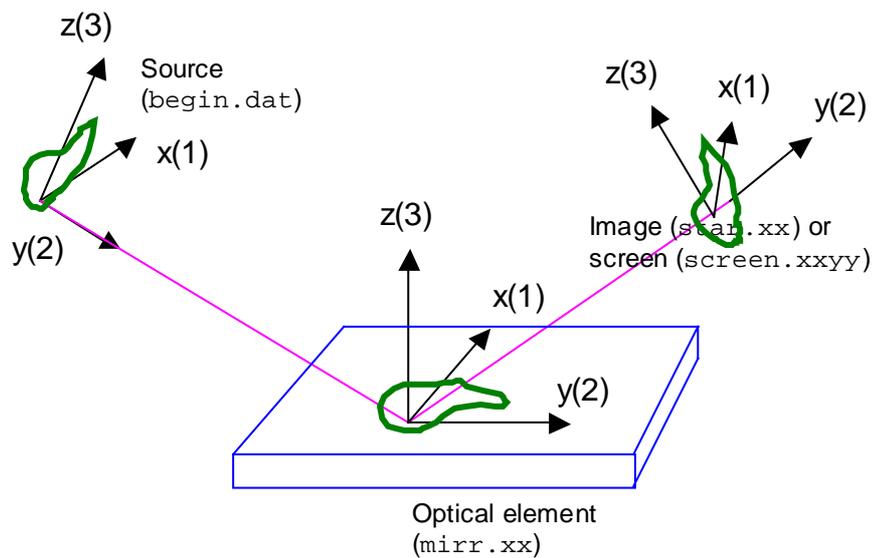


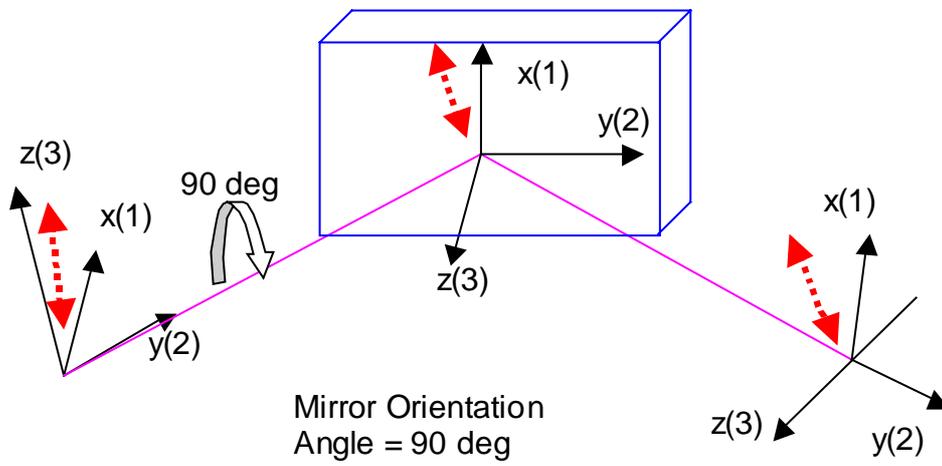
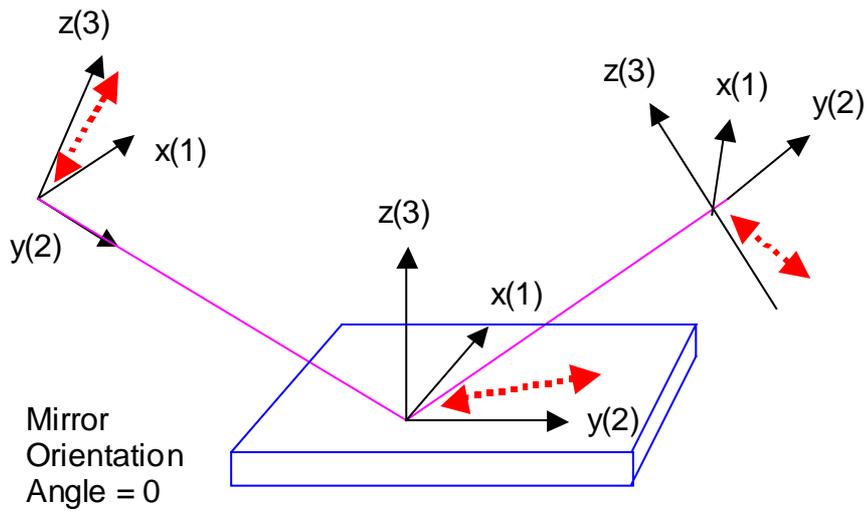
# XOP tutorial at ESRF - Session 3

## Introduction to ray-tracing

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## 1. Geometrical source. Learning reference frames.

You will:

- learn to define geometrical sources
  - understand the use of a macro for modifying an existing source
  - understand reference frames
- 
- i) Create a collimated (i.e., zero divergence) geometric source with elliptical shape with vertical semiaxis twice the horizontal semiaxis. Visualize it
  - ii) Apply the following macro, that keeps only the rays with positive values of X and Z. Visualize the new result.

```
a=ReadSh('begin.dat')
x = GetShCol(a,1)
z = GetShCol(a,3)
f = GetShCol(a,10)
bad1 = Where(x LE 0)
bad2 = Where(z LE 0)
f[bad1]=-100
f[bad2]=-1100
a.ray[9,*]=f
putrays,a,'begin.dat'
```
  - iii) Create a mirror optical element, with incident angle 45 degrees, and  $p=q=1\text{m}$ . Trace the system in two cases, with Mirror orientation angle 0 and 90 degrees. Verify the results with the pictures shown before.

Hints: you may load the workspace `session3_1.ws`, where this system is defined, for zero mirror orientation angle.

## 2. Synchrotron sources: Bending magnets.

You will learn to

- simulate bending magnets

i) Simulate the source for the ESRF bending magnet (full emission) at a fixed energy (e.g., 8 keV). Use one mrad of horizontal divergence. Visualize the cross section  $(x,z)$ , the divergence space  $(x',z')$ , top view  $(y,x)$  and phase space  $(z,z')$ . Make histograms of intensity (total,  $\sigma$ -polarized and  $\pi$ -polarized) as a function of the vertical divergence. Do the same at 18 keV.

ii) Simulate the same source but on a limited vertical divergence (e.g.,  $\pm 50 \mu\text{rad}$ ).

Hints: you may load the workspace `session3_2.ws`, where this system is defined, for full vertical emission.

## 3. Insertion devices

You will learn to

- Simulate wigglers and undulators

a) Simulate the standard wiggler for ID17 (medical beamline) the energy interval  $10000 \pm 10 \text{ eV}$ . Calculate the total horizontal divergence (width of the  $x'$  histogram) and visualize a top view of the emission  $(y,x)$  with finite emittance and source size, and without emittances (i.e., setting emittances and sigmas to zero).

Hint: you may use the workspace file `session3_3a.ws`

b) Simulate the U46 undulator at the energy corresponding to the third harmonic. Play with the maximum aperture angle to create many rings.

- No emittance, max aperture angle 0.15 mrad
- No emittance, max aperture angle 0.015 mrad
- The same with emittances.

Hint: you may use the workspace file `session3_3b.ws` which implements the case using emittances and max aperture angle of 0.015 mrad.

#### 4. Beam propagation (phase space (z,z') ellipses)

You will learn to

- Define screens and slits associated to optical elements

a) Using the already created bending magnet source, add an optical element with several screens at 0 (source position), 50, 75 and 100 cm from the source. See the tilt of the (z,z') diagram.

b) Define an aperture in the first screen (20  $\mu\text{m}$ ) and see its effect in screens #2 and #3.

Hints: Use the *Modify oe...* button to define the oe parameters (these parameters are not important at this moment). Use the *Screen Manager...* button in the oe window to create and define the screens/slits. Then Run shadow using the button “Run Shadow/trace”. Visualize the screens using the PlotXY facility and loading the files `screen.0101` for the first screen, `screen.0102` for the second, etc.

You may use the workspace files `session3_4a.ws` and `session3_4b.ws`. They also contain a macro for visualizing the four screen planes in a single screen.

## 5. Focusing with grazing incidence mirrors: effect of aberrations.

You will learn to

- Use a geometrical source to simplify the simulation of an undulator
- Use different mirror shapes in SHADOW
- Experience with the automatic calculation of the mirror parameters.
- Include mirror reflectivity by using the “prerefl” preprocessor
- Visualize results using contour curves.

Create a geometrical source with Gaussian shape ( $\sigma_x=57 \mu\text{m}$ ,  $\sigma_z=10.4 \mu\text{m}$ ) and Gaussian divergence ( $\sigma_x'=88.5 \mu\text{rad}$  and  $\sigma_z'=7.2 \mu\text{rad}$ ) to simulate the emission of a 1.65 m undulator at 10 keV in a Low beta section (these numbers are taken from the web).

a) Study the case of different mirror shapes (spherical, toroidal and ellipsoidal) for focusing the source with distances  $(p,q)=(30\text{m},10\text{m})$  (magnification 1/3) and  $(30\text{m},1\text{m})$  (magnification 1/30) for a grazing angle of 0.12 degrees. Study the effect of the spherical aberrations and its influence depending on the magnification factor. See also the dependence on mirror dimensions and incident angle.

b) Enter the effect of mirror reflectivity. Consider a Rh ( $\rho=12.4 \text{ g/cm}^3$ ) coating and a source with energy distribution in 5-45 keV (box-distribution). Visualize the results using both scattered plot and contour curves (including reflectivity). Plot also the intensity versus energy.

Hints. Use the oe menu to enter the mirror values. *The angles [in deg] are INCIDENT angle and not GRAZING angle.* Shadow can calculate the surface parameters (curvature radii, ellipse axes, etc). by selecting in the screen under the “Figure...” the “internal/calculated” entry. After running Shadow, calculate the spot sizes using either InfoSh or from the histogram widths. The resulting mirror parameters can be seen using the “MirInfo” button. You may also use the workspace files `session3_5a.ws` and `session5b.ws` which implement a toroidal mirror for magnification 1/3, considering and not considering, respectively, mirror reflectivity.

## 6. Kirkpatrick-Baez system

You will learn to

- define an optical system with two mirrors
- define a cylindrical mirror with circular or elliptical section
- tell SHADOW to calculate automatically the mirror parameters in the case that focal planes that do not coincide with continuations planes
- exercise with the mirror orientation angle.
- define mirror dimensions

Study the case of the previous exercise ( $M=1/30$ ) with a Kirkpatrick-Baez system with cylindrical (and later with elliptical) mirrors of length=40 cm and width=4 cm. Distance source-m1=29.5m; Distance m1-m2=1m; Distance m2-spot=9.5m. Use 25000 rays. Do not include the mirror reflectivity.

Hint: you may use the workspace file session3\_6.ws, which contains this case with cylindrical mirrors.

## 7. Double crystal monochromator.

You will learn to

- create crystal reflectivity data using the “bragg” preprocessor
- use the “autotuning” facility to align the crystal
- calculate the energy resolution for a crystal and a combination of systems
- optimize the source bandwidth
- play with the mirror orientation angle. Relate its values to the crystal dispersion ( (+,-) and (+,+) crystal combination)

Create a bending magnet source (starting from exercise 2) at  $8000\pm 25$  eV with 3 mrad horizontal divergence. Verify its energy dependence and horizontal and vertical divergence values.

a) Use the Bragg preprocessor to create the reflectivity data for a Si 111 crystal. Implement a flat Si 111 crystal at 30 m from the source. Verify the energy dependence and calculate resolution. Redefine the source energy bandwidth to optimize the calculation in order to obtain the energy dependence with the highest signal.

b) Add a second crystal 10 cm downstream from the first one in (+,-) and (+,+) configurations (play with the mirror orientation angle). Explain the obtained differences in energy resolution.

Hint: you may use the workspace file session3\_7.ws. Notice that the workspace file does not contain the file with the reflectivity for the crystal, so you will need to run the bragg preprocessor. Pay attention to the file name when you run bragg, because it also appears in the o.e. crystal menus. In this case, the file is called si5\_15.111.

## 8. Sagittal focusing

You will learn to

- define a cylindrical mirror for sagittal focusing
- define “externally” the optical element radius of curvature
- optimize the focal spot

a) Using the (+,-) system defined in the last exercise, bend sagittally the second crystal to focus in the horizontal plane at the sample position, placed 1000 cm downstream from the monochromator). Calculate horizontal spot size.

Use ShadowVUI|Results|ray\_prop to find the position of the best focus. Calculate its size.

b) Study the effect of the ratio between the distances mono-sample and source-mono in the transmitted intensity. Study the case of  $M=1/30$ . See the effects in energy resolution and system transmittivity. Explain these differences. Verify that ratio  $1/3$  is the optimum.

Hints: Use the program ShadowVUI|Utils|Optical|Tang and sag radii (rcil) to calculate the curvature radius:  $R_s(8\text{keV}, M=1/3)=371$  cm. You may use the workspace files `session3_8a.ws` and `session3_8b.ws`, corresponding to  $M=1/3$  and  $M=1/30$ , respectively.

## 9. Simulation of a complete beamline.

You will learn to:

- Combine several optical elements
- Obtain final results for a beamline in terms of flux, resolution and spot size.

Define the following elements in SHADOW:

Geometrical Gaussian source at  $10000\pm 10$  keV (box distribution) (like in exercise 5b, but changing the energy interval)

M1: Cylindrically collimating mirror in the vertical plane at 25 m. Grazing angle 0.12 degrees. Rh coating (density=12.4g/cc). Dimensions:

MONO: Double crystal monochromator, Si 111, with second crystal sagittally bent (focusing the source into the sample position in the horizontal plane), at 30 m ( $R_s=307.5$  cm)

M2: Re-focusing mirror at 35m, focusing at the sample position. Same angle as M1  
Sample at 40 m

Calculate:

- i) Beam geometry at the sample position
- ii) Energy resolution

- iii) Transmittivity of the whole beamline. Number of photons at the sample position supposing that at the source we have, at 10 keV, a flux of  $5 \cdot 10^{13}$  ph/sec/0.1%bw
- b) How are these results modified using a focusing first mirror and a flat second mirror?

Hint: you may use the workspace file `session3_9.ws`

## **Appendix 1- SHADOW introduction**

SHADOW is a ray-tracing program specially optimized for the design of the synchrotron radiation beamline optics. It has been developed by F. Cerrina et al. at the University of Wisconsin. SHADOW generates and traces *a beam* along the *optical system*. The beam is a collection of *rays* in a given point of the beamline which are stored in a disk file. The optical system is a collection of *optical elements (o.e.)* (mirrors, multilayers, slits, screens, etc.) placed in a sequential order. Each ray is an array of 18 (or 12) variables or *columns*. Each variable of column has a special physical meaning. The first six defines the geometry: spatial coordinates (Col. 1,2,3 or x, y and z, respectively) and the direction of the ray (cols. 4,5,6, or x',y' and z', respectively). The rest of the columns defines the history of the ray traversing the optical system (electric vector for s-polarization (cols. 7,8,9) and p-polarization (cols. 16-18), flag for lost ray (10), wavelength (11) etc.).

The *source* is the beam at the starting point. It is generated by SHADOW by sampling the spacial, angular, energy and other qualities of the synchrotron radiations sources (i.e., bending magnets, wigglers and undulators) into a finite number of rays, using a Monte Carlo method. At the source position the intensity of each ray (or better, its probability of observation) is set to 1. This intensity will decrease along the beamline because of the interaction of the ray with the optical elements. The source generated by SHADOW samples linearly the real source, which allows to scale the intensity with the number of photons. SHADOW traces the source sequentially through each individual optical element of the optical system. SHADOW solves the intercept of each ray at a given o.e., calculates the output direction and the decrease in intensity. This decrease is calculated for each ray using a physical model (i.e. Fresnel equations for mirrors, Dynamical Theory of the Diffraction for perfect crystals, etc.)

## **Appendix 2- SHADOW files**

The binary files containing the rays at different points are:

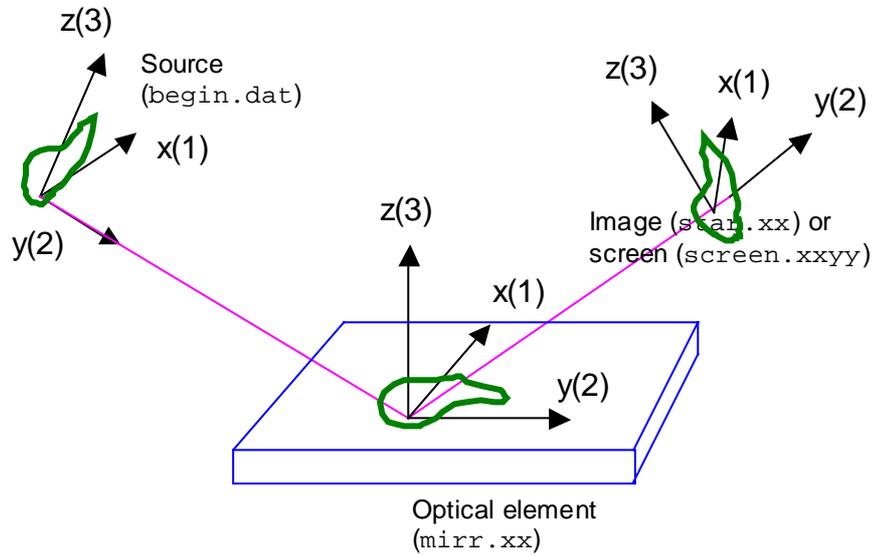
- `begin.dat` binary file containing the beam at the source position
- `mirr.xx` binary file containing the beam on each o.e. (i.e. `mirr.02` is the beam on the second o.e)
- `star.xx` binary files with the beam at the image created by each o.e. The image of a given o.e. is the source for the following o.e.
- `screen.xxyy` SHADOW can (optionally) create the image file in a different points of the beamline, or screens. Screens are associated to a given o.e., and can allow to define apertures (slits or beam stoppers) and absorbers (filters). `xx` refers to the o.e. and `yy` refers to the screen order (i.e. `screen.0204` means the fourth slit associated to the 2<sup>nd</sup> o.e.)

The files containing the list of variables used as input/output for SHADOW are:

- `start.xx` an ASCII file with the list of variables for the source or optical elements (`start.00` for the source, `start.01` for the first o.e, `start.02` for the second, and so on)
- `end.xx` the same as `start.xx` but with few parameters recalculated after the run

### Appendix 3- SHADOW frame

The coordinate system of SHADOW is (schematic):



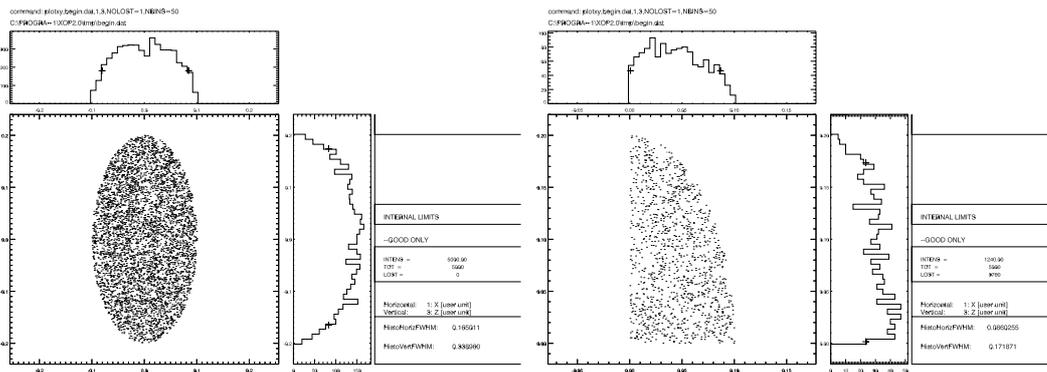
Note that:

- The  $y(2)$  coordinate is along the beam direction
- The frame is rotated if one o.e. is rotated
- The position, orientation, etc. of any o.e. is always referred to the previous one

## Answers

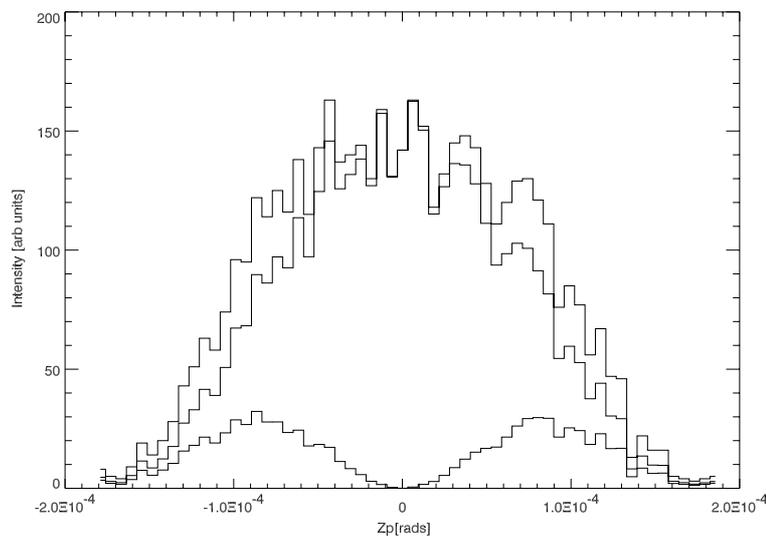
In general, use the corresponding workspaces files `session3_<exercise>.ws`

### 1 - Geometrical source. Learning reference frames.



### 2 - Synchrotron sources: Bending magnets

i) histograms of intensity (total,  $\sigma$ -polarized and  $\pi$ -polarized) at 8 keV:

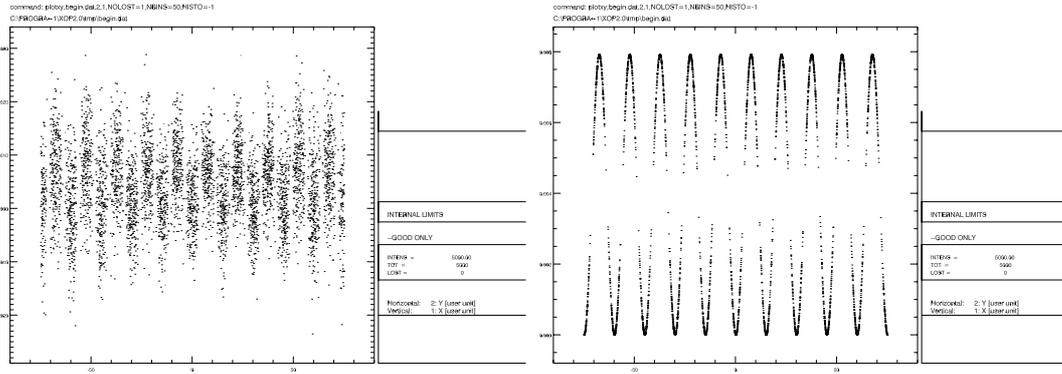


### 3 - Insertion devices

a)

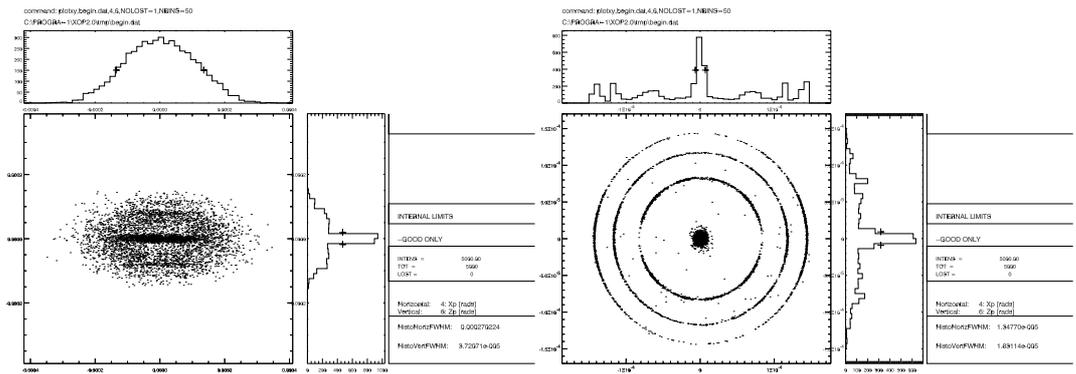
E [keV]	x' [mrad]	z' [mrad]
10	3.1	0.20

With/without emittances



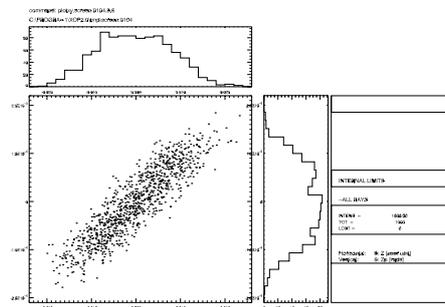
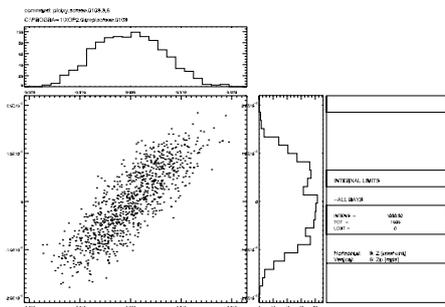
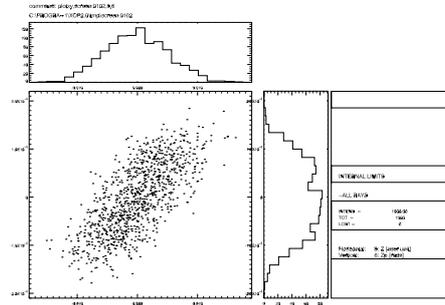
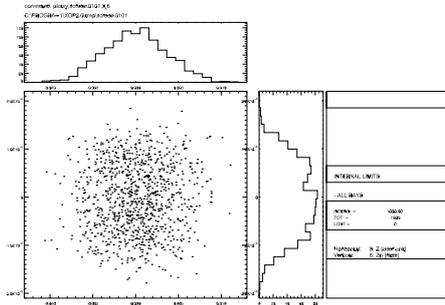
b)

With/without emittances

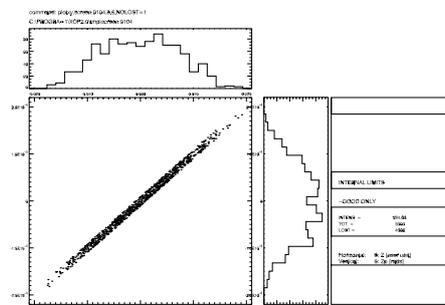
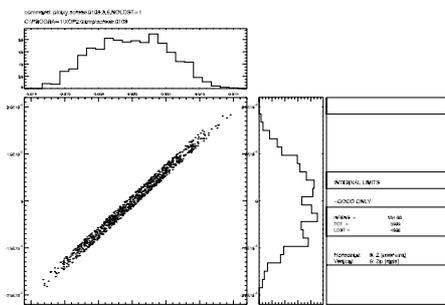
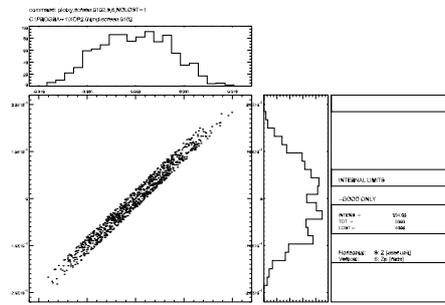
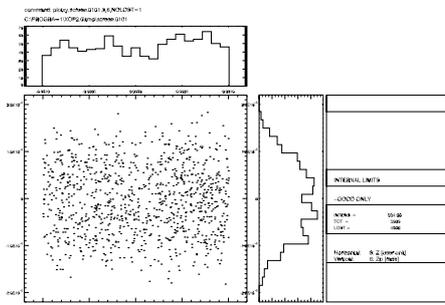


## 4 - Beam propagation (phase space $(z, z')$ ellipses)

a)

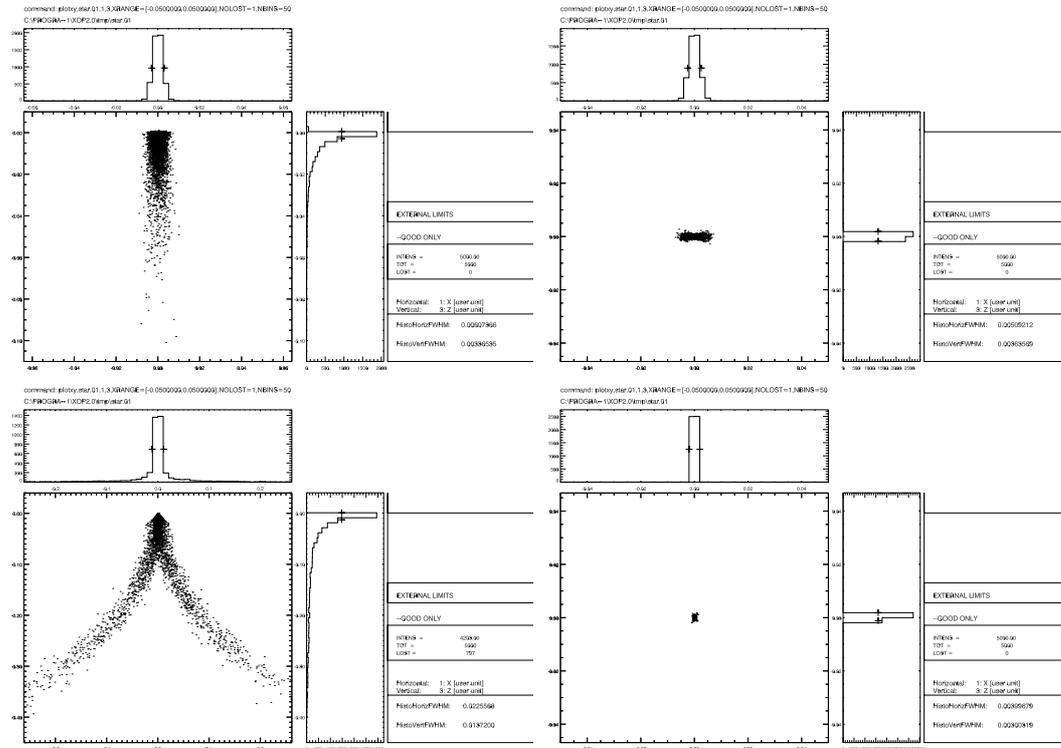


b)

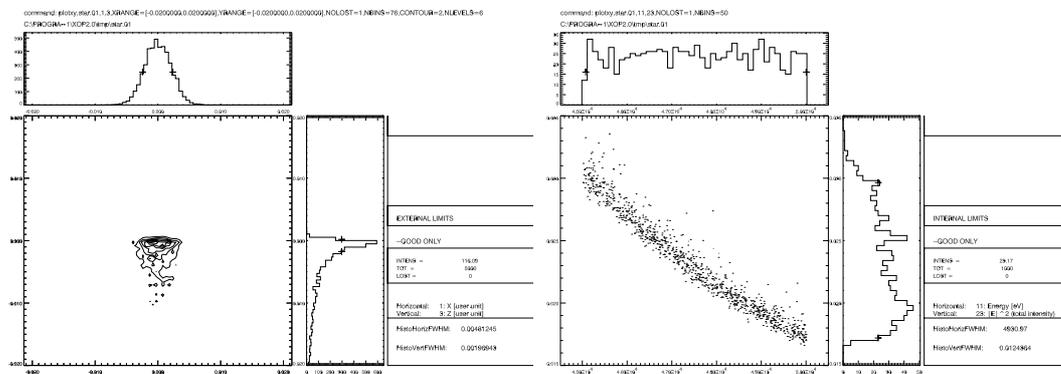


## 5 - Focusing with grazing incidence mirrors: effect of aberrations

a) M=1/3 toroidal (top left); M=1/3 ellipsoidal (top right); M=1/30 toroidal (bottom left); M=1/30 ellipsoidal (bottom right)

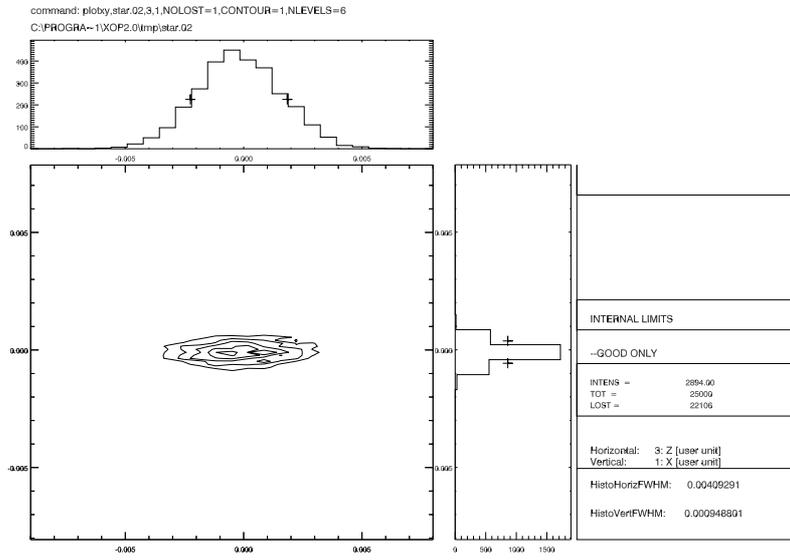


b) Spot (left); I(E) plot (right)



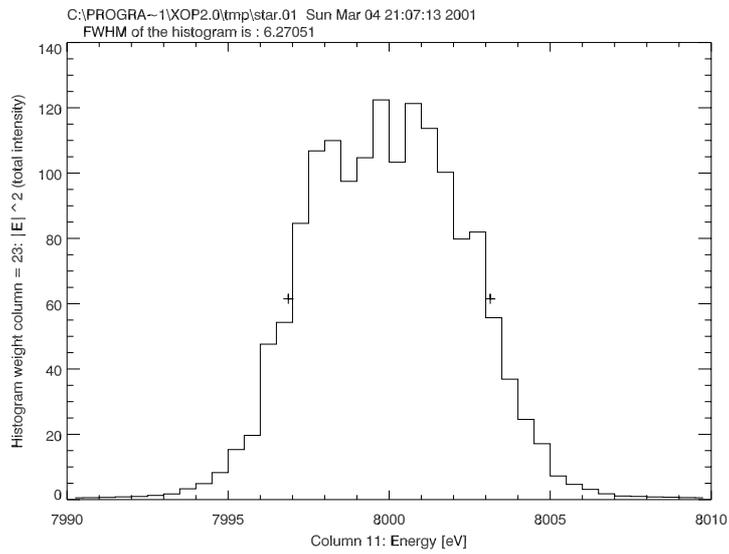
## 6 - Kirkpatrick-Baez system

### Spot with cylindrical mirrors:

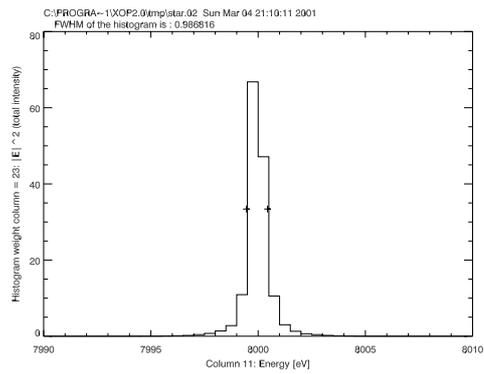
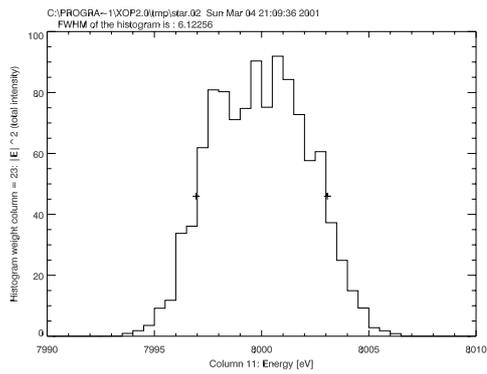


## 7 - Double crystal monochromator

a)

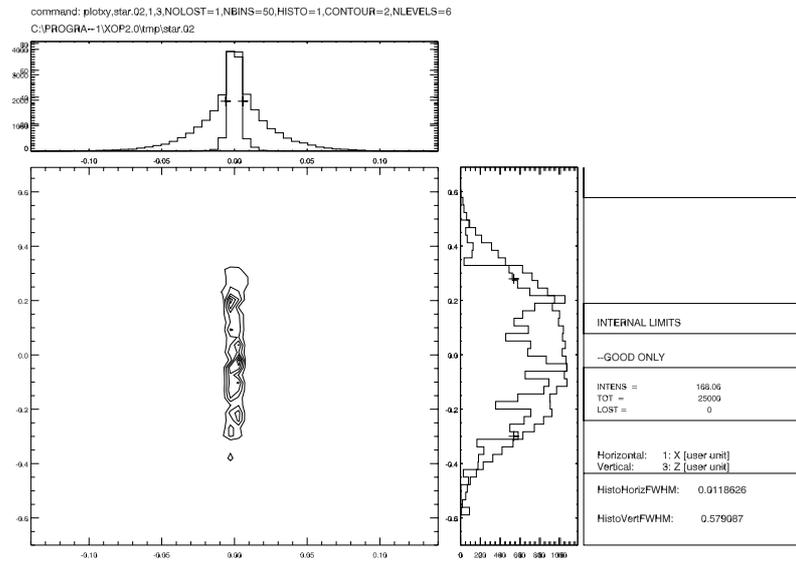


b) I) (+,-) MOA=180 (left); II) (+,+) MOA=0 (right)

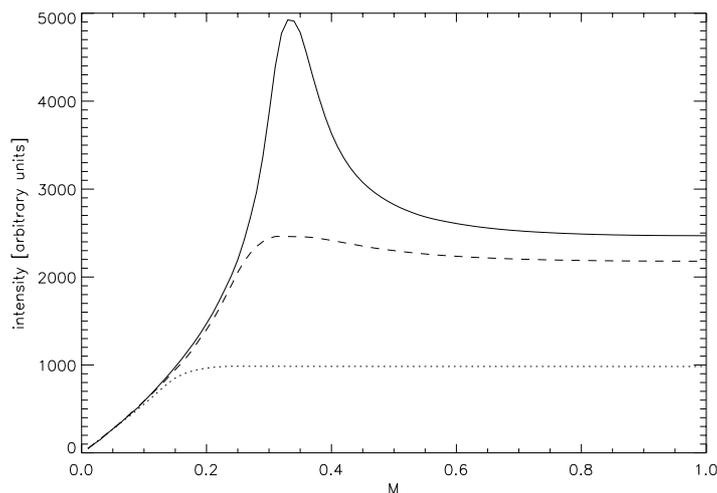


## 8 - Sagittal focusing

- a) Focusing system: Spot width=0.031 cm,  $I/I_0=1090/25000$ ,  $\Delta E=6$  eV  
 Non-focusing system: Spot width=12.0 cm,  $I/I_0=1090/25000$ ,  $\Delta E=5.8$  eV  
 Best focus at about 0.7 cm downstream the focal position. The spot size does not change appreciably.
- b)  $p=30$ m,  $q=1$ m,  $R_s=47.8$  cm, Spot width=0.012 cm,  $I/I_0=168/25000$ ,  $\Delta E=5.8$  eV



The study of the variation of the intensity as a function of the magnifications needs to run shadow for many points of M. It can be done manually or with a macro. The result should show an optimum magnification of  $M=1/3$  for large divergence values. Its effect can be seen in the following figure (M. Sanchez del Rio "Ray tracing simulations for crystal optics" SPIE proceedings, vol. 3448, 230-245, 1998)



Intensity (in arbitrary units) versus magnification factor M for a point and monochromatic ( $E= 20$  keV) source placed at 30 m from the sagittally bent crystals. Three beam divergences are considered: 1 mrad (dotted), 2.5 mrad (dashed) and 5 mrad (continuous). We clearly observe the maximum of the transmission at  $M=0.33$  when focusing the 5 mrad beam, as predicted by the theory

## 9 - Simulation of a complete beamline

$\Delta E_{\text{source}}=4 \text{ eV}$ ;  $\Delta E=1.3\text{eV}$ ;  $I/I_0=1420/5000$

Transmittivity in one eV= $T=(I/\Delta E) / (I_0/\Delta E_{\text{source}})(1420/1.3)/(5000/4)$

Number of photons at the source in one eV bandwidth = $N= 5 \cdot 10^{12}$

Total number of photons =  $N \times T \times \Delta E$

