Ray-Tracing of the Synchrotron Radiation Sources in Python

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Abstract

The present research is devoted to modeling of real Synchrotron Radiation Sources for Ray-Tracing. The modeling was implemented in Python for open source Ray-Tracer XRT licensed under the MIT License. The results obtained for Bending Magnet are in good agreement with theoretical studies. Also, the data precision is higher compared to the results obtained with analogous closed source program SHADOW.

Contents

1. Introduction

In the construction of a beamline at a synchrotron radiation facility, the understanding of the light source is important in order to design various components to be installed in the beamline. And in the last 20 years many computer software products have been developed for this purpose. Evolution of SR requires that simulation tools also evolve alongside the new sources. Whilst the generic and most prominent use of simulation tools is anticipating what to from an experimental arrangement and optimizing it, simulation tools may also be used for data analysis. To first order these tools may also be used to correct data for instrumental imperfections, but by including sophisticated sample models one may use simulations to determine the validity of the models, by matching experimental to simulated data. Another application of simulation tools in automatic beamline alignment (ABA) schemes. Since ABA requires that the simulation tool is closely linked to, for example, beemline control, the structure of the simulation tool also needs to be highly flexible from a computer science point of view.
Currently, a number of tools are available for simulating X-ray instrumentation and experiments, each with their own focus characteristics. Whilst all of these packages have their strengths, it can be difficult for the user community to drive the further development according to their needs. This a compelling reason for use open-source software, which aims to include the community in its mission to provide a practical and reliable platform into which users may easily inject their knowledge for their own benefit and for that of community as a whole[1]. Taking into account flexibility of the script and speed-in-action the most advanced open source ray-tracer is XRT, which was written in python. Nevertheless, this simulation software did not have any description of the real sources recently.
The purpose of this research was to extend the XRT library taking the real sources' parameters into consideration.

2. Theory

Synchrotron radiation (SR) is a relativistic effect and many features can be understood in terms of two basic processes – Lorentz contraction and Doppler shift. If an electron is moving with velocity v its relative velocity β is defined by
$\beta = v/c$.
As the total energy of electron is

$$‘E = \frac{m_0 \cdot c^2}{\sqrt{1-\beta^2}} = \gamma \cdot m_0 \cdot c^2$$

with m_0 the electron rest mass and c the velocity of light (in free space). γ is the relativistic Lorentz factor:

$$\gamma = \frac{E}{m_0 \cdot c^2}.$$

It is well known that the spatial radiation distribution of the non-relativistic electron is toroidal (Figure 1,a).

If the electron is relativistic, $\beta \to 1$, hence, $\gamma \gg 1$ and due to the Doppler shift all the radiation is emitted in a forward cone with aperture $\sim\frac{1}{\gamma}$ at a tangent to the direction of motion(Figure 1,b).

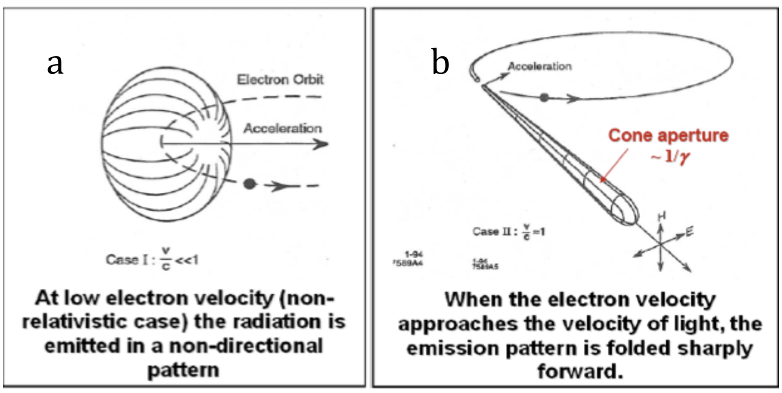

Figure 1. Spatial radiation distribution. a- non -relativistic and b- relativistic electron[6].

2.1 Radiation from a bending magnet

A bending magnet has a uniform magnetic field. The electron travels on the arc of a circle of radius set by the magnetic field strength as it is accelerated and forced to bend along a circular path. Schwinger[4] derives the number of photons N per second radiated in all vertical angles per current I and horizontal arc θ:

$$N(\lambda, t) = \frac{3^{3/2}}{40\pi} \cdot \frac{e\theta I \gamma^4}{h\rho} \left(\frac{\lambda_c}{\lambda}\right)^2 \int_y^\infty K_{5/3}(\eta)\, d\eta \qquad (1)$$

with y given by

$$y = E/E_c = \lambda_c/\lambda$$

where $\lambda_c = \frac{4\pi\rho}{\gamma^3}$ is the critical wavelength and E_c is the critical energy i.e. the value which splits the power spectrum for a bending magnet into two equal halves. Sokolov and Ternov[2] have examined the polarization of synchrotron radiation in considerable detail. The power radiated in the unit vertical angle was derived from their study by G.K.Green [3]:

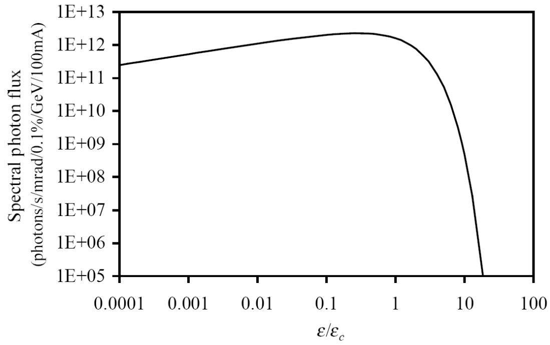

Figure 2 .Spectral photon flux vs photon energy (relative units)[6].

$$\frac{dP_i}{d\psi} = \frac{3e^2}{4\pi^2\rho}\left(\frac{\lambda_c}{\lambda}\right)^2 \gamma^2 \left\{(1+\gamma^2\psi^2)\left[l_2\, K_{2/3}(\xi) + l_3\, \gamma\psi\, (1+\gamma^2\psi^2)^{-1/2} K_{1/3}(\xi)\right]\right\}^2 \qquad (2),$$

$$\xi = \frac{\lambda_c}{2\lambda}(1+\gamma^2\psi^2)^{3/2}$$

where $K_\nu(x)$ are the modified Bessel functions of the 2nd kind for real order ν and real argument x; $l_2 = 1,\ l_3 = 0$ for the linear polarized radiation parallel to the orbital plane (σ -component of linear polarization) and $l_2 = 0,\ l_3 = 1$ for the linear polarized radiation perpendicular to the orbital plane (π -component).

Radiation emitted from a bending magnet has elliptical polarization which can be obtained if the phase shift between the components of linear polarization is known. Elliptical polarization may be presented as a sum of two circle components (right and left circle polarization). For the right circle polarization $l_2 = l_3 = \frac{1}{\sqrt{2}}$, for the left circle polarization $-l_2 = l_3 = \frac{1}{\sqrt{2}}$, and the phase shift between σ and π components is:

$$\sin\varphi = -\frac{|E_R|^2 - |E_L|^2}{2|E_\pi||E_\sigma|} \qquad (3).$$

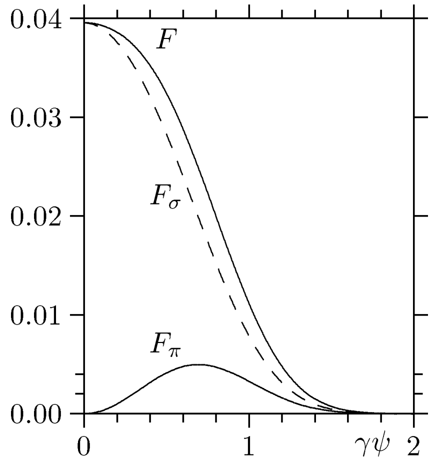

Figure 3. Total intensity(F) and components of sigma and pi polarization components vs vertical angle[6].

In the orbital plane the polarization is linear and parallel (has only σ -component). Out of the plane it is elliptical with a phase difference between components $\pm\frac{\pi}{2}$, so that the axes of the polarization ellipse are always parallel and perpendicular to the orbital plane.

Another way to get and to improve SR is to use insertion device such as wiggler and undulator. They are periodic magnetic structures that stimulate highly brilliant, forward-directed SR emission by forcing a stored charged particle beam to perform wiggles, or undulations, as they pass through the device. These two classes of id have a very little mechanical difference and criterion normally used to distinguish between them is the K-factor (deflection parameter) defined as:

$$\mathrm{K} = \frac{\mathrm{Be}}{\mathrm{mc}}\frac{\lambda_0}{2\pi}$$

where e is the charge of the particle passing through the ID, B is the peak magnetic field of ID, λ_0 is the period of the ID, m is the mass of the accelerated particle, and c is the speed of light.

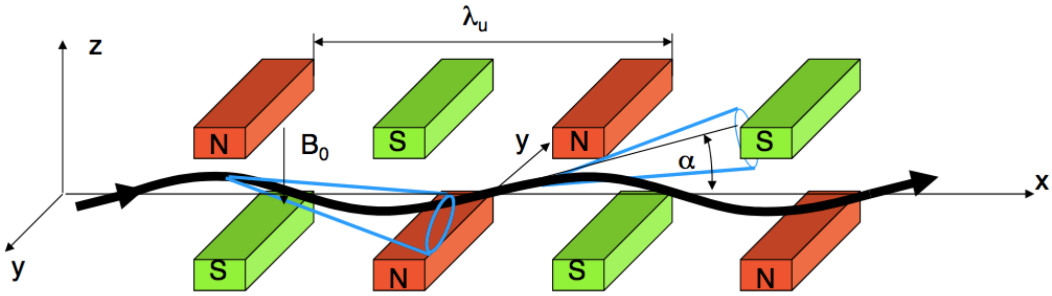

Figure 4. Schematic diagram of a wiggler. [5]

The case with K>>1 corresponds to a wiggler. In a wiggler period and strength of the magnetic field are not tuned to the frequency of radiation produced by the electrons. Thus every electron in the electron bunch radiates independently, and the resulting radiation spectrum is broad. A wiggler can be considered as a series of BM concatenated together, and its radiation intensity scales as the number of magnetic poles in the wiggler.
Undulators are deemed to have K<1. In an undulator source the radiation produced by the oscillating electrons interferes constructively with the motion of other electrons, causing the radiation spectrum to have relatively narrow bandwidth. Intensity of radiation scales as N^2, where N is the number of poles in the magnet array.

2.2 *Radiation from a* multipole wiggler (MPW)

Assuming small angular deflections ($\dot{x} \ll 1, \dot{y} \ll 1$) we can write equations of motion for the electrons travelling in s direction:

$$\frac{d^2x}{ds^2} = \frac{e}{\gamma mc}(B_y - \frac{dy}{ds}B_s)$$

$$\frac{d^2y}{ds^2} = \frac{e}{\gamma mc}(-B_x + \frac{dx}{ds}B_s)$$

If we have a MPW which only deflects in horizontal plane, i.e. only has vertical fields on axis.

$$\frac{d^2x}{ds^2} = \frac{e}{\gamma mc}(B_y), \quad \frac{d^2y}{ds^2} = 0$$

The B field is assumed to be sinusoidal with period λ_0
After integration of the equation (n) we obtain:

$$\frac{dx}{ds} = \frac{B_0 e}{\gamma mc}\frac{\lambda_0}{2\pi}\cos\left(\frac{2\pi s}{\lambda_0}\right) = \left(\frac{K}{\gamma}\right)\cos\left(\frac{2\pi s}{\lambda_0}\right)$$

$$x(s) = \left(\frac{K}{\gamma}\right)\frac{\lambda_0}{2\pi}\sin\left(\frac{2\pi s}{\lambda_0}\right).$$

Thus peak angular deflection is $\left(\frac{K}{\gamma}\right)$.
From Werner Brefeld the critical energy for MPW is defined by the following equation:

$$E_c = \frac{3}{2}\frac{hc^2}{e_0}BE^2$$

and the spectral flux is:
$N = 2.458 * 10^{10} * 2N * I_0[mA]E_e[GeV] * \frac{E}{E_c}\int_{\frac{E}{E_c}}^{\infty} K_{\frac{5}{3}}(\eta)d\eta$ [phot./(s mrad*0,1 *bandw.)].

Thus two clear advantages of the MPW is:
The critical energy can be set to suit the science need
The Flux is enhanced by twice number of periods

The total power emitted from a wiggler [6] with sinusoidal magnetic field is :

$$P = 1265.5 * E^2 I_b \int_0^L B(s)^2 ds = 632.8 * E^2 B_0^2 L I_b$$

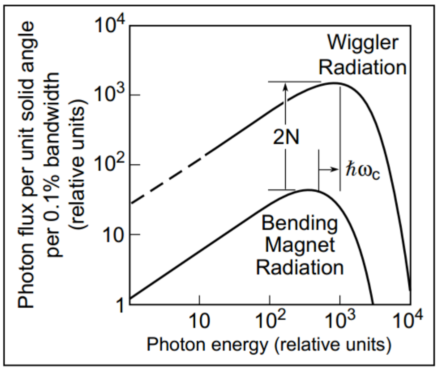

Figure 5.Photon flux vs photon energy for Wiggler and Bending magnet [6]

2.3 Radiation from an undulator

For the case of an elliptical trajectory ($\beta_z = \frac{K_x}{\gamma}\cos\frac{2\pi y}{\lambda_0}$, $\beta_x = \frac{K_z}{\gamma}\sin\frac{2\pi y}{\lambda_0}$) of N identical periods with periodicity λ_0 the radiation consists of a series of harmonics at frequencies:

$$\omega_n = n\frac{4\pi c\gamma^2}{\lambda_0(1 + K_x^2/2 + K_z^2/2 + \alpha^2)}, \qquad n = 1,2,3 \ldots$$

with intensity given by the following:

$$\frac{d^2 I}{d\Omega d\omega} = \frac{e\gamma^2 I}{4\pi\varepsilon_0 c}\left|\vec{A}_n(\alpha,\varphi)\right|^2 L\left(\frac{\Delta\omega}{\omega_1}\right),$$

where

$$L\left(\frac{\Delta\omega}{\omega_1}\right) = \sin^2\left(N\pi\frac{\Delta\omega}{\omega_1}\right)\Big/\sin^2\left(\pi\frac{\Delta\omega}{\omega_1}\right), \qquad \Delta\omega = \omega - \omega_n$$

$$\vec{A} = \xi(2\alpha\cos\phi\, S_0 - K_x(S_1 + S_{-1}), \qquad 2\alpha\sin\phi\, S_0 - iK_z(S_1 - S_{-1}), \qquad 0)$$

$$S_q = \sum_{p=-\infty}^{\infty} e^{\{-i(n+2p+q)\Phi\}} J_p(Y) J_{n+2p+q}(X)$$

$$\tan\Phi = \frac{K_z}{K_x}\tan\phi$$

$$X = 2\xi\alpha(K_x^2\cos^2\phi + K_z^2\sin^2\phi)^{1/2};$$

$$Y = \frac{\xi(K_x^2 - K_z^2)}{4}$$

$$\xi = \frac{n}{(1 + K_x^2/2 + K_z^2/2 + \alpha^2)}, \qquad \alpha = \gamma\theta.$$

The intensities of polarized radiation are conveniently described in terms of the Stokes parameters, involving differences in intensity between the radiation polarized in the x,z directions (S_1), in the $\pm 45°$. Directions (S_2) and circularly polarized with right and left helicity (S_3). S_0 is the total intensity.

$$S_0 = I_x + I_y = I_R + I_L = I_{45°} + I_{135°}$$
$$S_1 = I_x - I_y$$
$$S_2 = I_{45°} - I_{135°}$$
$$S_3 = I_R - I_L.$$

In practice, the Stokes parameters are calculated from the real (R) and imaginary (I) components of $\vec{A}$ as follows:

$$S_0 = A_{xR^2} + A_{xI^2} + A_{yR^2} + A_{yI^2}$$
$$S_1 = A_{xR^2} + A_{xI^2} - A_{yR^2} - A_{yI^2}$$
$$S_2 = 2(A_{xR}A_{yR} + A_{xI}A_{yI})$$
$$S_3 = 2(A_{xI}A_{yR} - A_{xR}A_{yI}).$$

Standard undulator ($K_z = 0$) emits linear polarization but the angle changes with observation position and harmonic order.

3. Modeling

Banding Magnet

Simulation of the Banding Magnet consists in creation array of energy, coordinates, direction and polarization for each photon. The following block-diagram showed algorithm of simulation.

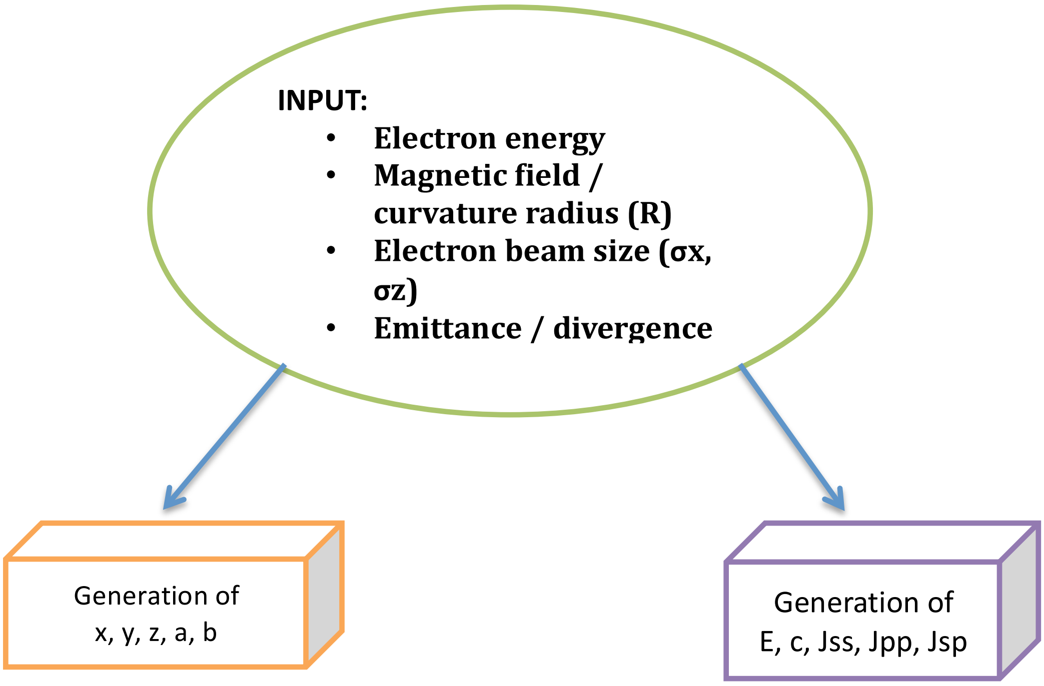

Figure 7. Block – diagram. There are showed inputs parameters and two main block of algorithm. x,y,z are arrays of coordinates ; a ,b, c are arrays coordinates of the k vector ; E is a photon energy array and Jss, Jpp, Jsp are arrays of the coherence matrix components.

Generation of coordinates and directions

Spatial distribution:

- θ – uniform
- r – normal
- $(r, \theta) \rightarrow (x, y)$
- z – normal

Angular distribution:

- φ – normal
- $a = \sin(\theta + \varphi)$
  $b = \cos(\theta + \varphi)$
- $c \equiv \psi$ – polarization dependence

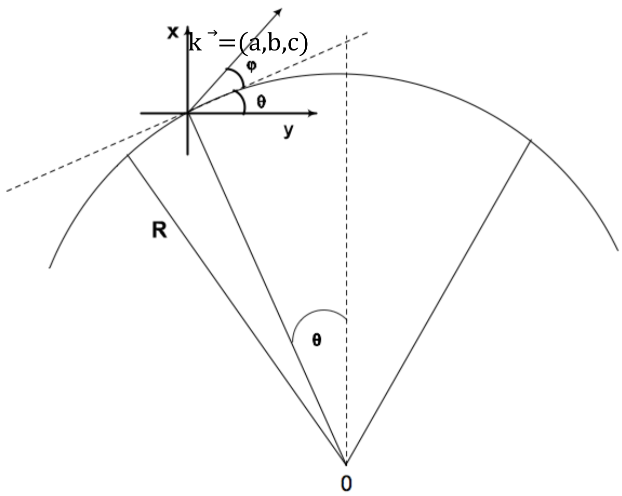

Figure 8. Schematic picture of photon emission at the arc of the bending magnet.

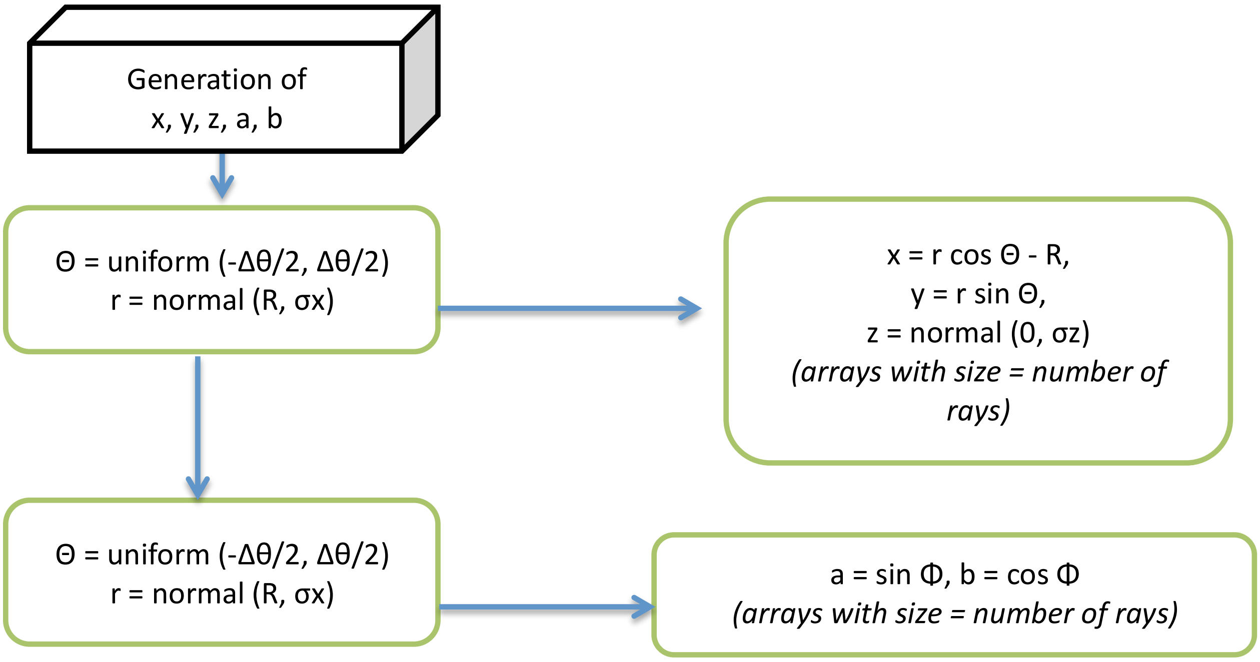

Figure 9. Block-diagram of module responsible for generation spatial and angular distribution of the photons.

Generation of energies and angular distributions

Dependence of the photon flux on the photon energy given by the equation (3). Therefore energy distribution can be obtained using the special algorithm (Figure 10).

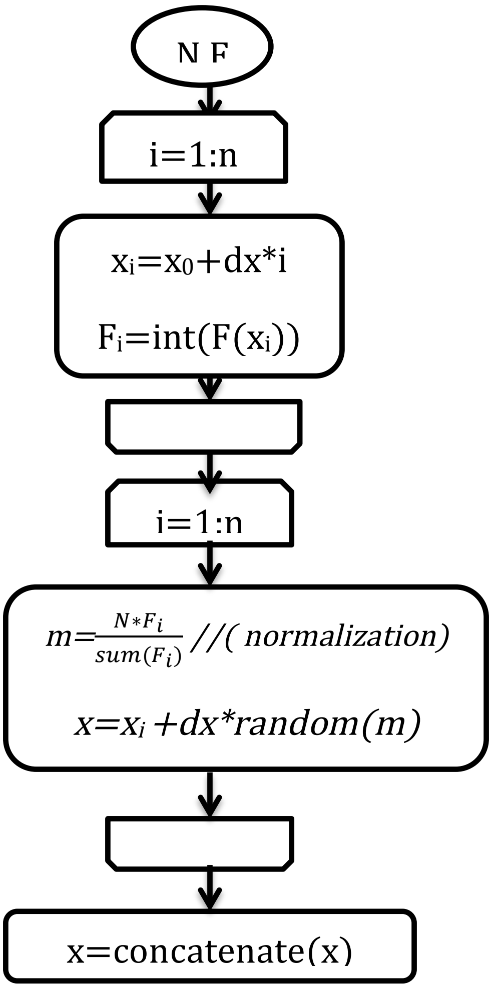

Figure 10. Block-diagram of the algorithm which makes distribution by x with the probability density as a given function F(x). n is a number of bins.

Further distribution of the vertical angle (θ) was obtained in a similar way. However, for making array values of c (c is vertical coordinate of k-vector) it is necessary to convolve angular distribution obtained by this method (from eq.(2)) and normal distribution for vertical angle with input divergence.
Components of coherence matrix is definite as:

$$Jss = \frac{Is}{Is + Ip}$$

$$Jpp = \frac{Ip}{Is + Ip}$$

$$Jsp = \sqrt{Jss * Jpp}(cos\varphi + isin\varphi)$$

where Is, Ip are intensities of π and σ polarization (eq. 2) for each vertical angle Θ and φ is a phase shift between σ and π components (eq. 3).

Wiggler and undulator:
It was written some scripts for these sources, but we have no time to debug it. Thus booth of them are in 'to do list' now.

4. Results

Results of our simulation of the BM were compared with the data from well-known ray-tracer "SHADOW". And in most cases our program gives values with better precision and distribution are smoother then SHADOW's one (Figure 11-15).

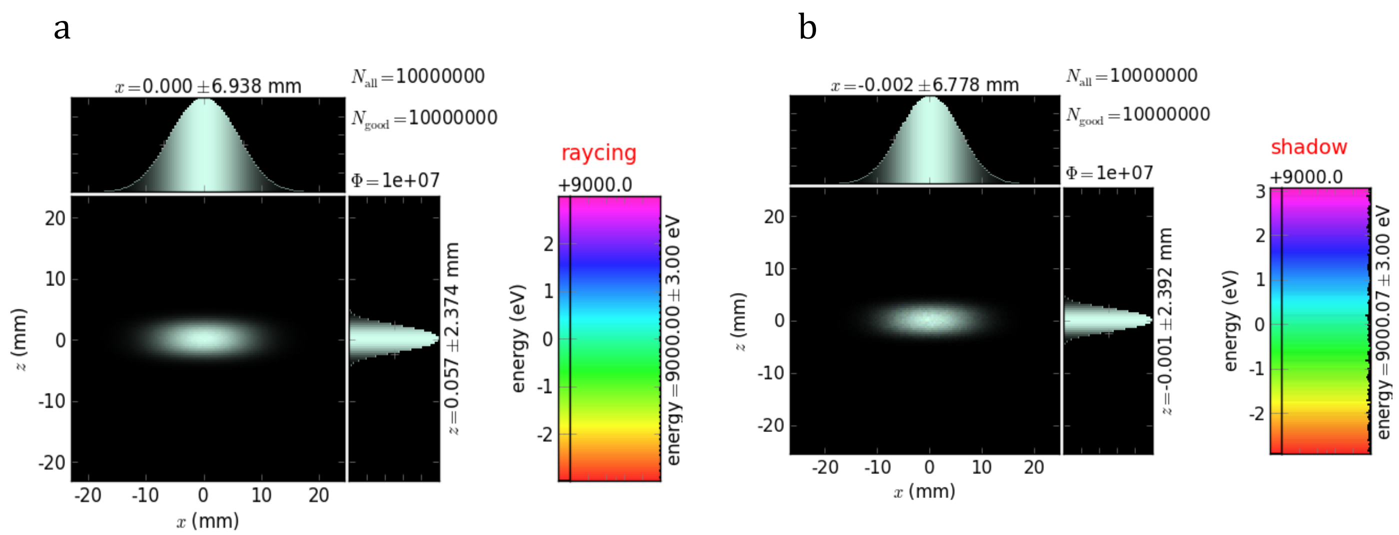

Figure 11. Comparison of x and z distributions for photon beam. a- results obtained with our script ; b- results of simulations in 'SHADOW'.

a b

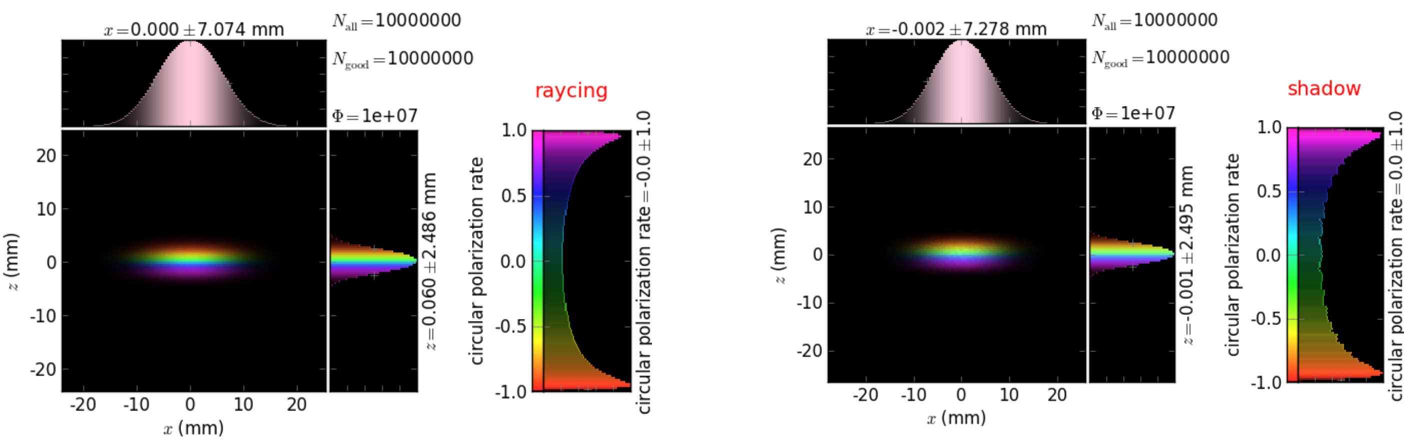

Figure 12. Comparison of circular polarization rate. . *a- results obtained with our script ; b- results of simulations in 'SHADOW'.*

a b

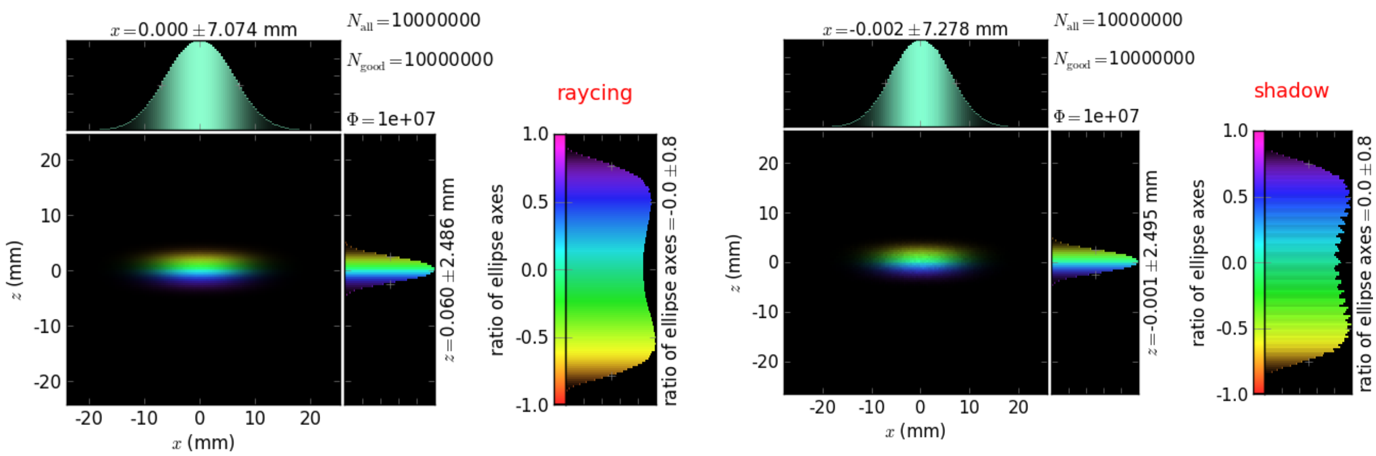

Figure 13. Comparison of ratio of ellipse axes. . a- results obtained with our script ; b- results of simulations in 'SHADOW'.

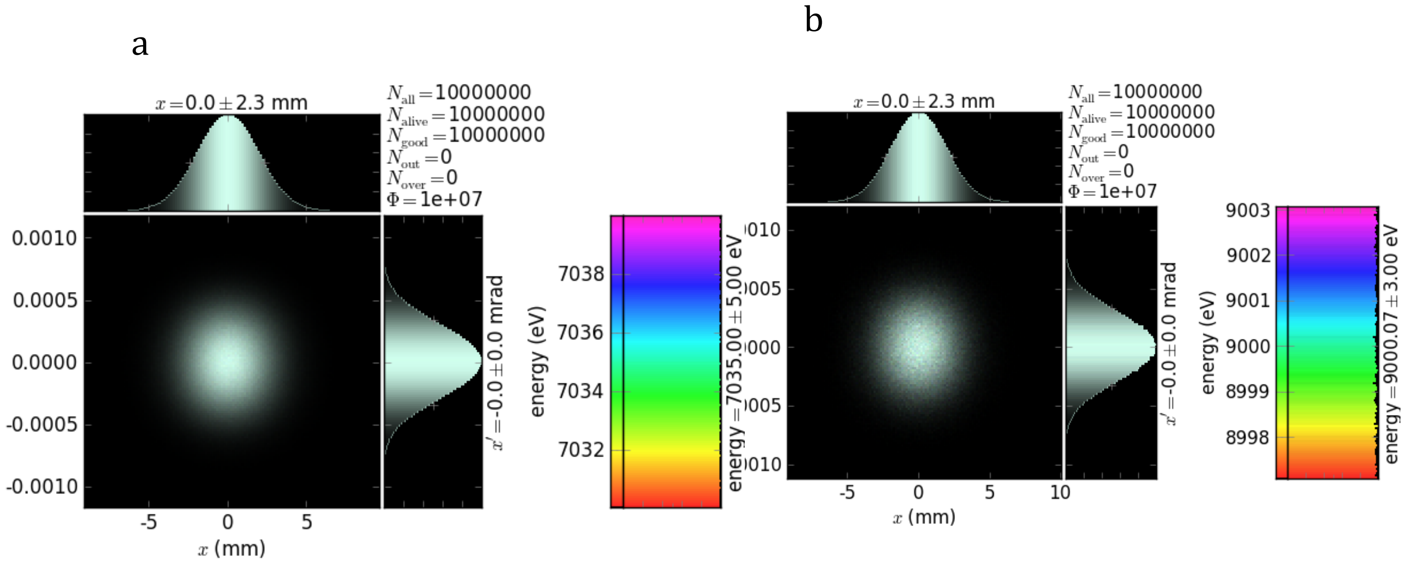

Figure 14. Comparison of x and x' distributions . a- result from our script . a- results obtained with our script ; b- results of simulations in 'SHADOW'

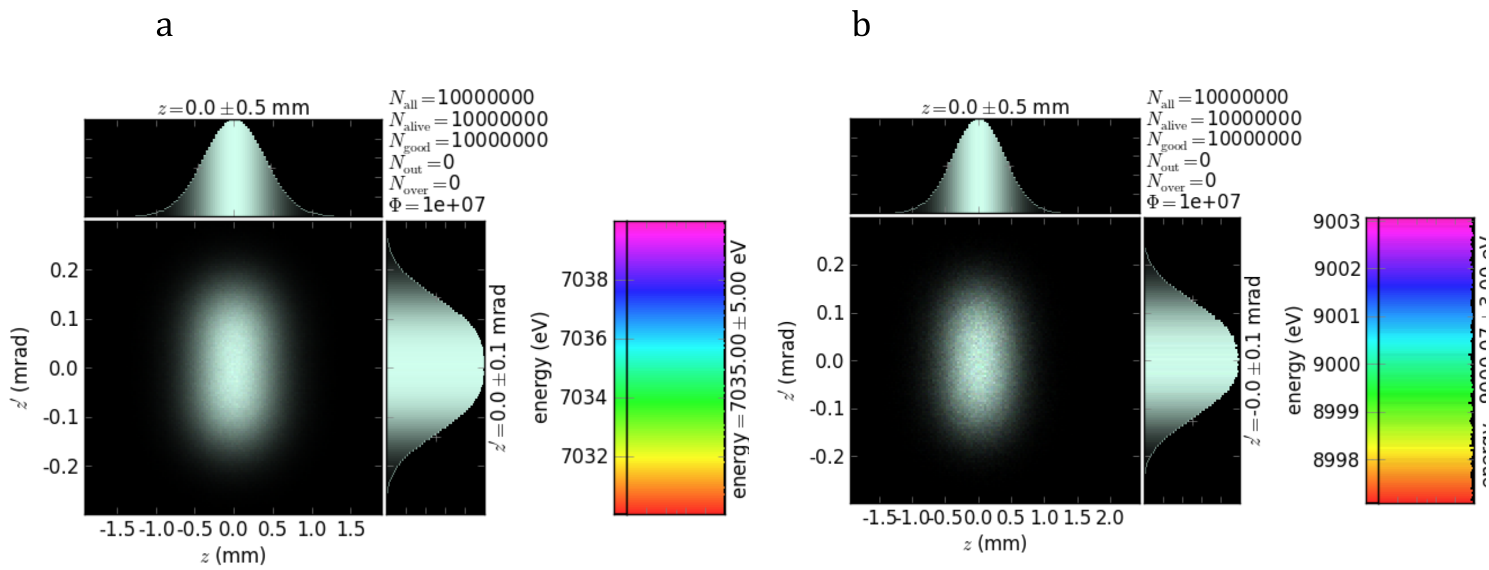

Figure 15. Comparison of z and z' distributions . a- results obtained with our script ; b- results of simulations in 'SHADOW'

5. Conclusion

During the poject the module which simulated real SR source (Bending Magnet) was written in python for open-source ray-tracer XRT. Moreover in python has been written a fast operation algorithm for building distributions with density of probability defined as difficult customer function. This algorithm will be useful in simulation of the others real SR sources such as wiggler and undulator . Futhemore have been done few steps in modeling of the wiggler and undulator and it will be in aslo usefull in the following work .
Results of the Bending Magnet simulation have been compared to the analogous ray-tracer SHADOW. As it was showed above the distributions have a similar characteristics values, but the distributions given by our simulation are more smoothly then distributions from SHADOW source in case of equal inputs parameters. Thus our modeling of a bending magnet takes priority over already existing simulation tools.
As well it is necessary to note that available now module of the Bending Magnet is only betta version and will be improved and developed soon.

6. Reference:

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