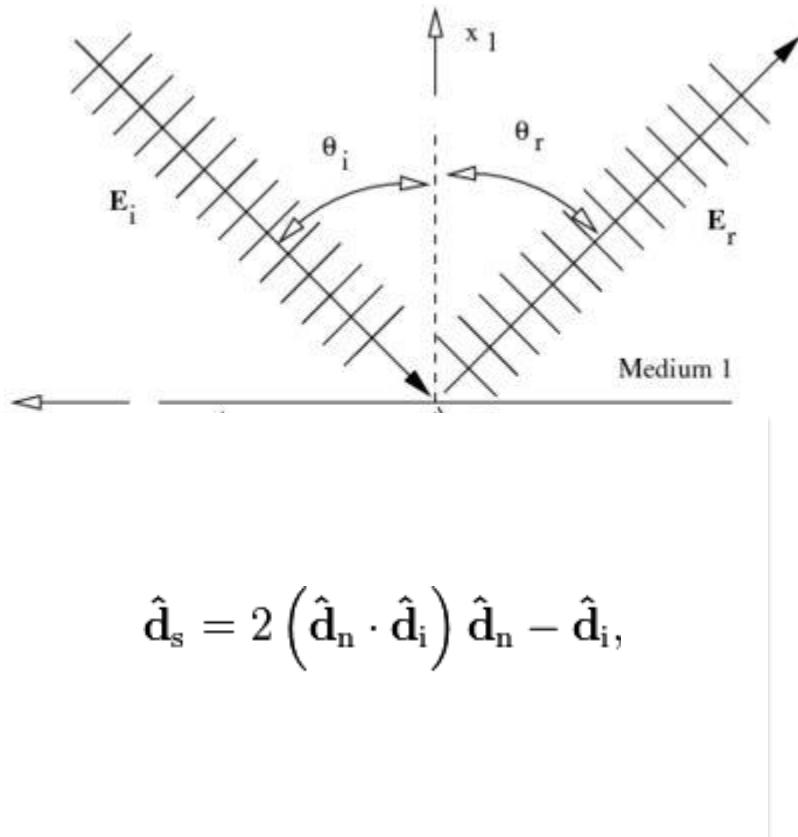
Fake Geometrical Source (Gaussian spatial + Gaussian divergency)



Optical Elements (mirrors)

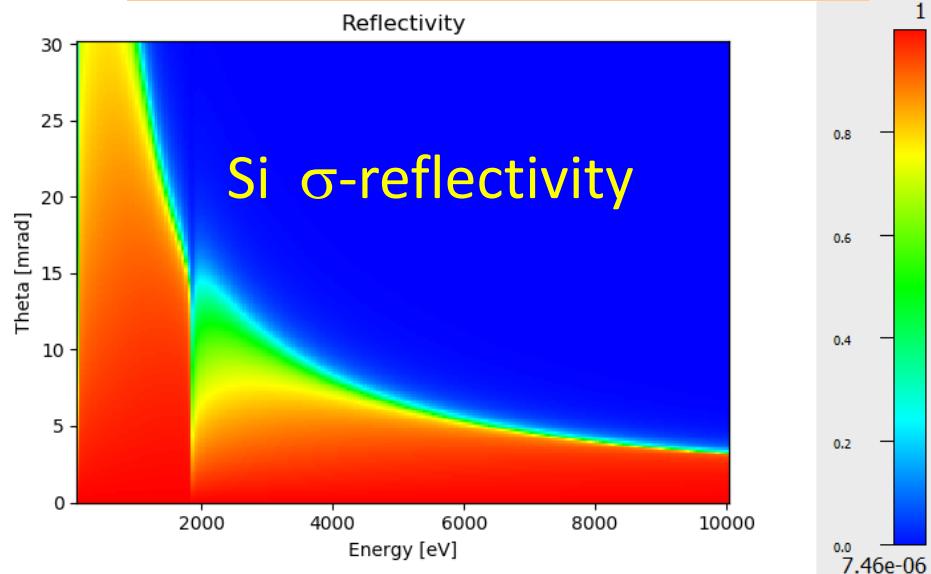
Geometrical model

Physical model



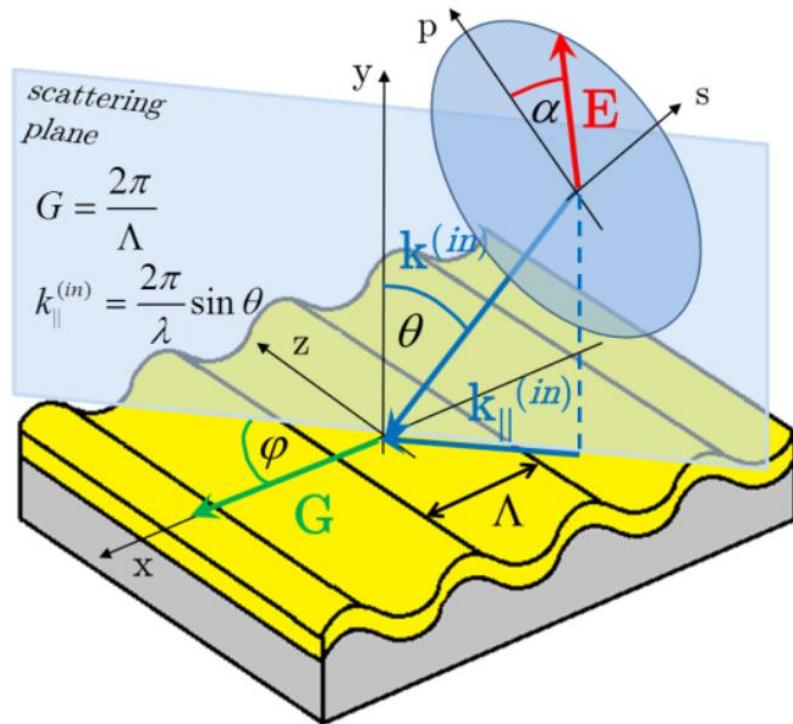
Fresnel equations give the reflectivity as a function of angle and photon energy. As a consequence, one gets the critical angle:

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



Optical Elements (gratings)

Geometrical model



Physical model

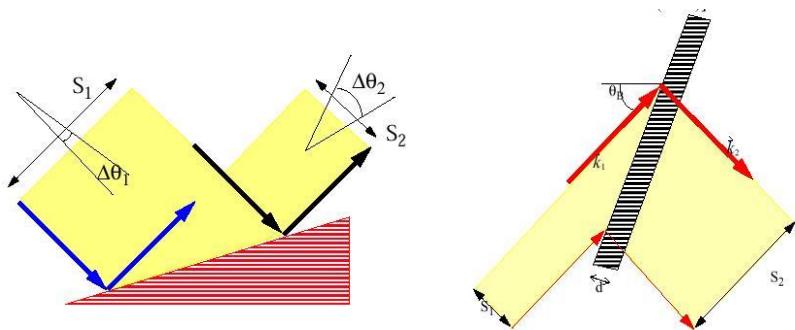
No model (yet) in SHADOW for grating efficiency

SHADOW uses Fresnel equations like for mirrors

Figure from doi.org/10.5772/51044

Optical Elements (crystals)

Geometrical model

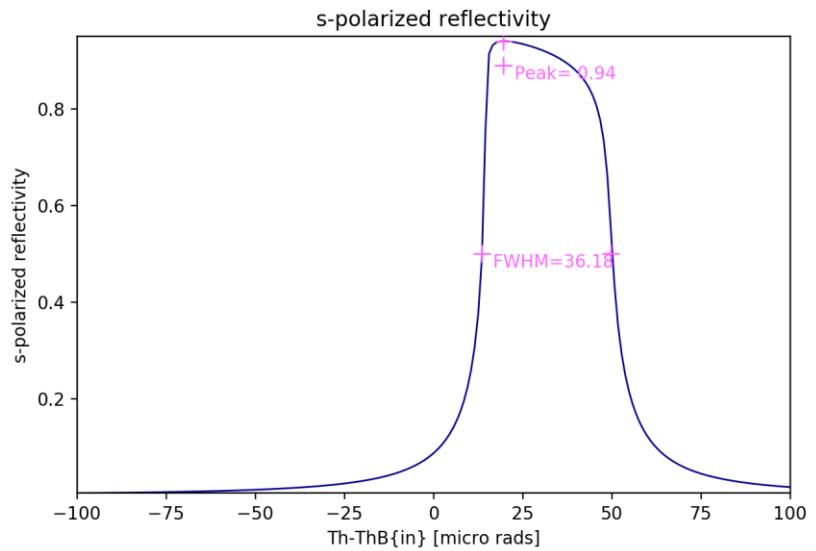


$$|\vec{k}_1| = |\vec{k}_2|$$

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

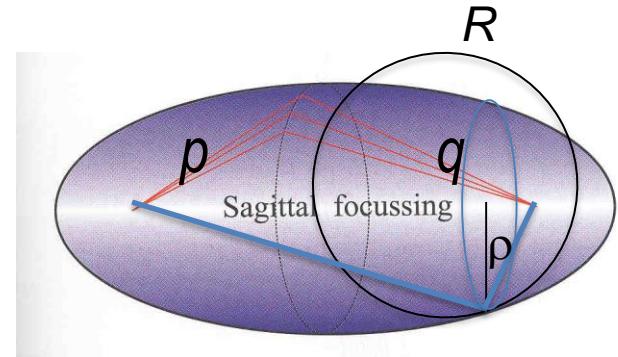
Physical model

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



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



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

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

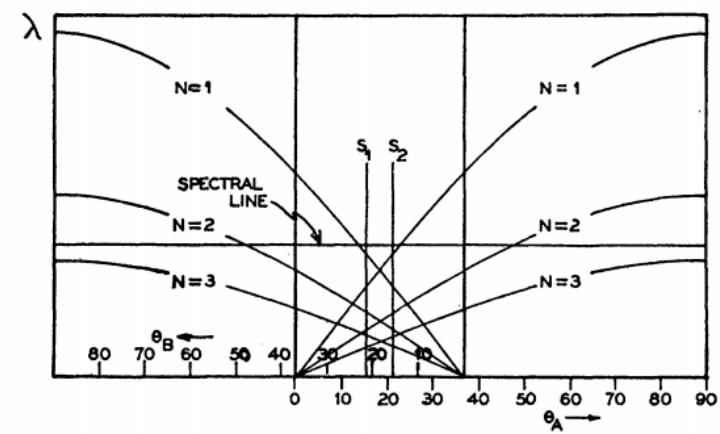
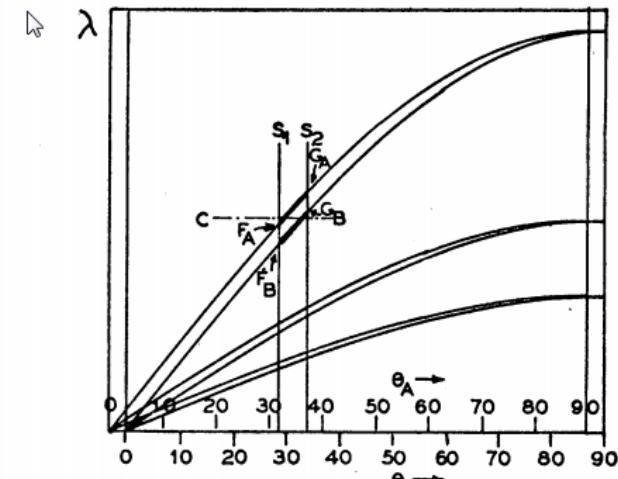
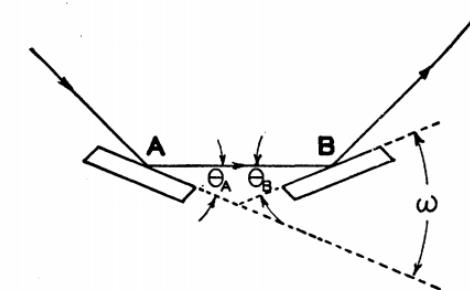
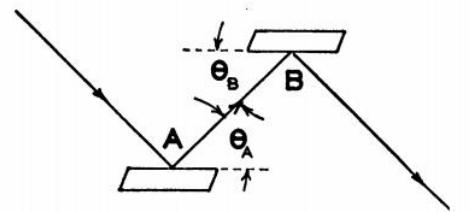
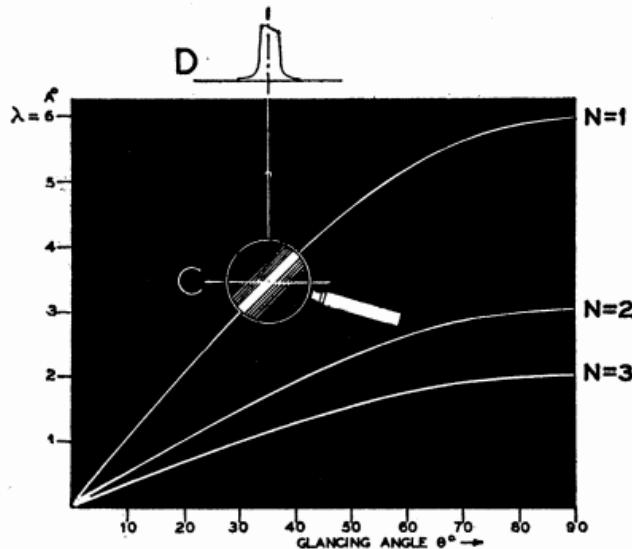
Crystal monochromators

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>



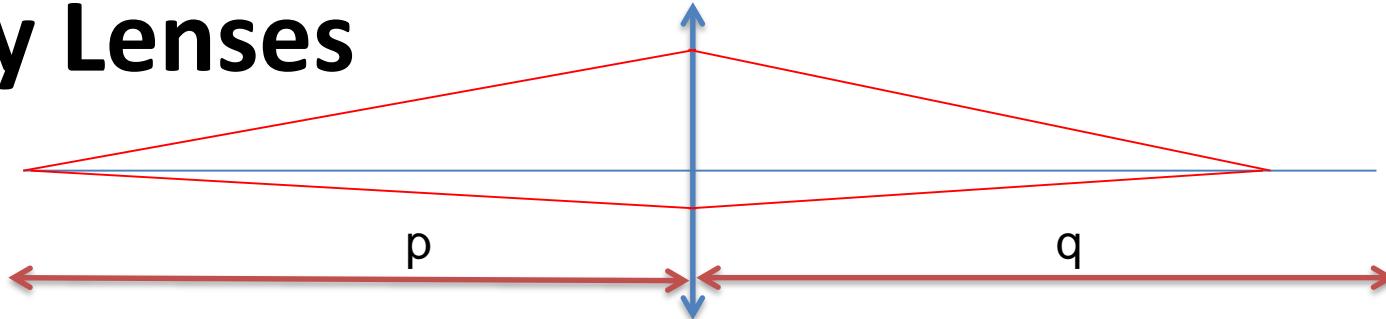
Crystal curvature and spectral resolution

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

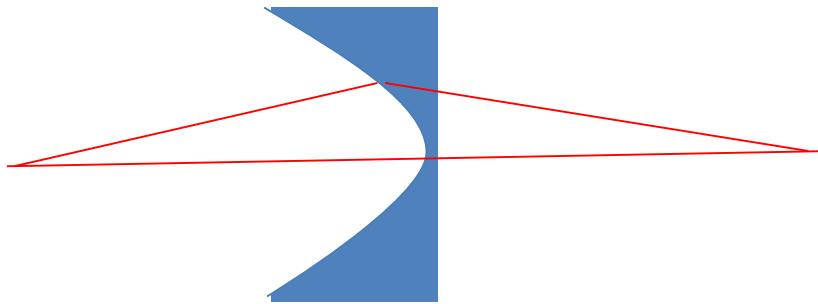
$$\frac{\Delta\lambda}{\lambda_0} = \frac{\Delta E}{E_0} \approx \sqrt{\omega_D^2 + (\Delta_{geom} + \Delta_{ss})^2} \cot \theta_0 = \sqrt{\omega_D^2 + \left[\left(\frac{p}{R \sin \theta_1} - 1 \right) \Delta_{src} + \frac{s_1}{p} \right]^2} \cot \theta_0$$

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

X-ray Lenses

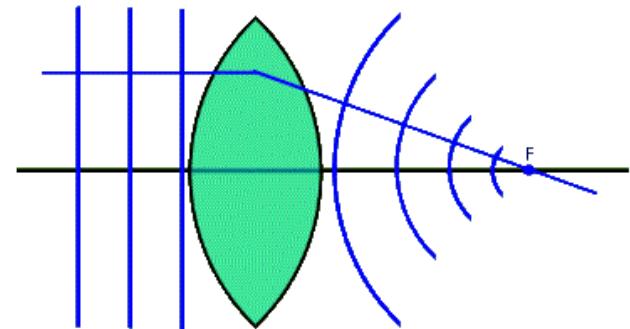


$$\frac{1}{F} = \frac{1}{p} + \frac{1}{q}$$



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

$$\frac{1}{F} = (n - 1) \left(\frac{1}{R_1} - \frac{1}{R_2} + \frac{(n - 1)d}{nR_1 R_2} \right) \approx \frac{\delta}{R_1}$$



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

CRL (COMPOUND REFRACTIVE LENSES) = replicate N lenses

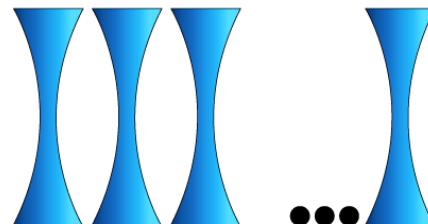
Single interface



Lens



Compound Refractive
Lens (CRL)

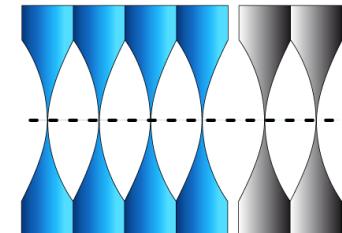


$$F = \frac{R}{\delta}$$

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

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

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



1996 Experimental demonstration of CRL

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

2011 Transfocator

Outline

- Introduction to OASYS
- XOPPY toolbox: Source emission and characteristics of optical elements. Power transport
- ShadowOUI: Ray tracing SR beamlines
 - Mirror aberrations
 - Crystal systems
 - Lenses
- WOFRY and SRW: coherent beam transport:
 - Simple examples with WOFRY
 - Introduction to Partial coherence

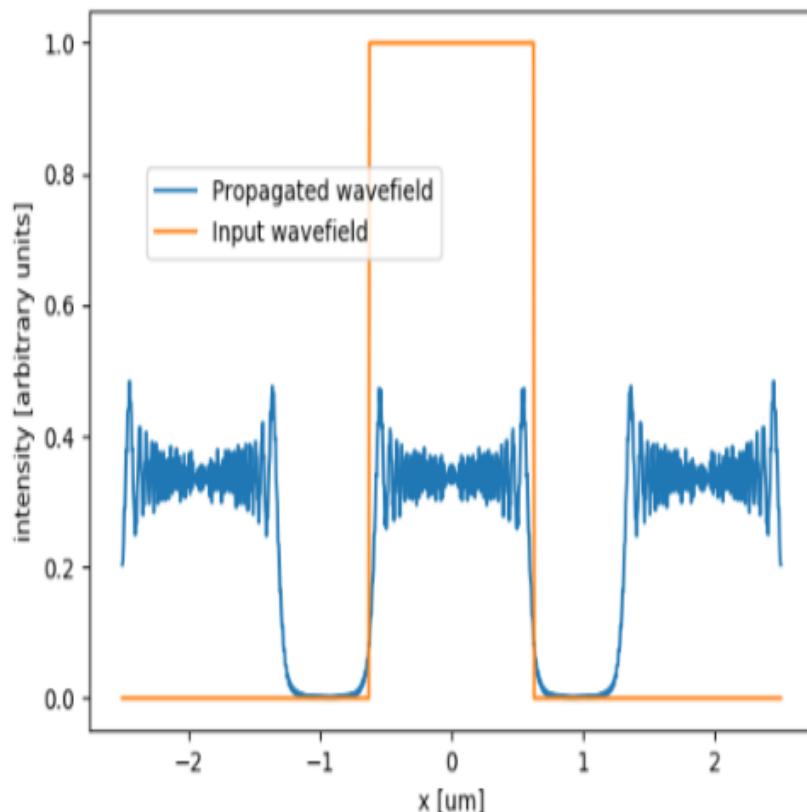
Wave optics

- Based on sampling a wavefront (monochromatoc and coherent), and propagate it (in free space and trough optical elements)
- 2D wavefront sampling is costly $\sim N^2$
- Propagation is expensive N^4 or N^2 if FFT
- Optical elements modelled as thin objects
- Parameter setting is complex

Wavefront and Propagator discretization

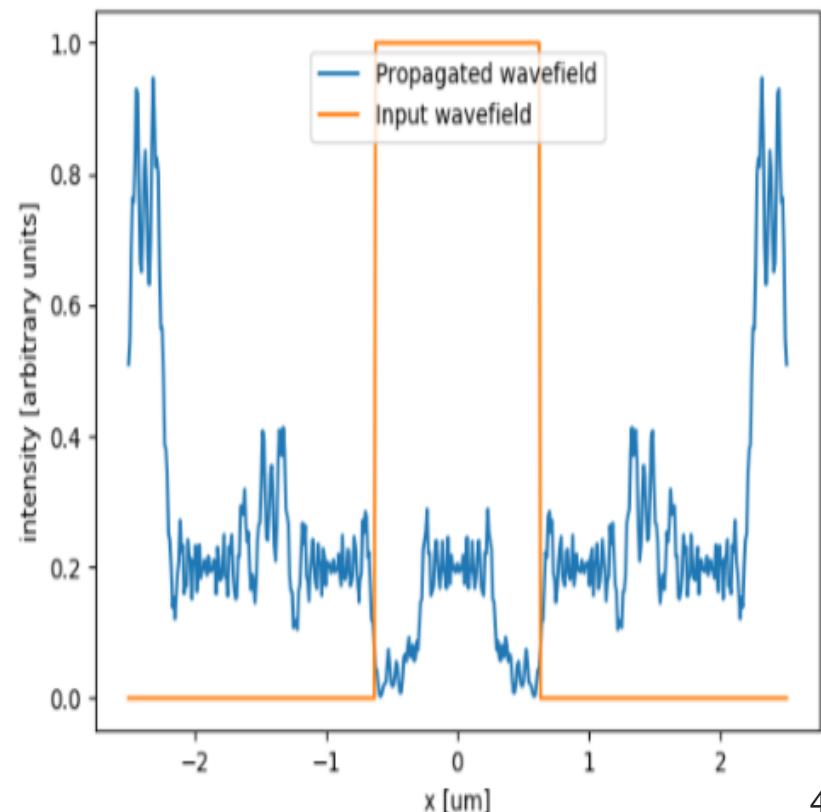
Effect of the discretization: Replicas

Replicas can be avoided by increasing the sampling or by isolating the main feature at the image plane, if the replica are well separated.



Effect of under-sampling: Aliasing

Under-sampling produces an overlapping of the replicas, thus completely distorting the expected result. This effect is called *aliasing*.



SRW (Oleg Chubar, BNL)

<https://github.com/ochubar/SRW>

Chubar, O. and Ellaume, P.: *Accurate and efficient computation of synchrotron radiation in the near field region*. Proceedings of the 6th European Particle Accelerator Conference - EPAC-98, pages 1177-1179

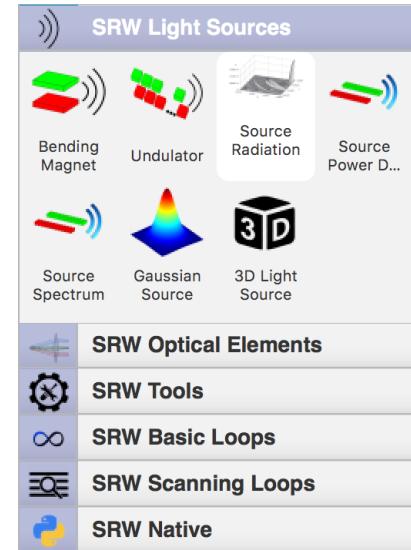
Chubar, O.: *Wavefront calculations*. Proc. SPIE, 4143:48-59 (2001)

Chubar, O., Berman, L., Chu, Y. S., Fluerau, A., Hubert, S., Idir, M., Kaznatcheev, K., Shapiro, D. Shen, Q. and Baltser, J.: *Development of partially-coherent wavefront propagation simulation methods for 3rd and 4th generation synchrotron radiation sources*. Proc. SPIE, 8141:814107 (2011)

Chubar, O.: *Recent updates in the "Synchrotron Radiation Workshop" code, on-going developments, simulation activities, and plans for the future.* Proc. SPIE, 9209:920907 (2014)

Chubar, O., Rakitin, M., Chen-Wiegart, Y.K., Chu, Y.S., Fluerau, A., Hidas, D. and Wiegart, L.: *Main functions, recent updates, and applications of Synchrotron Radiation Workshop code*. Proc. SPIE, 10388:1038805 (2017)

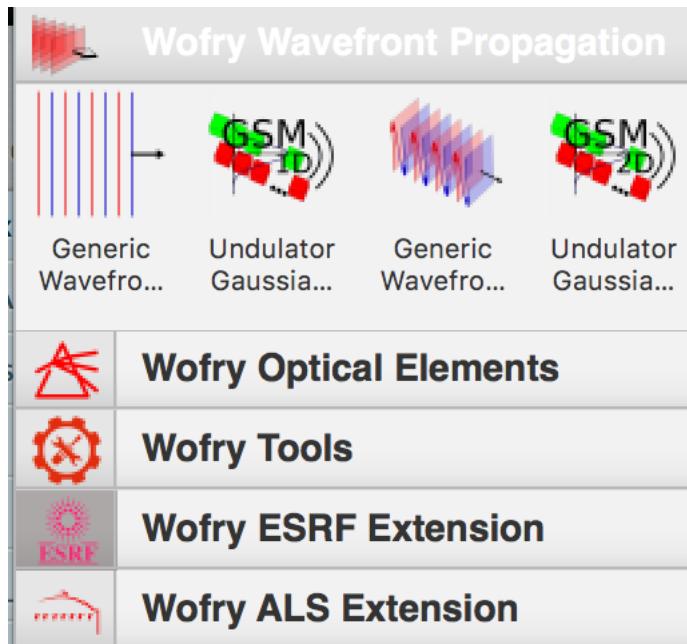
Chubar, O. and Celestre, R.: *Memory and CPU efficient computation of the Fresnel free-space propagator in Fourier optics simulation*. Opt. Express 27, 28750-28759 (2019)



OASYS interface by Luca Rebuffi

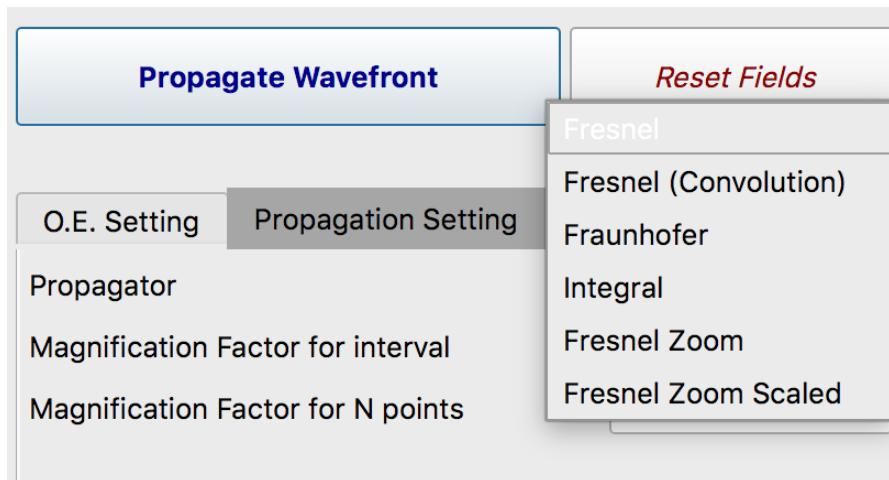
WOFRY (OASYS team)

- Simpler use
- Basic wavefronts (plane waves, spherical waves)
- 1D and 2D modes (less expensive)
- Approximated undulator sources
- Effective propagators
- Not as complete as SRW but growing fast
- Good for prototyping beamlines



Propagators

1D



Fresnel

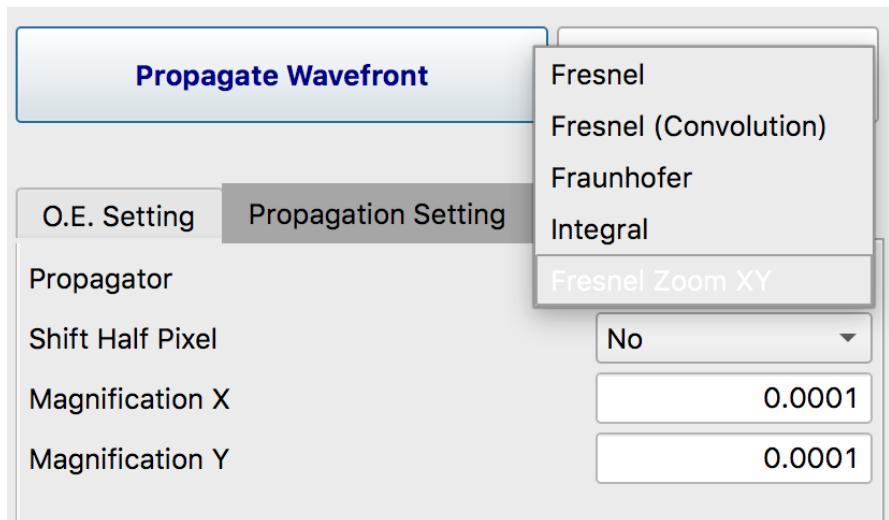
Fresnel (convolution)

Integral

Fresnel Zoom

Fresnel Zoom Scaled

2D



Zoom Propagator

$$U(x_2, y_2) = \frac{e^{ik\Delta z}}{\sqrt{m_x m_y}} e^{i \frac{k}{2\Delta z} [\frac{m_x - 1}{m_x} x_2^2 + \frac{m_y - 1}{m_y} y_2^2]} \\ \mathcal{F}^{-1} \left[\mathcal{F} \left[U(x_1, y_1) e^{i \frac{k}{2\Delta z} [(1-m_x)x_1^2 + (1-m_y)y_1^2]} \right] \times e^{-i\pi\lambda\Delta z (\frac{f_x^2}{m_x} + \frac{f_y^2}{m_y})} \right]$$

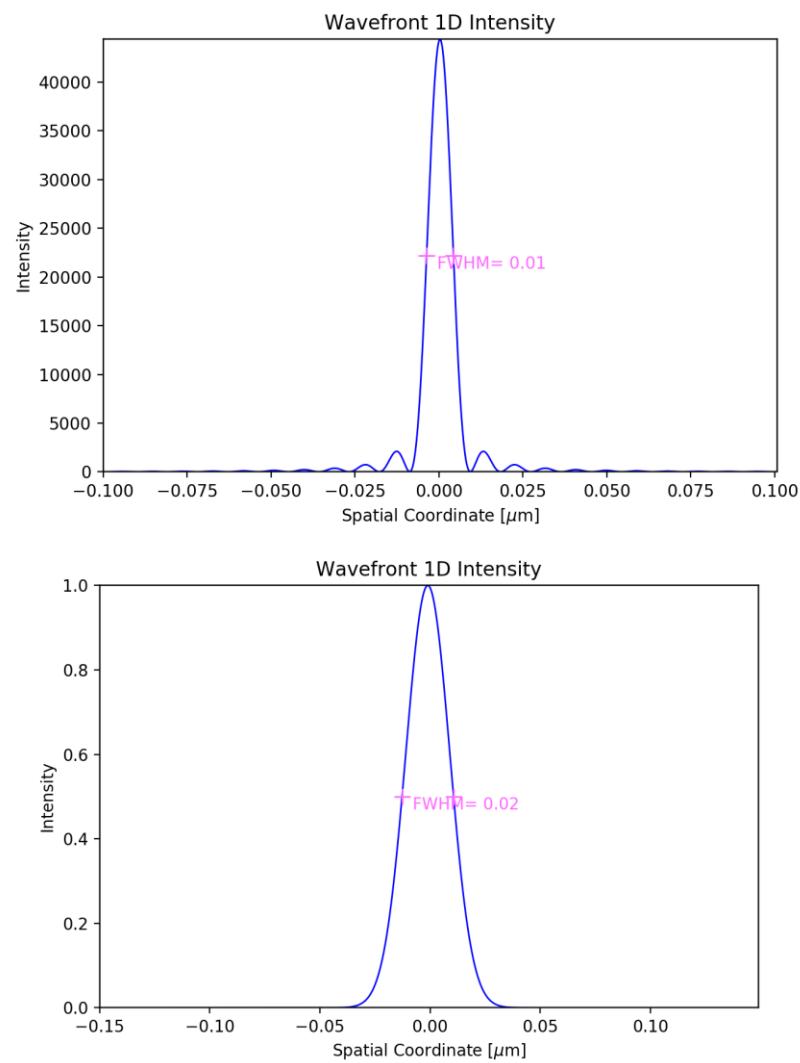
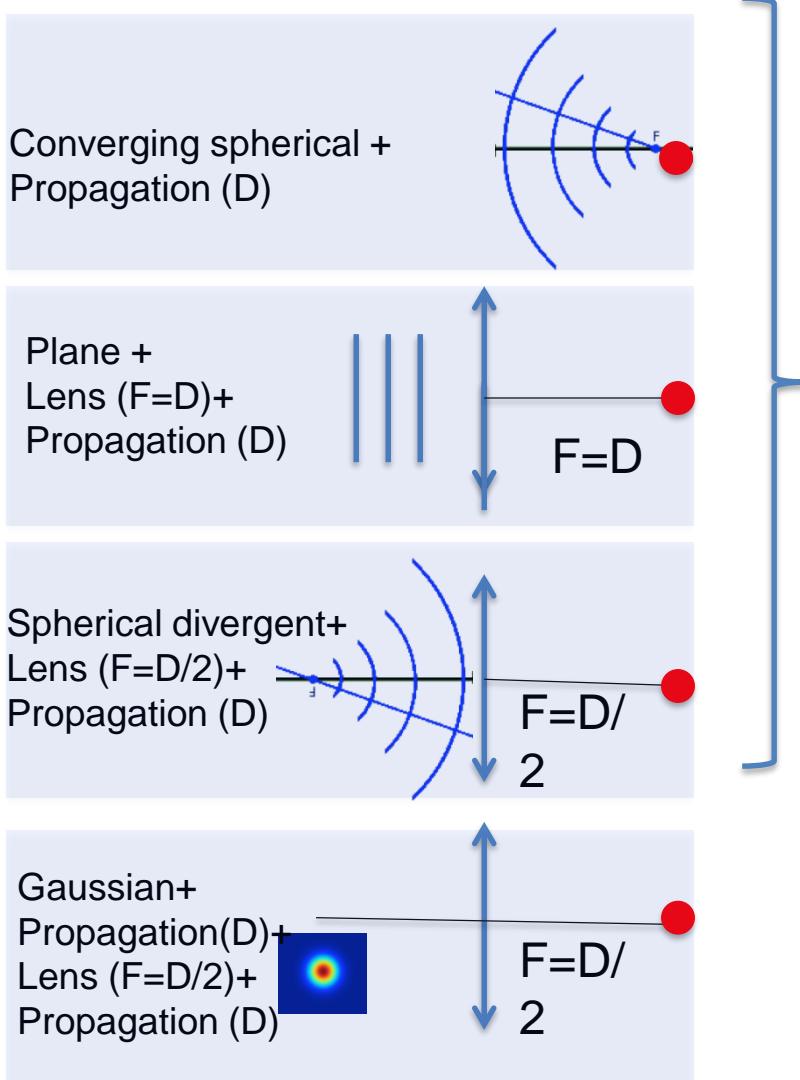
Jason D. Schmidt. *Numerical Simulation of Optical Wave Propagation*. SPIE Press, Bellingham, WA, USA, 2010.

G. Pirro, Master Thesis (2017)

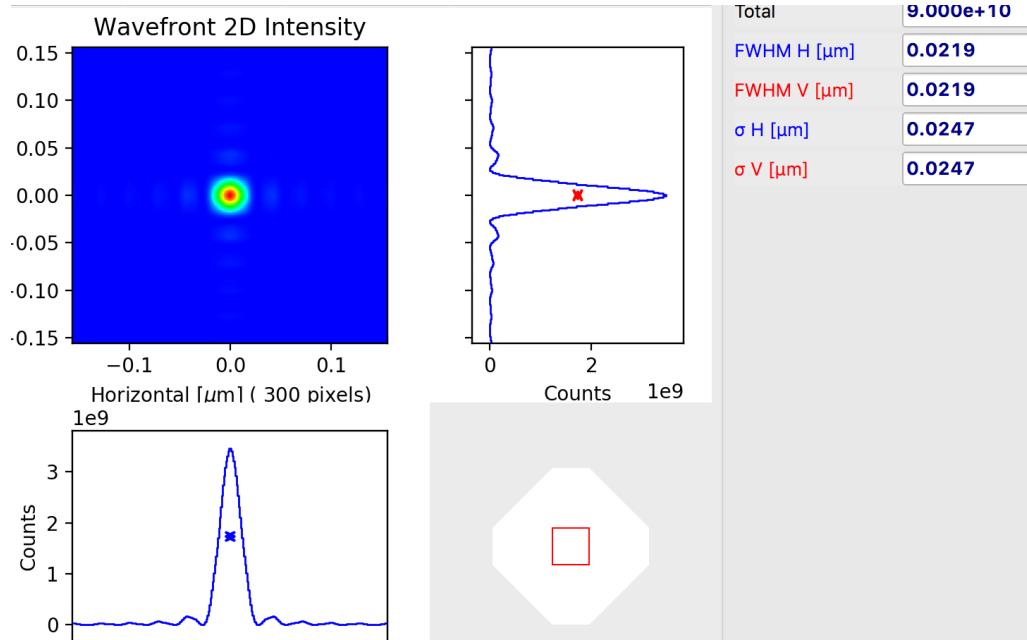
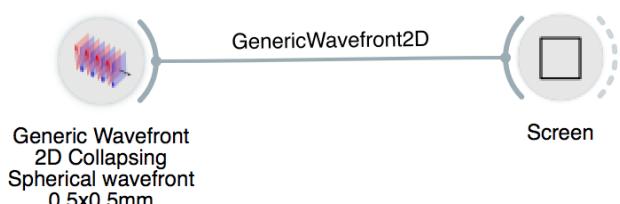
https://github.com/oasys-kit/documents/blob/master/zoom_propagator_pirro_thesis.pdf

wofry_examples.ows simple propagation cases

Aperture=0.4 mm, E=17225 eV, D=5cm



2D Oversimplified Beamline



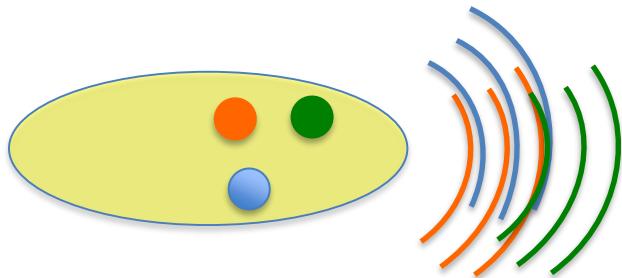
Theoretical consideration

The diffraction by a $D \times D$ square aperture of a collapsing spherical wavefront has an intensity distribution proportional to $\text{sinc}^2(kDx/2f) \text{ sinc}^2(kDy/2f)$, where $k=2\pi/\lambda$, $x(y)$ is the horizontal (vertical) coordinate, and f is the distance aperture-focus (D/f is the divergence). Considering that the FWHM of $\text{sinc}^2(x)$ is approximately 2.78, one obtains a $\text{FWHM}=0.885 * \text{wavelength} / \text{divergence}=18\text{nm}$

Partial coherence

Partial coherence is due to the electron beam emittance

Multielectron Calculation (SRW)

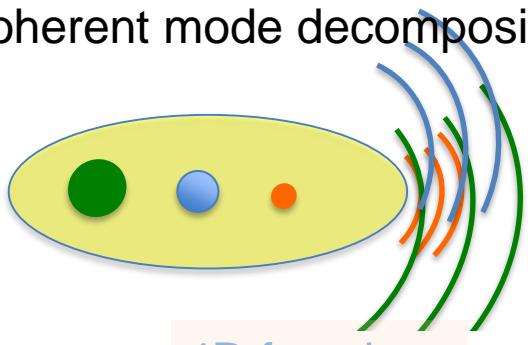


$$W(x_1, y_1, x_2, y_2, z, \omega) = \langle E^*(x_1, y_1, z, \omega) E(x_2, y_2, z, \omega) \rangle$$

$N_x, N_y \in [100, 1000]$

$W \sim 10^8 - 10^{12}$ (Gb-Tb)
Propagate: 4D integrals

Coherent mode decomposition



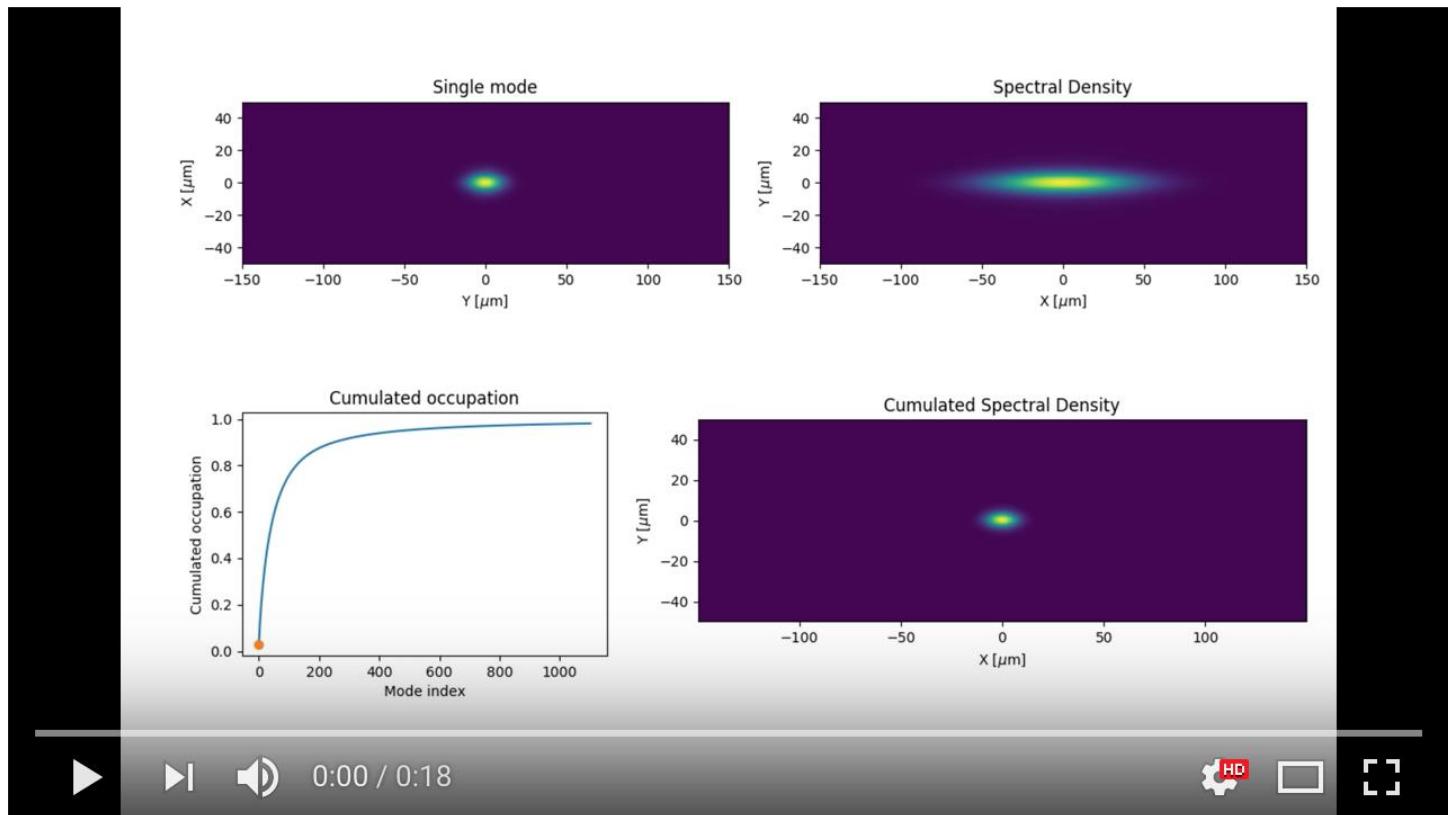
<http://dx.doi.org/10.1209/0295-5075/119/34004>

Mark Glass, Manuel Sanchez del Rio (2017) Coherent modes of X-ray beams emitted by undulators in new storage rings EPL (Europhysics Letters) 119

$$W(x_1, y_1, x_2, y_2, \omega) = \sum_m \lambda_m(\omega) \phi_m^*(x_1, y_1, \omega) \phi_m(x_2, y_2, \omega)$$

2D functions

Store $m \times N \times N$ Propagate: 2D integrals



Coherent modes of synchrotron radiation for EBS

<https://youtu.be/h24RrJZaQ80>

Example approximating the Undulator by the Gaussian Shell-model

SIMPLE CASE: 1D Gaussian SHELL-MODEL

$$W(x_1, x_2, \omega) = A^2 e^{-(x_1^2 + x_2^2)/(4\sigma_I^2)} e^{-(x_2 - x_1)^2/(2\sigma_\mu^2)}$$

Both **intensity (Spectral Density)** and **correlation (Spectral Degree of Coherence)** are Gaussians



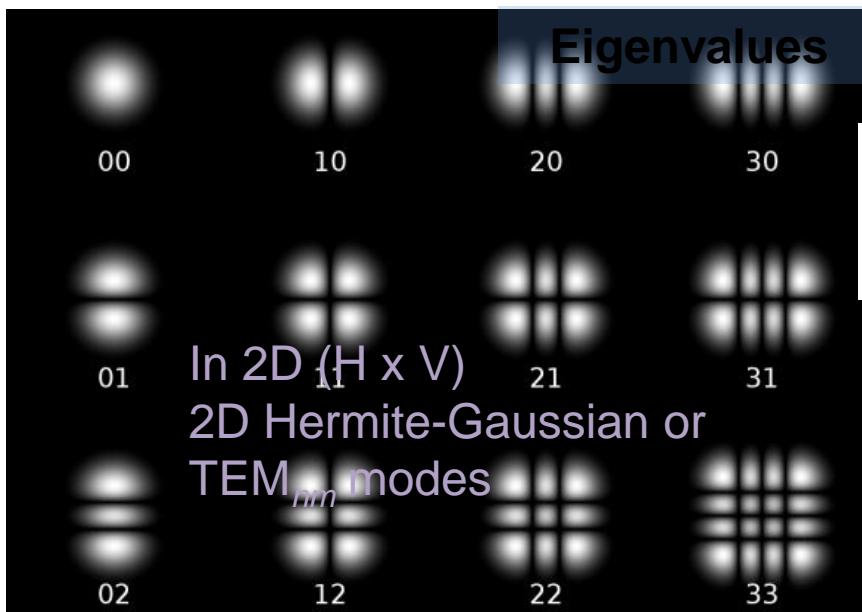
$\sigma_I \gg \sigma_\mu$ the source is mostly incoherent (quasi homogeneous)



$\sigma_I \ll \sigma_\mu$ is mostly coherent

$$W(x_1, x_2, \omega) = \sum_n \lambda_n(\omega) \phi_n^*(x_1, \omega) \phi_n(x_2, \omega),$$

$$\beta = \frac{\sigma_\mu}{\sigma_I}$$



Eigenfunctions
(Hermite-Gaussian modes)

$$\phi_n(x) = \left(\frac{2c}{\pi}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(x\sqrt{2c}) e^{-cx^2}$$

Magic property: Propagation invariance

In the first mode (Gaussian) :

$$S_x S_q = \frac{I}{4p}$$

The spectrum of coherent modes

Eigenvalues

$$a(\omega) = \frac{1}{4\sigma_I^2(\omega)}, \quad b(\omega) = \frac{1}{2\sigma_\mu^2(\omega)} \quad c = (a^2 + 2ab)^{1/2}$$

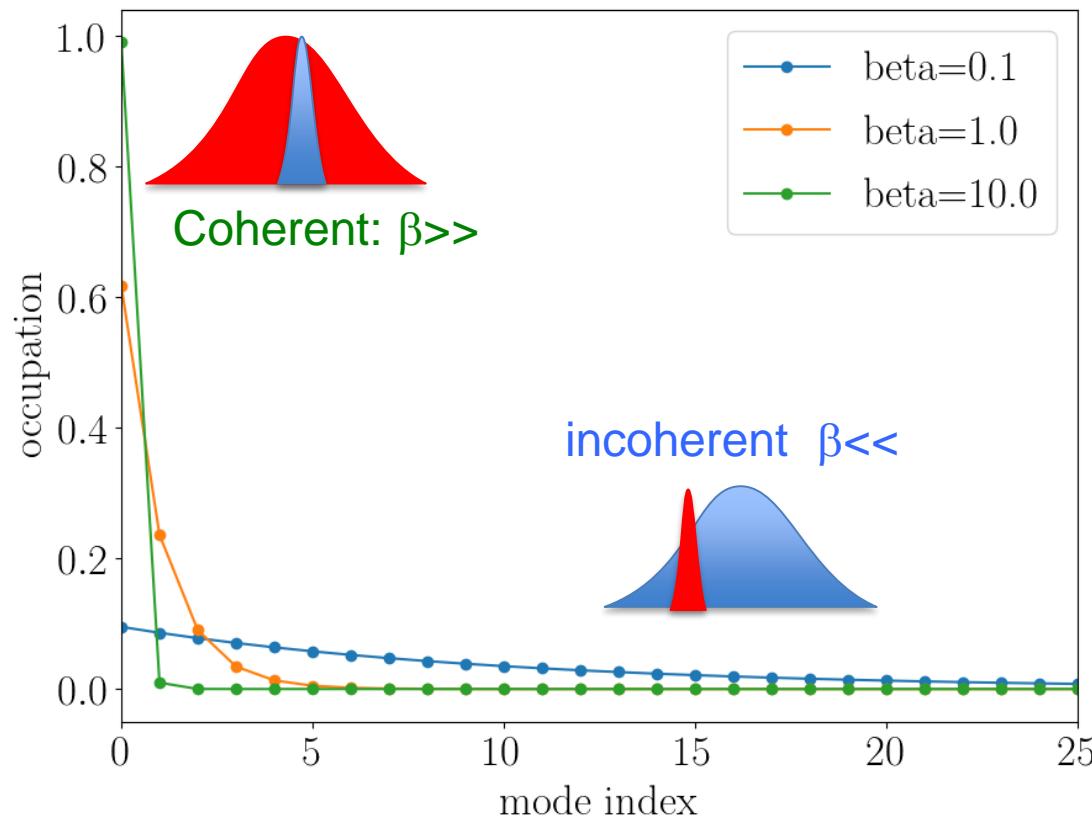
$$\lambda_n = A \left(\frac{\pi}{a+b+c} \right)^{1/2} \left(\frac{b}{a+b+c} \right)^n$$

Mode occupation:

$$\eta_i(\omega) = \frac{\lambda_i(\omega)}{\sum_{n=0}^{\infty} \lambda_n(\omega)}$$

Coherent fraction:

$$CF = \frac{\lambda_0}{\sum \lambda_n}$$



$$\beta = \frac{\sigma_\mu}{\sigma_I}$$

In general we cannot apply Gaussian Shell-model to synchrotron