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A Fast Method for Generating Synchrotron Radiation Ray Traces at the ALS

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Abstract. Ray tracing for radiation safety involves defining an envelope that contains all possible ray paths, accounting for the motion range of the optics. This is required for all x-ray beamlines at the Advanced Light Source. Traditionally, it would take days for designers to manually sketch the envelope using computer-aided design. We present a MATLAB-based program that generates 3D envelope models in seconds. The program tracks light propagation in the phase space using ray transfer matrices. We compared its results against the long-established RAY-UI ray tracing program, which requires extensive computation to achieve sufficient ray sampling and motion discretization. Both techniques yield nearly the same results for quasi-flat mirrors with small motion range, with differences of less than 0.5 mm. For more complex optics, a complementary hybrid approach takes over from the ray transfer matrix method, leveraging RAY-UI's capabilities to provide accurate yet efficient ray tracing.

1. Introduction

Synchrotron radiation ray traces are required to ensure the safe operation of x-ray beamlines at the Advanced Light Source (ALS), protecting both the users and equipment. These ray traces must demonstrate that all rays originating from the source remain within a safe envelope as they propagate through the beamline. Accurately generating these envelopes is challenging due to the need to account for the motions of all beamline components, often resulting in overly conservative assumptions.

Traditionally, ray tracing was performed manually in CAD, with a time-consuming and labor-intensive process. Existing ray tracing programs offer an alternative, but they require significant computation time to account for all optic positions with sufficient ray sampling and motion discretization to accurately capture all ray paths. For a typical ALS beamline—4 optics, 24 degrees of freedom—this process can take days.

With the ALS-Upgrade (ALS-U) project [1], approximately 40 beamlines require new ray traces to utilize the highly coherent beams, raising concerns about scalability. To address this, a fast method was developed to generate ray tracing envelopes in seconds.

2. Method

2.1 Ray transfer matrices

A single ray is expressed as a column vector (x, α, y, β), where x and y represent the positions, and α and β are the slopes relative to the optical axis. Ray transfer matrices (RTM) transform rays as they propagate through an optical system. Given the position and angle of a ray at one point, RTMs can determine its position and angle at a subsequent point, providing a simple tool for analyzing ray propagation [2-4].

For free-space propagation, the RTM is a shear transformation where the shear factor d is the travel distance. For mirrors, the RTM is defined by the tangential R_t and the sagittal R_s radii of curvature (ROC). The radii are calculated using the Coddington's equations. To account for optical misalignments, the RTM is augmented with ad hoc correction terms calculated based on geometrical optics considerations. These corrections are valid under the small-angle approximation. The mirror motions are defined in a local coordinate system, where the W-axis aligns with the projection of the beam on the optical surface, and the U-axis is normal to the surface. u, v, and w are the normal, sagittal, and tangential motions, while $\delta\theta$ and $\delta\psi$ represent the pitch and roll motions, respectively.

The RTM for a mirror, including these corrections, is expressed as:

$$M_{mirror} = \begin{pmatrix} -1 & 0 & 0 & 0 & 2u \\ \dfrac{2}{R_t \sin\theta} & -1 & 0 & 0 & \dfrac{-2u}{R_t \tan\theta} + 2\delta\theta - 2w/R_t \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & \dfrac{-2\sin\theta}{R_s} & 1 & 2\delta\psi\, sin\,\theta + 2v\, sin\,\theta/R_s \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

2.2 Phase space manipulations

Light is traced in the phase space. This method has been used before to model optical elements and x-ray beamlines [5-8]. Instead of using brute-force ray sampling, it enables tracing of only the boundary rays to describe all possible positions and slopes of light rays.

Figure 1 illustrates typical optical elements in the phase space. The phase space starts as a rectangular surface defined by four vertices, representing the position and slope of all possible rays at the source. As light propagates through vacuum, the free space propagation RTM shears the phase space. For apertures, the rays remain unchanged as long as they are within the opening. Thus, apertures are represented as two vertical cutting edges in the phase space. If the aperture cuts through a vertex, new vertices must be created to accurately capture the new boundaries. For a flat mirror, where R_t and R_s are infinity, the RTM is a simple reflection matrix with correction terms that translate the phase space. For example, a normal motion (u) translates the phase space horizontally by $2u$. A pitch motion ($\delta\theta$) translates it vertically by $2\delta\theta$.

A MATLAB-based program automates those phase space manipulations. It leverages MATLAB's polyshape library, a practical tool for manipulating polygonal surfaces. To analyze mirror reflections, nested loops iterate through the mirror's motion range. At each iteration, the effective aperture of the mirror is calculated based on its position and orientation. The cutting edges are inclined to accurately capture the slanted mirror surface. The mirror RTM transforms the input phase space, and once the loops are completed, the phase space is reconstructed by computing the convex hull of all transformed boundary rays.

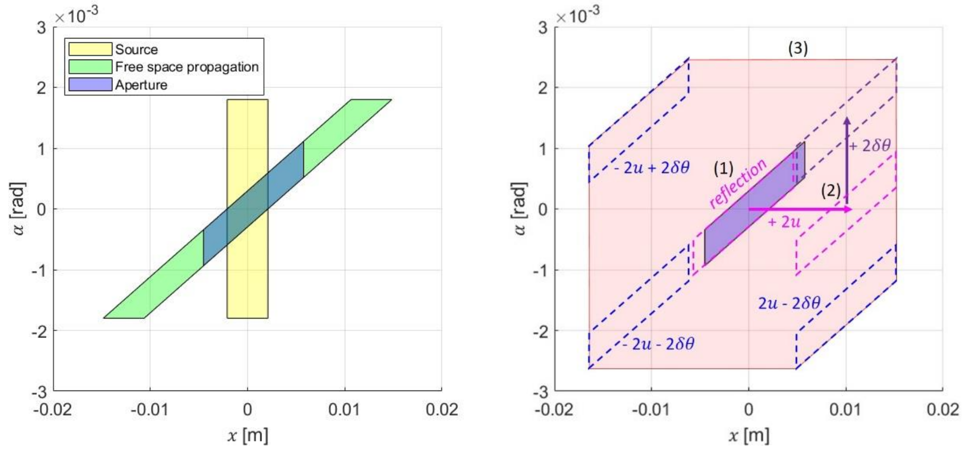

Figure 1. Phase space transformations of beamline elements: (Left) Source, free travel, aperture. (Right) Simplified step-by-step for mirrors: (1) Reflection, (2) Translation, (3) Reconstruction.

2.3 Process

1. **Prepare the input file**: an Excel table enables the user to define all relevant parameters for ray tracing. At this time, the types of beamline components include: source, aperture (or stop), mirror (or as premirror of gratings).
2. **Run *raytrace.m***: a MATLAB script reads the input file and automates ray tracing.
3. **Evaluate the results**: the program generates 2D plots of the ray tracing envelope. The program runs in a few seconds, allowing for quick iterations on the input parameters.
4. **Import in CAD**: the algorithm generates 3D models of the ray tracing envelope that can be imported into CAD for further verification.

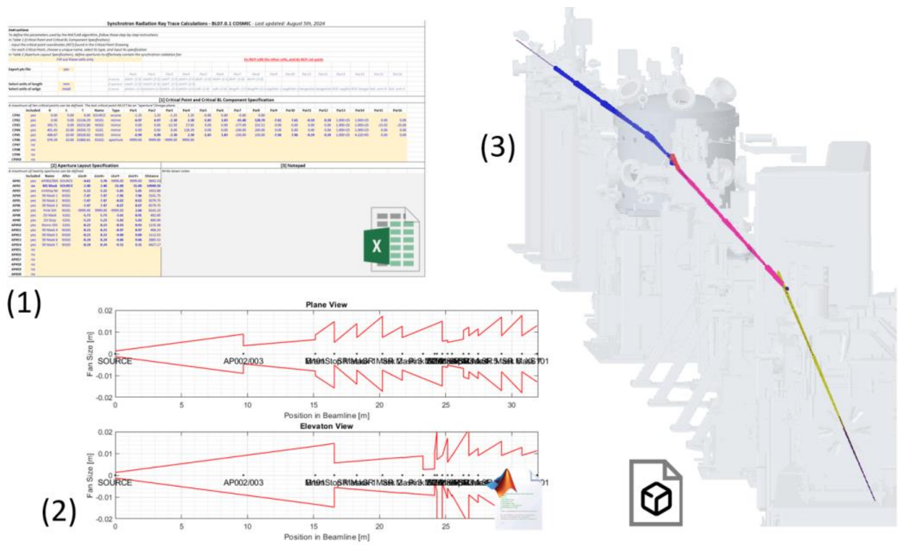

Figure 2. Automated ray tracing process: (1) Input preparation in Excel, (2) MATLAB execution and evaluation of 2D envelope plots, and (3) CAD integration for verification

3. Benchmarking

3.1 Results

The QERLIN beamline features a flat M1 mirror at 9.5 m from the source, a plane grating monochromator at 23 m and multiple apertures [9]. This beamline was used to benchmark our new program against the well-established RAY-UI ray tracing program [10].

In RAY-UI, we specified the source as a hard-edge point source with 100,000 rays, which take about 10 sec to trace. Using RAY-UI's looper tool, we ran multiple simulations varying the alignment parameters. For example, varying u: ±2.0 mm, $\delta\theta$: ±0.75 mrad, $\delta\psi$: ±5.00 mrad with 5 discretization points, results in 125 iterations, which takes about 20 minutes to complete.

We tested different beamline configurations, replacing the flat M1 mirror with paraboloid and toroidal mirrors found at ALS. The comparison showed a strong correlation between the two methods, with maximum differences ranging from 0.1 mm to 0.5 mm, well within the typical shielding design safety margin (5 mm). Figure 3 illustrates this— the two methods overlap so well that the red (our method) and blue (RAY-UI) lines yield a single purple line. The difference at each beamline element, plotted in orange, never exceed 100 µm.

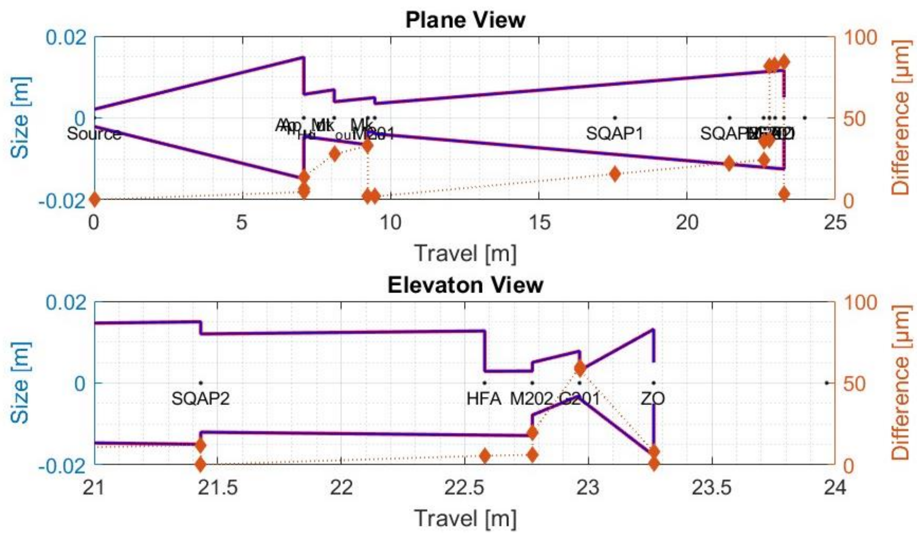

Figure 3. Comparison of ray tracing envelopes for BL06.0.2 QERLIN: calculated by our program (red) vs. RAY-UI (blue). M1 mirror: flat, 300 mm-long, fixed; PGM's premirror: flat, 300 mm-long, pitch motion -11 to 13 mrad; PGM's grating: flat, 200 mm-long, pitch motion ±10 mrad.

3.2 Limitations

The program performs well for simple mirrors with small motion range. However, limitations arise when dealing with more complex optics. To further evaluate the program, we varied all six degrees of freedom (DOF) independently by ±5 mm or ±5 mrad and compared the phase space after a pseudo-QERLIN M1 mirror. Figure 4 shows the RMS of the maximum differences in x, y, α, and β after the mirror, while varying the ROC. As the ROC decrease, the differences between the two methods increase. In such cases, a complementary method may be used.

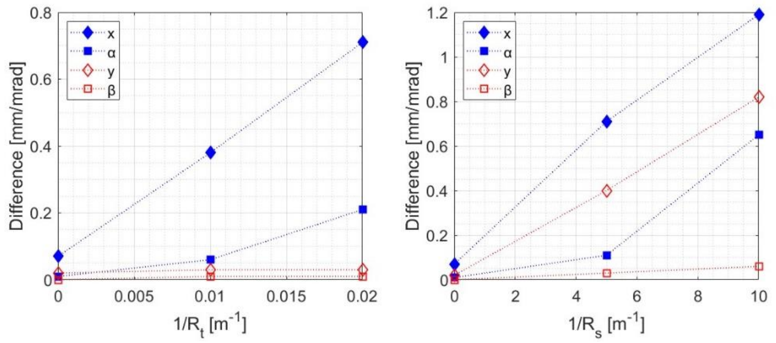

Figure 4. RMS of maximum differences in x, y, α, and β after the pseudo-QERLIN M1 mirror for each DOF varied ±5 mm or ±5 mrad. (Left) Tangential ROC varied while sagittal ROC is kept at infinity. (Right) Sagittal ROC varied while tangential ROC radius is kept at infinity.

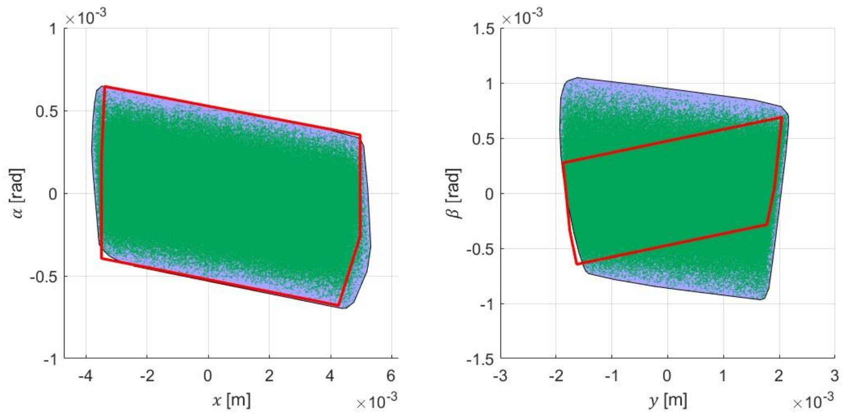

Figure 5. Comparison of the phase space after the BL08.3.1 M2 mirror moving by ±5.00 mrad in yaw: overlaps of the ray vectors traced in RAY-UI (green dots), and the phase space calculated by the RTM method (red) and reconstructed from the RAY-UI results (blue).

3.3 Integrated complementary method

Our program covers most mirrors at the ALS, but more complex optics, typically downstream after several reflections, require additional handling. For example, an ALS protein crystallography beamline features a M2 toroidal mirror with a sagittal ROC of 64.6 mm [11]. The mirror operates with two motorized motions: ± 0.32 mrad in pitch and ± 5.00 mrad in yaw.

The algorithm evaluates the bounds of applicability and flags the user if the estimated error exceeds 250 µm or 25 µrad. When this happens, the MATLAB routine pauses. Our program can generates ray vectors contained within the input phase space, readable by RAY-UI. RAY-UI performs ray-based tracing, and upon completion the MATLAB routine can resume, replacing the phase space with that derived from the RAY-UI results. Although more time-consuming, it eliminates previous constraints and enables accurate ray tracing for the most complex optics found at the ALS.

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Figure 5 shows the overlap between the phase space calculated by the RTM method, the reflected ray vectors from RAY-UI, and the reconstructed phase space from RAY-UI. Particularly, since the RTM does not directly account for yaw motion ($\delta\phi$), we applied two manual corrections:

- We increase the sagittal motion by $v = \pm l\delta\phi$ to factor in the lateral translation. Here, $2l$ is the mirror's total length.
- We increase the pitch motion by $p = \pm l.\sin^2 \delta\phi / R_s$ to account for the change in curvature in the tangential direction.

4. Conclusion

Our program received approval for usage at the ALS in December 2023. It is now in use in various beamline projects. With a simple user interface, it quickly generates a graphical output and a 3D model of the ray tracing envelope. The 3D model, when overlaid with beamline components, is easy to interpret. The efficiency gains allows our team to focus on collecting input parameters, which presents its own set of challenges for 20+ year-old beamlines. This tool also enables conceptualization of beam containment systems early in the design process.

Based on the RTM method, the program takes only seconds to run. Comparative analysis with the long established RAY-UI ray tracing program shows both techniques yield nearly identical results (<1 mm difference) for simple, quasi-flat mirrors with small motion ranges. For more complex optics, the program switches to a complementary method that leverages RAY-UI's capabilities to provide accurate ray tracing. This slower approach, which take minutes to hours depending on the DOF, may be triggered when the estimated errors exceed 250 µm or 25 µrad.

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