Coherence of x-ray sources and beams: From basic concepts to computer simulations

Manuel SANCHEZ DEL RIO

OUTLINE

- Waves and coherent optics
  - Wave representation. Effects: diffraction and interference
  - Coherent lengths
  - Diffraction: Fraunhofer, Fresnel, Fresnel-Kirchhoff
  - Codes

- Sources and Beams
  - Extended sources can be coherent
    - Coherent Fraction
    - SR sources (coherence & emittance)
  - Incoherent sources can produce coherent beams
    - Coherence by propagation: Complex Degree of Coherence, Van Cittert-Zernike
  - A quick insight in partial coherence

- Few ideas on calculations

- New software

I could not find a coherent definition of coherence….

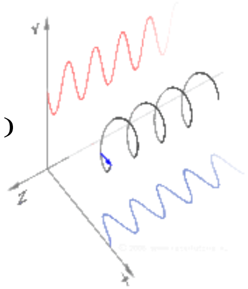
Although some optical coherence phenomena are known to all physicists, no general agreement exists on the precise meaning of the term "coherence," or on the domain encompassed by coherence theory.

Coherence Properties of Optical Fields
Rev. Mod. Phys. 37, 231
Mandel and Wolf

The ingredient: Waves

- Solutions of the Wave equation $\frac{\partial^2 u}{\partial t^2} = c^2 \nabla^2 u$ $\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}$
- Plane wave $\vec{E}(\vec{r},t) = \frac{\vec{k}}{|\vec{k}|} U(\vec{r},t);\quad U(\vec{r},t) = A_o e^{i(\vec{k}\cdot\vec{r}-\omega t+\varphi)}$
- Spherical wave $U(r,t) = \frac{A_o}{r} e^{i(kr-\omega t+\varphi)}$
- Polarization

$$\vec{E}(\vec{r},t) = \vec{E}_o e^{i(\vec{k}\cdot\vec{r}-\omega t+\varphi)};\quad \begin{pmatrix} E_x(z) \\ E_y(z) \\ 0 \end{pmatrix} = \begin{pmatrix} E_{x0} e^{i\varphi_x} \\ E_{y0} e^{i\varphi_y} \\ 0 \end{pmatrix} e^{i(kz-\omega t)}$$



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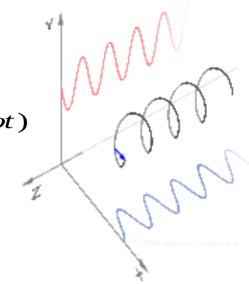
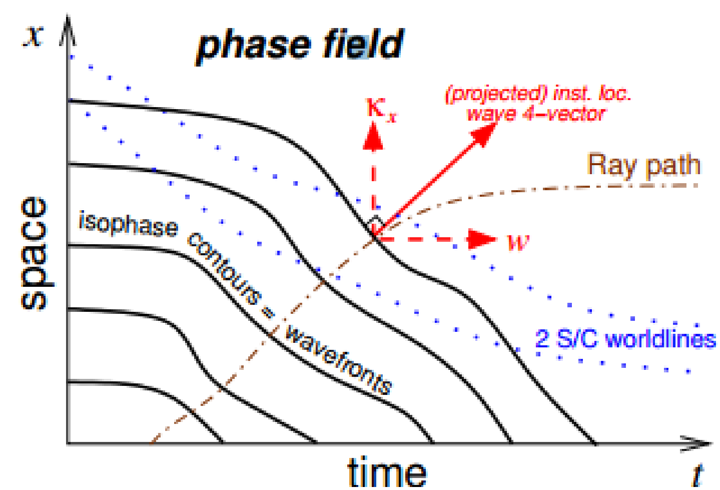
- Spherical wave $U(r,t) = \frac{A_o}{r} e^{i(kr - \omega t + \varphi)}$
- Polarization $\vec{E}(\vec{r},t) = \vec{E}_o e^{i(\vec{k}\cdot\vec{r} - \omega t + \varphi)}$; $\begin{pmatrix} E_x(z) \\ E_y(z) \\ 0 \end{pmatrix} = \begin{pmatrix} E_{x0} e^{i\varphi_x} \\ E_{y0} e^{i\varphi_y} \\ 0 \end{pmatrix} e^{i(kz - \omega t)}$



- Wavefronts: surfaces with constant phase,
  ϕ(x)=const

- Ray paths: trajectories which are everywhere orthogonal to the wavefronts.
  - Rays follow the wavefront normals ∇ϕ.
  - The local wavevector is κ(t, x) := −∇ϕ

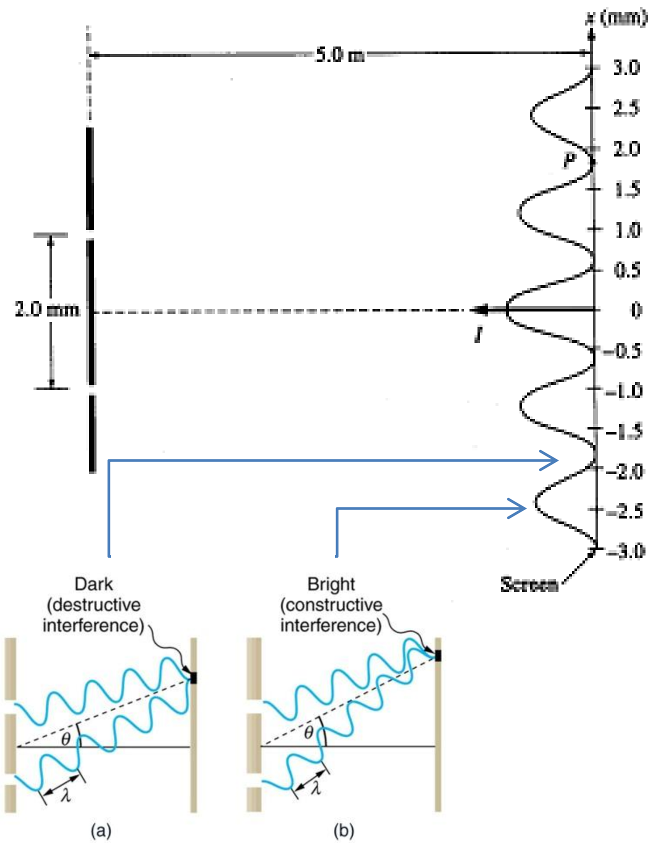


- A wave is always fully coherent (even with a wavy wavefront)

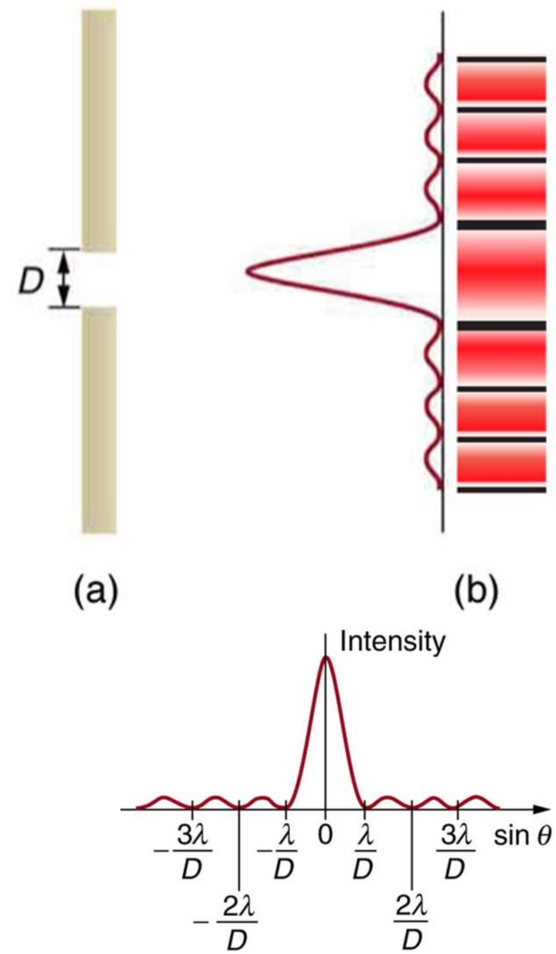
Coherent radiation produces interference patterns:

Coherence: “the property that enables a wave to produce *visible* interference and diffraction effects”

INTERFERENCE



DIFFRACTION



- **At least TWO waves are needed to define coherence lengths**
- **A beam is a collection of waves:**
  - **Described individually**
  - **Described as a sum of individual waves**
  - **Described collectively (statistical optics)**

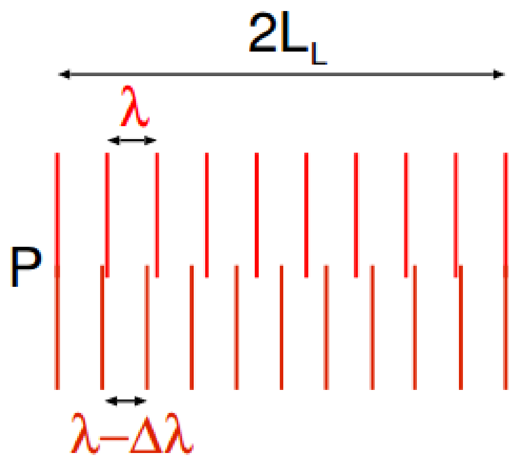
Coherence describes the correlation between WAVES at different points:

- Spatial coherence describes the correlation between waves at different points in space.

- Temporal coherence describes the correlation or predictable relationship between waves observed at different moments in time.

http://www.csrri.iit.edu/~segre/phys570/10F/lecture_04.pdf

Starting with TWO well defined (thus coherent) waves:



LONGITUDINAL COHERENCE LENGTH L_L

Definition: Distance over which two waves from the same source point with slightly different wavelengths will completely dephase.

$$2L_L = N\lambda$$
$$2L_L = (N+1)(\lambda - \Delta\lambda)$$

$$0 = \lambda - N\Delta\lambda - \Delta\lambda \longrightarrow \lambda = (N+1)\Delta\lambda \longrightarrow N \approx \frac{\lambda}{\Delta\lambda} \longrightarrow \boxed{L_L = \frac{\lambda^2}{2\Delta\lambda}}$$

- **Coherence time τ: $L_L = c\,\tau$**

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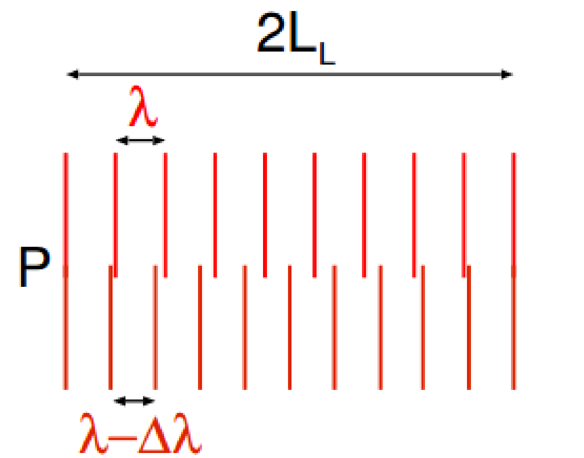

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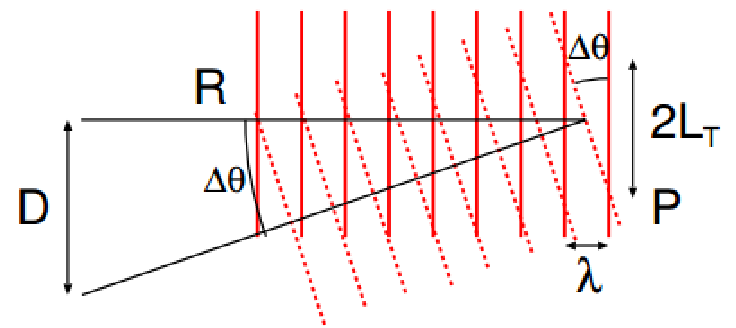
- **Coherence time τ: $L_L = c\,\tau$**

TRANSVERSE COHERENCE LENGTH L_T

Definition: The lateral distance along a wavefront over which there is a complete dephasing between two waves of the same wavelength, which originate from two separate points in space



$$\frac{\lambda}{2L_T} = \tan\Delta\theta \approx \Delta\theta \qquad \frac{D}{R} = \tan\Delta\theta \approx \Delta\theta$$

$$\boxed{L_T = \frac{\lambda R}{2D}}$$

For a typical 3rd generation undulator source we are typically R = 30m away with our experiment. If we assume a typical wavelength of λ = 1Å, and a monochromator resolution of $\Delta\lambda/\lambda = 10^{-4}$ we have:

$L_L = (1/2)\,(\lambda/\Delta\lambda)\,\lambda = 0.5 * 10^4 * 10^{-10} = 0.5\ \mu m$

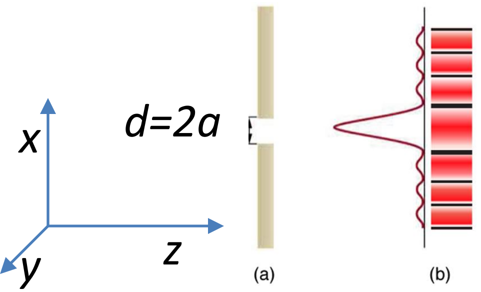
$L_T = \lambda R / (2D) = 1.5\ 10^{-9}/D$

	High beta	Low beta	ESRF-II
Vertical	$D = 3.5*2.35\mu m$	$D = 3.5*2.35\mu m$	$D = 3.4*2.35\mu m$
	-------------------------	L_T=185 μm	-------------------------------
Horizontal	$D=387.8*2.35\mu m$	$D=37.4*2.35\mu m$	$D=27.2*2.35\mu m$
	L_T~1.5 μm	L_T~15 μm	L_T~25 μm

Coherent beam(s) produce interference and <u>diffraction:</u>

- Far field (Fraunhoffer)
- Near field (Fresnel)
- Kirchhoff-Fresnel

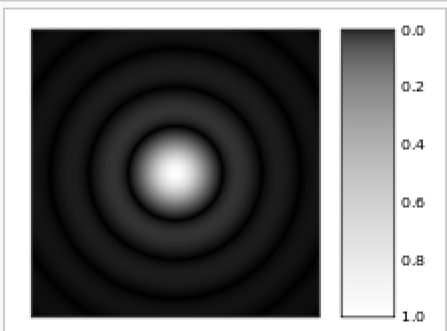
See for example: http://photonics.intec.ugent.be/download/ocs130.pdf



FRAUNHOFFER DIFFRACTION

$$U(x_0,y_0)=\frac{-e^{-jkz}}{j\lambda z}e^{-\frac{jk}{2z}[x_0^2+y_0^2]}\int\int_{-\infty}^{+\infty}U(x_1,y_1)e^{j\frac{2\pi}{\lambda z}[x_0x_1+y_0y_1]}dx_1dy_1$$

Fourier transform with conjugated variables:
x_1 ; $f_x=x/(\lambda\ z) \sim \sin\theta/\lambda$ (same for y)



Computer-generated image of an **Airy disk**. The gray scale intensities have been adjusted to enhance the brightness of the outer rings of the Airy pattern.

The **Airy disk** or **Airy pattern** is the diffraction pattern produced by a circular aperture

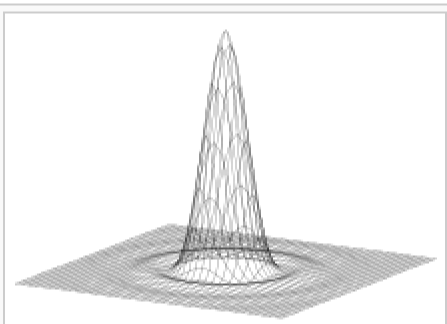
$$I(\theta)=I_0\left[\frac{2J_1(ka\sin\theta)}{ka\sin\theta}\right]^2$$

Far away from the aperture, the angular radius of the central ring (position of the first extinction measured from the direction of incoming light) is found at $(k\ a\ \sin\theta) = 1.22\ \pi$, thus given by the approximate formula:

$$\sin\theta\approx 1.22\frac{\lambda}{d}$$

or :

$$\boxed{\Delta_x\ \Delta_\theta\approx\frac{\lambda}{0.41}=30.7\frac{\lambda}{4\pi}}$$



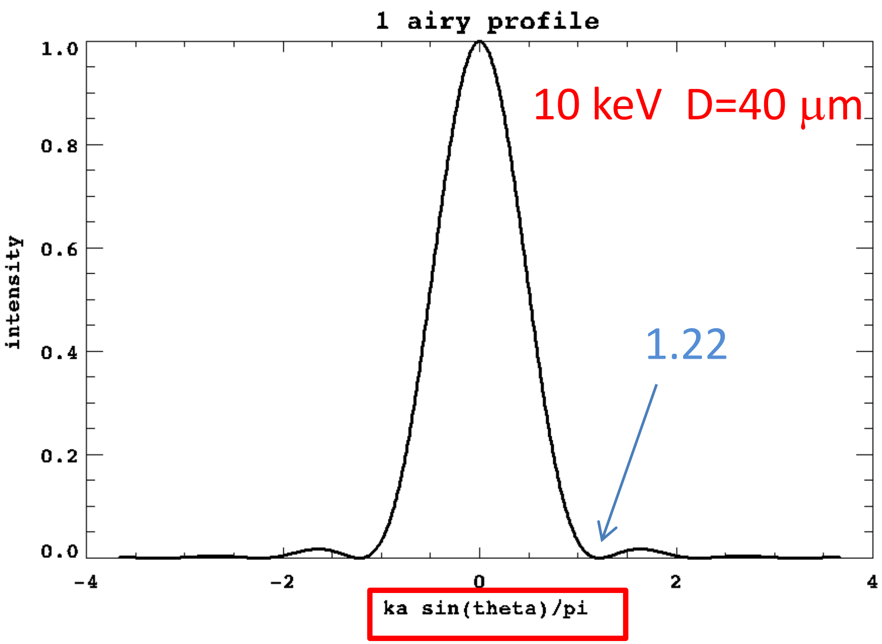
Surface plot of intensity in an **Airy disk**.

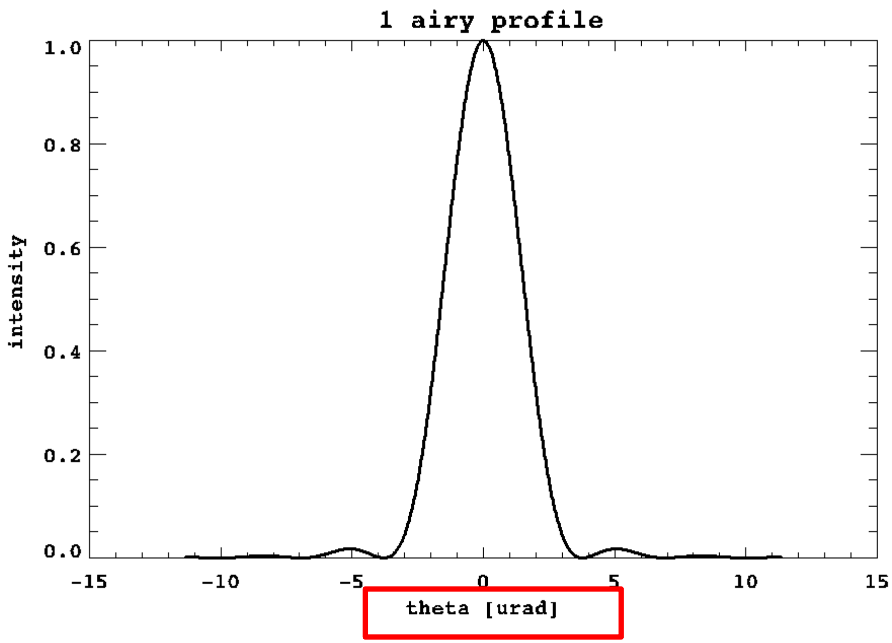
en.wikipedia.org/wiki/Airy_disk

FRAUNHOFFER DIFFRACTION
PYTHON CALCULATION GAUSSIAN APERTURE
/tmp_14_days/srio/seminar/airy_profile.py

```
from scipy.special import jv
import numpy

wavelength = 1.24e-10 # 10keV
aperture_diameter = 40e-6
x = (2*numpy.pi/wavelength) * (aperture_diameter/2) * sin_theta_array
electric_field = 2*jv(1,x)/x
intensity = electric_field**2
```

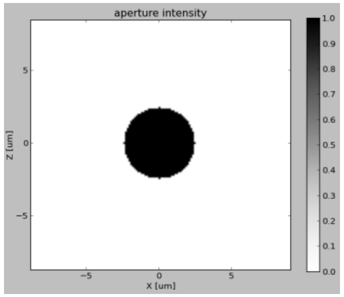


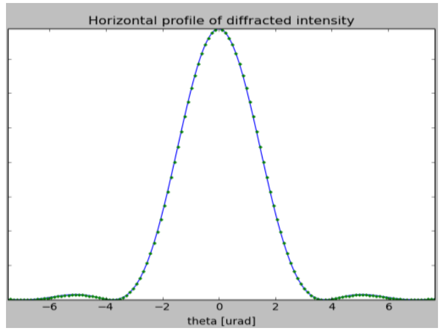


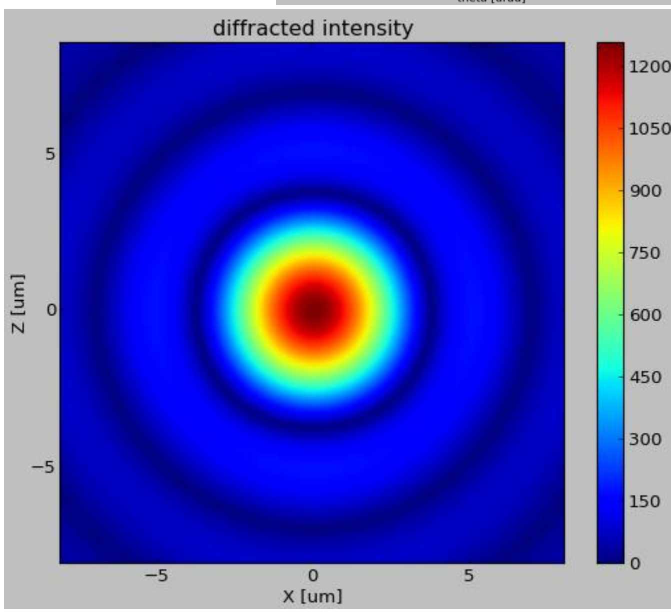
FRAUNHOFER DIFFRACTION : PYTHON CALCULATION OF FOURIER TRANSFORM

fraunhofer.py

```
F1 = np.fft.fft2(image)  # Take the Fourier transform of the image
```







$\Delta\theta\ \Delta x \sim 2 \text{ x}1.22\text{x } \lambda = \lambda\ /0.41$

A Gaussian profile with standard deviation $\sigma = 0.44\ \lambda\ /\ D$
has the same width as the Airy function.

Gaussian with same width:

$2.35\ \sigma x = d = \Delta x$; $\sigma_\theta\ \sigma_x \sim (0.44/2.35)\ \lambda \sim \lambda\ /5.34$

Numerical: $\sigma_\theta\ \sigma_x \sim \lambda\ /5.71$

FRAUNHOFFER DIFFRACTION : PYTHON CALCULATION OF FOURIER TRANSFORM

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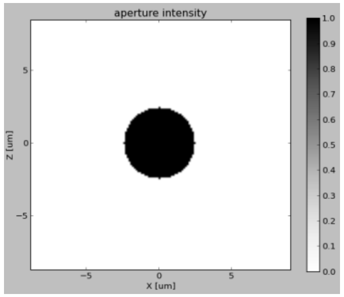
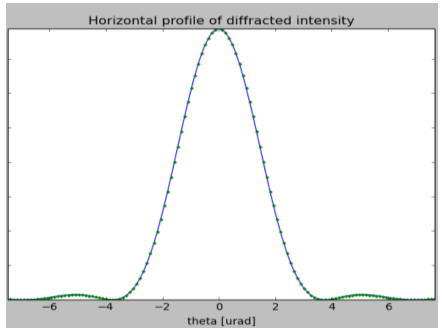
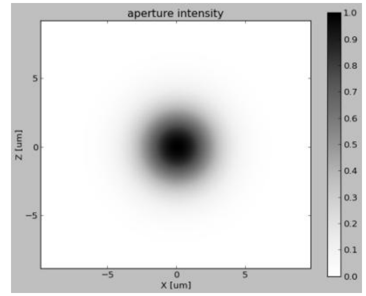
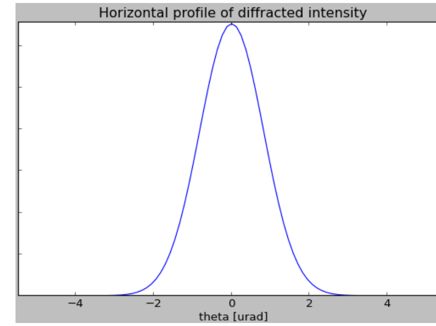
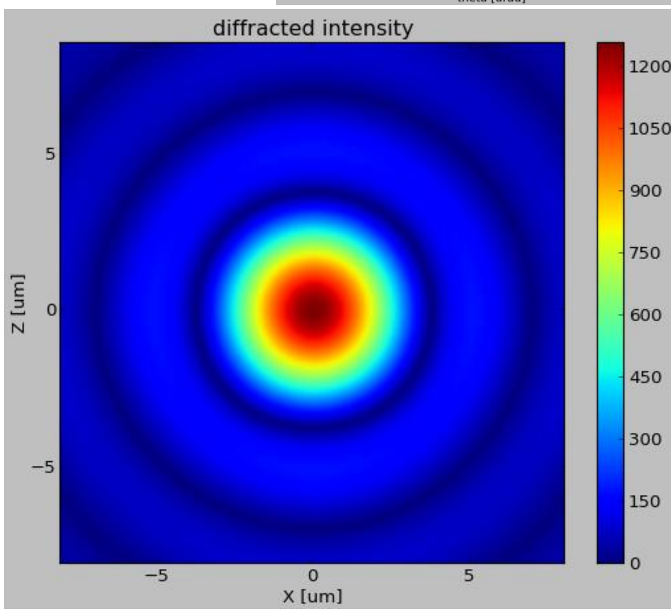
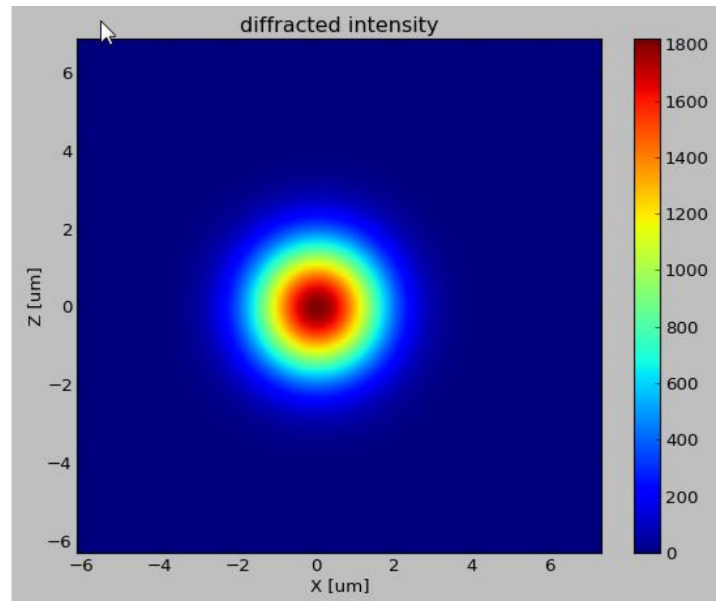












$\Delta\theta\ \Delta x \sim 2 \times 1.22 \times \lambda = \lambda / 0.41$

A Gaussian profile with standard deviation $\sigma = 0.44\ \lambda / D$ has the same width as the Airy function.

Gaussian with same width:

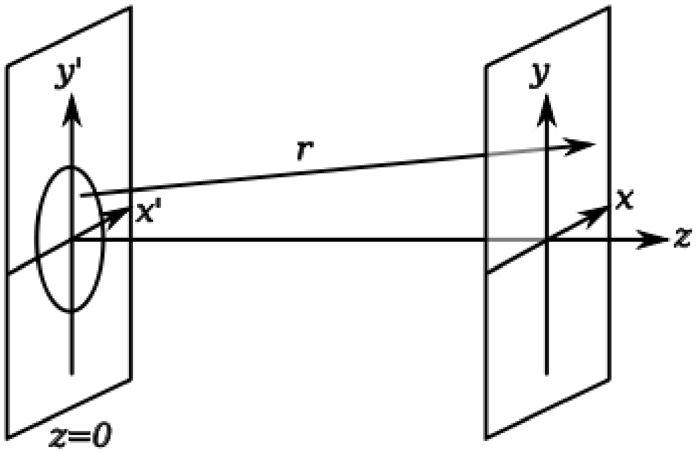
$2.35\ \sigma x = d = \Delta x$; $\sigma_\theta\ \sigma_x \sim (0.44/2.35)\ \lambda \sim \lambda / 5.34$

Numerical: $\sigma_\theta\ \sigma_x \sim \lambda / 5.71$

Numerical: $\sigma_\theta\ \sigma_x \sim \lambda / 14.40$

Theoretical: $\sigma_\theta\ \sigma_x \sim ?\ \lambda / (4\ \pi)$

FRESNEL DIFFRACTION



Fraunhofer diffraction occurs when:

$$F = \frac{a^2}{L\lambda} \ll 1$$

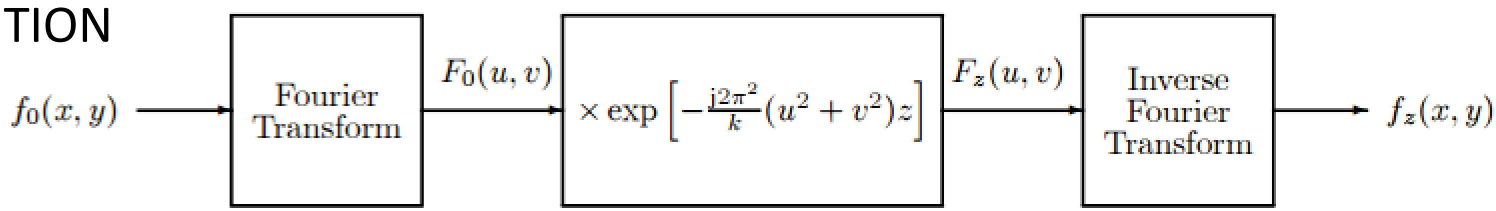
Fresnel diffraction occurs when:

$$F = \frac{a^2}{L\lambda} \geq 1$$

$$f_z(x,y) = \frac{1}{\mathrm{j}\lambda z}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f_0(x_0,y_0)\exp\left[\frac{\mathrm{j}k}{2z}\left((x-x_0)^2+(y-y_0)^2\right)\right]\mathrm{d}x_0\,\mathrm{d}y_0.$$

Numeric calculation:

CONVOLUTION



http://home.comcast.net/~szemengtan/LinearSystems/waves.pdf

KIRCHHOFF DIFFRACTION THEORY

Maxwell equations => Wave equation

$$\nabla^2 V = \frac{1}{c^2}\frac{\partial V}{\partial t}$$

Scalar monochromatic wave: V = U(x,y,z) exp(-iωt) => Helmholzt equation

$$\nabla^2 U + k^2 U = 0$$

Green solution= Integral theorem of Helmholtz and Kirchhoff

$$U(P_0) = \frac{1}{4\pi}\int\int_S \left(\frac{\partial U}{\partial n}\frac{e^{-jk|\mathbf{r}-\mathbf{r}_0|}}{|\mathbf{r}-\mathbf{r}_0|} - U\frac{\partial}{\partial n}\frac{e^{-jk|\mathbf{r}-\mathbf{r}_0|}}{|\mathbf{r}-\mathbf{r}_0|}\right) ds$$

Diffraction through an aperture in a planar screen
good boundary conditions => (Fresnel-Kirchhoff diffraction formula)

$$U(P_0) = \frac{1}{4\pi}\int\int_\sigma \frac{e^{-jk|\mathbf{r}_1-\mathbf{r}_0|}}{|\mathbf{r}_1-\mathbf{r}_0|}\left(\frac{\partial U}{\partial n} + jkU\cos(\mathbf{n},\mathbf{r}_1-\mathbf{r}_0)\right) ds_1$$

Better Green functions: Rayleigh Sommerfeld diffraction formula (Huygens-Fresnel principle):

$$U(P_0) = \frac{-1}{j\lambda}\int\int_\sigma U(P_1)\cos(\mathbf{n},\mathbf{r}_1-\mathbf{r}_0)\frac{e^{-jk|\mathbf{r}_1-\mathbf{r}_0|}}{|\mathbf{r}_1-\mathbf{r}_0|} ds_1$$

KIRCHHOFF DIFFRACTION THEORY II

Approximation:

$$
\begin{aligned}
|\mathbf{r}_1 - \mathbf{r}_0| &= \sqrt{z^2 + (x_1 - x_0)^2 + (y_1 - y_0)^2} \\
&\cong z\left[1 + \frac{1}{2}\left(\frac{x_1 - x_0}{z}\right)^2 + \frac{1}{2}\left(\frac{y_1 - y_0}{z}\right)^2\right]
\end{aligned}
$$

Fresnel (quadratic term, obliquity=1):

$$
\frac{-1}{j\lambda z} e^{-jk|\mathbf{r}_1 - \mathbf{r}_0|} \sim \frac{-e^{-jkz}}{j\lambda z} e^{-\frac{jk}{2z}\left[(x_1 - x_0)^2 + (y_1 - y_0)^2\right]}
$$

Fraunhofer (quadratic term neglected)

$$
z >> \frac{k\left(x_1^2 + y_1^2\right)_{\max}}{2}
$$

$$
U(x_0, y_0) = \frac{-e^{-jkz}}{j\lambda z} e^{-\frac{jk}{2z}\left[x_0^2 + y_0^2\right]} \int \int_{-\infty}^{+\infty} U(x_1, y_1) e^{j\frac{2\pi}{\lambda z}\left[x_0 x_1 + y_0 y_1\right]} dx_1 dy_1
$$

Numeric implementation of the Fresnel-Kirchhoff diffraction integral:

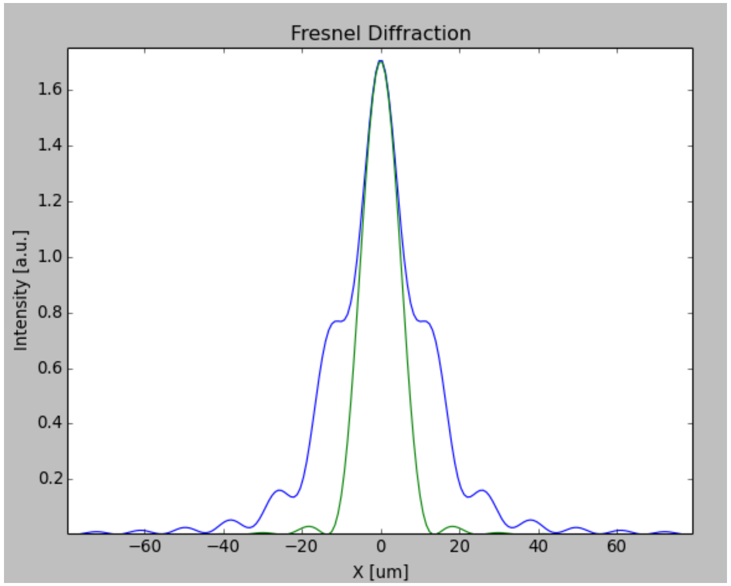
1) Sample points in aperture x_m and detector x_k
2) compute $r_{mk} = \sqrt{(x_m - x_k)^2 + (y_m - y_k)^2 + (z_m - z_k)^2} \sim \sqrt{(x_m - x_k)^2 + L^2}$
3) Evaluate exponential, and multiply by the field on the aperture U_m
4) Apply (if wanted) inclination and ~1/R term
5) sum (integral) : $I_k = |R_{mk} U_m|^2$

fresnel_fourier_1D.py

```
# FT
F1 = numpy.fft.fft(fields1)
wfou_fft = numpy.fft.fftshift(F1)

#propagate
wfou_fft *= numpy.exp(-1j * numpy.pi *
           wavelength * distance *
           wfou_fft_x**2 )

#back FT
fields2 = numpy.fft.ifft(wfou_fft)
fieldIntensity = numpy.abs(fields2)**2
```

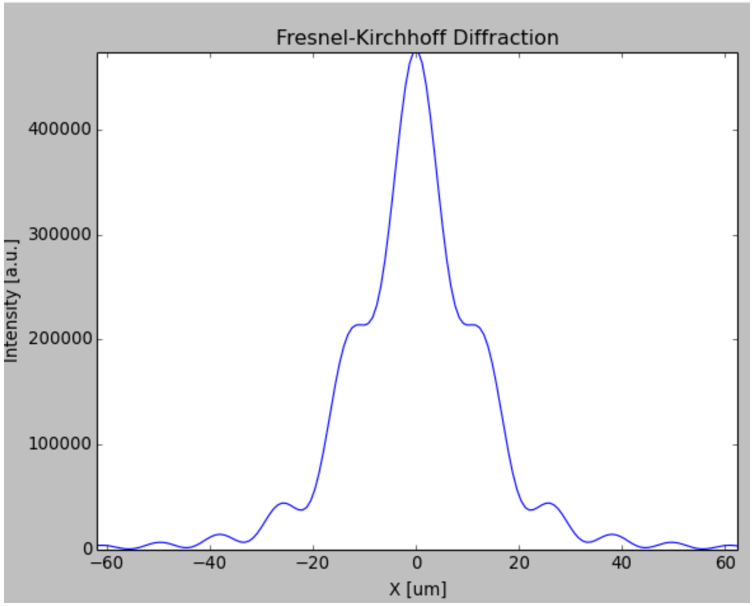


fresnel_kirchhoff_1D.py

```
def goFromTo(source,image,distance=1.0,lwavelength=1e-10):
    x1 = numpy.outer(source,numpy.ones(image.size))
    x2 = numpy.outer(numpy.ones(source.size),image)
    r = numpy.sqrt( numpy.power(x1-x2,2) + numpy.power(distance,2) )
    return numpy.exp(1.j * wavenumber *  r)


fields12 =
goFromTo(position1x,position2x,distance,wavelength=wavelength)

fieldComplexAmplitude = numpy.dot(numpy.ones(sourcepoints),fields12)
fieldIntensity = numpy.power(numpy.abs(fieldComplexAmplitude),2)
```



Exercise: do this in 2D

Some Computer Codes for Synchrotron Radiation and X-Ray Optics Simulation

Free

Spontaneous

- **Synchrotron Radiation**
  - URGENT (R .Walker, ELETTRA)
  - XOP (M.S. del Rio, ESRF, R. Dejus, APS)
  - SPECTRA (T. Tanaka, H. Kitamura, SPring-8)
  - WAVE (M. Scheer, BESSY)
  - B2E (P. Elleaume, ESRF, 1994)
  - SRW (O. Chubar, P. Elleaume, ESRF, 1997-…)
  - SRCalc (R. Reininger, 2000)

SASE (3D)

  - GENESIS (S. Reiche, DESY/UCLA/PSI, ~1990-…)
  - GINGER (W.M. Fawley, LBNL, ~1986-…)
  - FAST (M. Yurkov, E. Schneidmiller, DESY, ~1990-…)

- **Geometrical Ray-Tracing**
  - SHADOW (F. Cerrina, M.S. del Rio)
  - RAY (F. Schäfers, BESSY)
  - McXtrace (E. Knudsen, A. Prodi, P. Willendrup, K. Lefmann, Univ. Copenhagen)
- **Wavefront Propagation**
  - PHASE (J. Bahrdt, BESSY)
  - SRW (O. Chubar, P. Elleaume, ESRF, 1997-…)
  - Code of J. Krzywinski et. al. (SLAC)
  - Code of L. Poyneer et. al. (LLNL)

Commercial

- ZEMAX (Radiant Zemax)
- GLAD (Applied Optics Research)
- VirtualLab (LightTrans)
- OSLO (Sinclair Optics)
- Microwave Studio (CST)

Commercial codes are expensive, and yet don't have all functions required for SR / X-ray Optics simulations

Courtesy O Chubar

Some Computer Codes for Synchrotron Radiation and X-Ray Optics Simulation

- **Synchrotron Radiation**

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- **Wavefront Propagation**
  - PHASE (J. Bahrdt, BESSY)
  - SRW (O. Chubar, P. Elleaume, ESRF, 1997-...)
  - Code of J. Krzywinski et. al. (SLAC)
  - Code of L. Poyneer et. al. (LLNL)

Free

Commercial

- ZEMAX (Radiant Zemax)
- GLAD (Applied Optics Research)
- VirtualLab (LightTrans)
- OSLO (Sinclair Optics)
- Microwave Studio (CST)

Commercial codes are expensive, and yet don't have all functions required for SR / X-ray Optics simulations

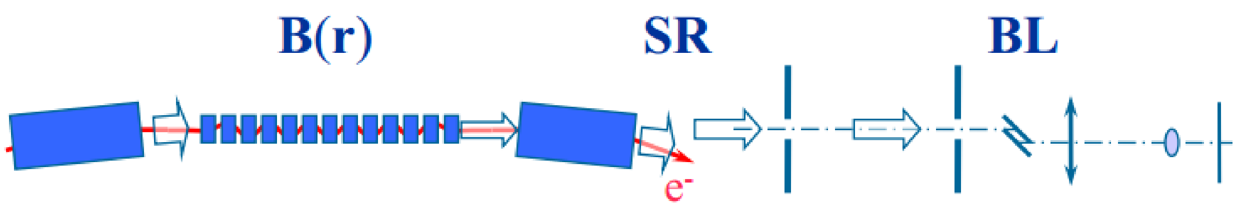
FULL BEAMLINES + OPEN SOURCE + PYTHON BINDING

Courtesy O Chubar

SRW (O. Chubar)

https://github.com/ochubar/SRW

General Motivation: Start To End Simulation



- Computation of **Magnetic Fields** produced by Permanent Magnets, Coils and Iron Blocks and in 3D space, optimized for the design of **Accelerator Magnets**, **Undulators** and **Wigglers**
- Fast computation of **Synchrotron Radiation** emitted by relativistic electrons in Magnetic Field of arbitrary configuration
- **SR Wavefront Propagation** (Physical Optics)
- Simulation of some **Experiments** involving **SR**

RADIA

ESRF

SRW

Started at ESRF thanks to Pascal Elleaume

Simulation

Known Object ⇒ Image

Direct Space

Reciprocal Space

OBJECT

multiplication wave with
transmission function

$T = e^{-B} e^{i\varphi}$

convolution

PROPAGATION

diffraction integral

multiplication FT wave with
propagator

$P_D = \exp(-i\neq\lambda D\mathbf{f}^2)$

INTENSITY

$I_D^{\mathrm{coh}}(x,y) = |u(x,y)|^2$

auto-correlation

COHERENCE / DETECTOR

convolution intensity with
projected source
PSF detector

multiplication FT intensity with
degree of coherence
detector transfer function

$|\propto_{12}(\lambda D\mathbf{f})|$

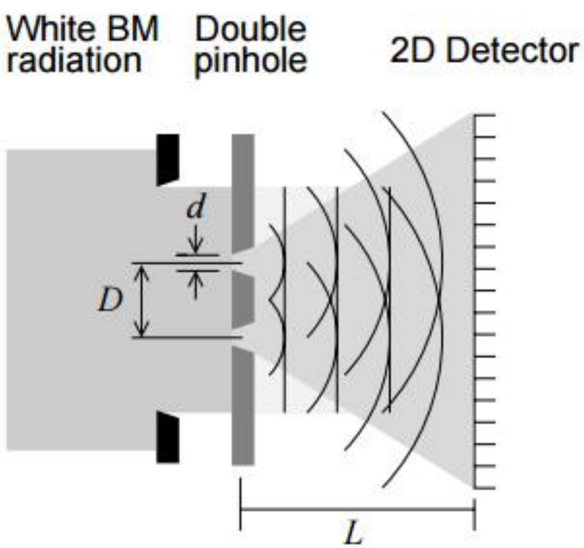
$R(\mathbf{f})$

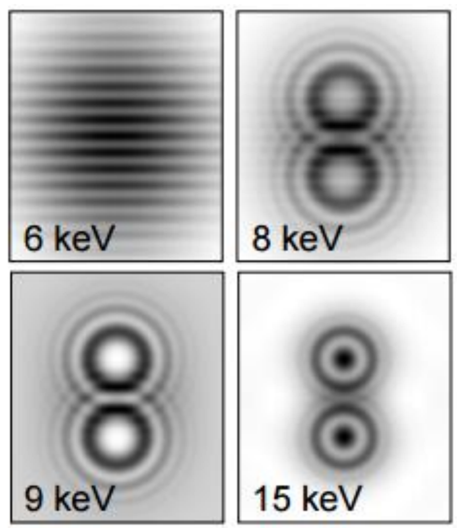
COURTESY: P Cloetens ID16A

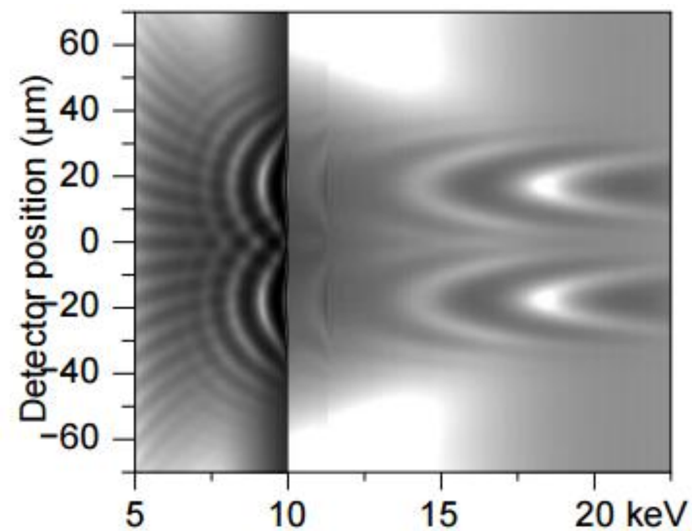
XWFP

Timm Weitkamp "XWFP: an x-ray wavefront propagation software package for the IDL computer language", *Proc. SPIE* 5536, (2004) doi:10.1117/12.56964

`IDL> w = OBJ_NEW('wavefront', KEV=15.0, NPIX=800, PIXSIZE=0.5e-3)`	Initialize wavefront of 800×800 pixels of 0.5 μm size at 15 keV
`IDL> w -> Planewave, 1e11`	Set field values to a plane wave, intensity 10^{11} photons / mm^2 / s
`IDL> w -> Sphere, 0.1, MATERIAL='B'`	Boron sphere, 100 μm diameter
`IDL> w -> Sphere, 0.05, MATERIAL='W', XOFFSET=0.05, YOFFSET=0.05`	Tungsten sphere, 50 μm diameter, off center
`IDL> w -> Display`	Show intensity
`IDL> w -> Display, /PHASE`	Show phase profile
`IDL> w -> Propagate, 2000`	Propagate by a distance of 2 m
`IDL> w -> Display`	Show intensity
`IDL> w -> Display, /PHASE`	Show phase
`IDL> w -> Display, PSF_WIDTH=5e-3, COUNT_TIME=0.1, DQE=0.01`	Show intensity with detector blurring and noise
`IDL> OBJ_DESTROY, w`	Delete object and free memory







Exercise: do this in Python

SHADOW3 - FRESNEL-KIRCHHOFF

M. Sanchez del Rio, N. Canestrari, F. Jiang and F. Cerrina "SHADOW3: a new version of the synchrotron X-ray optics modelling package"
J. Synchrotron Rad. (2011). 18, 708–716 doi: 10.1107/S0909049511026306

N. Canestrari, D. Karkoulis, M. Sanchez del Rio "SHADOW3-API: the application programming interface for the ray tracing code SHADOW", *Proc. SPIE* 8141, 814112 (2011) doi:10.1117/12.893433;

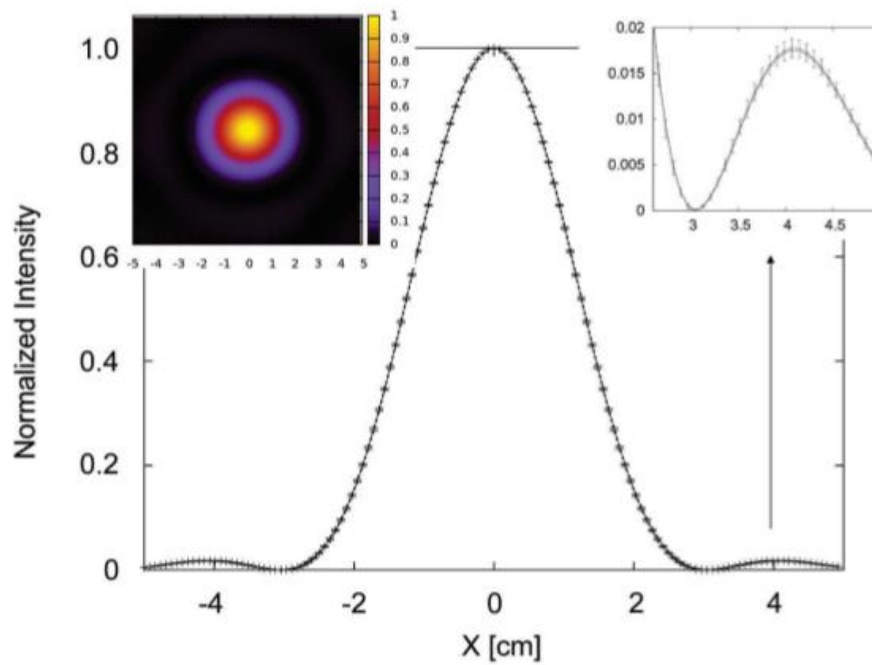
FFRESNEL is basically a numerical implementation of the *full* Fresnel-Kirchoff integral. It integrates over all the rays across a suitably located aperture. The priciple is discussed in B. Lai, K. Chapman and F. Cerrina, *SHADOW: New Developments*, Nucl. Instr. and Meth. **A266**, 544-549 (1988). Briefly, the FK integral can be written as:

$$A'(\vec{r}') = \frac{i\overline{u}}{\lambda}\int_S A(\vec{r})\frac{e^{ikR}}{R}d\vec{r} \tag{3.5}$$

where $R = |\vec{r} - \vec{r}'|$ and $r(r')$ is the position vector at the image (exit pupil) plane. $A(A')$ is the electric field at the same positions. SHADOW knows exactly $A(\vec{r})$ at the exit pupil while the mapping performed by the ray tracing operation has transformed the integral from a Riemann to a Stieltjes type. In order to do that, it must know for each ray the amplitude and phase of the electric field vector $\vec{A}$. In general, we separate $\vec{A}$ into two components :

$$\vec{A} = \vec{A}_s e^{i\theta_s} + \vec{A}_p e^{i\theta_p} \tag{3.6}$$

where s and p are the perpendicular and parallel component (respect to the plane of incidence). At the source, they are along the X and Z direction. Thus the $\vec{A}$ vector is defined



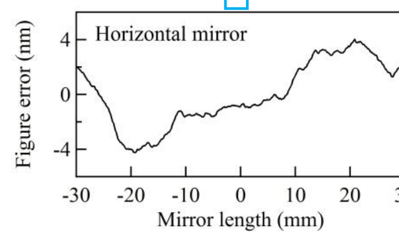
Limitation: only applicable to the LAST optical element

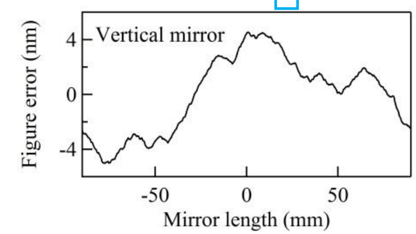
HYBRID METHOD IN SHADOW (X. Shi *et al.*)

Combining ray tracing and wavefront propagation

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

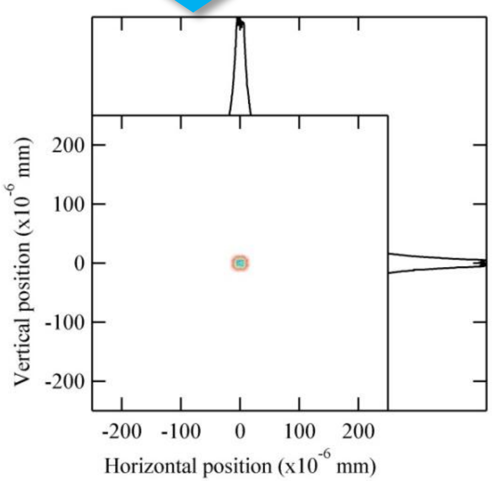
Ideal lens with focal lengths of f_x and f_z



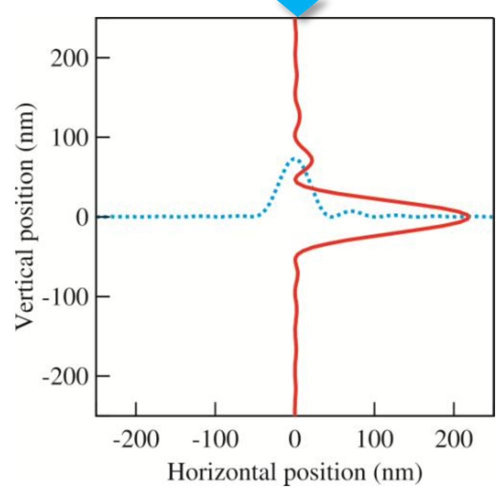


$$E(x,z) \rightarrow \boxed{\text{FFT}} \xrightarrow{\mathcal{F}(u,v)} \boxed{\times \exp\left[-\frac{i2\pi^2}{k}(u^2+v^2)y\right]} \xrightarrow{\mathcal{F}'(u,v)} \boxed{\text{Inverse FFT}} \rightarrow E(x',z')$$

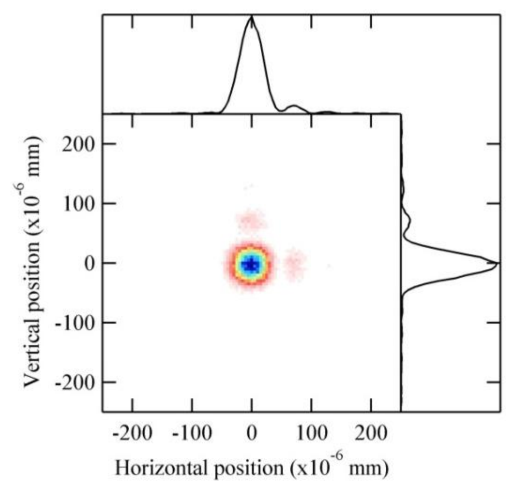
Ray tracing of the beamline



$\otimes$



$=$



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

So far…

- Wavefront representation = coherent optics calculations
- Fraunhofer - Fresnel – Fresnel-Kirchhoff => Propagators for wavefronts
- Codes for coherent optics and incoherent optics
- But:
  - Beams are not fully coherent
  - Wavefronts are not plane (source at infinity) or spherical (point source)
  - Coherent and incoherent optics are extreme cases. Real life cases are in between.

A point source does not exist but has an extended size

What is the minimum source size?

A <u>non rigorous </u>discussion based on Heisenberg principle:

$$\frac{\hbar}{2} \leq \Delta x \, \Delta p = p \, \Delta x \, \Delta x'$$

$$\Delta p \approx p \Delta x'$$

- For electrons ~ 6 GeV

$$E = \frac{mc^2}{\sqrt{1-\beta^2}} = \gamma mc^2$$

$$p = \frac{mv}{\sqrt{1-\beta^2}} = \gamma mv = \gamma m\beta c = \gamma mc(1-\gamma^{-2}) \approx \gamma mc$$

$$\frac{\hbar}{2} \leq \Delta x \, \Delta x' \; p \rightarrow \Delta x \, \Delta x' \geq \frac{\hbar}{2\gamma mc} = \frac{6.62\,10^{-34}}{4\pi \times 12000 \times 9.1\,10^{-31} \times \; 3\,10^{8}} = 0.16\,10^{-18} \approx 0.2 \text{ atto m}$$

- If 1e$^-$ -> Ne$^-$ (ergodic) this gives a physical lower limit for electron phase space volume (emittance).

What is the smallest photon source (Heisenberg)

$$E = \sqrt{p^2c^2 + m^2c^4}$$

$$p = \frac{E}{c} = \frac{h\nu}{c} = \frac{h}{\lambda} = \hbar k$$

$$\frac{\hbar}{2} \leq \Delta x\, \Delta x'\, p \rightarrow \Delta x\, \Delta x' \geq \frac{\hbar}{2\hbar k} \rightarrow \boxed{\Delta x\, \Delta x' \geq \frac{\lambda}{4\pi}}$$

This indicates how small (in phase space) a point source is

How small a source must be to produce a " real" spherical wavefront which can be considered a coherent source

Is this *approvimately* a "diffraction limited" source… Better: a "Heisenberg-limited" source

A source like this is coherent (if a point source is coherent, and this is like a point source, there is no reason to be incoherent)

Extended coherent sources are limited by Heisenberg, but nothing prevents them to be larger and still fully coherent. But not much much larger?

Can we define: DL source = coherent source ?

Extended sources can be coherent

Gaussian Beams

x and *x′* are conjugated pairs via FT

Plane and spherical waves are limiting cases

$$\boxed{\sigma_x \, \sigma_{x'} = \frac{\lambda}{4\pi}}$$

Gaussian Beams

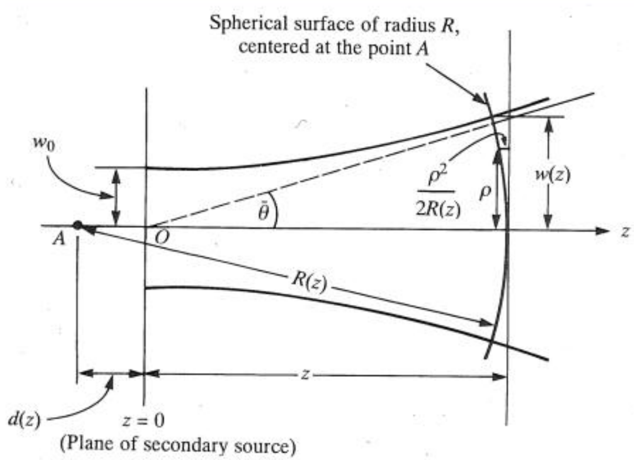
x and x' are conjugated pairs via FT

Plane and spherical waves are limiting cases

$$\boxed{\sigma_x \, \sigma_{x'} = \frac{\lambda}{4\pi}}$$

SO WHAT IS A GAUSSIAN LASER MODE?

ESRF



In the laser literature the width-angle product of a Gaussian mode are represented by the following expression [Yariv equation 2.5-18], [Mandel and Wolf equation 5.6-40]

We will recast this into "storage ring" notation:

At axial distance z from the beam waist, $w(z)$ is the off-axis distance at which the electric field E falls to $1/e$ of its on-axis value. At the waist, w_0 equals $w(0)$, while the beam angle, $[w(z)/z]_{\text{FAR FIELD}}$, is represented by $\bar{\theta}$.

Now suppose that the laser beam intensity depends only on the distance r from the axis, and thus

$I(r) = e^{-r^2/2\sigma_I^2}$ or $E(r) = e^{-r^2/4\sigma_I^2}$

so that $\sigma_E = \sqrt{2}\,\sigma_I$. Now E falls to $1/e$ when $r^2/2\sigma_E^2 = 1$ so that $r_{1/e}^{\text{field}} = \sqrt{2}\,\sigma_E = 2\sigma_I$ whence $w_0 = 2\sigma_I$. Similarly $\bar{\theta} = 2\sigma_{I'}$ where the prime implies the beam *angle*.

Substituting into the "laser" expression

$$\bar{\theta} = \frac{\lambda}{\pi w_0} \longrightarrow \boxed{\sigma_I \sigma_{I'} = \frac{\lambda}{4\pi}}$$

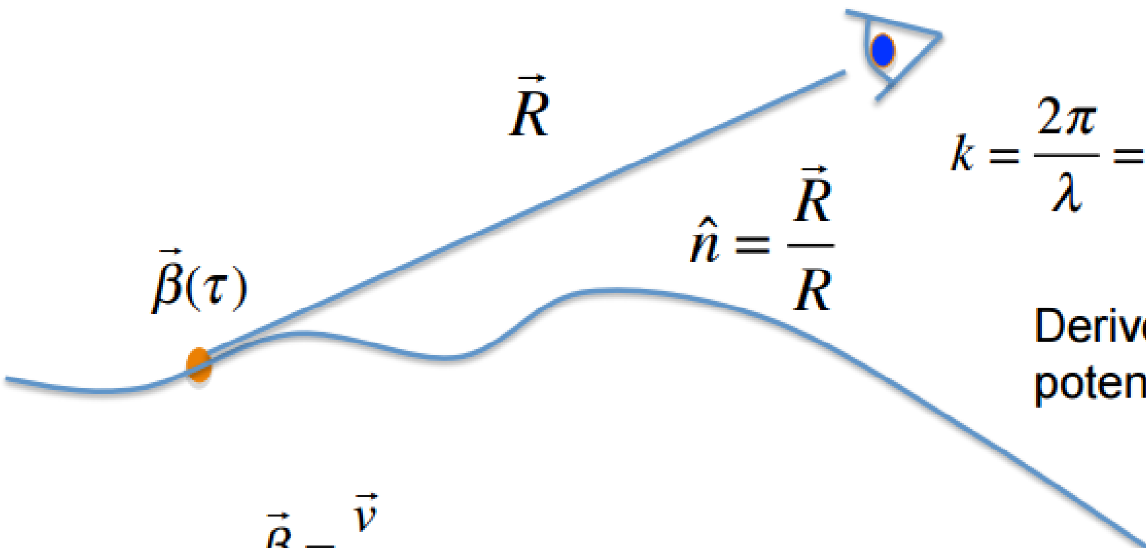
ESRF Lecture Series on Coherent X-rays and their Applications, Lecture 4, Malcolm Howells

Electron and Light emittances for SR sources

- BM, W, U: **Can be coherent?**
- **Are they (naturally) coherent?**
- **Is undulator light (naturally) coherent**

General expression for Radiation from a trajectory

$$\vec{E}(\vec{R},\omega) = \int_{-\infty}^{\infty} \left[\vec{\beta}(\tau) - \frac{\hat{n}(\tau)}{R}\left(1 + \frac{ic}{\omega R}\right)\right] e^{i\omega\left(\tau + \frac{R}{c}\right)} d\tau$$



$$k = \frac{2\pi}{\lambda} = \frac{\omega}{c}$$

Derived from Liénard-Wiechert potentials

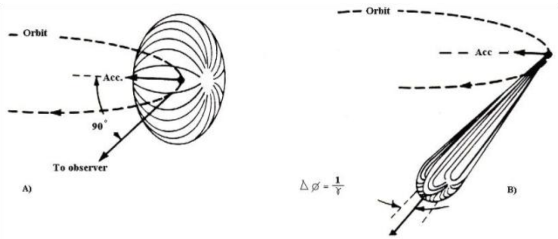
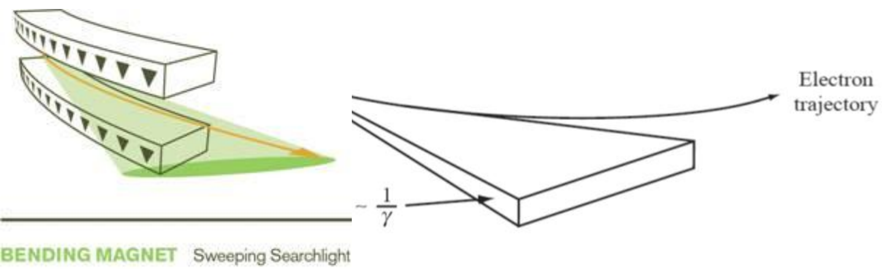
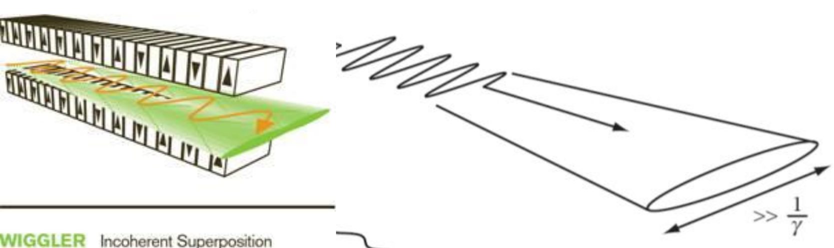
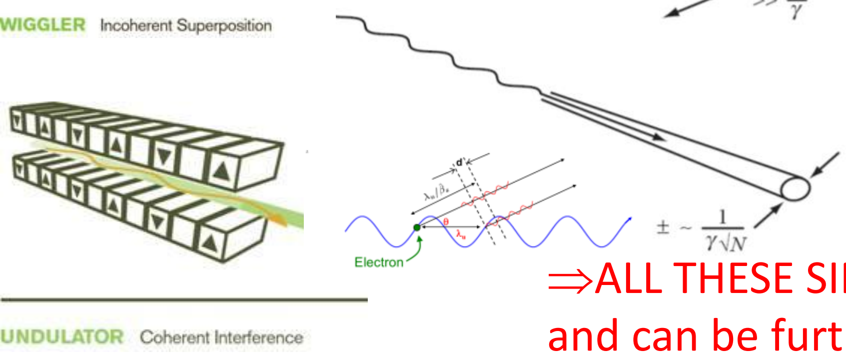
$$\vec{\beta} = \frac{\vec{v}}{c}$$

So, given the electron orbit, we can compute the radiated electric field at a given frequency

$\Rightarrow$AND IS COHERENT ….

Courtesy: Boaz Nash

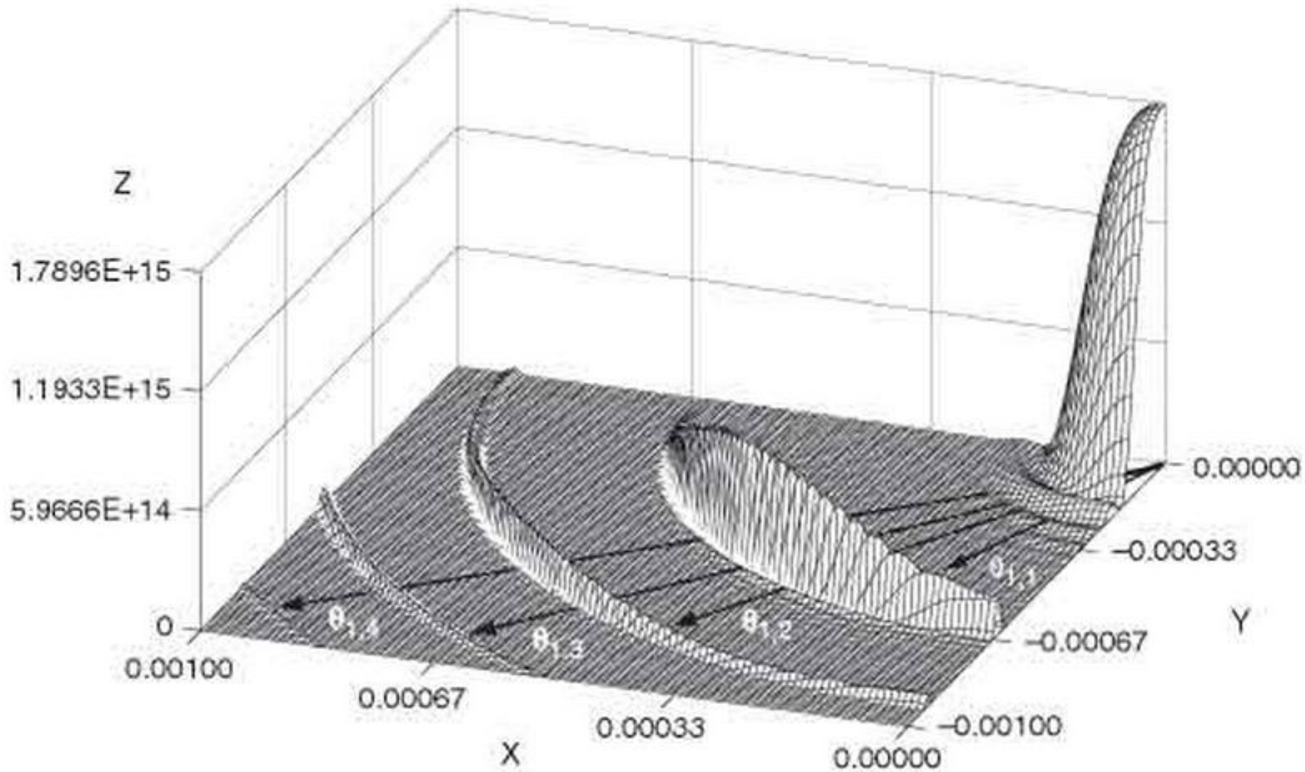
Divergence of photons produced by one electron

	H [rad]	V [rad]
	$1/\gamma$	$1/\gamma$
	$\Theta >> 1/\gamma$	$1/\gamma$
	$K/\gamma >> 1/\gamma$	$1/\gamma$
	$1/(\gamma N^{1/2})$	the same

$\Rightarrow$ALL THESE SINGLE ELECTRON EMISSIONS ARE COHERENT and can be further propagated by coherent optics (e.g., SRW)

Undulator radiation in more detail: angular emission at energy resonance

The angular distribution of fundamental (n = 1) undulator radiation for the limiting case of zero beam emittance. The x and y axes correspond to the observation angles **q** *and* **y** *(in radians), respectively, and the z axis is the intensity in photons·s^{-1}·A^{-1}·(0.1 mr)$^{-2}$·(1% bandwidth)$^{-1}$. The undulator parameters for this theoretical calculation were N = 14, K = 1.87, l_u = 3.5 cm, and E = 1.3 GeV. (Figure courtesy of R. Tatchyn, Stanford University.)*



A common tendency is to approximate this emission by a Gaussian shape and extrapolate results of Gaussian beams

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

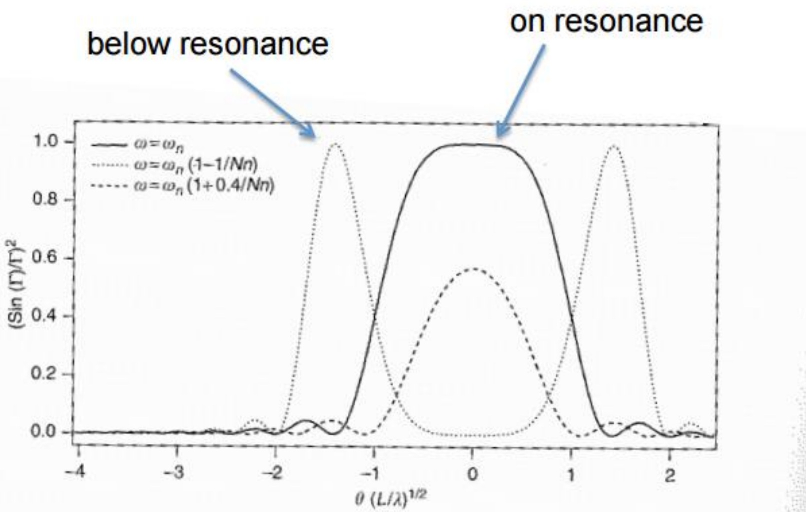


Figure 3.3 Graph of $(\sin(\Gamma)/\Gamma)^2$ as a function of the angle $\theta = \sqrt{\theta_x^2+\theta_z^2}$ for three different frequencies. ω_n is an abbreviation for $n\omega_1$ (0, 0).

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

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

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

below resonance

on resonance

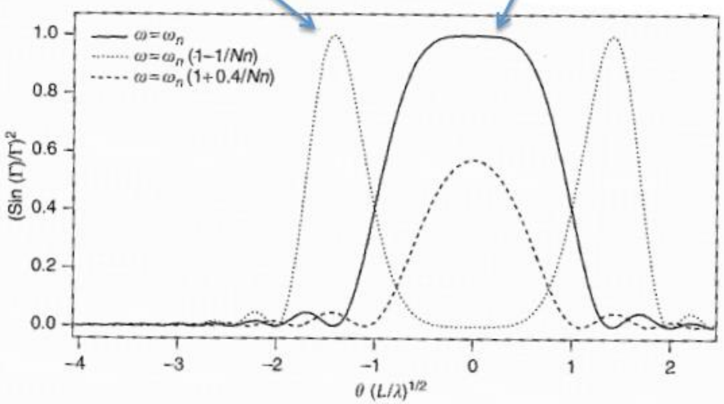


Figure 3.3 Graph of $(\sin(\Gamma)/\Gamma)^2$ as a function of the angle $\theta = \sqrt{\theta_x^2+\theta_z^2}$ for three different frequencies. ω_n is an abbreviation for $n\omega_1\,(0,0)$.

78 *P. Elleaume*

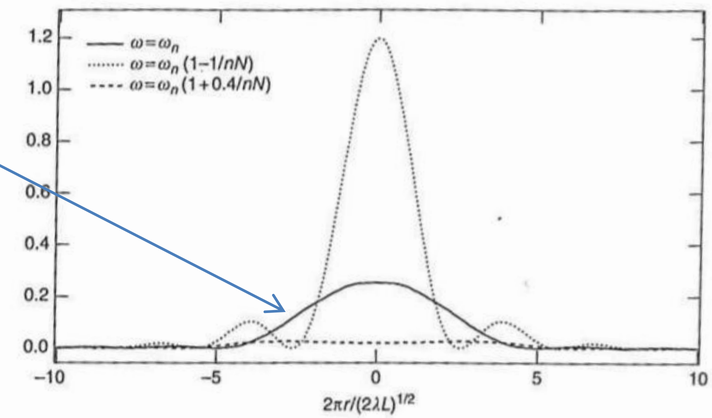


Figure 3.4 Spectral flux per unit surface in the middle of the undulator for three frequencies close to the on-axis resonant frequency $\omega_n = n\omega_1(0,0)$.

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

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

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

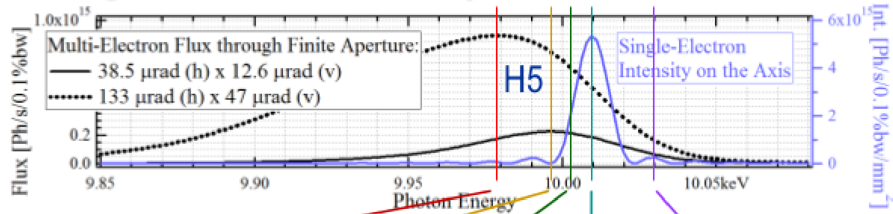
$$\sigma_r \sigma_{r'} = \frac{1.89\lambda}{4\pi} \approx \frac{\lambda}{2\pi}$$

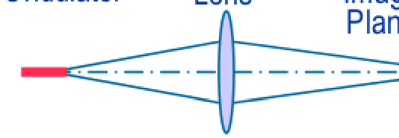
- Undulator beams are not Gaussian beams (even at resonances)
- Undulator emittance at resonance is twice as Gaussian beam but is fully coherent

Single-Electron (Fully Transversely-Coherent) UR Intensity Distributions "in Far Field" and "at Source"

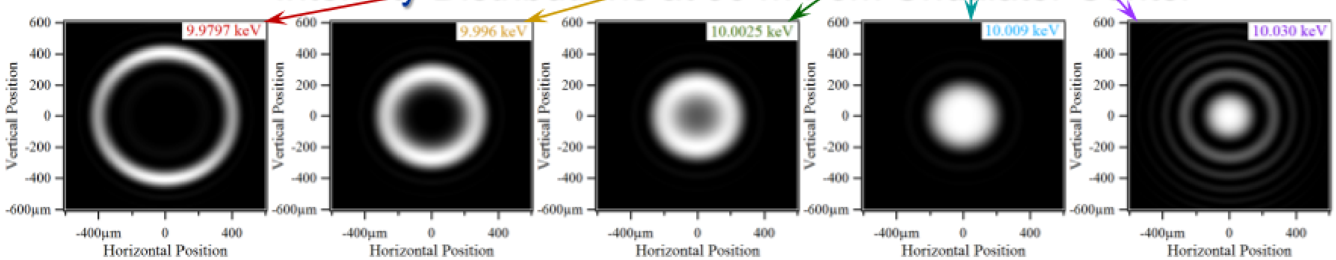
UR "Single-Electron" Intensity and "Multi-Electron" Flux

E-Beam Energy: 3 GeV
Current: 0.5 A
Undulator Period: 20 mm

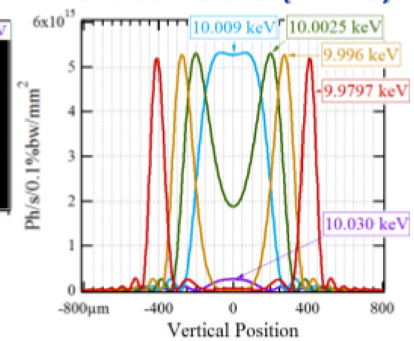




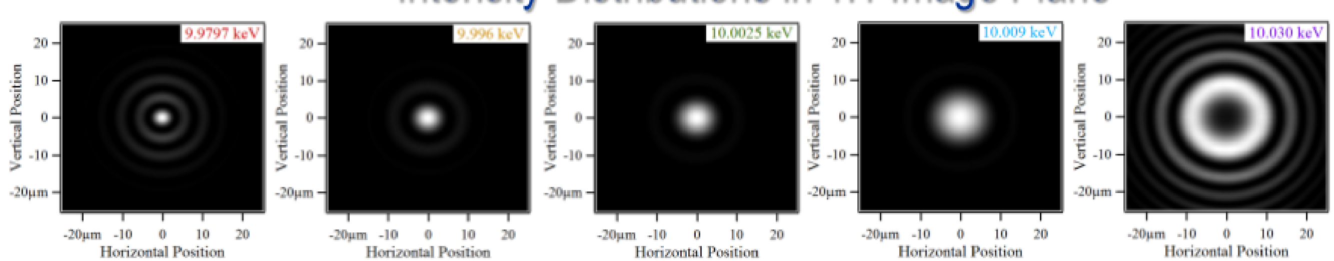
Intensity Distributions at 30 m from Undulator Center

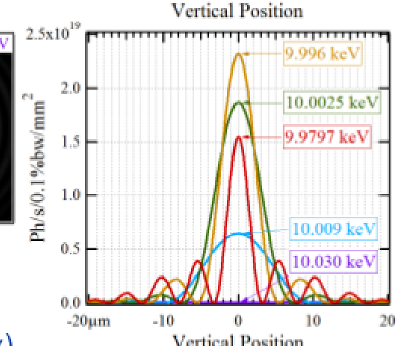


Vertical Cuts (x = 0)



Intensity Distributions in 1:1 Image Plane





"Phase-Space Volume" Estimation for Vertical Plane

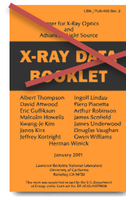
(RMS sizes/divergences calculated for the portions of intensity distributions containing 95% of flux)

$\sigma_y\sigma_y' \approx 7.7\dfrac{\lambda}{4\pi}$ $\quad 3.3\dfrac{\lambda}{4\pi}$ $\quad 1.9\dfrac{\lambda}{4\pi}$ $\quad 1.5\dfrac{\lambda}{4\pi}$ $\quad 9.2\dfrac{\lambda}{4\pi}$

Courtesy: O. Chubar

ATTENTION!!!!

WRONG value of $\sigma_{r'}$ in
KIM (NIM 1986, AIP Conf Proc. 1989)
and X-ray data booklet



$$\cancel{\sigma_r = \frac{1}{4\pi}\sqrt{\lambda L}} \quad , \qquad \cancel{\sigma_{r'} = \sqrt{\lambda / L}}$$

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

Corrected value of $\sigma_{r'}$ in > Kim 1995 (Optical Eng.) but forced emittance to be like Gaussian beam (half size than Elleaume). Same criterion used in Huang SLAC-PUB 15449 (2013), Tanaka, and others.

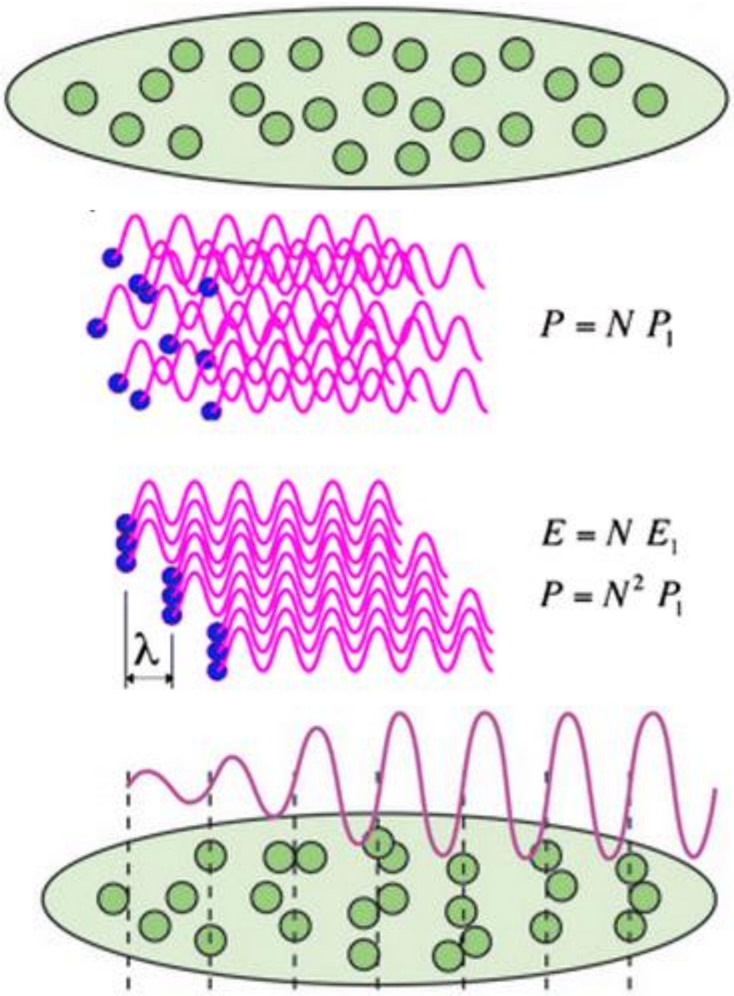
Coherent fraction

ratio of the photon phase space size over the phase space size of the coherent beam, multiplying H*V, but

- Use Gaussian beams $\lambda/4\pi$? <= (therefore max(CF)=0.25 with Elleaume size, 1 with Kim size)
- Use undulator emittance $\lambda/2\pi$ (therefore max(CF)=1)

e- do not travel alone but many electrons in bunches

bunch length



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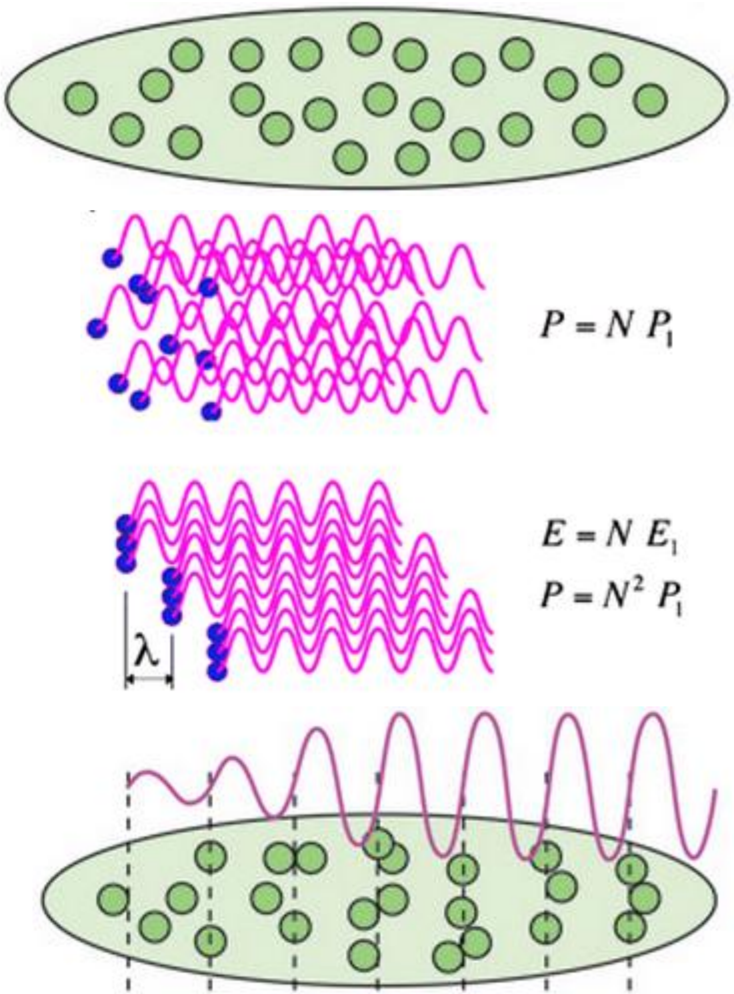
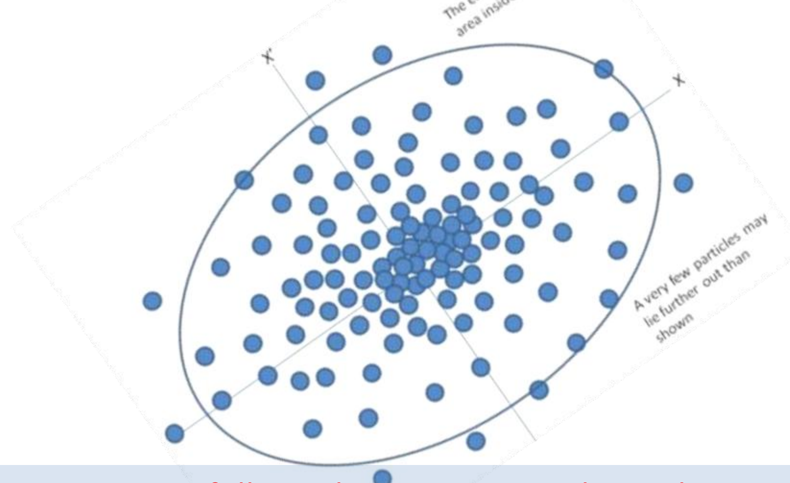


bunch cross section



For a given s, e- follow a bivariate Normal Distribution in (x,x') (H) and (z,z') (V)

$$f_{\mathbf{x}}(x_1,\ldots,x_k) = \frac{1}{\sqrt{(2\pi)^k|\boldsymbol{\Sigma}|}}\exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right),$$

$$\Sigma = \begin{pmatrix} \langle x^2 \rangle & \langle xx' \rangle \\ \langle xx' \rangle & \langle x'^2 \rangle \end{pmatrix} = \begin{pmatrix} \sigma_x^2 & \rho\sigma_x\sigma_{x'} \\ \rho\sigma_x\sigma_{x'} & \sigma_{x'}^2 \end{pmatrix}$$

=> in SR storage rings (not for XFELs) the different electrons emit incoherent photons

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):

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

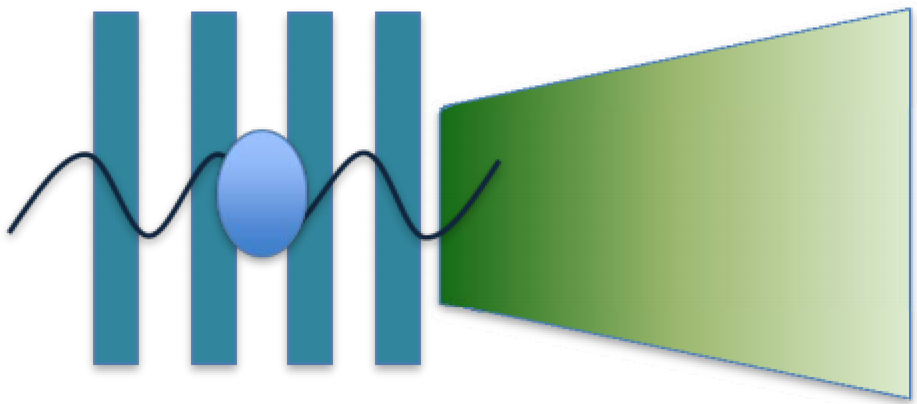
Photon beam size and divergence is determined by a combination of electron beam and single electron emission

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

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

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

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



Courtesy: Boaz Nash

(AT THE WAIST, AT THE UNDULATOR RESONANCE, AND SUPOSSING GAUSSIAN EMISSION)

Quantifying efficiency of the source to emit coherent radiation:

coherent fraction for SR lattices (Undulator emission)

$$\boxed{CF = CF_h CF_v = \frac{(\lambda/2\pi)^2}{\Sigma_x \Sigma_{x'} \Sigma_y \Sigma_{y'}}}$$

$$CF_{H,V} = \frac{\lambda/(2\pi)}{\sqrt{\sigma_\gamma^2 + \sigma_{H,V}^2}\sqrt{\sigma_\gamma'^2 + \sigma_{H,V}'^2}} = \frac{\lambda/(2\pi)}{\sqrt{\frac{\lambda L}{2\pi^2} + \sigma_{H,V}^2}\sqrt{\frac{\lambda}{2L} + \sigma_{H,V}'^2}}$$

$\lambda/(2\pi)$ *or* $\lambda/(4\pi)$?

Limits (zero emittance):

1 if λ/2π (Undulator emission)

0.25 if λ/4π (Gaussian beam)

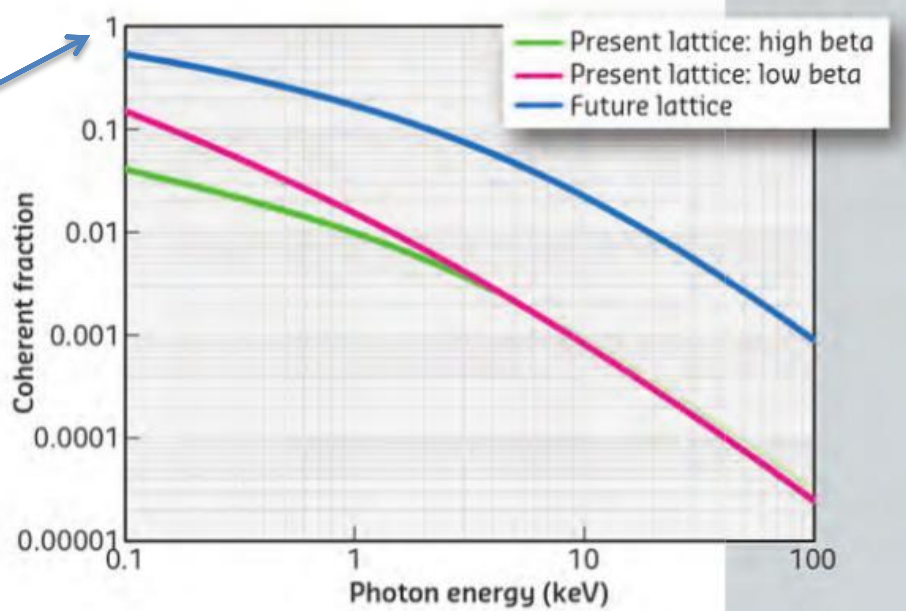
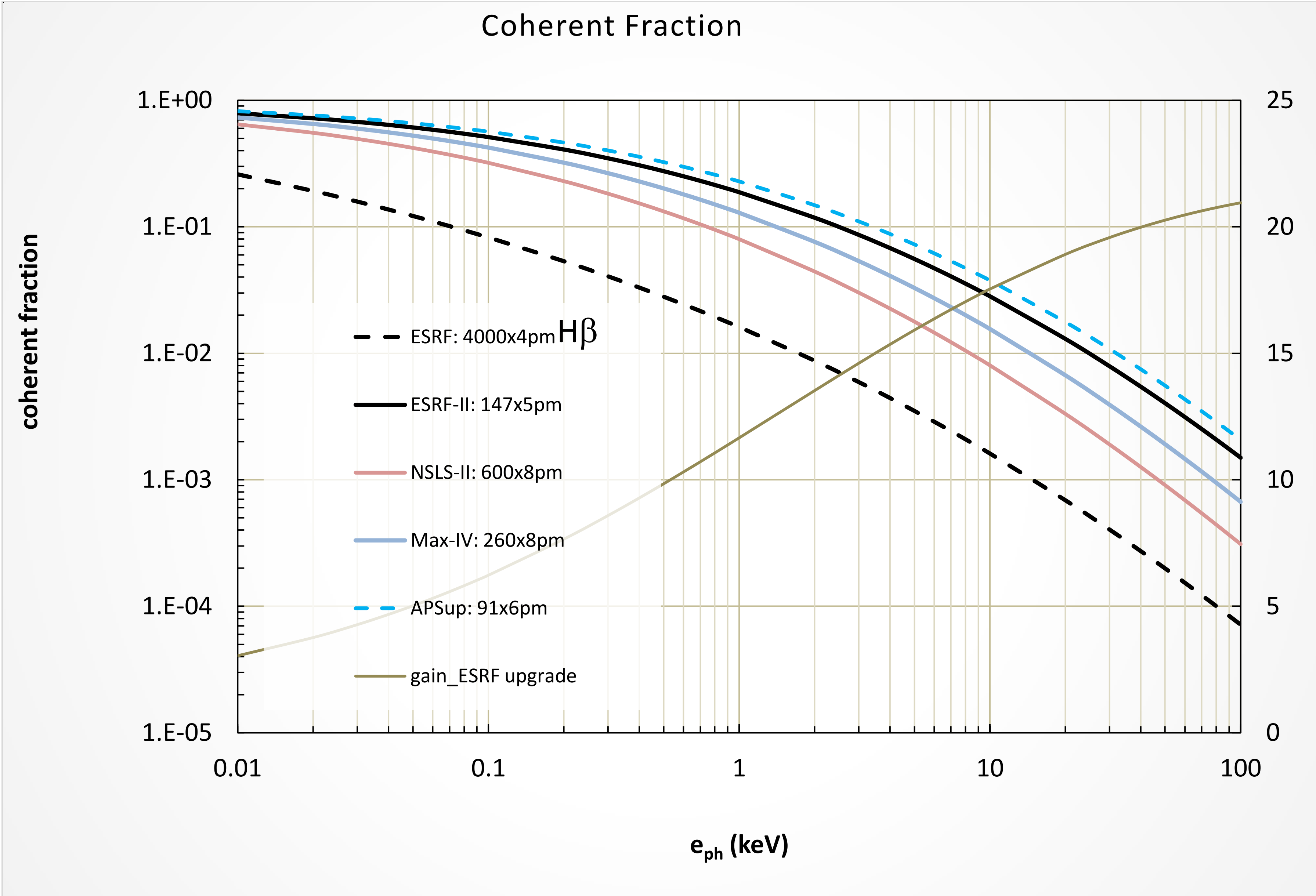


Figure 4.01: Comparison of the variation of the coherent fraction of X-ray emission with energy for the current insertion devices (low-β and high-β source points) and the proposed source.



Courtesy: L Zhang

Coherent beams produced by incoherent sources

- Thomson-Wolf

- Van Cittert-Zernike

Coherent beams produced by incoherent sources

Thomson & Wolf, JOSA 47, 895 (1957)

L=152 cm

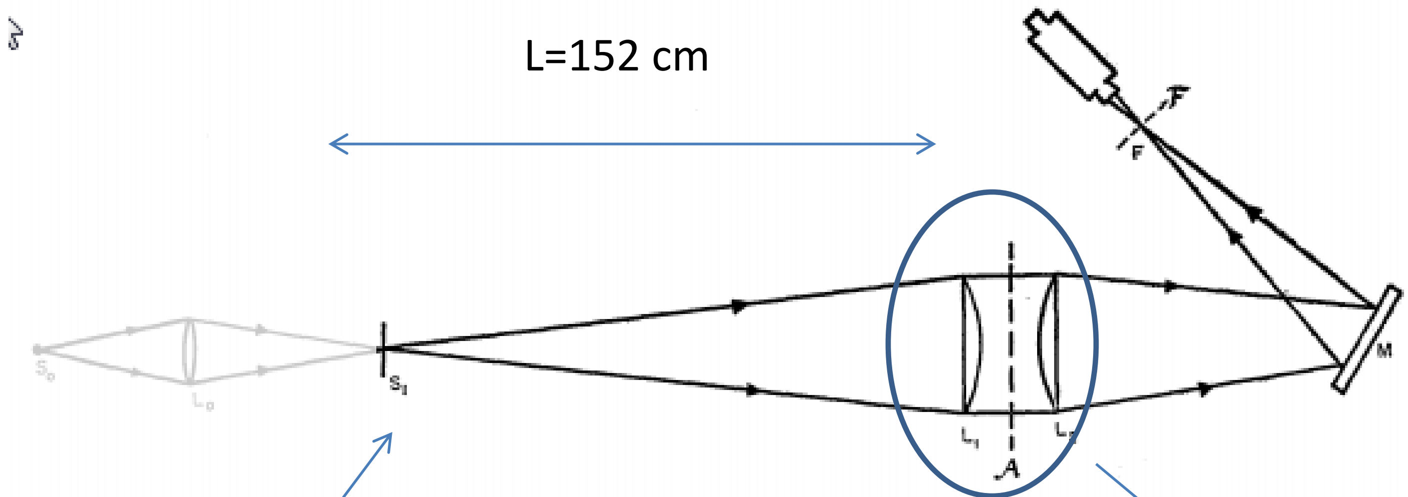
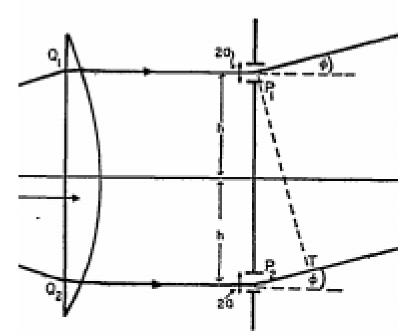


Fig. 3. The diffractometer.

L_1-L_2=14 cm

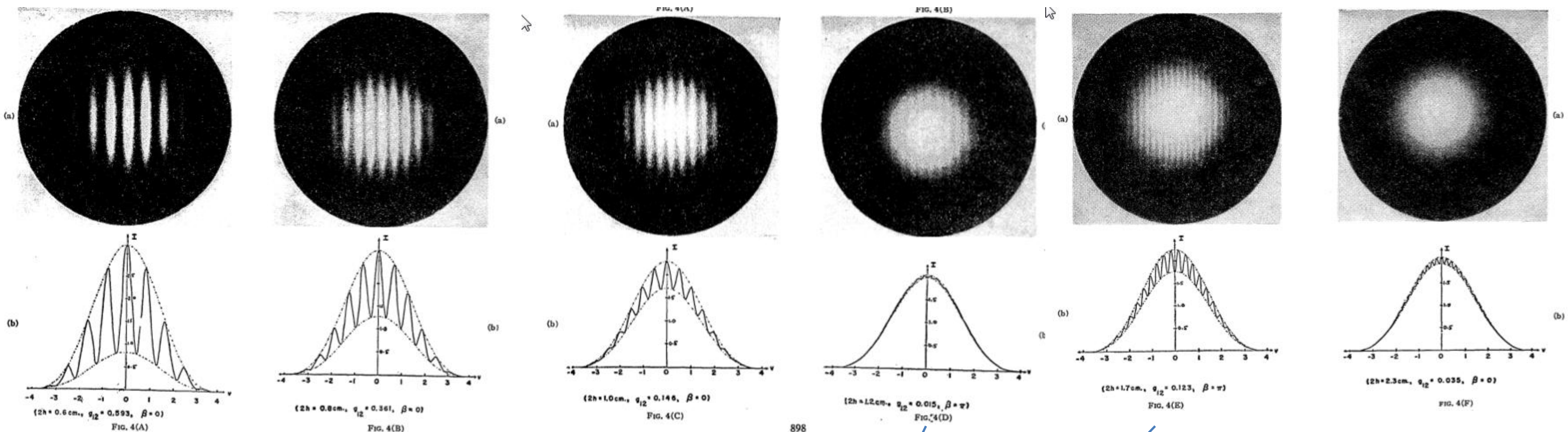
- S1 Disk INCOHERENT source (Ø=0, 90 um)
- λ=579 nm

- 2xPinhole Ø=0.14 cm
- 2h=0.6-2.5 cm



Thomson & Wolf, JOSA 47, 895 (1957)

Slit separation increases



Complex degree of coherence

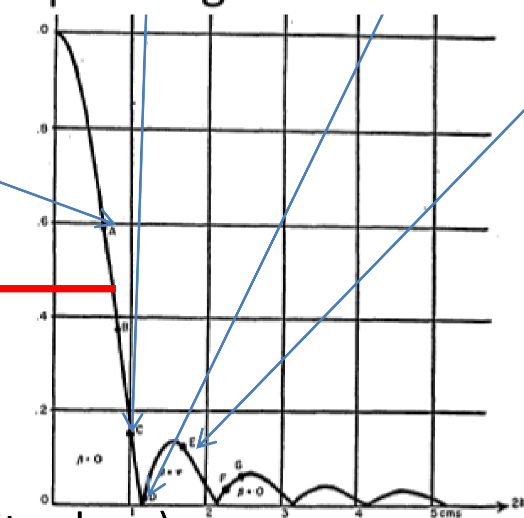


FIG. 6. The degree of coherence, as function of the separation 2h of the apertures at P_1 and P_2.

The COHERENCE LENGTH (at the slits plane) is usually related to this width

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Double pinhole diffraction of white synchrotron radiation

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Received 26 September 2002; accepted 12 December 2002

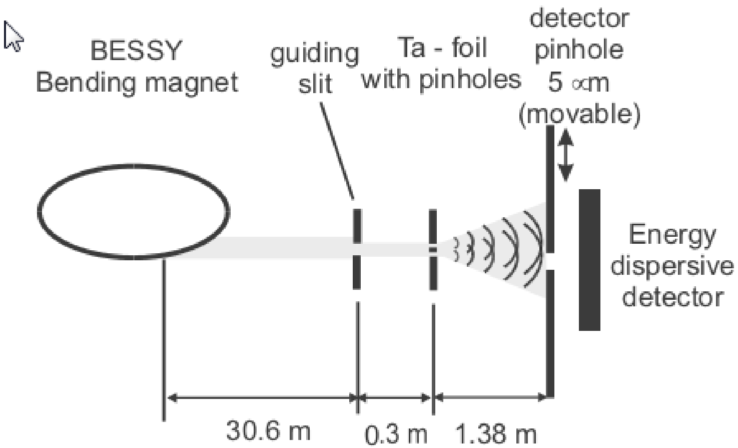


Fig. 1. Experimental set-up at the EDR-beamline at BESSY II.

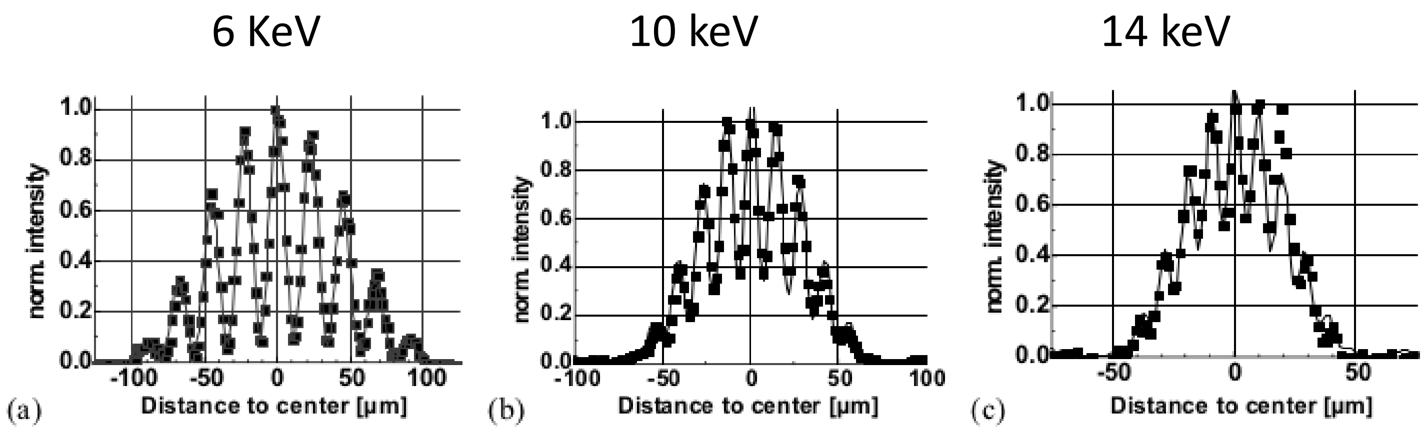


Fig. 4. Normalized interference fringes obtained with the double pinhole at three different energies (a)–(c) 6 keV, 10 keV and 14 keV. The squares indicate the measured data from Fig. 3 and the lines indicate the results of the best fit of Eq. (1).

Understanding coherence (statistical optics)

The cross correlation of two electric fields:

$$\Gamma_{12}(\boldsymbol{r}_1, \boldsymbol{r}_2; t_1, t_2) = \langle \boldsymbol{E}_1^*(\boldsymbol{r}_1, t_1)\, \boldsymbol{E}_2(\boldsymbol{r}_2, t_2) \rangle_{ensemble}$$

Complex degree of coherence:

$$\gamma_{12}(\boldsymbol{r}_1, \mathbf{r}_2; \mathrm{t}_1, \mathrm{t}_2) = \frac{\Gamma_{12}\,(\boldsymbol{r}_1, \boldsymbol{r}_2; t_1, t_2)}{\sqrt{\Gamma_{12}(\boldsymbol{r}_1, \boldsymbol{r}_1; t_1, t_1)}\sqrt{\Gamma_{12}(\boldsymbol{r}_2, \boldsymbol{r}_2; t_2, t_2)}} = \frac{\Gamma_{12}(\boldsymbol{r}_1, \boldsymbol{r}_2; t_1, t_2)}{\sqrt{\langle \mathrm{I}_1(\boldsymbol{r}_1, t_1\,) \rangle_e}\sqrt{\langle \mathrm{I}_2(\boldsymbol{r}_2, t_2) \rangle_e}}$$

$|\gamma| = 0$ incoherent

$0 < |\gamma| < 1$ partially coherent

$|\gamma| = 1$ coherent

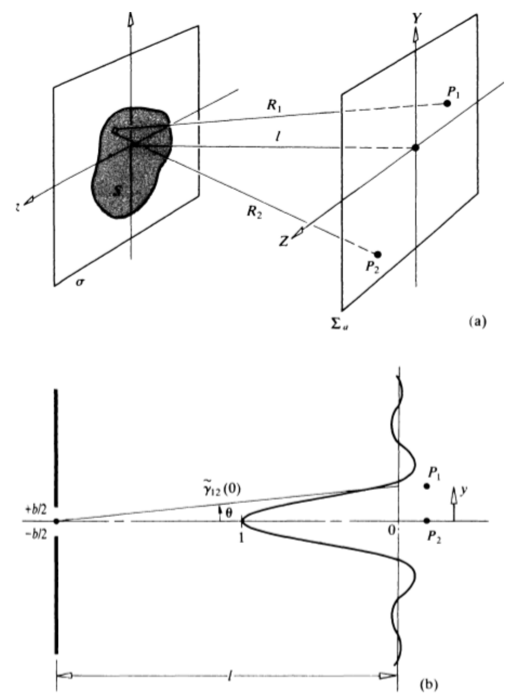
Interference equation:

$$\boxed{I = I_1 + I_2 + 2\sqrt{I_1 I_2}\,|\gamma_{12}|\cos(\phi) \quad \text{with:} \quad \phi = \arg(\gamma_{12})}$$

Van Cittert-Zernike theorem

$$\gamma_{12} = \frac{1}{(I_1 I_2)^{\frac{1}{2}}} \int\int_{\Sigma_0} \frac{I(x, y)}{R_1 R_2} e^{-ik(R_1 - R_2)} d\Sigma_0 ,$$

- Gives the Complex Degree of Coherence of radiation produced by an <u>extended</u> (quasi – monochromatic) <u>incoherent</u> source around a point P_2.
- The shape of CDOC is the same as the diffraction pattern produced by an aperture of the same form of the source emitting spherical waves converging to P_2.



So far…

- We can do coherence experiments with fully incoherent sources provided that the source is small and we go far away (VCZ). This is coherence by propagation. The price to pay is that we restrict the number of usable photons.

- Physics say that the extended photon source phase space cannot be smaller than $\lambda/4\pi$ ($\lambda/2\pi$ for undulator radiation). Thus it is useless (but in principle possible) to build storage rings with emittance much less than this values. "Diffraction limited storaged rings" (a not very meaningful term) exploit this fact to make sources with high CF.

- Undulator souces (one electron) have a certain natural size and divergence, and the emission is fully coherent. Source coherence drops when adding emittance. Beam coherence increases when we go away from the source.

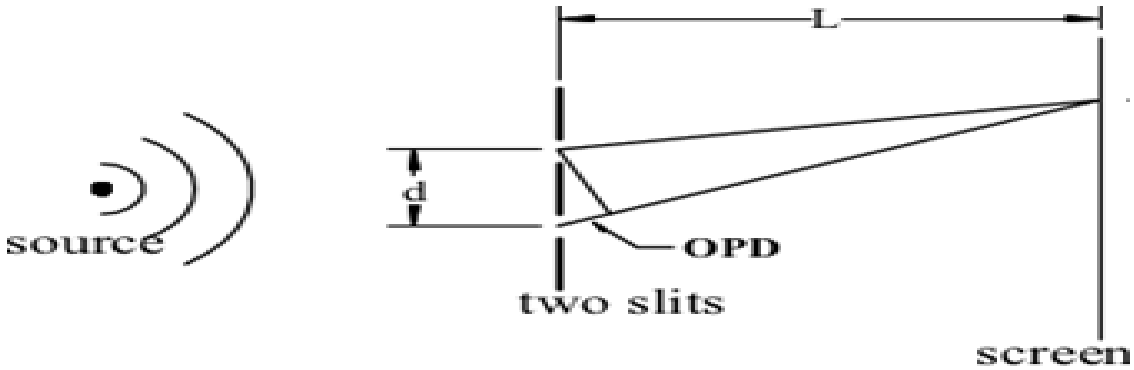
- Gaussian approximations and convolutions are dangerous!!

- Q: Are our beams coherent because of propagation only? Until which level? Can we exploit undulator coherence beyond VCZ?

- Statistical optics is needed to explain partial coherent. Several approximations are necessary (Wigner functions, coherent mode decomposition, propagation of mutual coherence function, Gauss-Schell approximations, numerical calculations)…

Few ideas on calculations

Calculating partial coherence by an ensemble average: Example: Thomson&Wolf



$$R_{nm} = e^{i\,k\,r_{nm}}$$

$$U_k = U_i R_{ij} R_{jk}$$

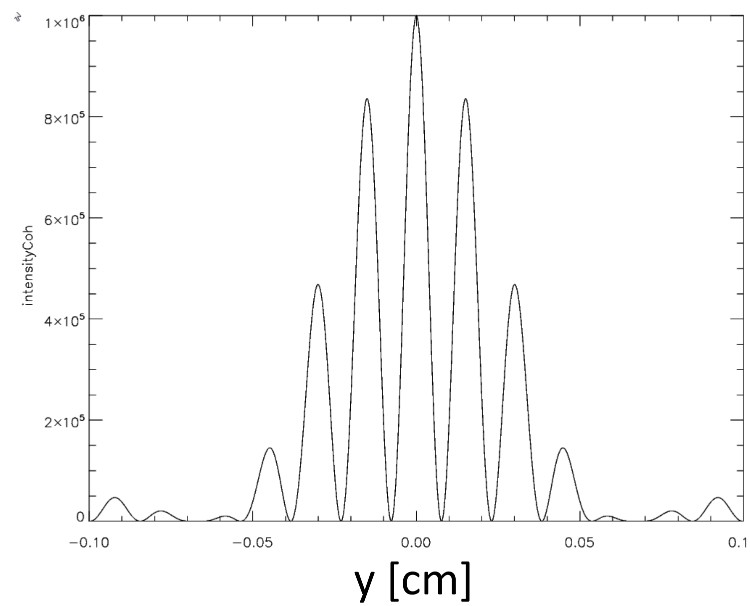
$$\text{coherent: } U_i = 1$$

$$I_k = \left|U_k\right|^2$$

x

x_i, U_i $\quad x_j$ $\quad x_k$

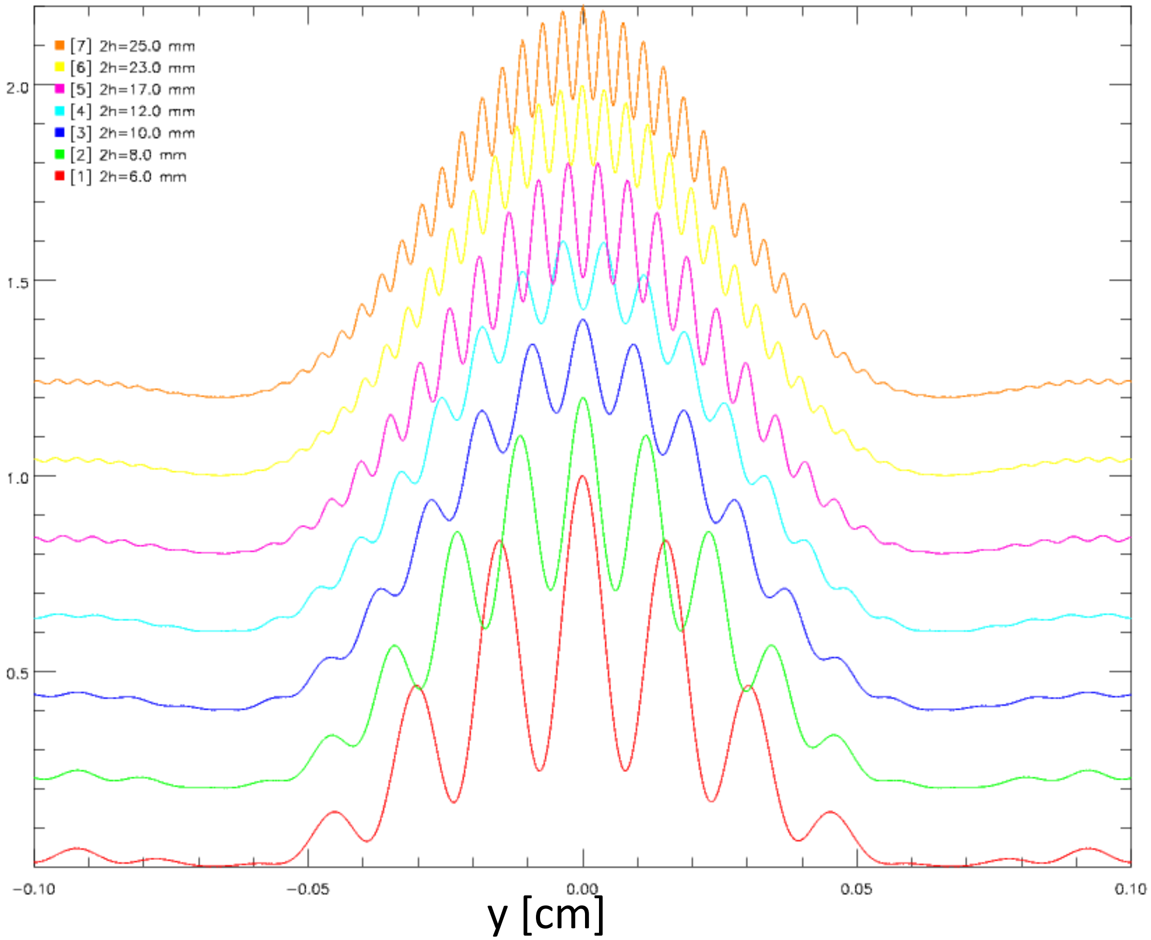
$$r_{mn} = \sqrt{(x_m - x_n)^2 + y_{mn}^2}$$



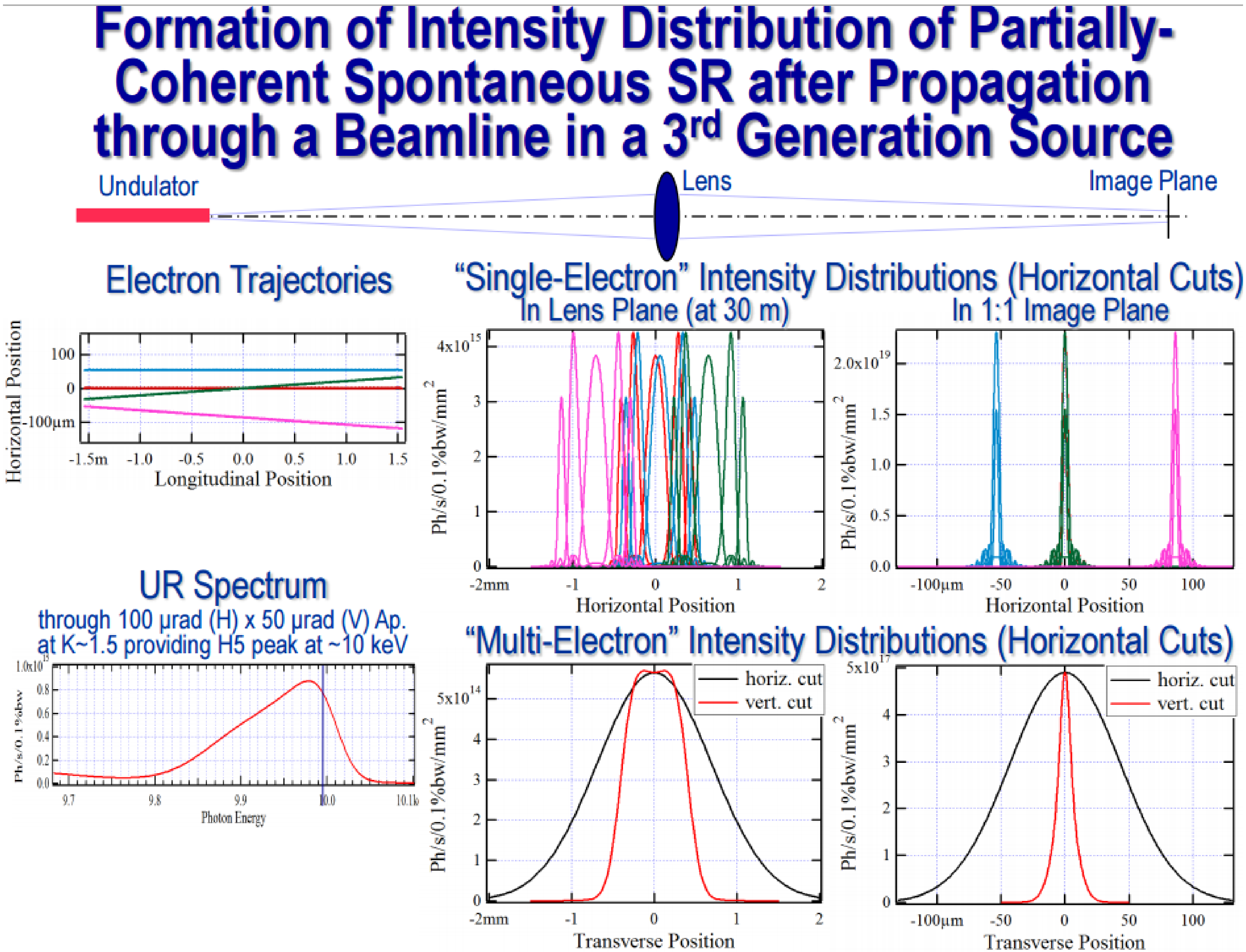
Incoherent source: $U_i = e^{i2\pi\zeta} \quad \zeta = random$

$$I_k = \sum_{r=1}^{R} \left\{ \left| U_k \right|^2 \right\}_r$$

See `thomson_wolf_1957.py` (R=1000)



Partial coherence using SRW: Multi electron calculation



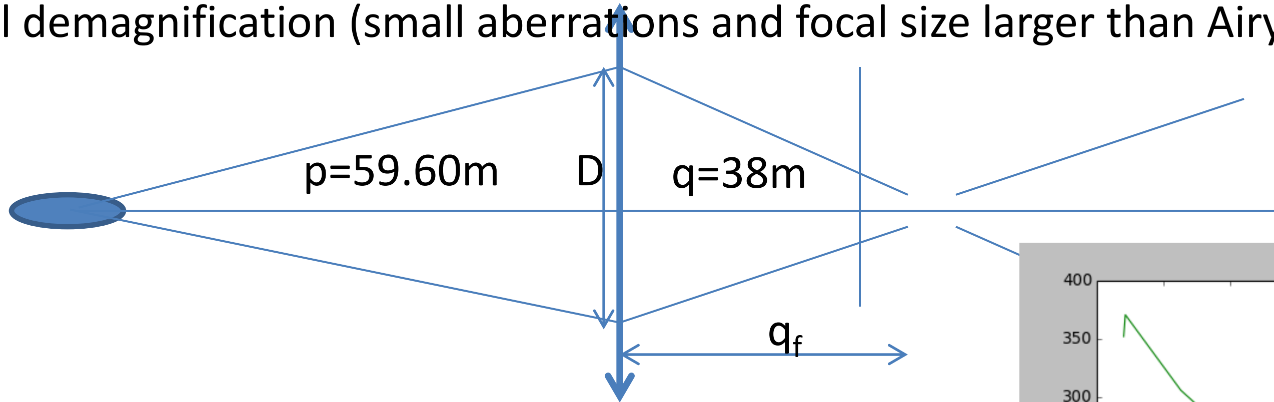
Courtesy: O. Chubar

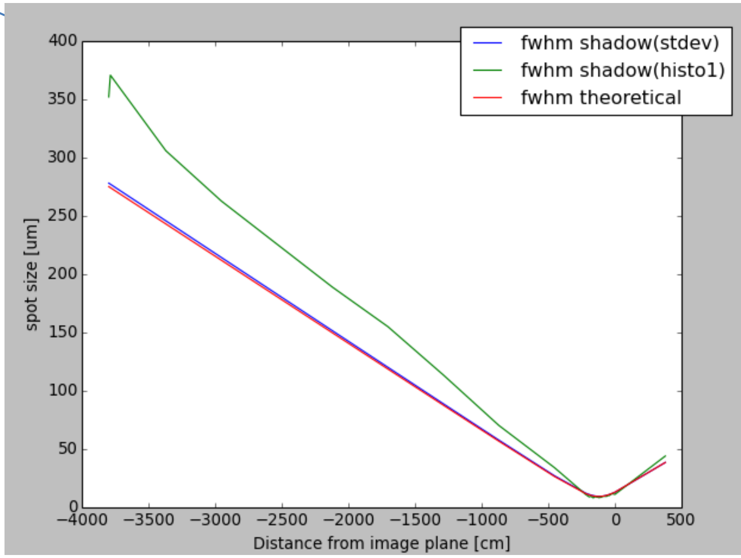
TF for ID30B

64.6μm x 4.29μrad ~λ/(0.3π);

E=14 keV => 5x50μm+2x100μm (D=500μm)=> F = 23.21m

Small demagnification (small aberrations and focal size larger than Airy disk)





Need to calculate on-focus and out of focus. By hand:

- On focus $s_2 = s_1\, q/p$
- Out of focus $s_2 = \theta(q-q_f)$; $\theta = D/q_f$

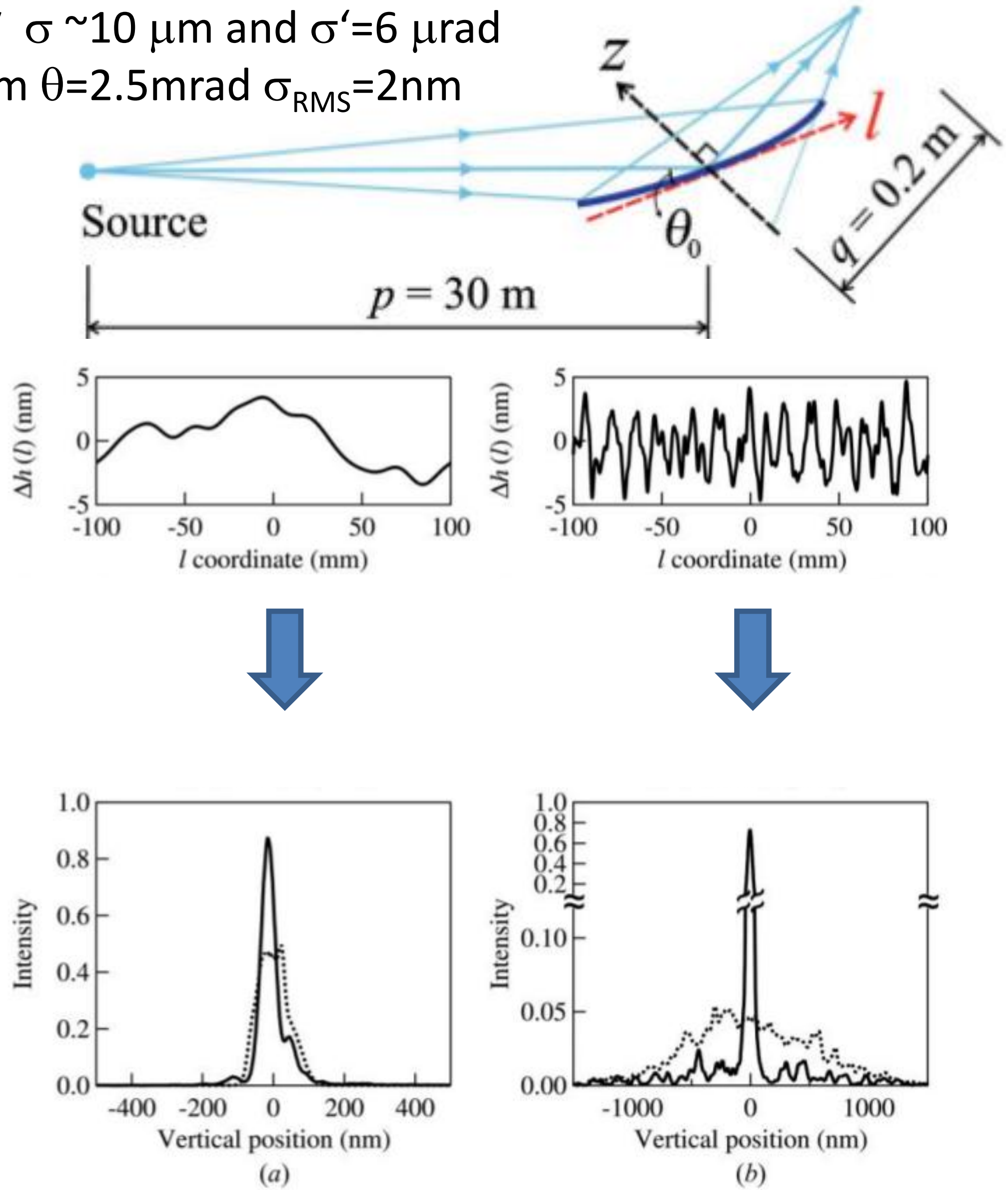
Physical optics

- Plane wave: wrong focal position
- Spherical wave (point): wrong focal size
- Gaussian beam, setting s_1 => good size at focus, bad size out of focus (underestimage divergence)
- Gaussian beam, setting s'_1 => good size out of focus, bad size at focus (underestimage source size)
- Needed multielectron approach (brute force)

Figure errors: Hybrid method in SHADOW

E=10 keV σ ~10 μm and σ'=6 μrad

L=200 mm θ=2.5mrad σ_{RMS}=2nm

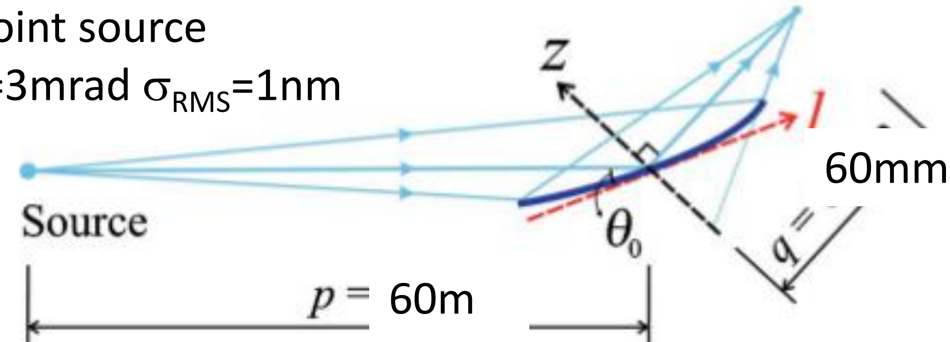


X. Shi, R. Reininger, M. Sanchez del Rio, L. Assoufid J. Synchrotron Rad. (2014) 21, doi:10.1107/S160057751400650X

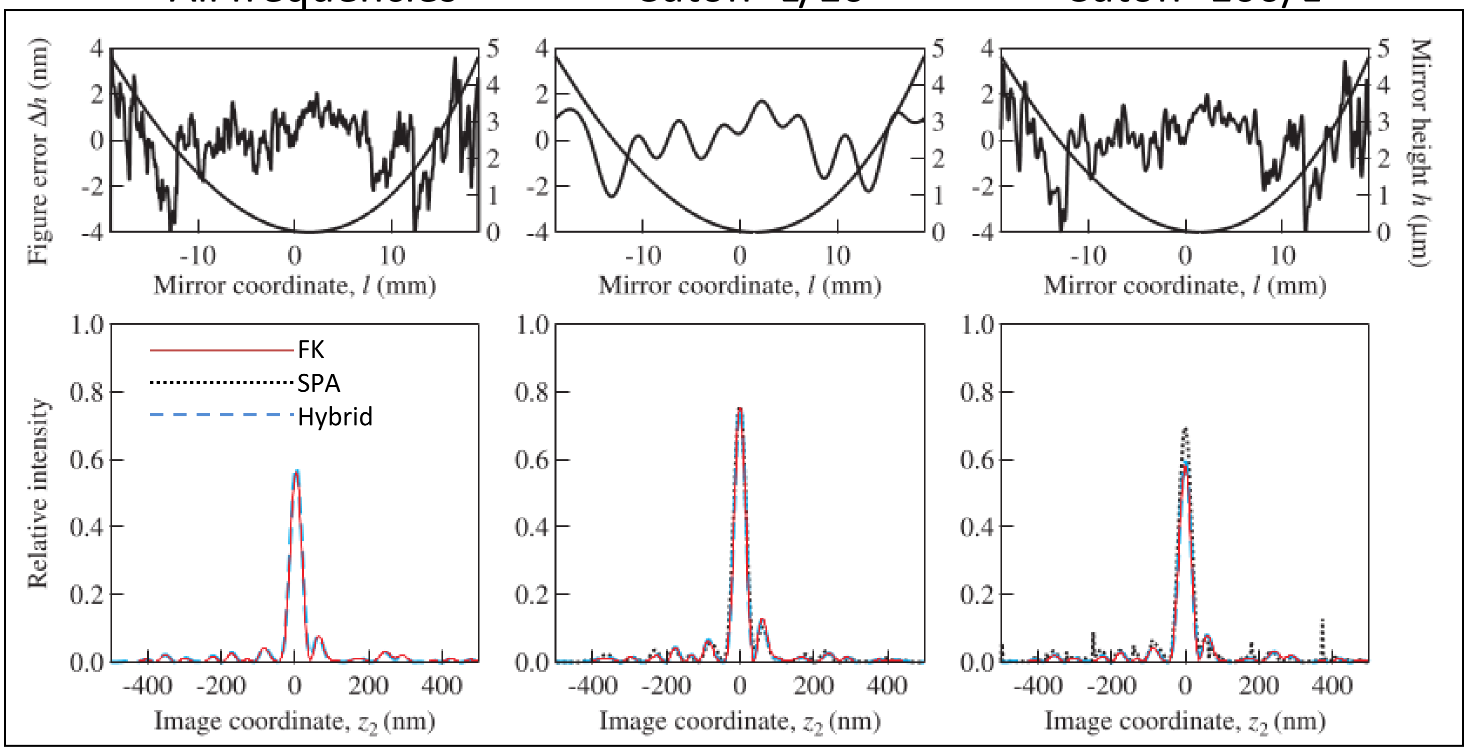
Figure errors: Hybrid method in SHADOW

E=15 keV point source

L=40 mm θ=3mrad σ_{RMS}=1nm

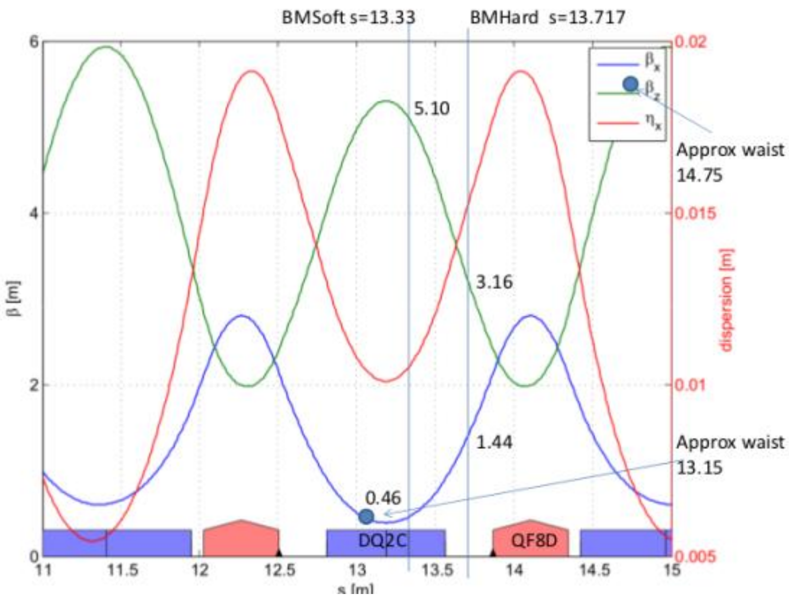


All frequencies | Cutoff=L/10 | Cutoff=100/L



X. Shi, R. Reininger, M. Sánchez del Río, J. Qian and L. Assoufid Proc. SPIE 9209, 920909 (2014); doi:10.1117/12.2061950

Using accurate electron beam values in Optics calculations:
Obtaining Twiss parameters (or moments) from electron tracking codes (like AT)



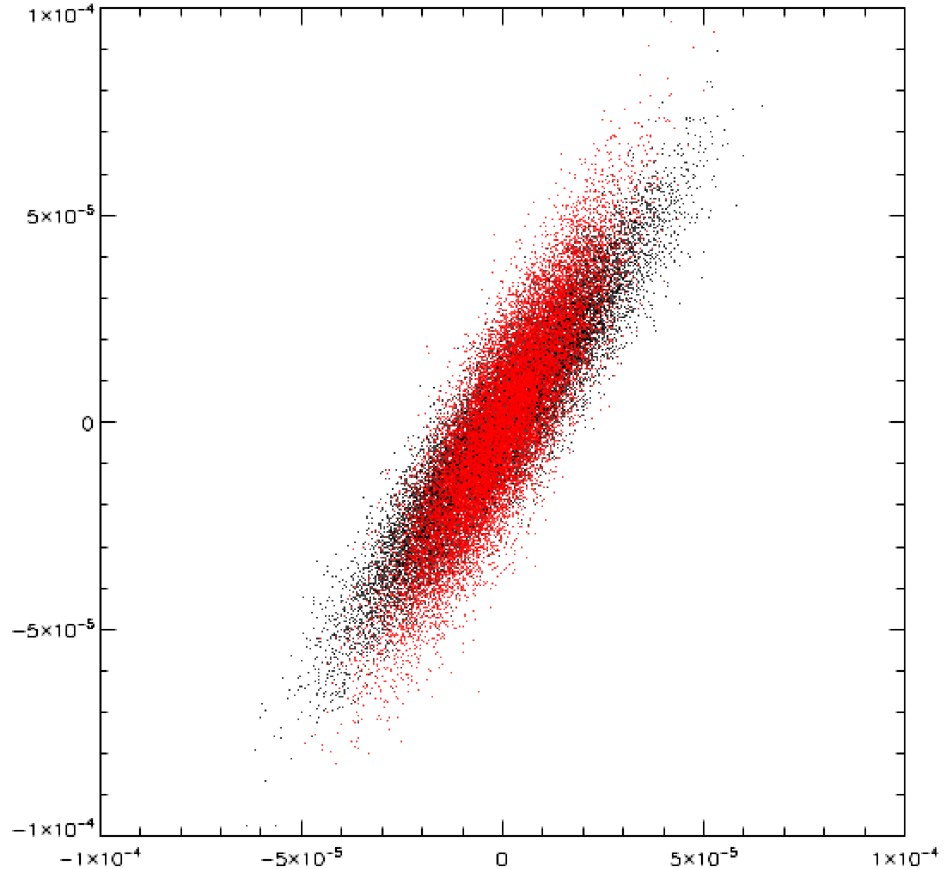


Figure 3: Monte Carlo sampling of the electron phase space $x'[rad]$ vs. $x[m]$ at the wiggler edges: $y = -0.1$ (red) and $y = 0.1$ (black).

Implementation in SHADOW: http://forge.epn-campus.eu/documents/784

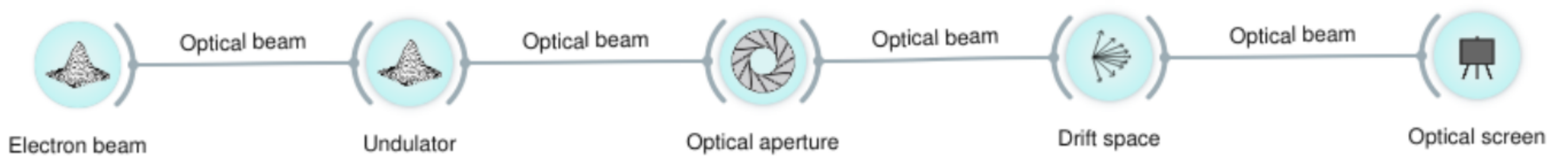
NEW SOFTWARE

- Combine incoherent optics (SHADOW) and coherent optics (SRW) in the same environment to simulate beamlines

- Extend the environment to the electron beam and to the samples to be able to calculate virtual experiments

Software development aspects

A framework for beamline simulation that is both easy to use and **generic**.



Written in modern programming languages and following today's programming paradigms.

Python 3

Orange framework

ESRF

The OASYS Project

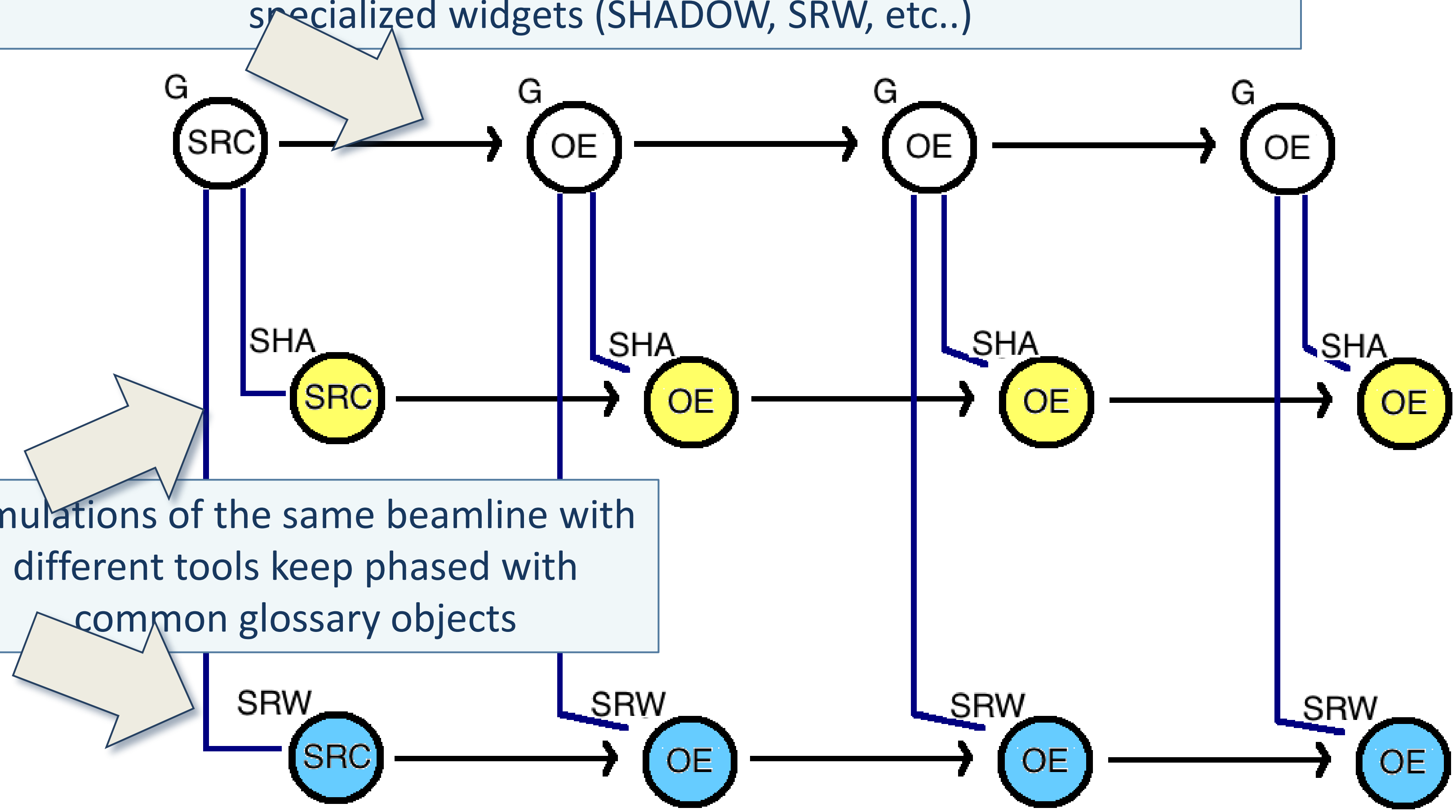
- ✓ OASYS = OrAnge SYnchrotron Suite
- ✓ A common platform to build synchrotron-oriented User Interfaces ***that communicate***
- ✓ The upper layer of the application presented to the user

M. Sanchez del Rio, L. Rebuffi, J. Demšar, N. Canestrari, O. Chubar, “A proposal for an Open Source graphical environment for simulating X-ray optics”, Proceedings of SPIE, Volume 9209 • New Advances in Computational Methods for X-Ray Optics III (2014).

L. Rebuffi & P. Scardi, “Calculation of the instrumental profile function for a powder diffraction beamline used in nanocrystalline material research”, Proceedings of SPIE, Volume 9209 • New Advances in Computational Methods for X-Ray Optics III (2014).

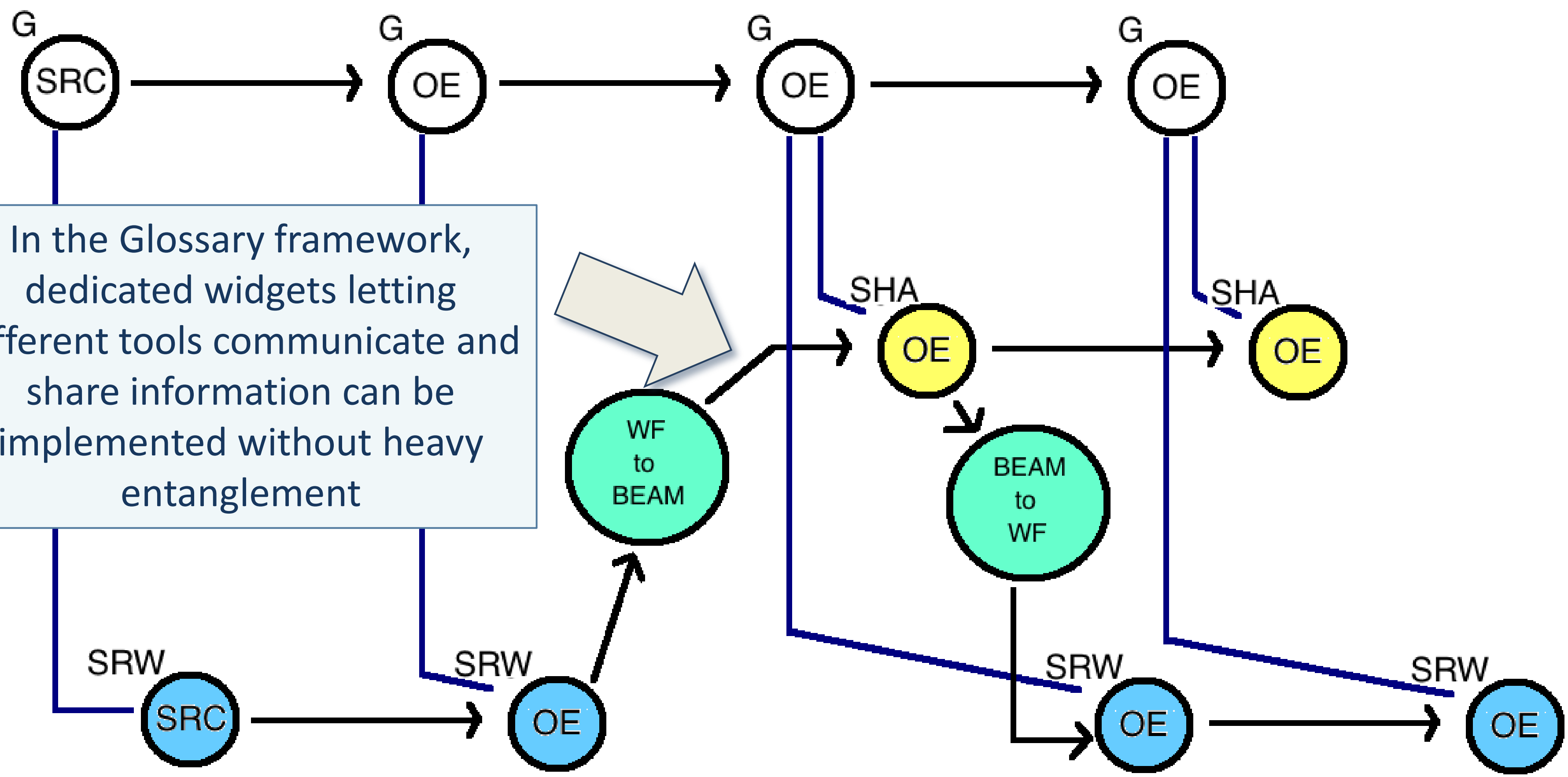
The OASYS Project

Glossary widgets will represent the beamline at the highest abstraction level and will send glossary objects to populate common information in the specialized widgets (SHADOW, SRW, etc..)



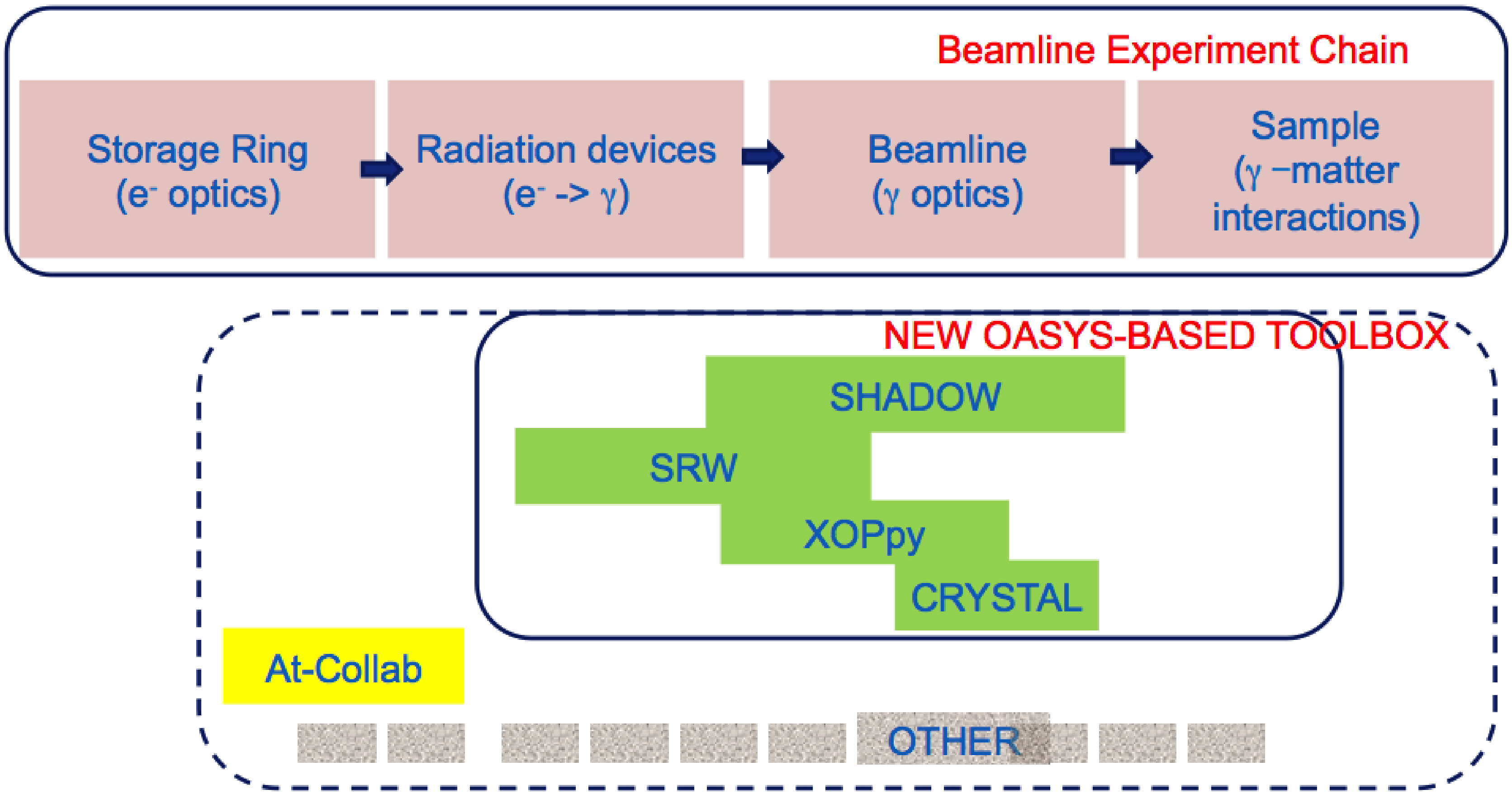
Simulations of the same beamline with different tools keep phased with common glossary objects

The OASYS Project



In the Glossary framework, dedicated widgets letting different tools communicate and share information can be implemented without heavy entanglement

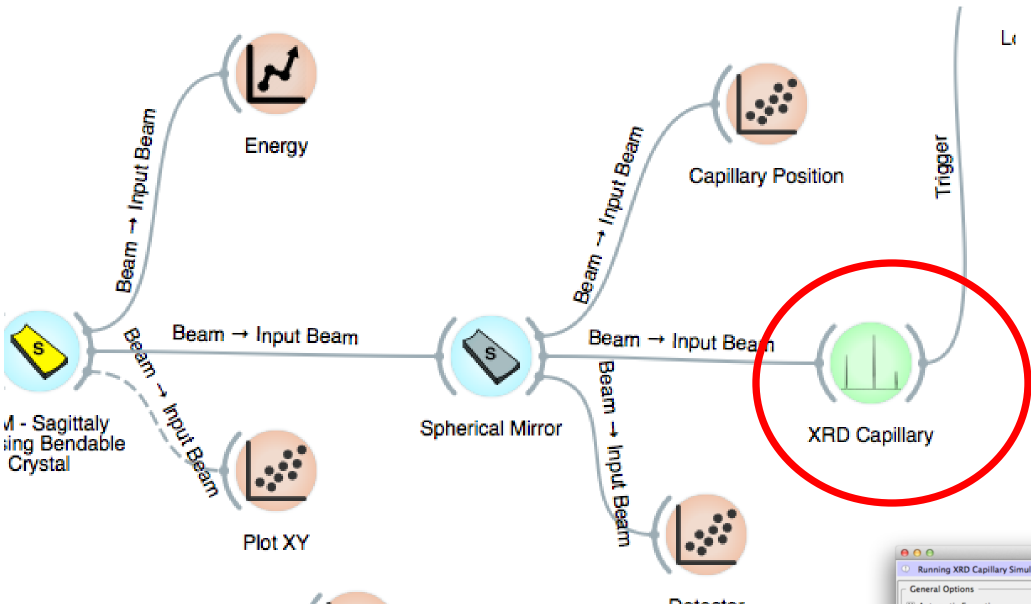
Towards Virtual Experiments

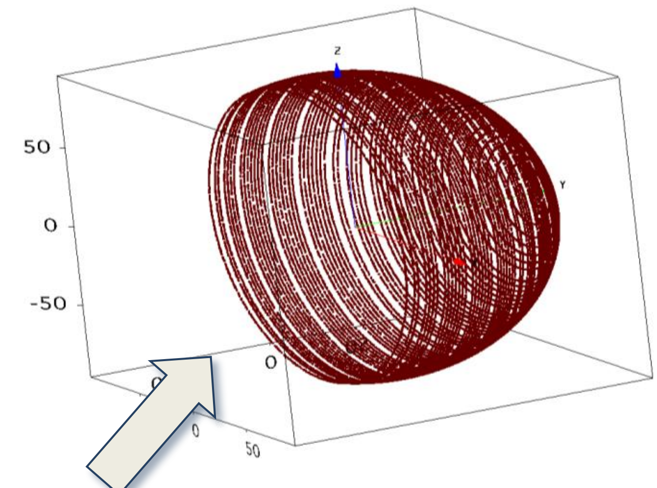


ON GOING

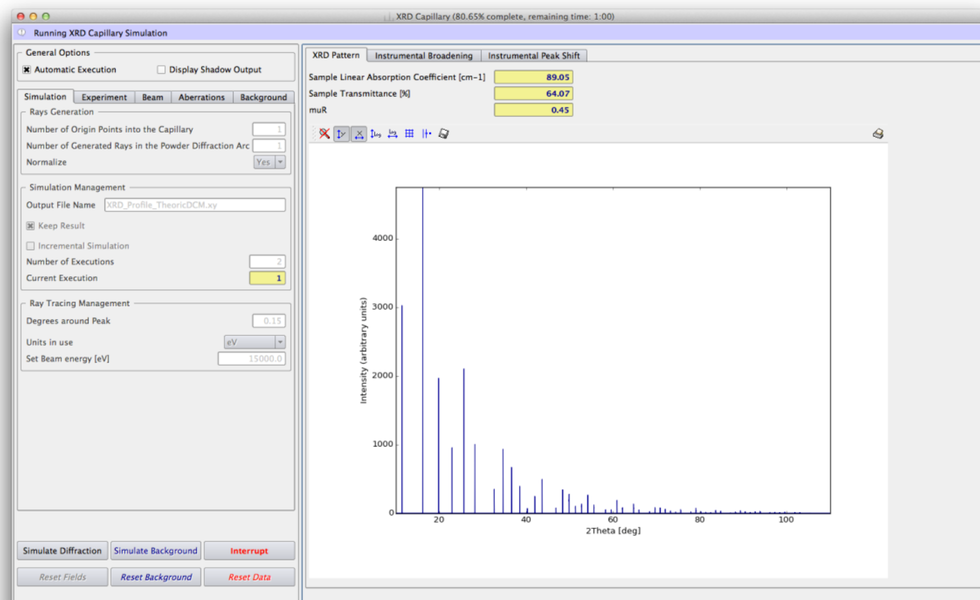
- A completely new User Interface for SHADOW is almost operational (L Rebuffi)
- A new SRW interface is planned; First tests done (M Glass)
- A new XOP under Oasys called XOPPY is under development (M Sanchez del Rio)
- An optics tools for crystals (including Stokes-based optics) is being coded (M Glass)

SAMPLE SIMULATION: EXAMPLE XPD





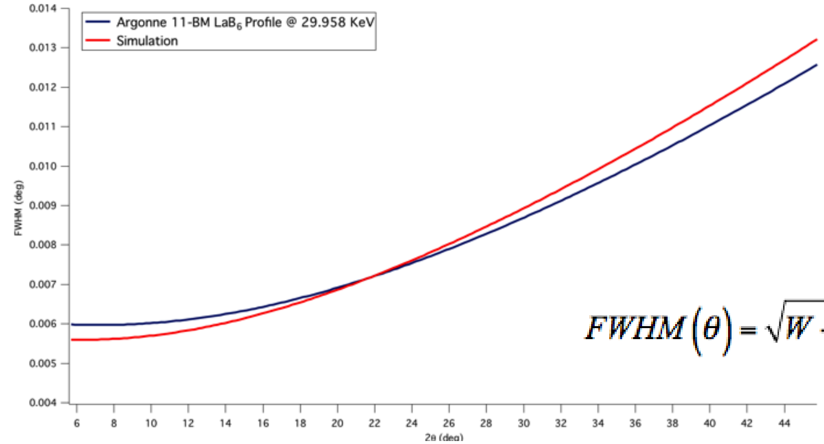
Debye Rings generated as SHADOW rays



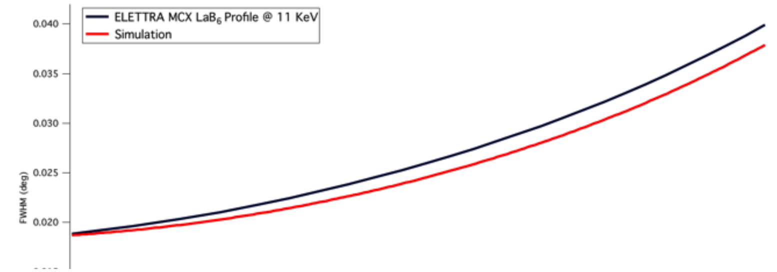
L Rebuffi, P Scardi and M Sanchez del Rio (2015) Powder Diffraction, 30, S56-S64 doi:10.1017/S0885715614001328.

Preliminary results: Ray-Tracing of LaB_6 Profile

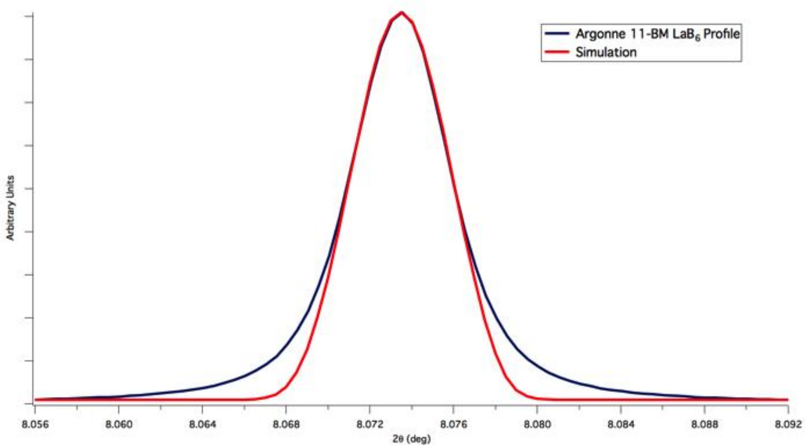
APS 11-BM

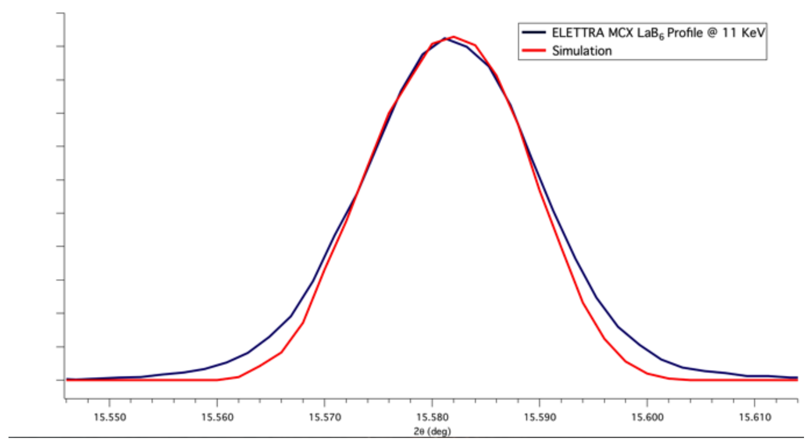


ELETTRA MCX

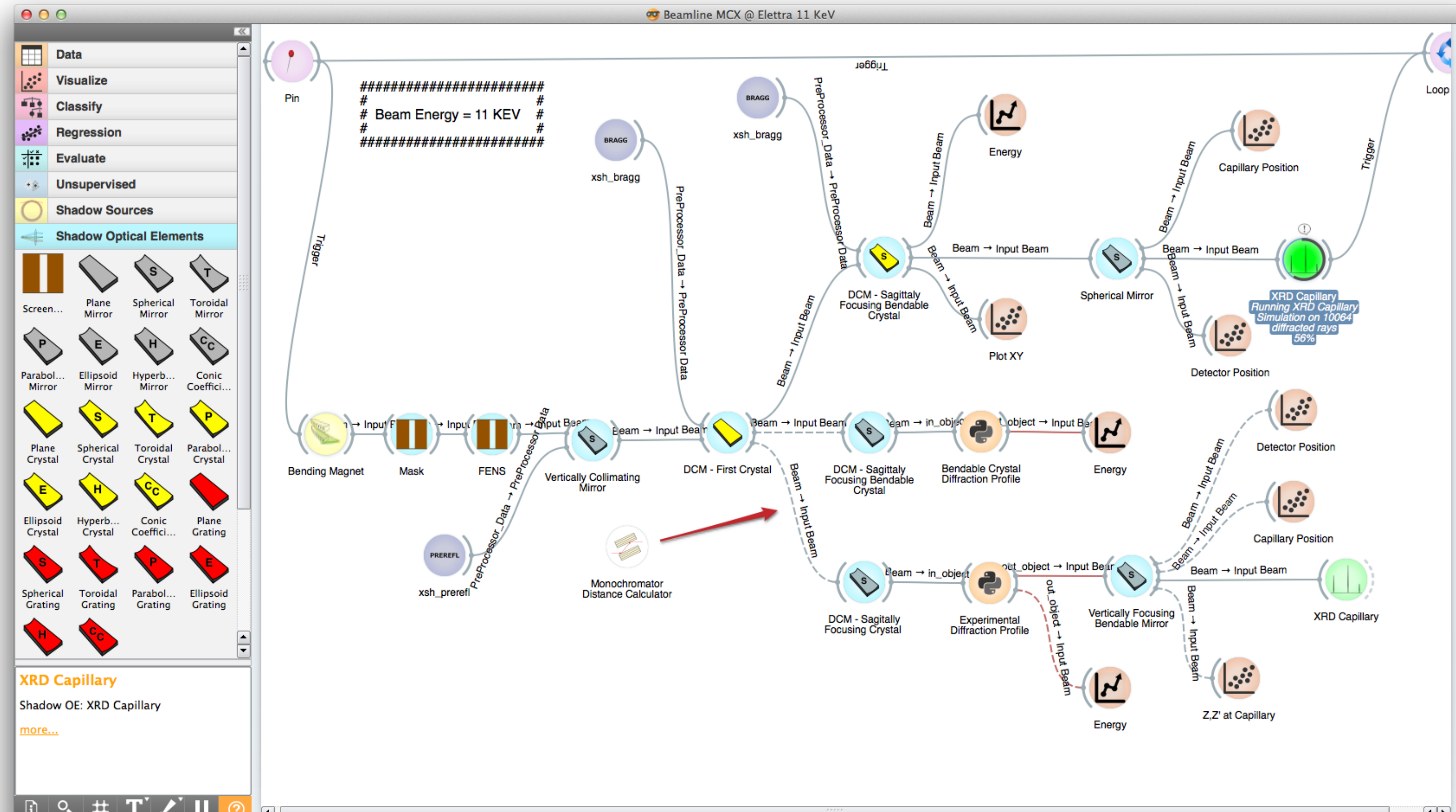


$$FWHM\left(\theta\right) = \sqrt{W + V\tan\theta + U\tan^2\theta}$$





New SHADOW interface
New XOPPY tools



Thank you

Mark Glass
Luca Rebuffi (Elettra)

Boaz Nash
Xianbo Shi (APS)
Ruben Reininger (APS)
Kwang-Je Kim (APS)
Oleg Chubar (NSLS-II)

And many others…