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Detailed X-ray Brightness Calculations in the Sirepo GUI for SRW

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Abstract. The brightness and coherence of modern light sources is pushing the limits of X-ray beamline design. The open source Synchrotron Radiation Workshop (SRW) provides physical optics based algorithms for correctly simulating such beamlines. We present new SRW capabilities to calculate source brightness and related quantities for undulator radiation. The Sirepo cloud computing framework includes a browser-based GUI for SRW. In addition to high-accuracy wavefront simulations, the Sirepo interface now supports analytical calculations for flux, photon beam size, divergence and photon brightness. We have included the effects of detuning from resonance and electron beam energy spread, which can be important in realistic operational conditions. We compare our results to features previously available in the Igor Pro interface to SRW, to analytical formulae available in the literature, and also to the results of simulated wavefront propagation. Differences between the various approaches are explained in detail, so that all the assumptions, conventions and ranges of validity can be better understood.

INTRODUCTION

Brightness of synchrotron radiation sources is one of the key parameters to measure performance. A synchrotron radiation calculation code should thus include utilities for such computations. At the same time, there exist a variety of formulae in the literature for the brightness.

The Synchrotron Radiation Workshop (SRW) is a physical optics code for precise calculation of synchrotron radiation from electron beams in bending magnet, wiggler and undulator devices in synchrotron light sources. Sirepo [5, 10, 11] is a web-browser based interface to SRW. It allows the setting up of source and beamline in a user-friendly way, with SRW doing the calculation on the server. We have added a fast calculation of brightness to the Sirepo interface so that one can quickly analyze a proposed SR source. The formulae used here were previously implemented in the Igor Pro interface to SRW. We describe this reimplementation and write down the analytic expressions for the formulae implemented, comparing them to ones in the literature, and also comparing to SRW wavefront computation for benchmarking purposes.

FLUX AND BRIGHTNESS FORMULAE

Formally, the brightness of a synchrotron radiation source is defined as the central value of the multi-electron Wigner function for the radiation [1], normalized by the total flux. In this paper, we will work with another often used approximate expression for the brightness:

$$B = \frac{\Phi}{4\pi^2 \epsilon_x \epsilon_y} \tag{1}$$

where Φ is the total flux (per unit time for a given current, and per 0.1% frequency bandwidth) and $\epsilon_{x,y}$ are the horizontal and vertical emittances of the photon wave front at the source location[1]. The horizontal and vertical emittances

[1] This equation requires that the photon distribution be Gaussian. Here, we use this result, even slightly off resonance where the Gaussian condition starts to be violated.

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of the emitted photon beam may be expressed as:

$$\epsilon_{x,y} = \Sigma_{x,y}\Sigma_{x',y'} \tag{2}$$

Here, $\Sigma_{x,y}$ are the RMS photon beam sizes including the effect of the electron beam distribution and likewise $\Sigma_{x',y'}$ represent the RMS divergences for the photon beam. Since we assume Gaussian distributions, these may be decomposed in quadrature as follows[2]:

$$\Sigma^2_{x,y} = \sigma^2_{x,y,eb} + \sigma^2_{r,\gamma} \tag{3}$$

$$\Sigma^2_{x',y'} = \sigma^2_{x',y',eb} + \sigma^2_{r',\gamma} \tag{4}$$

where $\sigma_{x,eb}$ and $\sigma_{y,eb}$ are the RMS horizontal and vertical electron beam sizes and $\sigma_{x',eb}$ and $\sigma_{y',eb}$ the RMS electron beam divergences. $\sigma_{r,\gamma}$ and $\sigma_{r',\gamma}$ are the photon beam divergences resulting from a single electron emission, potentially including an average over electron beam energy spread as well.

In the similar way that the electron beam size has a component coming from the electron beam energy spread, the single electron radiation emission also has a contribution from electron beam energy spread. This topic has been addressed in the paper by Tanaka and Kitimura [9]. Here we will provide different formulae [2] that were implemented in the Igor Pro interface to SRW since many years. In this proceeding we will give the formulae, though not the detailed derivations.

PHOTON BEAM FLUX

A well known formula for photon beam flux is given by K.J. Kim [6] (see also [7, 8]). The result is[3]

$$\Phi = \frac{\pi}{2} C_0 N_u I_b Q_n(K) \tag{5}$$

where N_u is the number of undulator periods, I_b is the beam current, n is the undulator harmonic number. The constant C_0 is

$$C_0 = \frac{\alpha d\omega/\omega}{q_e} = 4.5546497 \times 10^{13}\text{Coulombs}^{-1} \tag{6}$$

where a frequency bandwidth $d\omega/\omega$ of 0.01% has been used. α is the fine structure constant, 1/137, and q_e is the charge of the electron. The function $Q_n(K)$ is defined

$$Q_n(K) = \left(1 + \frac{K^2}{2}\right)\frac{F_n(K)}{n} \quad with \quad F_n(K) = \frac{4nq}{1+\frac{K^2}{2}} JJ^2(q). \tag{7}$$

We have defined

$$q = \frac{nK^2}{4+2K^2}. \tag{8}$$

The Bessel function factor JJ is given by

$$JJ = \left[J_{\frac{1}{2}(n-1)}\left(\frac{nK^2}{4+2K^2}\right) - J_{\frac{1}{2}(n+1)}\left(\frac{nK^2}{4+2K^2}\right)\right]. \tag{9}$$

K is the undulator deflection parameter which is related to the undulator parameters as

$$K = \frac{q_e B_0 \lambda_u}{2\pi m_e c} = 0.934\lambda_u[cm]B_0[T] \tag{10}$$

with λ_u the undulator period and B_0 the maximum undulator magnetic field.

[2] This is a good approximation when the electron beam sizes and divergences dominate. In the next generation "difraction limited" light sources, this is not the case and more care should be taken.

[3] Note that this is the result exactly on resonance. Other sources quote an equation larger by a factor of 2 for the flux. This is explained by the fact that the flux is larger by 2 at a slightly lower energy of $E_n = E_{n0}(1 - \frac{1}{nN_u})$. See also our Fig. 2b.

Generalization of Kim Formula

The Kim formula is generalized in several ways [2]. First, we accomodate elliptical undulators with a k_x in addition to k_y, along with relative phases ϕ_x and ϕ_y. Further, we allow the inclusion of the effects of energy spread and detuning from resonance. The energy spread and detuning effects will be accounted for by so-called "universal functions". The formula for flux is given by

$$\Phi = C_0 N_u I_b \frac{n k_1^2}{1+\frac{K^2}{2}} \overline{JJ}^2(qq) F_f(\Delta,\epsilon) G(\Delta, k_1, k_2) \tag{11}$$

The Bessel function factor is now a generalization of (9) given by

$$\overline{JJ}^2(qq) = \left[J_{\frac{n-1}{2}}(qq) - J_{\frac{n+1}{2}}(qq)\right]^2 + \frac{k_2^2}{k_1^2}\left[J_{\frac{n-1}{2}}(qq) + J_{\frac{n+1}{2}}(qq)\right]^2 \tag{12}$$

where

$$qq = \frac{n}{4}\frac{k_1^2 - k_2^2}{1+\frac{1}{2}(k_1^2+k_2^2)} \tag{13}$$

We have also defined

$$k_1^2 = k_y^2 \cos^2(\phi_x - \phi_0) + k_x^2 \cos^2(\phi_y - \phi_0) \tag{14}$$

$$k_2^2 = k_y^2 \sin^2(\phi_x - \phi_0) + k_x^2 \sin^2(\phi_y - \phi_0) \tag{15}$$

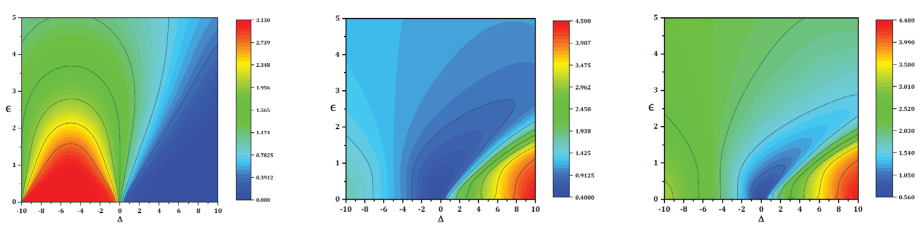
The phase ϕ_0 is given by

$$\phi_0 = \frac{1}{2}\tan^{-1}\left(\frac{k_y^2 \sin 2\phi_x + k_x^2 \sin 2\phi_y}{k_y^2 \cos 2\phi_x + k_x^2 \cos 2\phi_y}\right) \tag{16}$$

The quantities F_f and G in Eqn. (11) account for the detuning and energy spread effect. The universal function $F_f(\Delta,\epsilon)$ for the flux is a function of the normalized detuning and energy spread, which are defined thus:

$$\Delta = N_u n \frac{dE}{E_n}, \qquad \epsilon = N_u n \sigma_\delta. \tag{17}$$

Here, σ_δ is RMS relative energy spread of the electron beam and $dE = E - E_n$ is the detuning from the n^{th} resonant energy E_n. There are likewise universal functions for the beam size and divergence, notated as F_r and $F_{r'}$. These universal functions are plotted in Fig. 1.



(a) Flux correction (b) Beam size correction (c) Beam divergence correction

FIGURE 1: Universal functions of (a) photon flux, F_f (b) beam size, F_r and (c) divergence, $F_{r'}$. These contour plots provide the effect of energy spread and detuning from resonance on these quantities.

The factor G is an additional correction factor, higher order in the energy deviation.

$$G = \frac{1}{2}(1 + e^{\frac{a_\sigma^2}{2}})(1 - \mathbf{erf}(\frac{a_\sigma}{\sqrt{2}})) \tag{18}$$

$$a_\sigma = 2 m_a \frac{dE}{E}, \qquad m_a = \frac{n^2(k_1^2+k_2^2)}{w_f^2(1+\frac{1}{2}(k_1^2+k_2^2))} \tag{19}$$

w_f is a fitting parameter equal to 0.63276.

Reduction to Kim Formula

In the case of a horizontal planar undulator, such that $k_x = 0$, we find $\phi_x = \phi_0$, $k_1 = k_y$, and $k_2 = 0$. We then find

$$qq = \frac{nK^2}{4 + 2K^2} \equiv q \tag{20}$$

as in equation 8. The expression for flux, now reduces to the result in equation (5), noting that $F_f(0, 0) = \pi/2$.

PHOTON BEAM SIZES AND DIVERGENCES

For the brightness computation, and also for their intrinsic interest, we need the beam sizes and divergences. The single electron photon wavefront is not a Gaussian, so some care is required in defining the photon beam sizes and divergences. Expressions for RMS values are given as in reference [4], but with additional correction for energy spread and detuning via universal functions F_r and $F_{r'}$

$$\sigma_{r,\gamma} = \frac{1}{2}\sqrt{\lambda_n L_u}\ F_r(\Delta, \epsilon) \tag{21}$$

$$\sigma_{r',\gamma} = \sqrt{\frac{\lambda_n}{L_u}}\ F_{r'}(\Delta, \epsilon) \tag{22}$$

$$\lambda_n = \frac{\lambda_u}{2n\gamma^2}\left(1 + \frac{K^2}{2}\right) \tag{23}$$

the on-resonance spectral wavelength of the nth harmonic and L_u the undulator length, γ the average relativistic energy factor for the electron beam, and again, the universal functions are displayed in Fig. 1. We note that $F_r(0, 0) = 0.4717$ and $F_{r'}(0, 0) = 0.5795$.

BENCHMARKING WITH SRW

To test these formulae, we set up a simulation in SRW with an electron beam and undulator. We then compute total spectral flux and photon beam sizes and divergences at the center of the undulator. For the electron beam, we consider the case of the NSLS-II design parameters, with an energy of 3 GeV, a current of 500 mA, with a horizontal emittance of 0.9 nm and vertical emittance of 8 *pm*. We consider a low beta straight section with $\beta_x = 1.84m$ and $\beta_y = 1.17m$. The energy spread is $\sigma_\delta = 8.9 \times 10^{-4}$. We ignore dispersion in this calculation[4]. The corresponding electron beam sizes and divergences are as follows: $\sigma_{x,eb} = 40.7\ \mu m$, $\sigma_{x',eb} = 22.1\ \mu rad$, $\sigma_{y,eb} = 3.06\ \mu m$, $\sigma_{y',eb} = 2.61\ \mu rad$. For our example undulator, we consider a 3 *m* U20:

$$\lambda_u = 2cm \quad L_u = 3m \quad N_u = 150 \tag{24}$$

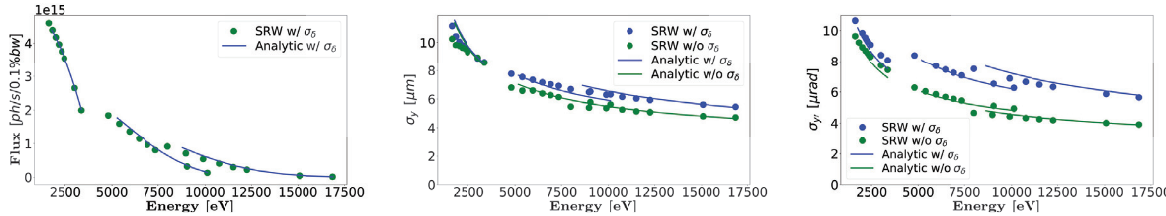
This undulator has a maximum K value of 1.828, and $n = 1$ resonant energy of 1.601 keV.

Opening the undulator gap reduces the K value (see Eqn. (10)) and we set the minimum K at 0.7. We refer to these plots as K-tuning curves. Since our formulae have the ability to capture flux, beam sizes and divergences away from the resonance, we may also cross check these quantities. In order to compute beam sizes, we set up 1:1 imaging optics, with a lens at 30 meters with focal lengths of 15 meters, and our observation plane at a total distance of 60 meters. We then compute beam sizes via the RMS value of the resulting transverse intensity profile. For the divergences, we simply allow a drift of 30 meters, and divide the resulting RMS beam sizes by the propagation length of 30 meters. The RMS values computed depend on the collection aperture size used. We have attempted to use a size such that 95% of the flux is captured. The same condition was used in the computation of the universal functions in the analytic formulae.

Fixing K and varying the energy from the resonance will be referred to as a "spectral detuning curve"[5]. The flux, beam sizes and divergences may then be combined to test the brightness using Eq. (1). All simulation results are shown in Figs. 2, 3, and 5.

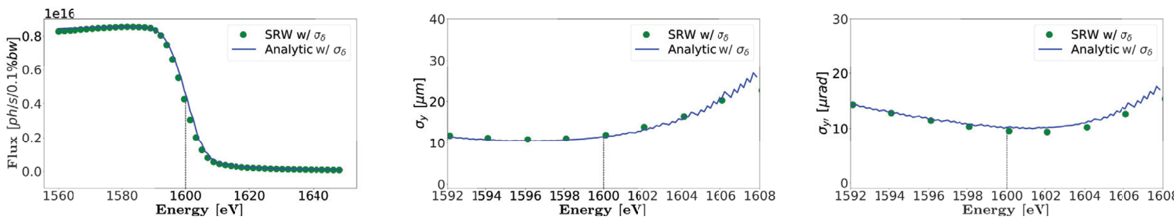
[4]We note that the effect of dispersion when coupled with energy spread is an increase in electron beam size, or divergence for a dispersion derivative. Energy spread is included in single photon beamsizes and divergences by averaging the resulting radiation patterns over the different energies. The effect on the size due to the resulting transverse offsets is included in the electron beam component in Eqs. (3).

[5]The jagged fluctuations present in the analytic spectral detuning plots in these figures are also found in the details of the universal functions in Fig. 1. This is an artifact of the numerical computation involving an FFT. We foresee improved accuracy to ameliorate this issue in the future.



(a) (b) (c)

FIGURE 2: K-tuning plots, on-resonance, K ranges from 1.828 to 0.7:(a) Photon flux, (b) beam size, and (c)divergence.

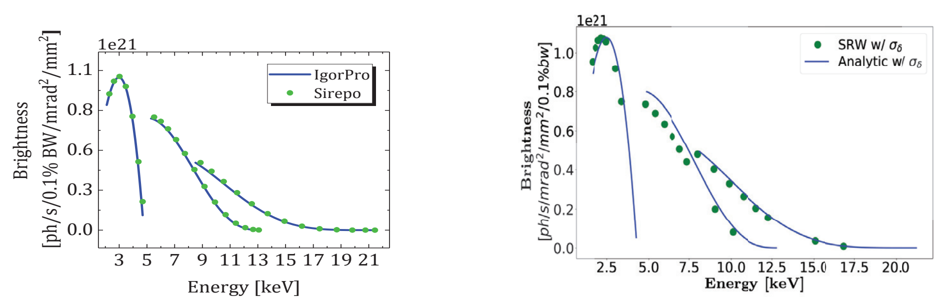


(a) (b) (c)

FIGURE 3: Spectral detuning plots (K = 1.828): (a) Photon flux, (b) beam size, and (b) divergence. Vertical dotted lines demarcate resonant energy.

SRW-SIREPO Integration

The formulae described in this proceeding and previously implemented in Igor-Pro have been integrated into Sirepo. The equations use the electron beam and undulator as defined within the Sirepo interface. We have cross checked that the resulting formulae implemented in Python for use with SRW and Sirepo give the same results as in Igor pro. This comparison is also shown in Fig. 4a. A screen-shot showing this brightness report in Sirepo is given in Fig. 5.



(a) (b)

FIGURE 4: (a) Comparison between Igor Pro and Sirepo brightness implementations.(b) Brightness K-Tuning plot with analytic and SRW calculations.

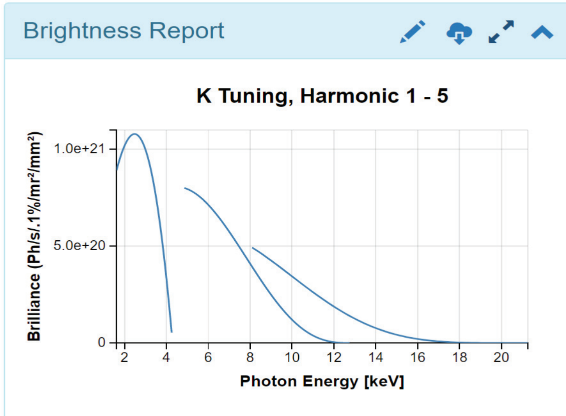


FIGURE 5: Screenshot of implementation of brightness report in Sirepo. Report types include flux, angular flux, brilliance, horizontal RMS angular divergence, vertical RMS angular divergence, horizontal RMS source size, and vertical RMS source size. Furthermore, both K tuning and spectral detuning plots are available for each quantity. The URL for the SRW Sirepo interface is given in reference [11].

CONCLUSION

We have described the implementation of undulator brightness formulae in the Sirepo interface to SRW and have benchmarked these formulae via SRW wavefront propagation computations. The Python implementation of analytic brightness formulae were benchmarked both against the previous implementation in Igor Pro and SRW wavefront propagation calculations. We have found good agreement in this benchmarking giving confidence in the validity of the expressions. They allow the inclusion of energy spread and detuning from resonance as we have shown. Derivations for these expressions will be provided elsewhere. These fast calculations should augment the usefulness of the Sirepo interface. Similar calculations for bending magnets and wigglers are still under development.

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