

Ray tracing Laboratory
School on Synchrotron Radiation
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A. Bianco, D. Cocco

Introduction

Ray tracing is a powerful tool to estimate and understand the behaviour of a complicated object. When in optic one have to deal with a lot of elements (may be lenses, mirrors, diffractive objects and so on) it's surely possible to estimate the final behaviour of the system by first principle (i.e. simply satisfy complicated equations) but...

There are so many parameter to take into consideration, misalignment, slope errors, high order aberrations, residual astigmatism and many other and, practically, it's impossible to estimate carefully the final system performances.

On the other hand, a ray-tracing program, even if it is a very good program, is not able to substitute an optical designer in the definition of the parameter of a beamline.

For this reason, the equations at the basis of the optics for synchrotron radiation must not be forgotten but perfectly understood.

In particular, in the case of the synchrotron radiation, the following statements must be recorded. Since we have to deal with soft or hard x-ray, the transmission of the elements is negligible or useless, so, no lenses can be used. Nevertheless, the reflectivity of every material in both these ranges drop down faster with the increasing of the grazing angle of incidence. Therefore, very grazing angle is necessary. Typical values could be $1-2^0$ for the soft X-ray range and $0.2-0.3^0$ for the hard X-ray radiation. This introduces further problems. The radiation becomes "sensible" to any surface imperfection. For this reason acceptable difference between the real and desired slope could not exceed few μrad RMS on a 1-m length mirror.

Another problem is the high power radiation impinging on the mirrors. This causes an unavoidable heat load that increases the deformation of the mirrors.

All this problems and boundaries condition must be strictly taken into consideration before run a ray tracing program, because great difference between simulated and real value are easy to be obtained.

So, we can conclude saying that ray tracing is fundamental for a good design of a beamline but is not only useless, but also dangerous, if is not used properly.

How a ray-tracing program works

As mentioned above, the ray-tracing program must "simulate" the behaviour of a photon during its travel. Even if a rigorous quantistic description (involving wave functions) should be used, we can approximate the photons as object travelling along a straight line (exactly as made in the geometrical optics). The only thing to take into consideration is the effect on the trajectory of the optical elements. In fact, a mirror can be perfectly simulated by this representation. The photons arrive on the surface, the surface is locally simulated as a plane mirror and a specular reflection takes part. This is exactly what a ray-tracing program does, even if the physic behind this simple process is quite complicated. Another story is the problem of the efficiency (i.e. how many photons are reflected by the mirror and how many are adsorbed) but this is out of the scope of these notes.

Therefore, we now can simulate the behaviour of a photon on a mirror, but, following it step by step, we must start from the source. First, we need to know the characteristic of the source. The programs, typically, are able to simulate point sources, rectangular sources, gaussian (both in angular and spatial), monochromatic, polychromatic (some different line of energy), continuous energy range, and sometimes also to simulate a real synchrotron source, a bending magnet, an undulator or a wiggler. Practically it generates a series of photons any one with a defined position in the space, a trajectory, energy, and in some cases the polarisation degree (a value useless and meaningless for single photons).

To generate real synchrotron sources some complicated equation must be solved or, alternatively, the electron trajectory and the emission from any electron must be simulated. This procedure is quite complicated and in most of the cases is not necessary. For instance, to simulate an undulator source without the aid of external programs, a gaussian distribution is a good approximation. The gaussian shape should be defined by the following equations:

$$(1) \quad \Sigma_x = (\sigma_x^2 + \sigma_R^2)^{1/2} \quad \Sigma_y = (\sigma_y^2 + \sigma_R^2)^{1/2}$$

$$(2) \quad \Sigma'_x = (\sigma'_x{}^2 + \sigma_R^2)^{1/2} \quad \Sigma'_y = (\sigma'_y{}^2 + \sigma_R^2)^{1/2}$$

where Σ_x Σ_y Σ'_x Σ'_y are the spatial and angular divergence of the photon beam, σ_x is the nominal electron beam size in the horizontal direction (Elettra case is typically 0.24 mm), σ_y is the nominal electron beam size in the vertical direction (Elettra case is 0.04 mm), σ'_x is the nominal electron beam divergence in the horizontal direction (Elettra case is 0.03 mrad), σ'_y is the nominal electron beam divergence in the vertical direction (Elettra case is 0.017 mrad). The dependence of the emitted radiation from the energy is related to following relations:

$$(3) \quad \sigma_R = 0.15 (\lambda L)^{1/2} \quad \text{and} \quad \sigma'_R = 1.30 (\lambda/L)^{1/2}$$

L is the undulator total length and λ is the selected photon wavelength.

The energy distribution of the source is fundamental to understand the behaviour of the beamline. The first step is the simulation of a perfect monochromatic source. In this way one have the exact idea of what happen at the selected energy. Another important parameter is the divergence. The ideal divergence of a synchrotron source is quite small. Nevertheless, the angular distribution is big enough to light the full optics and to introduce errors induced by the divergence (i.e. non-paraxial approximation necessary). For this reason, a real beamline and also a simulated one should have a pinhole some meter after the source to adsorb all the radiation out of a specified distribution cone (typical divergence accepted by a beamline is less then 0.05 mrad^2 for the

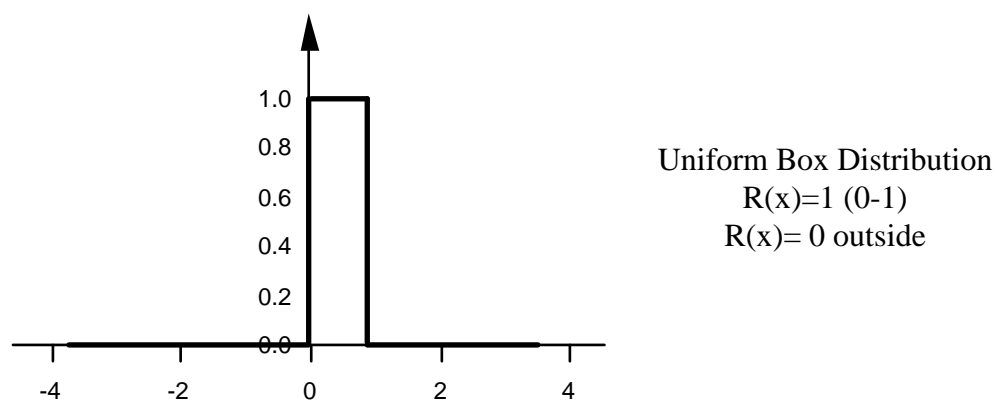


Fig. 1 Random box distribution.

soft x-ray beamline and some mrad^2 for the HXR ones). In any case, also a gaussian distribution could not be so easy to be simulated. Let us consider the possibility to write a program by ourselves. In this case, a standard programming language gives a random distribution inside a box (typically 0-1). It is necessary to use a random distribution because the number of photons used in a simulation could not be too high. The use of 5000-10000 ray is already a number great enough, but only if the rays are randomly distributed. The box distribution ($R(x)$) is easily defined as a function that is equal to 1 inside the range 0-1 and is zero outside, i.e. as shown in fig.1. Vice versa, the Gaussian distribution is defined by the equation in fig. 2

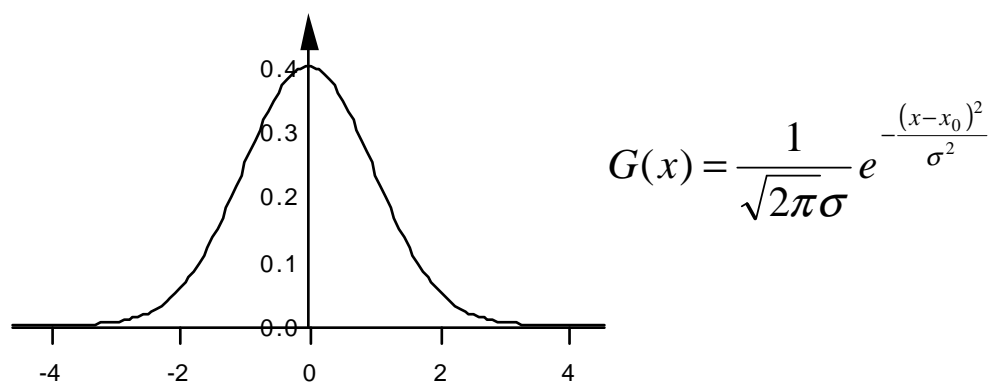


Fig. 2 Gaussian distribution with the equation that define it.

Now, the probability to found a photon (or whatever) gaussian distributed in the interval between $-\infty$ and x_1 is:

$$(4) \quad P(x)[-\infty; x_1] = \int_{-\infty}^{x_1} G(x) dx$$

Since the probability to found a value between $-\infty$ and $+\infty$ for a gaussian distribution is 1, the easiest way to random distribute elements with gaussian shape is the following. First, found a value V between 0 and 1 for the equation $R(x)$ and impose this value to the probability distribution $P(x)$ i.e.

$$(5) \quad R(x) = V[0 - 1] = P(x)[-\infty; x_1] = \int_{-\infty}^{x_1} G(x) dx$$

Now, the value x_1 is the value assigned to our photons. Following this procedure for every photon, one defines exactly a gaussian distribution.

Let us now spend some more words about the mirrors. Every program has a collection of shapes available. Typical shapes are Plane, Spherical, Elliptical, Cylindrical, Toroidal, Parabolic, and so on. All these shapes have to be defined (by the programmer) with his geometrical equation typically quite complicated.

Once the rays are defined, everyone with its direction and position in the space, it could be traced up to meet the following mirror surface. Practically, the only equation to solve is the intersection between a line (the ray path) and a geometrical function describing the optical surface of the mirror. At the intersection point, one should calculate the normal at the optical surface, and reflect the ray respect it. In this way the mirror, locally, can be approximated with a plane surface, and the result is just a simple reflection (easy to treat).

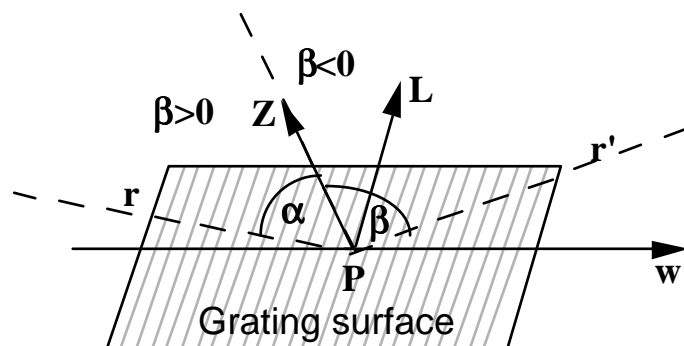
In this way, every aberration introduced by the optics, every error of focus will be shown in the final image obtained. It is easy to introduce slope errors (just modifying the geometrical equation describing the optical surface); it is easy to simulate misalignment (just moving the pole of the optical surface) and so on.

In reality, behind this simple concept of reflection, some complicate equations take into consideration the aberrations, the focal property and so on. However, instead of treat its as the “case of the mirrors”, we will treat as a simplifications of the more general case of the grating.

The grating, as a prism or a crystal, is a dispersive object. We will consider only the grating. The case of the crystal will be discussed in another section of this school. The basic equations for gratings is:

$$(6) \quad d(\sin\alpha - \sin\beta) = n\lambda$$

Where the following reference system was adopted.



But, to have a deep knowledge of the property of a grating/mirror, the Fermat's principle must be applied. This principle, widely used in optics, can be summarised as follow: the light travel between two different points in the shortest possible time. Therefore, it is necessary to recover the optical path F of a ray passing trough a grating (the case of the mirror is a sub-case) and then derives this path respect the time t . The minimum time condition is fulfilled when:

$$(7) \quad \frac{\partial F}{\partial t} = 0$$

Any deviation from this condition can be called “aberration”, i.e. distortion from the ideal value.

To found the minimum time path is equal to found the minimum distance path, since the photon travels always in the same medium (i.e. vacuum). One must therefore define the optical path F of a ray passing trough a general point P (of co-ordinate w, k, l) on the grating as a function of w, k , and l and found the minimum distance path respect these co-ordinates. The general optical path can be written as:

$$(8) \quad F = \overline{AP} + \overline{PB} + \frac{n\lambda}{d}$$

Where the dispersive term is introduced to take into account the dispersive property of the grating.

The co-ordinate of the point A and B will be respectively $(x, y, z$ and $x', y', z')$ and thus the distance AP and PB could be re-written as follow:

$$(9) \quad \overline{AP} = \sqrt{(x - w)^2 + (y - k)^2 + (z - l)^2}$$

$$(10) \quad \overline{PB} = \sqrt{(x' - w)^2 + (y' - k)^2 + (z' - l)^2}$$

Now, the co-ordinate x, y and z (as x', y', z') can be re-written as a function of r (distance source-pole of the grating), r' (distance pole of the grating-image) and of the angles α and β , i.e.:

$$(11) \quad x = -r \cdot \cos \alpha$$

$$(12) \quad y = r \cdot \sin \alpha$$

$$(13) \quad x' = r' \cos \beta$$

$$(14) \quad y' = r' \sin \beta$$

$$(15) \quad z' = -z \frac{r'}{r}$$

The last point to know is the relation between k , w and l . Practically it is necessary to know the geometrical equation describing k as a function of w and l . This equation should be written in the following form:

$$(16) \quad k = \sum_{i,j} K_{ij} w^i l^j$$

Of course, this equation is different for the different geometrical shapes. Nevertheless, there is a case, the toroidal, which describe more than 90% of the cases of mirror and gratings (probably 100% of the gratings).

For this case, of a toroidal grating, this relation is:

$$(17) \quad k = \frac{1}{2R} w^2 + \frac{1}{2\rho} l^2 + \frac{1}{4R^2 \rho} w^2 l^2 + \frac{1}{8R^3} w^4 + \frac{1}{8\rho^3} l^4$$

Where R is the major radius of curvature of the toroidal shape and ρ the minor radius of curvature.

With the previous relations (8-15) it is easy to re-write the equation 8 as a polynomial series, still as a function of w and l , i.e.:

$$(18) \quad F = \sum_{i,j} F_{ij} w^i l^j$$

Each term of the equation 18 can be obtained from equation 8 simply by deriving it:

$$(19) \quad F_{i,j} = \frac{1}{(i+j)!} \left[\frac{\partial^{(i+j)} F}{\partial w^i \partial l^j} \right]_{w,l=0}$$

In principle, one must satisfy the following two equations to found the “no aberration” condition for a grating:

$$(20) \quad \frac{\partial F}{\partial w} = 0 \quad ; \quad \frac{\partial F}{\partial l} = 0$$

Nevertheless, practically, this condition is more or less impossible to found for a general grating shape. The operative approach is to set independently to zero as much terms as possible of the equation 18. In this way, even if are not equal to zero, the equations 20 become small enough. The word «enough» depends on a lot of parameter, the shape, the divergence of the incoming radiation, the illuminated area of the grating and so on. For this reason is important to know the influence of each term to final image shape, to set to zero the most important ones and minimise the others. For instance, the term F_{00} (which can be set at any value because his derivative respect w and l is always zero) is simply the amount of path travelled ($r+r'$). F_{10} take into account the dispersive property of the grating, i.e. the equation 6.

The high order terms, vice-versa, describe the focal property as the residual aberration introduced by the optical component.

Let us consider, for instance, the terms F_{20} . This term is the second derivative of the optical path function F , i.e. from equation 19:

$$(21) \quad F_{2,0} = \frac{1}{2} \left[\frac{\partial^2 F}{\partial w^2} \right]_{w,l=0}$$

Since the first derivative is zero (as a boundary condition to have diffraction), this term is an indicator of how much the optical path function differs from zero moving out from the ideal working condition, i.e. out from the centre of the grating. If this term is set to zero, this means that every ray, even if it does not hit the grating in its pole, still satisfies the minimum time path (at least in the second order approximation). This is exactly the focal condition of an object, i.e. the main term that contributes to the presence or not of aberration.

The same consideration can be made for the term F_{02} . Nevertheless, since F_{20} describes the focal condition in the “tangential plane” (the plane defined by the outgoing ray and the normal to the grating surface), the term F_{20} describes the focal condition in the orthogonal plane, the sagittal one (described by the outgoing radiation direction and the groove direction (for a grating)).

Let us see the form of these terms, always in the case of a toroidal grating:

$$(22) \quad F_{2,0} = \left(\frac{\cos^2 \alpha}{r} - \frac{\cos \alpha}{R} \right) + \left(\frac{\cos^2 \beta}{r'} - \frac{\cos \beta}{R} \right)$$

$$(23) \quad F_{0,2} = \frac{1}{r} + \frac{1}{r'} - \frac{\cos \alpha - \cos \beta}{\rho}$$

The further terms will describe the residual (or absence of) aberrations. Of course, the higher the order of the aberration, the lower is the influence of this on the final image. So, for practical reasons, only the term F_{30} will be considered.

$$(24) \quad F_{3,0} = \left(\frac{\cos^2 \alpha}{r} - \frac{\cos \alpha}{R} \right) \frac{\sin \alpha}{r} + \left(\frac{\cos^2 \beta}{r'} - \frac{\cos \beta}{R} \right) \frac{\sin \beta}{r'}$$

Let us now see how we can estimate the effect of these terms in the final image. As explained above, the optical path function describes the optical characteristics of the final image. So, with the knowledge of the terms $F_{i,j}$, one can write the optical path function as a function of w and l , when w and l are, this time, the half dimension of the photon spot on the grating surface. This will give an estimation of the contribution at the final image of the most distant rays from the pole of the grating, i.e. the rays that mostly contribute to the final imperfection of the image. Therefore,

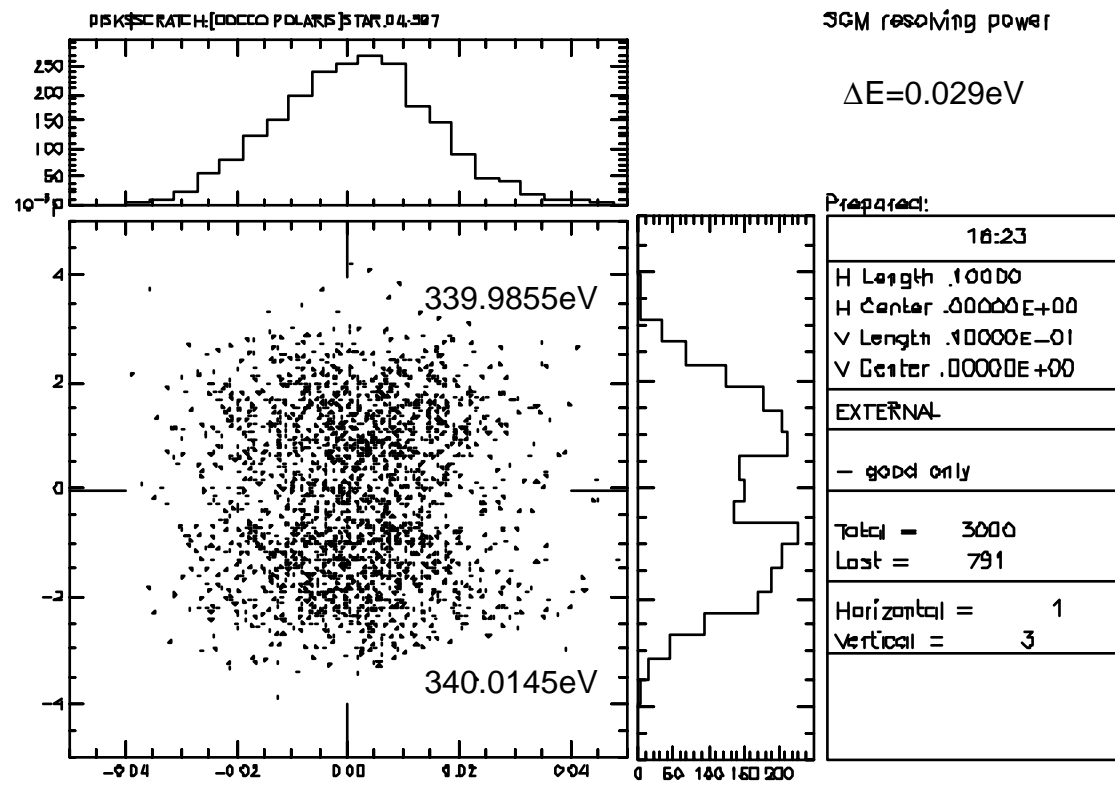
$$(25) \quad \left[\frac{\partial F}{\partial w} \right]_{w=l=0} \cdot W = \frac{3}{2} W^3 F_{30} + \dots$$

will give an idea of the enlargement of the final image due to the F_{30} contribution. The aberration due to this term is called “primary coma”. Typically, it is quite difficult or impossible to set to zero the term F_{30} . Therefore, one must try to minimise it considering that the equations 6 and 22 must be absolutely set to zero. Nevertheless, at the end, to have a more evident (and precise) view of the effect of the residual slope errors, ray tracing is the ideal solution.

Let us see now which information we can obtain. Other than the shape of the final image, another important information could be the number of rays lost or, alternatively, the dimension of the optics required. In fact, one

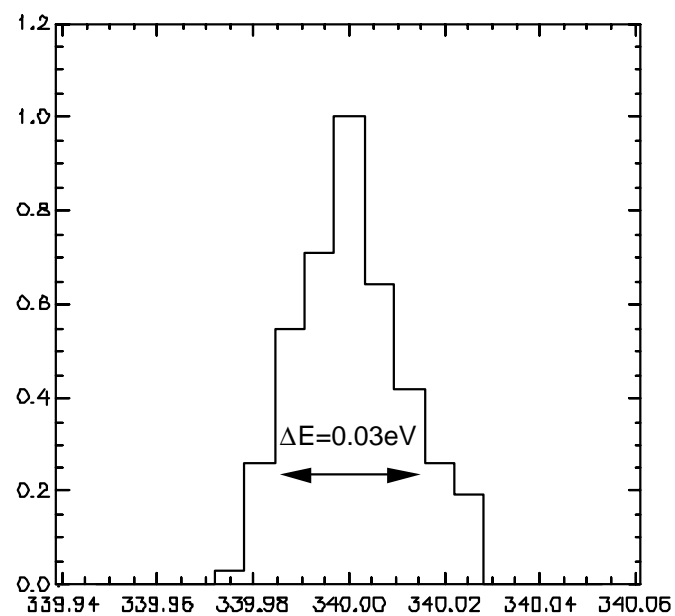
can also have a look at the spot on the mirror surface. If one want to have a particular divergence accepted by the beamline, should have the optics big enough to accept it. Very important is also the resolving power of a beamline. There is different method to estimate it. Let us consider two.

In the first case, one can define a source with an energy distribution made by two single lines. The source will pass the optics, (mirrors and the grating) and arrive in the plane where there will be the exit slit. Evidently the two line are *resolved* when are visible and the resolving power will be defined by the energy separation between the two lines, i.e. as in the following picture:



In this case, the resolving power will be 12000 ($340/0.029$) with an exit slit of $20 \mu\text{m}$ (the separation between centre of the two image, i.e. the dimension of the monochromatic spot).

A different approach can be adopted introducing a real exit slit. The source now should be defined as a continuous energy distribution. In particular, one should define an energy interval great enough to have an



energy distribution well defined after the exit slit, but small enough to do not loose too much ray in the slits. One should now be able to plot the energy distribution after the slit and the result, for the same system above is:

Another information that one can obtain is the effect of the slope errors on the focal property of an element. One can introduce the slope errors in one or more optics and compare the result with the ideal case. Alternatively, one can simulate different mirror shape to found the best solution for his purpose.

Two examples

1) Demagnification with a single mirror

In the first example, let us consider the case of the demagnification of a square source ($50 \times 50 \mu\text{m}^2$). We will use a single mirror, focusing only in the vertical direction. There are numerous possible choices. We will limit at the cases of spherical, cylindrical and elliptical mirror.

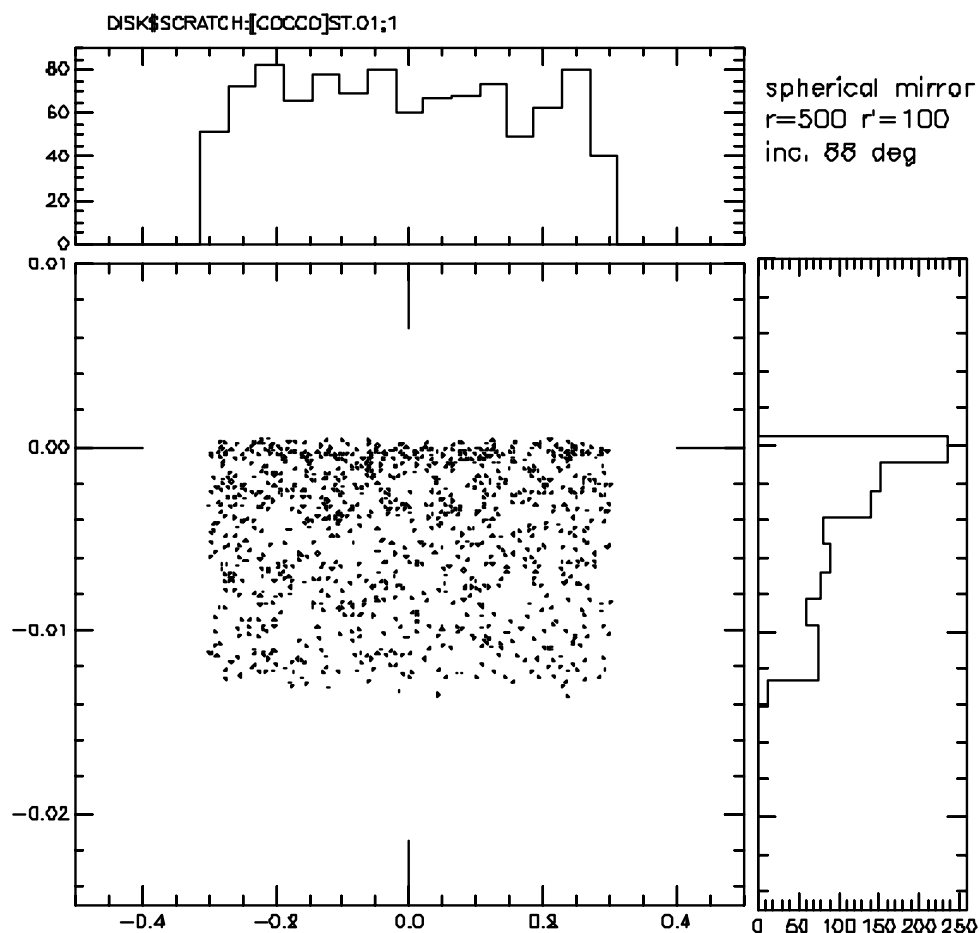
The divergence of the source is 0.5×0.5 mrad. This is a typical value for a synchrotron radiation beamline. The idea is to create a $10 \mu\text{m}$ vertical dimension spot. Another constrain is the incidence angle. Above 2° grazing incidence (88° normal) the reflectivity drop down rapidly. Therefore, 2° will be our choice.

The Program used is SHADOW, later described. In the first case, the mirror is spherical; the radius (that can be calculated by the program) is defined by the equation

$$(26) \quad \left(\frac{1}{r} + \frac{1}{r'} \right) \frac{\cos \vartheta}{2} = \frac{1}{R}$$

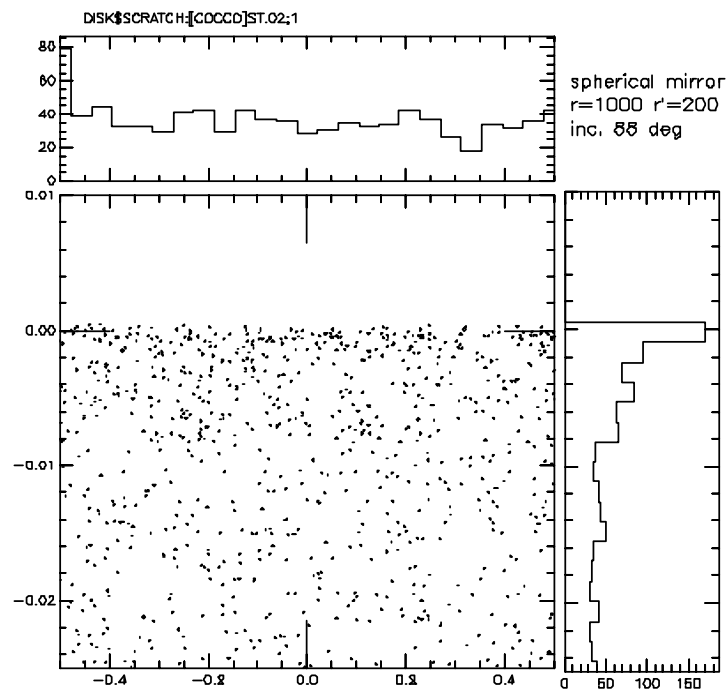
Where the angle θ is respect the normal to the surface.

In this case $r=500\text{cm}$, $r'=100\text{cm}$ and $R=4775\text{cm}$. A demagnification 5:1 should give us a $10\mu\text{m}$ vertical dimension, but the result is the following:



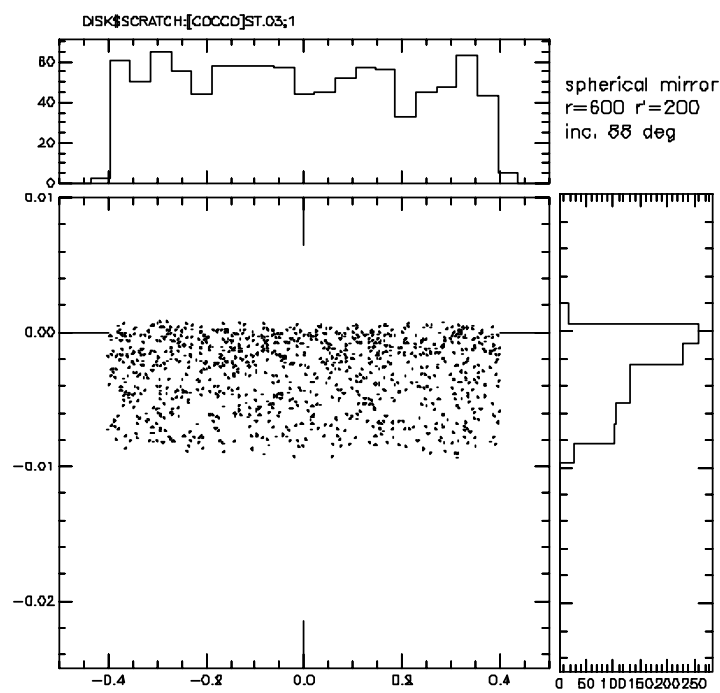
The units are cm. As can be seen, the final spot is not a stripe of 10 μm but has a big tail due to a lot of aberration, induced by the combination of the strong demagnification and the high divergence of the beam.

The second case is identical to the first except for the distances that are doubled, i.e. $r=1000\text{cm}$ $r'=200\text{cm}$. The final image is:

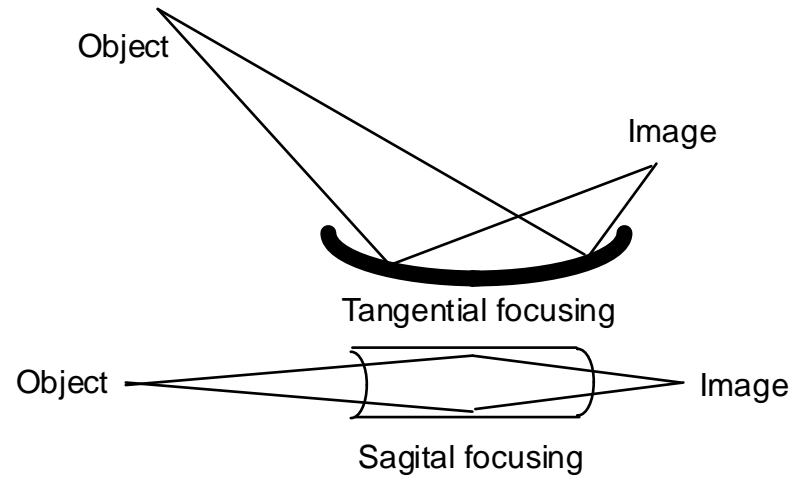


The width of the graph is always the same. It is evident that there is an enlargement of the tail. This is due to the increasing of the lightened part of the mirror, i.e. the parameter W of the aberration theory. As explained the aberration is proportional to the same power of W and this explain the enlargement of the image aberration.

The third case is no more a 5:1 demagnification but a 3:1. Even in this case we will use a spherical mirror but with $r=600$, $r'=200$. The expected image height is about 15 μm , but, considering the reduced demagnification, i.e. the reduction of aberrations, the result is better than the first case. The spot become:



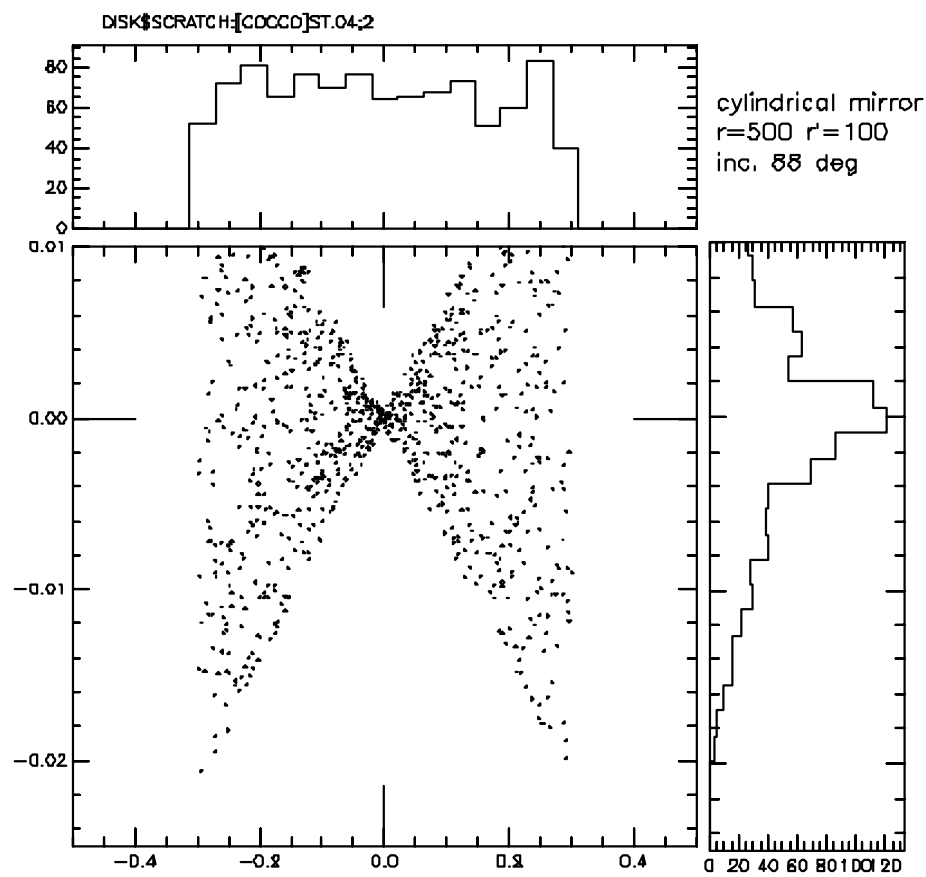
Up to now, the mirror(s) was placed with the reflecting surface faced up, i.e. in tangential focusing mode (see next picture). Now, let us consider a sagittal cylinder. This is a cylinder with the reflecting surface face left (or right) focusing still in the vertical direction (see figure).



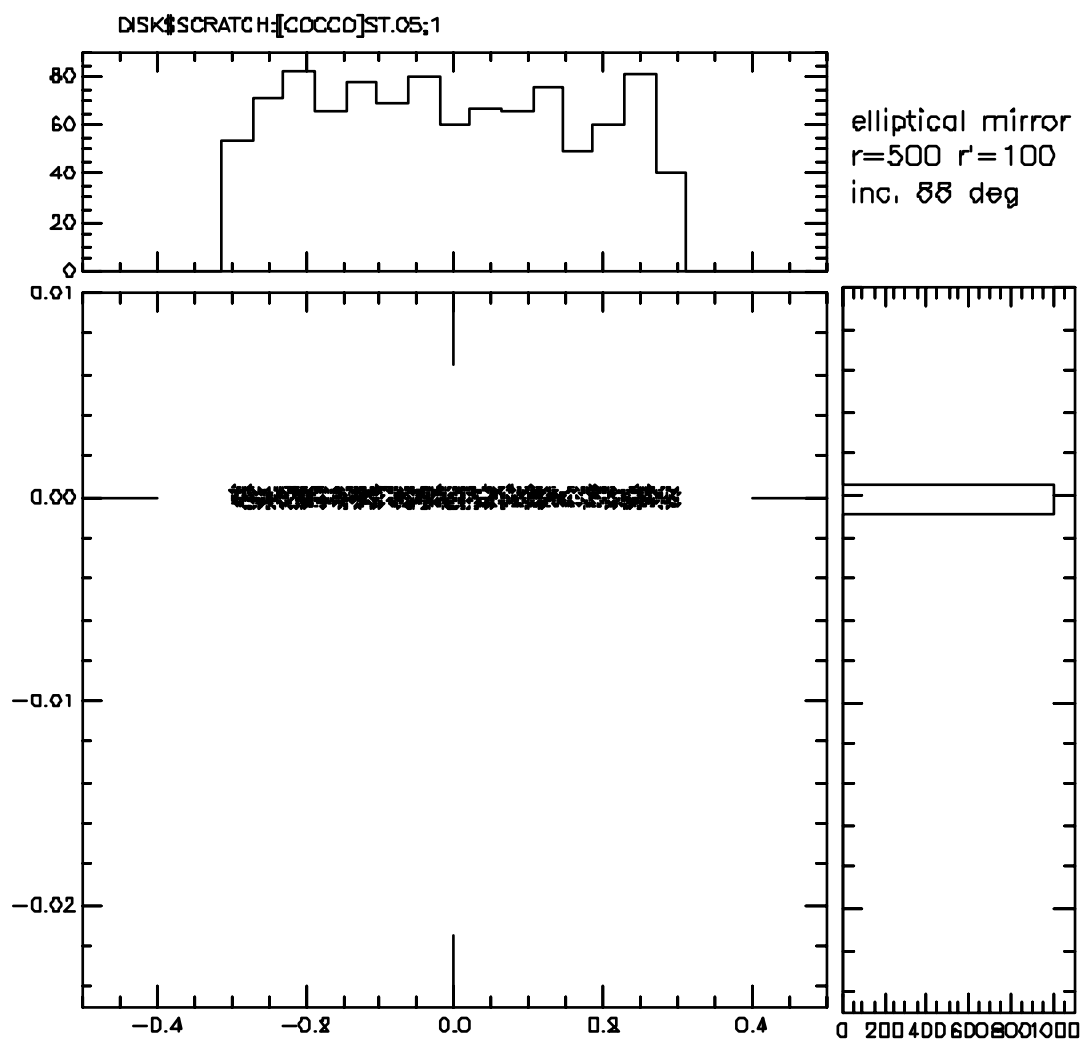
From the geometrical theory of aberration it come out that there is an enlargement of the final spot dimension. Always considering an entrance arm $r=500$ cm and $r'=100$, with the radius of curvature ρ calculated (from eq. 23) as:

$$(27) \quad \left(\frac{1}{r} + \frac{1}{r'}\right) \frac{1}{2 \cos \vartheta} = \frac{1}{\rho}$$

The final image will be:



The final case is the case of a plane-elliptical mirror. This is a mirror with elliptical shape in the tangential direction and plane in the sagittal. This still focus in tangential direction and the great advantage is the absence of aberration due to the width of the spot. This is because the ellipsoid always focuses a point in a point even if the divergence is quite large. Of course, this is true if the aberrations are not considered. Without aberrations the final image is:



Therefore, in principle, the elliptical shape is the best choice.

2) Spherical grating

This second example will introduce the use of the program SHADOW. We will consider a spherical grating again working in tangential mode. The grating will have a radius of curvature $R=2000$ cm. The groove density is 6000 l/cm, the distance source grating is 400 cm and the distance grating-image (grating-exit slit) is 150 cm.

By satisfying eq. 22, i.e. $F_{20}=0$ a table of energy and angle of the grating is:

Photon energy (eV)	Incident angle	Diffraction angle
500	83.04834	83.79230
300	82.63818	83.84556
100	80.94452	84.25400
50	79.01137	85.23461

In this case, we are working with the external orders, for SHADOW the positives.

Before creating the grating, we must create the source. Both source and optical elements must be create in window mode.

The source must be described carefully, trying to avoid forgetting some parameters. We will simulate a source of $240 \times 10 \mu\text{m}^2$ (see the first of the 3 figures appended to this notes).

The energy distribution should be a multi-line or continuous introducing an exit slit to define the resolution. Once al the parameters are defined, we can define the optical element, the grating.

We use now the photon energy of 100 eV. Even in this case, the window mode is quite easy to be used. One must insert the right parameter, in the main menu and in the sub menu. Once that everything is defined, the program should trace the rays (processing the data) and to visualise the results is possible to use both the internal plot system (pressing on the button plot) or using the post-processor (under the menu tools).

Briefly, SHADOW defines as **STAR.XX** the image of the element XX (01,02 etc...). The image in the mirror surface is defined as: **MIRR.XX** and, if a screen is defined, the image on the screen is **SCREEN.XXYY** where XX is related to the optical element on which the screen is appended and YY is the number of the screen. Vice-versa the source is recorded in the file **BEGIN.DAT**.

The post-processors are sub-programs useful to analyse the data. They work in prompt mode; i.e. an answer is expected for any question the program formulates. In particular, **histo1** generate a histogram to see the mono-dimensional distribution of photons (in space or energy). Remember that the column for SHADOW are defined as follow:

1	X
2	Y
3	Z
4	X'
5	Y'
6	Z'
11	Energy

In addition, the reference system is the following:

