McXtrace - modern ray-tracing package for X-Ray instrumentation

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McStas ESRF McXtrace DTU SAXSLAB

Abstract

Ray-tracing is a well established simulation method to characterize optical elements with geometrical approximation. Within the field of X-ray studies the most used simulation package - Shadow - is limited in its development because of the code structure. Therefore we present a new state of the art ray-tracing package, that will be faster, modular and more flexible.

Thanks to the many simularities in propagation of neutron and photon beams, we can adopt all the relevant frameworks from McStas (existing ray-tracing neutron package) and integrate it within McXtrace.

NEUTRON	*X-RAY PHOTON*
n=(**r**,**v**,p,t,**s**)	$\vec{p} = (\mathbf{r}, \mathbf{k}, p, t, \phi, \mathbf{E})$
$\longrightarrow$ time domain prop.	$\longrightarrow$ freq. domain prop.
magnetic field/ spin polarization	optical polarization
gravitational polarization	phase propagation wave optics

Structure

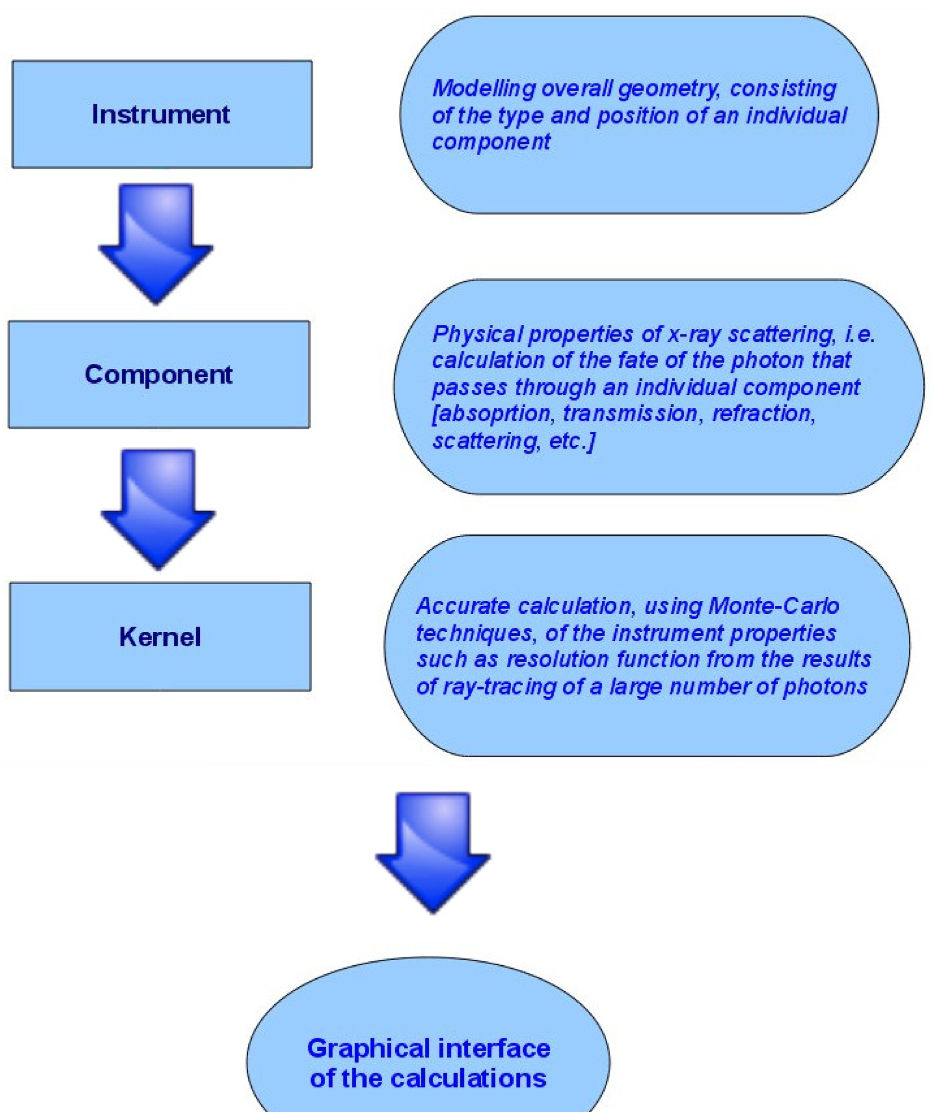

Figure 1: Three levels of the code structure.

- *Modular.* Users can easily build an *instrument* (to be simulated) by simply choosing its building blocks from existing library of tested *components.*
- *Powerful.* New *components* are maintained by McXtrace team (but also can be developed by the user community) to respond to the needs of state of the art development in synchrotron radiation devices, i.e. in multilayer mirrors, partially coherent sources, compound refractive lenses, etc. No knowledge of the low-level code implementation is required to develop a McXtrace component.
- *Faster.* As in McStas, at each run the meta-language describing the simulation is automatically translated into ANSI-C code. This allows the user to choose between C-compilers and optimization options and tailor it to a specific platform. This can speed up the simulation significantly.

The weight factor

An important part of speeding up the calculation is to introduce the ˝photon weight˝. If, for example, the reflectivity of a certain component is 10 %, and only reflected photons are considered later in the simulation, the photon weight will be multiplied by 0.1 when passing through the component. The resulting weight factor for the photons after passage through the whole instrument becomes the product of all contributions:

$$p = p_{ph} = p_0 \prod_{j=1}^{n} \pi_j$$

Example of a component definition - compound refractive lens (CRL)

When simulating a CRL within McXtrace, a user is to specify the lens parameters in accordance with fig.2, where *R* is half of the lens aperture, *w* is the depth of the profile along the propagation axis and *d* is the distance between the apices of the profiles. Such convention correlates well with the manufacturing parameters of the lens through $2R = 2(2R_0 w)^{\frac{1}{2}}$ [3].

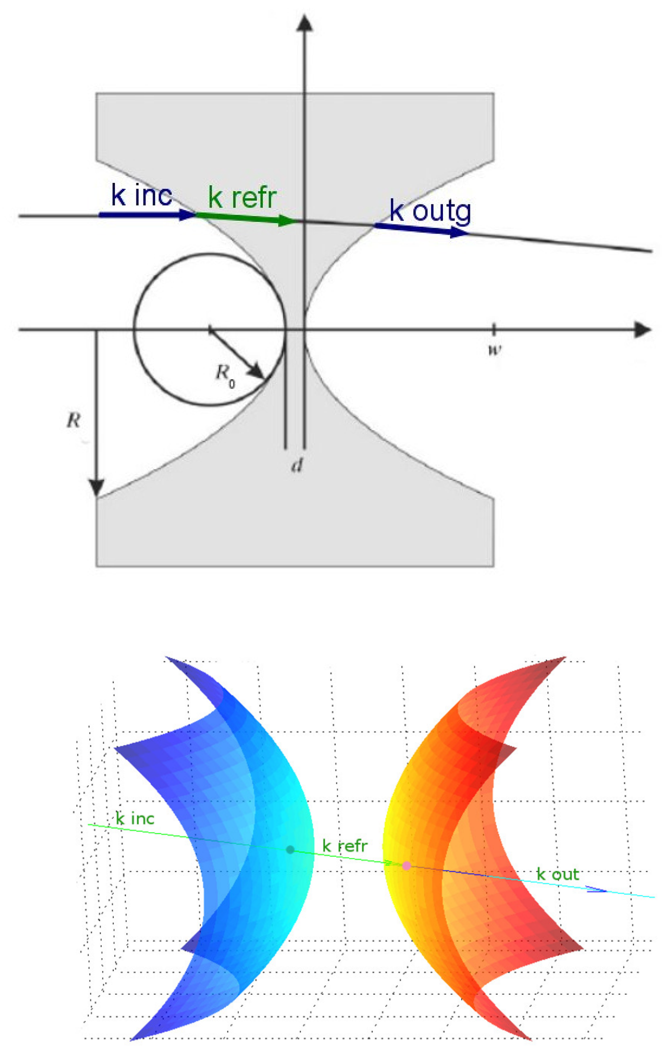

Figure 2: Schematic illustration of a model of a photon's interaction with a CRL [3].

At the point of intersection we determine the incident angle and by applying Snell's law $\sin\theta = \frac{n}{n'}\sin\theta'$ can then calculate the second intersection point with the adjacent surface, whilst in the meantime absorption processes inside the material of the lens are also accounted for. This routine is repeated as many times, as there are lenses in a stack, allowing tracing the photon's fate through the device.

Advantages of the CRL modelling within McXtrace

- The Focusing properties are simulated, not derived by exact results from the theory.
- The surface of the lens is not limited to have just a parabolic profile $\frac{x^2}{r^2} + \frac{y^2}{r^2} \pm \frac{z}{w} = 0$, but instead is user-defined and thus can be elliptical or cylindrical.
- The lens material is set by a user and correspondent absorption properties are taken from existing database.
- Surface imperfections such as roughness and waviness can be accounted for.

Virtual set-ups

A simple idea of a low-budget monochromator [4] comprises usage of an in-vacuum transfocator (IVT). Due to chromatic nature of focusing, it is possible, by sliding the slit along the axes within δf for different energies, to cut off the required energy from a white beam, thus monochromatizing radiation:

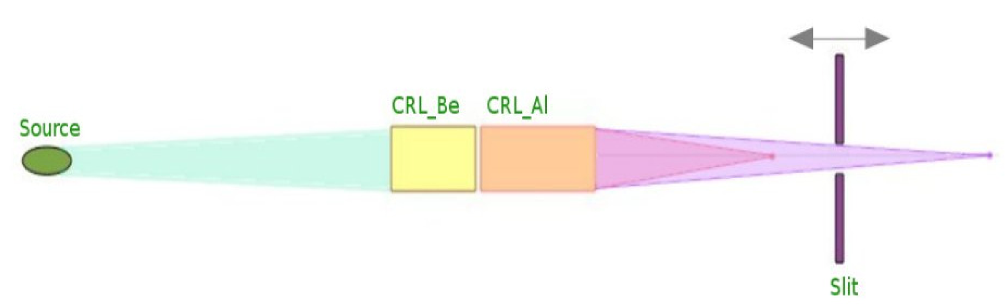

Figure 3: Model of monochromatization of the white beam through IVT: a consecutive set of Be and Al CRLs allows focus tunability to 18-45 keV.

Verification of experimental data

We have performed a virtual experiment of an Al CRL in accordance with the real one described in [3] that was carried out at ID22 at the European Synchrotron Radiation Facility (ESRF). The source size is 297x14.9 μm^2 (HxV), its divergence is 30x20 μrad^2 (HxV), the distance between the source and the CRL L=63m. With the photon energy of 15 keV, that corresponds to 0.826 Å, lens aperture 2R=0.87 mm, distance between the apices of the profiles d=54 μm and number of lenses N=33, the focusing of the beam is at f=1.26m.

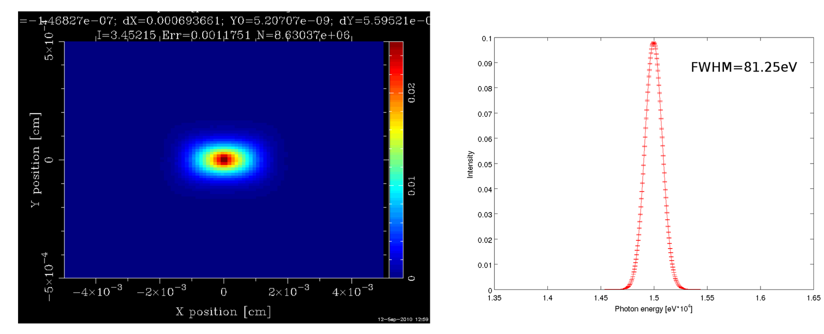

Figure 4: Simulation of the undulator source at ID22 [3] at the focal spot. Left figure is a PSD, right figure is energy distribution.

As it can be observed at the figure 4 the beam size at the focal spot in the horizontal plane is $\sigma_h = 6.94\mu m$ and $\sigma_v = 0.5\mu m$ in the vertical plane. The FWHM is 81.25 eV. The simulation results we have obtained coincide quite well with the theory, yet we're debugging the codes to eliminate the last bugs and thus achieve precision.

Double slit virtual experiment

A first attempt of a phase coherent simulation, tested on a double slit experiment, showing 2D intereference fringes from two point sources placed in 2 cm from each other and recorded on a 20x20 cm 2D position-sensitive detector. The detector is situated 1 m downstream from the source assembly [1].

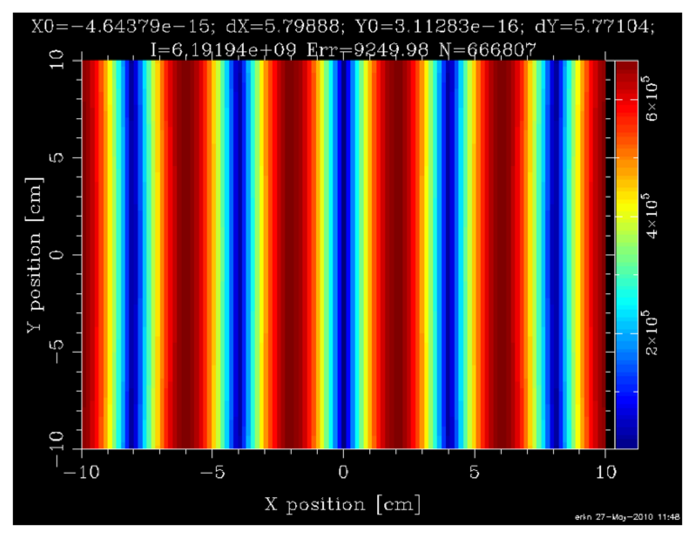

Figure 5: Real 2D interference fringes from two point sources on a 2D PSD.

Conclusion

We're expecting a coming release of McXtrace to have all the basic components like multilayers (not presently available anywhere else), pinholes, partially coherent source (this component will probably be released in later versions), etc. We are interested in characterizing the beamlines at ESRF ID-09 and ID-11.

References

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