

SHADOW
User's Guide

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Contents

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)*:

$$N(\mathbf{r}_i) = p(\mathbf{r}_i) \cdot N_0 \quad (1.1)$$

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. 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

Figure 1.1: Example of Deterministic and Stochastic Functions
Notice change of spacing in lower panel

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:

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

Figure 1.2: Example of Stochastic Sampling
The solid curve is the CDF of the distribution shown.

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 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:

$$\mathbf{A}_i(\text{after}) = \mathbf{A}_i(\text{before}) \cdot \mathbf{R}_i \quad (1.3)$$

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:

$$\langle E \rangle = \sum_{i=1}^N E_i \cdot A_i^* A_i \quad (1.4)$$

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 :

$$y = F(x) \quad (1.5)$$

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):

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

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:

$$\langle A \rangle = \int dx A(x) F(x) = \int d\left(\int_{x'} dx' F(x')\right) A(x) = \int dYA(x(Y)) \quad (1.7)$$

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:

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

where p_1, \dots, 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 $N = 11$ $M = 3.6 \cdot 10^8$). 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).

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.,

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

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, 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

¹For 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.

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:

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

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 stored². 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 of the losses³. In other cases, the ray may happen to be definitively lost:

²There 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.

³This 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.

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 ($\phi_G = \text{Optical Path}/\lambda$) 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*.

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:

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

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:

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

where (x, y, \dots) 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.

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, $\omega = e_0 H c / E$. 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

⁴Over 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

⁵For 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.

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 rise 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 from 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:

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

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.,

$$\delta_w = \frac{K}{\gamma} = \frac{e}{\gamma mc^2 \beta} \frac{\gamma_0 B_0}{2\pi} \quad (1.14)$$

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:

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

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.

1.5.5 Source Optimization

In some cases it may happen that a given source is ill-matched to an optical system, so that only a few rays survive the propagation. In terms of phase space this means that the etendue of the system does not overlap that of the source. This can be easily verified for example by reverse ray-tracing, i.e., tracing from the final image (such as the exit slit of a monochromator) back through the optical system to the equivalent source plane. Then one can display simultaneously the two phase spaces and verify the overlap. In the case of a mismatch, the etendue of the system will typically be much smaller than that of the source. It is in principle possible to use this information to improve the statistics, by rejecting the rays that fall outside the etendue of the OS. However, storage problems (the phase space of interest is really 7-dimensional) restrict the application to the case of systems with independent sub-spaces in $\{x, y, z\}$. In order to use this feature, a first run is made without optimization. Then a utility program is run to generate the histograms that represent the etendue of the system as a fraction of the source and the resulting file passed to `SHADOW`. This process may be repeated a couple of times to improve the analysis, but should always be used with caution.

Figure 1.3: Preliminary programs for wiggler and undulator

1.6 Preliminary Programs

As said before, some of the source models implemented in SHADOW cannot be scaled or defined exactly because of their computationally intensive nature. This is particularly true for the case of the insertion devices. It is then necessary to run some utilities to generate the files needed by SHADOW. This utility is called MAKE_ID, and is activated by the command MAKE_ID. Although the prompts are not too dissimilar, the algorithms implemented differ profoundly for the two cases. This is true also of their computational efficiency (the Undulator case is much more time consuming than the Wiggler). Transparently to the user, the MAKE_ID activates several different programs in the right sequence. Although SHADOW is a self-contained program, it may be the case that the user has available some local code to generate undulator sources spectra. If this is the case, the program will have been installed by the system manager and will be activated by selecting the proper flag during the execution of MAKE_ID. At the outset the user is prompted to select Undulator vs. Wiggler source. Once the selection is

made and the rest of the parameters specified, the program activates the EPATH module; this computes the trajectory of the electron in the insertion device. However, for calculation efficiency in the case of the Undulator only one period is computed and the data stored in a binary array (not printable or plottable). The trajectory of the Wiggler is stored in a formatted file that can be easily printed or plotted ⁶.

1.6.1 Wiggler Source

After the trajectory has been computed a module called NPHOTON is activated. This module computes the radiation spectrum over the range (in energy) specified in the I/O session, to finally generate an unformatted file that contains the source description to be used by SHADOW in the module SOURCE. When running in PROMPT mode, the user will notice that the only inputs requested in the case of the wiggler source are the name of the file that contains the source description and the specification of the electron beam parameters. The user will also notice that several files will have been generated in the process; they are the *trajectory*, *source* and *parameters* files. Their meaning is explained in detail in the example (and in the DEMO section) below.

1.6.2 Undulator Source

As explained, the Undulator source is much more complex because of its strong chromaticity. One of the parameters used in the I/O requires some explanation of its use, and that is the *End Field Correction Factor*. Its use is best explained by following the example in the DEMO section on the Undulator source; briefly, it is used to fine tune the source spectrum. The suggested procedure is to run the on-axis case using the utility USER_UNDUL on the trajectory file obtained from MAKE_ID when exiting before computing the photon source, and then to plot out the spectrum on a logarithmic scale, using TopDrawer. Ideally, the spectrum should be formed by a series of peaks at the harmonics and look like in Fig. 1.4. If some extra features such as the extra dip shown in Fig. 1.5 should appear, in this case between first and third harmonic, then the value of the factor should be changed until the extra feature disappears and the spectrum becomes “nice” (the default correction factor is 1.0). See also page 60. Make a note of that factor and enter it when running MAKE_ID. We notice that the effect of the correction is apparent only in the region where there are very few photons (its a logarithmic plot) so that the effect on the overall distribution is small; in the majority of the cases there will be no need of “fiddling” with the correction factor. In any case, there are some more important points to be made. The first is the *Internal* vs. *External* case selection; as explained earlier, this refers to the case of which program is used to generate the source (SHADOW’s vs. the “Home recipe”). After this decision is made, the program will ask the user about the size array to use. For more on the arrays, see page 59. Which one to use depends on the available computing resources and the type of modelling; for example, a source spanning a narrow photon energy range and a small angle spread will be quite well described by the *small* model. In other cases, such

⁶If you want to plot out the trajectory of the electrons in an undulator, as computed by SHADOW, run the *wiggler* case with the parameters appropriate to the *undulator*. This will give you a plottable file

Figure 1.4: Correction factor of 0.9925

as broad band calculations spanning several harmonics it will be necessary to use the larger array. Some experimentation will be quite useful. Another important concept is that of the “*improved*” source (we reserve the term “*optimized*” for the case discussed earlier). The source model is improved by generating a stochastic representation rather than a deterministic one for the source. This is achieved by performing several passes of calculations. The first is used to determine a first estimate of the radiation spectrum. In the second, a stochastic representation of the *total* flux is generated. From this, a new set of spectra at deterministic angles is computed and the cycle repeated for the other two variables (θ and ϕ). The cost of an improved source calculations is then that of a factor of three in computational time; in some cases (very narrow harmonics) this may be a necessary price to pay. Normally, after a few trial runs to make sure that the parameters are setup properly, a batch job is the best way of computing the source file.

Figure 1.5: Correction factor of 1.0

Chapter 2

Detailed Input Description

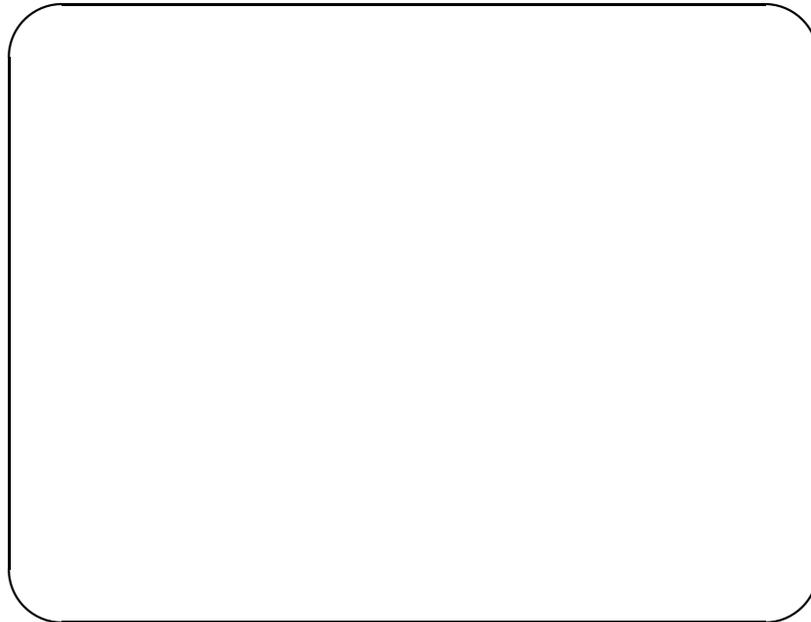
This section of the Guide will go through the SOURCE part of SHADOW in detail. We will show the screen output for both the PROMPT and MENU modes, explain what is being asked for, and give examples of uses for each choice. If applicable, we will then show a three dimensional “picture” of what’s going on. The following page will show the contents of the Binary Output File used by PLOTXY and the output PLOTXY gives. The last page lists informal notes, errata or bugs.

After starting SHADOW, the following screens will appear.

PROMPT:

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MENU:

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Source Sampling – Random

Source Sampling	Random
-----------------	--------

RANdom in REAL Space:

Points in (X, Y, Z) space where the rays originate are pseudo-randomly generated. The distributions are chosen by the user in the $X - Z$ *Plane source type* section and the *Source depth* section. The number of random rays to be generated along with a seed for the random number generator are supplied by the user.

RANdom in MOMENTUM Space:

Points in (X', Z') space where the rays originate are randomly generated. As with real space the distributions are selected by the user, although the nature of the angle distributions are different than those of position.

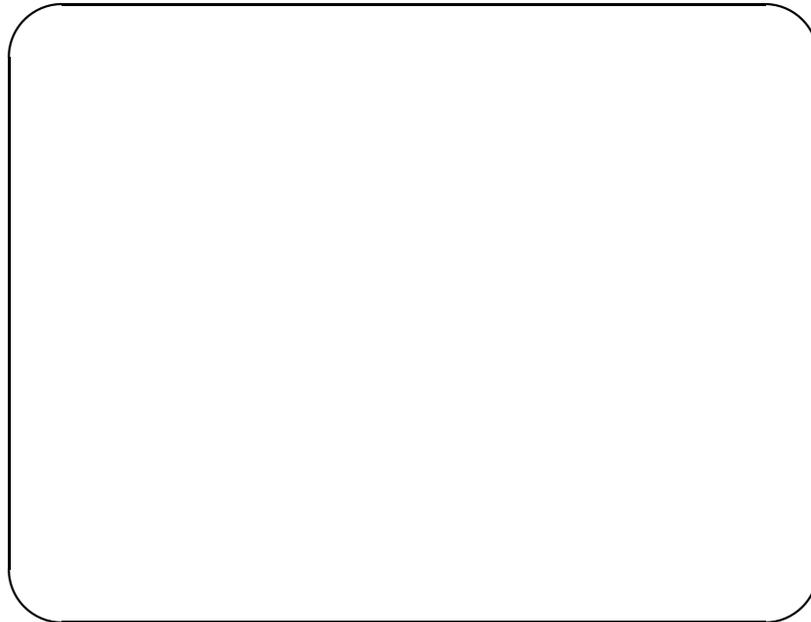
Example:

In most cases the source modelling type will be RAN/RAN – since sources radiate according to stochastic processes. Generally the rays are distributed independently in the \bar{X}, Y, Z, X', Z' directions. This is demonstrated by the graphs on page 28 in the phase space plot. Note the lack of correlation between X and X' . However, in other cases this may not be true. For example, in a synchrotron source X and X' will not be independent.

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MENU:

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Source Sampling – Grid

Source Sampling Grid

GRID in REAL Space:

Points in (X, Y, Z) space are generated in a regular fashion according to a selected distribution (e.g. elliptical). The number of points along each direction is supplied by the user.

GRID in MOMENTUM Space:

Points in (X', Z') space are generated following the source angle distribution selected by the user. The number of points in the X' and Z' directions are given by the user. In the menu mode VX and VZ refer to X' and Z' respectively. In prompt mode “Number of Points in the Vertical” refers to the number of points in the grid along Z' . Similarly, “Number of Points in the Horizontal” refers to X' .

Example:

Grid sources may be used to determine the image defects (aberrations) of an optical system. They are also useful for plotting the wavefront of a bundle of rays, and determining interference and diffraction patterns by keeping track of phases at points on a uniform grid. The graphs on page 29 illustrate GRID/GRID sources in the laboratory reference frame and in (X, X') phase space. The total number of rays generated in a GRID/GRID source is $NX * NY * NZ * NX' * NZ'$, where NX is the number of points in the X -direction etc. This product must be less than 5000.

Laboratory Reference Frame for a RAN/RAN Source:

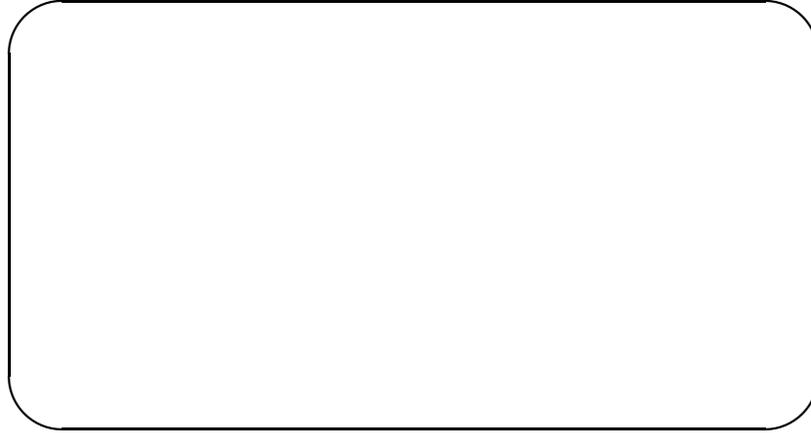
PLOTXY Result:

Laboratory Reference Frame for a GRID/GRID Source:

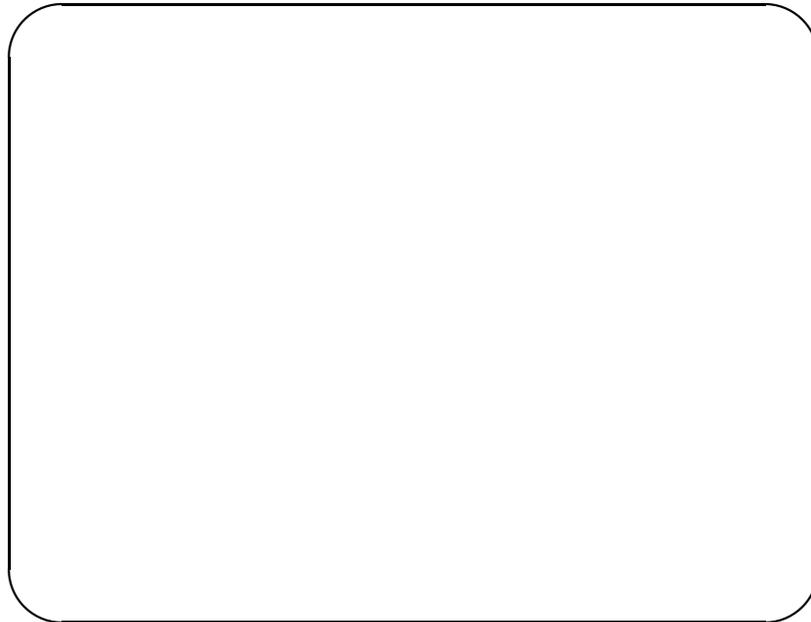
Source Sampling

PLOTXY Result:

PROMPT:

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MENU:

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Source Sampling – Grid/Ran Example

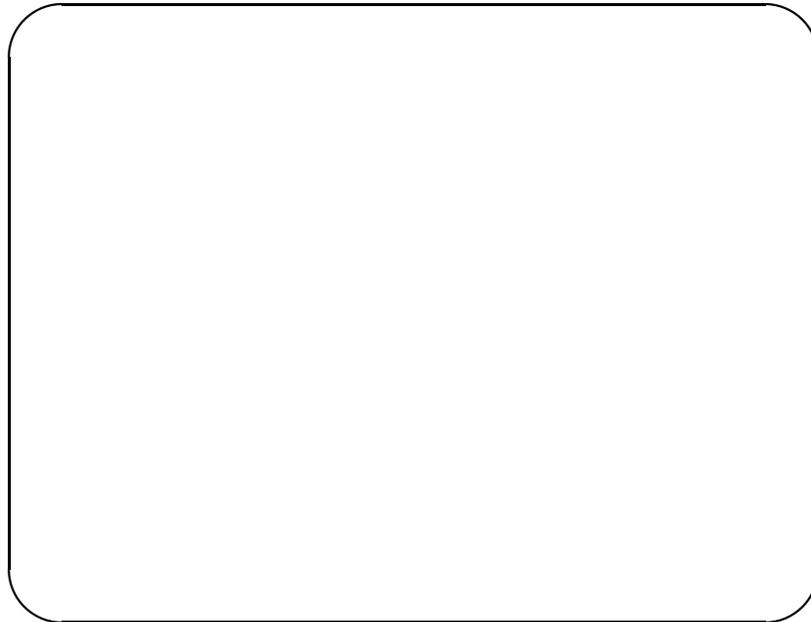
Source Sampling	Grid/Ran
-----------------	----------

This source is useful for “searchlight” studies. The graphs on page 34 illustrate GRID/RAN sources. Note that the points are spaced regularly in the XZ plane, but the directions X', Z' are randomly generated according to the desired distribution. However, for each point in real space the random directions are identical. This is most clearly shown in the phase space plot. The total number of rays generated in a GRID/RAN source is $(NX * NY * NZ * \text{NUMBER OF RANDOM RAYS})$. Note the phase space duality between GRID/RAN and RAN/GRID.

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MENU:

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Source Sampling – Ran/Grid Example:

The graphs on page 35 demonstrate RAN/GRID sources. The points in the XZ plane are positioned randomly – according to the chosen distribution. From each point the directions of the rays are generated in a regular fashion according to the chosen GRID distribution. The number of points in a RAN/GRID source is (NUMBER OF RANDOM POINTS * NX' * NZ')

Source Sampling Ran/Grid

Laboratory Reference Frame for a GRID/RAN Source:

PLOTXY Result:

Laboratory Reference Frame for a RAN/GRID Source:

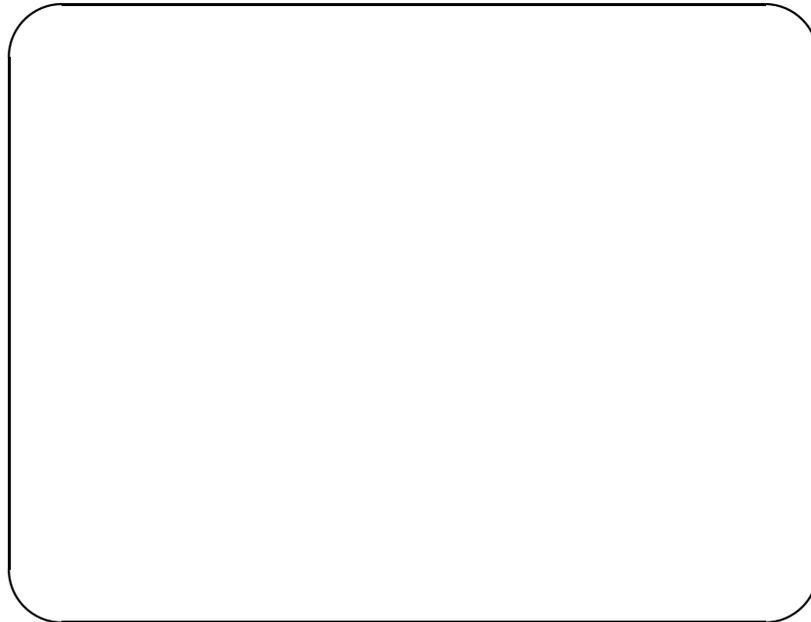
Source Sampling

PLOTXY Result:

PROMPT:

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MENU:

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ELLipse in Phase space:

Points in the two phase spaces, (X, X') and (Z, Z') , are independently generated along ellipses. The following parameters are supplied by the user:

1. σ (Standard deviation) in X
2. σ in X'
3. The number of σ Levels in X - Phase space
4. The value in multiples of $(\sigma_X, \sigma_{X'})$ for the ellipse of each level.

The first two parameters define a two dimensional independent gaussian distribution in one of the phase spaces. The number of "Levels" is just the number of ellipses to be generated on the gaussian surface. The value in multiples of σ defines where on the gaussian surface the ellipses are to be generated. For example, if we chose the value of one of the levels to be $2 * \sigma$ then 68% of the defined phase space would lie inside of this ellipse. Points along the ellipse can be generated at random positions or in a grid fashion (corresponding to ELLI/RAN or ELLI/GRID in source description menu).

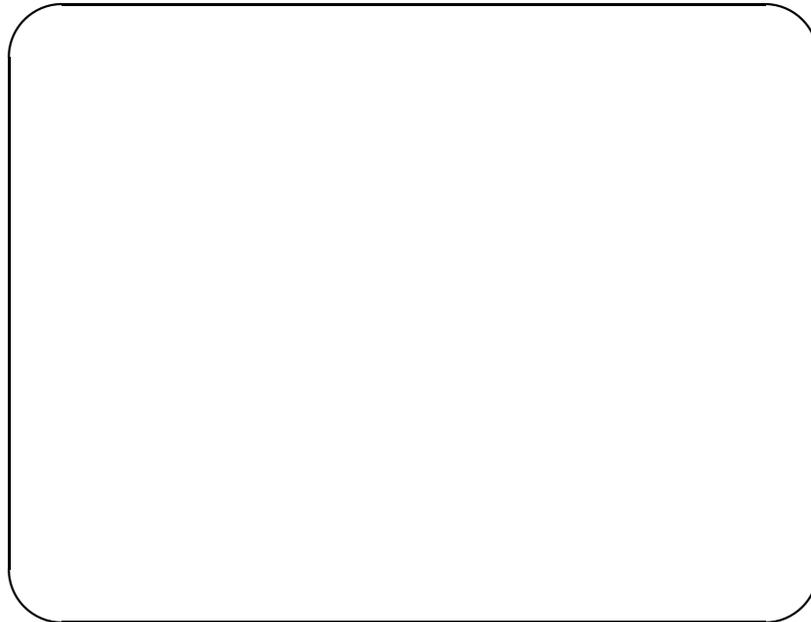
Example:

Phase space ellipses depict the correlation between position and momentum space in one dimension, say X and X' . Such a representation is useful for determining the dynamics of the beam, i.e. if it is focused, converging or diverging. Some optical elements may cause distortions in the ellipse, but the area is conserved throughout the system. The number of rays generated in an ELLI/RAN source is $(\text{NUMBER OF RANDOM RAYS})^2 * (\text{NUMBER OF } \sigma \text{ LEVELS IN } X) * (\text{NUMBER OF } \sigma \text{ LEVELS IN } Z)$ On page 40 notice how the ellipses are regularly spaced, but points are random around each ellipse.

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Source Sampling – Elli/Grid Example

Source Sampling Elli/Grid

ELLI/GRID is more useful than ELLI/RAN for determining exactly how a phase space ellipse has been transformed by an optical element. The number of rays generated in an ELLI/GRID source is (NUMBER OF POINTS ON EACH ELLIPSE IN X) * (NUMBER OF σ LEVELS IN X) * (NUMBER OF POINTS ON EACH ELLIPSE IN Z) * (NUMBER OF σ LEVELS IN Z). In the Phase space plot on page 40 notice the similarity to a GRID/GRID source. A more thorough description of phase space ellipses is on page 37 .

PLOTXY Result for a ELLI/RAN Source:

PLOTXY Result for a ELLI/GRID Source:

A Grid/Ran source may be used to study cases where the image is more dependent on the position in the XZ plane than on the divergence (for very small angles). An example would be to examine how an image of an off-axis point compares to the on-axis image. This example was traced with a 3x3 grid centered on axis, incident on a toroidal mirror. The image is shown below.

Source Sampling

A Ran/Grid source may be used to discriminate between images that are more dependent on the divergence than the source shape. An example would be to create a slit source in real space and a few discrete angles in momentum space, shine the beam on a diffraction grating, and examine the relationship between image position (and shape) and divergence angle. This example was traced with 5 discrete angles. The diffracted image is shown below.

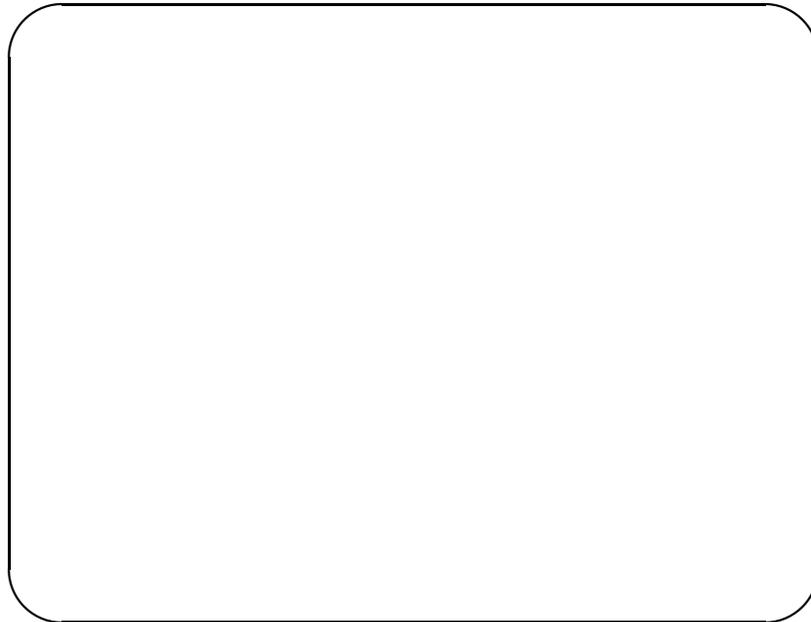
NOTES:

- A note about GRID sources: the number of rays can get very high if you're not careful. A source with a 20 X 20 grid in the $X - Z$ plane and 10 points in depth along with a 10 X 10 array in X' and Z' doesn't seem to be a very fine grid, but it will generate 400,000 rays! The maximum number of rays that SHADOW should normally generate is 5,000. The program will stop if the number is greater than 5000.
- For random models, the number generator requires an ODD number with at least 8 digits for the seed.
- All PLOTXY results in the source modelling section were from the actual sources generated by the prompt/menu examples.
- All laboratory reference frame plots contain only a few rays for the purpose of clarity – these do not show the same source as in the PLOTXY graphs.

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Optimization**Optimization**

Sometimes when a system is traced, a substantial number of rays may be lost due to vignetting or mismatch of system and source etendue. High losses are undesirable since reliability of ray statistics and CPU time are sacrificed. The user may wish to have a more efficient source without altering the parameters. This can be achieved by flagging that area of phase space in which source rays are lost, then regenerating the source with no rays occupying the flagged phase space regions. The file used for the source optimization is generated by the utilities REFLAG or SHADOWIT followed by HIST03. Refer to the documentation on these routines for more information. Generation of an optimized source follows the example.

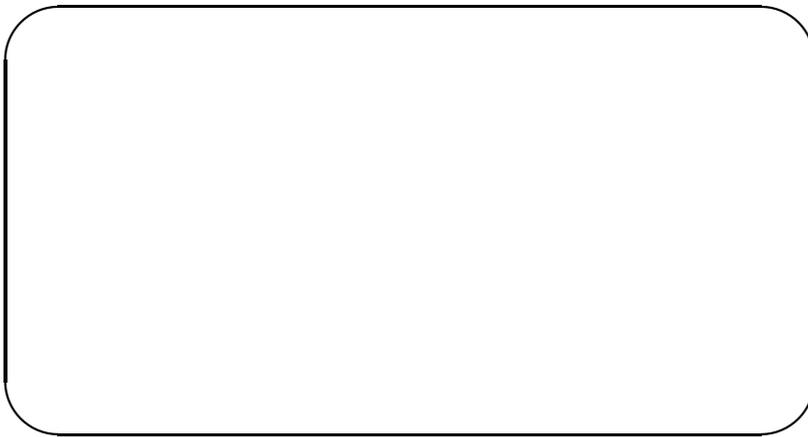
Example:

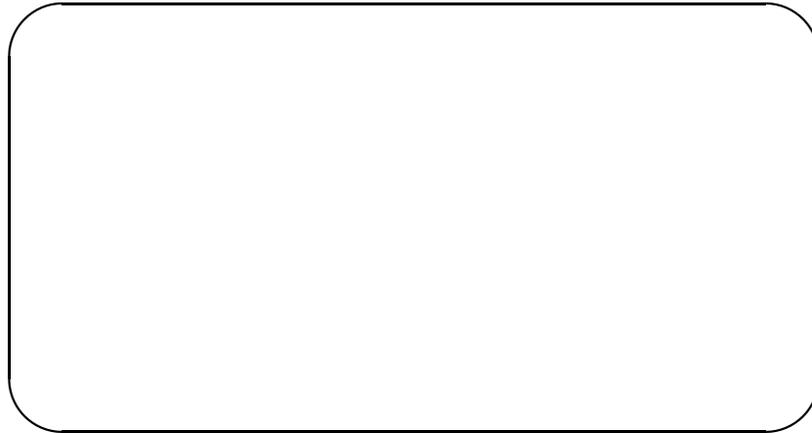
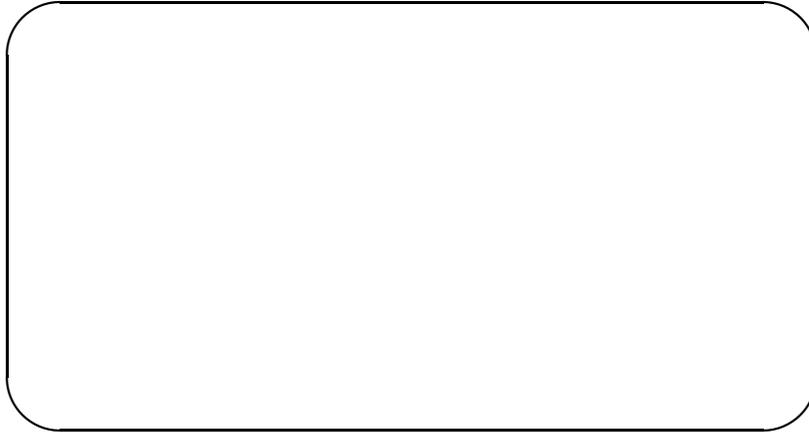
An example in which the source optimization is useful is with a monochromator where the entrance or exit slits block a large number of the rays. The source can be regenerated so that all rays pass through both slits, yielding better statistics when analyzing the system characteristics such as resolution.

Output from SOURCINFO:

Output from SYSINFO:

SOURCINFO and SYSINFO describe the source used and the system it was traced through to demonstrate optimization. Notice above in the output from MINMAX, the large number of lost rays. The following shows the process of optimizing the source. The source must then be regenerated using the file created with REFLAG and HISTO3 and retraced.





Notice the difference in the messages in this case compared to the normal source output. We then retrace the system to see if we get fewer lost rays. The output from MINMAX is below. Notice a decrease in the number of lost rays.

Optimization

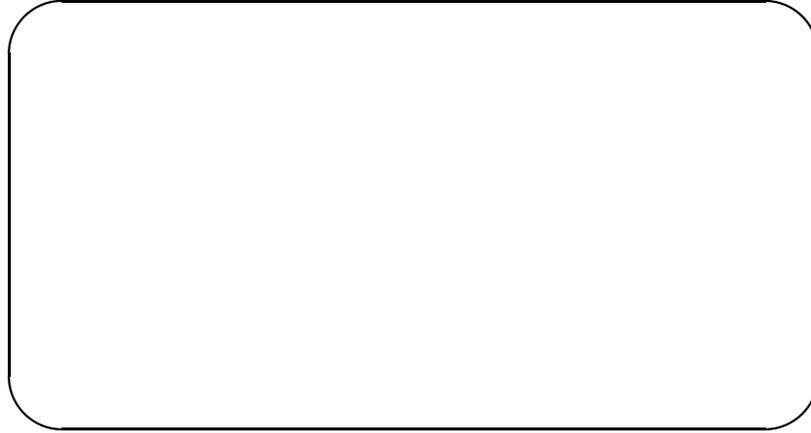
No Optimization

Optimization

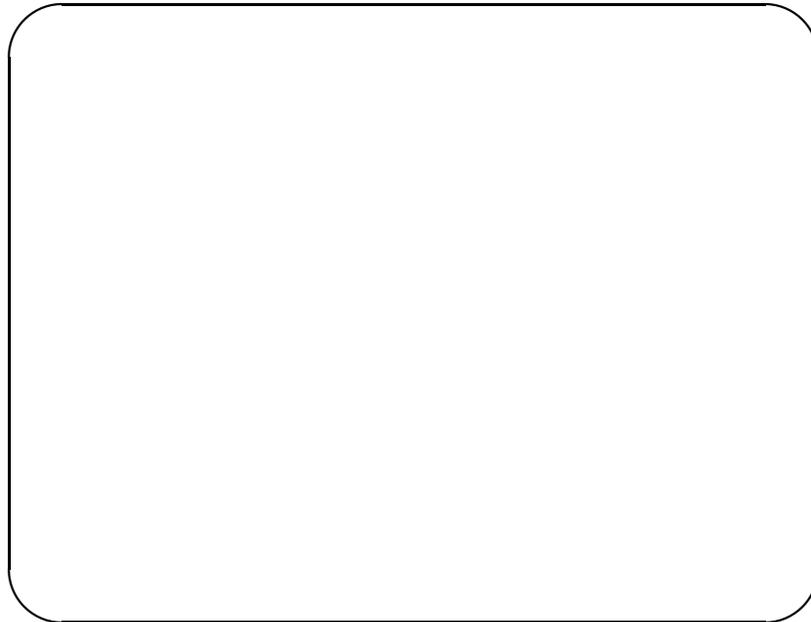
NOTES:

- For disk and memory economy, SHADOWIT flags phase spaces (X, X') , (Y, Y') , and (Z, Z') independently of each other. This independence does not necessarily exist in the system, i.e. with a synchrotron source. For this reason, optimization should be used with caution (see page 18)
- Optimization will only work for *RANDOM* sources.

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For insertion devices with large K, SHADOW uses the wiggler source. It basically assumes incoherent emission processes, thus the wiggler can be approximated by bending magnets of changing magnetic radius. Then the task is divided into computing: a) electron trajectory, b) photon radiation. They are both computed by the procedure MAKE_ID which must be called before running SOURCE.

The correction field factor is used to adjust the end magnetic fields so there is smooth transition in and out of the wiggler. The output of this first part is in WIGGLER.PAR and WIGGLER.TRAJ. The first file simply stores the parameters for the trajectory, while the second file stores the actual trajectory in the following format:

X	Y	Z
β_x	β_y	1/R

where (X,Y,Z) is the usual SOURCE reference frame, $\beta=v/c$, R the instantaneous radius of curvature. They are both formatted files and metric units (meter) are used.

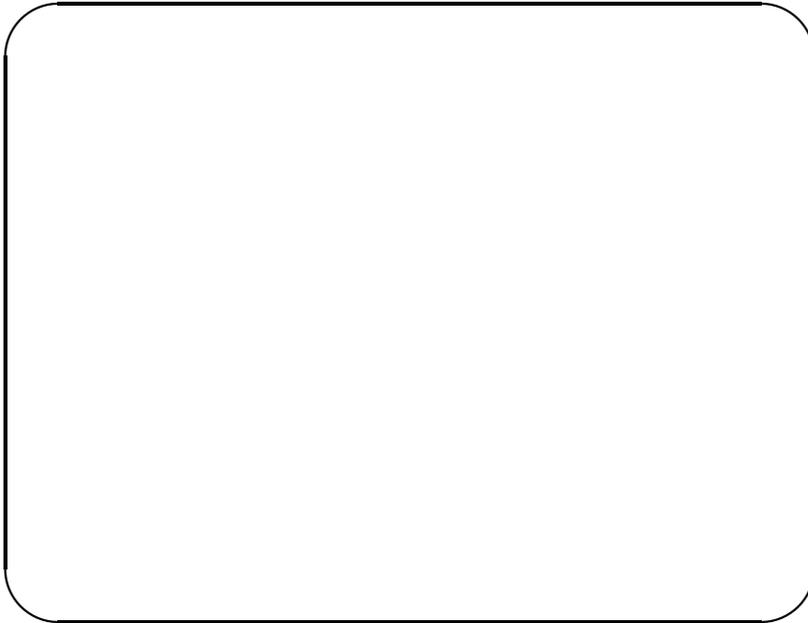
The second part uses the trajectory file (WIGGLER.TRAJ) from the first part and computes the radiation at each point, within the photon energy range specified by the user. The output file (RADIAT.DAT) then stores the CDF of photon emission along the wiggler in binary form ready for input to SOURCE. Note that the highest critical energy ω_c is determined by the smallest radius of curvature.

MAKE_ID



MAKE_ID

Wiggler Source



Example:

For the example here, $N=10$ periods, $\lambda=10$ cm, $K=14.94$, $E=1$ GeV. Typically, 101 points is sufficient to describe the trajectory of *each period*. For the SOURCE part, we use finite emittance to demonstrate its effects which can be seen at both the top view and the cross view. The electrons come to a waist at the middle of the wiggler, as we have specified in SOURCE. Most photons are clearly generated near turning points, giving rise to the two loops when viewing the wiggler head on. Note the entire wiggler is offset to the positive x-axis. The photon energy range, on the other hand, is taken from MAKE_ID (1-100 eV).

Binary Output File Data:

Col	Par	Minimum:	Maximum:	Center:	St. Dev.:
1	X	-0.22843E-01	0.47147E-01	0.11786E-01	0.12239E-01
2	Y	-49.962	49.985	0.84569	29.300
3	Z	-0.17584E-01	0.22624E-01	0.86574E-05	0.59984E-02
4	X'	-0.78173E-02	0.80459E-02	-0.10372E-03	0.45388E-02
5	Y'	0.99997	1.0000	0.99999	0.00000E+00
6	Z'	-0.47680E-02	0.49928E-02	0.97529E-05	0.13851E-02
11	Photon Energy (eV)		1.0478	99.523	
20	Numerical Aperture		0.11507E-03	0.80810E-02	

Top View of Wiggler:

Cross View of Wiggler:

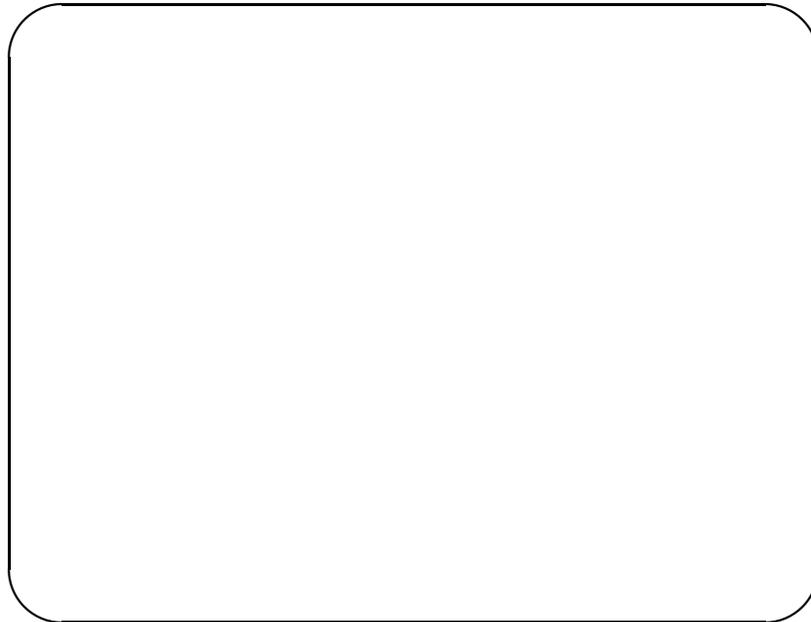
Wiggler Source

NOTES:

PROMPT:

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MENU:

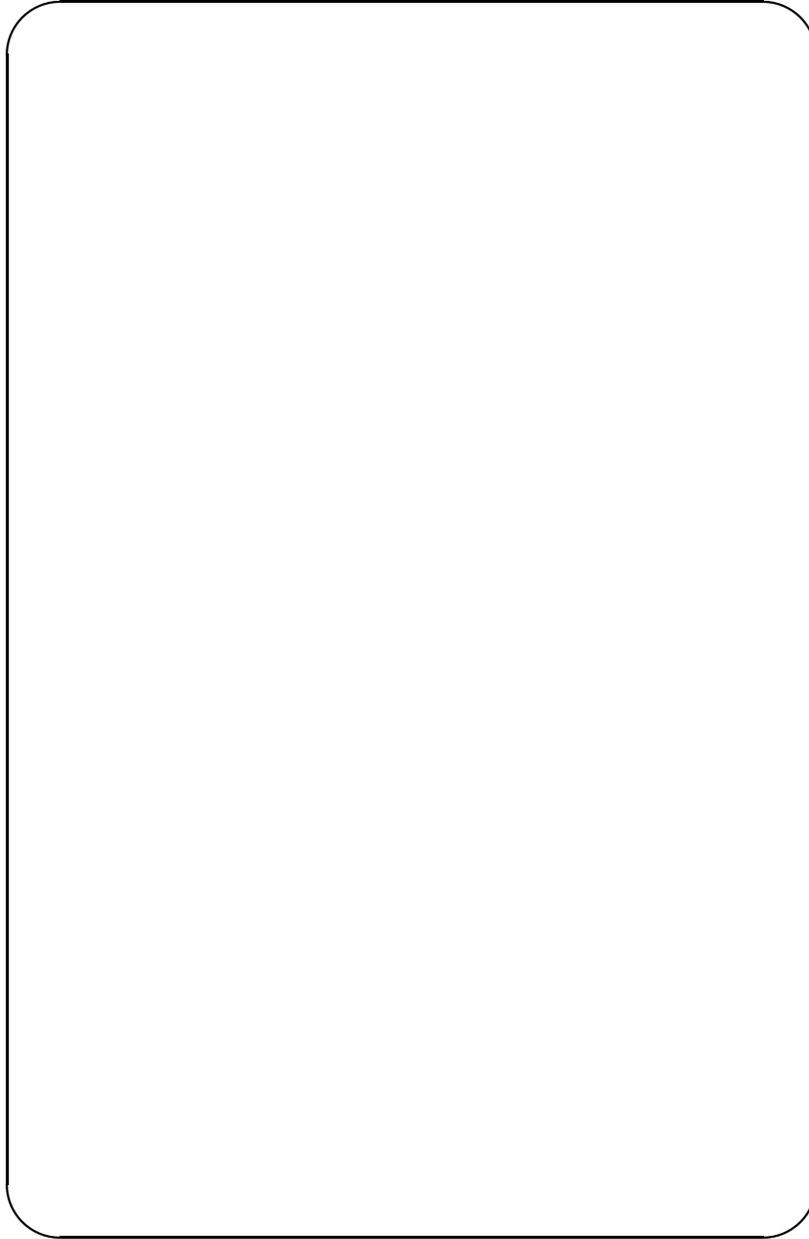
A large, empty rounded rectangular box with a thin black border, intended for a menu.

Undulator Source is the small K case for insertion devices. It is similar to the Wiggler Source in that both are generated by calling MAKE_ID, which first generates the single electron trajectory for both cases. Then they diverge when computing the photon radiation. Since no simple scaling relations exist for an undulator, the photon distribution is function of $(\hbar\omega, \theta, \phi)$ where θ and ϕ are the polar and azimuthal angles respectively referred to the SOURCE Y-axis (forward direction). Thus the distribution must be recomputed every time the photon energy range or the polar angle range is changed (ϕ is always taken from 0 to 2π), even though the physical parameters of the undulator are the same.

This process makes the undulator calculation very computer time-consuming, so we limit the $(\hbar\omega, \theta, \phi)$ array to a maximum size of (51,31,31). If the user is only looking at the peak of a harmonic, ≈ 5 array points in ω is sufficient (at least 2 points are needed for the interpolation scheme to work). For a good description of an entire harmonic, ≈ 10 to 30 points should be used to cover the wider energy range. Finally to cover more than one harmonic, the full 51 points should be used. For the angular part, we recommend using the (31,31) points whenever possible. This is especially true for the θ array because it has more structures, while the features are usually not as sharp in the azimuthal ϕ direction.

For the Undulator Radiation part, the user can choose between entering the parameters from terminal (TT:) or a namelist file. At the end of each run a namelist file called UPHOT.PAR is always created; this can be used (ITER must be reset to 0 though, see appendix for User's Program) by the user if he needs to run the program again. For the first pass, we can only use the interactive process here.

MAKE_ID

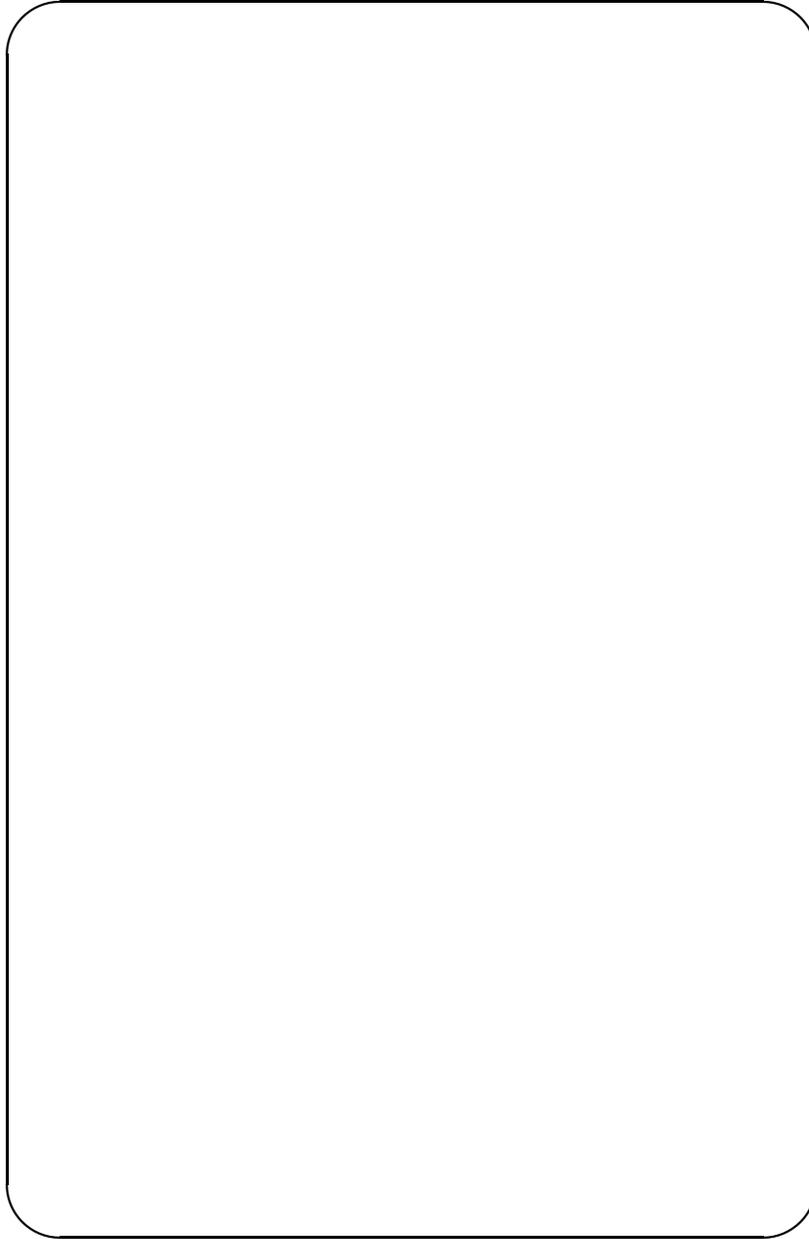


Undulator Source:

We provide a general purpose program to compute the undulator radiation distribution, which is sufficient for most cases; but the user can use his own program if he finds our program insufficient for his needs (see appendix for User's Program). To make better use of the array $(\hbar\omega, \theta, \phi)$, its not equally spaced in the variables; rather we put them where there are more photons. This involves computing the angular "rings" at each energy for the first pass, and what we called the optimization for the latter passes. At the end of the first pass, we know the approximate photon distribution. The optimization process then comes in: it finds out where there are higher emission of photons according to the existing distribution, relocates the array points in $(\hbar\omega, \theta, \phi)$, and then recomputes the entire photon distribution for the new array using either the radiation program we provided or the User's Program. The upper and lower limits on the three variables are of course unchanged. This procedure can be repeated as many time as needed, we do it four times for the example. The angular patterns as a result of each optimization are shown as X'-Z' plots below. We note that the overall features are fairly evident even before optimization, while the plot after the last optimization looks more realistic. So the last distribution (stored in CDF100.DAT;5) should be used in subsequent ray tracing. A warning here about artifact: a higher amount of rays may be generated between the rings due to the linear interpolation scheme used.

The essential output files of MAKE_ID is in CDF100.DAT (CDF100.DAT;1 is before optimization, CDF100.DAT;5 after fourth optimization). It contains the integrated probability distribution function (CDF) ready as input to SOURCE. An unintegrated version is found in RN100.DAT:*

MAKE_ID



Undulator Source:

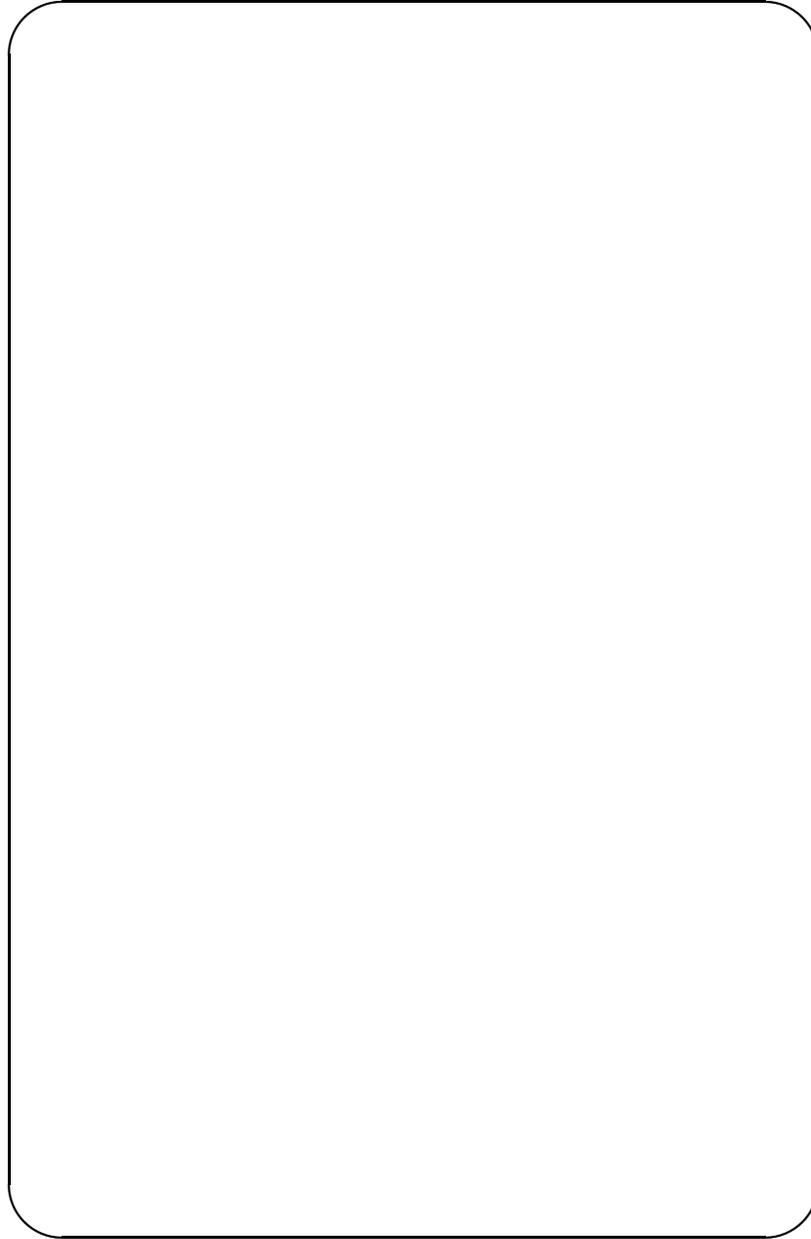
They are both unformatted files and use exactly the same format. For SOURCE, we select a zero emittance source. Since the photon energy and the angle range are already pre-determined by MAKE_ID, there is no need to specify them in SOURCE.

Example:

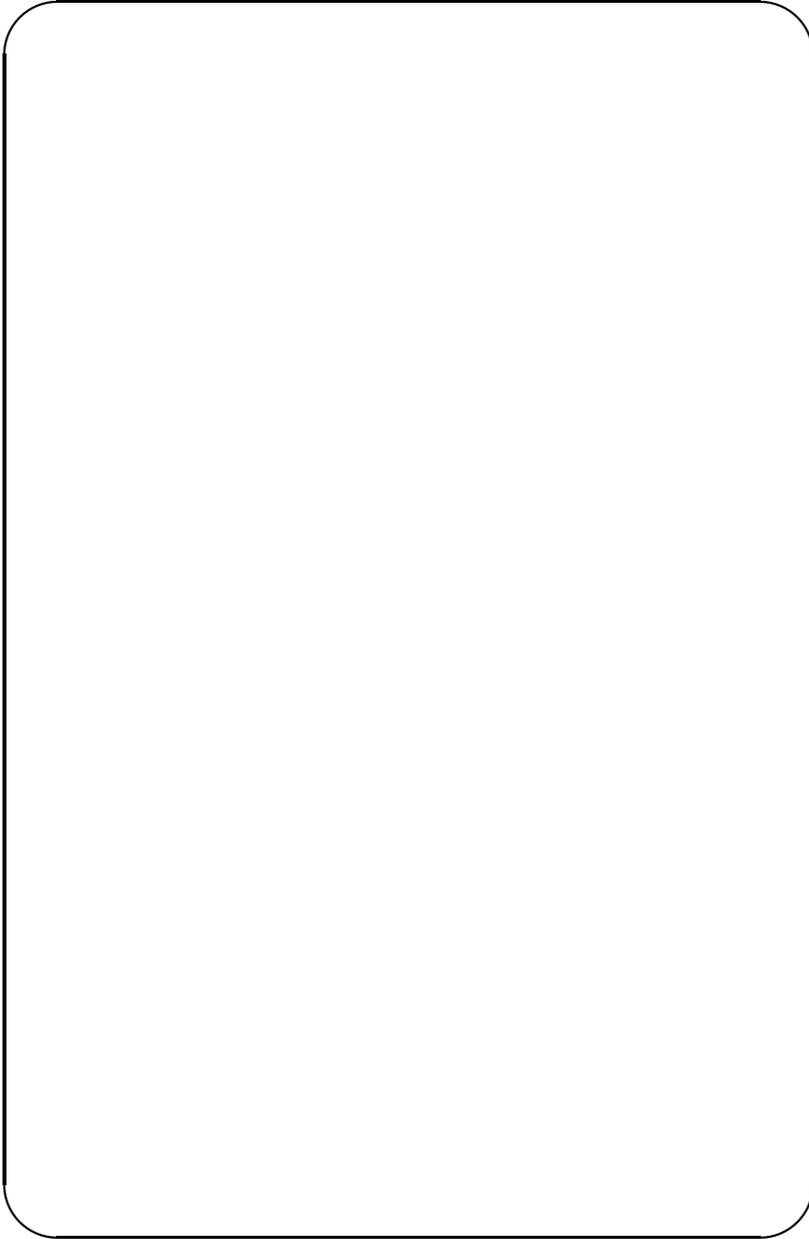
In the example below, we take an undulator of $\lambda = 3.5\text{cm}$, $K=1.87$, $E=1.3\text{Gev}$. The correction field factor modifies the magnetic fields at the two ends so that the electron trajectory transits smoothly in and out of the undulator. 101 points are used for each period. The trajectory is now fully defined, and its parameters are stored in the file SSRL.PAR and the trajectory itself in SSRL.TRAJ. An optional plottable file SSRL.PLOT is also created for demonstration, which is a formatted 5 columns file in $(X, \beta_x, Y, 1 - \beta_y, t)$ where (X, Y, Z) is the usual SOURCE coordinates, β is v/c , and t the time. The computation uses metric units and are equally spaced in the Y-axis.

In this example we are centered at the peak of the first harmonic, so 7 points in energy is enough. From the parameters of the trajectory file we note that the first harmonic is at 166.81 eV, and so we take the range from 166.6 to 166.9 eV which is still narrower than the width for a 100 periods undulator. For θ we go from 0 to 1.0 mrad. Now the calculation is fully defined which involved 6727 ($7 \times 31 \times 31$) points, and the user can tell our program to update on the screen whenever it finishes every 20 or 50 points.

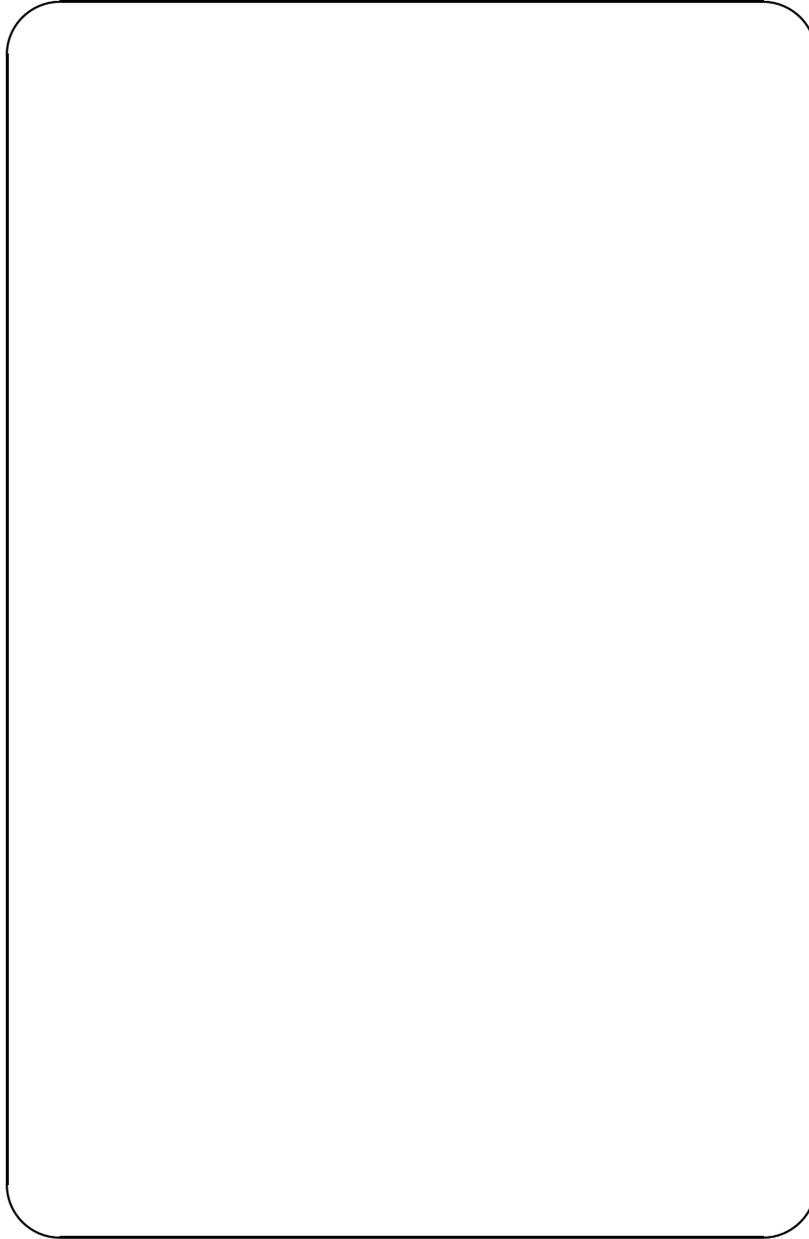
MAKE_ID



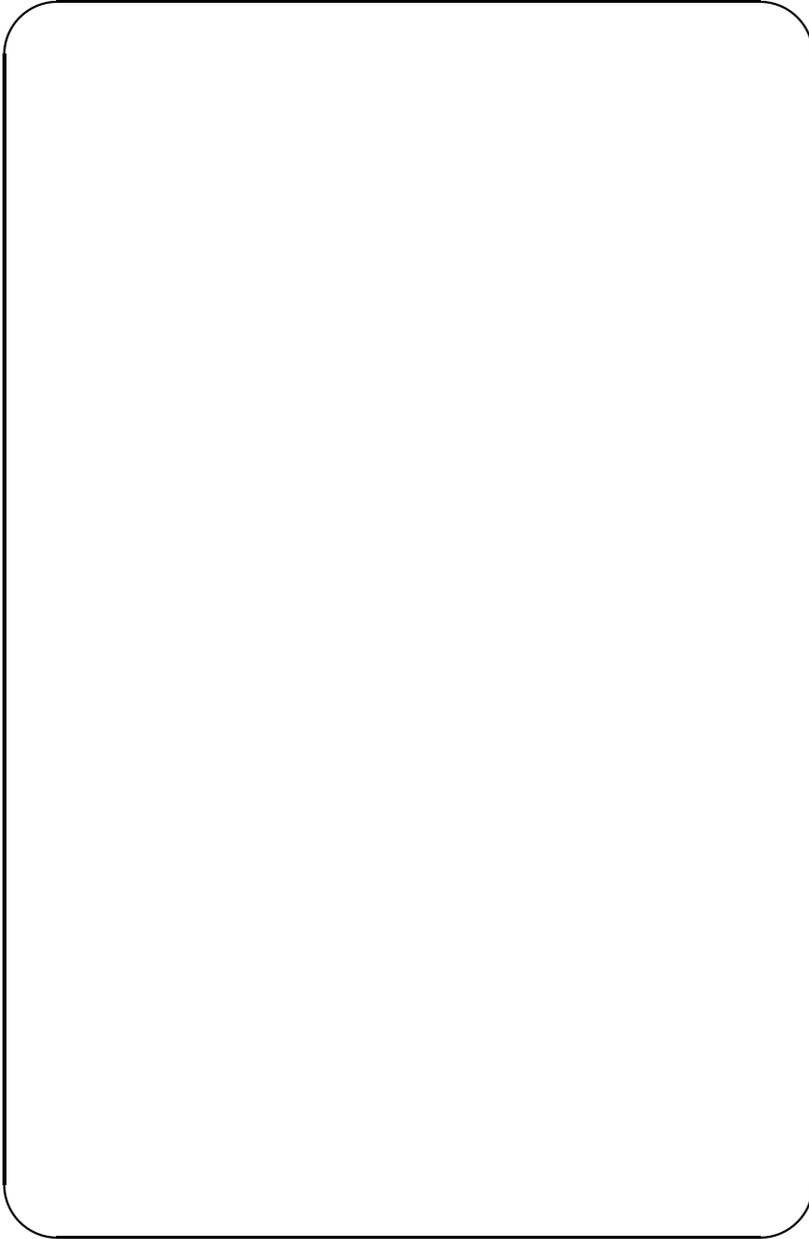
Undulator Source



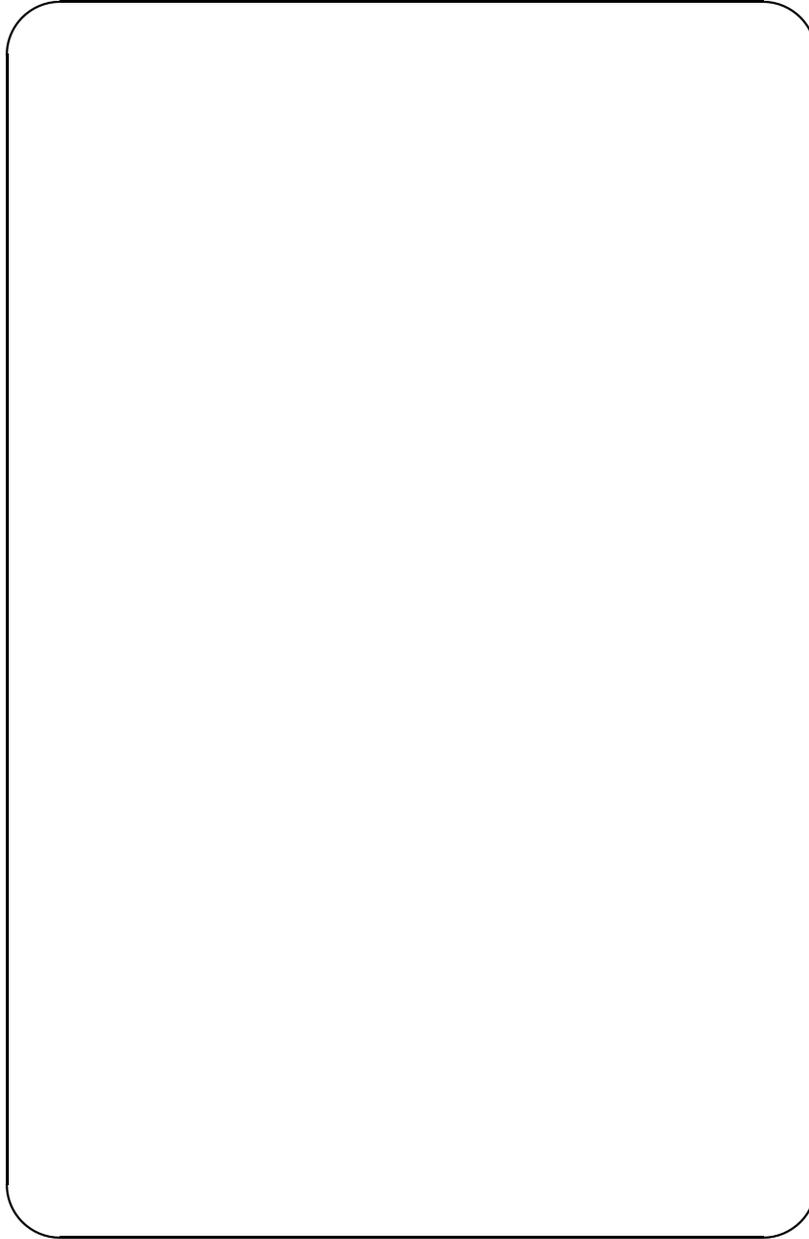
MAKE_ID



Undulator Source



MAKE_ID



Binary Output File Data:

Undulator Source

Col	Par	Minimum:	Maximum:	Center:	St. Dev.:
1	X	-0.18902E-01	0.15474E-01	0.69256E-04	0.49395E-02
2	Y	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
3	Z	-0.16522E-01	0.22615E-01	0.60388E-04	0.50354E-02
4	X'	-0.98957E-03	0.99296E-03	0.46751E-05	0.44681E-03
5	Y'	1.0000	1.0000	1.0000	0.34527E-03
6	Z'	-0.98606E-03	0.98558E-03	-0.46301E-05	0.46783E-03
11	Photon Energy (eV)		166.60	166.90	
20	Numerical Aperture		0.76118E-07	0.99957E-03	

No Optimization:

First Optimization:

Second Optimization:

Third Optimization:

Undulator Source

Fourth Optimization:

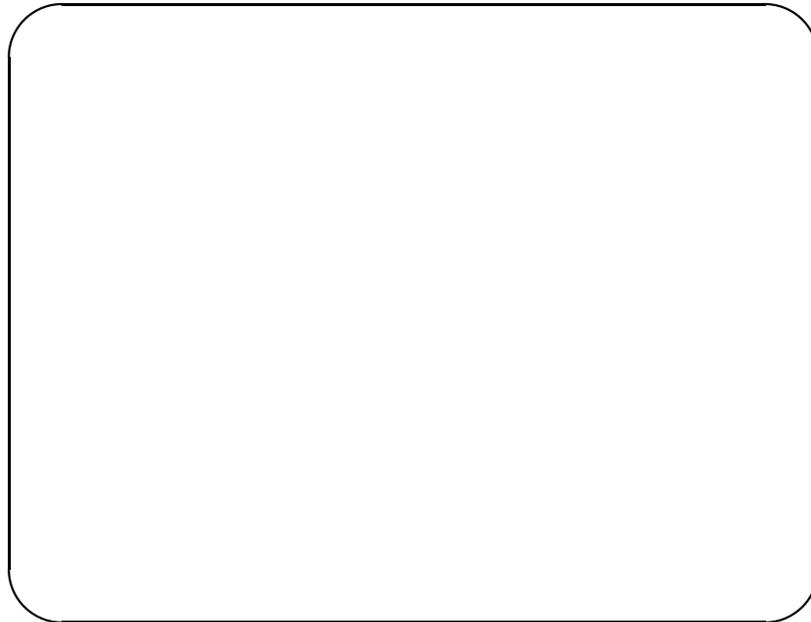
NOTES:

- A separate utility USER_UNDUL is also provided for easy inspection of the spectra. Its very similar to the second part of MAKE_ID where the photon distribution is computed; it reads in the trajectory file (SSRL.TRAJ) and then computes the photons/sec/rad²/eV or photons/sec/rad²/bandpass. For this utility, the user can use as many points as he likes in both energy and angles since the spectra is computed point by point and no arrays are used. Cartesian angles are used though, where θ_x and θ_z are the angles projected onto the x and z-axis. The output is stored in a 5 columns formatted file: energy, θ_z , θ_x , no. of photons, degree of polarization.

PROMPT:

A large, empty rounded rectangular box with a thin black border, intended for a prompt.

MENU:

A large, empty rounded rectangular box with a thin black border, intended for a menu.

Point Source Type

Point Source Type

All rays are generated from a single point in the $X - Z$ plane. The depth of the source (Y -direction) is prompted for and user-specified in the source depth.

Example:

One use of a point source is to determine the point spread function of an optical system (the image of a point), which gives information about the imaging quality of the system. For a true point source, NO DEPTH is used along with either a FLAT, UNIFORM, or CONICAL angle distribution.

Laboratory Reference Frame:

Binary Output File Data:

Col	Par	Minimum:	Maximum:	Center:	St. Dev.:
1	X	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
2	Y	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
3	Z	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
4	X'	-0.49970E-01	0.49957E-01	0.28123E-03	0.29015E-01
5	Y'	0.99872	1.0000	0.99956	0.00000E+00
6	Z'	-0.99809E-02	0.99672E-02	0.14161E-03	0.58881E-02
11	Photon Energy (eV)		0.00000E+00	0.00000E+00	
20	Numerical Aperture		0.20755E-02	0.50672E-01	

PLOTXY Result:

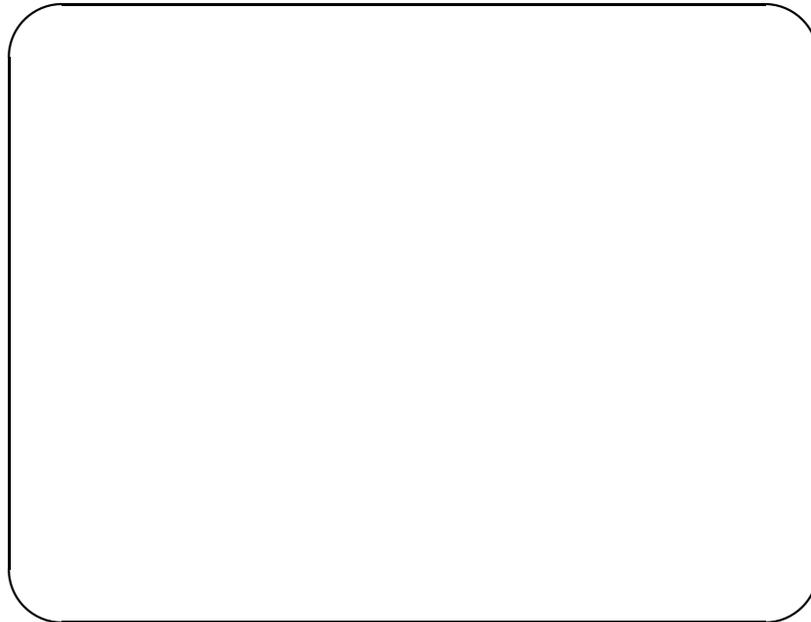
NOTES:

- For verification purposes, if you want to plot the $X - Z$ plane of a point source with PLOTXY, be sure to use external limits for the scaling option and input numbers on the order of ± 0.001 for the maximum and minimum values, otherwise you will not get a plot.

PROMPT:

A large, empty rounded rectangular box with a thin black border, intended for a prompt.

MENU:

A large, empty rounded rectangular box with a thin black border, intended for a menu.

Rectangular Source Type

Rectangular Source Type

Rays in the $X-Z$ plane originate within the boundaries of a rectangle. The user supplies the width (in X) and the height (in Z). The depth, in Y , is specified later.

Example:

A RECTANGULAR source may be used to model a source that uniformly illuminates a slit (or is a slit). A ribbon filament could be another example. The source shown in the example is 2mm by 3mm.

Laboratory Reference Frame:

Binary Output File Data:

Col	Par	Minimum:	Maximum:	Center:	St. Dev.:
1	X	-0.99988	0.99985	-0.40605E-01	0.56542
2	Y	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
3	Z	-1.4994	1.4997	-0.16572E-01	0.88398
4	X'	-0.49680E-01	0.49957E-01	0.15356E-02	0.28606E-01
5	Y'	0.99870	1.0000	0.99957	0.00000E+00
6	Z'	-0.99941E-02	0.99798E-02	-0.85504E-04	0.60022E-02
11	Photon Energy (eV)		800.00	800.00	
20	Numerical Aperture		0.30107E-03	0.50949E-01	

PLOTXY Result:

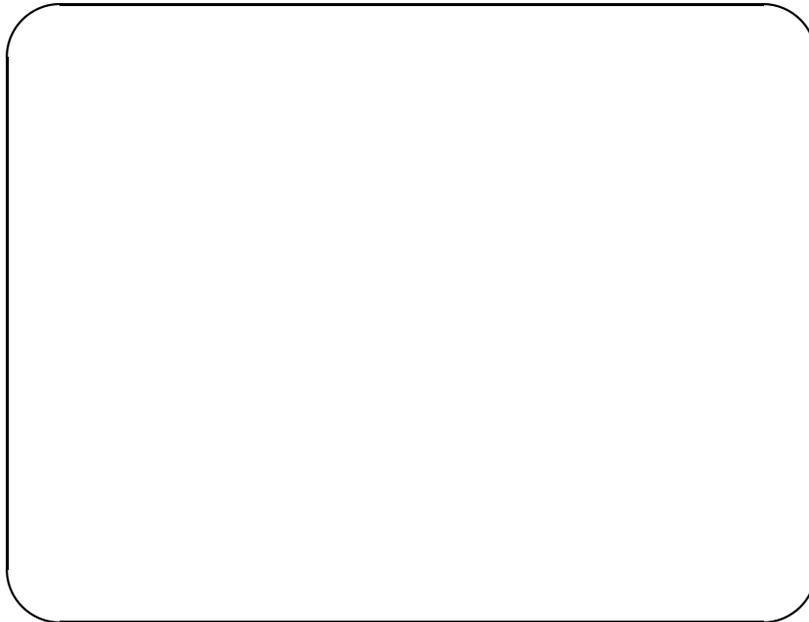
NOTES:

- When plotting a source that is rectangular but not square, use cartesian or external limits for the scaling option if you want to preserve the shape of the source.

PROMPT:

A large, empty rounded rectangular box with a thin black border, intended for a prompt.

MENU:

A large, empty rounded rectangular box with a thin black border, intended for a menu.

Elliptical Source Type

Rays in the $X - Z$ plane are generated within an ellipse. The user supplies the major axis of the ellipse as the width in X , and the minor axis of the ellipse as the height in Z . Also, if the source model is GRID in real space the user gives the number of concentric ellipses along with the number of points around each ellipse.

Example:

The ELLIPTICAL source type is well suited to applications involving the illumination of a pinhole or circular aperture. The plot shown below is in GRID with 16 concentric ellipses with 10 points on each ellipse, and with 3mm by 2mm major and minor axes respectively.

Laboratory Reference Frame:

Binary Output File Data:

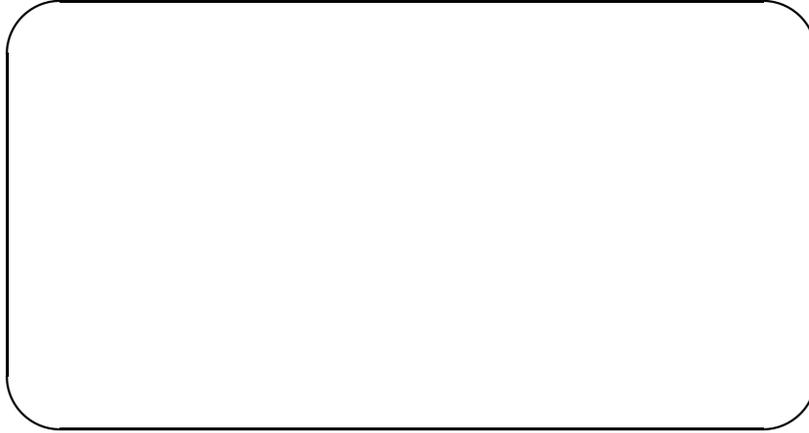
Col	Par	Minimum:	Maximum:	Center:	St. Dev.:
1	X	-3.0000	3.0000	0.12885E-07	1.5000
2	Y	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
3	Z	-1.9021	1.9021	0.49070E-07	1.0000
4	X'	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
5	Y'	1.0000	1.0000	1.0000	0.00000E+00
6	Z'	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
11	Photon Energy (eV)		0.00000E+00	0.00000E+00	
20	Numerical Aperture		0.00000E+00	0.00000E+00	

PLOTXY Result:

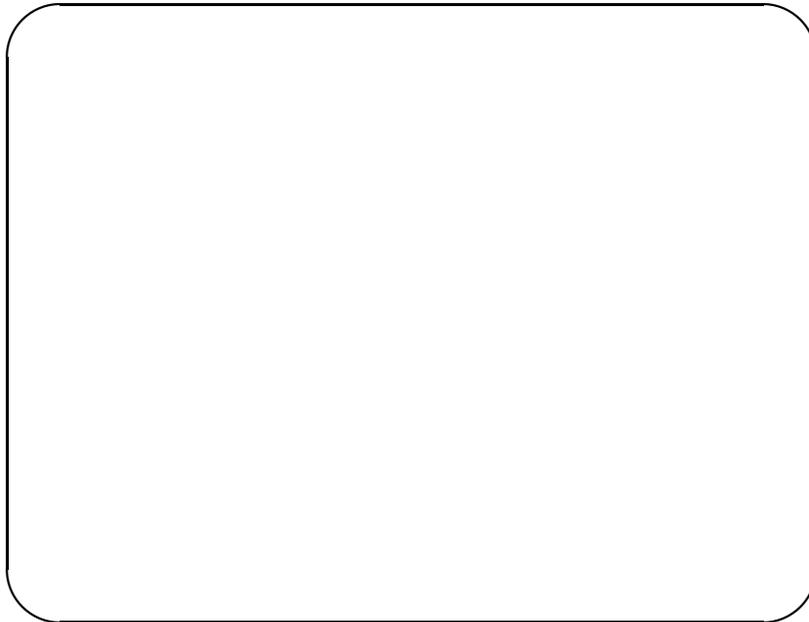
NOTES:

- To preserve the source shape when plotting with PLOTXY, use the cartesian or external limits scaling option. Otherwise ellipses will tend toward circles in appearance which may be misleading.
- The radial density of rays in the ellipse increases radially to maintain constant surface energy density.

PROMPT:

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MENU:

A large, empty rounded rectangular box with a thin black border, intended for a menu.

Gaussian Source Type

Gaussian Source Type

The cross section of the beam in the $X - Z$ plane has a gaussian distribution which is characterized by the standard deviations in the X and Z directions (no correlation between X and Z). The mean of both of the distributions is zero by default, i.e is centered on the Y axis. The mean may be offset by moving the source in the TRACE mode. This plane source type is generated only in RANdom real space.

Example:

The GAUSSIAN Plane Source Type is used to model a gaussian beam. Possible examples are a laser or a synchrotron radiation source, both of which may have gaussian intensity distributions in their cross sections.

Laboratory Reference Frame:

Binary Output File Data:

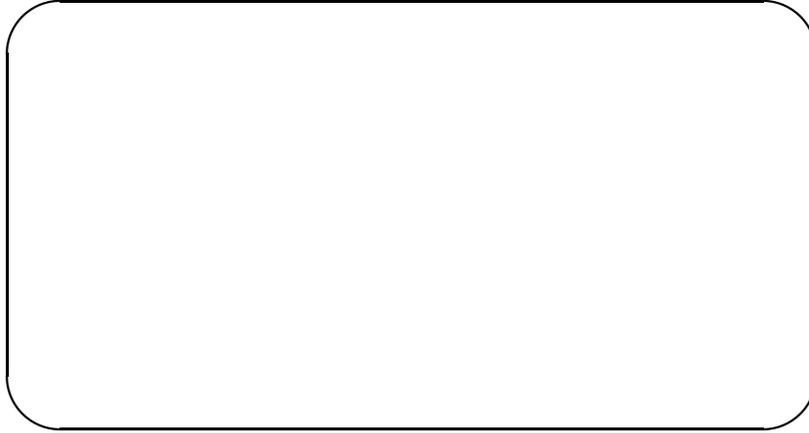
Col	Par	Minimum:	Maximum:	Center:	St. Dev.:
1	X	-1.5768	1.4417	0.10786E-01	0.48496
2	Y	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
3	Z	-0.89408	0.79141	0.75340E-02	0.25315
4	X'	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
5	Y'	1.0000	1.0000	1.0000	0.00000E+00
6	Z'	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
11	Photon Energy (eV)		0.00000E+00	0.00000E+00	
20	Numerical Aperture		0.00000E+00	0.00000E+00	

PLOTXY Result:

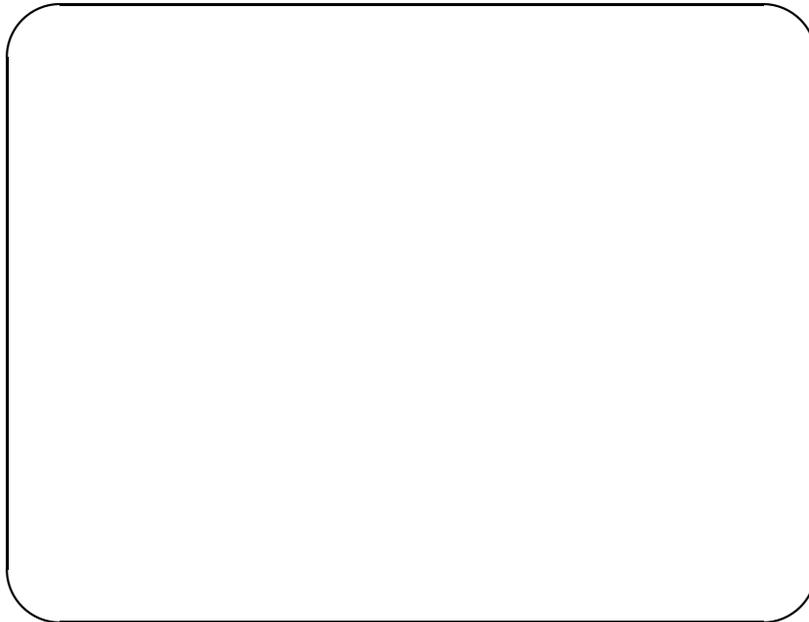
NOTES:

- Notice the correspondence in the value specified and those “measured” by PLOTXY (in the “St. Dev. ”column): $\sigma_x = 0.5 \rightarrow 0.485$, $\sigma_z = 0.25 \rightarrow 0.251$.

PROMPT:

A large, empty rounded rectangular box with a thin black border, intended for a prompt.

MENU:

A large, empty rounded rectangular box with a thin black border, intended for a menu.

No Source Depth

No Source Depth

The source depth is the spread of the source in the Y direction in real space. If the source model is GRID, the number of points along the depth must be given to SHADOW, and be equal to at least 1. For the no depth option, the rays are generated with no variation in Y at the source. In MENU mode, this option is specified as OFF.

Example:

A ribbon filament source has no depth because the radiation is emitted at the surface of the ribbon. The same is true for a black-body cavity. These sources would be created with the depth OFF. The plot below shows the $X - Y$ plane to demonstrate that the distribution of rays is in a single plane in the Y -direction.

Laboratory Reference Frame:

Binary Output File Data:

Col	Par	Minimum:	Maximum:	Center:	St. Dev.:
1	X	-1.4964	1.4974	0.22205E-01	0.87818
2	Y	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
3	Z	-0.99976	0.99586	0.12581E-01	0.57292
4	X'	-0.49921E-01	0.49903E-01	0.14935E-03	0.27602E-01
5	Y'	0.99872	1.0000	0.99960	0.00000E+00
6	Z'	-0.99815E-02	0.99857E-02	0.19558E-03	0.57881E-02
11	Photon Energy (eV)		0.00000E+00	0.00000E+00	
20	Numerical Aperture		0.87375E-03	0.50688E-01	

PLOTXY Result:

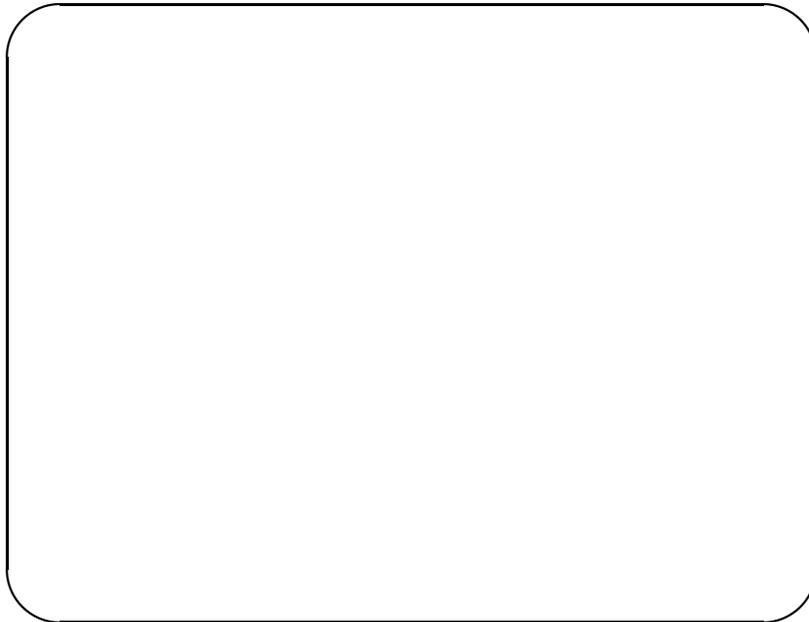
NOTES:

No Source Depth

PROMPT:

A large, empty rounded rectangular box with a thin black border, intended for a prompt.

MENU:

A large, empty rounded rectangular box with a thin black border, intended for a menu.

Flat Source Depth

Flat Source Depth

The rays are positioned according to a uniform depth distribution, i.e. a ray has equal probability of being assigned any value of Y within a user specified interval. This interval is the depth of the source. In MENU mode this distribution is noted as UNIFORM.

Example:

Suppose the user wants to model a gas or a transparent three dimensional object that is radiating uniformly. The FLAT depth distribution is a suitable model for these sources. Shown below is a plot of a source with a uniform depth of 0.15 mm.

Laboratory Reference Frame:

Binary Output File Data:

Col	Par	Minimum:	Maximum:	Center:	St. Dev.:
1	X	-1.4988	1.4996	-0.80459E-02	0.87779
2	Y	-0.74852E-01	0.74854E-01	0.11277E-02	0.42812E-01
3	Z	-0.99601	0.99913	-0.40586E-02	0.58142
4	X'	-0.49771E-01	0.49909E-01	-0.12477E-02	0.28820E-01
5	Y'	0.99871	1.0000	0.99957	0.42286E-03
6	Z'	-0.99748E-02	0.99606E-02	0.43271E-04	0.57035E-02
11	Photon Energy (eV)		0.00000E+00	0.00000E+00	
20	Numerical Aperture		0.20702E-03	0.50819E-01	

PLOTXY Result:

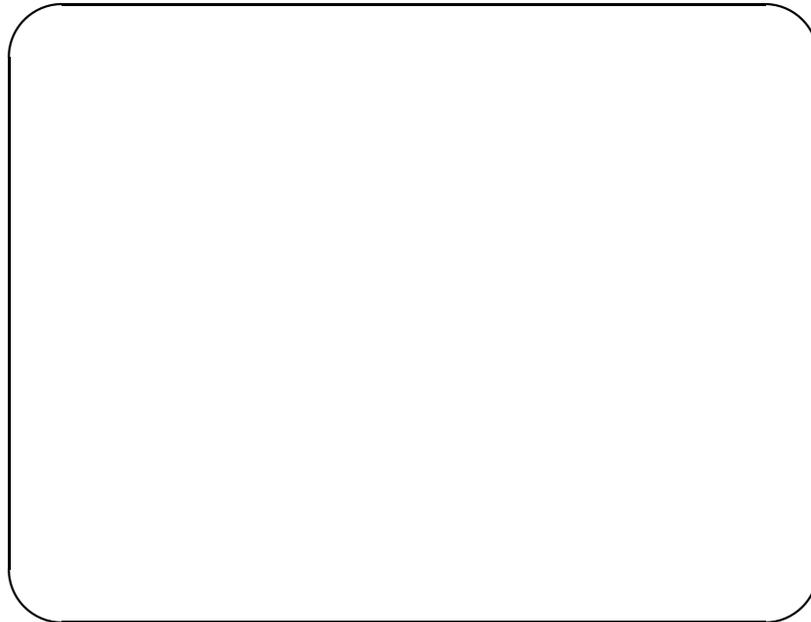
Flat Source Depth

NOTES:

PROMPT:

A large, empty rounded rectangular box with a thin black border, intended for a prompt.

MENU:

A large, empty rounded rectangular box with a thin black border, intended for a menu.

Gaussian Source Depth**Gaussian Source Depth**

The depth is determined by a gaussian distribution with mean zero and standard deviation (σ_Y) supplied by the user. The mean may be changed in TRACE mode by offsetting the source in the Y direction.

Example:

An example of a gaussian depth could be a single bunch of electrons in an electron storage ring. Notice that using a gaussian source in (X, Y, Z) with the same σ will give a spherical gaussian source.

Laboratory Reference Frame:

Binary Output File Data:

Col	Par	Minimum:	Maximum:	Center:	St. Dev.:
1	X	-0.99873	0.99844	0.12886E-01	0.58235
2	Y	-1.5463	1.6991	0.60299E-02	0.49791
3	Z	-0.99923	0.99983	-0.63615E-02	0.58969
4	X'	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
5	Y'	1.0000	1.0000	1.0000	0.00000E+00
6	Z'	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
11	Photon Energy (eV)		0.00000E+00	0.00000E+00	
20	Numerical Aperture		0.00000E+00	0.00000E+00	

PLOTXY Result:

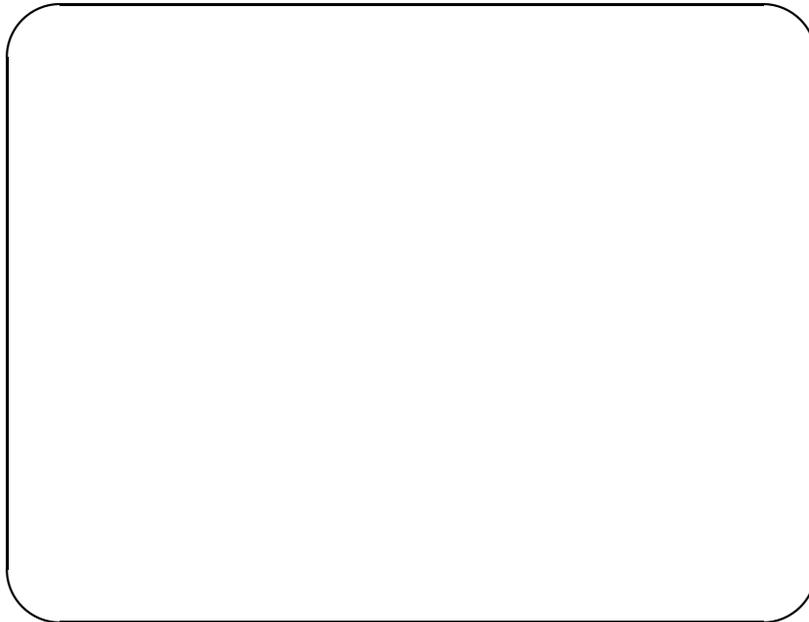
NOTES:

Gaussian Source Depth

PROMPT:

A large, empty rounded rectangular box with a thin black border, intended for a prompt.

MENU:

A large, empty rounded rectangular box with a thin black border, intended for a menu.

Synchrotron Source Depth

The depth of a synchrotron source is characterized by the geometry of the system. The parameters are the machine radius and the horizontal (X') beam divergence; the depth increases with increasing machine radius and increasing divergence. The exception here is that the depth is NOT independent of the divergence. The synchrotron depth was designed to be used in conjunction with the synchrotron angle distribution. The machine and beam parameters are to be specified in the angle distribution section. A synchrotron source is typically used with a gaussian $X - Z$ plane source distribution, although others are equally valid.

Example:

This model is applicable to radiation emitted by charged particles being accelerated in a circular trajectory.

Laboratory Reference Frame:

Binary Output File Data:

Col	Par	Minimum:	Maximum:	Center:	St. Dev.:
1	X	-1.8622	2.0817	0.21170E-01	0.66697
2	Y	-20.815	20.832	-0.17096	12.167
3	Z	-1.1886	1.0742	0.45658E-03	0.36646
4	X'	-0.99905E-02	0.99998E-02	-0.82015E-04	0.58405E-02
5	Y'	0.99995	1.0000	0.99998	0.00000E+00
6	Z'	-0.88765E-03	0.88991E-03	-0.14414E-05	0.28656E-03
11	Photon Energy (eV)		400.16	4962.7	
20	Numerical Aperture		0.76989E-04	0.10011E-01	

PLOTXY Result:

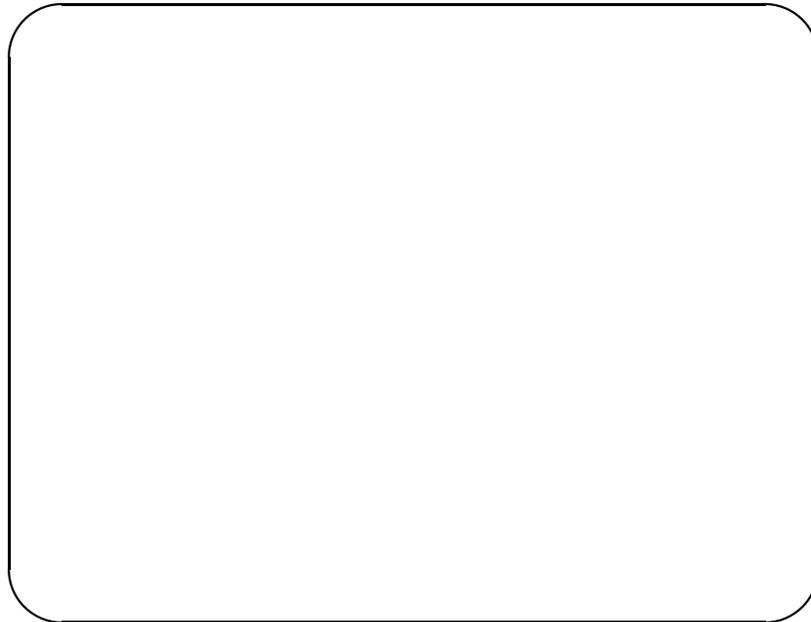
NOTES:

Synchrotron Source Depth

PROMPT:

A large, empty rounded rectangular box with a thin black border, intended for a prompt.

MENU:

A large, empty rounded rectangular box with a thin black border, intended for a menu.

Flat Angle Distribution

The source angle distribution dictates how the rays in momentum space will be generated. If GRID is chosen as the model in momentum space the user must supply the number of points in the X' and Z' directions. In Flat angle distribution, the rays have an equal probability of being assigned any angle within the user specified interval of horizontal and vertical half-divergences (in radians). This source will *not* illuminate uniformly a sphere centered on it, but rather a plane.

Example:

Flat source angle distribution models a uniformly illuminated *plane* or portion of a *plane*.

Laboratory Reference Frame:

Binary Output File Data:

Col	Par	Minimum:	Maximum:	Center:	St. Dev.:
1	X	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
2	Y	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
3	Z	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
4	X'	-0.39958E-01	0.39785E-01	0.72294E-03	0.22674E-01
5	Y'	0.99920	1.0000	0.99974	0.00000E+00
6	Z'	-0.49836E-02	0.49873E-02	0.11776E-04	0.28893E-02
11	Photon Energy (eV)		0.00000E+00	0.00000E+00	
20	Numerical Aperture		0.60951E-03	0.40103E-01	

PLOTXY Result:

NOTES:

PROMPT:

A large, empty rounded rectangular box with a thin black border, intended for a prompt.

MENU:

A large, empty rounded rectangular box with a thin black border, intended for a menu.

Uniform Distribution

With a uniform distribution, the intensity of the source incident on a plane varies as the cosine of the angle of the ray with respect to the optical axis, following Lambert's law. This means a uniform *brightness* source, where the flux flowing into a solid angle $d\Omega$ from an area dA is independent of the observation angle. In general, $\frac{dN}{d\theta} = \cos \theta$. For the case of an *isotropic* source, see the "Conical Source" case.

Example:

The Uniform source angle distribution models a radiating gaseous sphere such as the sun, a frosted glass sphere or a black-body cavity.

Laboratory Reference Frame:

Binary Output File Data:

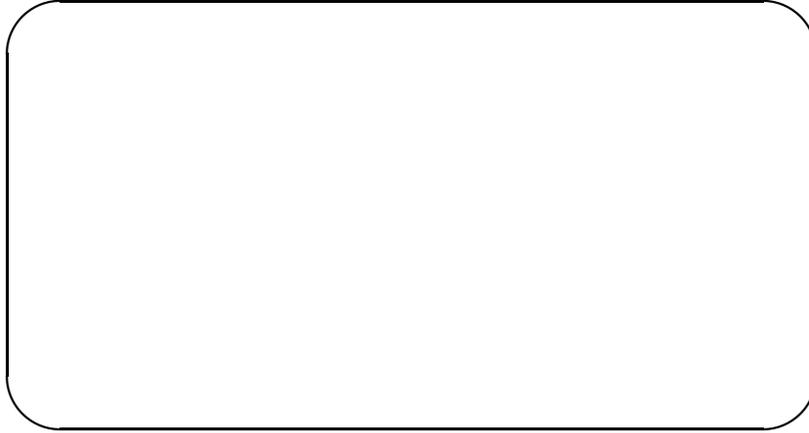
Col	Par	Minimum:	Maximum:	Center:	St. Dev.:
1	X	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
2	Y	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
3	Z	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
4	X'	-0.49971E-01	0.49834E-01	-0.39708E-03	0.28406E-01
5	Y'	0.99871	1.0000	0.99958	0.00000E+00
6	Z'	-0.99941E-02	0.99945E-02	-0.26348E-03	0.57903E-02
11	Photon Energy (eV)		0.00000E+00	0.00000E+00	
20	Numerical Aperture		0.15102E-02	0.50852E-01	

PLOTXY Result:

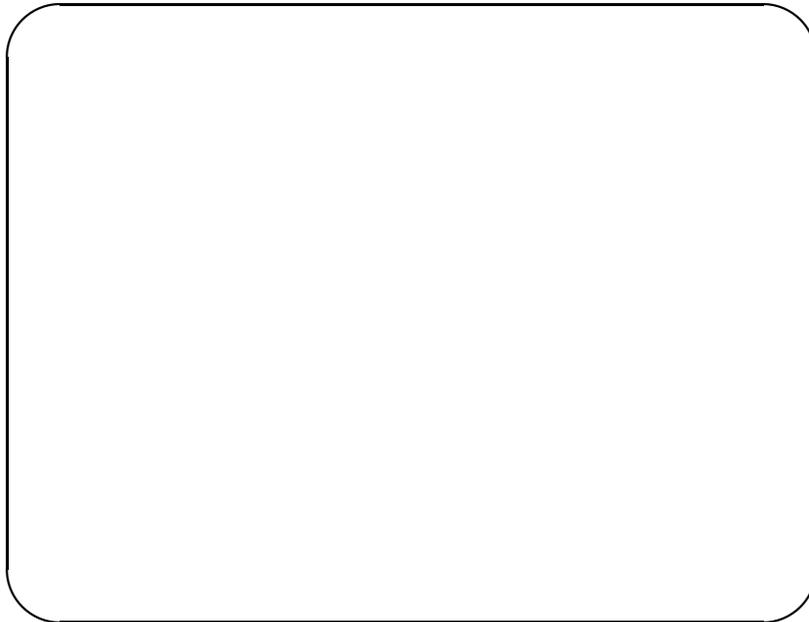
Uniform Distribution

NOTES:

PROMPT:

A large, empty rounded rectangular box with a thin black border, intended for a prompt.

MENU:

A large, empty rounded rectangular box with a thin black border, intended for a menu.

Gaussian Angle Distribution

The gaussian angle distribution is characterized by four parameters, the standard deviation in X' and Z' ; the maximum divergence in X' and Z' . The mean of the distributions is zero by default. The standard deviations determine the spread of the angle distributions while the maximum divergence acts as a cutoff.

Example:

This source angle distribution would be appropriate in the modelling of a laser or an undulator.

Laboratory Reference Frame:

Binary Output File Data:

Col	Par	Minimum:	Maximum:	Center:	St. Dev.:
1	X	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
2	Y	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
3	Z	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
4	X'	-0.38049E-01	0.29802E-01	-0.14766E-03	0.99368E-02
5	Y'	0.99920	1.0000	0.99990	0.64594E-03
6	Z'	-0.37165E-01	0.37051E-01	-0.48994E-03	0.10293E-01
11	Photon Energy (eV)		0.00000E+00	0.00000E+00	
20	Numerical Aperture		0.60327E-03	0.40032E-01	

PLOTXY Result:

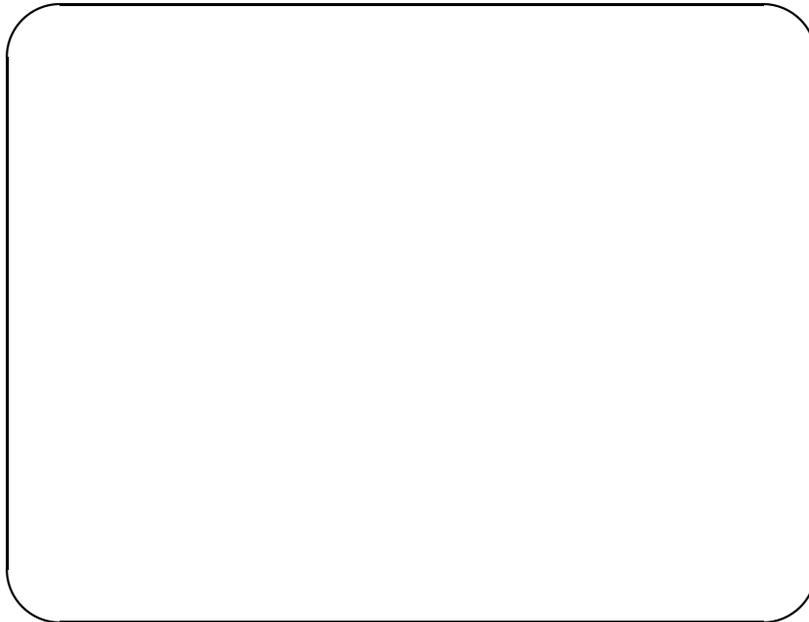
NOTES:

- The maximum divergence is ignored in the current version of SHADOW. Thus the only parameter that dictates the distribution is the standard deviation. This will be fixed in a later release.

PROMPT:

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MENU:

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Synchrotron Angle Distribution

Synchrotron Angle Distribution

(4) Synchrotron (Interpolated)

Divergences: These represents the limits within which the rays will be generated in the vertical and horizontal directions.

Machine parameters

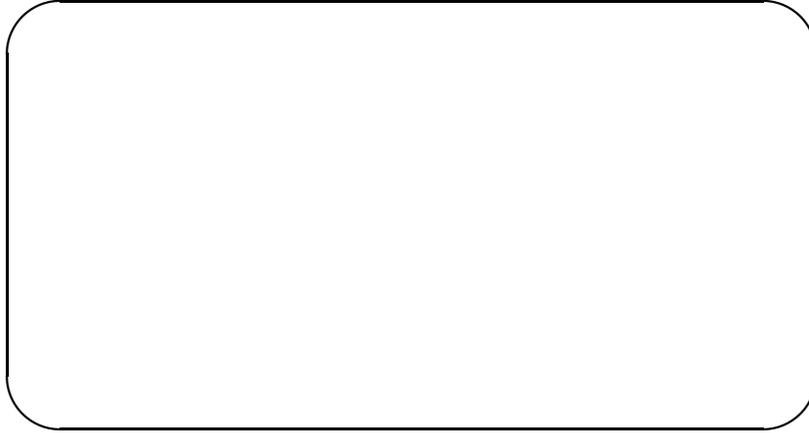
Magnetic Radius: This value needs to be in meters because of the algorithm used to generate the photon distribution.

Orbit Radius: Same as above, but in user units. SHADOW needs to know the units used by the user so that the radius of the orbit will have appropriate values. Notice that in principle this value may be different from the magnetic radius, although such a source would be meaningless. Note a negative orbit radius signifies a storage ring with electrons running in the CCW direction when viewed from the top, while a positive value represents a CW direction

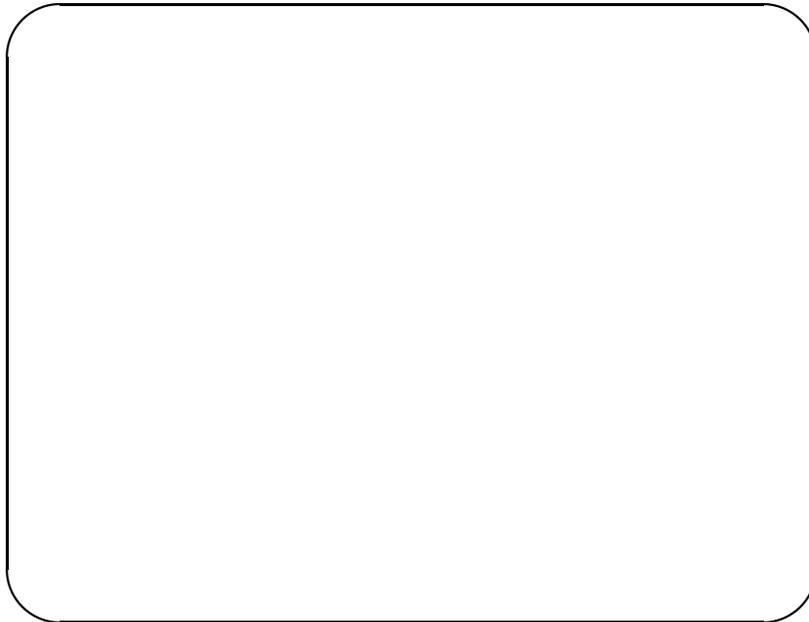
Emittance Y/N: Used to specify effects of finite e-beam size and angle spread. If not selected the electron beam is assumed to be perfectly collimated, with all orbits parallel to the central one. If selected, the beam is treated as a gaussian beam propagating along the magnet, assumed without focusing actions. This is certainly true for the short arcs typical of bending magnets sources (a few milliradians). The effect of finite beam angle divergence depends on its value relative to the radiation FWHM; it should be small on low-energy machines, noticeable on high-energy ones. The values should be obtained from the machine group for the particular magnet under study. The emittance is the product of the spatial and angle standard deviation:

$$\epsilon_{x,z} = \sigma_{x,z} \cdot \sigma_{x',z'} \quad (2.1)$$

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and it is often specified in *meters · radians*. (Notice that our definition does NOT include a factor of 2π – verify with the source of your data if their definition does; if so, divide the numbers by 2π).

Here you will have to use the same units of length (i.e. *cm, mm*) that you are planning to use in the TRACE part of SHADOW, times *radians*. Notice that $\sigma_{z,x}$ was specified earlier; it can be zero.

Emittance at waist. The electron may be converging, diverging or at a focus (waist) at the source tangent point. In the case that it is not, the SOURCE needs to take that into account in order to compute the correct model. The new standard deviation becomes:

$$\sigma_{x,z}^2(s) = \sigma_{x,z}^2(s=0) + \sigma_{x',z'}^2 s^2 \quad (2.2)$$

where s is the distance from the waist. The inclusion of the emittance effects will result in a tilted phase space (see example). The distance sign from the waist means:

$$\begin{aligned} \text{positive} &\rightarrow \text{downstream} \\ \text{negative} &\rightarrow \text{upstream} \end{aligned} \quad (2.3)$$

and, as usual, must be in user's units. Thus, positive values mean a diverging electron beam.

Electron beam energy. The machine energy, in GeV. No energy spread is assumed.

Polarization. This flag selects which of the polarization components SHADOW will create. In general, use [3].

Photons/Power. This directs SHADOW to use either one of two possible stochastic models. In the first, the probability of finding a ray at photon energy E is obtained from the $N(E)$ curve, in the second from the $P(E) = N(E)E$ curve. The two models are not too different over a small photon energy range; not so over a large range.

The choice between the two depends for what purpose the calculation is being setup. If you are interested in computing power densities, for examples, then you should select [1] but be sure to read the part on power density calculation in the relative section of the UG. In any other case, you should select [0].

Example:

The model uses a set of precomputed vertical angle distributions and then interpolates the data to find the distribution corresponding to the specified photon energy. The data are stored in the file SRSPEC.DAT and contain an (exact) source at 1000 photon energies between $0.000001 \epsilon_c$ and $10 \epsilon_c$. These limits define the photon energy range within which the photon energy can be specified; other values will cause an error. A longer discussion is available in the Introduction and should be read carefully.

The example shown refers to Aladdin, the electron storage ring of the University of Wisconsin (although the values of emittance and waist positions are only for illustration purposes). It is instructive to run the same case with a fictitious machine of 5 GeV beam energy.

Notice that SOURCE does not ask any question about beam current; this is because of the sampling scheme discussed in the Introduction – whatever the current in the machine, the number of rays specified represents a linear fraction of the total flux. The current stored is of importance for the case of power densities and its value is normally asked by the post-processor programs (such as PWR_DENS).

Binary Output File Data:

Synchrotron Angle Distribution

Col	Par	Minimum:	Maximum:	Center:	St. Dev.:
1	X	-0.37723	0.44268	0.12268E-01	0.11205
2	Y	-10.406	10.383	0.14166E-01	6.0394
3	Z	-0.32709E-01	0.35049E-01	-0.33003E-03	0.11223E-01
4	X'	-0.50643E-02	0.51778E-02	0.34638E-05	0.29040E-02
5	Y'	0.99999	1.0000	1.0000	0.00000E+00
6	Z'	-0.10511E-02	0.12995E-02	-0.13872E-04	0.35709E-03
11	Photon Energy (eV)		300.09	4784.6	
20	Numerical Aperture		0.88542E-04	0.51837E-02	

Photon Energy vs Z':

PLOTXY Result: A synchrotron source in X and Z .

PLOTXY Result: X phase space of a synchrotron angle distribution.

Synchrotron Angle Distribution

PLOTXY Result: Z phase space of a synchrotron angle distribution.

PLOTXY Result: Far Field Plot:

Synchrotron Angle Distribution

PLOTXY Result: A synchrotron source in X and Y .

The next example corresponds to the case of:

$$\varepsilon_X = 0.1E - 03 \quad \varepsilon_Z = 0.1E - 03$$

$$\sigma_X = 0.1 \quad \sigma_Z = 0.1$$

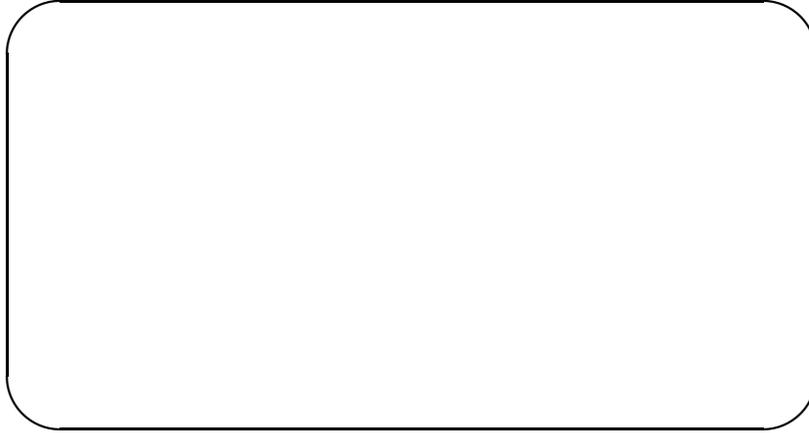
$$s_X = -10000 \quad s_Z = 10000$$

Notice how in horizontal the beam is broadened relative to the former case. (FWHM $\cong 20$ vs. $\cong 0.3$). This is due to the gaussian electron beam propagation by s_X . It is interesting to notice that in X we have essentially a zero-thickness line (complete correlation between X, X' at large s) while in Z there is still a thickness (because of the additional angles introduced by the SR opening.)

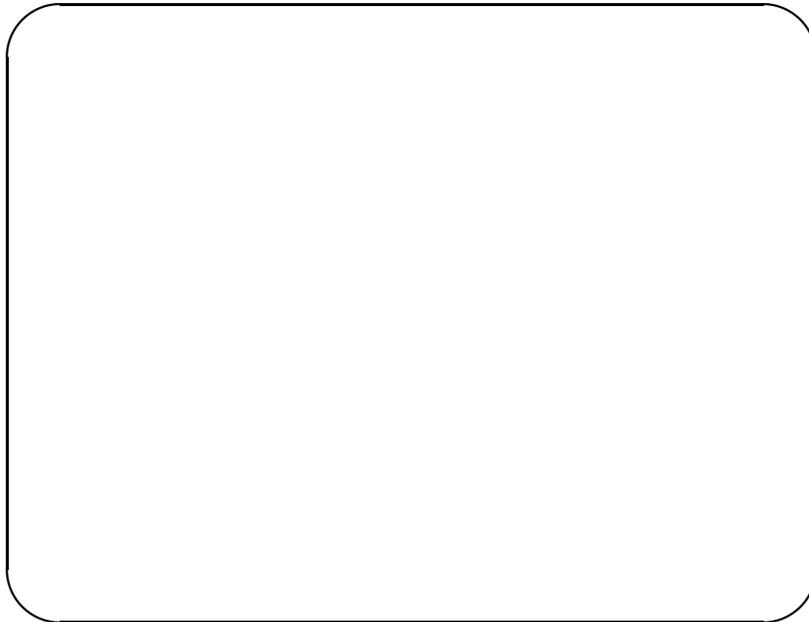
Synchrotron Angle Distribution when out of focus as shown in PLOTXY result below:

NOTES:

PROMPT:

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MENU:

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Conical Angle Distribution**Conical Angle Distribution**

This distribution has the angles of the rays uniformly generated between a minimum and maximum absolute value. The minimum can be zero. The distribution of rays in the angle θ is uniform, i.e. a spherical surface will be uniformly illuminated by this source placed at its center. This is in contrast to the case of a uniform source.

Example:

If used with a point source and the depth OFF, conical source angle distribution is good for testing the image quality of a system with circular symmetry. It will also model a section of a spherical wave with rotational symmetry. Illustrated below is a GRID source model with maximum and minimum divergences being 0.1 and 0.05 radians.

Laboratory Reference Frame:

Binary Output File Data:

Col	Par	Minimum:	Maximum:	Center:	St. Dev.:
1	X	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
2	Y	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
3	Z	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
4	X'	-0.99998E-02	0.99998E-02	-0.40445E-12	0.55901E-02
5	Y'	0.99995	0.99999	0.99998	0.00000E+00
6	Z'	-0.99998E-02	0.99998E-02	0.19647E-09	0.55901E-02
11	Photon Energy (eV)		0.00000E+00	0.00000E+00	
20	Numerical Aperture		0.50000E-02	0.10000E-01	

PLOTXY Result:

A source with a conical angle distribution was traced through the following system and plotted to show the aberrations present in the system.

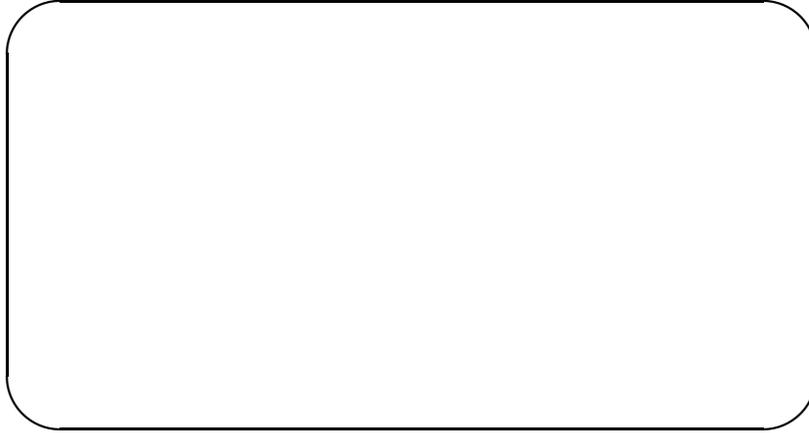
Conical Angle Distribution

X phase space and Z phase space plots showing the aberrations in the system:

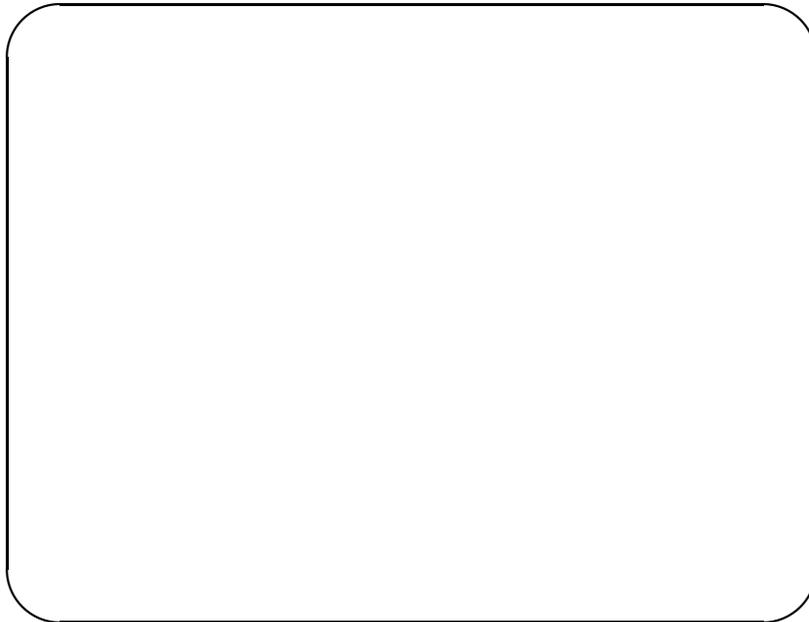
NOTES:

Conical Angle Distribution

PROMPT:

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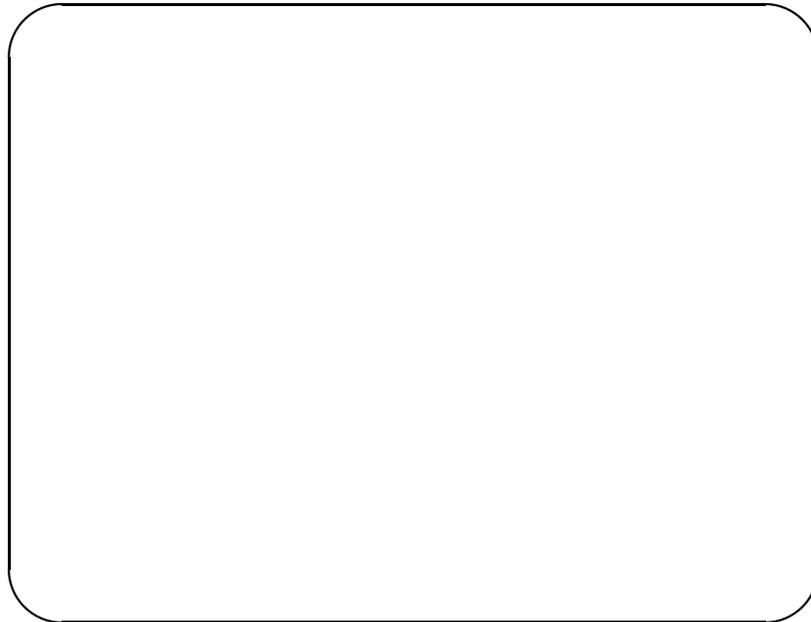
MENU:

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PROMPT:

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MENU:

A large, empty rounded rectangular box with a thin black border, intended for a menu.

Example:

In the example here, we again use ALADDIN at 1 GeV whose critical energy is 1065 eV. In order to show the structures in the angular distribution, we choose a low photon energy (65 eV), where photons are emitted within a few milliradians. If the vertical divergence (3 mrad) is decreased, the emission will be truncated and also will take more time to generate all the rays. In the diagram, the histogram is obtained by running HISTO1 on BEGIN.DAT and is compared to the computed spectra (solid lines) of the total component.

Binary Output File Data:

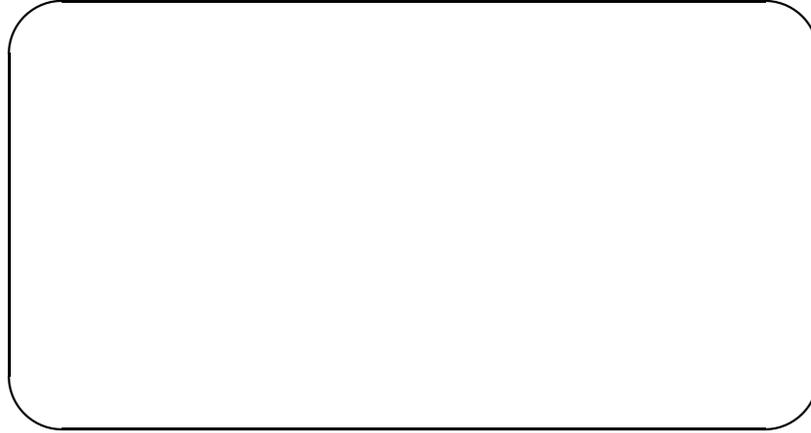
Col	Par	Minimum:	Maximum:	Center:	St. Dev.:
1	X	-1.8019	1.8880	0.25297E-01	0.50842
2	Y	-10.407	10.409	-0.51080E-02	6.0346
3	Z	-0.70149	0.70996	0.28179E-02	0.24185
4	X'	-0.50042E-02	0.50033E-02	-0.18401E-05	0.28957E-02
5	Y'	0.99999	1.0000	1.0000	0.00000E+00
6	Z'	-0.24190E-02	0.24913E-02	-0.21035E-04	0.87633E-03
11	Photon Energy (eV)		65.000	65.000	
20	Numerical Aperture		0.85980E-04	0.52392E-02	

HISTO1 on BEGIN.DAT

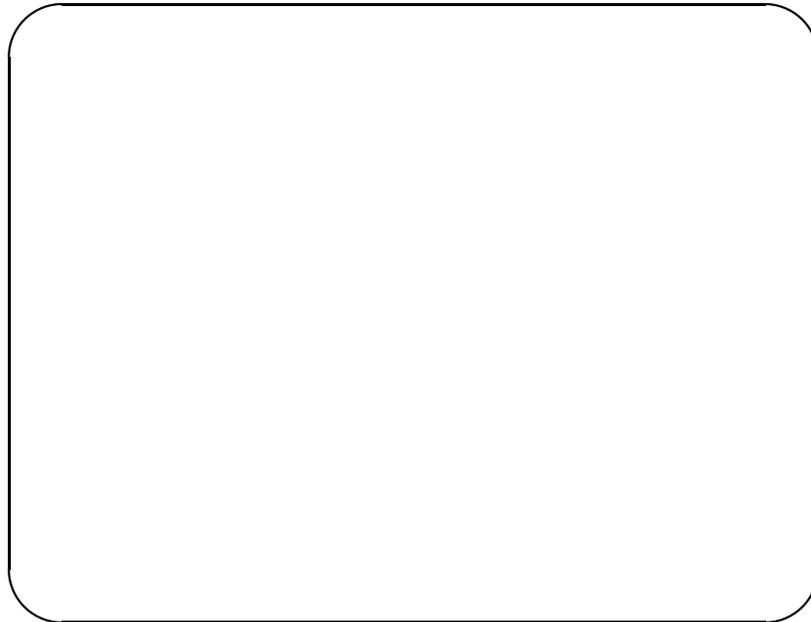
NOTES:

- **WARNING** Since the Exact Synchrotron Distribution is more computationally intense, it can be done only at one single photon energy. Also, this distribution should be used only if the user is not satisfied with the Synchrotron Angle Distribution results (e.g. photon energy is outside the range that it can interpolate).

PROMPT:

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MENU:

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Single Line Photon Energy

Single Line Photon Energy

If the user wishes, a photon energy of a single line can be specified (SLINE in menu). The photon energy of a source can be given in electron-volts or can be given as the wavelength in Angstroms. The rays will be generated with only one energy.

Example:

This type of source is used to study dispersing or absorbing optical systems. In conjunction with a point uniform source it will provide the point spread function of a monochromator or a spectrograph.

Laboratory Reference Frame:

Binary Output File Data:

Col	Par	Minimum:	Maximum:	Center:	St. Dev.:
1	X	-1.4995	1.4953	-0.50441E-01	0.86828
2	Y	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
3	Z	-0.99534	0.99885	0.14181E-01	0.57256
4	X'	-0.49902E-01	0.49555E-01	0.17977E-03	0.29625E-01
5	Y'	0.99871	1.0000	0.99955	0.00000E+00
6	Z'	-0.99937E-02	0.99958E-02	-0.19550E-03	0.57042E-02
11	Photon Energy (eV)		800.00	800.00	
20	Numerical Aperture		0.13587E-03	0.50786E-01	

PLOTXY Result:

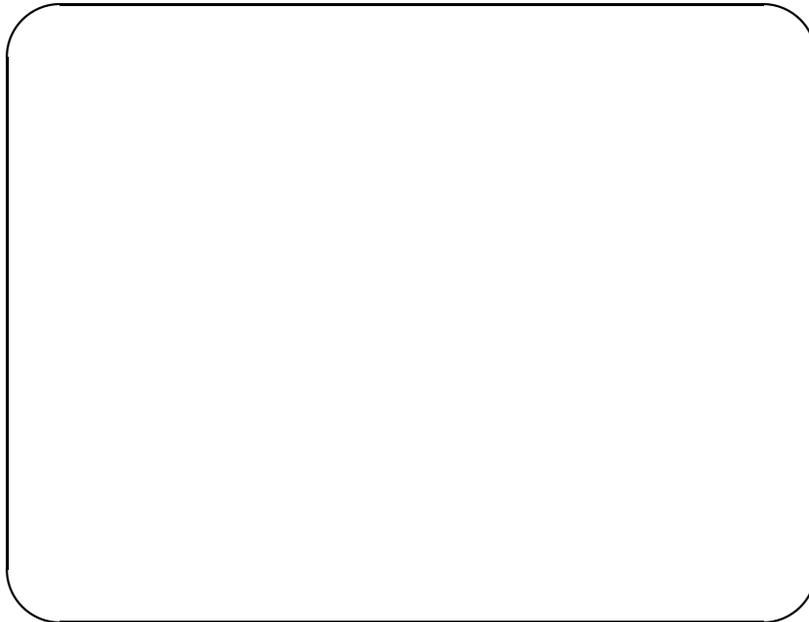
NOTES:

- For best results when plotting photon energy with PLOTXY, plot column 11 in the horizontal and column 1 - or whichever spatial variable you decide to use, in the vertical. This way the program will plot histograms in photon energy to show the distribution.

PROMPT:

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MENU:

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Multiple Line Photon Energy

If the user wishes, a photon energy consisting of several lines can be specified (MLINE in menu). The photon energy of a source can be given in electron-volts or can be given as the wavelength in Angstroms. Up to ten discrete energies can be chosen and each energy can have any value (not necessarily equispaced). All specified energies will be generated with equal intensity.

Example:

Multiple line photon energy is useful in the representation of emission spectra resulting from the excitation of a gas, and for testing the resolution of monochromators and spectrometers. After running a case at a given wavelength, to compare the response of a monochromator or other system at a different photon energy, you may use the utility RECOLOR. It will reset the photon energies in a source to other values without affecting other variables.

Laboratory Reference Frame:

Binary Output File Data:

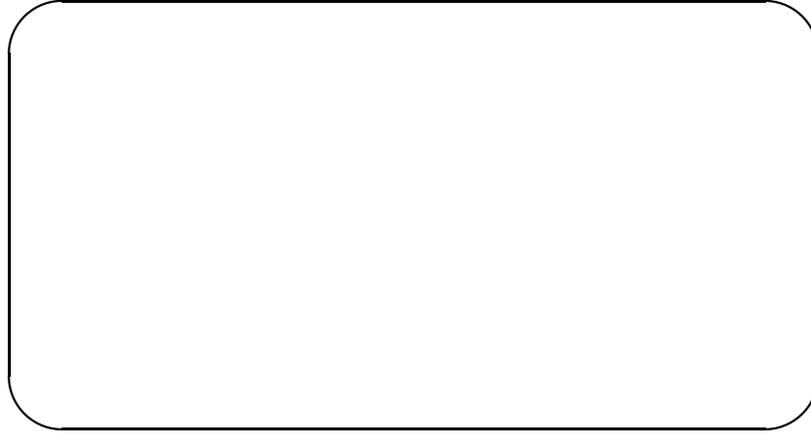
Col	Par	Minimum:	Maximum:	Center:	St. Dev.:
1	X	-1.4995	1.4953	-0.50441E-01	0.86828
2	Y	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
3	Z	-0.99534	0.99885	0.14181E-01	0.57256
4	X'	-0.49902E-01	0.49555E-01	0.17977E-03	0.29625E-01
5	Y'	0.99871	1.0000	0.99955	0.00000E+00
6	Z'	-0.99937E-02	0.99958E-02	-0.19550E-03	0.57042E-02
11	Photon Energy (eV)		398.00	404.00	
20	Numerical Aperture		0.13587E-03	0.50786E-01	

PLOTXY Result:

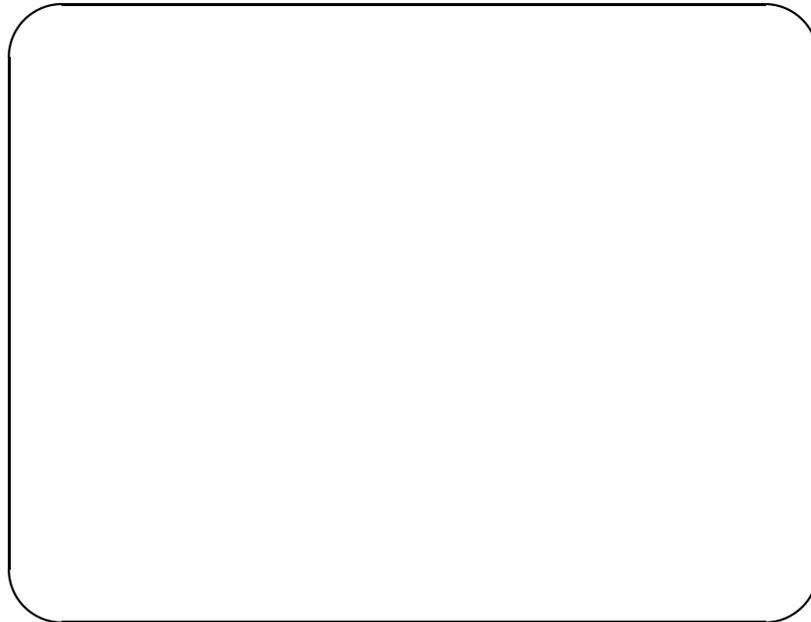
NOTES:

- For best results when plotting photon energy with PLOTXY, plot column 11 in the horizontal and column 1 - or whichever spatial variable you decide to use, in the vertical. This way the program will plot histograms in photon energy to show the distribution.

PROMPT:

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MENU:

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Continuous Photon Energy

If the user wishes, a uniform photon energy can be specified (CONTINUOUS in menu). The photon energy of a source can be given in electronvolts or can be given as the wavelength in Angstroms, but the rays are always uniform in energy rather than in wavelength. The minimum and maximum of a uniform distribution are supplied by the user. The rays have equal probability of having any energy within the interval.

Example:

A continuous photon energy represents a general or white light source. It is also useful in the modelling of a synchrotron source, and in the study of monochromator and other dispersive optical systems. For example, plotting column 3 (Z) vs. 11 will give the dispersion of a monochromator.

Laboratory Reference Frame:

Binary Output File Data:

Col	Par	Minimum:	Maximum:	Center:	St. Dev.:
1	X	-1.4995	1.4953	-0.50441E-01	0.86828
2	Y	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
3	Z	-0.99534	0.99885	0.14181E-01	0.57256
4	X'	-0.49902E-01	0.49555E-01	0.17977E-03	0.29625E-01
5	Y'	0.99871	1.0000	0.99955	0.00000E+00
6	Z'	-0.99937E-02	0.99958E-02	-0.19550E-03	0.57042E-02
11	Photon Energy (eV)		200.21	599.58	
20	Numerical Aperture		0.13587E-03	0.50786E-01	

PLOTXY Result:

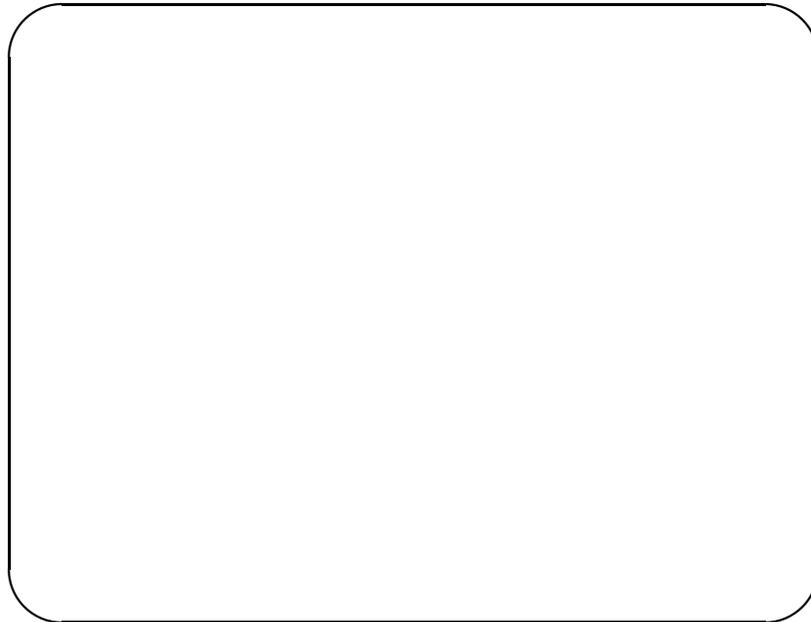
NOTES:

- For best results when plotting photon energy with PLOTXY, plot column 11 in the horizontal and column 1 - or whichever spatial variable you decide to use, in the vertical. This way the program will plot histograms in photon energy to show the distribution.

PROMPT:

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MENU:

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Optical Path Length**Optical Path Length**

The Optical path of a ray is given by the distance a ray travels weighted by the index of refraction in the medium it is traveling through. This scalar quantity is accumulated at the end of each optical element. It is set to zero at the source point for each ray.

Example:

One use of the optical path length is to study aberrations in an optical system. In a stigmatic imaging system a point is imaged onto a point. This means that a diverging spherical wave is transformed into a converging spherical wave, and that the optical path lengths of all the rays are equal. In a non-ideal system the optical path lengths depend on some parameter such as the angle that the ray makes with the optical axis or the mathematical description of the surface of the element. The optical path is also useful for determining the phases of the electric field vectors at a given point in the system. These phases can be used to compute an interference or diffraction pattern.

Laboratory Reference Frame:

A point source was generated saving the optical paths and traced through a toroidal mirror. The following is information on the source and the system from SOURCINFO and SYSINFO respectively.

Optical Path Length

Plots of optical path vs. Z and Z'

Optical Path Length

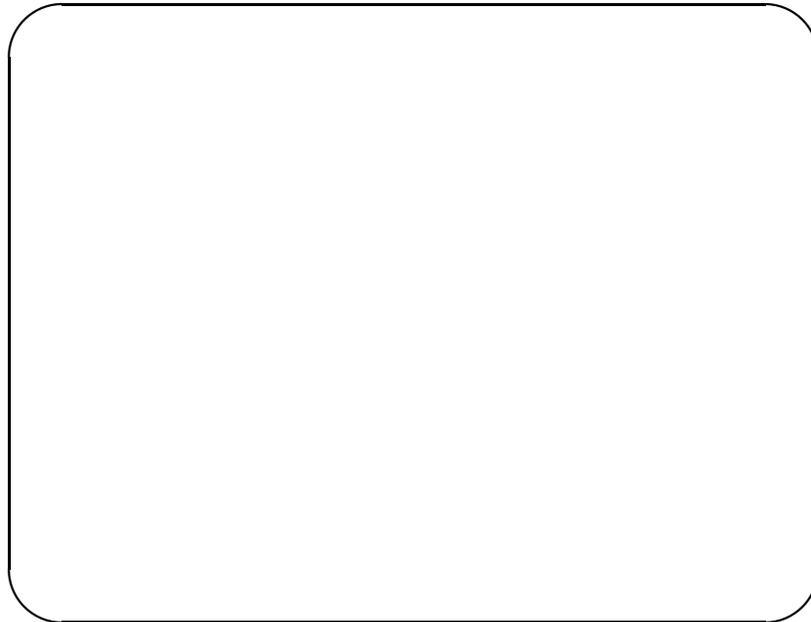
NOTES:

- Storing the optical path length will increase the number of rows for each ray from 12 to 13, hence more storage space is needed.

PROMPT:

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MENU:

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Electric Field Vectors

The electric field of the propagating wavefront can be expressed as

$$(As_x + As_y + As_z) \exp(j * \phi_s) + \\ (Ap_x + Ap_y + Ap_z) \exp(j * \phi_p)$$

where the s and p vectors are perpendicular and parallel to the plane of incidence respectively and ϕ is the phase of each vector. At the source, s is defined to be horizontal (x-axis) and p is vertical (z-axis) to the electron itself; also

$$(A_s)^2 + (A_p)^2 = 1$$

. SHADOW prompts the user for the phase difference in degrees between ϕ_s and ϕ_p . The Degree of polarization determines the relative amplitude of the s and p vectors according to the relation :

$$\text{Degree of polarization} = \cos(\theta) / (\cos(\theta) + \sin(\theta))$$

where θ is the angle of polarization from the A_s axis.

Example:

Some examples of polarization states:

- Linearly polarized:

Phase difference = 0

Degree of polarization = whatever the above expression is when the desired value of θ is plugged in.

for $\theta = 45$ deg, $DOP = 0.50$

for $\theta = 30$ deg, $DOP = 0.63$

- Circularly polarized:

Phase diff = +90 (for Right), -90 (for Left)

Degree of Polarization = 0.5

Linearly Polarized Electric Field:

Circularly Polarized Electric Field:

NOTES:

- Generating the A vectors automatically forces storing the optical path length. Thus the number of rows will increase to 18 for each ray.
- If this A vector option is disabled, the full representation (18 instead of 12 rows) will not be used and rows 7, 8, and 9 will just contain the unpolarized electric field vector pointing in the horizontal (x-axis). Its magnitude is still normalized to 1. The only exceptions are the two synchrotron cases where the vector is either horizontal or vertical depending on the degree of polarization for that particular ray.
- There may be an overall phase factor $\exp(j * \phi)$ from one ray to another. If the source is specified coherent, this phase factor is set to 1. For incoherent sources, ϕ is varied randomly between 0 and 2π .

Appendix A

User's Program

The user's program must compute the photons/sec/rad²/eV at each point of the $(\hbar\omega, \theta, \phi)$ array and store the result on disk. The procedure is the following – MAKE_ID first writes the array in the file called UPHOT.DAT, all real values are in REAL*8 precision. The User's program should contain the READ statements:

```
OPEN (20, FILE='UPHOT.DAT', STATUS='OLD', FORM='UNFORMATTED')
READ (20) NE, NT, NP
READ (20) (ENER(K), K = 1, NE)
READ (20) ((THETA(J,K), J = 1, NT), K = 1, NE)
READ (20) (((PHI(I,J,K), I = 1, NP), J = 1, NT), K = 1, NE)
```

where NE, NT, NP are the number of points in ω, θ, ϕ respectively. It may be a good idea to use the IMPLICIT REAL*8 statement. Note that the file must remain open for writing later on. The user's program, after computing the photon distribution at the values specified by these ENER, THETA, PHI arrays, should append it to the file UPHOT.DAT:

```
WRITE (20) (((RN0(I,J,K), I = 1, NP), J = 1, NT), K = 1, NE)
WRITE (20) (((POL_DEG(I,J,K), I = 1, NP), J = 1, NT), K = 1, NE)
CLOSE (20)
```

where RN0 is the photons/sec/rad²/eV and POL_DEG the degree of polarization defined by:

$$\text{Degree of Polarization} = \frac{A_x}{A_{total}} = \frac{A_x}{A_x + A_z}$$

The User's program may read (or compute) whatever trajectory file is appropriate. If the user wants to use the trajectory computed by MAKE_ID, the following information is available. The needed parameters for the user's program can be obtained from the namelist file UPHOT.PAR (see the example for a listing). In particular, the variables have the following meaning :

NCOMP = number of periods
RCURR = electron beam current (Amp.)
FTRAJ = file name of electron trajectory
IOPT = number of optimization
ITER = number of optimization completed

The remaining information is then obtained from the trajectory file which is read by the statements :

```
OPEN ( 21 , FILE=FTRAJ , STATUS= ' OLD ' , FORM= ' UNFORMATTED ' , READONLY )  
READ ( 21 ) N0 , RLAU , ENERGY1  
READ ( 21 ) RLA1 , RK , GA0 , BETA0  
READ ( 21 ) BETAX0 , BETAZ0 , BETAY0  
READ ( 21 ) B0 , ER , RLEN , NPOINT
```

```
READ ( 21 ) PHI_E , THE_E  
READ ( 21 ) TAU , Y0 , YSTEP  
C  
C the following loop reads the trajectory itself.  
C  
DO I = 1 , NPOINT  
  READ ( 21 ) X(I) , Z(I) , Y(I)  
  READ ( 21 ) BETAX(I) , BETAZ(I) , BETAY(I)  
  READ ( 21 ) T(I)  
END DO  
CLOSE ( 21 )
```

where :

N0	= ignored
RLAU	= wavelength of undulator (m)
ENERGY1	= fundamental energy (Joule)
RLA1	= fundamental wavelength (m)
RK	= deflection parameter K
GA0	= γ , E/mc^2
BETA0	= β , $\sqrt{1 - \frac{1}{\gamma^2}}$
BETAX0,BETAZ0,BETAY0	= initial $\beta_x, \beta_z, \beta_y$
B0	= peak magnetic field (Tesla)
ER	= electron energy E (Joule)
RLEN	= ignored
NPOINT	= number of points for the trajectory
PHI_E	= ignored
THE_E	= ignored
TAU	= ignored
Y0	= ignored
YSTEP	= ignored
X(I),Z(I),Y(I)	= instantaneous (X,Y,Z) coordinate
BETAX(I),BETAZ(I),BETAY(I)	= instantaneous $\beta_x, \beta_z, \beta_y$
T(I)	= instantaneous time t(y)

As usual (X,Y,Z) is the reference frame of SOURCE (Y is the undulator axis). Given this information, the User's Program will be called by MAKE_ID whenever it needs to calculate the photon spectra, either in the first pass or subsequent optimizations.

Appendix B

Bibliography

In the course of writing the code and this documentation, we have drawn on much published material and feedback from our users. The following list is by no means exhaustive but represent texts and papers that we found particularly useful.

For general optics, the following books are excellent material:

1. Max Born and Emil Wolf. *Principles of Optics: Electromagnetic Theory of Propagation Interface and Diffraction of Light*. Pergamon Press, sixth edition 1980.
2. H. P. Brueggemann. *Conic Mirrors*. The Focal Press, 1968.
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6. Orestes N. Stavroudis. *The Optics of Rays, Wavefronts, and Caustics*. Academic Press, 1972.

For Monte-Carlo and Stochastic Processes:

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4. Athanasios Papoulis. *Systems and Transforms with Applications in Optics*. McGraw-Hill Book Company, 1968.
5. Reuven Y. Rubinstein. *Simulation and the Monte Carlo Method*. John Wiley & Sons, 1981.

6. N. G. Van Kampen. *Stochastic Processes in Physics and Chemistry*. North Holland, 1981.

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1. K. Green. *BNL Internal Report 50522*. Upton, 1976.
2. *International Conference on Insertion Devices for Synchrotron Sources*. SPIE Proceedings **582**, 1985.
3. E. Koch (Ed.). *Handbook on Synchrotron Radiation 1a*. North Holland, 1983.
4. Giorgio Margaritondo. *Introduction to Synchrotron Radiation*. Oxford Press, 1988.
5. *Proceedings of Synchrotron Radiation Instrumentation Conferences*. Nucl. Instr. and Methods. North Holland 1982, 1984, 1986, 1988.
6. Herman Winick and S. Doniach. *Synchrotron Radiation Research*. Plenum Press, 1980.

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1. Alan G. Michette. *Optical Systems for Soft X Rays*. Plenum Press, 1986.
2. D. Sayre, M. Howells, J. Kirz, and H. Rarback (Eds.). *X-Ray Microscopy II*. **56** Springer-Verlag, 1988.
3. G. Schmall and D. Rudolph (Eds.). *X-Ray Microscopy*. **43** Springer-Verlag, 1984.

Also there are several SPIE proceedings on x-ray and geometrical optics, in particular:

1. *Space Optics Imaging X-Ray Optics Workshop*. **184** 1979.
2. *Ultra Violet and Vacuum Ultra Violet Systems*. **279** 1981.
3. *Reflecting Optics for Synchrotron Radiation*. **315** 1981.
4. *High Resolution Soft X-Ray Optics*. **316** 1981.
5. *Science with Soft X-Rays*. **447** 1983.
6. *International Conference on the Application, Theory, and Fabrication of Periodic Structures, Diffraction Gratings and Moire Phenomena II*. **503** 1984.
7. *Geometrical Optics*. **531** 1985.
8. *Applications of Thin-Film Multilayered Structures to Figured X-Ray Optics*. **563** 1985.
9. *Grazing Incidence Optics*. **640** 1986.
10. *X-Ray Calibration: Techniques, Sources, and Detectors*. **689** 1986.

11. *X Rays in Materials Analysis: Novel Applications and Recent Developments.* **690** 1986.
12. *X-Ray Imaging II.* **691** 1986.
13. *Soft X-Ray Optics and Technology.* **733** 1986.
14. *Reflective Optics.* **751** 1987.