Computational Simulation of Diffraction Patterns Using Numerical Integration and Monte Carlo Methods

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Abstract

This report explores the simulation of Fresnel and Fraunhofer diffraction for various aperture configurations, including rectangular, circular, and square apertures. A Monte Carlo method is employed for circular diffraction approximations. The report highlights the ability to customize aperture parameters and diffraction regimes (Fresnel, Fraunhofer, or custom settings). Simulation results illustrate key diffraction phenomena and validate theoretical expectations for each regime. The enhanced menu interface allows flexible parameter adjustments, showcasing how numerical methods capture complex diffraction patterns efficiently.

1 Introduction

Diffraction is a fundamental phenomenon in wave optics, providing insight into wave propagation through apertures. The study of Fresnel (near-field) and Fraunhofer (far-field) diffraction patterns has applications in optical systems, wave analysis, and imaging technologies. This report investigates diffraction patterns for various aperture shapes, employing numerical methods to simulate their intensity distributions.

Four diffraction scenarios are simulated: 1D Fresnel and Fraunhofer diffraction for a slit aperture, 2D rectangular diffraction with customizable aperture height, 2D circular diffraction for Fresnel and Fraunhofer regimes, and Monte Carlo simulations for circular apertures. The report examines the influence of aperture parameters and diffraction regimes on intensity distributions, validating the results with established theoretical predictions.

2 Theory and Methods

2.1 Theory

2.1.1 Diffraction Overview

Diffraction is the bending of light as it passes through an aperture or around an obstacle, resulting in characteristic intensity patterns. It is fundamental to wave optics and is governed by the *Huygens-Fresnel principle*, which states that each point on an aperture acts as a secondary source of spherical waves. The total electric field at a point on the observation screen is computed by integrating contributions from all points on the aperture. Fresnel and Fraunhofer diffraction represent two primary regimes, distinguished by the distance between the aperture and the observation screen.

2.1.2 Fresnel and Fraunhofer Diffraction

Fresnel diffraction describes near-field diffraction, where the observation screen is close enough that the curvature of the wavefront cannot be ignored. In this regime, wavefronts retain curvature and are modeled as parabolic rather than planar. Conversely, Fraunhofer diffraction characterizes far-field diffraction, where the observation distance is sufficiently large for the wavefronts to be approximated as planar due to the parallel nature of light rays. The transition between these regimes is quantified by the *Fresnel number*:

$$N = \frac{a^2}{z\lambda}, \tag{1}$$

where a is the aperture width, z is the distance to the observation screen, and λ is the wavelength of light. A Fresnel number $N > 1$ indicates Fresnel diffraction, while $N \ll 1$ signifies Fraunhofer diffraction.

2.1.3 Governing Integrals for Diffraction

The electric field at the observation screen due to an aperture is governed by the Fresnel diffraction integral:

$$E(x, y, z) = \frac{e^{ikz}}{i\lambda z} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} E(x', y') \exp\left(i\frac{k}{2z}\left[(x - x')^2 + (y - y')^2\right]\right) dx'dy', \tag{2}$$

where $E(x', y')$ represents the electric field in the aperture plane, $k = \frac{2\pi}{\lambda}$ is the wave number, and z is the distance from the aperture to the screen.

For Fraunhofer diffraction, the phase terms simplify due to the large z, transforming the integral into a Fourier transform of the aperture function. This simplification allows for computational efficiency and is widely used for far-field diffraction modeling.

2.1.4 Numerical Computation of Diffraction Patterns

To compute diffraction patterns numerically, the real and imaginary parts of the integral are separated:

$$\mathrm{Re}(E) = \frac{kE_0}{2\pi z} \int_{\text{aperture}} \cos\left(\frac{k}{2z}\left[(x - x')^2 + (y - y')^2\right]\right) dx'dy', \tag{3}$$

$$\mathrm{Im}(E) = \frac{kE_0}{2\pi z} \int_{\text{aperture}} \sin\left(\frac{k}{2z}\left[(x - x')^2 + (y - y')^2\right]\right) dx'dy'. \tag{4}$$

The intensity of the diffraction pattern is proportional to the square of the electric field magnitude:

$$I(x, y) = |E(x, y, z)|^2 = \mathrm{Re}(E)^2 + \mathrm{Im}(E)^2. \tag{5}$$

These integrals are evaluated using numerical techniques, such as `scipy.integrate.dblquad`, or approximated via Monte Carlo methods for complex geometries. These approaches provide robust tools for simulating and visualizing diffraction patterns across different regimes and geometries.

2.2 Methods

2.2.1 Implementation of Governing Integrals

The numerical computation of diffraction patterns is central to the implementation. The Fresnel and Fraunhofer diffraction integrals are solved using numerical methods. Specifically:

- For rectangular apertures, the integration is carried out over a defined aperture area using the `dblquad` function from `scipy.integrate`. This function computes double integrals with high accuracy by evaluating both the real and imaginary parts of the electric field independently.
- For circular apertures, the same governing equations are adapted to polar coordinates, and integration limits are adjusted to reflect the circular geometry.
- The Monte Carlo method is employed as an alternative for circular apertures, where random sampling is used to approximate the diffraction pattern.

2.2.2 Program Structure and Workflow

The implementation is divided into five main parts, each corresponding to a different aspect of diffraction:

- **1D Diffraction (Part 1):** This section computes and visualizes 1D diffraction patterns for both Fresnel and Fraunhofer regimes. It includes error analysis and provides options for user customization of parameters such as aperture width and observation distance.
- **2D Rectangular Diffraction (Part 2):** This section extends the computation to 2D rectangular apertures. Users can visualize normalized intensity patterns and adjust parameters like screen resolution, aperture dimensions, and plot range.
- **2D Circular Diffraction (Part 3):** Diffraction from circular apertures is modeled using both Fresnel and Fraunhofer regimes. Double numerical integration is employed, with normalization applied to produce relative intensity values.
- **Monte Carlo Diffraction (Part 4):** For scenarios involving circular apertures with complex geometries or high computational costs, Monte Carlo methods provide an efficient alternative to direct integration.
- **Efficiency Analysis (Part 5):** A comparative study of the computational efficiency of Monte Carlo sampling and numerical integration techniques is performed. Results are plotted to illustrate runtime versus accuracy trade-offs for both methods.

2.2.3 User Interaction and Customization

An interactive menu system enables user control over the simulation parameters:

- Users can select predefined Fresnel or Fraunhofer modes or input custom values for parameters such as aperture width, screen distance, plot range, and resolution.

- For Monte Carlo simulations, the number of samples can also be customized, allowing a trade-off between computational time and precision.
- Input validation ensures that invalid entries do not cause crashes, with error messages prompting users to retry.

2.2.4 Efficiency Comparison

To evaluate the computational performance of the different methods:

- Runtime and accuracy are recorded for varying grid resolutions and sample sizes.
- Log-log plots of efficiency versus runtime highlight the trade-offs inherent to each method.
- Insights gained from the efficiency comparison guide the selection of appropriate methods for different diffraction scenarios.

3 Results and Discussion

3.1 Overview

This section presents the results generated by the numerical simulations of diffraction patterns, as implemented in the code. The results are divided into subsections corresponding to different parts of the program, with a focus on the computed diffraction patterns, error analyses, and computational efficiency.

3.2 1D Diffraction Patterns

3.2.1 Fraunhofer Diffraction

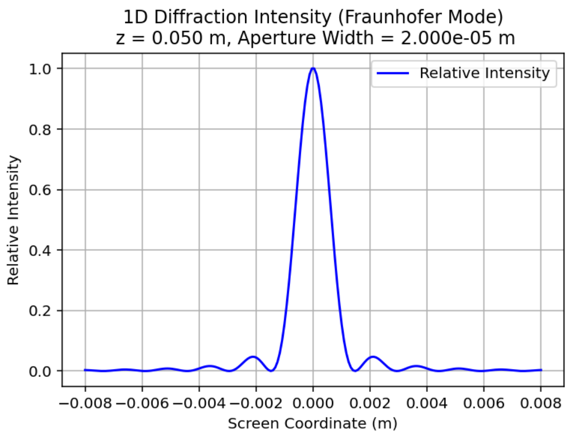

Figure 1: 1D Fraunhofer diffraction

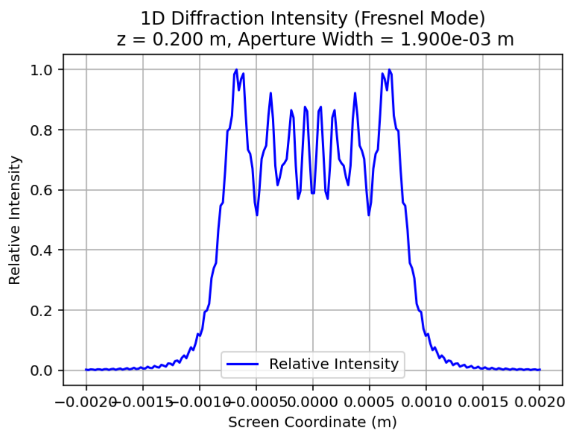

Figure 2: 1D Fresnel diffraction

The results validate the expected behavior for far-field diffraction. he results for Part 1 effectively illustrate the differences between Fresnel and Fraunhofer diffraction patterns. The Fraunhofer regime (Fig. 1), characterized by sharp peaks and nulls, reflects the predictable far-field interference from parallel wavefronts. In contrast, the Fresnel regime

(Figure 2) shows smoother intensity transitions, consistent with near-field diffraction where wavefront curvature is significant (Fn = 30). These patterns align with theoretical expectations, as governed by the Fresnel number $N = \frac{a^2}{z\lambda}$, confirming the accuracy of the implemented methods in reproducing these distinct regimes.

3.2.2 Error Analysis for 1D Diffraction Patterns

To evaluate the accuracy of the numerical integration methods used in simulating 1D diffraction patterns, error analysis was conducted for both Fresnel and Fraunhofer diffraction. Two key metrics were plotted:

- **Absolute Error:** This measures the deviation of computed intensity values due to numerical approximations.
- **Relative Error:** This indicates the error scaled by the computed intensity, highlighting regions with significant inaccuracies.

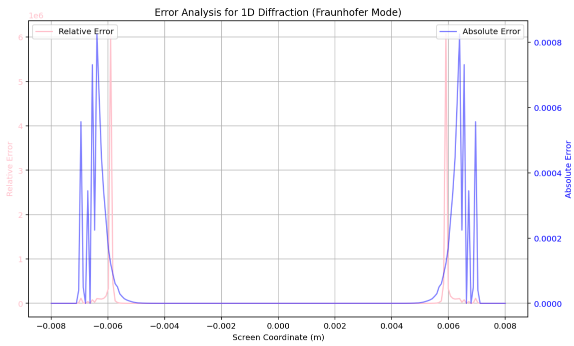

Figure 3: 1D Fraunhofer Error analysis

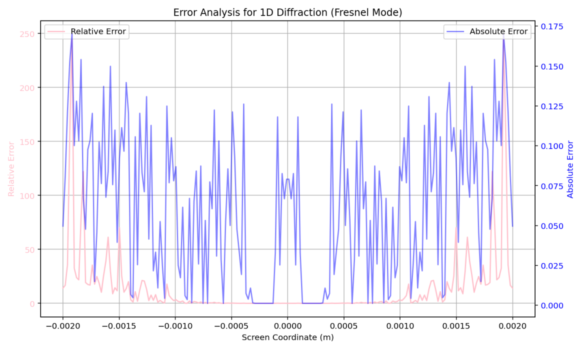

Figure 4: 1D Fresnel Error analysis

The error analysis reveals key insights. For Fraunhofer diffraction (Figure **??**), errors remain consistently low, reflecting the computational stability of far-field approximations. In the Fresnel regime (Figure 4), relative errors increase in regions of rapid intensity variation, highlighting the challenges of resolving near-field wavefront curvature. Absolute errors are more prominent in low-intensity regions, where numerical uncertainties have a proportionally greater impact. While the integration method is effective, further refinements, such as adaptive grid resolution or optimized solvers, could improve accuracy, particularly for Fresnel diffraction.

3.3 2D Diffraction Patterns

3.3.1 Rectangular Aperture

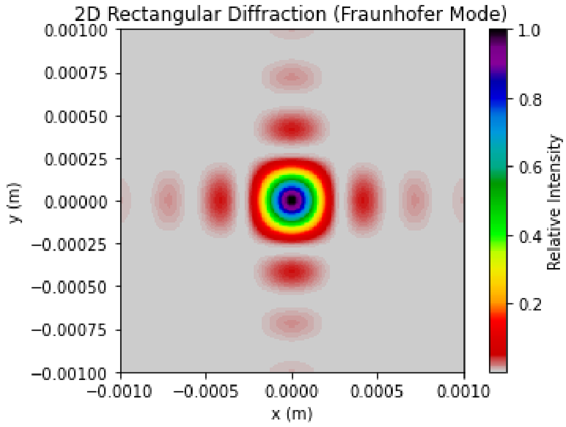

Figure 5: 2D Fraunhofer diffraction pattern - rectangular apeture

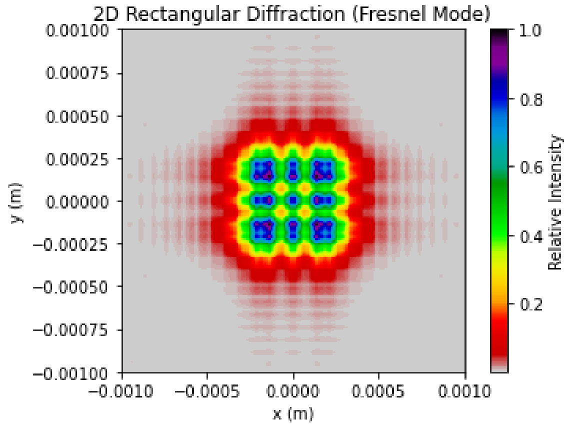

Figure 6: 2D Fresnel diffraction pattern - rectangular apeture

Figures 5 and 6 are 2D versions of the 1D plots above, providing clear insights into the expected behavior in Fresnel and Fraunhofer regimes. For the Fraunhofer diffraction case (5), the simulation produced a central bright fringe flanked by symmetrically distributed side lobes. This pattern aligns with theoretical predictions for far-field diffraction, where the intensity distribution results from the constructive and destructive interference of planar wavefronts. In contrast, the Fresnel regime (Fig. 6) demonstrated more intricate, localized intensity variations and curved fringes, characteristic of near-field diffraction. These patterns illustrate the impact of wavefront curvature and proximity to the aperture.

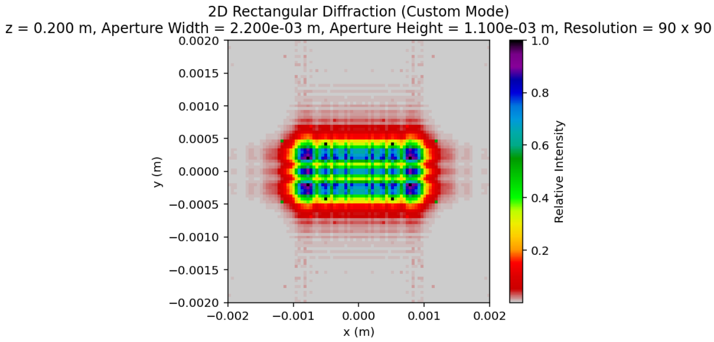

Figure 7: 2D Custom diffraction pattern

*T*he custom configuration plot (Fig. 7) shows how user-defined parameters influence the diffraction pattern, demonstrating the flexibility of the simulation. This result underscores the model's adaptability to explore apetures of varying widths and heights, revealing unique diffraction geometries and variations

3.3.2 Circular Aperture

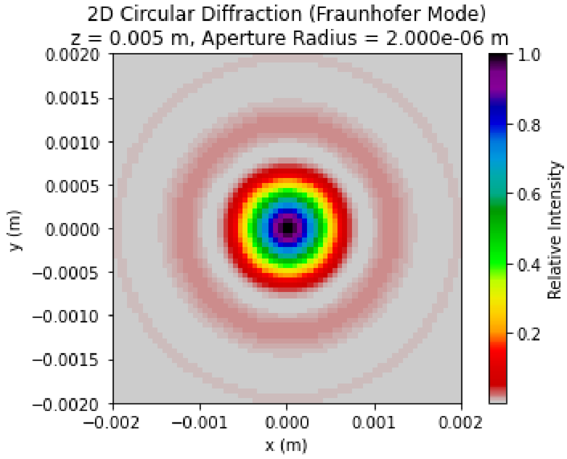

Figure 8: 2D Fraunhofer diffraction pattern - circular apeture

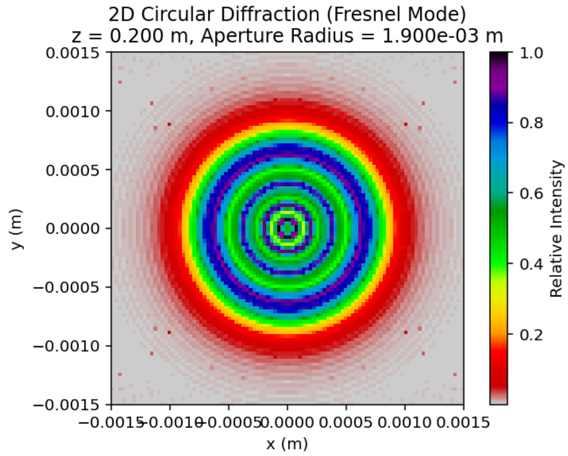

Figure 9: 2D Fresnel diffraction pattern - circular apeture

The diffraction patterns for a circular aperture are illustrated in Fig. 8 and Fig. 9, representing the Fraunhofer and Fresnel regimes, respectively. These results highlight the distinct characteristics of Fraunhofer and Fresnel diffraction regimes for circular apertures. The Fraunhofer pattern (8) clearly demonstrates the Airy disk surrounded by concentric rings, a well-known feature of far-field diffraction. This pattern aligns with theoretical expectations, capturing the spatial coherence and symmetry that arise from the planar wavefronts in this regime. In contrast, the Fresnel diffraction pattern (9) displays a more intricate intensity structure, reflecting the curved wavefronts and near-field effects inherent to this regime. Interestingly, the Fresnel number for Figure 9 matches that of the rectangular aperture in Figure 2, underscoring the consistency of Fresnel diffraction characteristics across different aperture geometries. This highlights the importance of the Fresnel number in determining the diffraction behavior, regardless of aperture shape.

The numerical integration process for circular apertures in Part 3 posed additional challenges due to the need to account for radial symmetry. Nevertheless, the resulting patterns exhibited minimal error, as evidenced by the sharpness and clarity of the visualized intensity distributions. The normalization of intensity values further ensured that the results were independent of absolute scaling, allowing for meaningful comparisons between the Fresnel and Fraunhofer regimes. However, the computational demands of double integration over a circular aperture were significant, particularly for high-resolution plots. Future improvements could involve the implementation of more efficient numerical techniques, such as adaptive mesh refinement or Monte Carlo sampling methods (explored in Part 4). Additionally, studying the transition between the Fresnel and Fraunhofer regimes by systematically varying the aperture size and screen distance could yield further insights into the underlying diffraction phenomena.

3.4 Monte Carlo Simulations

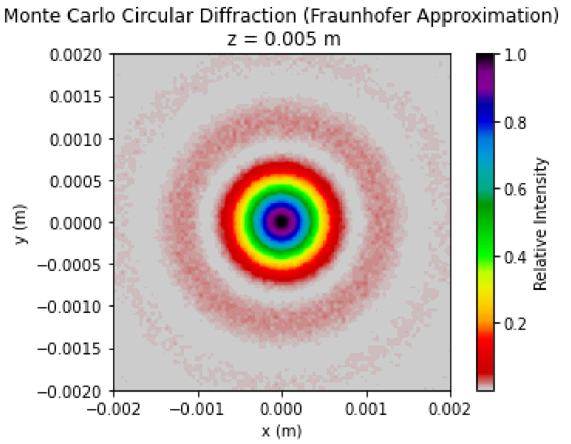

Figure 10: 2D Fraunhofer diffraction pattern computed using Monte Carlo methods

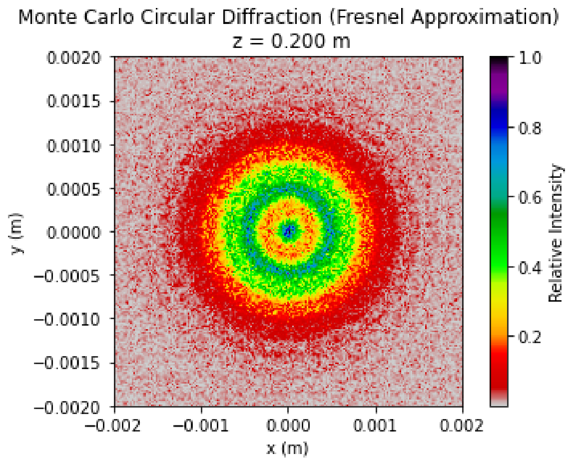

Figure 11: 2D Fresnel diffraction pattern computed using Monte Carlo methods

The Monte Carlo simulations provided an alternative and flexible approach to understanding the diffraction behavior of circular apertures. These simulations effectively captured the distinct features of both the Fresnel and Fraunhofer diffraction regimes, as depicted in Figures 11 and 10. The Fraunhofer diffraction plot (Figure 10) exhibited the expected Airy disk structure, with a bright central maximum surrounded by progressively dimmer concentric rings. In contrast, the Fresnel plot (Figure 11) showed more intricate intensity variations, highlighting the complex interference effects arising from the wavefront curvature in the near-field regime.

One limitation observed was the computational cost associated with achieving high accuracy. For both Fresnel and Fraunhofer simulations, increasing the number of random samples improved the resolution and fidelity of the intensity patterns but at the expense of significantly increased runtime. This trade-off between precision and performance is inherent in the Monte Carlo method. The Fresnel simulations, in particular, required higher sample sizes due to the increased sensitivity of near-field interference patterns. These observations suggest that further optimization, such as parallel processing or variance reduction techniques, could enhance the efficiency of Monte Carlo simulations for diffraction studies.

3.5 Efficiency Comparison

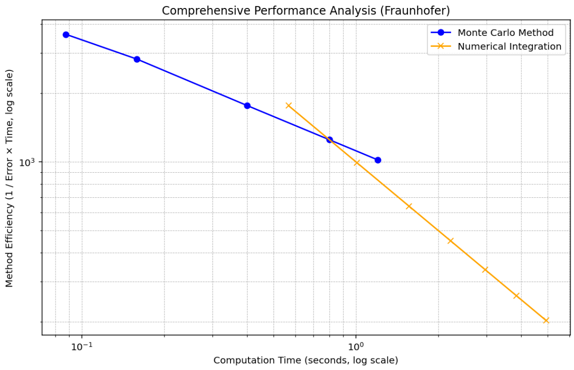

Figure 12: Efficiency comparison - Fraunhofer

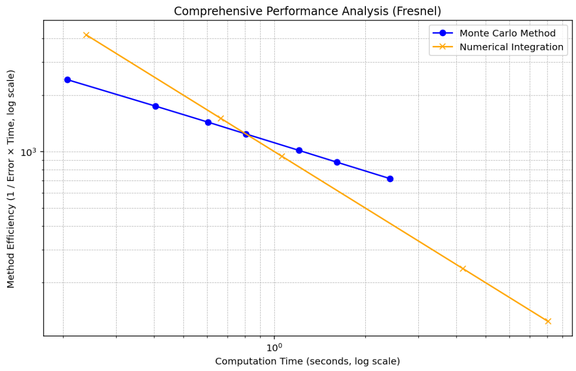

Figure 13: Efficiency comparison - Fresnel

In Part 5, the efficiencies of Monte Carlo sampling and numerical integration (`dblquad`) methods are compared for circular aperture diffraction patterns in both Fresnel and Fraunhofer regimes.

In the Fraunhofer regime 12, Monte Carlo sampling demonstrates increasing efficiency with runtime, particularly for larger sample sizes, due to its ability to approximate stochastic integrals efficiently. Numerical integration, while precise at lower grid resolutions, plateaus in efficiency as computational demands grow with finer grids.

For the Fresnel regime 13, Monte Carlo retains utility at high sample sizes, though its efficiency gains are less pronounced due to the complexity of near-field wavefront curvature. Numerical integration remains reliable for coarse grids but struggles with diminishing returns in efficiency for higher resolutions.

These results highlight the complementary strengths of the methods: Monte Carlo is ideal for rapid approximations over large domains, while `dblquad` excels in high-accuracy simulations with defined integration limits. Further optimization, such as adaptive sampling or advanced grid strategies, could enhance both approaches.

4 Conclusion

This project successfully simulated and analysed diffraction patterns for various apertures and regimes, providing valuable insights into the interplay between physics and computational methods. By employing numerical integration and Monte Carlo techniques, we were able to plot Fresnel and Fraunhofer diffraction patterns and compare their computational efficiencies.

The simulations confirmed the expected physical behaviors, such as the appearance of Airy disks in circular apertures and the distinct central maxima and side lobes in rectangular apertures. The Fresnel number proved to be a key factor in distinguishing between near-field and far-field plots, with patterns and efficiencies aligning closely with theoretical predictions.

The comparison of Monte Carlo and numerical integration methods revealed their respective strengths: Monte Carlo excelled in approximating stochastic integrals efficiently for large domains, while numerical integration provided reliable precision for well-defined geometries. However, both methods faced trade-offs in accuracy and runtime, particularly in the Fresnel case's computationally intensive scenarios.

References

[1] E. Hecht, *Optics*, 5th ed., Pearson, 2016.

[2] P. Virtanen, et al., "SciPy 1.0: Fundamental Algorithms for Scientific Computing in Python," *Nature Methods*, vol. 17, no. 3, pp. 261–272, 2020.

[3] S. Hanna, *Intro to Computational Physics Exercise 2*, PHYS20035: Computational Physics and Data Science, PHYS20037: Laboratory and Computational Skills, PHYS30038/42, University of Bristol, 2024.

Appendix: Code Explanation

Overview

The code simulates diffraction patterns using numerical integration and Monte Carlo sampling across multiple parts, each focusing on different regimes and geometries. A menu-driven system allows users to select diffraction types, customize parameters, and visualize results.

Part 1: 1D Fresnel and Fraunhofer Diffraction

Overview

Part 1 simulates 1D Fresnel and Fraunhofer diffraction patterns, allowing for error analysis and detailed visualization of relative and absolute intensity distributions.

Key Functions

- `part1_1d_diffraction_with_error` (Line 47):
  - *Functionality:* Computes diffraction intensities and error estimates.
  - *Inputs:* Screen coordinates (`x_vals`), fixed height (`y`), screen distance (`z`), aperture width (`aperture_width`).
  - *Process:*
    * Double integration using `dblquad` calculates the real and imaginary components of the electric field.
    * Intensity is computed as the square of the field magnitude.
    * Absolute errors are derived from integration uncertainties, and relative errors are calculated.
  - *Outputs:* Arrays for intensities, absolute errors, and relative errors.
- `plot_1d_diffraction` (Line 77):
  - *Functionality:* Generates intensity and error plots.
  - *Modes:* Handles predefined Fresnel/Fraunhofer regimes and allows for custom user inputs.
  - *Error Analysis:* Calls `part1_1d_diffraction_with_error` for error metrics.
  - *Visualization:*
    * Intensity is normalized for relative comparison.
    * Error metrics are plotted with dual y-axes for clarity.

Key Features

- Accurate numerical integration using `dblquad`.
- Integrated error analysis provides reliability insights.
- Modular structure supports future extensions.

Part 2: 2D Rectangular Diffraction

Overview
Part 2 extends the simulation to 2D rectangular apertures, generating heatmaps of diffraction intensity for Fresnel or Fraunhofer models. Users can customize parameters like aperture dimensions, plot range, and resolution.

Key Functions

- `part2_2d_diffraction` (Line 144):
  - *Functionality:* Computes and visualizes diffraction patterns.
  - *Inputs:* Mode (`mode`), screen distance (`z`), aperture dimensions (`aperture_width`, `aperture_height`), plot range (`x_range`), resolution.
  - *Process:*
    - Predefined or custom parameters set simulation conditions.
    - Double integration (`dblquad`) calculates the electric field for each screen coordinate.
    - Intensity is computed as the magnitude squared of the field and normalized.
  - *Visualization:* A 2D heatmap is created using `imshow`, with clear axis labels and color bars.
- **Menu Integration:**
  - Users can simulate predefined modes or input custom parameters.
  - Errors are handled to prevent crashes.

Key Features

- Heatmaps offer clear visualizations of diffraction patterns.
- Normalization ensures interpretability.
- Supports Fresnel/Fraunhofer modes with flexible customization.

Part 3: 2D Circular Diffraction

Overview
Part 3 simulates 2D diffraction for circular apertures using Fresnel and Fraunhofer models, providing visual intensity distributions with customizable parameters like aperture radius and screen distance.

Key Functions

- **Phase Functions:**
  - `fresnel_circular_phase` (Lines 222–223): Computes the Fresnel phase shift for a circular aperture.
  - `fraunhofer_circular_phase` (Lines 225–226): Computes the Fraunhofer phase shift.

- `part3_2d_circular_diffraction` (Line 228):
  - *Functionality:* Simulates circular diffraction patterns.
  - *Inputs:* Mode, screen distance (`z`), aperture radius (`aperture_radius`), plot range (`x_range`, `y_range`), resolution.
  - *Process:*
    - Predefined or custom parameters configure the simulation.
    - Double integration computes the electric field for each screen coordinate.
    - Intensity is calculated as the field magnitude squared and normalized.
  - *Visualization:* Heatmaps display normalized intensity distributions with axis labels and color bars.

Key Features

- Flexible support for circular apertures in Fresnel and Fraunhofer regimes.
- Accurate intensity computation via double integration.
- Normalized heatmaps for visual clarity.

Part 4: Monte Carlo Circular Diffraction

Overview
Part 4 uses Monte Carlo sampling to simulate 2D diffraction patterns for circular apertures, offering an alternative to numerical integration.

Key Functions

- `monte_carlo_circular_diffraction` (Line 310):
  - *Functionality:* Simulates diffraction patterns using Monte Carlo methods.
  - *Inputs:* Mode, number of samples (`N`), screen distance (`z`), aperture radius (`aperture_radius`), plot range (`x_range`, `y_range`), resolution.
  - *Process:*
    - Random points (`xp`, `yp`) are sampled within the aperture.
    - For valid points, phase values are calculated based on the selected mode.
    - The intensity at each screen coordinate is derived from averaged samples.
  - *Normalization and Visualization:* Results are normalized and visualized as heatmaps.
- **Menu Integration:**
  - Users can choose predefined modes or customize parameters like sample size.

Key Features

- Monte Carlo sampling is efficient for complex scenarios.
- Customization enables flexibility in simulations.
- Heatmaps provide intuitive visualizations.

Part 5: Extended Efficiency Comparison

Overview
Part 5 compares the computational efficiency of Monte Carlo sampling and `dblquad` integration for circular diffraction patterns in Fresnel and Fraunhofer regimes.

Key Functions

- `comprehensive_method_comparison_` (Line 383):
  - *Functionality:* Evaluates efficiency for varying sample/grid sizes.
  - *Inputs:* Mode, sample sizes for Monte Carlo, and grid sizes for `dblquad`.
  - *Process:*
    * Monte Carlo samples are generated to compute efficiency as the reciprocal of runtime and error.
    * `dblquad` integration calculates efficiency based on grid resolution.
  - *Visualization:* A log-log plot compares runtimes and efficiencies for both methods.

Key Features

- Highlights trade-offs between Monte Carlo and `dblquad` approaches.
- Log-log plots provide clear visual comparisons.
- Supports user interaction for mode selection.

Conclusion
The code provides a comprehensive toolkit for simulating and analysing diffraction patterns using both numerical integration and Monte Carlo methods. The modular design ensures flexibility and extensibility, while visual outputs aid in interpretation and reporting. Potential improvements include optimisation of numerical computations and enhanced user interactivity through GUI-based parameter adjustments.