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SCHOOL ON THE USE OF SYNCHROTRON RADIATION IN SCIENCE AND TECHNOLOGY:
"John Fuggle Memorial"

3 November - 5 December 1997

Miramare - Trieste, Italy

Introduction to ray tracing

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Introduction to ray tracing

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The only way to estimate if a beamline will work or not is the ray tracing procedure. Some very few simple optical principle are involved in a ray tracing program, reflection, diffraction and, sometimes, absorption. The simple basic idea is to follow one by one the photons imagined as straight line. One should modelling the source, the optical surfaces, introduce the diffraction principles and the goal is reached.

In this way, one can simulate a real beamline, introducing errors on the surface, slits, misalignment, different solutions and have a look at the performances of his design.

For this reason, a lot of people write his own program, usually to watch at particularly problems not common to the other programs. Practically, regarding the synchrotron radiation beamline, there is two main program quite well diffused in the world, RAY and SHADOW. We will use the second one, of which there is copy of a part of the manual added at this notes.

Let's summarise now what is the knowledge necessary to run a ray-tracing program and which information we can have from it.

First of all we need to know the characteristic of our sources. The programs are able to simulate point source, rectangular sources, gausssian (both in angular and spatial), monochromatic, polychromatic (some different line of energy), continuos energy range, and sometimes also to simulate a real synchrotron source, a bending magnet, an undulator or a wiggler. If this option is not available, one can use, for example in the undulator case, a gaussian shape, defined by the equation:

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

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

where σ_x is the nominal electron beam size in the horizontal direction (Elettra case is 0.24 mm), σ_y is the nominal electron beam size in the vertical direction (Elettra case is 0.043

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), and

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

with L=the undulator total length and λ is the selected photon wavelength. (see figure UNDULATOR/GAUSSIAN SOURCE)

The energy distribution of the source is fundamental to understand the behaviour of the beamline. As a first step is necessary to simulate a perfect monochromatic source. In this way one have the exact idea of what happen at the radiation selected.

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. For this reason, a real beamline and thus also a simulated one, should have a pin-hole some meter after the source to adsorb all the radiation out of a specified divergence (typical divergence accepted by a beamline is less then half mrad.

Let's now speak about the mirrors. Every program has a collection of shapes available. Typical shapes are Plane, Spherical, Elliptical, Cylindrical, Toroidal, Parabolic, and so on. Every of this shape have to be defined (by the programmer) with his geometrical equation, typically very complicated (see the figure SHAPE DEFINITION). Now, we have our ray, everyone with his divergence and position in the space. We should trace it up to meet the mirror surface. At this position we should calculate the normal at the surface, and reflect the ray respect it. Very simple. In this way we do not use standard formulas or approximations, but simply we go to see where every ray has gone. Every aberration introduced by the optics, every error of focus will be emphasised by the final image obtained. For instance, one can see which is the difference in the focus obtained with a toroidal mirror respect an elliptical one, or a Kirkpatrick Baez configuration (2 spherical mirrors) at equal demagnification ratio (see figure DEMAGNIFICATION COMPARISON).

At the end, one can obtain information useful to design the beamline, but one should know the optical principles to have a reasonable starting point.

A particular care must be taken in the dispersive object. We will consider only crystal and gratings which working equation are:

$2d\cos\theta = n\lambda$ for the crystal, and

$$d(\sin\alpha - \sin\beta) = n\lambda$$ for the grating (see figure DISPERSIVE OBJECT)

Nevertheless, the dispersive elements introduce a great distortion in the incoming radiation, change the divergence, modify the optical path and so on. It's quite impossible to reach a real result from a ray tracing program, without know the exact behaviour of every object. In particular, for the grating case, one should apply the Fermat's principle. This can be expressed by the sentence that the light travel the space between two point in the minimum possible time. Mathematically speaking, it mean that we should calculate every the equation which describe the optical path and minimise the time to travel it (see figure GEOMETRICAL ABERRATION THEORY). Now is not important to know the exact meaning of each terms. Let's only know that real important is the equation F_{20} which describe the focus condition of a grating. This equation, should be solved a priory to have a good starting point.

The ray tracing program take in to account a dispersive element, introducing a phase shift in the optical path. The dispersion is made only in the plane perpendicular to the groove, while in the other direction there is a simply reflection. Thus, the program divide the angular component of the incoming radiation, diffract the one perpendicular to the groove and reflect that one parallel to the groove (the third component is obtained as a consequence of the firsts two) and recombine those after the grating.

Let's see now which information we can obtain.

First of all we can see which is the image of our source in any part of the beamline. We can introduce screen, slit and so on and follow, step by step the shape of the radiation. In this way one can see if his optics focus well or not, if the spot size is the desired one or not and so on.

Another important information is the number of ray 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's consider two.

In the first case one can define a source with an energy distribution made by two single line. The source will pass the optics, the grating and arrive in the plane where there will be the exit slit. One know that the two line are *resolved* when are visible distinguished (see figure RESOLVING POWER) and the resolving power will be defined by the energy separation between the two lines.

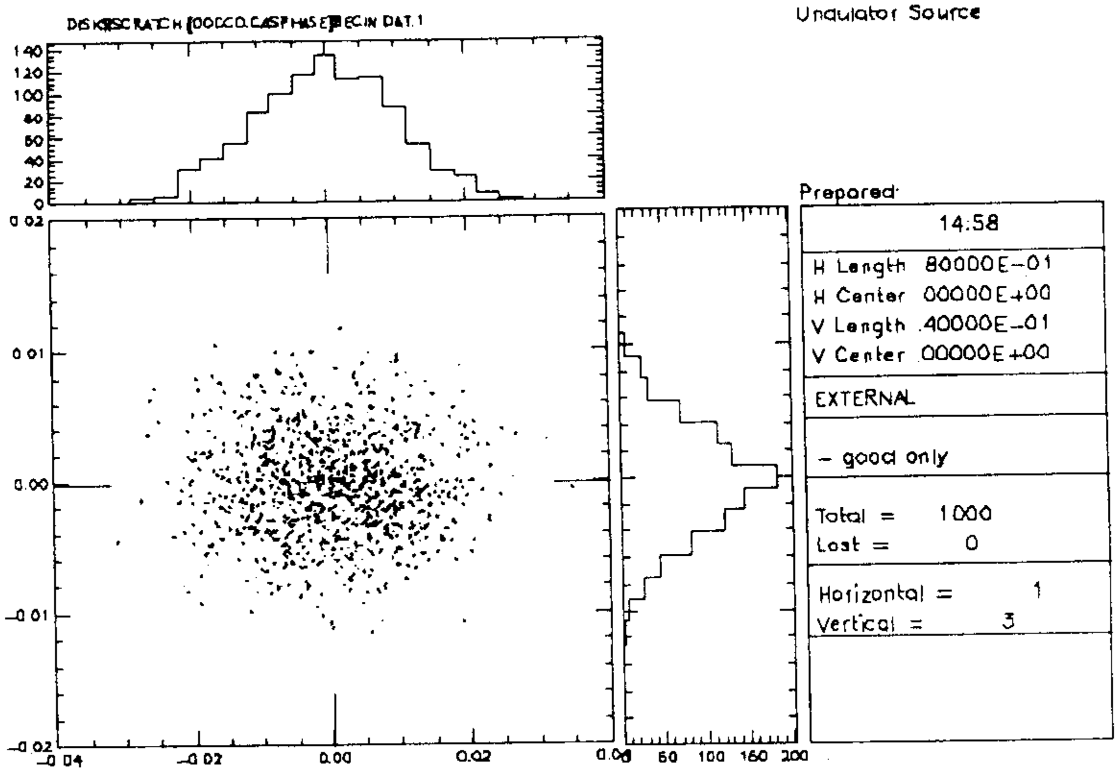
Much more faster is to introduce a real exit slit and define the source as a continuos energy distribution. In particular one should define an energy interval great enough to permit to have a energy distribution well defined after the exit slit, but small enough to do not loose too much ray in the slits (an energy distribution the is 4 times greater than the expected resolving power is a good choice). One run the ray-tracing program and analyse the energy distribution after the exit slit (see figure RESOLVING POWER). All the good programs has a tool to permit it (in the case of SHADOW the subroutine is called HISTO1).

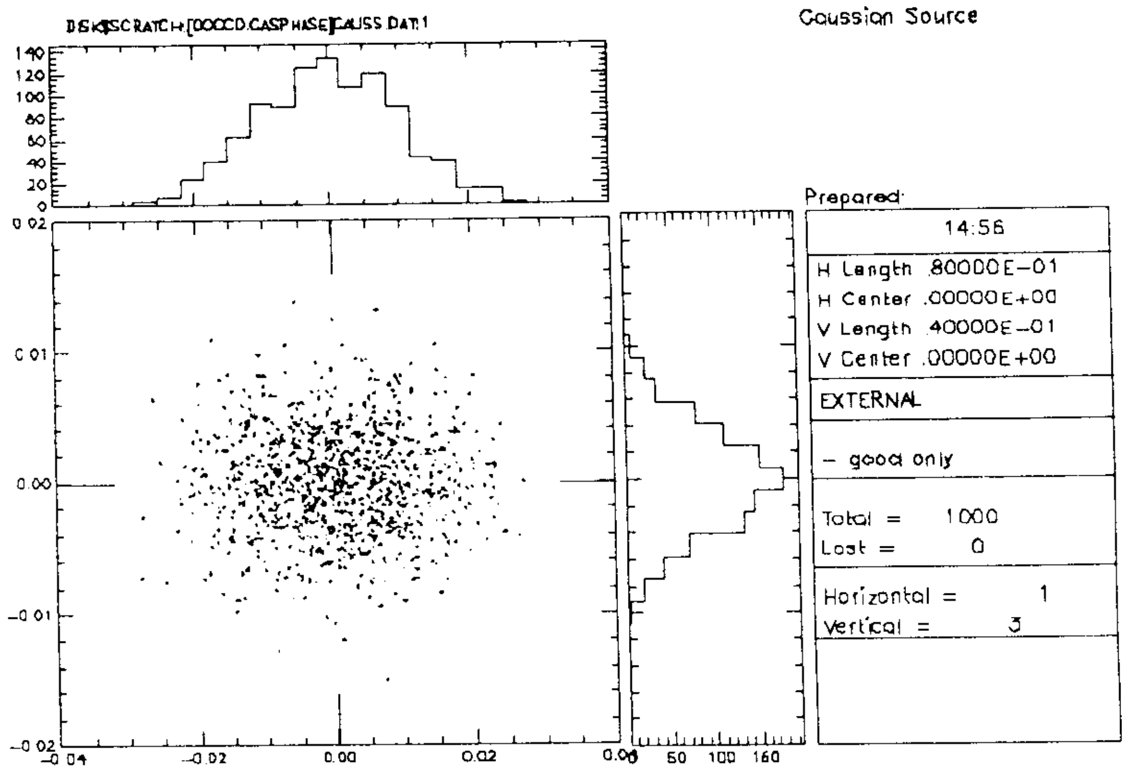
Another information that one can obtain is the effect of the slope errors on the focal property. One can introduce the slope errors in one or more optics and compare the result with the perfect case. Another source of error can be the shape error of the optics. Changing a little bit the radius of a sphere, what is the results? And any other source of error can be estimated.

At this point we can start to use the program SHADOW, written by F. Cerrina at the Madison University.

After the previous mentioned figure, you will find a copy of part of the instruction manual of SHADOW which explain more precisely in which way work SHADOW and how extract information from it.

UNDULATOR AND GAUSSIAN SOURCE

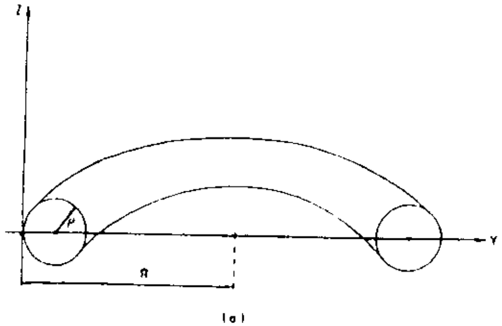




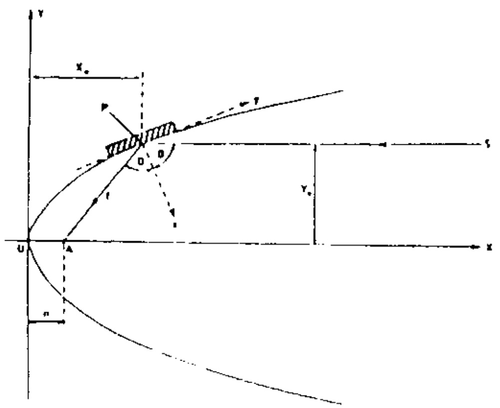
$\Sigma x=(\sigma x^2+\sigma R^2)^{1/2}$ $\Sigma y=(\sigma y^2+\sigma R^2)^{1/2}$ $\sigma R = 0.15\,(\lambda L)^{1/2}$

$\Sigma' x=(\sigma' x^2+\sigma' R^2)^{1/2}$ $\Sigma' y=(\sigma' y^2+\sigma' R^2)^{1/2}$ $\sigma' R = 1.30\,(\lambda/L)^{1/2}$

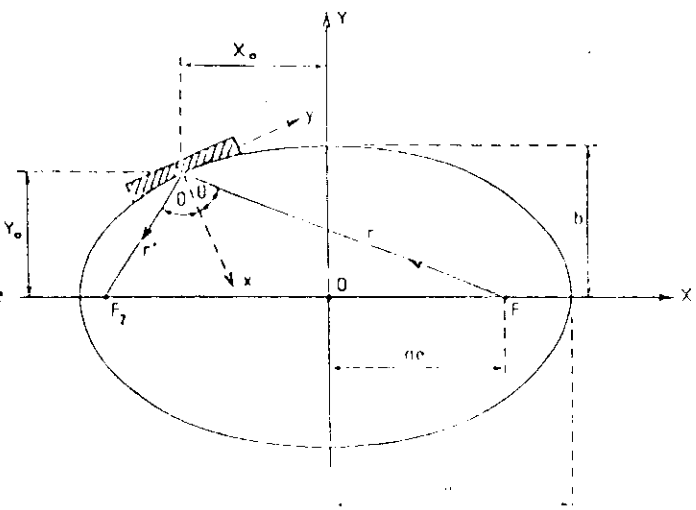
urface defined as: $\xi = \sum_{i=o}^{\infty} \sum_{j=o}^{\infty} a_{ij} w^i \mu^j$ w and l are the coordinate in the x and y direction



Toroid



Parabola



Ellipse

Toroid Note: For a sphere, ρ = R

$a_{02} = \frac{1}{2\rho}$ $a_{20} = \frac{1}{2R}$ $a_{22} = \frac{1}{4R^2\rho}$

$a_{40} = \frac{1}{8R^3}$ $a_{04} = \frac{1}{8\rho^3}$.

Ellipsoid Note: $f = \left[\frac{1}{r} + \frac{1}{r'}\right]^{-1}$

$a_{02} = \frac{1}{4f\cos\theta}$; $a_{20} = \frac{\cos\theta}{4f}$; $a_{04} = \frac{b^2}{64f^3\cos^3\theta}\left[\frac{\sin^2\theta}{b^2} + \frac{1}{a^2}\right]$

$a_{12} = \frac{\tan\theta(e^2 - \sin^2\theta)^{1/2}}{8f^2 \cos\theta}$; $a_{30} = \frac{\sin\theta}{8f^2}(e^2 - \sin^2\theta)^{1/}$

$a_{40} = \frac{b^2}{64f^3\cos\theta}\left[\frac{5\sin^2\theta\cos^2\theta}{b^2} - \frac{5\sin^2\theta}{a^2} + \frac{1}{a^2}\right]$

$a_{22} = \frac{\sin^2\theta}{16f^3\cos^3\theta}\left[\frac{3}{2}\cos^2\theta - \frac{b^2}{a^2}\left(1 - \frac{\cos^2\theta}{2}\right)\right]$

Paraboloid

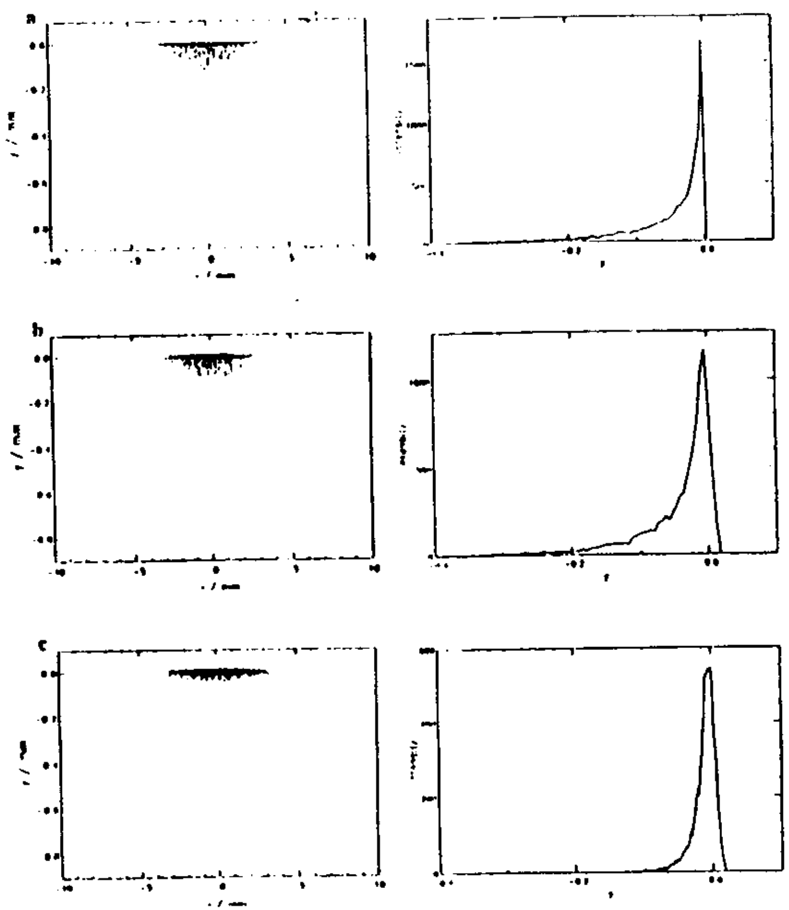
$a_{02} = \frac{1}{4f\cos\theta}$; $a_{20} = \frac{\cos\theta}{4f}$; $a_{04} = \frac{\sin^2\theta}{64f^3\cos^3\theta}$

$a_{12} = -\frac{\tan\theta}{8f^2}$; $a_{30} = -\frac{\sin\theta\cos\theta}{8f^2}$

$a_{[illegible]} = \frac{5\cos\theta\sin^2\theta}{f^3}$; $a_{22} = \frac{3\sin^2\theta}{32\cos\theta f^3}$

[illegible]

$R = \infty$; $\rho = \infty$; $a_{ij} \equiv 0$!



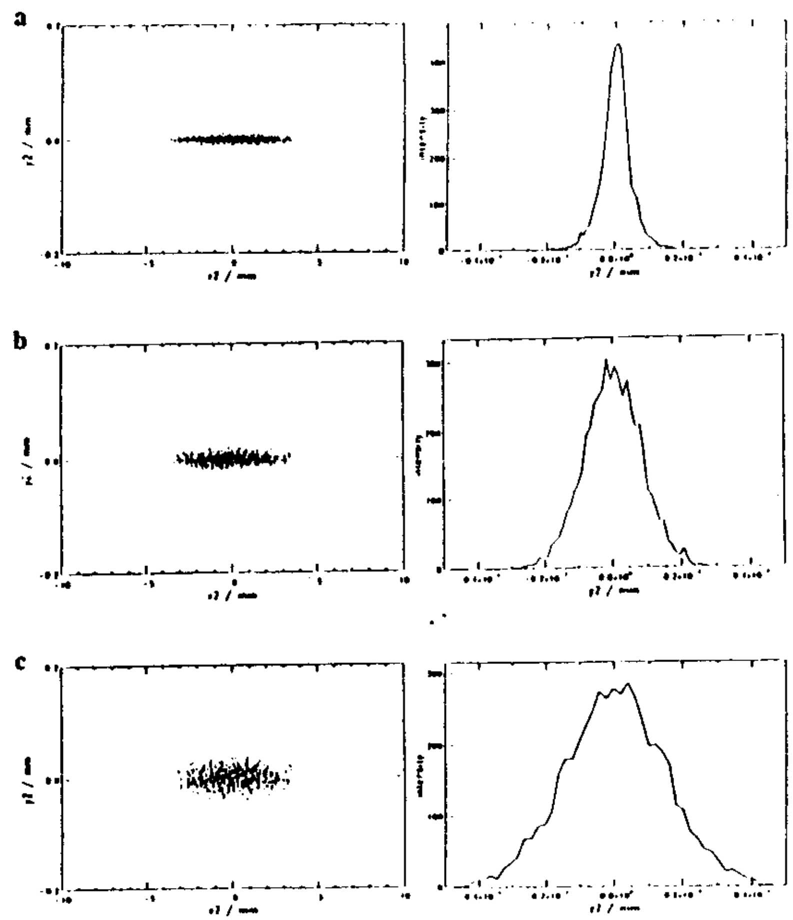
Focussing Characteristics of a Spherical Mirror

To the left the spot diagram. To the right the integrated vertical profile. Angle of incidence $\theta = 87.5°$.

a) Demagnification = 24, σ_{TE} = 0, σ'_{VSR} = 80 µrad

b) Demagnification = 24, σ_{TE} = 1 sec, σ'_{VSR} = 80 µrad

c)) Demagnification = 24, σ_{TE} = 1 sec, σ'_{VSR} = 40 µrad



Focussing Characteristics of a Plane Elliptical Mirror

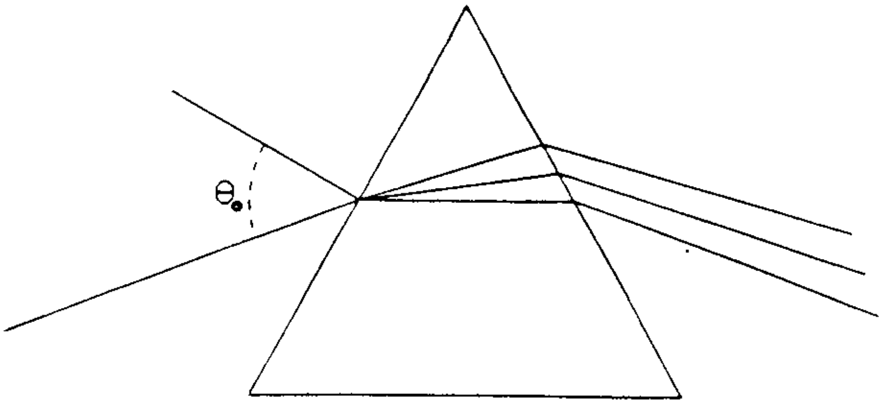
To the left the spot diagram. To the right the integrated vertical profile. Angle of incidence $\theta = 87.5°$.

a) Demagnification = 24, σ_{TE} = 0, σ'_{VSR} = 80 µrad

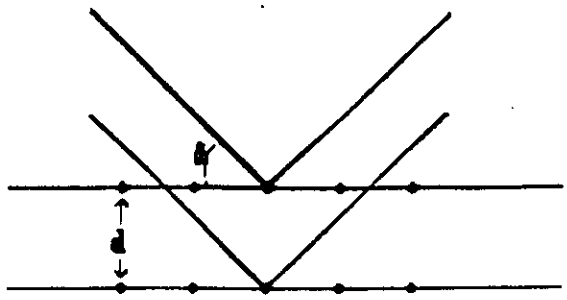
b) Demagnification = 24, σ_{TE} 1 sec, σ'_{VSR} = 80 µrad

c) Demagnification = 24, σ_{TE} = 2 sec, σ'_{VSR} = 80 µrad

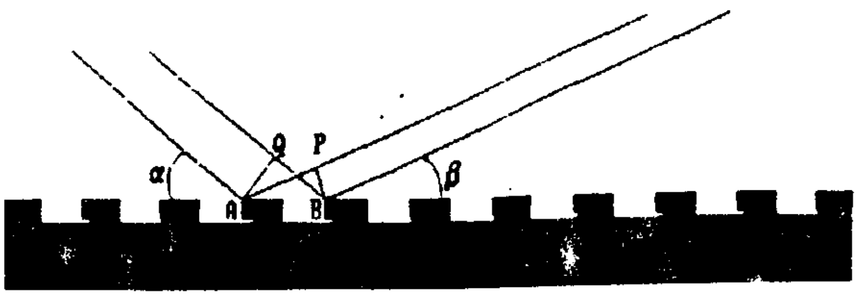
DISPERSIVE OBJECTS



$$\frac{sen\theta_1}{sen\theta_0} = \frac{n_0}{n_1}$$ Visible

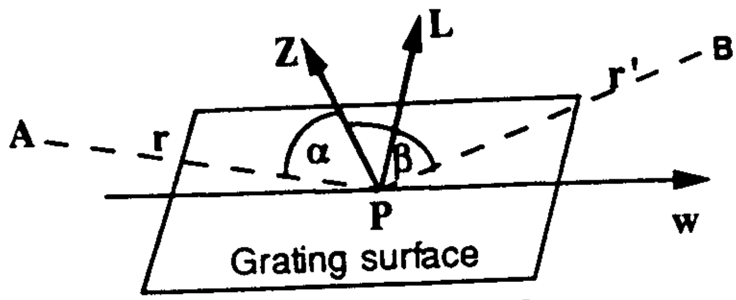


$$2sen\theta = \frac{n\lambda}{d}$$ Hard X-ray



$$d\left(cos\beta - cos\alpha\right) =$$ Soft X-ray

Geometrical Aberation Theory



$\beta>0$ if same side of α

Optical path function: $F=AP+PB+Nk\lambda$

Fermats Principle $\delta F/\delta w=0$ meridional focus
$\delta F/\delta l=0$ sagital focus

Re-writing the optical path as a function of w and l one obtain:

$$F=F_{000}+wF_{100}+1/2w^2F_{200}+1/2l^2F_{020}+1/2w^3F_{300}$$
$$+1/2w^2lF_{120}+1/8w^4F_{400}+\ldots\ldots$$

or, more precisely:

$F_{000}=r+r'$

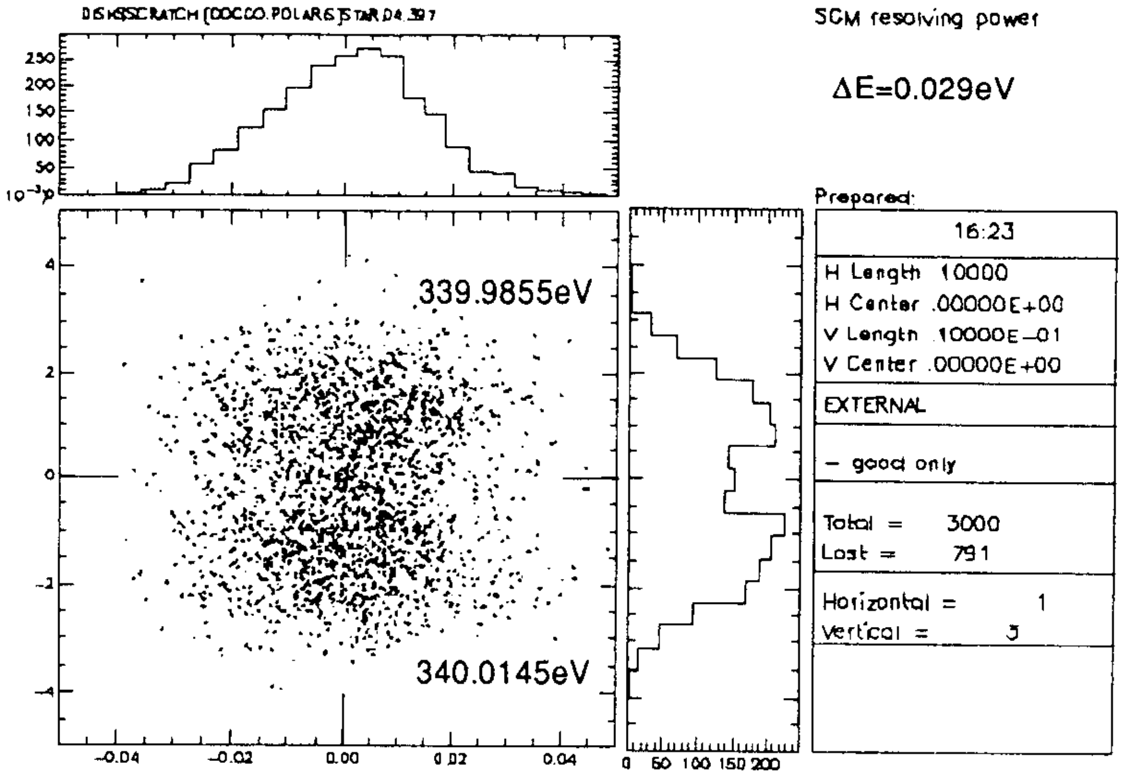
$F_{100}=Nk\lambda-(\sin(\alpha)+\sin(\beta))$ Grating equation

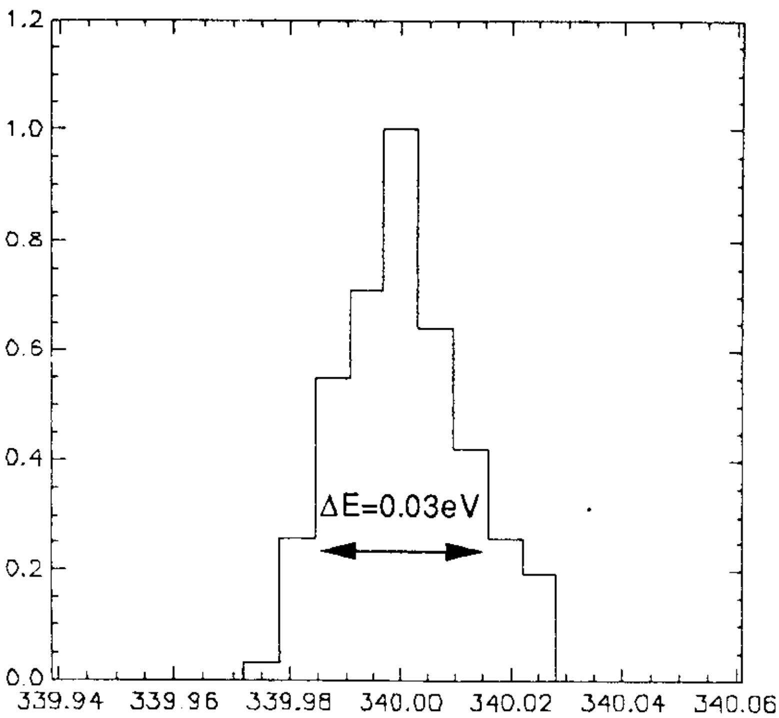
$F_{200}=\cos^2(\alpha)/r+\cos^2(\beta)/r'-2a_{20}(\cos(\alpha)+\cos(\beta))$ Meridional focus

$F_{020}=1/r+1/r'-2a_{02}(\cos(\alpha)+\cos(\beta))$ Sagital focus

F_{300} Primary Coma F_{120} Astigmatic Coma

RESOLVING POWER





SGM beamline
1200 l/mm
R=70 m
r'=2.4m

Comparison between different methods to evaluate the resolving power

An example of the use of SHADOW

Let's consider the two similar optical system designed in the next page (page 12). Both are single direction focusing element, one sphere, which focus tangentially and a cylinder with his focus in the sagital plane. We, step by step, will create with SHADOW the SOURCE, and then the spherical mirror. After that we will modify the sphere to have the cylinder.

The first step is to know the SHADOW reference system. This is shown in the following figure (page 13). Every time we define an optical element or a source, we have always to refer to his reference system and not to the previous one, except that for the relative orientation of the two surfaces.

Let's start entering the program with the command GO.

We find (page 14) 6 possible choice each explained. We should define the source and so we will write **source**. At this level there is 3 possible choice (menu, prompt and batch). We select **prompt** that correspond to the direct questions mode. After that some question will be appear on the screen. Bolded are the answer we should give it to has a rectangular source with gaussian angular distribution of 1 mrad x 1mrad (up to page 16).

In page 17 we found the output of the program after the source definition. BEGIN that is the file which contain the photon parameter one by one (position, divergence), END which contain the parameter to modify the source and START.00 which is the file to use in MENU and BATCH mode.

At this point we will see the shape of the source. Let's use the program **plotxy** (page 17). Also in this case we have to answer to some question, remembering that the file with the photon position is begin.dat and the reference system. At the end we have the plot of the source in the X-Z plane (page 19).

Let's comeback to the SHADOW program and go to the **trace** level. This level is used to trace the photons into the beamline. We still use the easiest option **prompt**. We also here have to answer to some evident questions, always remembering that the reference system is that of the mirror we are defining (up to page 24). At page 24 there is the actual file created. The news are MIRR.01 which contain the photon spot on the mirror, STAR.01 which contain the spot on the final position (called continuation plane), and the equivalent of the source, with the extension 01 (and so far for the following optical element.

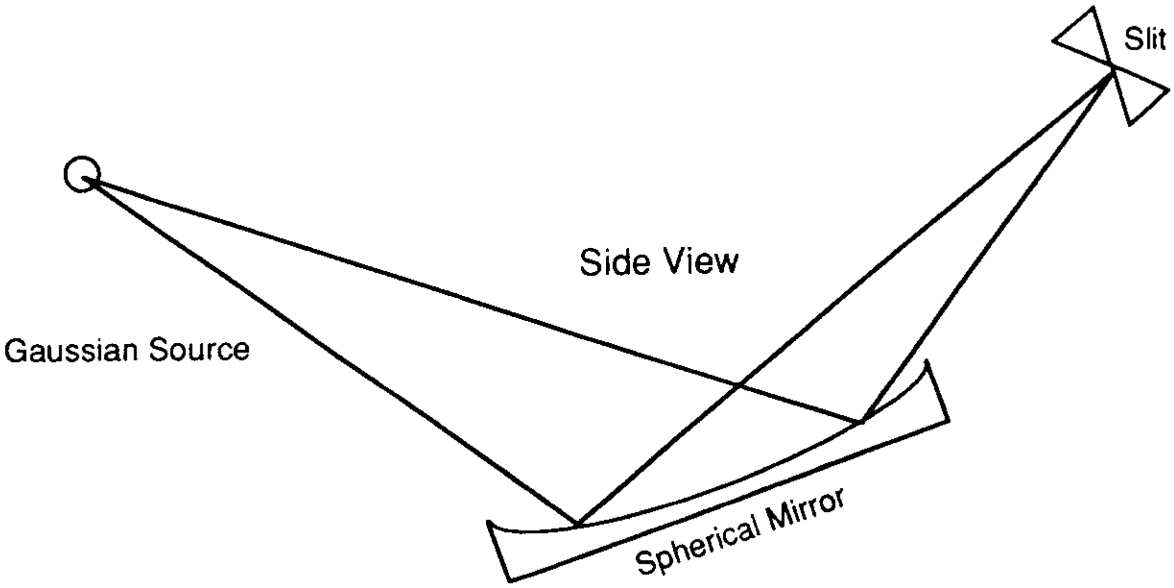
From this page to page 26 we have the command for the program plotxy and the obtained image (page 26). It's evident the tail in the focal spot of the spherical mirror, typical for this kind of large spot on the mirror.

Now we want to see how large is the spot on the mirror. For this reason we run again the program **plotxy** but analysing the file **mirr.01** (page 27-28) and we found a spot of 100x1 mm.

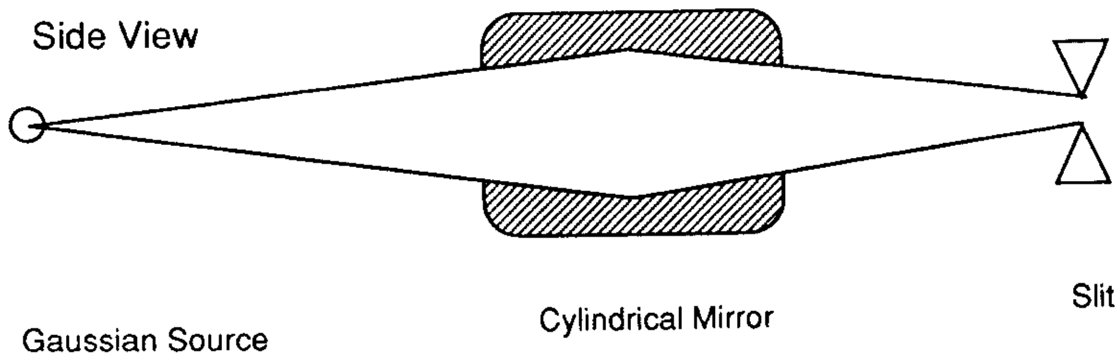
Let's now modify the mirror to define a cylindrical one. We enter the program SHADOW and use the option MENU (page 29). In menu, there is some windows that you can modify accordingly your request. For instance at the bottom of page 29 we have the original window for the spherical mirror and in page 30 the modified version for the cylinder. Some of this option has a sub-menu. For instance at page 30 we enter the sub-menu ***figure*** to define the radius and the orientation of the cylinder, and so on ***for mirror parameter*** and ***external parameters define***.

At page 31, after the menu definition of the element, we use the option **batch** to trace the photons. This option use the already defined mirror parameter to trace the photons along the beamline. As input the START.XX file are requested. Using **plotxy** (page 32) we are able to plot the continuation plane of the cylinder and to have a look of the great difference of the spot of a sphere in tangential focusing position and of a cylinder in the sagital one.

Systems considered

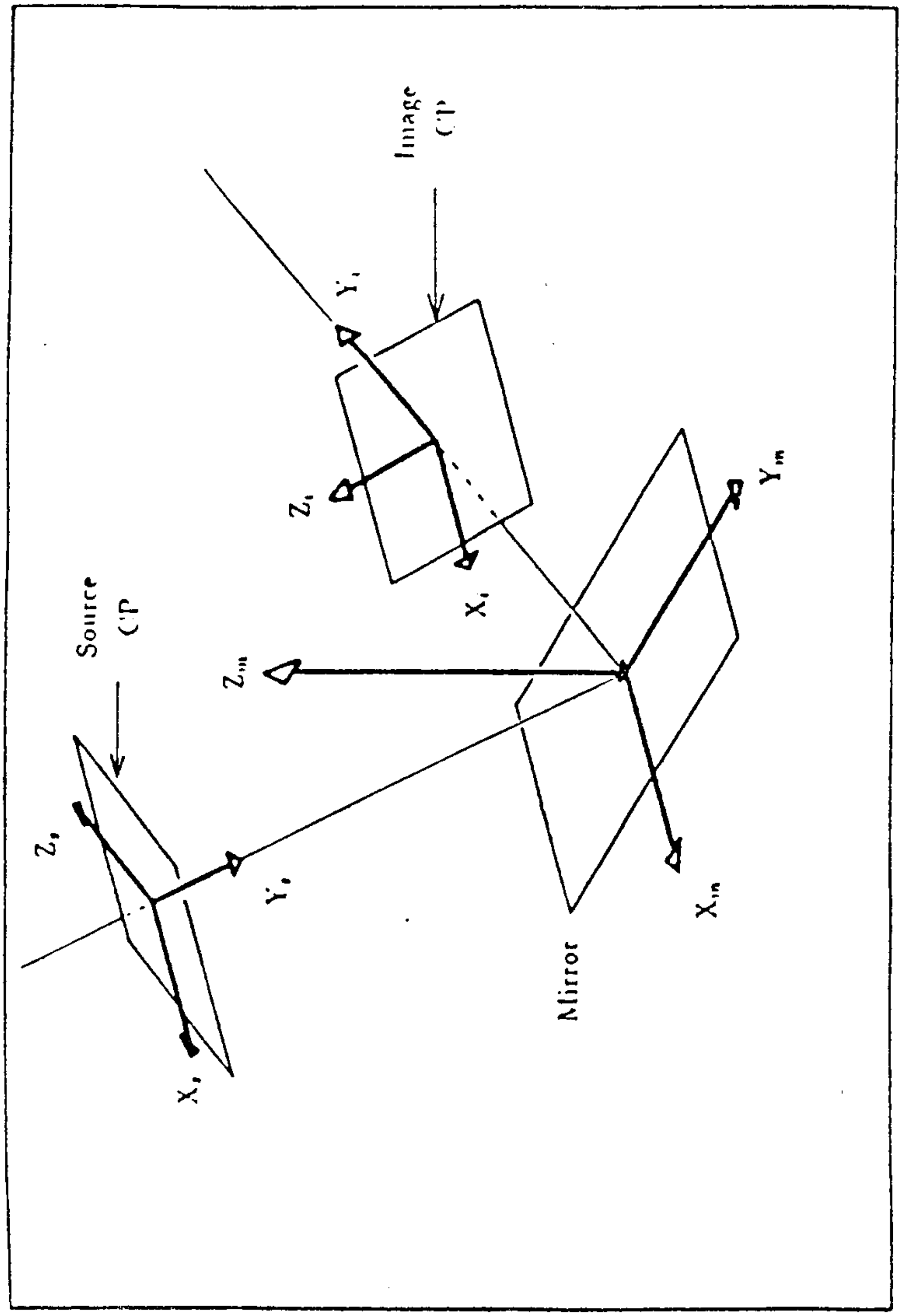


Tangential focussing Spherical Mirror
Source dimension 1x0.5 mm
divergence 1x1 mrad
Distance source mirror 2m
mirror image 0.4m



Sagital focussing Cylindrical Mirror
Source dimension 1x0.5 mm
divergence 1x1 mrad
Distance source mirror 2m
mirror image 0.4m

SHADOW Reference system



DEFINE THE SOURCE **The answer of the operator are BOLDED**

S H A D O W

Commands Available at this level:

HELP More informations on the following commands
SOURCE Generates a source file
TRACE Starts the tracing of an Optical System from a specified source file
MENU Begin the process of defining an optical system.
SETDIR Defines the destination for SHADOW output files.
EXIT Returns to shell

Shadow:: **source**

SOURCE selected. Begin procedure.

This procedure generates a SOURCE for SHADOW.
Mode selected [? <ret> for HELP] ? : **<ret>**
What ? Unrecognized input.
Enter :
MENU for screen-driven menus
PROMPT prompted session
BATCH file-oriented session
This procedure generates a SOURCE for SHADOW.
Mode selected [? <ret> for HELP] ? : **prompt**
Call to INPUT
-------------------------------- S H A D O W ------------------------------
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Defining source :
When prompted for a yes/no answer, you may enter:
for YES answer Y, 1
for NO answer anything else

Do you want a verbose [1] or terse [0] output ?**1**

------------- SOURCE SPECS -----------------
Options available:
Random in BOTH REAL and MOMENTUM space 0
Grid BOTH 1
Grid REAL, random MOMENTUM 2
Random REAL, grid MOMENTUM 3
Ellipses in PHASE space, random around each ellipse 4
Ellipses in PHASE space, grid around each ellipse 5

Source modelling type [0-5] ? **0**

How many rays [1 - 5 000] ? **1000**

Seed [odd, 1000 - 1 000 000] ? **12345**

Do you want to optimize the source ? **n**

--------------------------------- S H A D O W -----------------------------
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Source type : [0] regular source
[1] normal wiggler
[2] undulator
[3] elliptical wiggler

Then ? **0**

--------------------------------- S H A D O W -----------------------------
July 1995 F.Cerrina CXrL/ECE - UW

The source is specified in the laboratory reference frame. The program will the
n rotate the set of
rays in the mirror frame.

Type of source,now.

use (0) for point source
(1) for rectangular s.
(2) for elliptical s.
(3) for gaussian s.

X-Z plane source type [0-3] ? **1**

Source Width [x] ? **.1**

Height [z] ? **.05**

--------------------------------- S H A D O W -----------------------------
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Source depth. The actual source will be centered on the no-depth position. Use
(1) for no depth,
(2) for flat depth distribution,
(3) for gaussian depth distribution,
(4) for a synchrotron source depth distr.

Then ?

Source Depth [1-4] ? **1**

```
O.K., got it so far.
     Source distribution now. We may use
        ( 1 ) for a flat source
        ( 2 )     uniform  s.
        ( 3 )     gaussian  s.
        ( 4 )     synchrotron
        ( 5 )     conical
        ( 6 )     exact synchrotron

Source Angle Distribution [ 1-6 ] ? 3
Horizontal half-divergence [ (+)x, rads ] ? .5e-3
                  [ (-)x, rads ] ? .5e-3
Vertical             [ (+)z, rads ] ? .5e-3
                  [ (-)z, rads ] ? .5e-3
Vertical sigma [ rads ] ? .5e-3
Horizontal          ? .5e-3
Do you want a Photon energy [ Y/N ] ? y
We have these choices :
Single line ......................... 1
Several lines ....................... 2
Uniform source...................... 3
Energy distribution [ 1-3 ] ? 1
Photon Energy [ 0 ] or Angstroms [ 1 ] ? 0
Energy [ eV ] ? 200
```

---------------------------------- S H A D O W ------------------------------
July 1995 F.Cerrina CXrL/ECE - UW

```
Do you want to store the optical paths (OPD) [Y/N] ? y
Do you want to generate the A vectors (electric field) [Y/N]?
Exit from INPUT_SOURCE
Generated        250 rays out of       1000
             500
             750
             1000
Exit from SOURCE
SOURCE => Source has been succesfully generated.

SOURCE procedure completed.

Shadow:: exit

Exit to DCL
```

Directory DISK$SCRATCH:[COCCO.SHADOW]

```
BEGIN.DAT;2        211  29-OCT-1997 11:58:24.80  (RWED,RWED,RE,)
END.00;2             7  29-OCT-1997 11:58:25.28  (RWED,RWED,RE,)
START.00;2           7  29-OCT-1997 11:58:24.38  (RWED,RWED,RE,)
```

Total of 3 files, 225 blocks.

$ plotxy

PLOT> Input file? **begin.dat**
PLOT> Options --- Enter
PLOT> 0 for excluding the losses
PLOT> 1 for including only the losses
PLOT> 2 for including all the rays.
PLOT> Then ? **0**
PLOT> Comment for plot [80 char] ?
******************/******************/
******************/******************/

gaussian source

PLOT> File read OK. Full specifications:
DISK$SCRATCH:[COCCO.SHADOW]BEGIN.DAT;2
Was created : 29-OCT-1997 11:58

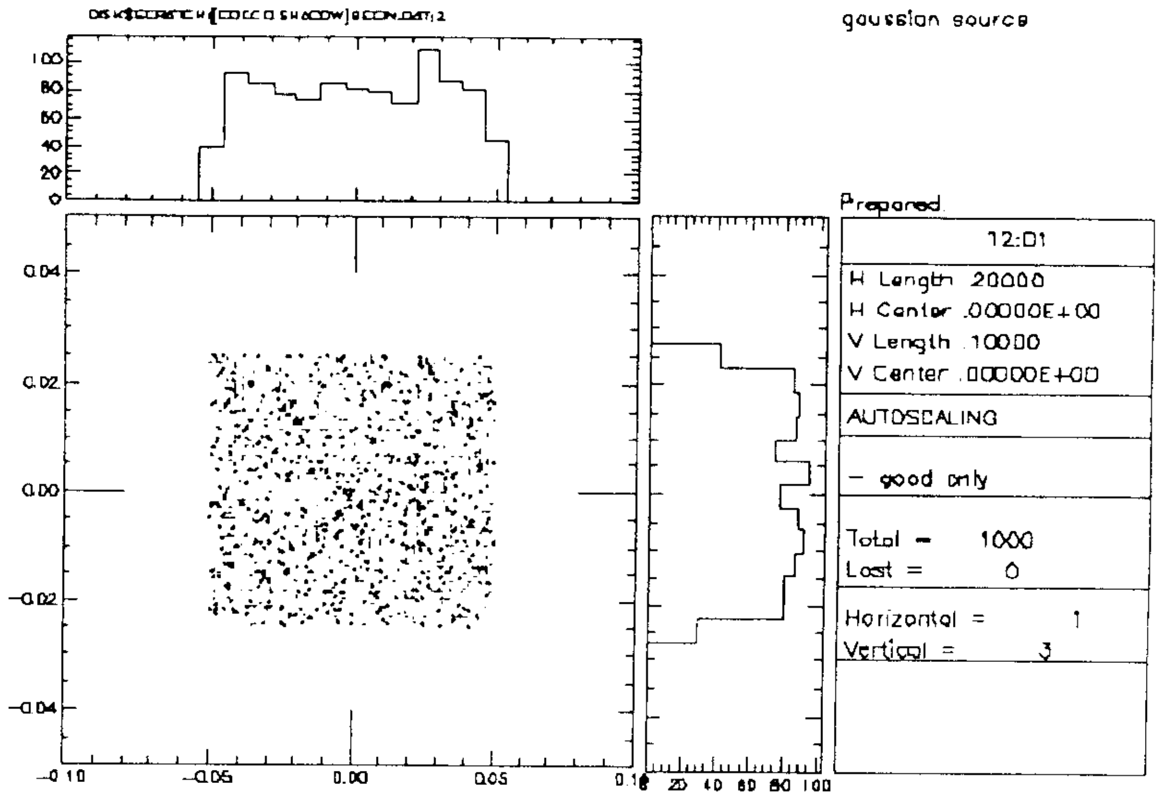
PLOT> Found 1000 good points out of 1000
PLOT> The following columns are defined for each ray :
1) the regular columns [1-12]
2) optical path [13]

Col	Par	Minimum:	Maximum:	Center:	St. Dev.:
1	X	-0.49881E-01	0.49915E-01	0.74016E-03	0.29273E-01
2	Y	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
3	Z	-0.24994E-01	0.24896E-01	0.31451E-03	0.14323E-01
4	X'	-0.16255E-02	0.15863E-02	-0.67975E-06	0.47507E-03
5	Y'	1.0000	1.0000	1.0000	0.24414E-03
6	Z'	-0.15775E-02	0.16320E-02	0.14188E-04	0.49406E-03
11	Photon Energy (eV)	200.00	200.00		
20	Numerical Aperture	0.11363E-04	0.17405E-02		

PLOT> Options. You may plot any two rows from
the above list versus each other.
You may also plot any of them versus the
ray Numerical Aperture. N.A. -- enter 20.

PLOT> Rows to use for plot :
PLOT> for horizontal axis ? **1**
PLOT> for vertical axis ? **3**

```
PLOT> Scaling options. Enter

    0  For automatic scaling
    1  For cartesian scaling
    2  For external limits
PLOT> Then ? 0
PLOT> Plotting options :
    0  For scattered plot
    1  For connected plot
    2  For contour plot
PLOT> Then ? 0
PLOT> Hairline at [ 0,0 ] ?
PLOT> Overlay a mirror/slit ?
PLOT> Ready for histograms. Enter:
   -1      to skip
    0   for same limits as plot
    1            3*stdev
    2            external
PLOT> ?
PLOT> Number of bins for X axis [default = 25] :
PLOT> Number of bins for Y axis [default = 25] :
Display type:
 [ 0 ] Xwindow
 [ 1 ] Tektronix
 [ 2 ] Postscript file
Terminal type: 1
```



DISK$CCRSTCH:[CDCCD.SHADOW]BCON.DAT;2
gaussian source
Prepared
12:01
H Length .20000
H Center .00000E+00
V Length .10000
V Center .00000E+00
AUTOSCALING
– good only
Total = 1000
Lost = 0
Horizontal = 1
Vertical = 3

DEFINE THE SPHERICAL MIRROR

SHADOW

Commands Available at this level:

```
HELP        More informations on the following commands
SOURCE        Generates a source file
TRACE        Starts the tracing of an Optical System from a specified
          source file
MENU        Begin the process of defining an optical system.
SETDIR        Defines the destination for SHADOW output files.
EXIT        Returns to shell
```

Shadow:: **trace**

Ray Tracing Selected. Begin procedure.

Mode selected [? <ret> for HELP] ? : **prompt**
PROMPT selected.
Call to RESET
Exit from RESET
Mode selected is:
PROMPT
Options: to start anew [0]
to restart from a given OE [1]
Then ? **0**
Call to INPUT_OE
---------------------------------- S H A D O W -----------------------------
July 1995 F.Cerrina CXrL/ECE - UW

When prompted for a yes/no answer, you may enter:
for YES answer Y, **1**
for NO answer anything else

Defining Optical Element: **1**
Continue ? [^Z or %EXIT to terminate OS]

Do you want a verbose [1] or terse [0] output ?**1**
You may save disk space by not writing out the
intermediate STAR or MIRR data files. In general you will not
need them unless you have specific needs (footprints, etc.)

Files to write out. Options:
All.......................... [0]
Mirror only....................[1]
Image at CP only...............[2]
None...........................[3]
Then ? **0**

Let's define the optical or central axis of the system for this particular optical element.

By this I mean a "virtual" line that runs throughout the optical system. Along this line are located the "continuation" planes, where the OS is subdivided in the individual OE. This line does not have to coincide with the true optical axis, as it is used mainly for bookeeping the data, but it helps greatly in the data analysis if this identity is preserved as everything in the program is referredto it.

Once established, you still have complete freedom of "moving" around the mirrors.

In the case of a grating, you will have several choices. The program may override your specifications for the central axis and locate the source and image at the "best" position.
You will be prompted later for this option.
It is recommended to use CM as units. This is not critical for most cases, but it is in the case of diffraction elements.
Optical Element definition:
Incidence Angle ? **88**
Source Distance ? **200**
Reflection Angle? **88**
Image Distance ? **40**
Reflector [0] or refractor [1] ? **0**

---------------------------------- S H A D O W ------------------------------
July 1995 F.Cerrina CXrL/ECE - UW

A segmented mirror is formed by M by N independent mirrors
Is this a segmented mirror system?**n**
Kumakhov lens are formed from tube arrays
their packing pattern are Wigner-Seitz type cell.
A capillary would be the central tube of a kumakhov lens.
Is this a Kumakhov system?**n**
Compound mirrors (or lenses) are formed
by several smaller mirrors (facets) combinedtogether.
A: Is this mirror faceted [Y/N] ?**n**
Lets define the mirror. I may compute its parameters, like the radius or the axes. This will not affect the rest of the calcu lations; all the geometrical parameters may be modified later.
Or, you may wish to specify the mirror parameters yourself.

What kind of surface are we dealing with ?
spherical = 1
elliptical = 2
toroidal = 3
paraboloid = 4
plane = 5
Codling slit = 6
hyperbolical = 7
cone = 8
polynomial = 9

Mirror surface [1-9] ? **1**

Do you want to specify the mirror parameters ?**n**
Is the mirror Cylindrical ? **n**
Is this optical element a Fresnel Zone Plate ? **n**
Are we dealing with a Grating ? **n**

Are we dealing with a crystal [Y/N] ? **n**
Is the mirror convex [Y/N] ? **n**
Reflectivity of Surface. SHADOW may solve the Fresnel equations
locally. Available options:No reflectivity 0
Full polarization dependence 1
No " " 2
Reflectivity mode [0,1,2] ? **0**

---------------------------------- S H A D O W ------------------------------
July 1995 F.Cerrina CXrL/ECE - UW

Mirror orientation angle. Angles are measured CCW, in deg,
referring to the mirror normal. Alpha=0 is the mirror
sitting at the origin, facing up. Alpha = 90 is the
mirror standing at your right and facing left when you
look along the beam STANDING ON THE PREVIOUS MIRROR
and so on.
Orientation Angle [Alpha] ? **0**

---------------------------------- S H A D O W ------------------------------
July 1995 F.Cerrina CXrL/ECE - UW

Mirror Dimensions finite [Y/N] ?**n**

---------------------------------- S H A D O W ------------------------------
July 1995 F.Cerrina CXrL/ECE - UW

The mirror will be computed from the optical parameters
that you supply. For example,in the case of a spherical mirror
I will compute the radius of the mirror to satisfy the equation
1/p + 1/q = 2/(R*cos(theta)) given p,q and theta.
This will NOT affect in any way the placement of the mirror in
the optical element.
Focii placed at continuation planes [Y/N] ? **y**

---------------------------------- S H A D O W ------------------------------
July 1995 F.Cerrina CXrL/ECE - UW

It may be helpful to save the exact incidence and reflection
angles for each ray. The saved file contains the index of the
ray, the incidence angle (in degrees), and the reflection
angle for each ray hitting this element.
Save incidence and reflection angles to disk? **y**

The Optical Element and the the relative mirror are now fully defined. The mirror pole is now located at the "center" of the optical element. It is possible to override this situation and "move" the mirror without affecting the rest of the system.
It is also possible to move the "source" without affecting the rest of the system.
The movements are expressed in the DEFAULT Mirror Ref. Frame.
so that if you move BOTH source and mirror the relative movement is the vector sum of the individual ones.
A word of caution: SOURCE movements and MIRROR movements are NOT equivalent from the point of view of the whole system.
Do you want to move the Source [Y/N] ? **n**

--- Mirror rotations and position. ---
We define three angles, as rotations around the three axis.
These rotation are defined in the program as corrections to the mirror nominal position; that is, they modify the mirror position relative to the Default Mirror Reference Frame, where all the calculations are performed. Remember that rotations do NOT commute. I apply them in the same order of entry.
CW ROTATIONS are (+) angles. A translation can be also applied to the mirror.
Do you want to move the mirror itself [Y/N] ? **n**
Distorted surface [Y/N] ? **n**
Do you want to include surface roughness [Y/N] ? **n**
---------------------------------- S H A D O W ------------------------------
July 1995 F.Cerrina CXrL/ECE - UW

Any screens in this OE [Y/N] ? **n**
---------------------------------- S H A D O W ------------------------------
July 1995 F.Cerrina CXrL/ECE - UW

Slit at continuation plane [Y/N] ? **n**
Extra Image plates [Y/N] ? **n**
File containing the source array ? begin
Exit from INPUT
Tracing optical element # 1
Call to SETSOUR
Exit from SETSOUR
Call to IMREF
Exit from IMREF
Call to OPTAXIS
Exit from OPTAXIS
Call to MSETUP
Exit from MSETUP
Call to RESTART
Exit from RESTART
Call to MIRROR
Exit from MIRROR
Call to IMAGE
Exit from IMAGE
Call to RESET
Exit from RESET
Do you want to change input mode ? **n**
Call to INPUT_OE

```
Defining Optical Element: 2
Continue ? [ ^Z or %EXIT to terminate OS ] Exit
End of session

Procedure completed. Return to COMMAND level


Procedure completed.

Shadow:: exit


Exit to DCL
Directory DISK$SCRATCH:[COCCO.SHADOW]

ANGLE.01;1          196  29-OCT-1997 12:17:43.19  (RWED,RWED,RE,)
BEGIN.DAT;2         211  29-OCT-1997 11:58:24.80  (RWED,RWED,RE,)
EFFIC.01;1            1  29-OCT-1997 12:17:43.10  (RWED,RWED,RE,)
END.00;2              7  29-OCT-1997 11:58:25.28  (RWED,RWED,RE,)
END.01;1             15  29-OCT-1997 12:17:44.23  (RWED,RWED,RE,)
HISTSIDE.DAT;1        5  29-OCT-1997 12:01:27.83  (RWED,RWED,RE,)
HISTTOP.DAT;1         4  29-OCT-1997 12:01:27.77  (RWED,RWED,RE,)
MIRR.01;1           211  29-OCT-1997 12:17:42.60  (RWED,RWED,RE,)
OPTAX.01;1            2  29-OCT-1997 12:17:42.16  (RWED,RWED,RE,)
PLOTXY.COM;1          5  29-OCT-1997 12:01:27.50  (RWED,RWED,RE,)
SCATTER.DAT;1        63  29-OCT-1997 12:01:27.55  (RWED,RWED,RE,)
STAR.01;1           211  29-OCT-1997 12:17:43.75  (RWED,RWED,RE,)
START.00;2            7  29-OCT-1997 11:58:24.38  (RWED,RWED,RE,)
START.01;1           15  29-OCT-1997 12:17:42.02  (RWED,RWED,RE,)

$ plotxy
PLOT> Input file? star.01
PLOT> Options --- Enter
PLOT>  0  for excluding the losses
PLOT>  1  for including only the losses
PLOT>  2  for including all the rays.
PLOT> Then ? 0
PLOT> Comment for plot [ 80 char ] ?
******************/******************/
******************/******************/
mirror image
PLOT> File read OK. Full specifications:
   DISK$SCRATCH:[COCCO.SHADOW]STAR.01;1
   Was created : 29-OCT-1997 12:17

PLOT>  Found        1000 good points out of        1000
PLOT>  The following columns are defined for each ray :
     1) the regular columns [1-12]
     2) optical path [13]
```

Col	Par	Minimum:	Maximum:	Center:	St. Dev.:
1	X	-0.43141	0.38218	0.57636E-03	0.11803
2	Y	-0.13839E-13	0.13353E-13	-0.98337E-16	0.45051E-14
3	Z	-0.68382E-01	0.48359E-02	-0.51807E-02	0.80935E-02
4	X'	-0.16127E-02	0.15750E-02	-0.70984E-06	0.47158E-03
5	Y'	0.99996	1.0000	1.0000	0.00000E+00
6	Z'	-0.88410E-02	0.78338E-02	0.57532E-04	0.25250E-02
11	Photon Energy (eV)	200.00	200.00		
20	Numerical Aperture	0.64246E-04	0.88458E-02		

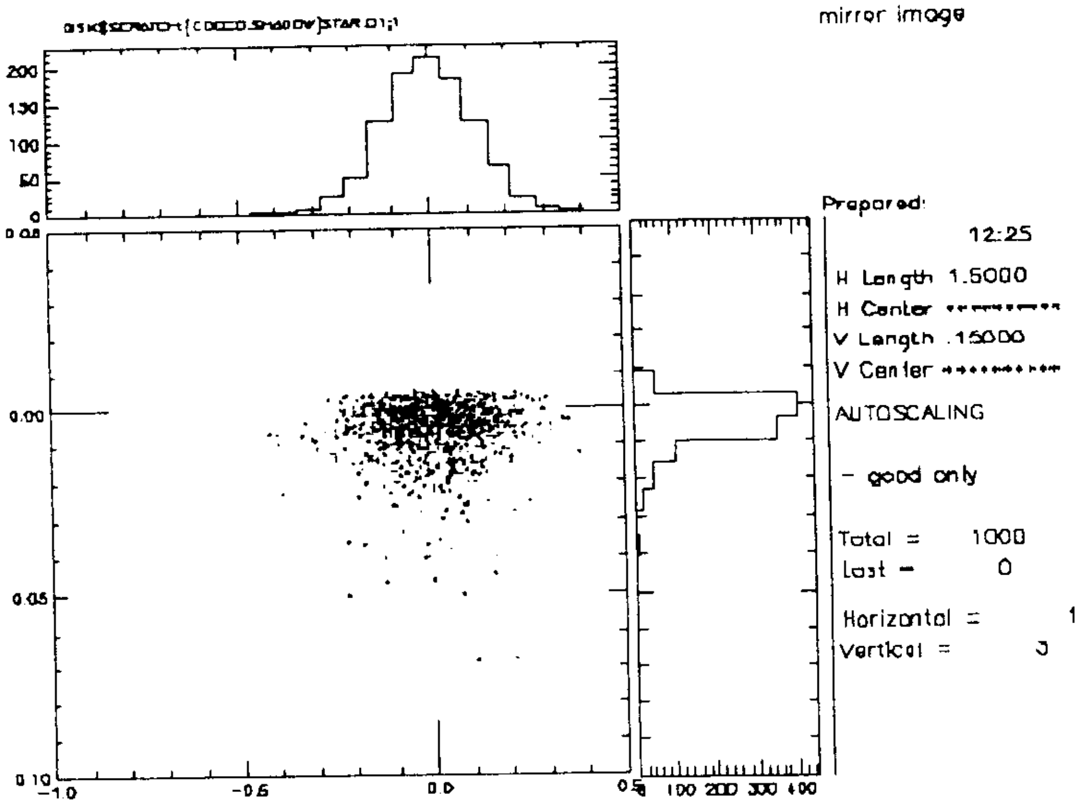
PLOT> Options. You may plot any two rows from
the above list versus each other.
You may also plot any of them versus the
ray Numerical Aperture. N.A. -- enter 20.

PLOT> Rows to use for plot :
PLOT> for horizontal axis ? **1**
PLOT> for vertical axis ? **3**

PLOT> Scaling options. Enter

0 For automatic scaling
1 For cartesian scaling
2 For external limits
PLOT> Then ? **0**
PLOT> Plotting options :
0 For scattered plot
1 For connected plot
2 For contour plot
PLOT> Then ? **0**
PLOT> Hairline at [0,0] ?
PLOT> Overlay a mirror/slit ?
PLOT> Ready for histograms. Enter:
-1 to skip
0 for same limits as plot
1 3*stdev
2 external
PLOT> ?
PLOT> Number of bins for X axis [default = 25] :
PLOT> Number of bins for Y axis [default = 25] :
Display type:
[0] Xwindow
[1] Tektronix
[2] Postscript file
Terminal type: **1**

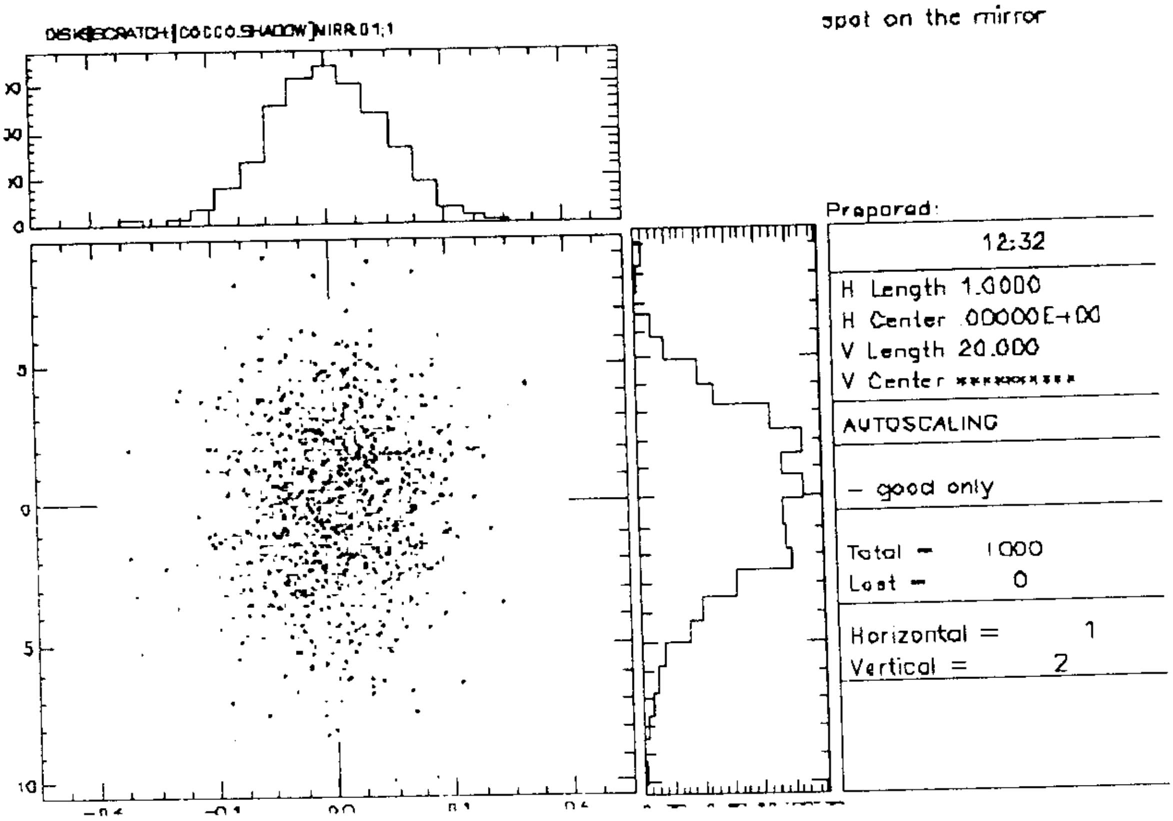
mirror image



LET'S SEE WHICH IS THE SHAPE OF THE SPOT ON THE MIRROR

```
$ plotxy
PLOT> Input file? mirr.01
PLOT> Options --- Enter
PLOT>  0  for excluding the losses
PLOT>  1  for including only the losses
PLOT>  2  for including all the rays.
PLOT> Then ? 0
PLOT> Comment for plot [ 80 char ] ?
******************/******************/
******************/******************/
spot on the mirror
PLOT> File read OK. Full specifications:
   DISK$SCRATCH:[COCCO.SHADOW]MIRR.01;1
   Was created : 29-OCT-1997 12:17

PLOT>  Found       1000 good points out of      1000
PLOT>  The following columns are defined for each ray :
     1) the regular columns [1-12]
     2) optical path [13]


Col Par Minimum:    Maximum:    Center:    St. Dev.:

 1 X  -0.37113     0.33087     0.67061E-03  0.99903E-01
 2 Y  -9.9510      8.9101      0.68456E-01  2.8778
 3 Z  0.42985E-06  0.25921E-01  0.21715E-02  0.30685E-02
 4 X' -0.16127E-02  0.15750E-02  -0.70984E-06  0.47158E-03
 5 Y' 0.99909      0.99966      0.99939     0.00000E+00
 6 Z' 0.26063E-01  0.42727E-01  0.34957E-01  0.25238E-02
11  Photon Energy (eV)   200.00     200.00
20  Numerical Aperture   0.26073E-01  0.42769E-01

PLOT> Options. You may plot any two rows from
    the above list versus each other.
    You may also plot any of them versus the
    ray Numerical Aperture. N.A. -- enter 20.

PLOT> Rows to use for plot :
PLOT>   for horizontal axis ? 1
PLOT>   for vertical axis  ? 2

PLOT> Scaling options. Enter

    0  For automatic scaling
    1  For cartesian scaling
    2  For external limits
PLOT> Then ?
PLOT> Plotting options :
    0  For scattered plot
    1  For connected plot
    2  For contour plot
```

PLOT> Then ?
PLOT> Hairline at [0,0] ?
PLOT> Overlay a mirror/slit ?
PLOT> Ready for histograms. Enter:
-1 to skip
0 for same limits as plot
1 3*stdev
2 external
PLOT> ?
PLOT> Number of bins for X axis [default = 25] :
PLOT> Number of bins for Y axis [default = 25] :
Display type:
[0] Xwindow
[1] Tektronix
[2] Postscript file
Terminal type: **1**



CYLINDRICAL MIRROR, Using MENU and BATCH procedures
A *bolded italic* and an arrow mean the sub-menu selected

S H A D O W

Commands Available at this level:

HELP More informations on the following commands
SOURCE Generates a source file
TRACE Starts the tracing of an Optical System from a specified source file
MENU Begin the process of defining an optical system.
SETDIR Defines the destination for SHADOW output files.
EXIT Returns to shell

Shadow:: **menu**

Prepare MENU ...
Ready:: **load sys**
Load Optical System Description

Directory name SYS$START:
File name START

Reading from file SYS$START:START.01
The system consists of 1 OE.

Ready:: **sel oe**
Number of Element: **1**
ORIGINAL

MAIN MENU	Optical Element 1
Files to write out	ALL
Source plane distance	200.
Image plane distance	40.
Incidence angle	88.
Reflection angle	88.
Mirror Orientation Angle	0.0
Source file	begin
Type of element (+)	REFLECTOR
Figure (+)	SPHERICAL
Diffraction (+)	MIRROR
Crystal (+)	NO
Mirror movement (+)	NO
Exit Slit (+)	NO
Modified Surface (+)	NO
Source Movement (+)	NO

MODIFIED

MAIN MENU	Optical Element 1
Files to write out	ALL
Source plane distance	200.
Image plane distance	40.
Incidence angle	88.
Reflection angle	88.
Mirror Orientation Angle	**90.**
Source file	begin
Type of element (+)	REFLECTOR
Figure (+)	SPHERICAL
Diffraction (+)	MIRROR
Crystal (+)	NO
Mirror movement (+)	NO
Exit Slit (+)	NO
Modified Surface (+)	NO
Source Movement (+)	NO

ORIGINAL

Mirror parameters (+)	INTERNAL
Surface curvature	CONCAVE
Cylindrical	NO
orient. [CCW from X axis]	n/a 0.0
Reflectivity (+)	OFF
Limits check (+)	NO

MODIFIED

Mirror parameters (+)	**EXTERNAL**
Surface curvature	CONCAVE
Cylindrical	**YES**
orient. [CCW from X axis]	**90.00**
Reflectivity (+)	OFF
Limits check (+)	NO

Type selected	SPHERICAL
External paramters define (+)	0.0000000000000E+00
Focii and Continuation Planes	COINCIDENT
Object side focal distance	n/a 0.0
Image side focal distance	n/a 0.0
Incidence angle	n/a 0.0
File with SPLINE/ POLYNOMIAL	n/a NONE SPECIFIED
Focus location	n/a SOURCE
Toroidal mirror pole location	n/a LOWER/OUTER
Codling Slit length	n/a 0.0
width	n/a 0.0

Type selected	SPHERICAL
Spherical radius	**2.327**
Ellipse major Axis	n/a 0.0
minor Axis	n/a 0.0
Angle of MajAx and Pole [CCW]	n/a 0.0
Paraboloid param.	n/a 0.0
Hyperbola major Axis	n/a 0.0
minor axis	n/a 0.0
Angle of MajAx and Pole [CCW]	n/a 0.0
Torus major Radius	n/a 0.0
minor Radius	n/a 0.0
Cone half-aperture [deg]	n/a 0.0

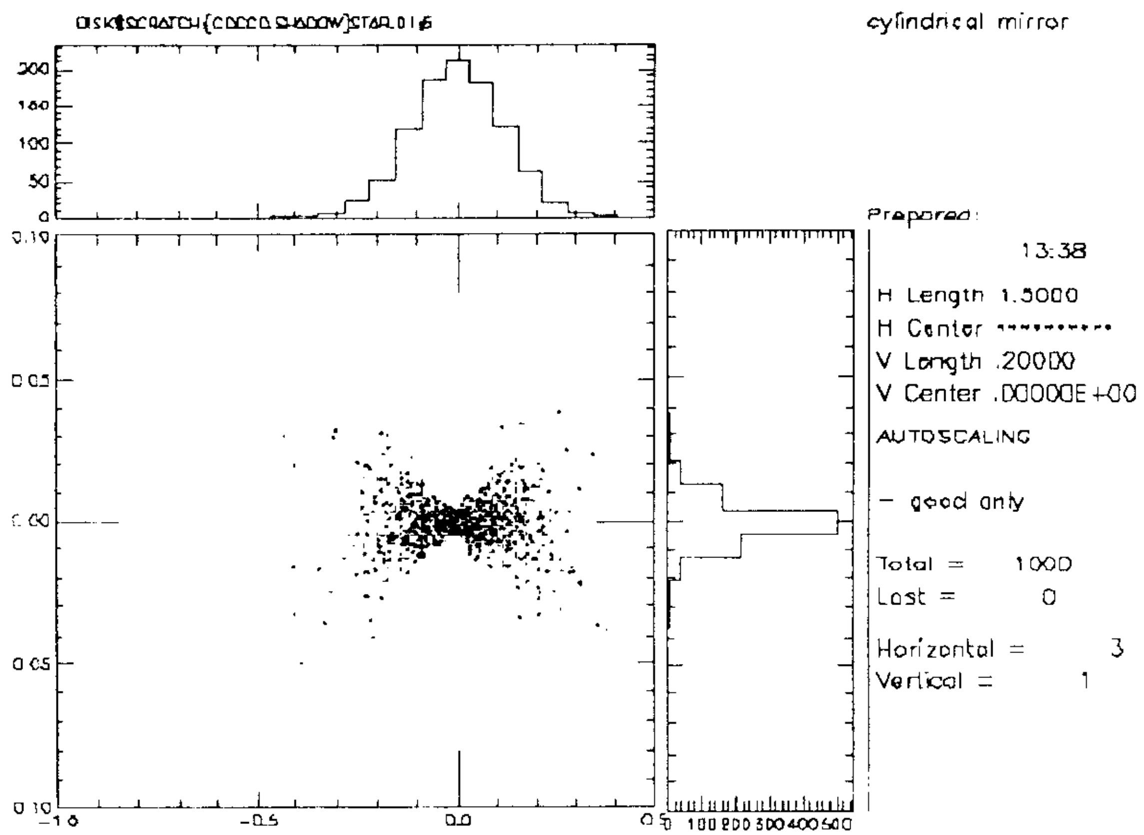
Ready:: **save sys**
Save Optical System Description
Directory name SYS$START:
File name START
Writing to file SYS$START:START.01
Ready:: **exit**
Exit from MENU to SHADOW COMMAND level
Shadow::
Shadow:: **trace**

Ray Tracing Selected. Begin procedure.
Mode selected [? <ret> for HELP] ? : **batch**
BATCH selected.
Call to RESET
Exit from RESET
Mode selected is:
BATCH
Options: to start anew [0]
to restart from a given OE [1]
Then ? **0**
Input file [^Z or %EXIT terminates OS] ?**start.01**
Tracing optical element # 1
Call to SETSOUR
Exit from SETSOUR
Call to IMREF
Exit from IMREF
Call to OPTAXIS
Exit from OPTAXIS
Call to MSETUP
Exit from MSETUP
Call to RESTART
Exit from RESTART
Call to MIRROR
Exit from MIRROR
Call to IMAGE
Exit from IMAGE
Call to RESET
Exit from RESET

```
Do you want to change input mode ? exit
Input file [ ^Z or %EXIT terminates OS ] ? Exit

Procedure completed. Return to COMMAND level

Procedure completed.

Shadow:: exit

Exit to DCL

$ plotxy
PLOT> Input file? star.01
PLOT> Options --- Enter
PLOT>  0  for excluding the losses
PLOT>  1  for including only the losses
PLOT>  2  for including all the rays.
PLOT> Then ? 0
PLOT> Comment for plot [ 80 char ] ?
******************/******************/
******************/******************/
cylindrical mirror
PLOT> File read OK. Full specifications:
   DISK$SCRATCH:[COCCO.SHADOW]STAR.01;5
   Was created : 29-OCT-1997 13:37

PLOT>  Found        1000 good points out of       1000
PLOT>  The following columns are defined for each ray :
     1) the regular columns [1-12]
     2) optical path [13]

Col Par Minimum:      Maximum:      Center:      St. Dev.:

 1 X   -0.49514E-01  0.56631E-01  -0.50388E-03  0.90261E-02
 2 Y   -0.12785E-13  0.13585E-13   0.66442E-16  0.45872E-14
 3 Z   -0.43011      0.38258       0.13971E-02  0.11785
 4 X'  -0.79914E-02  0.84145E-02  -0.80138E-04  0.25165E-02
 5 Y'   0.99996      1.0000        1.0000       0.00000E+00
 6 Z'  -0.17774E-02  0.14500E-02  -0.88289E-04  0.49173E-03
11  Photon Energy (eV)   200.00     200.00
20  Numerical Aperture   0.66032E-04  0.84439E-02

PLOT> Options. You may plot any two rows from
    the above list versus each other.
    You may also plot any of them versus the
    ray Numerical Aperture. N.A. -- enter 20.

PLOT> Rows to use for plot :
PLOT>    for horizontal axis ? 3
PLOT>    for vertical axis   ? 1
```

PLOT> Scaling options. Enter

0 For automatic scaling
1 For cartesian scaling
2 For external limits
PLOT> Then ?
PLOT> Plotting options :
0 For scattered plot
1 For connected plot
2 For contour plot
PLOT> Then ?
PLOT> Hairline at [0,0] ?
PLOT> Overlay a mirror/slit ?
PLOT> Ready for histograms. Enter:
-1 to skip
0 for same limits as plot
1 3*stdev
2 external
PLOT> ?
PLOT> Number of bins for X axis [default = 25] :
PLOT> Number of bins for Y axis [default = 25] :
Display type:
[0] Xwindow
[1] Tektronix
[2] Postscript file
Terminal type: **1**



Chapter 1

INTRODUCTION

The PRIMER describes the basic features of the programs and provides the user with the first hands-on experience. It is intended for the newcomer to the programs and provides annotated examples as a 'guided tour'. The reader should refer to the User's Guide for more in-depth coverage of the topics. The Glossary may also be quite helpful. In order to run the examples indicated below, we will assume that SHADOW has been installed and is successfully running.

In this PRIMER we will describe how to access SHADOW and some utility programs. Further examples can be found in the DEMO section of the documentation, where some more advanced cases are illustrated, and in the USER's GUIDE (hereafter UsG) where specific examples for each program are given.

1.1 SHADOW structure

SHADOW is a software package that is designed to study the propagation of a photon beam through an optical system. The program is general, but is optimized for the case of X-rays and reflective optics such as those encountered in the XUV and in Synchrotron Radiation. The code is designed to be simple and reliable, with prompt- and menu-driven programs. It resides on a VAX computer running the operating system VMS. It will not run under UNIX.

SHADOW is formed by a main core of programs and by a collection of utilities used to process the output from the main programs. As shown in Fig. 1.1, there are three groups of programs falling under the confines of SHADOW. The first group is used in the I/O session to define the characteristics of the source and of the optical system. The second is the one performing the actual calculations, i.e., generating and tracing the photon beam through the optical system. The third includes analysis programs necessary to interpret the results of the calculations performed earlier. The programs are run sequentially by the user in an interactive I/O session; they can also be run in batch mode.
The communication between different programs is via disk files. The files are normally created in the current directory [see INIT, below] and may be quite large, so that we strongly recommend to PURGE the disk area often. Some files have default names (like the ones indicated above), other have names that are supplied by the user. Briefly, we will encounter:

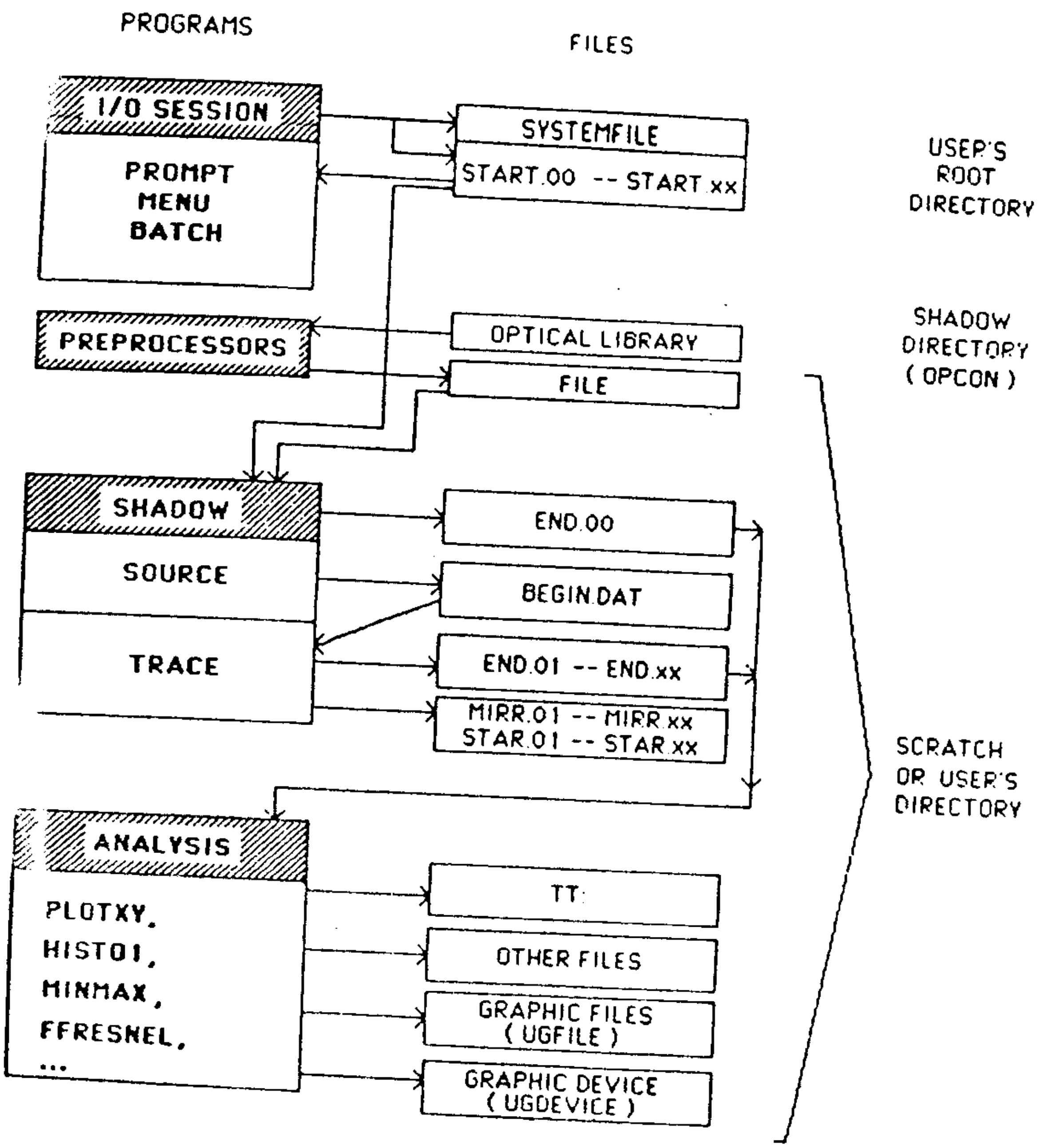


Figure 1.1: SHADOW structure

1.1.1 Data files:

They are normally in binary (unformatted) for accuracy and speed of disk access. NON printable. Typical names are MIRR.xx (where xx is a number from 01 to 20), STAR.xx and they are quite large (in excess of 189 blocks for a 1000 rays file).

1.1.2 Parameter Files:

Typically START.xx, NAMELIST format. They list the values of the parameters used by SHADOW in setting up a calculation of a source or of an optical system. They can be EDITED (but we do not recommend it); the DIFFERENCE (VAX DCL) utility may be useful in checking modifications. These files should seldomly concern the user directly.

1.1.3 Analysis Files:

They are created by the analysis program and vary widely in type and internal structure. Refer to the USER's GUIDE for a description of the files generated by each program.

Notice that the internal structure of the files used by SHADOW is rigid, in particular for the DATA ones, and cannot be modified.

1.2 Definitions and Nomenclature

When in doubt, look up the GLOSSARY. Here we describe the most commonly used terms in the code which are necessary in order to correctly set-up the calculations. SHADOW operates on an OPTICAL SYSTEM, which is in turn formed by a SOURCE and by (one or more) OPTICAL ELEMENTS. The following picture (Fig. 1.2) illustrates an OPTICAL SYSTEM, formed by two mirrors.

The solid line represents the 'central axis' or 'optical axis'; it connects the poles of the mirrors and defines the 'backbone' of the system.

The photon beam generated at the source is traced on the first mirror to the 'continuation plane', where an intermediate image is generated. This image becomes the source for the next mirror and is traced through to the final image position. SHADOW allows great flexibility in specifying the position and the type of mirrors used in the calculations. DATA files are generated at each 'critical' position in the optical element, i.e., at the mirror and at the continuation planes; more, if some options are selected.

In this way, many OE's can be concatenated together (up to 20). The files are automatically numbered to keep track of what belongs where.

Before beginning the description of a session, it is necessary to define briefly the geometry used by the programs [more in the UsG]. SHADOW works in a cartesian reference frame, always using the full specification of the vectors. Most programs refer the components to the optical axis but, although cheaper in terms of storage, this solution is rigid and makes exotic geometries impossible to implement. We thus define the geometry shown in figure 1.3. Notice that this geometry is somewhat different from other codes (in particular machine physics conventions). Notice also how for an off-center system the

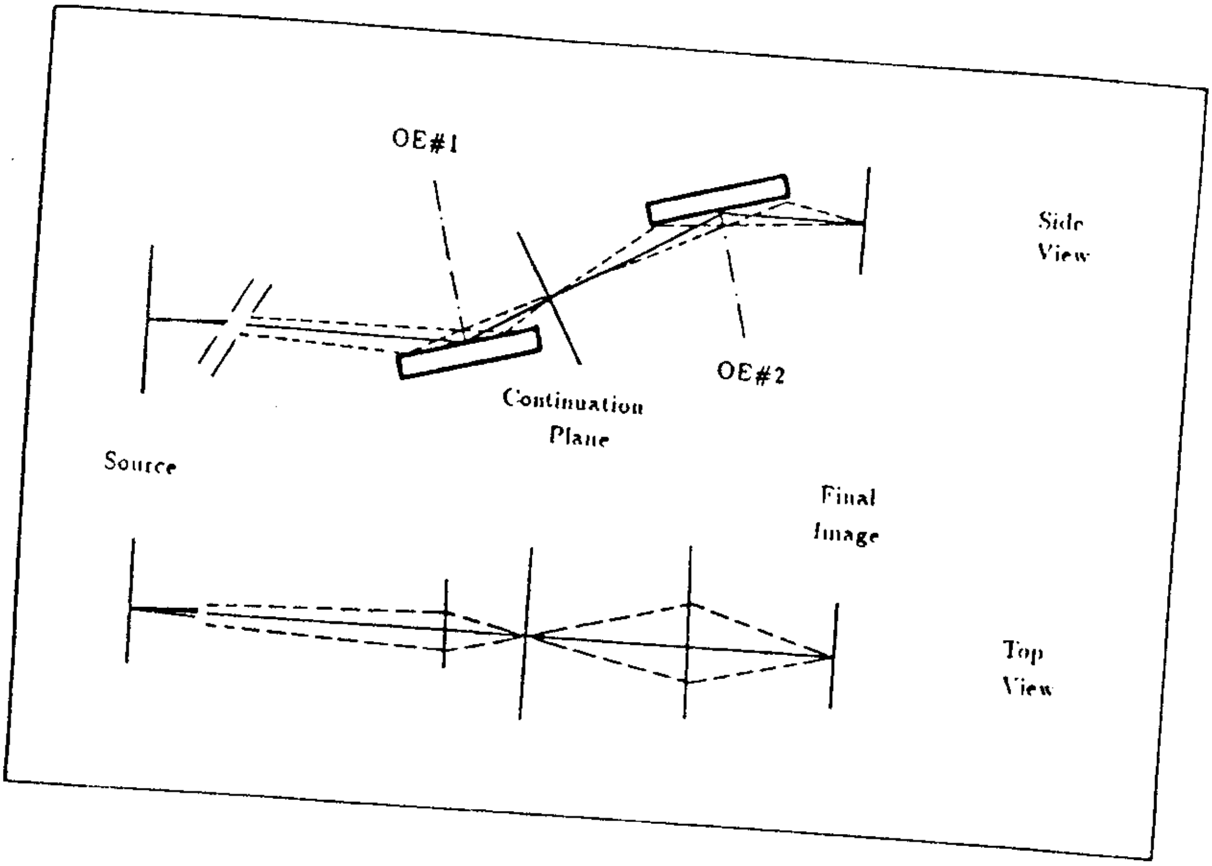


Figure 1.2: Two-mirrors Optical System

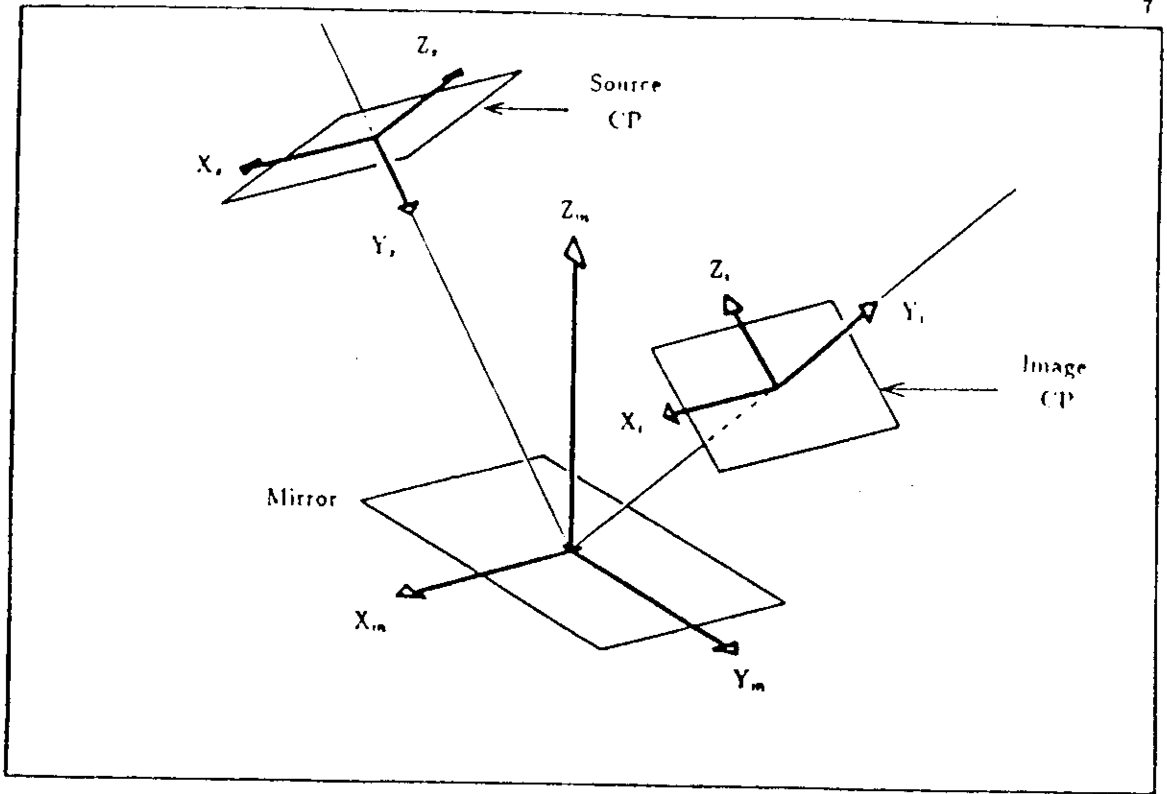


Figure 1.3: Optical Element Geometry and Continuation Planes

reference frame of the source flows in that of the mirror.

This is all that is needed for a first run of SHADOW. We will define other terms as needed.

Chapter 1

Source Modelling

1.1 Introduction

This chapter will describe the physical and mathematical models on which the source generation in SHADOW is based. The type of sources that can be modelled are those of interest for synchrotron radiation optics, although many classical ones are also implemented. The terminology reflects this choice. Furthermore, the manual is *not* an optics textbook, so that we may have taken some liberties with the standard definitions to adapt them to our purposes. The optics books from which we have more heavily drawn are listed in the bibliography.

1.2 Stochastic Processes

The generation of photons from an object that is self-luminous is a stochastic process both in time and in space. We assume a steady state process, i.e., time independent and concentrate on the spatial and angle properties of the source. In a real radiation source, photons are generated randomly with a frequency described by deterministic physical laws. In other words, on a space of variables $\mathbf{r_i}$ the frequency of observation of photons is obtained from the *probability density function (pdf)*:

$$N(\mathbf{r_i}) = p(\mathbf{r_i}) \cdot N_o \tag{1.1}$$

where p describes a probability distribution law (e.g., a gaussian, a constant, etc.) and N_0 is the total number of photons included in the sample. A computational model that describes the generation of photons must therefore be based on the distribution law 1.1 in order for the model to be physical.

4c

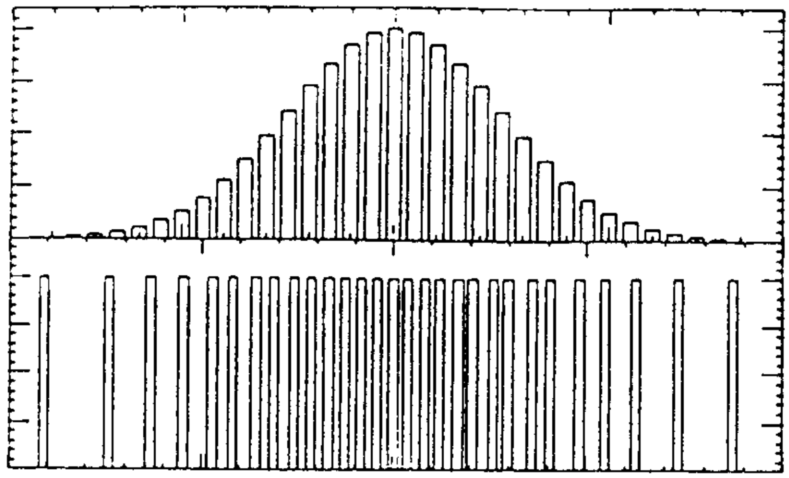


Figure 1.1: Example of Deterministic and Stochastic Functions

Notice change of spacing in lower panel

This can be achieved in either of two ways. In the first, deterministic, approach a function table is generated so that the source is described by a table of values of the function 1.1 over an equispaced grid. This is nothing more than the traditional definition of a function over a domain of an independent variable. The value of the probability can then be interpreted as an *amplitude* of the source at that particular point. The source generated this way may be quite inefficient from a computational point of view, since several of the rays generated will have a very small amplitude and thus computer time will be wasted computing trajectories that will not affect the final image. The other approach is based on the idea of generating a source, i.e., an array of numbers whose *frequency* of observation depends on the *pdf* itself. This is illustrated in fig. 1.1, where the two cases are compared. This second source is clearly much more efficient computationally, because the cpu time is spent where the rays physically are. This approach requires however a change of perspective that goes beyond a simple change of variables. For example, the normal integration process of a function (as pertaining to the Riemann definition of integral), must be replaced by the more general Stieltjes integral.

1.2.1 Ray Intensity and Ray distribution.

Following these initial guidelines, we must spend some time discussing the meaning of these definitions and how they can be implemented in a computational code. As a practical example, let us consider the case of a polychromatic radiation source, for simplicity point-like and collimated, with a photon energy distribution defined by a gaussian, so that:

$$P(\omega) = P_0 \frac{1}{2\pi\sigma} \exp - \frac{(\omega - \omega_0)^2}{2\sigma^2} \qquad (1.2)$$

and let us suppose that we want to generate 1000 rays to describe that source. This equation is normally interpreted to signify the repartition of energy among the different wavelengths; in wave optics it can be used to obtain the amplitude of the electric field for each wavelength. In an analytical representation we can say that the source has a larger intensity in the region around ω_0. In ray, or particle, optics the same equation can be used instead to infer the number of photons that are emitted at each photon energy. Even in this case there are two different interpretations of the same equation, since in a deterministic model, Eq. 1.2 will lead for example to the case of Fig. 1.1 (upper panel), where the distribution is sampled at 31 points and to each point is assigned a value described by Eq. 1.2. This could be interpreted by saying that each ray is generated with a different amplitude (or intensity). In a stochastic model the 31 rays are generated so that their frequency of observation will be described by Eq. 1.2 and *each ray will have the same amplitude*. This very important point is easily understood on the basis of physical intuition, if we remember that a photon is a quantum of energy of the electromagnetic field. What this mean is that a large intensity corresponds to a large number of photons of same amplitude, not to "a photon of large amplitude". Thus, a stochastic description is more physical than a deterministic one: the concept of a continuous amplitude must be replaced with that of a granular probability of observation.

These ideas are quite intuitive for the case of the description of a source, but how to extend them to include the case of physical optics? For example, how to deal with reflectivity from a surface? This problem can be easily solved if we stop to think about the meaning of reflectivity. To set $R = 0.6$ means that a fraction of the rays equal to 0.6 will be reflected and the balance absorbed. The total number of photons decreases then as the beam

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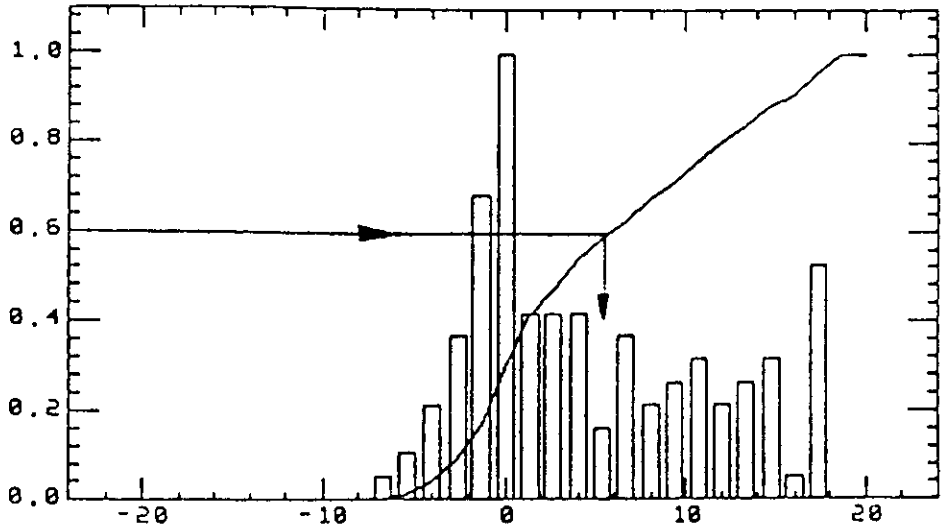

Figure 1.2: Example of Stochastic Sampling

The solid curve is the CDF of the distribution shown.

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propagates through the optical system. We can say that to each photon is associated a probability of observation I_i, which is set to one at the origin. Then, as the ray progresses through the system, the interactions will decrease its probability of "survival" and I_i will be less than 1; after the above reflection, it could be for example 0.6. It is easy to recognize the connection between I_i and the electric field (or vector potential) A_i of the photon. We identify the module of the amplitude of the electric field (normalized to 1 at the origin) with the probability of observation of the photon, i.e., its wave function. Thus the effect of reflectivity can be taken in account by scaling the electric field by the corresponding amount:

$$A_i(after) = A_i(before) \cdot R_i \tag{1.3}$$

where R_i would be the reflectivity as computed at the intercept point of the $i-th$ ray. Quite often, in the documentation, we use the two terms amplitude and probability interchangeably.

It is important to distinguish at this point between the probability density function that generates the source and the probability of transmission through the optical system. The first describes the source model itself and is independent of the optical system, while the second is independent of the source model. The first operates on the distribution of the rays among the spatial and angle coordinates, while the second affects the amplitudes only and may have only a weak dependence on the spatial characteristics of the rays.

The meaning of the amplitude is then not dissimilar from that of wavefunction in quantum mechanics when interpreted in the statistical framework: it represents the probability of finding a ray at a given position and can be used in obtaining the expected value of physical observables, such as energy:

$$< E >= \sum_{i=1}^{N} E_i \cdot A_i^* A_i \tag{1.4}$$

where the sums extends over all the rays.

1.3 Computational Models

All the models implemented in SHADOW follow the idea of a stochastic process, so that the rays are all generated with equal amplitude but with a spatial frequency determined by the model describing the source. This approach is not restricted to the case of random sampling. When we use a regular sampling of the source variable space we refer to it as a "grid", while we reserve the term Monte Carlo for the case in which each ray is generated independently accordingly to a pseudo-random number generator. Following standard texts, there are two main ways of generating random variates following a given distribution law. They are the *transformation* and the *inversion* method. We try to stay away from the *acceptance/rejection* methods because of their inefficiency and their incompatibility with the "grid" source. In the transformation method, one needs to find a functional form such that the random variable Y:

$$y = F(x) \tag{1.5}$$

will have the required *pdf* when the random variate x is uniform. This task is not easy since there are no general guidelines in finding the generating function F; however, several cases have been worked out and we refer the interested reader to the published work. This method is by far the most efficient once F is found, in particular for multidimensional random variables. The second method is the most general, since it is possible to generate efficiently random variates with *pdf* given by any law as long as it can be put in a table format. The basic idea is the following. Consider the probability *distribution* function, PDF (often called *cumulative distribution function*, CDF - we will use the two interchangeably):

$$Y(x) = \int_{-\infty}^{x} F(t)\, dt \tag{1.6}$$

Now generate a uniform Y variate and *invert* each point. Compare this with Fig. 1.2. It is clear that the majority of points will fall in the region where the slope of the PDF is the largest, i.e., where the *pdf* is large. It is easy to show that the *frequency distribution* is given indeed exactly by the *pdf*. The meaning of this approach is profound. Physically, it means that we sample in a uniform way the distribution space rather than the variable space, thus setting ourselves automatically in the framework of Stieltjes integrals and statistical analysis. After all, it is easy to rewrite the standard expectation value integral of the observable A as:

$$< A > = \int dx\; A(x)\, F(x) = \int d(\int_{x'} dx'\; F(x'))\; A(x) = \int dY\, A(x(Y)) \tag{1.7}$$

where Y is the random variable whose *pdf* is given by $F(x)$. The power of this approach will be revealed fully in the discussion of the diffraction effects in the image formation (Fresnel-Kirchhoff integral) and in the power density calculations.

Monte Carlo

In the case of the MC method, a relatively large number of rays is generated by either inverting or transforming uniform random variables. This is particularly useful when the source (or the system) depends on several parameters and one wants to study the dependence on each one of them. Let us consider the case of a system whose transfer function is such that:

$$\vec{R}_{out} = F(\vec{R}_{in}; p_1, p_2, ..., p_N) \tag{1.8}$$

where $p_1, ..., p_N$ is a set of parameters describing the source. If we use an MC generator to create M rays *each* of the parameters will be sampled M times, thus allowing a very effective study of the system. Another point of view is that of considering the dependence of F over a given variable as a *projection* of the source on that coordinate. In the case of the MC method the projection will have all the M rays to sample that coordinate. The MC method is thus very effective for complex sources depending onto a large number of parameters, such as the various synchrotron sources. The MC method should be used as the normal working case, unless specific functional dependences are sought.

Discrete Sampling

In the case of discrete sampling (*grid*, in the language of SHADOW) the distribution is sampled by generating a regularly spaced Y variate and an X variate from it. In this case it is easy to show that it is the distance between points that depends (inversely) on the *pdf*: points more closely spaced will correspond to region of large *pdf*. Again, this is exactly in line with the definition of Stieltjes integral and provides an automatic and powerful tool for the computation of that class of integrals. The case of a uniformly spaced grid correspond to that of constant probability and is useful to assess first order properties of an optical system, in particular in terms of aberrations. The problem of grid sampling is that it is not an efficient way of obtaining a projection over a large set of parameters. For example, if a source is a function of six different variables, the total number of rays needed to provide a sampling of N in each variable is $M = 6^N$, a number that becomes rapidly very large (for $N = 11$ $M = 3.6\ 10^8$). The grid sampling should be reserved for those cases in which it is necessary to obtain an in-depth study of the dependence of an output variable on a source variable (optical aberration studies) or when post-processing is critically dependent on the cancellation of some terms (Fresnel-Kirchhoff integral).

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Mixed cases

Sometimes it is instructive to mix random and grid cases. For example, one may want to generate a bundle of random rays originating at an ordered grid; this is useful in the study of optical systems with extended fields of view. SHADOW replicates the specified number of random rays at the grid location, so that care must be taken not to exceed the number of allowed rays (5000).

1.4 Physical Models

1.4.1 Spatial and Angle Distribution

A source is described by a collection of rays originating in a region of space; by *ray* we define a straight line originating at a point and propagating without changes until it intersects a ***surface*** or ***optical element***. The ensemble of rays constitutes a ***beam***. The source is three-dimensional and is characterized by the distribution of rays in the region of space that intuitively defines the source itself, i.e.,

$$Source = \{\vec{r}_i, \vec{v}_i;\ i = 1, N\} \tag{1.9}$$

The distribution of the ***directions*** of the rays describe the propagation characteristics of the beam. SHADOW works in a cartesian coordinate reference frame (see below). The probability distribution densities that describe the ray distribution in space and in angle form the source physical model; these *pdf's* may be independent or not. The boundaries of the source specify the region of space within which the rays are generated and may have different shape (rectangular, elliptical, etc.) [1].

Phase Space

The statistical nature of the stochastic models lead to the introduction of other results from the domain of statistical mechanics. We recall that given a spatial variable, it is possible to define its canonical momentum from Hamilton's law of motion for a given mechanical system that can be described by a Lagrangian. In general the formulation is quite more complicated than just the familiar set of coordinates $\{x, y, z\}$ and $\{v_x, v_y, v_z\}$ typical of free-space motion. We always assume that $|v| = 1$; furthermore,

[1] For some source models the full algorithm that allows the separation between model and boundaries has not yet been implemented. For example, a lambertian source is easily implemented for a conical source (circular boundaries) but not so easily for a rectangular one.

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we also often use the notation x' for v_x (and so on). The conjugate variables depend directly on the forces that act on the material point (ray). In the case of an optical system, these forces can be thought of as being acting only at the optical surface and be characterized by a suitable Dirac δ-function, in order to justify the abrupt change of direction. Although it is certainly true that in the free-space propagation between optical surfaces the couples $\{x_i, v_{x_i}\}$ are canonical conjugates, this is not so for the whole optical system, unless all the surfaces are cylindrical and orthogonal to each other. What happens is that the effect of the reflection (or refraction) from surfaces mixes the coordinates thus requiring the definition of a new set of canonical variables, in general quite complex. The set of coordinates that describe a beam form its *phase space*, where each ray represents a point. In general the phase space will then be 6-dimensional and only if the coordinates are independent the phase space can be decomposed in sub-spaces, one for each pair of independent conjugate variables. The representative position of each ray in these sub-spaces does not depend on the value of the other coordinates (of the same ray). In general this is only approximately true. In the case of "normal" optical system, the transverse coordinate y and the angle from the optical axis form the conjugate set. The definition of phase space shows again the power of the statistical interpretation of the generation and propagation of photon beams; in particular, the applicability of Liouville's theorem leads to very important consequences. The theorem states that the density in phase space is conserved throughout the evolution of the beam in its propagation. This leads directly to the Smith-Helmoltz invariant and to the magnification law. The study of the distribution of the rays in phase space is one of the most important tools of optical system designs, in particular for complex sources such as those typical of soft X-ray Optics.

Wavefront Sampling

The idea of wavefront applies to the case of a coherent source, where the different fields are radiated with a precise phase relationship between different parts of the source. The perturbation created by a source propagates with a field described by the wave equation and is fully specified by its amplitude and phase. The surfaces of constant phase describe the *wavefront*; the amplitude is not necessarily constant across the wavefront. In an analogy with the quantum-mechanical wavefunction, the wavefront can be interpreted as defining the probability of observing a photon at a given position with a set of parameters (polarization, wavelength, etc.). The next step is to remember that the direction of propagation is by definition given by the *normal* to the wavefront along the wavefront itself. Furthermore, using the statistical interpretation of QM, we can say that the number of photons per unit area will be proportional to the intensity of the wavefront (normalized to 1) at that point. The meaning of the source model generated by SHADOW should be at this point clear: the *distribution of rays generated by* SHADOW *represents a stochastic sampling of the source wavefront.* Some cases are discussed below from in this framework. SHADOW generates coherent sources by keeping a precise phase relation between different rays. Incoherent sources are generated by adding a random phase to each ray.

1.4.2 Coordinate Space and Ray representation.

After the discussion of the source generation process it may be useful to re-discuss the meaning of the coordinates and variables that define a ray belonging to a given source. SHADOW uses for each ray the following variables:

$$\{x, y, z; v_x, v_y, v_z; A_{s,x}, A_{s,y}, A_{s,z}; flag, \frac{2\pi}{\lambda}, ray_{id}; \phi_G, \phi_s, \phi_p; A_{p,x}, A_{p,y}, A_{p,z}\} \tag{1.10}$$

totaling up to 18 double-precision values. Normally SHADOW uses only a subset of 12 (up to ray_{id}). Because of the way Fortran stores arrays, to each variable is associated a *row* of the memory area where the rays are stored [2]. As the rays propagate through the systems, the first 6 values define the origin and direction of the ray itself; although one variable is clearly redundant (since $|v| = 1$) the gain in mathematical simplicity by far outweighs the extra demand on storage. What is the meaning of the other variables? They do represent the "history" of the ray in traversing the optical system. For example, the value of *Flag* distinguishes between an "ordinary" ray (to which nothing peculiar has happened) from other cases. Initially, the flag is set to 1. If the ray has fallen outside the aperture of a slit or the physical dimensions of a mirror, the ray is labelled as *lost*, so that the (geometrical) efficiency of the optical system can be determined. However, the ray would be still good for another optical system with, say, a wider slit or a larger mirror so that SHADOW will keep tracing it – in this way the user can for example decide if it is indeed worthwhile losing all those rays to improve the image quality by simply comparing two graphs (*"goodonly"* vs. *"all"*. in PLOTXY or other graphics programs). In these cases the flag is set to $-11,000 \cdot OE_{number}$ so that it is possible to keep track

[2] There is some confusion in the documentation and in the language of the utilities about columns/rows. This will be cleared as the documentation work progresses.

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of the losses[3]. In other cases, the ray may happen to be definitively lost: for example, it may fall completely outside a mirror to the point that the intercept is complex - clearly it would not make sense to continue tracing that ray and the loss is considered "hard".
The set of A's represents the electric field of the ray (set to $|A| = 1$ at the origin) and is progressively attenuated when the ray is reflected or transmitted by a material medium. SHADOW uses only the set A_s for unpolarized light, while the full set of A_s, A_p are needed for the more general case of an elliptically polarized beam. The set of ϕ refers to the phase of the ray. This is an essential ingredient in the calculation of the properties of coherent and polarized optical sources. The total phase of a ray will contain a term due to the geometrical optical path ($\phi_G = Optical\ Path/\lambda$) and a term due to the phase shifts occurred under reflection or refraction. The first can be activated independently of the other, while the last automatically activate the geometrical phase shift.

Sampling and Number of Rays.

What is the relationship between the number of rays used in SHADOW and a real source? The relation is linear: if a source is generating for example 10^{18} *photons/sec* and SHADOW is using 5000 rays, then each ray represents a sample of $2 \cdot 10^{14}$ photons per second. Furthermore, these 5000 rays are generated accordingly to the specified distribution and represent a faithful and reduced model of the real source. Since the relation is linear, the scaling principle applies to all issues of power density, flux, etc.

1.5 Specific models

1.5.1 Simple sources

The case of simple sources include those in which the *pdf* is given by a simple law. For example, in the case of an *isotropic* source the emission intensity is independent of the emission angle while in the case of lambertian (uniform) source the emission angles varies with the cosine of the angle from the surface normal. These sources are discussed in the later sections of this *Users Guide*.

[3] This counter is automatically overridden by the most recent loss. If a ray is out a mirror in OE 1 and out a slit in OE 2, the flag will be -22000. For a careful analysis of losses it is better to use SHADOWIT rather than SHADOW.

1.5.2 Gaussian Beams

The discussion of gaussian beams is important for the following sections. By gaussian beam we intend here a beam of photons (not necessarily coherent) described by the density law:

$$\begin{aligned} N(x,x') &= \frac{2\pi}{\sigma_x \sigma_{x'}} \exp -(\frac{x^2}{2\sigma_x^2} + \frac{x'^2}{2\sigma_{x'}^2}) \\ \sigma_x &= \sigma_{x_0} + s\sigma_{x'} \end{aligned} \quad (1.11)$$

where σ_u refers to the standard deviation of the relative variable (σ_{u_0} is the standard deviation at the waist itself) and s is the distance from the beam's waist. Such a law is typical of a beam of electrons in a storage ring [4] and will describe as well the distribution of photons if we imagine that these will be emitted along an extremely narrow cone centered along the electron direction. Here we hit one of the central ideas of the modelling of electron-beam based photon sources: since the electrons are assumed to be radiating incoherently from each other (power proportional to current I, rather than I^2) the photon distribution will be given by the convolution of the two distributions:

$$N_{final}(x', y', \ldots) = \int dx\, dy\, \ldots \rho_{electrons}(x, y, \ldots) N_{photons}(x, y, \ldots; x', y', \ldots) \quad (1.12)$$

where $(x, y, \ldots)$ are any (relevant) variable. The effect of these convolutions *in first approximation* is only that of redistributing the flux, not of modifying its value [5]. If the electrons have a gaussian distribution, then the convolution becomes very simple. This effects are indeed observed in storage rings: in the case of machines of small γ's (see below) the natural divergence of the radiation dominates and the electron opening angles have little effect. In the opposite case of machines with large γ's the radiation angle can be so small that the electron angles dominate.
SHADOW allows the specification of gaussian distributions in spatial and angle coordinates independently, i.e., one could specify a point source with gaussian angle distribution. The distance from the waist is used however only in the case of the bending magnet source. We notice that the double gaussian source, both in coordinate and angle, is the one typical of electron beams.

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[4] Over small distances, e.g., an arc of a bending magnet of a few milliradians, the σ can be considered constant; this is not true anymore for relatively long arcs of bending magnet

[5] For example, electrons that are travelling off-plane will see a different magnetic field and focusing effects, so that the simple free-space propagation of the gaussian beam does not apply anymore.

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1.5.3 Bending Magnet Radiation

The detailed theory of the emission of radiation from bending magnets is beyond the scope of this work. We refer the interested reader to the publications listed in the Bibliography. In the implementation of the code for SHADOW, we have drawn heavily on the work of K.Green and his excellent summary of equations and formulae. In our opinion, the best way of visualizing the far-field emission from relativistic electrons is that of considering the storage ring as a large dipolar antenna. The straight and focussing parts of the lattice are immaterial to this discussion, so that we can consider the ESR to be a circle of radius R where electrons of energy $E = \gamma m_0 c^2$, are kept in a stable orbit. Let us consider first the case of an observer located exactly in the orbit's plane. For low energy electrons, the observer will "see" a dipole with the electrons oscillating between $-R$ and R; the radiation frequency will be the Larmor frequency, $\omega = e_0 Hc/E$. The first effect to become apparent at relativistic energies will be a blue shift of the radiation, because of the Doppler effect. The typical lobe pattern will be folded in a cone of opening $1/\gamma$ centered along the electron velocity, so that the observer will be able to detect a radiation only when "looking" along the tangent of the orbit to the incoming electrons. We notice that the cone limits the observation time to a very short interval, of the order of $1/\gamma$. The Doppler shift provides a factor of the order of γ^2, while the Fourier transform of the pulse of radiation will contain terms well above $1/\gamma$. All in all, the radiation will be shifted by a factor $1/\gamma^3$. The fact that an electron storage ring is essentially a well-tuned X-ray antenna explains why these sources are the most efficient in the production of X-rays. This simple model explains well the elliptical nature of the radiation emitted by a storage ring. If our observer moves slightly off the orbit plane, he will "see" an elliptical orbit rather than a single oscillator. The motion can be decomposed in two orthogonal oscillations with a 90° phase shift: the vertical oscillation will give raise to a vertical polarization component of the radiation, just as the horizontal one. The characteristics of the synchrotron radiation are fairly complex from a mathematical point of view. The source is characterized by a continuous spectrum extending over a wide photon energy range; a set of utilities, described in the *Utilities* section of the UG, is provided to study the photon distribution in angle and energy. From our point of view, the main conclusion is that the number of photons emitted by the source in vertical (the synchrotron orbit being assumed horizontal) is given by a law $N(\theta, \hbar\omega)$. Since the form is complex and not reducible to closed form, SHADOW uses the inversion method to generate the source distribution. Furthermore, since the "sweeping" effect of the orbital motion averages out the emission in horizontal, the SR source is assumed to be uniform in the horizontal direction.

Exact Model

In this method the exact function $N(\theta, \hbar\omega)$ is computed at a selected $\hbar\omega$. Since the process involves the integration from scratch of Bessel functions of fractional order, it should be used only for verification purposes. Typically, it may take up to 10 minutes of CPU to generate an exact source. Once generated, the *pdf* is integrated to form the *CDF* that will be used by an inversion algorithm to generate the random variate.

Interpolated Model

This model makes use of the scaling properties of the synchrotron radiation. It can be shown that the spectrum emitted by relativistic electrons can be written in function of the reduced variables $(\hbar\omega/\epsilon_c, \gamma\theta)$ while its value is scaled by the factor E. In this way it is possible to precompute an accurate two-dimensional distribution of the photon energy fro the generation of the source spectrum. A file called SRSPEC.DAT is included in the SHADOW distribution tape and contains the SR spectrum CDF's computed from 0.000001 to 10 in ϵ_c units. When an SR source needs to be generated, SHADOW reads SRSPEC, scales it to the new units and then generates the photon distribution by inversion of the CDF's. Since the distribution is two-dimensional (in θ and $\hbar\omega$) and the two variables are not independent, the following steps are taken. First a photon energy ω_0 is generated by inverting the *angle integrated* spectrum $N(\hbar\omega)$ (after scaling). Then the two CDF's relative to $N(\theta, \omega_1)$ and $N(\theta, \omega_2)$ are interpolated to obtain that of $N(\theta, \omega_0)$ which is then used to generate the angle. The process is highly efficient, to the point that several thousands rays are typically created in a few seconds of CPU. In this model the user can specify any photon energy range extending between the above limits.

Electron Emittances

The electron emittance effects, i.e., the fact that the electrons are not all moving on the ideal central orbit but are rather distributed around it with a distribution law given by eq. 1.12, can be taken in account easily if one notices that the formulae describing the radiation emission are shift-invariant in the angle coordinates. That means that Eq. 1.12 reduces to the more tractable:

$$N(x', y') = \int dx dy \, \rho(x, y) \, N(x - x', y - y') \qquad (1.13)$$

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on the velocity variables. In other words, the photon emission is aligned to the electron direction. It is thus possible to generate the photon energy and angle independently from the electron direction and then simply shift the emission angles along the orbit of that particular electron. In this way a convolution between the two distributions is automatically obtained. The fact that an electron is moving at an angle z' from the orbit plane also implies that the magnetic field seen by the electron is $H_0 cos(z')$, thus leading to a slight red shift. This effect is normally not appreciable because of the broadband nature of the emission but if a monochromatic synchrotron source with non-zero emittances is specified, the user will notice a broadening of the photon energy spectrum generated by SHADOW.

1.5.4 Insertion Devices

Insertion devices are special radiation sources made by a periodic array of dipolar magnetic fields that impart to the electron beam a snake-like, undulating, trajectory. We refer the user to specialized literature for a full discussion of their properties. SHADOW includes a module, EPATH, for the computation of the trajectory of an electron in a sinusoidal magnetic field. This trajectory is computed by solving the electron equations of motion and stored in a user-specified file for use by other programs. The trajectory is computed only for electrons launched on-axis and includes end correcting fields.

An important parameter that is used to define insertion devices is the so-called deflection parameter K. The maximum angle of deflection of the electron for sinusoidal motion is observed when the electron crosses the undulator axis, i.e.,

$$\delta_W = \frac{K}{\gamma} = \frac{e}{\gamma m c^2 \beta} \frac{\gamma_0 B_0}{2\pi} \tag{1.14}$$

From the user's point of view, there is a main difference between the case of insertion devices and that of the bending magnet. In this last case, the user needs to specify only the machine's radius and energy since all the spectral information is already pre-computed in the file SRSPEC.DAT. In the case of IDs no simple scaling relations exist so that the user itself will have to generate the equivalent of SRSPEC.DAT, by running the MAKE_ID facility.

Large K: Wigglers

Briefly, ID's can be divided in two classes, wigglers and undulators. In the first, the magnetic field is so large that the amplitude of oscillation is not small and the angle relative to the ID axis is as well large. From the point of view of an observer located at a distance D, the overlap between the fields created at each bend will be small so that the wiggler will appear as as formed by N_p independently emitting bending magnets. The radiation can then be easily computed using: a) the scaling properties of the radiation and b) the knowledge of the trajectory radius of curvature at any point. The overall spectrum will be then N_p times more intense than that of a bending magnet of same field. SHADOW computes the source by using the following algorithm. Most of the photons will be emitted in the regions of high curvature and very few in the region between poles. A utility program, EPATH (see below) is used to compute the trajectory in the wiggler. Then, the total number of photons emitted at each point of the trajectory is computed, integrated and normalized to obtain the CDF of the total photon emission. This CDF is used to select from which point in the trajectory a photon will be emitted by using the usual inversion algorithm and the radius of curvature of the trajectory at that point, ρ, is then computed. From now on the source is treated as a conventional bending magnet of radius ρ and convoluted with the electron emittances, if specified. The overall properties of the source are not too dissimilar from that of a bending magnet, but for the fact that the source is (horizontally) more extended. The source is treated as fully incoherent, while the polarization is that of the synchrotron source.

Small K: Undulators

The case of the source model for undulators is quite more complicated than that of the bending magnet case and again we refer the reader to specialized work. SHADOW includes an insertion device source model that is adequate for most cases; however, for sophisticated calculation ad-hoc sources should be generated. The undulator sources are characterized by relatively small values of magnetic field so that the angle of the trajectory with the central orbit remains always small: this means the loss of the factor of $1/\gamma$ due to the short duration of the radiation pulse so that the fundamental wavelength is blue shifted only by γ^2. However, the small angles also mean that the field radiated along the trajectory overlap strongly giving raise to interference patterns, whose sharpness depends on the number of poles of the undulator. The interference process leads to the formation of peaks in the spectrum at energies:

$$\lambda_m = \frac{\lambda_u}{2m\gamma^2}(1 + \gamma^2\theta^2 + \frac{K^2}{2}) \tag{1.15}$$

with width of the order of $1/N_p$. Similar to the case of a diffraction grating or a crystal, the radiated spectrum contains two terms: the form (or structure) factor that depends on the details of the trajectory within each period and the grating term which is of the form $sin(N_p x)/sin(x)$. The spectrum is thus formed by a series of narrow harmonics centered at λ_m, whose relative intensity decreases with m. On axis, symmetry arguments force all of the even harmonics to be zero. The source is not invariant under any simple transformation, as was the case for the bending magnet. The calculations of this type of source are fairly computer intensive and require carefully optimized code. The source is still shift invariant in the angles (the magnetic field is assumed to be uniform so that the cross section does not matter). Since no general scaling relationships exist for this case, it is unfortunately necessary for the user to recompute the source for each case under examination. The basic idea is similar to that of the bending magnet, i.e., to generate a set of tables that contain the source CDF's in energy and in the angles. Because of the geometry, the source is now function of (θ, ϕ, ω) and larger arrays are necessary. From the point of view of the user it is necessary then to generate a file, similar in principle to SRSPEC.DAT described before, that can be used by SHADOW to generate the random variate describing the undulator source. Since the peaks can be fairly sharp, it is a good idea to limit the range of photon energy generation to a narrow region around the harmonic of interest.

Improved and External Sources.

The source is improved by two passes of linearization in Y. Because of space limitation, the maximum size of the array used to compute the source has been limited to (31,31,51) in (θ, ϕ, ω). The finite sampling frequency may cause problems (aliasing) if the peaks are too narrow, as often may be the case. For this reason the source is linearized twice in Y, in order to improve the sampling precision. An initial range and number of points is defined, say 10 eV and 51 points. A spectrum is computed and from it a first set of CDFs. These are now used to compute the position of 51 points equispaced in Y, so that the regions of rapid variations (peaks) are now sampled much better. New CDF's are computed and the process repeated, to insure a good convergence. The result is a set of CDFs already linear in Y that can be very easily inverted to generate the photon distribution; most importantly, the mathematical model concentrates on the regions of actual photon generation, in complete agreement with the philosophy of the stochastic model. SHADOW can use arbitrary external sources, as long as they are specified in a format usable by the code.

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