Parallel simulations of partially coherent wavefront propagation from a finite emittance electron beam

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Abstract. Hard X-ray undulator radiation at 3rd generation storage rings falls between the geometrical and the fully coherent limit. This is a result of the small but finite emittance of the electron beam source and means that the radiation cannot be completely modelled by incoherent ray tracing or by fully coherent wave propagation. We have developed using the wavefront propagation code Synchrotron Radiation Workshop (SRW) running in a Python environment, a parallel computer program using the Monte Carlo method for modelling the partially coherent emission from electron beam sources taking into account the finite emittance of the source. Using a parallel computing cluster with in excess of 500 cores and each core calculating the wavefront from in excess of a 1000 electrons, a source containing millions of electrons could be simulated. We have applied this method to the Diamond X-ray Imaging and Coherence beamline (I13).

1. Introduction

Synchrotron Radiation Workshop (SRW) [1, 2] is a versatile code with a library of routines written in C++ which is able to model the path of electrons through complex magnetic structures such as undulators and to calculate the resulting electric field in the frequency domain using the retarded potential [3]. SRW propagates the electric field using the Fresnel-Kirchoff equation [4]. Recently, SRW has been interfaced to the python programming language allowing the SRW routines to be called directly from python code. This gives great flexibility in developing new applications as wrapper code can be written in python to simulate new arrangements while retaining the speed and efficiency of the original SRW routines. The code can then take advantage of the available python code libraries for data processing and visualisation.

Complete coherence between two points on a wavefront implies a fixed phase relationship between the fields. Transverse coherence is therefore measured by the correlation between the electric field at two spatially separated points \( r_1 \), \( r_2 \) for waves with the same frequency \( \omega \). The definition of the cross-spectral density is [5]

\[
W(r_1, r_2, \omega) \delta(\omega - \omega') = \langle V^* (r_1, \omega) V(r_2, \omega') \rangle
\]  

(1)
Where \( \langle \ldots \rangle \) denotes an ensemble average and \( V(\mathbf{r}, \omega) \) is a component of the photon field with angular frequency \( \omega \) at position \( \mathbf{r} \). By definition, the spectral density at position \( \mathbf{r} \) is given by \( I(\mathbf{r}, \omega) = W(\mathbf{r}, \mathbf{r}, \omega) \). We then express the field in Eq. 1 as a summation over the field from each electron: \( V(\mathbf{r}, \omega) = \sum_i v_i(\mathbf{r}, \omega) \). When the resulting double summation is separated into a single summation of terms from the same electron and a double summation of terms from different electrons, this leads to

\[
W(\mathbf{r}_1, \mathbf{r}_2, \omega) \delta(\omega - \omega') = \left( \sum_i v_i^*(\mathbf{r}_1, \omega) v_i(\mathbf{r}_2, \omega') \right) + \left( \sum_{i \neq j} v_i^*(\mathbf{r}_1, \omega) v_j(\mathbf{r}_2, \omega') \right)
\]

If electron bunch length is much longer than the X-ray wavelength, the phase of the field from different electrons is uncorrelated and the double summation term averages to zero giving

\[
W(\mathbf{r}_1, \mathbf{r}_2, \omega) \delta(\omega - \omega') = (N_e/N) \sum_i v_i^*(\mathbf{r}_1, \omega) v_i(\mathbf{r}_2, \omega')
\]  \hspace{1cm} (2)

Where the ensemble averaging has been incorporated into the summation. The spectral degree of coherence at frequency \( \omega \) is given in terms of the cross-spectral density

\[
\mu(\mathbf{r}_1, \mathbf{r}_2, \omega) = W(\mathbf{r}_1, \mathbf{r}_2, \omega)/ \left( W(\mathbf{r}_1, \mathbf{r}_1, \omega) W(\mathbf{r}_2, \mathbf{r}_2, \omega) \right)^{1/2}
\]  \hspace{1cm} (3)

The normalisation in Eq. 3 ensures that \( \mu(\mathbf{r}, \mathbf{r}, \omega) = 1 \) independent of \( \mathbf{r} \). The spectral coherence also satisfies \( 0 \leq |\mu(\mathbf{r}_1, \mathbf{r}_2, \omega)| \leq 1 \) with 0 corresponding to complete lack of coherence and 1 to complete coherence (e.g. the field from a single electron). For emission from a realistic electron bunch, we must take account of the fact that the radiation field is generated by a large number of electrons which have some known distribution in phase space. The coordinates of the electron phase space are horizontal transverse position and angle \((x, x')\), vertical transverse position and angle \((y, y')\) and energy \(E\).

2. The Monte-Carlo method

The Monte-Carlo method can be used to perform the summation over the electrons in Eq. 2. In this method electrons are generated randomly with phase space coordinates conforming to the known electron distribution function. By generating sufficient numbers of electrons, the average will approach the required ensemble average in Eq. 1 as \( N^{-1/2} \) where \( N \) is the number of electrons generated. The multi-electron Monte-Carlo calculation is more demanding of computing power than single electron calculations as the computing time required scales as \( N \) which can be in excess of a hundred thousand. Fortunately, computer power has increased and the availability of parallel compute clusters containing hundreds of cores makes this approach possible. There are efficient routines available for generating a sequence of values of a set of uncorrelated random variables given their distribution function.

3. Modelling of the electron beam

SRW is able to model the trajectories of relativistic electrons through an undulator given starting values for the phase space coordinates. We assume that horizontal motion \((x, x')\), vertical motion \((y, y')\) and energy \((E)\) are uncorrelated so the distribution can be separated - \( p(x, x', y, y', E) = p_x(x, x') p_y(y, y') p_E(E) \). At an electron beam waist, \( p_x(x, x') \) and \( p_y(y, y') \) can be separated into the product of a distribution over position and over angle which allows efficient generation of phase space coordinates. In general however the horizontal and vertical phase space coordinates must separately be transformed, using an orthogonal matrix \( \mathbf{M} \) which depends on the electron beam Twiss parameters \([6]\), to a new coordinate system \((\xi, \xi')\) where the distribution can be written as \( p_\xi(\xi) p_\xi'(\xi') \). We assume normal distributions in \( \xi \) and in \( \xi' \)
and use standard python library routines to generate random coordinates for each electron. The matrix $M$ is then used to transform the new coordinates back to the original coordinate system giving the initial values for $(x, x', y, y')$ at the center of the undulator. We also model the energy spread using a normal distribution allowing values for the electron energy to be generated.

4. Code
The python code is split into four parts as follows:

(i) A program that schedules the multiple wavefront simulation processes and passes a unique random number seed to each.

(ii) A program to perform the wavefront simulation – reads in a configuration file and calls the SRW library routines to run the simulation code on a single processor. The program takes a single parameter – an integer, which is used to generate an output file name and to seed the python random number generator. The program stores the sums over a number of electrons of the mutual intensity function (Eq. 2) in the output file.

(iii) A program that combines all of the output files generated by the processes in part (ii) to produce the mutual intensity function and the complex degree of coherence. Runs on a single processor only.

(iv) A program to analyse and plot the data.

The code is run at a single X-ray energy to calculate the wavefront at a grid of positions on the image plane. In general, the spectral coherence is a function of 4 parameters - two positions on the plane $(x_1, y_1)$ and $(x_2, y_2)$. Although it would be computationally feasible to calculate the full two dimensional wavefront, in order to simplify interpretation, two separate one dimensional calculations were performed - for positions along a vertical and along a horizontal line through the beam axis.

5. Modelling of the Diamond coherence beamline
The Diamond I13 beamline is situated on one of the long straight sections of the storage ring and has two separate undulators feeding a coherence and an imaging branch. The electron
Figure 2. Magnitude of the spectral coherence in vertical direction 20 eV below the undulator peak energy (left) and 30 eV below (right).

optics consists of a mini beta section to get optimised electron focusing at each undulator. The beam emittance under normal conditions is 2.74 nm horizontally and 0.0274 nm vertically (1% coupling) and the Twiss parameters at the center of the coherence undulator are horizontally $\alpha = 0.97$, $\beta = 22.53$, $\gamma = 0.086$ m$^{-1}$ and vertically $\alpha = -0.028$, $\beta = 1.44$, $\gamma = 0.086$ m with energy spread $\Delta E/E = 1.00 \times 10^{-3}$. Fig. 1 shows the spectral degree of coherence along a vertical and a horizontal line through the center of the undulator radiation cone. The effect of varying the X-ray energy were also investigated and the results at two energies – one 50 eV below and one 50 eV above the peak energy are shown in Fig. 2.

6. Conclusions
As expected the simulations (Fig. 1) show a greater degree of coherence between points separated vertically in the undulator beam compared to points separated horizontally. The simulation for horizontally separated points is however more demanding of computer time as it required a finer mesh of points on the wavefront to capture the narrow feature at $(x_1 - x_2)/2 = 0$. This shows that the calculations becomes easier as a source approaches the coherent limit.

The calculations also show that the coherence is greatest at the vertical center of the undulator beam as gauged by the width in $(y_2 - y_1)/2$ of the spectral coherence at $(y_2 + y_1)/2 = 0$. There is also significant variation coherence as a function of X-ray energy (Fig. 2) for example the lobes in evidence at the undulator peak energy disappear as the X-ray energy is reduced. These features are not predicted by applying the Van Cittert-Zernike theorem to fully coherent single electron emission.

References
[1] O Chubar. Accurate and efficient computation of synchrotron radiation in the near field region. proc. of the EPAC98 Conference, pages 1177–1179, 1998.
[2] O Chubar. Precise computation of electron-beam radiation in nonuniform magnetic fields as a tool for beam diagnostics. Review of Scientific Instruments, 66(2):1872, 1995.
[3] I D Landau and E M Lifshitz. The classical theory of fields, volume 2 of Course of theoretical physics. Butterworth-Heinemann, 1980.
[4] M Born and E Wolf. Principles of Optics, volume 10. Cambridge University Press, 1999.
[5] Leonard Mandel and Emil Wolf. Optical Coherence and Quantum Optics. Cambridge University Press, 1995.
[6] Richard Talman. Accelerator X-Ray Sources. Wiley-VCH, 2006.