New challenges in ray tracing simulations of X-ray optics

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Abstract. The construction of new synchrotron sources and the refurbishment and upgrade of existing ones has boosted in the last years the interest in X-ray optics simulations for beamline design and optimization. In the last years we conducted a full renewal of the well established SHADOW ray tracing code, ending with a modular version SHADOW3 interfaced to multiple programming languages (C, C++, IDL, Python). Some of the new features of SHADOW3 are presented. From the physics point of view, SHADOW3 has been upgraded for dealing with lens systems. X-ray partial coherence applications demand an extension of traditional ray tracing methods into a hybrid ray-tracing wave-optics approach. The software development is essential for fulfilling the requests of the ESRF Upgrade Programme, and some examples of calculations are also presented.

1. Introduction

The first step before the construction of any X-ray system, such as a synchrotron beamline, is an accurate conceptual design of the optics. The beam should be transported to a given image plane (usually the sample position) and its characteristics should be adapted to the experimental requirements, in terms of flux, energy bandwidth, beam divergence, focal size, time structure, etc. Today, optical design relies more and more on computer simulation and optimization. These programs can be divided in two groups, those based on the propagation of rays along well defined optical paths, and those that propagate waves. The first ones are based on geometrical optics whereas the second ones rely on physical or wave optics. Some optical effects are better described by a geometrical model (sometimes extended by associating electric fields to each ray) like aberrations, errors in the optical surfaces, beam dimensions, role of critical angle in beam intensity, etc., whereas others, like interference and diffraction, are better explained using a wave model. Wave optics methods are computationally more expensive, as usually one has to finely grid the phase space. Hybrid methods permitting to switch from one description to another and vice versa would be ideal. The present trend [1] is the co-existence of software tools that allow treating the same system from two points of view. The integration of these two approaches into a single computer environment is a challenge that will certainly be developed in the near future. This paper describes the recent developments in ray tracing, mainly in connection with the SHADOW [2] code. At the end of the paper, some ideas of integration of ray tracing and wave optics are discussed, and some collaborative effort is on progress.

2. The SHADOW3 code

For synchrotron radiation applications, the code SHADOW has become the de facto standard because i) it is modular and flexible, capable of adapting to any optical configurations, ii) it has demonstrated its reliability during more of 25 years of use, as shown in hundreds of publications, iii) is simple to
use, specially under the ShadowVUI interface [3], and iv) it is in open source. Indeed, almost all of the synchrotron beamlines today in existence have in some way benefit from the help of SHADOW. The latest version SHADOW3 contains a major upgrade from the computational point of view. The code has been restructured following new computer engineering standards, ending with a modular Fortran 2003 structure and an Application Programming Interface (API). The new code conserves the original file-oriented SHADOW philosophy, but simplifying the compilation, installation and use. In addition, users can now become programmers using the newly designed SHADOW3 API for creating scripts, macros and programs; being able to deal with optical system optimization, image simulation, and also low transmission calculations requiring a large number of rays. SHADOW3 is open source, the code source is maintained using git and can be freely downloaded (e.g., git clone git://git.epn-campus.eu/repositories/shadow3).

3. Recent results of applications for the ESRF upgrade and new developments

3.1. X-ray lenses (single and compound)

Single and compound refractive lenses are frequently used at the synchrotron beamlines. Shaping the lens to a correct ideal profile for a perfect point-to-point focusing is essential for preparing X-ray micro- and nano-probes. The smaller spot size in a standard lens is limited by the size of the Airy disk (proportional to $\lambda/NA$) but the accepted numerical aperture $NA$ is limited by total reflection on the lens surface. This limitation can be overcome: Evans-Lutterodt et al. (2007) [4] demonstrated that kinoform lenses are not limited by the critical angle, and Schroer & Lengeler (2005) [5] proposed an adiabatically focusing lens, an array of lenses with increasing curvature from the entrance to the exit lens. Ray tracing is a very powerful tool to study aberrations. Ray tracing simulations [6] confirmed that elliptical lenses should be preferred to parabolic lenses for nano-focusing, in particular for large lens apertures. The major differences are not on the FWHM spot size, but in the intensity of the tails and therefore in the peak intensity (related to gain). Simulations (Fig. 1) also suggest that for highly demagnifying optics, it could be beneficial to use lenses with a profile that follows the Cartesian oval, to reduce the tails and obtain the ideal Gaussian focus. In fact, a lens for point-to-point focusing must be shaped following the Cartesian oval, as suggested by Descartes in the XVII century.

![Figure 1](image_url)

**Figure 1.** Simulations [6] of focal spot versus lens diameter for parabolic and elliptical shapes. The source is a typical Diamond undulator at $E = 8$ keV (approximated with Gaussian source of $\sigma_y=7$ µm, $\sigma_y'=8$ µrad). The theoretical broadening due to diffraction (Airy disk) is also shown, as well as the "theoretical" spot size obtained by applying the geometrical demagnification to the source dimension.
Compound refractive lenses are already implemented in SHADOW3, permitting the simulation of arrays of ellipses or parabolas, and the full control of the interface parameters, like varying curvatures. As an example, a parabolic CRL for the MASSIF Upgrade Beamline at the ESRF, made of 10 Be lenses of $R=500\,\mu m$, focusing in the vertical plane (focal distances $p=41.081$ m, $q=16.518$ m, thus $F=11.761$ m, demagnification $p/q=2.49$, at $E=12900$ eV, $\delta=2.04927 \times 10^{-6}$). The evolution of the beam divergence inside the CRL is shown in Fig. 2.

![Figure 2. Beam vertical divergence RMS when the beam traverses the individual lenses in a CRL.](image)

### 3.2. Coherence and partial coherence

Many experimental techniques exploit the good lateral coherence of the third generation synchrotron beams, and the excellent properties of the fourth generation. Light coherence originates interference and diffraction of X-ray beam and it is usually treated by wave optics methods, a formalism well adapted for totally coherent beams. However, the X-ray beam is not fully coherent, but partially coherent, thus the need of simulation tools that go beyond the physical models for treating these limit cases (wave and geometrical optics). A workshop “Partially coherent X-ray beam propagation: theory and computation” held in San Diego on August 23th 2012 discussed these issues [1]. The theory for the emission and propagation of partially-coherent synchrotron radiation exists, but there is an increasing need for its CPU-efficient algorithmic implementations.

The problem of simulating partially coherent beams for synchrotron application is twofold. On one side one has to know the intrinsic coherence of the source. We can suppose that the source is fully incoherent, totally coherent, or partially coherent. The propagation of a beam also originates coherence, as a result of the van Cittert-Zernike theorem, that relates the spatial coherence to the intensity distribution of the incoming radiation (e.g., source size). In fact, for several applications of 3rd generation synchrotron sources, the undulator source can be considered as a fully (but small) incoherent source and coherence is originated by propagation.

SHADOW includes a postprocessor \texttt{ffresnel} that can be used for wave-optics propagation of a beam calculated by ray tracing. It implements the Kirchhoff -Fresnel integral:

$$U(\vec{r}_f) = \frac{i k L}{4 \pi} \int_{S} U(\vec{r}_i) \frac{e^{ik|\vec{r}_f-\vec{r}_i|}}{|\vec{r}_f-\vec{r}_i|} dS,$$

(1)
where $U$ is the electric field, $\vec{r}_j$ is a point on the detector, $\vec{r}_i$ is a point on the aperture $S$, $k = 2\pi/\lambda$, and $I$ is an inclination factor ($-2 \cos \delta$, $\delta$ the angle between incident and output directions). This wave-optics application permits the calculation of the diffraction pattern, for example, from a slit or double-slit from a fully coherent beam (Fig. 3). SHADOW3 contains a 2D version of the Fresnel-Kirchhoff propagator, and a parallel version using GPUs is also available [7].

![Figure 3. Interference and diffraction from pinhole/apertures (Ø=0 or 200 μm). Left: rays on the apertures, right: intensity profiles at $L=1$ m from aperture, wavelength $\lambda=500$ nm](image)

It is remarkable that in most interesting cases the oscillations in the detector plane come from the variations in the optical path (the exponential term). Therefore, similar diffraction patterns can then be obtained using the approximation:

$$U_j = U(\vec{r}_j) \approx \sum_{i=\text{source}} U_i e^{i k r_{ij}} = M^{ij} U_i$$

(2)

Where $M$ is the ‘optical path matrix’, $r_{ij} = |\vec{r}_i - \vec{r}_j|$, and the source is just the aperture. For calculating a system made of several optical elements, the $M$ matrix is calculated for each element to the next one, and Eq. 2 can be used for propagating the source to the detector using a matrix $M$ that results from the
multiplication of the individual matrices. For two elements, a source propagated to the first optical element gives $M_{01}$, from first to second $M_{12}$, thus from source to detector $M_{03}=M_{01}M_{12}M_{23}$. $M$ matrices can be calculated using ray tracing because the coordinates of the points at a given element $r_i$ and at the next one $r_j$ are known by ray tracing. As an example, following the experiment in Leitenberger et al. [8], we simulated a source (140 µm, $E=10$ keV) projected on a plane at 30.9 m with two pinholes ($\Omega=2$ µm) separated 11.3 µm, and detected in a plane 1.38 m downstream from the beam. The intensity profile calculated using Eq. (2) for $U=1$ is shown in Fig. 4a. This is the diffraction pattern for a fully coherent beam. If one wants to calculate the intensity given by a partially coherent beam, or a totally incoherent beam, one can make $m$ realisations of $\{U_j\}$ with phase correlated according a given coherence degree and mutual distribution function, and calculate the intensity at the detector:

$$I_j = \sum_m \left\{ |U_j|^2 \right\}.$$  

Using a completely incoherent source, i.e., $U_j=\exp(i \theta)$, $\theta$ a random angle in [0,2π), we obtained the pattern in Fig. 4b. It shows less visibility than the one for a full coherent beam (Fig. 4a) and the visibility is originated by the beam coherence ‘created by propagation’, as a consequence of the van Cittert-Zernike theorem. This result is in good agreement with the experimental results shown in [8]. A very similar approach is used in [9]; the implementation given there seems to be more efficient using pre-calculated basic-fields that do not need to be re-propagated.

**Figure 4.** Diffraction using a fully coherent source (left) and fully incoherent source (right).

### 3.3. Others

The multilayer (ML) model in SHADOW3 has been upgraded to include the interlayer roughness following the Nevot-Croce formalism, and the input for laterally graded multilayers has been simplified. As an example, Fig. 5 shows the reflectivity versus ML coordinate for the laterally graded ML of MASSIF BL.

Some variance reduction tools have been implemented. The source simulation can now discard rays not arriving into a defined slit, a method that can be very useful for beamlines using wigglers and undulators. For visualization purposes in systems with low reflectivity, it is sometimes interesting to resample the final beam to reduce the number of rays. It can be done using the following algorithm: for each ray generate a random number $r$ in (0,1); if $r<=I$, keep the ray and its intensity one $I=1$, otherwise reject the ray. This allows 2D intensity plots of simulations with $3\times10^5$ rays, as shown in [10]. Other improvements include the use of external simulation codes such as SRW [11] for sampling rays to be used by SHADOW, as proposed in [12], python scripts for scanning mirror rotation and
translations and then compute allowed tolerances in these movements, the use of patterned screens [10], and scripts for reading FEA simulations for thermal and mechanical deformations [13].

Figure 5. ML reflectivity for rays reflected by the MASSIF ML versus the coordinate along the ML. Red: graded multilayer, black: non-graded ML.

4. Towards an integrated hybrid simulation environment
A collaborative work has started to bring together different simulation codes into a common environment. A first step consists in implementing an API (application programming interface) that will permits to run SRW and SHADOW from a python session. McXtrace [14], a new ray tracing software is proposed as an alternative for users that want to code their own elements, and for performing calculations with very high number of rays (like for 2D imaging). Last, but not least, I want to thank N. Canestrari, A. Prodi and O. Chubar for very fruitful interactions.

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