

GAUSSIAN RANDOM FIELD GENERATOR SERVAL: A NOVEL ALGORITHM TO SIMULATE PARTIALLY COHERENT UNDULATOR RADIATION

A. Trebushinin*, G. Geloni, and S. Serkez[†]

European XFEL, Schenefeld, Germany

Abstract

Wavefront propagation codes play pivotal roles in the design of optics at synchrotron radiation sources. However, they usually do not account for the stochastic behavior of the radiation field originating from shot noise in the electron beam. We propose a computationally efficient algorithm to calculate a single statistical realization of partially coherent undulator radiation fields at a given frequency under the approximation of quasi-homogeneity of the source. The proposed algorithm relies on a method for simulating Gaussian random fields. This algorithm is consistent with other well-established approaches, and, in addition, it possesses an advantage in terms of computational efficiency. It can be extended to other types of sources that follow Gaussian statistics. Finally, the demonstration of the algorithm is well suited for educational purposes.

INTRODUCTION

The wave optics approach allows to straightforwardly account for the effects related to fully coherent radiation. Nevertheless, the case of partially coherent radiation remains a sophisticated problem. The characteristics of synchrotron radiation heavily depend on the presence of the shot noise in an electron beam. Because of it, amplitudes and phases of the radiation exhibit stochastic fluctuations. In other words, radiation fields distributions change from realization to realization, and in order to obtain statistically meaningful intensities and correlation functions one needs to average over a statistical ensemble, so that the framework of statistical optics becomes quite natural.

Approaches for simulating partially coherent undulator radiation are proposed in several codes and in plenty of publications. Based on the framework of statistical optics, one can consider propagating the cross-spectral density function of the electric field by exploiting coherent mode decomposition methods, e.g. [1]. An alternative type of methods is based on Monte-Carlo-like simulations. One of the most well-known wave-optics simulation toolkits, Synchrotron Radiation Workshop (SRW) [2, 3] where the intensities are being summed up to form an intensity of the synchrotron radiation.

The algorithm we propose here relies on the generation of instances of the stochastic process, instead of dealing with ensemble-averaged quantities like correlation functions or averaged intensities. The method we propose is based on

Gaussian random field generator. In practice, we restrict complex Gaussian noise by the effective size and divergence of the radiation field. Introducing Gaussian noise, we effectively emulate the contribution of the shot noise accounting for all electrons at once. As a result the algorithm provides complex amplitude of a multimode field of the undulator radiation, suitable for propagation through a beamline. We call this method SERVAL (Synchrotron Emission Rapid eVALuator)¹. The results reported in this contribution were published in [4].

THEORETICAL BACKGROUND ON UNDULATOR RADIATION STATISTICAL PROPERTIES

Undulator radiation has an intrinsic stochastic structure caused by random distribution of electrons in a volume of 6D phase space. This distribution follows the shot noise statistics as the number of electrons located in the finite volume of the electron beam phase space is *discrete* and *random*. This shot noise is imprinted in the radiation structure. It manifests itself as longitudinal and transverse spikes in the radiation pulse as illustrated in Fig. 1. By its nature, those fields follow the same statistics as *thermal light*: both are described in terms of Gaussian random processes [5].

However in contrast with thermal sources, which are fully incoherent and whose coherent spot-size at the source is about the radiation wavelength, undulator sources are partially coherent, and they exhibit a coherent spot size equal to the single-electron diffraction size.

For the case of the thermal light, the relation of the spiky structure in the far zone with the source size is described by Van Cittert-Zernike theorem [6, 7]. This theorem relates the cross-spectral density in the far zone with the intensity distribution at the source via Fourier transform. For undulator radiation this theorem is only applied to the special case of quasi-homogeneous sources. Applicability of Van Cittert-Zernike theorem to undulator radiation was thoroughly reviewed in [8]. To assess the coherence properties of the source one should compare the natural size and divergence of the radiation from a single electron with the size and divergence of the electron beam.

Field Correlation

The electron beam length $c\sigma_T$ (c is the speed of light and σ_T is the electron beam duration) is almost always much

¹ This is a backronym. From the beginning we came up with this name SERVAL and only then decided that it stands for Synchrotron Emission Rapid eVALuator.

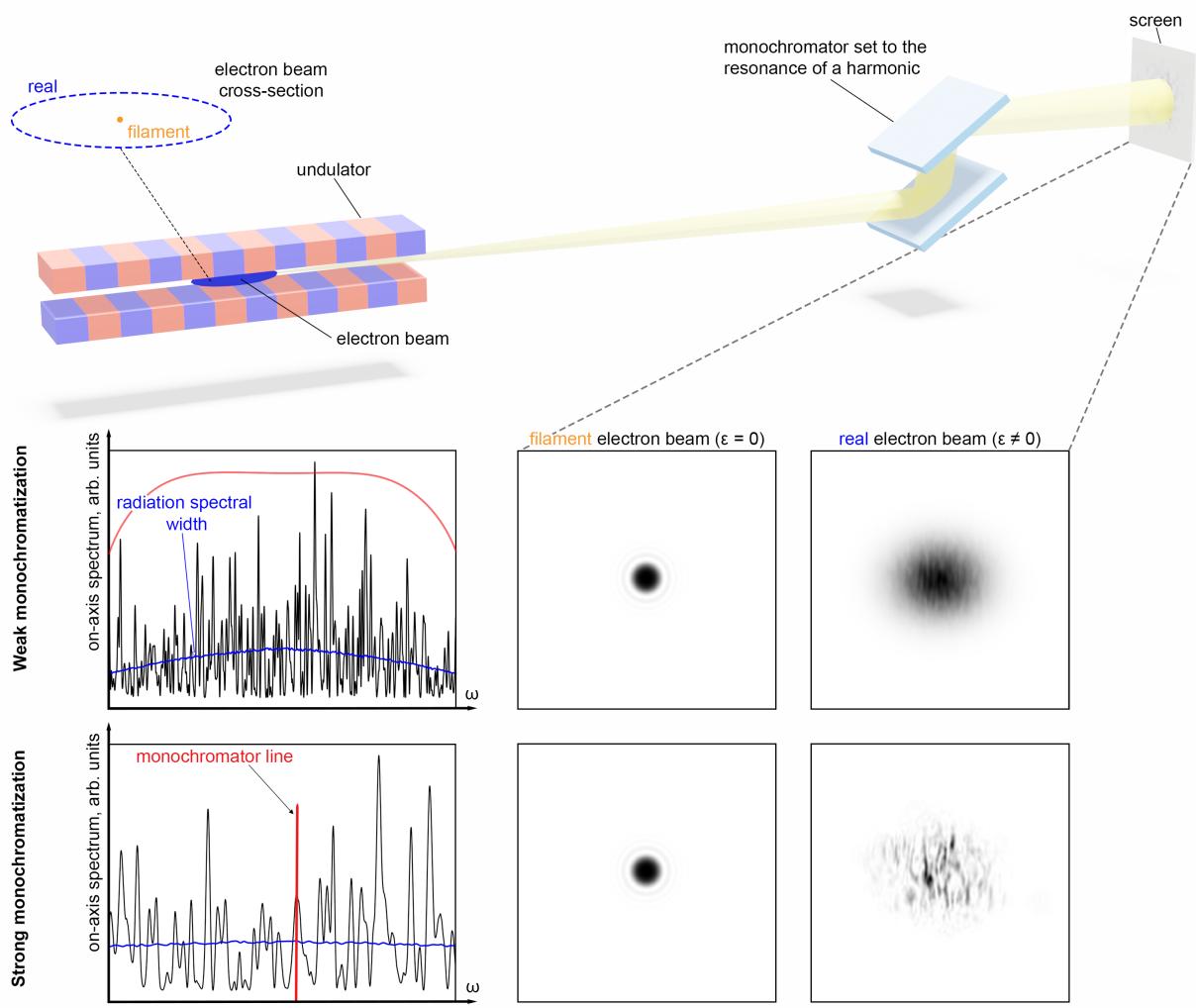


Figure 1: Spiky structure of synchrotron radiation. We compare radiation from a filament electron beam and from an electron beam with non-zero emittance. Figures on the left contain a single realization of spectrum (black lines) and ensemble-averaged spectrum (blue lines). Red lines represent the resolving power of monochromators. The plot on the top row illustrates a typical monochromatization incapable of resolving spectral spikes. To obtain the intensity observed at a detector (after a single passage of the electron beam) one needs to average over these frequencies/realizations. This is justified as the different spikes in the spectrum are not correlated both in time and, correspondingly, in the frequency domain. The bottom plot represents the resolving power of a monochromator that allows to resolve a single spectral spike of undulator radiation revealing its transverse spiky structure. Four figures on the right represent transverse intensity distribution upon monochromatization.

larger than the radiation wavelength ($\omega\sigma_T \gg 1$), this we call "long" electron beam approximation, and under this assumption we can express the spatial correlation separately from the longitudinal correlation, via the *cross-spectral density function* G at fixed frequency ω (see e.g. Eq. (12) in [8]):

$$G(z, \vec{r}_1, \vec{r}_2, \omega) \equiv \langle \bar{E}(\vec{\eta}, \vec{l}, z, \vec{r}_1, \omega) \bar{E}^*(\vec{\eta}, \vec{l}, z, \vec{r}_2, \omega) \rangle, \quad (1)$$

where $\langle \dots \rangle$ denotes averaging over the ensemble of fields $\bar{E}(\vec{\eta}_k, \vec{l}_k, z, \vec{r}, \omega)$ emitted by electrons with the deflections $\vec{\eta}_{1,\dots,N_e}$ and offset \vec{l}_{1,\dots,N_e} at fixed frequency ω . We represent the field of undulator radiation in the $\omega\vec{r}$ -domain by a function $\bar{E}(z, \vec{r}, \omega)$, where the radiation field is considered at a given frequency ω . $\bar{E}(z, \vec{r}, \omega)$ is related with the field

$E(z, \vec{r}, t)$ in the $t\vec{r}$ -domain by an inverse Fourier transform. Then, it is customary to define a normalized version of G , the *spectral the degree of coherence* $g(z, \vec{r}_1, \vec{r}_2)$, as:

$$g(z, \vec{r}_1, \vec{r}_2) = \frac{G(z, \vec{r}_1, \vec{r}_2)}{\sqrt{\langle |\bar{E}(\vec{\eta}, \vec{l}, z, \vec{r}_1)|^2 \rangle \langle |\bar{E}(\vec{\eta}, \vec{l}, z, \vec{r}_2)|^2 \rangle}}. \quad (2)$$

Starting from here we will omit ω in the equations for brevity of the notation.

Quasi-homogeneous Sources

Quasi-homogeneity is the transverse equivalent of quasi-stationarity. It means that at different transverse positions

across the radiation beam intensity $\bar{I}(z, \vec{r})$ transverse modes have the same "shape". It allows us to factorize cross-spectral density of the virtual source (located at $z = 0$):

$$G(0, \vec{r}, \Delta\vec{r}) = \bar{I}(0, \vec{r})g(0, \Delta\vec{r}), \quad (3)$$

here we introduced two new variables: $\vec{r} = (\vec{r}_1 + \vec{r}_2)/2$ and $\Delta\vec{r} = (\vec{r}_1 - \vec{r}_2)$.

Quasi-homogeneous sources are characterized by a special relation², which is strictly related to the van Cittert-Zernike theorem [6, 7] between source-intensity distribution $\bar{I}(0, \vec{r})$ and spectral³ degree of coherence in the far zone $g(z_0, \Delta\theta)$, where z_0 denotes position in the far zone. Namely, these two quantities form a Fourier pair. Note that the factorization presented in Eq. (3) is possible if:

- (i) intensity of the radiation at the source varies slowly at the scale of coherence length (i.e. large number of transverse modes)
- (ii) transverse coherence length does not depend on the transverse position (i.e. similar shape of transverse modes)

SERVAL ALGORITHM

We shape the transverse distribution of the field from an undulator as a Gaussian Random Field (GRF) in a manner similar to those mathematically described in [9], explained in simple words in [10], and exploited in imitating spectra and power distributions of free-electron laser in the linear regime [11, 12].

The SERVAL field at the center of undulator ($z = 0$) can be written in the following form:

$$\phi(\vec{r}) = \mathcal{F}^{-1} \left\{ \sqrt{\hat{I}(\vec{\theta})} \mathcal{F} \left\{ \sqrt{\bar{I}(\vec{r}')} \mathcal{W}(\vec{r}') \right\}(\vec{\theta}) \right\}(\vec{r}), \quad (4)$$

where $\mathcal{F}\{\cdot\}(\vec{\theta})$ and $\mathcal{F}^{-1}\{\cdot\}(\vec{r})$ are direct and inverse Fourier transforms, $\mathcal{W}(\vec{r}) = X(\vec{r}) + iY(\vec{r})$ is a complex Gaussian white noise where $X(\vec{r})$, $Y(\vec{r})$ follow the normal distribution with a mean is equal to zero and a variance is equal to unity. Finally,

$$\bar{I}(\vec{r}) = |\bar{E}_b(0, \vec{r})|^2 = \int_{\mathbb{R}^2} f_l(\vec{l}) |\bar{E}(\vec{\eta}, \vec{l}, 0, \vec{r})|^2 d\vec{l}, \quad (5)$$

$$\hat{I}(\vec{\theta}) = |\hat{E}_b(0, \vec{\theta})|^2 = \int_{\mathbb{R}^2} f_\eta(\vec{\eta}) |\hat{E}(\vec{\eta}, \vec{l}, 0, \vec{\theta})|^2 d\vec{\eta}, \quad (6)$$

are the intensity distributions of the radiation from the whole electron beam in \vec{r} -domain and inverse-spatial $\vec{\theta}$ -domain domains, correspondingly. The fields $\bar{E}(\vec{\eta}, \vec{l}, 0, \vec{r})$ and $\hat{E}(\vec{\eta}, \vec{l}, 0, \vec{\theta})$ are calculated with a help of Eq. (39) and Eq. (40) from [13]. $f_l(\vec{l})$ and $f_\eta(\vec{\eta})$ represents (smooth)

² Following the reasoning from [8].

³ Despite the word "spectral", this degree of coherence determines coherence properties in *real* or *inverse* space domain at given frequency ω , which is implied.

distribution functions of offsets and deflections of transverse electron beam phase space. The physical idea behind Eq. (4) is that the resulting field $\phi(\vec{r})$ should follow Gaussian statistics and obey the correct first order cross-spectral density function $g(0, \vec{r}_1, \vec{r}_2)$ under the quasi-homogeneous approximation, as we show in Appendix A of the original publication [4]. Following Eq. (4), the proposed algorithm consists of four steps: (i) creating complex Gaussian white noise, (ii) constraining it by the radiation distribution in the spatial domain at the source location, (iii) Fourier transform to inverse-spatial domain, and (iv) constraining the resulting field in the inverse-spatial domain. \vec{r} and $\vec{\theta}$ are assumed to be uncorrelated. Here we discuss these steps in more details:

- (i) Creating complex Gaussian white noise $\mathcal{W}(\vec{r}) = X(\vec{r}) + iY(\vec{r})$ in spatial domain.
- (ii) Constraining the complex Gaussian white noise by multiplication of the effective distribution of the radiation at the source expressed by Eq. (5). The result of this step is depicted at Fig. 2b.

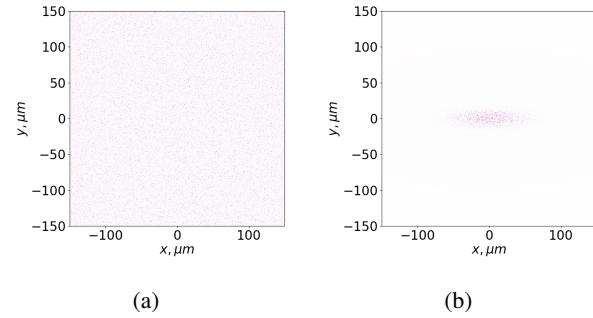


Figure 2: Intensity of the complex Gaussian white noise in spatial domain before (a) and after constraining (b) by the effective field size.

- (iii) Fourier transforming to the inverse-spatial domain (Fig. 3a). At this stage, we have a fully incoherent light source bounded in space akin to a *thermal light source*.
- (iv) Constraining the inverse-spatial distribution at Fig. 3a by multiplication with the effective radiation divergence following Eq. (6). This field is ready for propagation through free space, as the free space propagator works in the inverse-space domain.

After an inverse Fourier transform of the field in Fig. 3b back to real space one obtains the intensity distribution at the source, presented in Fig. 4.

As a result Fig. 4 and 3b depict a single realization of undulator radiation distribution at the source (in the center of the undulator cell), seen through a monochromator capable of resolving beyond the width of a single spike in the frequency domain.

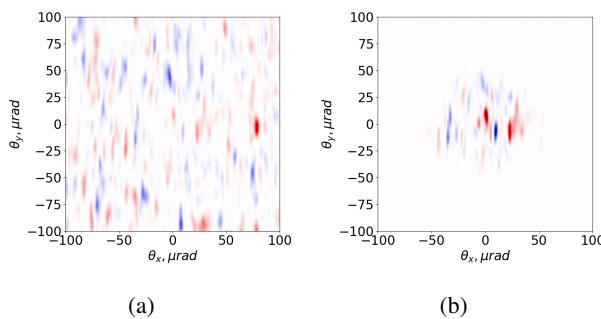


Figure 3: Angular intensity distribution of the field before (a) and after applying radiation divergence constraints (b).

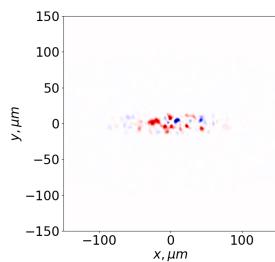


Figure 4: Radiation distribution at the source in real space.

Underlining Assumptions and Approximations

As it was said in the present section and demonstrated in Appendix A of the original publication [4], SERVAL is mathematically well-founded for quasi-homogeneous sources, where the cross-spectral density at the source factorizes Eq. (3). This is a strong restriction. In the Appendix A we show to which extent we can apply SERVAL when quasi-homogeneity (large number of spikes) does not hold. However, we found numerically that our method is satisfactorily applicable if a source is not strictly quasi-homogeneous.

When using SERVAL we consider single-cell undulators: the single source must have only one waist. This basically implies no quadrupoles, phase shifters, etc. in the magnetic structure of the insertion device. For the magnetic structure with imperfections, one can calculate the intensity distributions from a filament beam (Eq. (5) and (6)) numerically for a given magnetic structure and then convolve them with the electron beam phase space. If we simulate the radiation with SERVAL the effects of the electron beam emittance (along with energy spread) are accounted for in $\bar{I}(\vec{r})$ and $\hat{I}(\vec{\theta})$, Eq. (4).

Under these assumptions SERVAL accurately calculates synchrotron radiation pulses with computational advantages over Monte-Carlo-like methods. The SERVAL algorithm is not exclusively restricted to undulators sources, as $\bar{I}(\vec{r})$ and $\hat{I}(\vec{\theta})$ do not impose any additional restrictions except quasi-homogeneity. Thus, this Gaussian random field generator can be used to simulate the stochastic properties of other types of radiation sources.

CONCLUSION

In this contribution, we propose a novel computationally efficient algorithm, SERVAL, for simulating partially coherent synchrotron radiation emitted by an undulator at a specific harmonic. The proposed method is based on generating a Gaussian random field followed by application of constraints in real and inverse space domains. The result exhibits multimode structure which qualitatively corresponds to a radiation "slice" along the radiation pulse or which could be observed experimentally upon extreme monochromatization.

The algorithm yields a radiation field at the source position, which is usually in the middle of the undulator. One can propagate this field through an optical beamline to the sample location by conventional methods and codes for coherent radiation propagation. The proposed algorithm may be exploited for educational purposes when explaining basics of coherence. For more details, see the original publication [4].

ACKNOWLEDGEMENTS

We thank Evgeny Saldin for the initial discussions on the realization of the proposed method and his guiding support. We thank Serguei Molodtsov for his interest in this work.

REFERENCES

- [1] A. Singer and I. A. Vartanyants, "Modelling of partially coherent radiation based on the coherent mode decomposition", in *Advances in Computational Methods for X-Ray Optics II*, Sep. 2011, vol. 8141, p. 814106. doi:10.1117/12.893618
- [2] O. Chubar, Available: <https://github.com/ochubar/SRW>
- [3] O. Chubar and P. Elleaume, "Accurate and efficient computation of synchrotron radiation in the near field region", in proc. of the *EPAC98 Conference*, 1998, pp. 1177–1179.
- [4] A. Trebushinin *et al.*, "Gaussian random field generator for simulating partially coherent undulator radiation", *Optica*, vol. 9, no. 8, pp. 842–852, Aug. 2022, <https://doi.org/10.1364/OPTICA.460902>
- [5] J. W. Goodman, "Statistical Optics". Wiley, 2015.
- [6] P. H. van Cittert, "Die Wahrscheinliche Schwingungsverteilung in Einer von Einer Lichtquelle Direkt Oder Mittels Einer Linse Beleuchteten Ebene", *Physica*, vol. 1, no. 1, pp. 201–210, Jan. 1934, doi:10.1016/S0031-8914(34)90026-4
- [7] F. Zernike, "The concept of degree of coherence and its application to optical problems", *Physica*, vol. 5, no. 8, pp. 785–795, Aug. 1938, doi:10.1016/S0031-8914(38)80203-2
- [8] G. Geloni, *et al.*, "Transverse coherence properties of X-ray beams in third-generation synchrotron radiation sources", *Nucl. Instrum. Methods Phys. Res., Sect. A*, vol. 588, no. 3, pp. 463–493, Apr. 2008, doi:10.1016/j.nima.2008.01.089
- [9] A. Lang, "Simulation of stochastic partial differential equations and stochastic active contours", Ph.D. Thesis (Universität Mannheim, 2007) <http://ub-madoc.bib.uni-mannheim.de/1770>

- [10] G. Goon, "Cosmic Microwave Background simulations", Available: <https://github.com/garrett361/cmbpy>
- [11] T. Pfeifer *et al.*, "Partial-coherence method to model experimental free-electron laser pulse statistics", *Opt. Lett.*, OL, vol. 35, no. 20, pp. 3441–3443, Oct. 2010, doi:10.1364/OL.35.003441.
- [12] OCELOT collaboration, Available: <https://github.com/ocelet-collab/ocelet>
- [13] G. Geloni *et al.*, "Fourier treatment of near-field synchrotron radiation theory", *Optics Commun.*, vol. 276, no. 1, pp. 167–179, Aug. 2007, doi:10.1016/j.optcom.2007.03.051.