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An overview of numerical methods for modeling x-ray propagation through a multi-lens system

Szymon Tokarski, Paweł Wojda

Faculty of Applied Physics and Mathematics, Gdansk University of Technology,
Narutowicza 11/12, 80-233, Gdansk, Poland

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Abstract

This article offers a comprehensive examination of the field of X-ray optics and the methods employed to simulate X-ray propagation through multi-lens systems. The publication presents three distinct approaches to address X-ray optics problems, including the utilization of oriented Gaussian beams, the fast Fourier transform, and the second-order Runge-Kutta method. It also provides an in-depth analysis of the paraxial wave equation used in X-ray optics and how the paraxial approximation can be employed to reduce computational complexity. Finally, the article provides a detailed mathematical description of the concave lens used in X-ray focusing.

Furthermore, the article offers a comparative analysis of each method's advantages, disadvantages, and limitations. It also highlights the differences in computation speed, required data points, and precision of each approach.

Keywords:

X-ray wave, X-ray optics, X-ray propagation

1. Introduction

The field of X-ray optics is rapidly evolving due to the potential of visualizing microscopic objects. To achieve this visualization, it is necessary to focus X-rays onto the object of interest. Currently, the most popular method of achieving this is by using lenses with a concave profile, either spherical or parabolic. However, the materials used for X-ray focusing have complex refractive indices, denoted as $n = 1 - \delta + i\beta$, where δ is responsible for X-ray refraction in lenses and β for attenuation of the X-ray intensity [1]. The ideal material for X-ray lenses should have a high refractive value and low absorption coefficient while being durable and inexpensive [1]. Unfortunately, meeting these requirements simultaneously is challenging. Beryllium is a commonly used material for X-ray focusing, but the production cost of a beryllium lens is approximately €5,000 [2]. Additionally, the lens material oxidizes during use, requiring periodic replacements. Achieving high magnification with short-distance X-ray focusing necessitates complex optical systems consisting of several lenses, making experiments costly. To reduce these costs, cheaper and more efficient lens materials must be found or developed, and more extensive theoretical research must be conducted [2].

This publication aims to present and compare three numerical methods used to calculate the propagation and focusing of X-ray waves through a multi-lens system. The publication outlines a method based on fast Fourier transform (FFT), finite differences, and oriented Gaussian beams.

2. Mathematical description of propagation

In the field of X-ray optics, the paraxial wave equation has emerged as a reliable method for computing the electric wave field. The aforementioned equation is derived from the Helmholtz equation, which provides an approximate solution. Over time, the paraxial equation has gained widespread acceptance due to its accuracy and efficacy in computing the electric wave field. The Helmholtz equation can be expressed as follows [3–5]:

$$\nabla_{\perp} E + \frac{d^2 E}{dx^2} - k^2 E = 0. \tag{1}$$

The equation Eq. 1 features the wave number, denoted by the symbol k. In the case of an electromagnetic wave propagating through a vacuum at the speed of light, k is defined as $k = \frac{\omega_0}{c_0}$, where ω_0 represents the angular frequency and c_0 is the speed of light in a vacuum [3].

The second derivatives that arise in equation Eq. 1 substantially influence the computation time. In order to mitigate the computational complexity, we propose to employ the paraxial approximation [3].

In geometric optics, the paraxial approximation describes the propagation of light via geometric rays. This approximation assumes that the angle θ between the rays and the propagation axis of the optical system remains small, i.e., $\theta \ll 1$ [5].

Since we are considering propagation in the direction of the OX axis, it is reasonable to assume that $|A_{xx}| \ll |kA_x|$. This implies that the angle θ between the wave and the z axis is very small, and consequently, the expression $u_{xx}e^{ikx}$ contributes insignificantly to the calculation. As a result, this expression can be neglected without impacting the accuracy of the computation. The paraxial Helmholtz equation can be expressed as follows [3, 5]:

$$\nabla_{\perp} E + 2ikE_x = 0. \tag{2}$$

For each methodology, we shall exclusively consider the values of the function at appropriately chosen points within the domain. These points shall be represented by spatial steps denoted by Δx and Δy, which correspond to the X and Y axes, respectively. The function values at the chosen points shall be denoted by $A_{i,j} = A(i\Delta x, j\Delta y)$, where $i, j \in N$ [3].

In order to establish the initial condition, we will consider the function as follows [3]:

$$E_0(y) = \frac{1}{2\pi\sigma^2} \exp[-y^2/(2\sigma^2)]. \tag{3}$$

This expression denotes the probability density function of a normal distribution with zero mean and standard deviation of σ. It is noteworthy that the function satisfies the normalization condition and is symmetric with respect to the y-axis. In addition, this function is continuous and differentiable. These features make it a suitable initial condition for a wide range of applications in various fields of science and engineering.

2.1. Description of the concave lens

Modern X-ray lenses adopt parabolic concave surfaces to eliminate aberrations commonly seen in lenses with spherical concave surfaces. Due to the low refractive index, the focusing effect of a single lens is minimal, and a multiple-lens system is often used to achieve a significant focusing effect. When the lenses are arranged in a row, one after the other, the lens system operates as a single lens and is referred to as a compound refractive lens (CRL) [1, 2, 4].

The lens at a point (x, y) is described by the function $B(x, y) = \frac{\omega_0}{c_0}(i\delta + \beta)d(x, y)$, where δ denotes the refractive index, and β represents the absorption coefficient. Addi-

tionally, the function $d(x,y)$ is defined by the formula [6]:

$$d(x,y) = \begin{cases} 1 & \text{if the ray is in the lens.} \\ 0 & \text{if the ray is not in the lens.} \end{cases}$$

To provide a geometrical description of the lens, we shall employ the functions denoted as $F(y,z)$ and $\frac{\Delta F(y_m,z_l)}{\Delta y}$. These functions are defined by the following formulas [6, 7]:

$$X_L(y) = max\{-0.5Ry^2 + 0.5(W - W_{sm}), 0\},$$

$$X_R(y) = min\{0.5Ry^2 + 0.5(W + W_{sm}), W\},$$

$$F(y) = X_R(y) - X_L(y),$$

$$\frac{\Delta F(y_m)}{\Delta y} \simeq \frac{F(y_{m+1}) - F(y_{m-1})}{2h}.$$

In this context, R denotes the curvature of the lens, W refers to the maximum thickness of the lens, and W_{sm} denotes the minimum thickness of the lens.

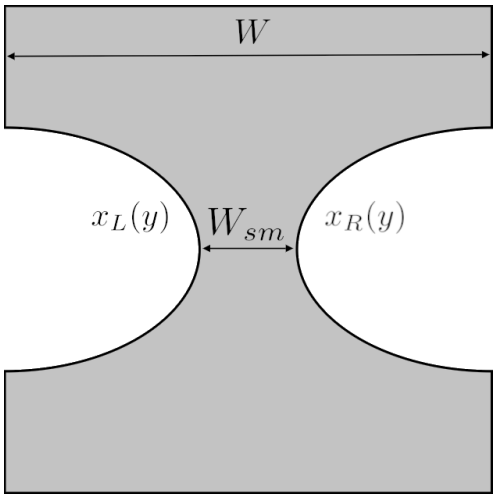

Figure 1: Diagram of a concave lens.

3. Mathematical description of the methods used

The paraxial wave equation in X-ray optics can be solved through various methods, including the finite difference method, the fast Fourier transform method, and the method based on oriented Gaussian beams.

3.1. Finite difference method

The system of ordinary differential equations indicated by equation Eq. 2 can be effectively solved through the use of a variety of standard numerical methods that are well-suited to this purpose. Among the available methods, the second-order Runge-Kutta method is a particularly universal approach that yields reliable and accurate results. The second-order Runge-Kutta method is given by the equations [6]:

$$y_{n+1} = y_n + hf\left(t_n + \frac{h}{2}, \frac{1}{2}(y_n + y_{n+1})\right),$$

$$y_{n+\frac{1}{2}} = y_n + \frac{1}{2}hf\left(t_n + \frac{h}{2}, y_{n+\frac{1}{2}}\right).$$

The computational framework for the Runge-Kutta method with an intermediary point consists of two steps [6].

- In the first step, intermediate points are calculated using an iterative scheme. The following equations are utilized to calculate the intermediate points:

$$A^{(0)}_{i+\frac{1}{2},j} = \frac{A_{i,j} + r(A_{i,j+1} + A_{i,j-1})}{1 + \frac{\Delta x}{2}B_{i+\frac{1}{2},j} + 2r},$$

$$A^{(n+1)}_{i+\frac{1}{2},j} = \frac{A_{i,j} + r\left(A^{(n)}_{i+\frac{1}{2},j+1} + A^{(n)}_{i+\frac{1}{2},j-1}\right)}{1 + \frac{\Delta x}{2}B_{i+\frac{1}{2},j} + 2r}. \quad (4)$$

  The parameters k and r are defined as $k = \frac{\omega_0}{c_0}$ and $r = \frac{i\Delta x}{4k(\Delta y)^2}$, respectively.
- In the second step, grid points values are calculated using equation:

$$A_{i+1,j} = 2A^{(m)}_{i+\frac{1}{2},j} - A_{i,j}.$$

  Here, m is the last iteration made using formula Eq. 4

3.2. Method based on the fast Fourier transform

The paraxial wave equation is commonly solved using the fast Fourier transform (FFT), which is highly efficient. However, as the exact solution of the paraxial equation is in the form of an infinite Fourier series, truncation is necessary when using the FFT, which can lead to errors. While methods for estimating the truncation error of the Fourier series are well-developed for analytically determined functions, they are difficult to apply to functions that are digitized on a grid, as is the case in X-ray optics [8]. The Nyquist principle is useful for determining the necessary frequency of digitization but does not estimate the truncation error of the Fourier series. Fur-

thermore, research shows that different focus characteristics are sensitive to the quality of calculations to varying degrees [8].

The fast Fourier transform is an algorithm for determining the discrete Fourier transform and its inverse. The algorithms for computing the discrete Fourier transform are based on the divide-and-conquer method, which recursively divides a transform of size $N = N_1 N_2$ into transforms of size N_1 and N_2 [9]. The Cooley-Tukey algorithm is commonly used, as it is highly efficient in terms of execution time. However, the input sample vector must have a length of N = 2^k, where k is a natural number. The computational complexity of the algorithm used is $O(N\log_2(N))$, which is significantly better than the $O(N^2)$ complexity resulting from a naive implementation [9].

The calculation procedure for the fast Fourier transform-based method is divided into two steps:

1. In the first step, the signals before the lens and on the lens are calculated:
   (a) Firstly, the input signal for the discrete Fourier transform is computed using the equation Eq. 3. The Fourier transform is then applied to this signal to obtain $A_m(0)$.
   (b) In the subsequent step, the inverse discrete Fourier transform is computed for $x = x_c$, where x_c represents the geometric center of the lens. The following equation is employed for this purpose:

$$A_j(x) = \frac{1}{N}\sum_{m=-\frac{N}{2}}^{\frac{N}{2}-1} A_m(0) e^{\frac{ic_0 x}{\omega_0 \Delta y^2}(cos(\frac{2\pi}{N}m)-1))} e^{i\frac{2\pi}{N}mj}.$$

   (c) Following that, $A_j(x)$ is multiplied by $e^{(-B(x,y)F(y_j))}$, and the discrete Fourier transform is applied. This yields the new initial condition, $A'_m(0)$.
2. In the second step, the signal after the lens is calculated using $A'_m(0)$ as a new initial condition:

$$A_j(x) = \frac{1}{N}\sum_{m=-\frac{N}{2}}^{\frac{N}{2}-1} A'_m(0) e^{\frac{ic_0 x}{\omega_0 \Delta y^2}(cos(\frac{2\pi}{N}m)-1))} e^{i\frac{2\pi}{N}mj}.$$

3.3. Method based on oriented Gaussian beams

The Helmholtz equation Eq. 2 is closely approximated by Gaussian beams, which have widths that are substantially larger than the wavelength of X-rays. As a result, the superposition of Gaussian beams can be considered nearly exact solutions to the aforementioned equation [2]. In practice, virtually all solutions to X-ray optics problems can be constructed using specially chosen sums of Gaussian beams [2].

In our work, we utilize oriented Gaussian beams, which are Gaussian beams that propagate at specific angles to the optical axis of the optical system. This approach combines the properties of geometrical optics, which provide Gaussian beams with clear wave propagation directions and localized transverse directions, with wave optics, which demonstrate that Gaussian beams are nearly exact solutions to the Helmholtz wave equation [2]. We find that this method is particularly well-suited for addressing multi-lens problems and enables us to calculate the focus with a high degree of accuracy [2].

The present study proposes a methodology based on oriented Gaussian beams to calculate the propagation of electromagnetic waves through a thin lens. The calculation scheme involves several steps that are described below [7].

- First, E_{0m} is obtained by discretization of the initial condition Eq. 3.
- Next, the propagation value at the geometric center of the lens in front of the lens denoted by x_c, is calculated for the vector position $r_m = (x_0, y_0)$.

$$E(\mathbf{r}) = \sum_m E_{0m} G(\mathbf{r}, \mathbf{r}_m, \mathbf{e}_{\mathbf{1},m}).$$

  Here, G is a function defined by equation:

$$G(\mathbf{r}, \mathbf{r}_m, \mathbf{e}_{\mathbf{1},m}) = \exp[ik_0(\mathbf{r}-\mathbf{r}_m)\mathbf{e}_{\mathbf{1},m}] \times \frac{h}{(2\pi\{\sigma^2 + i[(\mathbf{r}-\mathbf{r}_m)\mathbf{e}_{\mathbf{1},m}]/k_0\})^{\frac{1}{2}}} \times \exp\left(-\frac{[(\mathbf{r}-\mathbf{r}_m)\mathbf{e}_{\mathbf{2},m}]^2}{2\{\sigma^2 + i[(\mathbf{r}-\mathbf{r}_m)\mathbf{e}_{\mathbf{1},m}]/k_0\}}\right), \quad (5)$$

  where $\mathbf{e_{1,m}} = (x, y_m)$ is the direction of wave propagation and $\mathbf{e_{2,m}}$ is a vector perpendicular to $\mathbf{e_{1,m}}$.
- In the next step, the propagation value at x_c behind the lens and the new directional vectors are calculated using equations:

$$E(\mathbf{r})^+ = E(\mathbf{r})\exp[ik_0(-\delta + i\beta)F(y)],$$

$$e^+_{1,m,y} = e_{1,m,y} - \delta\frac{\Delta F(y_m)}{\Delta y},$$

$$e^+_{1,m,x} = 1 - \frac{(e^+_{1,m,y})^2}{2}.$$

- Finally, the final directional vectors for calculating propagation outside the lens should be calculated

using equations:

$$e'_{1,y} = \Re\{-i\frac{D_y[E(\mathbf{r})]}{E(\mathbf{r})}\}/k_0,$$

$$e'_x = 1 - \frac{e'^2_{1,y}}{2}.$$

Here, $D_y[E(\mathbf{r})]$ is defined as follows with vector $r_m = (x_0, y_m)$:

$$D_y[E(\mathbf{r})] = \sum_m ik_0\mathbf{e}_{\mathbf{1},m}E_{0ml}G(\mathbf{r},\mathbf{r}_m,\mathbf{e}_{\mathbf{1},m}).$$

3.4. Estimating the accuracy of numerical simulations: a modified Runge's rule for estimating errors in numerical simulations

The Runge method is a technique used to estimate the precision of a finite difference simulation by comparing the computations executed with different spatial steps. The method involves calculating the quotient of the difference between results obtained with two different spatial steps, normalized by a factor that depends on the accuracy of the method. The Runge method is expressed by the following equation [3]:

$$Q(h_1) = \left|\frac{Z_{h_1} - Z_{h_2}}{(h_2/h_1)^n - 1}\right|. \quad (6)$$

Here, Z_{h_1} and Z_{h_2} represent the outcomes of a numerical approximation with spatial steps h_1 and h_2, respectively, where $h_2 < h_1$. The accuracy of the method is denoted by n [3].

Estimating errors in FFT-based methods is challenging, especially when the initial function under consideration is not sufficiently smooth. However, when dealing with propagation through a lens, for instance, and the function is continuous but not differentiable, the possibility of error estimation is nonexistent. The Runge rule is also inapplicable in such cases due to the lack of spatial steps, which makes it impossible to determine the method's order [3]. The inability to estimate errors is a significant limitation of FFT-based methods that must be addressed to enhance their efficacy.

In the context of methods utilizing oriented Gaussian beams, the Runge method Eq. 6 can also be applied [7].

4. Results

The present study involved simulations with an initial beam width of 0.0001 meters, using concave lenses with a curvature of $\frac{1}{15000}m^{-1}$. The lenses in question had a maximum width of 0.001 meters and a minimum width of 3×10^{-5} meters. The refractive index was set at 2.216×10^{-6}, while the absorption coefficient was 3.18×10^{-10}. Those parameters correspond to a concave lens made of beryllium.

4.1. Results with 1 lens

The interval $[-0.000256, 000256]$ meters was utilized to perform the calculations with a spatial step of $\Delta_y = 2.5 \times 10^{-7}$ meters along the OY axis. Moreover, for the Runge-Kutta method, an additional spatial step of $\Delta_x = 0.001$ meters was included.

The results of the analysis are presented in Figures Fig. 2, Fig. 3, and Fig. 4, where the findings obtained from the FFT, oriented Gaussian beam, and Runge-Kutta methods are displayed, respectively.

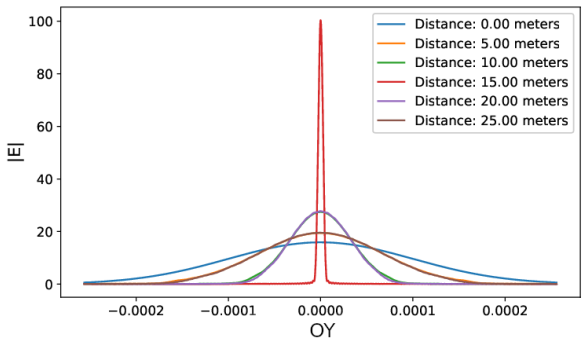

Figure 2: Results obtained using the FFT method at 0, 5, 10, 15, 20, and 25 meters. The values are given in millions.

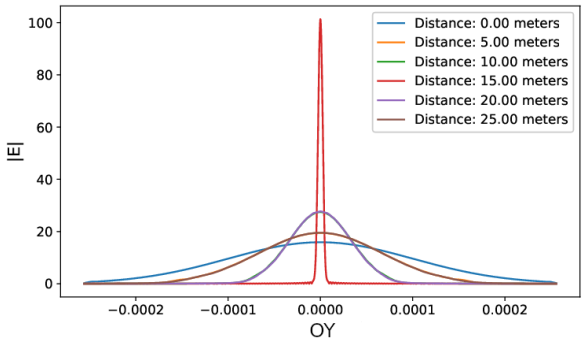

Figure 3: Results obtained using the oriented Gaussian beam method at 0, 5, 10, 15, 20, and 25 meters. Function values are given in millions.

It can be observed that using a single lens produces similar results across all methods. Theoretical analysis has shown that the maximum focus value is approximately 15.04 meters. The methods yield the following results:

- The Runge-Kutta method has a focus point at 15.69 m with a Runge rule of 1.64% and a relative error of 4.31% based on the focus point. The relative error based on the maximum value at the focus point is 0.20%.

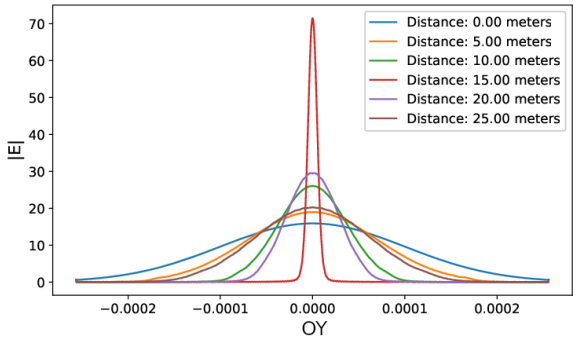

Figure 4: Results obtained using the Runge-Kutta method at 0, 5, 10, 15, 20, and 25 meters. Function values are given in millions.

- The FFT method has a focus point at 15.10 m with a relative error of 0.39%, based on the focus point. The relative error based on the maximum value at the focus point is 0.00%.
- The Gaussian beam method has a focus point at 15.03 m with a Runge rule of 0.00% and a relative error of 0.08%, based on the focus point. The relative error based on the maximum value at the focus point is 0.04%.

It is worth noting that the Runge rule and relative error for the maximum value at the focus point were calculated using different spatial steps of Δ_y, which were $2.5 \times 10^{-}7$ meters and $2 \times 10^{-}7$ meters respectively.

4.2. Results with 5 lenses

The interval $[-0.000256, 000256]$ meters was utilized to perform the calculations with a spatial step of $\Delta_y = 6.25 \times 10^{-8}$ meters along the OY axis. Moreover, for the Runge-Kutta method, an additional spatial step of $\Delta_x = 0.0001$ meters was included.

The results of the analysis are presented in Figures Fig. 5, Fig. 6, and Fig. 7, where the findings obtained from the FFT, oriented Gaussian beam, and Runge-Kutta methods are displayed, respectively.

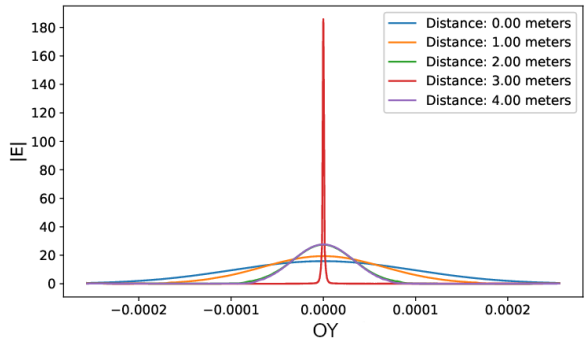

Figure 5: Results obtained using the FFT method at 0.0, 1.0, 2.0, 3.0 and 4.0 meters. The values are given in millions.

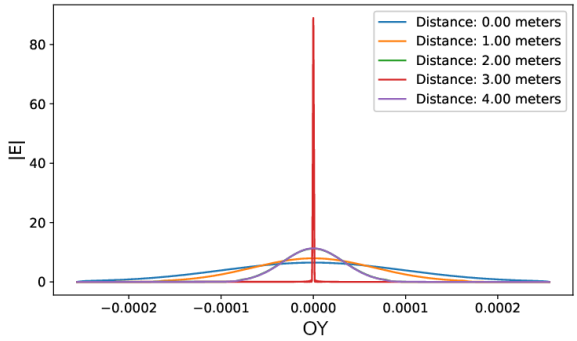

Figure 6: Results obtained using the oriented Gaussian beam method at 0.0, 1.0, 2.0, 3.0 and 4.0 meters. The values are given in millions.

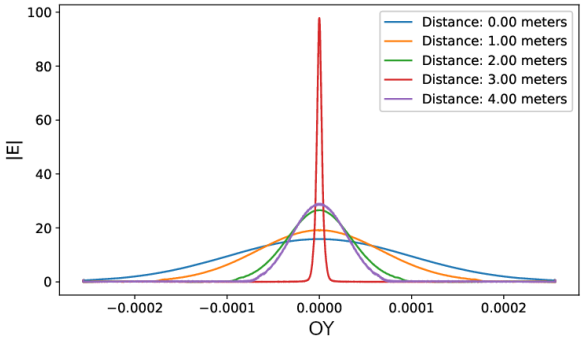

Figure 7: Results obtained using the Runge-Kutta method at 0.0, 1.0, 2.0, 3.0 and 4.0 meters. The values are given in millions.

It can be observed that using a five lenses produces different results across all methods. Theoretical analysis has shown that the maximum focus value is approximately 3.00 meters. The methods yield the following results:

- The Runge-Kutta method has a focus point at 3.09 m with a Runge rule of 4.12% and a relative error of 2.71% based on the focus point. The relative error based on the maximum value at the focus point is 3.55%.
- The FFT method has a focus point at 3.02 m with a relative error of 0.38%, based on the focus point. The relative error based on the maximum value at the focus point is 3.86%.
- The Gaussian beam method has a focus point at 3.01 m with a Runge rule of 0.00% and a relative error of 0.05%, based on the focus point. The relative error based on the maximum value at the focus point is 0.90%.

It is worth noting that the Runge rule and relative error for the maximum value at the focus point were calculated using different spatial steps of Δ_y, which were 6.25×10^{-8} meters and 3.125×10^{-8} meters, respectively.

4.3. Results with 10 lenses

The study involved performing calculations on the interval $[-0.000256, 000256]$ meters with a spatial step Δ_y of 3.125×10^{-8} meters for the *OY* axis.

The results of the analysis are presented in Figures Fig. 8 and Fig. 9, where the findings obtained from the FFT and oriented Gaussian beam methods are displayed, respectively.

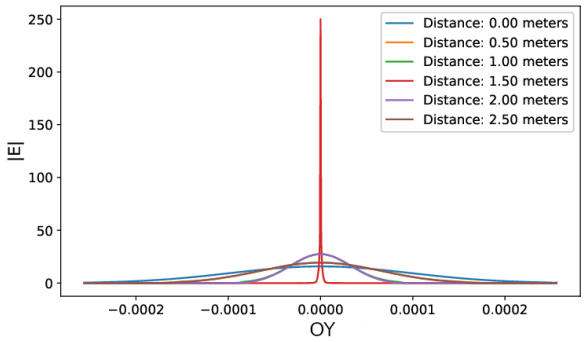

Figure 8: Results obtained using the FFT method at 0.0, 1.0, 1.5, 2.0 and 2.5 meters. The electric field strength module is given in millions.

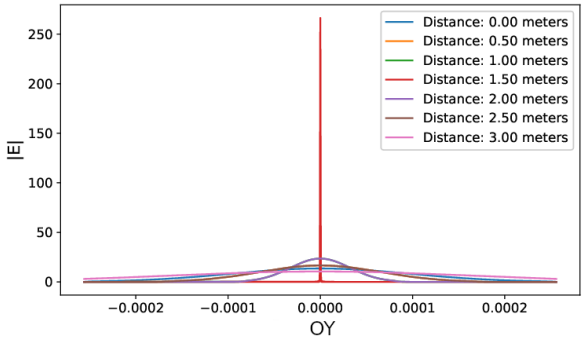

Figure 9: Results obtained using the oriented Gaussian beam method at 0.0, 1.0, 1.5, 2.0, 2.5 and 3.0 meters. The electric field strength module is given in millions.

It can be observed that using ten lenses produces different results across all methods. Moreover, it was not possible to obtain reliable results for the Runge-Kutta method. Theoretical analysis has shown that the maximum focus value is approximately 1.50 meters. The methods yield the following results:

- The FFT method has a focus point at 1.52 m with a relative error of 1.05%, based on the focus point. The relative error based on the maximum value at the focus point is 9.20%.
- The Gaussian beam method has a focus point at 1.51 m with a Runge rule of 0.01% and a relative error of 0.39%, based on the focus point. The relative error based on the maximum value at the focus point is 1.76%.

It is worth noting that the Runge rule and relative error for the maximum value at the focus point were calculated using different spatial steps of Δ_y, which were 3.125×10^{-8} meters and 1.5625×10^{-8} meters, respectively.

5. Conclusion

This research article presents three distinct methods for simulating radiation propagation using concave lenses. The study explores the relative error for each method and calculates the Runge rule. The results indicate that, for a single lens, all methods provide comparable outcomes. However, the method based on the Runge-Kutta scheme presents the highest error, which is notably greater than the other methods. Nonetheless, the accuracy of the calculation is still acceptable.

With five lenses and ten lenses, the test results are similar to those with one lens. However, it is crucial to note the larger error of the Runge-Kutta method, which is attributed to an insufficient number of Δy points. Despite the increase in calculation error, the other methods present themselves favourably. It is noteworthy that the Runge-Kutta-based method for 10 lenses failed to provide reliable outcomes, owing to the enormous error incurred in the computations caused by an excessively large variable Δ_y.

The time required to determine the maximum focus point is the highest for the directed Gaussian beam method (6 minutes 55 seconds). The fastest method turned out to be the FFT-based method (about 1 second), while the calculation time for the Runge-Kutta method is close to the FFT method (about 2 seconds). On the other hand, the time required to reach the maximum focus point is completely different. For the FFT-based method for 5 and 10 lenses, the calculations were completed in about 1 second. However, there is a significant increase in calculation time for the Runge-Kutta method for 5 lenses (22 minutes 38 seconds), which is very close to the method based on oriented Gaussian beams (22 minutes 53 seconds). For 10 lenses, the time required to obtain the maximum focus point for the method based on oriented Gaussian beams is 55 minutes 43 seconds.

In summary, the Gaussian beam method is the most accurate and stable. However, its disadvantage is the significant increase in calculation time, relative to the number of lenses used, because the computational complexity is N^2. On the other hand, the method based on the fast Fourier transform is the fastest. This is due to the fast Fourier transformation algorithm, which reduces the computational complexity to a $Nlog_2(N)$. Although this method is not as accurate as the method based on Gaussian beams, the calculation error is at a low level. How-

ever, the disadvantage of this method is the limited number of Δ_y points we can consider due to the instability of the solution if these points are too close to each other. The second-order Runge-Kutta method is the least favourable of the methods presented, as it is much less accurate than the Gaussian beam method and much slower than the FFT-based method. Furthermore, computing the next step x_i for the parallax axis requires determining the step x_{i-1} first, which results in greater memory complexity. This makes the method not very effective for X-ray propagation applications.

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