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FOCUS: FAST MONTE CARLO APPROACH TO COHERENCE OF UNDULATOR SOURCES

M. Siano*, B. Paroli, M. A. C. Potenza, Università degli Studi di Milano, Milan, Italy
G. Geloni, European XFEL, Schenefeld, Germany
D. Butti, T. Lefevre, S. Mazzoni, G. Trad, CERN, Geneva, Switzerland
U. Iriso, A. A. Nosych, L. Torino, ALBA-CELLS, Cerdanyola del Vallés, Spain

Abstract

We present *Fast Monte-CarlO approach to Coherence of Undulator Sources* (FOCUS), a new GPU-based code to compute the transverse coherence of X-ray radiation from undulator sources. The code relies on scaled dimensionless quantities and analytic expressions of the electric field emitted by electrons in an undulator. A consistent use of Fourier optics and statistical optics naturally leads to the core structure of the code, which exploits GPUs for massively parallel computations. We validate our approach by direct comparison with *Synchrotron Radiation Workshop* (SRW), evidencing a reduction in computation times by up to five orders of magnitude on a consumer laptop. Finally, we show examples of applications to beam size diagnostics.

INTRODUCTION

Computational tools are or fundamental importance at current synchrotron radiation facilities. The high complexity of modern X-ray beamlines and the need to properly characterize the emitted X-ray wavefronts as a function of the source parameters demand for accurate numerical codes.

To this aim, several software packages have been developed, based either on ray tracing or on wave optics [1–4]. Among them, *Synchrotron Radiation Workshop* (SRW) has been extensively validated at different facilities, and has become a reference in the accelerator and X-ray optics communities.

Simulations of the transverse coherence of X-ray beams are among the most challenging tasks and must rely on a statistical description of wave optics. The standard approach involves multi-electron simulations based on Monte Carlo sampling techniques. More recently, the coherent-mode decomposition method [5] has been applied to describe the transverse coherence properties of X-ray beams from undulator sources [6]. However, both methods are quite demanding in terms of computer resources and computation times.

Here we describe a new code, natively running on GPUs, to compute the transverse coherence of undulator X-ray radiation as a function of the electron beam parameters [7]. The code is named *Fast Monte CarlO approach to Coherence of Undulator Sources* (FOCUS) and relies on analytic expressions of the electric field obtained in free space. A consistent use of Fourier optics and statistical optics naturally leads to the massively parallel code implementation. FOCUS is written in C++ language accelerated with CUDA to harness the compute capabilities of modern GPUs. Compared to multi-electron SRW simulations running with multi-threading parallelization, FOCUS achieves a remarkable reduction in computation times by up to five orders of magnitude on a consumer laptop. This enables fast and accurate characterization of the transverse coherence properties of the emitted X-ray beam as a function of the electron beam parameters.

THEORETICAL BACKGROUND

Let $\vec{E}(\vec{x}, z)$ be the slowly-varying envelope of the Fourier transform of the electric field (hereafter, simply the field) emitted by an ultra-relativistic electron moving through a planar undulator. Here $\vec{x} = (x, y)$ denotes transverse coordinates over an observation plane at a distance z from the undulator center. In the ultra-relativistic regime $\gamma \gg 1$, γ being the Lorentz factor, the field $\vec{E}(\vec{x}, z)$ is determined by solving paraxial Maxwell equations [8]. In addition, under the so-called resonant approximation, the vertical polarization component can be neglected and the vector field reduces to a scalar quantity [8]. For distances $z \gg L_w$, L_w being the undulator length, the following general expression for the horizontally polarized field is valid [8]:

$$\hat{E}(\hat{\vec{\theta}}, \hat{z}) = \frac{e^{i\phi_s}}{\hat{z}} \operatorname{sinc}\left(\frac{\hat{C} - \hat{\delta}_E}{2} + \frac{\zeta^2}{4}\right). \tag{1}$$

In Eq. (1) we have defined scaled quantities and dimensionless parameters as follows [8]:

$$\hat{E} = -\frac{2c^2\gamma}{K\omega e A_{JJ,h}} E$$
$$\hat{\vec{x}} = \vec{x}\sqrt{\frac{\omega}{L_w c}} \qquad \hat{z} = \frac{z}{L_w} \qquad \hat{\vec{\theta}} = \frac{\hat{\vec{x}}}{\hat{z}}$$
$$\hat{\vec{l}} = \vec{l}\sqrt{\frac{\omega}{L_w c}} \qquad \hat{\vec{\eta}} = \vec{\eta}\sqrt{\frac{\omega L_w}{c}}$$
$$\hat{C} = 2\pi N_w \frac{\omega - h\omega_1}{\omega_1} \qquad \hat{\delta}_E = 4\pi N_w h \frac{\delta\gamma}{\gamma}$$
$$\phi_s = \frac{\hat{z}}{2}\left|\hat{\vec{\theta}} - \frac{\hat{\vec{l}}}{\hat{z}}\right|^2 \qquad \zeta = \left|\hat{\vec{\theta}} - \frac{\hat{\vec{l}}}{\hat{z}} - \hat{\vec{\eta}}\right|. \tag{2}$$

In Eq. (2),

- ω is the angular frequency of the emitted radiation
- $\lambda = 2\pi c/\omega$ is the radiation wavelength

* mirko.siano@unimi.it

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- c is the speed of light
- K is the undulator strength parameter
- $-e$ is the electron charge
- h is the harmonic number of the radiation emitted by the undulator
- $A_{JJ,h} = (-1)^{(h-1)/2}[J_{(h-1)/2}(u) - J_{(h+1)/2}(u)]$
- $u = hK^2/[2(2+K^2)]$
- J_n is the Bessel function of the first kind of order n
- N_w is the number of undulator periods
- $\omega_1 = 4\pi\gamma^2 c/[\lambda_w(1+K^2/2)]$ is the first harmonic of the undulator
- λ_w is the undulator period
- $\vec{l}$ and $\vec{\eta}$ are the electron offset and deflection, respectively
- $\Delta\gamma/\gamma$ is the relative energy deviation due to the finite energy spread of the electron beam.

Thanks to the paraxial approximation, ensured by the ultra-relativistic regime, we can apply Fourier optics methods to determine the electric field at any $\hat{z}$ [9]. In particular, the field in Eq. (1) can be described as a laser-like beam originating from a virtual source located at the undulator center and exhibiting a plane wavefront, similarly to the waist of a laser beam [8]. The field distribution of such virtual source is related to the inverse Fourier transform of the far-field pattern in Eq. (1), while the field at any $\hat{z}$ downstream the undulator center can be expressed as [8]:

$$\hat{E}(\hat{\vec{\theta}}, \hat{z}) = e^{i\phi_s} e^{-i\frac{\hat{z}}{2}\zeta^2} \left[\mathrm{Ei}\left(\frac{i\hat{z}^2\zeta^2}{2\hat{z}-1}\right) - \mathrm{Ei}\left(\frac{i\hat{z}^2\zeta^2}{2\hat{z}+1}\right)\right], \quad (3)$$

where Ei is the exponential integral function. Equation (3) is valid at perfect resonance $\hat{C} = 0$ and in the absence of energy spread. It reduces to Eq. (1) in the far-field limit $\hat{z} \gg 1$.

The transverse coherence properties of the emitted X-ray radiation are described by the two-point field correlation function known in statistical optics as the Spectral Degree of Coherence (SDC) [5]:

$$\mu(\hat{\vec{\theta}}_1, \hat{\vec{\theta}}_2, \hat{z}) = \frac{\langle \hat{E}(\hat{\vec{\theta}}_1, \hat{z})\hat{E}^*(\hat{\vec{\theta}}_2, \hat{z})\rangle}{\langle |\hat{E}(\hat{\vec{\theta}}_1, \hat{z})|^2\rangle^{1/2} \langle |\hat{E}(\hat{\vec{\theta}}_2, \hat{z})|^2\rangle^{1/2}}, \quad (4)$$

where angular brackets denote ensemble averages over the phase space density of the electron beam at the undulator center. For $\lambda \ll l_{\mathrm{bunch}}$, being l_{bunch} the bunch length, each electron emits independently on the others. This naturally leads to a description of the radiation SDC in terms of single-electron contributions only, which is particularly suitable for massively parallel implementations based on Monte Carlo sampling techniques:

$$\langle f(\hat{\vec{\theta}}, \hat{z})\rangle = \frac{1}{N_e} \sum_{k=1}^{N_e} f(\hat{\vec{\theta}}, \hat{z}, \hat{\vec{l}}_k, \hat{\vec{\eta}}_k, \hat{\delta}_k), \quad (5)$$

where $f(\hat{\vec{\theta}}, \hat{z})$ denotes quantities between brackets on the right-hand side of Eq. (5) and N_e is the number of electrons in the beam.

STRUCTURE OF THE CODE

FOCUS exploits the analytical expressions of the electric field in Eqs. (1) and (3) to compute the ensemble averages in Eq. (5). Since terms in the summations refer to different electrons, they can be simultaneously evaluated through the concurrent execution of many parallel threads.

The general workflow of FOCUS is sketched in Fig. 1, where we also highlight operations running either on the CPU or on the GPU.

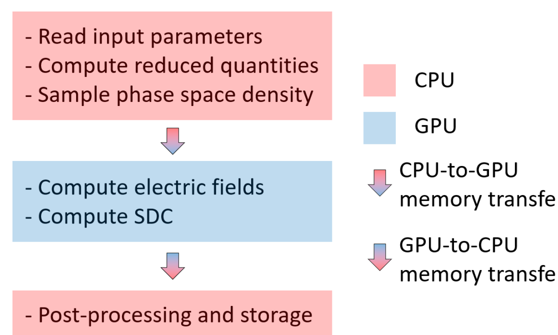

Figure 1: General FOCUS workflow.

First, the main parameters required to run the simulation are imported from external text files, which makes data input quite easy and flexible. Reduced parameters are derived based on Eq. (2). Then the phase space density of the electron beam is sampled either by an internal method relying on random number generators, or by reading values from a user-supplied file. This latter option is useful for benchmark purposes, as well as to assess the influence of non-gaussian beams on the coherence properties of the emitted X-ray beam. Computation is then moved from the CPU to the GPU. The terms in the summations in Eqs. (4) and (5) are computed in parallel through the concurrent execution of many threads on the processing cores residing on the graphic card. The final sum in Eq. (5) is also computed on the GPU by means of a parallel algorithm. Results are then transferred back onto the CPU for final post-processing and storage.

BENCHMARK WITH SRW

We validate FOCUS by direct comparison with SRW for N_e varying from 10 to 10^5. SRW simulations are run in parallel by exploiting multi-threading parallelization on the CPU. For each simulation, the same electron offsets, deflections and relative energy deviations are used in both FOCUS

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and SRW. To showcase the results of such comparison, we consider the NCD-SWEET undulator source at the ALBA Synchrotron Light Source as a typical case study for current third-generation machines. The main parameters are summarized in Table 1.

Table 1: Main Parameters of the NCD-SWEET Undulator Source

Quantity	**Parameter**	**Value**
Electron beam energy	E	3 GeV
Undulator parameter	K	1.56
Number of periods	N_w	92
Period length	λ_w	21.6 mm
Harmonic number	h	7
Observation distance	z	33 m
Hor. beam size	$\sigma_{\mathrm{beam,x}}$	130 μm
Hor. beam divergence	$\sigma'_{\mathrm{beam,x}}$	48 μm
Ver. beam size	$\sigma_{\mathrm{beam,y}}$	6 μm
Ver. beam divergence	$\sigma'_{\mathrm{beam,y}}$	5 μm
Energy spread	Δ_E	$1.05 \cdot 10^{-3}$

We report in Fig. 2 examples of the simulated horizontal and vertical profiles of the SDC. FOCUS results match SRW simulations, even reproducing the spurious fluctuations of the SDC at large Δx and Δy due to the relatively low number of sampled electrons. Results also show that increasing the number of electrons in the beam to values in the order of 10^4 or larger is effective in suppressing such oscillations.

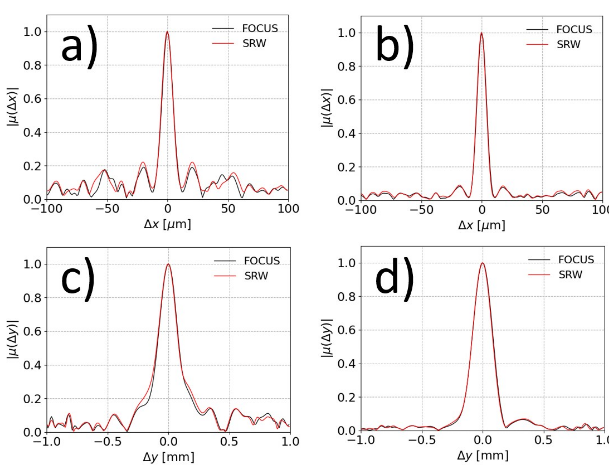

Figure 2: Benchmark of FOCUS with SRW. Results for the horizontal (a,b) and vertical (c,d) profiles of the SDC are shown, for $N_e = 10^3$ (a,c) and $N_e = 10^4$ (b,d).

We compare FOCUS and SRW computation times in Fig. 3. FOCUS achieves a remarkable reduction in computation times by up to five orders of magnitude with respect to SRW simulations. We also notice that the computation time of FOCUS does not scale linearly with N_e, opposite to the SRW case. Thanks to the concurrent execution of many parallel threads, the computation time of FOCUS is roughly constant for $N_e < 10^4$, and scales linearly with N_e only when all GPU resources are fully utilized, for N_e in the order of 10^5 or larger. For $N_e = 10^6$, FOCUS simulations require 3-4 seconds, whereas the same SRW computations would take 5 days.

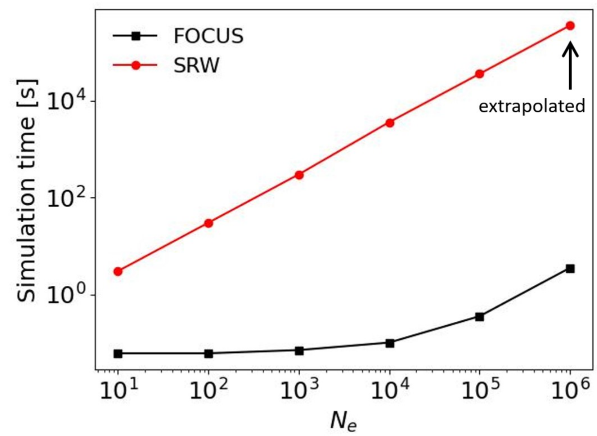

Figure 3: Comparison between FOCUS and SRW simulation times.

These results refer to a consumer laptop with a dual-core CPU and a NVIDIA GeForce 940MX graphic card with 512 CUDA cores. More modern, high-end GPUs with more CUDA cores and dedicated graphics memory can in principle achieve even better performances.

APPLICATIONS TO BEAM DIAGNOSTICS

Interferometric beam size measurements rely on the application of the well-known van Cittert and Zernike theorem to retrieve the electron beam size from the measured transverse coherence of X-ray radiation [5]. However, applicability of the van Cittert and Zernike theorem to undulator sources is highly debated, especially along the vertical direction in presence of beam emittances comparable to, or smaller than, the radiation wavelength [10–12].

Here we take advantage of the computation speed of FOCUS and thoroughly investigate the validity of the van Cittert and Zernike theorem for the NCD-SWEET undulator source. To this aim, we compute the horizontal and vertical profiles of the SDC for different beam sizes by performing accurate FOCUS simulations with $N_e = 10^6$-10^7 to limit random fluctuations in the results to a few per mils or less. Coherence profiles are then fitted to a Gaussian function to extract the transverse coherence length, here defined as the rms width of the SDC. Results are reported in Fig. 4, alongside with predictions based on the van Cittert and Zernike theorem.

Along the horizontal direction, the rigorous statistical optics approach and the van Cittert and Zernike theorem perfectly agree. The same applies along the vertical direction for beam sizes in the order of tens of micrometers. Opposite to these cases, deviations arise as the beam size is decreased to a few micrometers. Discrepancies are larger for smaller beam sizes. For example, for a vertical beam size of 3 μm the van

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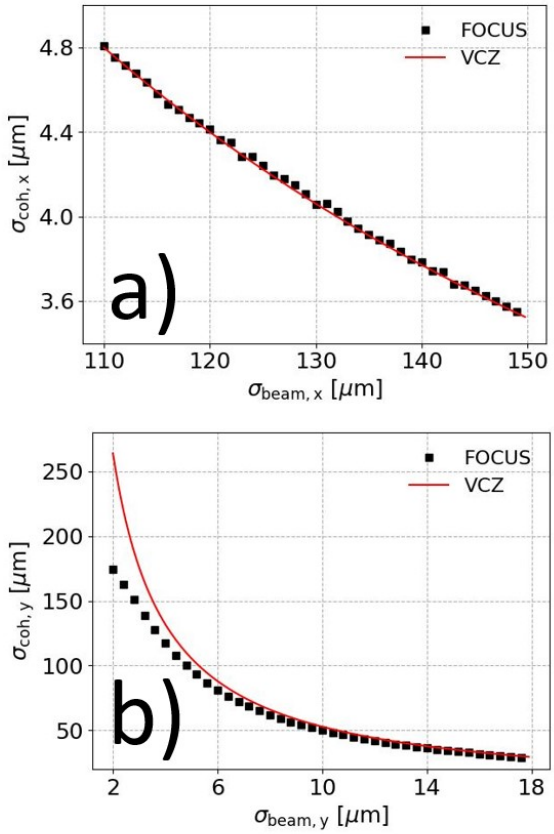

Figure 4: Simulated horizontal (a) and vertical (b) transverse coherence length as a function of the beam size for the NCD-SWEET undulator source, and comparison with predictions based on the van Cittert and Zernike theorem (VCZ).

Cittert and Zernike theorem would over-estimate the transverse coherence length by roughly 25% (175 µm, compared to 140 µm). On the other way around, this implies that interferometric beam size measurements based on the van Cittert and Zernike theorem would overestimate the beam size by roughly 25%, since a vertical beam size of 3.8 µm would be inferred from a measured transverse coherence length of 140 µm. Notice that such relative error of roughly 25% would then propagate to a relative error of roughly 50% in the emittance estimation. Therefore, although deviations between the two models are small for current third-generation facilities, they are however indicative of larger deviations which will become evident in future fourth-generation synchrotron light sources with micron-sized electron beams, especially close to the diffraction limit.

CONCLUSIONS

We have described *Fast Monte CarlO approach to Coherence of Undulator Sources* (FOCUS), a new GPU-base simulation code to compute the transverse coherence of X-ray radiation from ultra-relativistic electrons in an undulator source. We have validated FOCUS through a direct comparison with multi-electron SRW simulations. Besides accurately reproducing SRW results, FOCUS achieves a remarkable reduction in computation times by up to five orders of magnitude on a consumer laptop. Finally, we have shown an example of application to beam size measurements in presence of small beam emittances. These results might be of interest in view of next-generation light sources close to the diffraction limit.

We remark that FOCUS is complementary to existing codes like SRW. In particular, the aim of FOCUS is to fast evaluate the transverse coherence properties of the emitted X-ray beams as a function of the electron beam parameters, to support and help preparing more advanced and detailed simulations with traditional codes like SRW.

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