# DEVELOPMENT OF AN OPTICAL SIMULATION TOOLKIT FOR TRANSVERSE BEAM PROFILE CHARACTERIZATION

Xin-ru Gao\*, Yong-bin Leng National Synchrotron Radiation Laboratory (NSRL), University of Science and Technology of China, Hefei, China

Abstract

The increasing demands for high-resolution beam diagnostics necessitate advanced simulation tools capable of modeling complex wave-optics phenomena. We present an optical simulation toolkit based on the angular spectrum propagation method, validated through comparisons with SRW. For synchrotron radiation interferometer simulations, the toolkit demonstrates excellent agreement with SRW results. The toolkit's unique capabilities are further demonstrated through three key application case studies. Through its physics-based modeling and wave-optics simulation capabilities, the simulation toolkit provides support for both optimized hardware design and methodology research to enhance the accuracy of beam profile characterization.

## INTRODUCTION

High-precision diagnostics of particle beams are critical for improving accelerator performance. As beam quality requirements continue to rise, advanced optical simulation tools are required for high-precision beam diagnostics. Geometric optics models fail to capture key wave-optics phenomena (e.g., diffraction, coherence, and wavefront distortion), leading to deviations in beam profile characterization. Current wave-optics simulation frameworks (SRW [1], SHADOW3 [2]) provide robust capabilities for modeling radiation fields according to key parameters and wavefront propagation for synchrotron radiation. However, they exihibit a few limitations in simulating complex optical systems, which include:

- Restricted wavefront propagation capabilities for complex optical elements (e.g. X-ray pinhole camera with more precise 3-D pinhole structure)
- Limited capabilities of modeling multiphysics coupling phenomena (e.g., thermal/mechanical-induced wavefront distortions)

To bridge these gaps, we develop a versatile optical simulation toolkit based on angular spectrum propagation theory. Its design prioritizes both high-precision propagation through arbitrary optical paths (lenses, drift spaces, apertures or other complex optical elements) and extensibility, which allows for modulations of multiphysics coupling effects

## **METHODOLOGY**

Angular Spectrum Propagation

Angular spectrum method models optical wavefront propagation by decomposing an input electric field E(x, y, 0) at plane z = 0 into a superposition of plane waves via Fourier transform [3]:

$$A(f_x, f_y, z) = \mathcal{F}\{E(x, y, 0)\},\tag{1}$$

where  $A(f_x, f_y, 0)$  is the angular spectrum, and  $f_x, f_y$  denote spatial frequencies. The propagated spectrum to plane z is calculated by

$$A(f_x, f_y, z) = A(f_x, f_y, 0) \cdot H(f_x, f_y, z), \tag{2}$$

with the transfer function H defined as

$$H(f_x, f_y, z) = \exp\left(i\frac{2\pi z}{\lambda}\sqrt{1 - (\lambda f_x)^2 - (\lambda f_y)^2}\right). \tag{3}$$

The output field E(x, y, z) is then reconstructed by inverse Fourier transform:

$$E(x, y, z) = \mathcal{F}^{-1} \{ A(f_x, f_y, z) \}. \tag{4}$$

This method was selected as the computational core of our toolkit due to its unique capabilities as follows:

- The transfer function of ASM strictly satisfies the Helmholtz equation without Fresnel or Fraunhofer approximations, enabling precise simulations regardless of distance and non-paraxial effects.
- Propagation through multi-element systems is simulated by cascading transfer functions of each element(e.g., drift space → lenses → masks):

$$H_{total} = H_{drift} \cdot H_{lens} \cdot H_{masks}, \tag{5}$$

which allows for flexibility in compound optical system.

• Thermal/mechanical distortions are incorporated as phase modulators  $\phi(x, y)$  in the spatial domain:

$$E_{pertubed}(x, y) = E(x, y) \cdot exp(i\phi(x, y)),$$
 (6)

which enables direct analysis of multiphysics coupling impacts on beam profile diagnostics.

## Toolkit Framework

The toolkit employs a modular three-layer architecture (Fig. 1) designed for optical simulation and extensibility.

<sup>\*</sup> gaoxinru@mail.ustc.edu.cn

Core Layer ASM Engine FFT Libraries GPU Acceleration Interface Laver Drift Space Optical Ele-Calculator ment Builder Basic Opti-User-defined cal Elements Element Application Layer Wave Propaga-Optical System tor(ASM Engine) Simulator Optical Path Multiphysics Coupling Analyzer Designer

Figure 1: Three-layer architecture of the wave-optics toolkit: Core computational layer, interface element builder, and application-specific modules.

## **VALIDATION RESULTS**

# Synchrotron Interferometer Benchmark

To validate the accuracy of our wave-optics simulation toolkit, a standard double-slit synchrotron radiation interferometer was simulated using both our toolkit and the wellestablished Synchrotron Radiation Workshop (SRW) code. The simulation parameters, including the source properties, slit geometry, and propagation distances, were kept identical in both models to ensure a direct comparison.

The simulated interferogram generated by SRW is shown in Fig. 2a, and the result from our toolkit is shown in Fig. 2b. Visually, the two patterns exhibit excellent agreement.

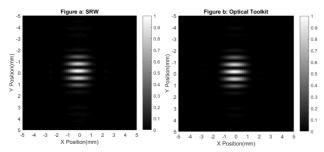


Figure 2: The simulated interferogram generated by SRW (left), and the result from our toolkit (right).

For a quantitative assessment, the Structural Similarity Index Measure (SSIM) was calculated between the two images. The SSIM value reached 0.973. This high degree of similarity demonstrates that our toolkit achieves a high level of accuracy in simulating complex wave-optics phenomena like interference and diffraction, providing a reliable foundation for the subsequent application case studies.

#### APPLICATION CASE STUDIES

## Complex Mask Interferometry

As the spatial frequency coverage of a traditional double silt is fixed and narrow, double-silt interferometers, while effective, are restricted in their capabilities for beam profile characterization. Consequently, novel aperture designs have been explored to improve synchrotron radiation interferometers, such as the non-redundant mask approach for two-dimensional beam profile monitoring successfully implemented at the ALBA synchrotron light source [4].

This case study demonstrates the toolkit's capability to model interferometers equipped with arbitrarily shaped complex masks. An outline of the optical system is shown in Fig. 3.

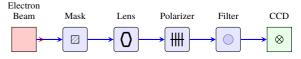


Figure 3: A brief outline of the complex mask SR interferometer.

Figure 4 shows two representative masks and their simulation results. Compared with a double-slit interferogram, the complex mask interferogram (Fig. 4) is intricate and non-periodic, which contains a broader spatial frequency spectrum, thus make the interferogram a richer data source for beam profile characterization.

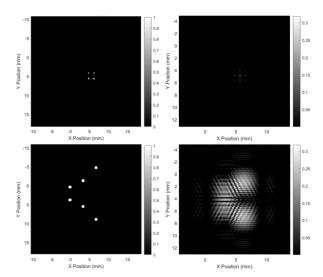


Figure 4: The transmittance grid of two representative complex masks (left) and their simulation results (right).

The toolkit enables the performance prediction of novel aperture designs before experimental setup and commissioning by providing a flexible environment to simulate such state-of-the-art configurations.

## X-ray Pinhole Camera Optimization

X-ray pinhole cameras are widely used in beam profile characterization due to their structural simplicity and high sensitivity [5]. However, geometric optics-based simulations often fail to accurately capture wave-optics effects, especially when dealing with thick pinhole structures made of materials like tungsten [6].

To address this, our simulation toolkit incorporates a waveoptics approach enabling precise modeling of the pinhole's 3D structure and its interaction with X-ray radiation.

Figure 5 demonstrates the mechanical design and dimensions of the tungsten pinhole mask via third-angle projections. X-ray pinhole consists of two 10 mm thick tungsten plates whose alignment forms a precise, square effective aperture of  $25 \times 25 \ \mu m^2$  at the intersection.

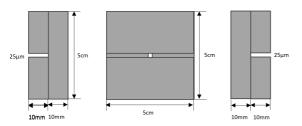


Figure 5: The third-angle projection of the pinhole: side (left), front (middle), isometric (right).

Figure 6 shows the simulation result of the PSF of the pinhole camera with the distance from source point to pinhole camera d = 6.19 m and the distance from pinhole camera to detector D = 9.25 m.

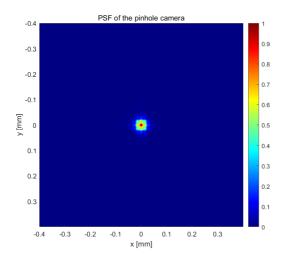


Figure 6: PSF of the X-ray pinhole camera.

# Thermal Distortion Impact

In practical environment, optical elements (e.g., lenses, mirrors) absorb energy, leading to temperature gradients. This causes thermal effects, resulting in wavefront distortions that degrade measurement accuracy.

Our simulation toolkit integrates a multi-physics simulation module to model this effect. Simulations quantitatively predict the wavefront error and its impact on the measured beam profile by heat load analysis and thermal-structure analysis.

A brief layout of the optical system is demonstrated in Fig. 7 with a focusing lens that is subjected to heat load.

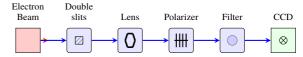


Figure 7: A brief outline of a SR interferometer.

Two scenarios were simulated and compared (Fig. 8), including an ideal case without wavefront distortion (left) and a thermal case (middle) considering the thermal effect. The quantitative difference map clearly visualizes the wavefront error introduced by the thermal load.

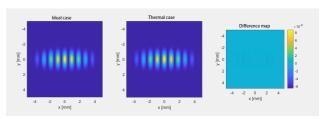


Figure 8: An ideal interferogram without wavefront distortion (left), a thermal case (middle) considering the thermal effect and the quantitative difference map (right).

This case study provides a clear, quantitative visualization of how thermal effects can affect interferometric measurements, which can be used to interpret experimental data accurately under high-heat-load conditions, ensuring the reliability of beam diagnostics.

## CONCLUSION

This work presents the development of a wave-optics simulation toolkit based on the angular spectrum method for advanced beam diagnostics. The toolkit was rigorously validated against established codes such as SRW, showing excellent agreement in simulating synchrotron radiation interferometers. Its practical value was demonstrated through several application case studies, including complex mask interferometers, X-ray pinhole cameras with 3D structure, and thermal effects in SRI. The current version requires long computation times for complex systems, a limitation we plan to address through future optimizations, a graphical interface, and better software compatibility. Despite this, the toolkit already provides a powerful and physics-based approach that helps optimize beam profile monitor design and improve beam characterization accuracy at advanced light sources.

#### REFERENCES

- [1] O. Chubar, A. Fluerasu, L. Berman, K. Kaznatcheev, and L. Wiegart, "Wavefront propagation simulations for beamlines and experiments with 'Synchrotron Radiation Workshop'", *J. Phys.: Conf. Ser.*, vol. 425, no. 16, p. 162001, Mar. 2013. doi:10.1088/1742-6596/425/16/162001
- [2] M. Sanchez del Rio, N. Canestrari, F. Jiang, and F. Cerrina, "SHADOW3: a new version of the synchrotron X-ray optics modelling package", J. Synchrotron Radiat., vol. 18, no. 5, pp. 708–716, Jul. 2011. doi:10.1107/s0909049511026306
- [3] J. W. Goodman, Introduction to Fourier Optics 3rd ed., Greenwood Village, CO, USA: Roberts and Company Publishers, 2005.
- [4] U. Iriso, L. Torino, B. Nikolic, C. Carilli, and N. Thyagarajan, "New interferometric aperture masking technique for full transverse beam characterization using synchrotron radiation", in *Proc. IBIC*'24, Beijing, China, Sep. 2024, pp. 178-181. doi:10.18429/JACOW-IBIC2024-TUP56
- [5] M. J. Boland and M. J. Spencer, "Vertical Beam Profile Measurement and Analysis with X-ray Pinhole", in *Proc. EPAC'08*, Genoa, Italy, Jun. 2008, paper TUPC009, pp. 1059–1061.
- [6] L. Bobb, "Diagnostics X-ray beamline at Diamond Light Source", presented at DEELS'18 Workshop, Diamond Light Source, Didcot, UK, Apr. 2018.