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Mahmoud Mohamed Reda Ahmed Elsawy

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University of L'Aquila, University of Nice Sophia Antipolis, Gdansk University of Technology

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Finite-difference model and numerical simulation for X-ray focusing

Author: **Mahmoud Mohamed Reda Ahmed Elsawy**

Born on September 7, 1988. Alexandria. Egypt

Supervisors:

Prof. Sergey Leble Dr. Pawel Wojda

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Abstract

Imaging with X-rays have developed rapidly over the last few years. X-ray microscopy, and micro-analysis have many applications in basic science and technology [1]. There are different ways to focus X-rays including focusing with mirrors, Fresnel zone plates, and CRLs (Compound refractive lenses) [1]. In our model we consider the propagation of X-rays from the undulator sources installed at the third-generation storage rings at the ESRF a high β undulator [1] through compound refractive lenses made of AL with parabolic profile. We use here the finite difference approach, and the implicit Runge Kutta method of the second order to solve the wave equation inside, and outside the CRLs. The program written in FORTRAN to compute the focal distance, and the spot size. We consider two cases, the first one for 33 Al lenses, and the second one for a few number of lenses up to 15 lenses. For the first case, we consider only the one dimensional case, as the numerical investigations showed that we need to use more than 50000 points in each direction which can not be done using the personal computer. We perform two dimensional simulation for the second case with few number of lenses. The design of the lenses is considered as in [1] and we use the same data to compare the results with the experimental data.. Our results give good agreement with the experimental data for the focal distance, and for the intensity at the focal plane while, for the FWHM we have smaller FWHM than in the experimental data. We believe that is because we use perfect parabolic lenses without any defects.

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1 Introduction

After the discovery X-rays in the late of 1895 by a German physicist, W. C. Roentgen they become an important tool to examine, and investigate several phenomena in different fields of science like Biology, Geology, Medicine, and materials science [21]. X-rays have a lot of applications nowadays in different parts of science. Most of the applications based on their ability to penetrate the materials. X-rays with lower energy are called soft X-rays, while X-rays with energy above 15Kev are called hard X-rays. Soft X-rays can be used in medical imaging for dental cavities, bone fractures, and diseased such as cancer. In materials science there is a need to investigate, and examine the structure of the samples. So, there is a demand to focus the X-ray beams that will allow us to study, and investigate the details of the materials with high resolution. Focusing X-ray beams becomes very essential in modern science to understand the Biological, chemical, and Physical systems [21]. There are different ways to focus X-rays like: grazing mirrors, Fresnel plates, and compound refractive lenses. We will introduce briefly the grazing mirrors, Fresnel plates, and we will consider the compound refractive lenses [2] in more detail as this method is the core of our work.

1.1 Focusing X-rays with mirrors

Focusing X-rays with mirrors was the first way to focus the X-ray beams. The idea of using the mirrors based on the reflection of X-rays off metallic surfaces. The most important thing is the incident angle. The incident angle should be very small. This kind of focusing X-ray beams with mirrors is efficient with metals with high density such as gold. For hard X-rays with small wavelength the incident angle should be very small [20]. This kind of mirror can be adapted to reach the required focusing. X-ray reflection does not occur except for very small incident angles, below the critical value $(2\delta)^{1/2}$, where 1-δ is the real part of the index of refraction n=1-δ+iβ. This means that it will be difficult

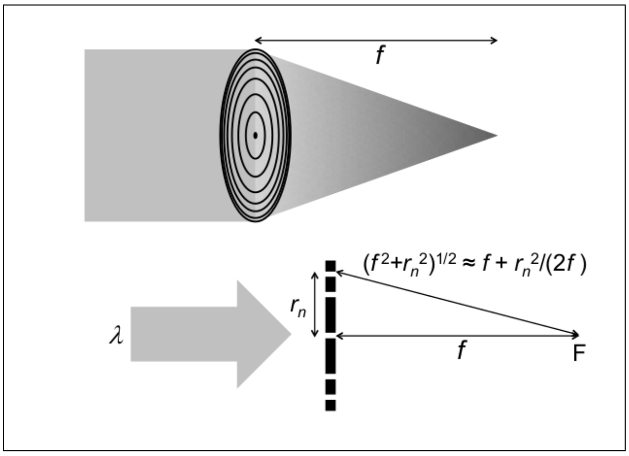


Figure 1: Focusing X-rays with zone plates. This figure form [22]

to obtain small incident angle for hard X-rays, for example $\delta = 2.414 \times 10^{-6}$ for AL at 15Kev. This is the main issue for such kind of focusing X-rays based on the mirrors [20].

1.2 Fresnel zone plates

The second way to focus X-rays is Fresnel zone plates. It consists of series circular zones made of an X-ray absorbing material. It focuses the incoming X-ray beams to a point focus. As it is shown in [22], we can see form figure (1) that the X-rays pass through the zones let's say the n-th zone of radius r_n, and the optical pass can be written as in [22] in the following way $F = (f^2 + {r_n}^2)^{1/2}$. Where f is the focal point. Which can be written as

$$(f^2 + {r_n}^2)^{1/2} - f = n\lambda$$

with wavelength λ, and n is the number of zones [22]. Now if we consider hard X-rays with small wavelength the last relation can be written as $(f^2 + {r_n}^2)^{1/2} = f + r_n^2/2f$ and $r_n = (2n)^{1/2}$ [22]. So, focusing X-rays with zone plates depends on the width of the zone, which depends on the way to fabricate it. In general, Fresnel zone plates can be used for soft X-rays with very low energy.

1.3 Compound refractive lenses

For the visible light, we can use lenses to focus the light. Refractive lenses can be used for visible light that will give us short focal distance, strong refraction, and weak absorption. But, for the X-rays the situation is different because the index of refraction n for X-rays is given by n=1-δ+iβ. The real part in the index of refraction $1-\delta$ is close to one. Although β is small number compared to one, the absorption can't be negligible. Basically in order to focus X-rays with refractive lenses we will have strong absorption, long focal distance, and the lens must take a concave shape [23]. This led to the observation that there is no way to fabricate refractive lenses for X-rays. However, the problems can be solved by stacking many lenses behind each other [23] by setting the radius of curvature to be small (e.g. 0.2 mm) [1], and by choosing a low-Z lens material like AL, and Be [1]. The first trial with CRLs was in [2] by considering a bulk of low-Z material with an array of cylindrical holes. The cylindrical holes play an important role for point focusing. The design of such CRLs is very easy to fabricate, but it causes spherical aberrations which produce a blurry image. So, in [1] they fabricated another kind of CRLs, to avoid the problem in [2]. The new lenses have a parabolic profile and rotational symmetry around the optical axis so, they focus in two directions and because of the parabolic shape they don't have spherical aberrations as in [2]. We will consider the parabolic shape of the lenses to focus X-rays using the finite difference method. But, we need to mention that we use here ideal lenses without any defects. In the last section we will compare our results with the experimental data in [1]

1.4 The general equations

Our starting point is Maxwell's Equations which can be written in the following form

$$
\begin{aligned}
\nabla \cdot \vec{D} &= \rho \\
\nabla \cdot \vec{B} &= 0 \\
\nabla \times \vec{E} &= -\tfrac{\partial \vec{B}}{\partial t} \\
\nabla \times \vec{H} &= \vec{J} + \tfrac{\partial \vec{D}}{\partial t}
\end{aligned}
\tag{1.1}
$$

Where, $\vec{E}$ is the electric field (V/m), $\vec{D}$ is the electric displacement, $\vec{J}$ is the current density, ρ is the volume charge density, and $\vec{B}$ is the magnetic field.

We can write the $\vec{D}$, and $\vec{B}$ as:

$$\vec{D} = \epsilon_0 \vec{E} + \vec{P}$$

and

$$\vec{B} = \mu_0 \vec{H} + \vec{M}$$

Where $\epsilon_0 = 1/(36\pi) \times 10^{-9}$ (F/m), and $\mu_0 = 4\pi \times 10^{-7}$ (H/m) are the permittivity and permeability of free space. $\vec{P}$ is the polarization, and $\vec{M}$ is the magnetization of the medium [14]. The other variables do not depend on the optical medium only $\vec{P}$, and $\vec{M}$ give us information about how the optical medium behaves when the electromagnetic wave propagate through it.

The vectors $\vec{D}$, and $\vec{B}$ are functions of $\vec{E}$, and $\vec{H}$ respectively. Assuming that the current $\vec{J}$ is also a function of the electric field $\vec{E}$, and the medium is linear we can obtain the following constitutive relations [14]

$$\vec{D} = \vec{f}(\vec{E})$$
$$\vec{J} = \vec{g}(\vec{E})$$
$$\vec{B} = \vec{h}(\vec{H})$$

The Polarization can be written as $\vec{P} = \epsilon_0 \chi_e(\omega_0)\vec{E}$ where $\chi_e(\omega_0)$ is the electric susceptibility. In general $\chi_e(\omega_0)$ is a second rank tensor but, we consider only isotropic medium so, we can write the electric displacement $\vec{D}$ as:

$$\boxed{\vec{D} = \epsilon_0\vec{E} + \epsilon_0\chi_e(\omega_0)\vec{E} = \epsilon_0(1 + \chi_e(\omega_0))\vec{E} = \epsilon_1(\omega_0)\vec{E}} \tag{1.2}$$

Such that $\epsilon_1(\omega_0)$ is the dielectric constant or the electric permittivity of the medium, and ω_0 is the frequency of the electromagnetic wave (in our model we assume that the frequency is fixed). The linear relation between the current $\vec{J}$ and the $\vec{E}$ for isotropic medium can be written as:

$$\vec{J} = \sigma\vec{E}$$

It means that the current $\vec{J}$ at point $\vec{r}$ depends only on the electric field $\vec{E}$ at that point and the conductivity σ. By the same way for the magnetic field

$$\vec{M} = \mu_0\chi_m(\omega_0)\vec{H}$$

where $\chi_m(\omega_0)$ is the magnetic susceptibility of the medium and the magnetic field $\vec{B}$ can be expressed as:

$$\boxed{\vec{B} = \mu_0 \vec{H} + \mu_0 \chi_m(\omega_0) \vec{H} = \mu_0 (1 + \chi_m(\omega_0)) \vec{H} = \mu_1(\omega_0) \vec{H}}$$

In the following subsections we will make some assumptions according to our model.

2 Our model

We consider the propagation of X-rays through CRLs with parabolic profile, we need to calculate the focal disatnce and the spot size. First we consider the propagation in free space (from the source to the lenses), then we consider the propagation inside the lenses. We solve the wave equation in free space, and inside the lenses using the finite-difference method, and implicit Runge Kutta of the second order. The considered medium inside the lenses is homogeneous, linear, non-magnetic, and isotropic.

2.1 Maxwell's equations in free space

In free space $\vec{P} = 0$ and $\vec{M} = 0$. So, we can write $\vec{D} = \epsilon_0 \vec{E}$, and $\vec{B} = \mu_0 \vec{H}$. Maxwell's equations can be written as:

$$\begin{aligned} \nabla \cdot \vec{E} &= 0 \\ \nabla \cdot \vec{B} &= 0 \\ \nabla \times \vec{E} &= -\frac{\partial \vec{B}}{\partial t} \\ \nabla \times \vec{B} &= \epsilon_0 \mu_0 \frac{\partial \vec{E}}{\partial t} \end{aligned} \tag{2.1}$$

2.1.1 Wave equation in vacuum

Since $\vec{E}$, and $\vec{B}$ generate each other, it will be enough to derive single differential equation to describe the propagation of X-rays by only $\vec{E}$.

$$\nabla \times \left(\nabla \times \vec{E}\right) = \nabla \times \left(-\frac{\partial \vec{B}}{\partial t}\right) = -\frac{\partial}{\partial t}\left(\nabla \times \vec{B}\right)$$

Using Faraday's law

$$\nabla \times \left(\nabla \times \vec{E}\right) = -\frac{\partial}{\partial t}\left(\epsilon_0 \mu_0 \frac{\partial \vec{E}}{\partial t}\right)$$

But,

$$\nabla \times \left(\nabla \times \vec{E}\right) = \nabla\left(\nabla \cdot \vec{E}\right) - \nabla^2 \vec{E}$$

and

$$\nabla \cdot \vec{E} = 0$$

So, we reach the following wave equation:

$$\boxed{\nabla^2 \vec{E} = \epsilon_0 \mu_0 \frac{\partial \vec{E}}{\partial t}} \tag{2.2}$$

Following the same procedure to eliminate $\vec{E}$ from Maxwell's equations we get:

$$\boxed{\nabla^2 \vec{H} = \epsilon_0 \mu_0 \frac{\partial \vec{H}}{\partial t}} \tag{2.3}$$

If we compare the last two equations with the general form of the wave equation

$$\nabla^2 \vec{F} = \frac{1}{v^2}\frac{\partial \vec{F}}{\partial t}$$

where v is the phase velocity, we will obtain the speed of the electromagnetic wave in vacuum:

$$v = \frac{1}{\sqrt{\epsilon_0 \mu_0}} \approx 3 \times 10^8 m/s$$

2.1.2 The propagation of X-rays in vacuum

We will consider now the equation (2.2) for the propagation in vacuum

$$\left(\nabla^2 - \frac{1}{c_0^2} \frac{\partial^2}{\partial t^2} \right) \vec{E}(\vec{r}, t) = 0 \tag{2.4}$$

With speed

$$c_0 \approx \frac{1}{\sqrt{\epsilon_0 \mu_0}} = 3 \times 10^8 m/sec$$

Where

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

So, the equation (2.4) can be written as:

$$\left(\frac{\partial^2 \vec{E}}{\partial x^2} - \frac{1}{c_0^2} \frac{\partial^2 \vec{E}}{\partial t^2} \right) = - \left(\frac{\partial^2 \vec{E}}{\partial y^2} + \frac{\partial^2 \vec{E}}{\partial z^2} \right) \tag{2.5}$$

We consider here monochromatic plane wave, and the optical axis along x-axis so, we can search for a solution for the wave equation in the following form:

$$\vec{E}(\vec{r}, t) = \vec{A}(\vec{r}, t) \exp(i(k_0 x - \omega_0 t)) + c.c \tag{2.6}$$

Where c.c is the complex conjugate, $k_0 = \frac{\omega_0}{c_0}$ is the wave number in a vacuum, and $\vec{A}$ is the complex amplitude which is slowly dependent on $\vec{r}$ and t. By differentiating equation (2.6) we get:

$$\frac{\partial \vec{E}}{\partial x} = \left(\frac{\partial \vec{A}}{\partial x} + ik_0\vec{A} \right) \exp(i(k_0x - \omega_0 t)) + c.c$$

$$\frac{\partial \vec{E}}{\partial t} = \left(\frac{\partial \vec{A}}{\partial x} - i\omega_0\vec{A} \right) \exp(i(k_0x - \omega_0 t)) + c.c$$

$$\frac{\partial^2 \vec{E}}{\partial x^2} = \left(\frac{\partial^2 \vec{A}}{\partial x^2} + 2ik_0\frac{\partial \vec{A}}{\partial x} - k_0^2 A \right) \exp(i(k_0x - \omega_0 t)) + c.c$$

$$\frac{\partial^2 \vec{E}}{\partial t^2} = \left(\frac{\partial^2 \vec{A}}{\partial t^2} - 2i\omega_0\frac{\partial \vec{A}}{\partial t} - \omega_0^2 \vec{A} \right) \exp(i(k_0x - \omega_0 t)) + c.c$$

Now, we can substitute into equation (2.5)

$$\left(\frac{\partial^2 \vec{A}}{\partial x^2} + 2ik_0\frac{\partial \vec{A}}{\partial x} - k_0^2 \vec{A} \right) - \frac{1}{c_0^2}\left(\frac{\partial^2 \vec{A}}{\partial t^2} - 2i\omega_0\frac{\partial \vec{A}}{\partial t} - \omega_0^2 \vec{A} \right) = -\left(\frac{\partial^2 \vec{A}}{\partial y^2} + \frac{\partial^2 \vec{A}}{\partial z^2} \right) \tag{2.7}$$

If we put $k_0 = \frac{\omega 0}{c_0}$ into the equation (2.7), it becomes:

$$\left(\frac{\partial^2 \vec{A}}{\partial x^2} + 2i\frac{\omega_0}{c_0}\frac{\partial \vec{A}}{\partial x} \right) - \frac{1}{c_0^2}\left(\frac{\partial^2 \vec{A}}{\partial t^2} - 2i\omega_0\frac{\partial \vec{A}}{\partial t} \right) = -\left(\frac{\partial^2 \vec{A}}{\partial y^2} + \frac{\partial^2 \vec{A}}{\partial z^2} \right) \tag{2.8}$$

We will assume that the field varies progressively along x-axis only (Paraxial approximation) which means that

$$\left| 2\frac{\omega_0}{c_0}\frac{\partial \vec{A}}{\partial x} \right| >> \left| \frac{\partial^2 \vec{A}}{\partial x^2} \right|$$

and we consider here a stationary wave so, equation (2.8) becomes:

$$\frac{2i\omega_0}{c_0}\frac{\partial \vec{A}}{\partial x} = -\left(\frac{\partial^2 \vec{A}}{\partial y^2} + \frac{\partial^2 \vec{A}}{\partial z^2} \right)$$

We finally get:

$$\boxed{\frac{\partial \vec{A}}{\partial x} = \frac{ic_0}{2\omega_0}\left(\frac{\partial^2 \vec{A}}{\partial y^2} + \frac{\partial^2 A}{\partial z^2}\right)} \tag{2.9}$$

We will solve the equation (2.9) numerically by using the finite difference method in the following sections. Now we need to find the dispersion relation for equation (2.9) because it will give us a quantitative estimation for the space steps. The minimal scale l_x along x-axis can be estimated as:

$$l_x = \frac{\omega_0}{c_0} h_r^2$$

Where h_r is the space step in y, z direction, we should take

$$h_x = constant * \frac{\omega_0}{c_0} h_r^2 << l_x$$

where $constant \leq 1$ we can find this constant only empirically. We need to choose that constant carefully such that the error associated with h_x be negligible. Consequently, the following condition must be satisfied for the propagation in free space

$$\boxed{h_x <<< \frac{w_0 h_r^2}{c_0}}$$

2.2 Maxwell's equations inside the lenses

We will use Aluminum or Beryllium lenses, so we need Maxwell's equations inside the metal with the following properties for the medium:

- conducting, with $\vec{J} = \sigma \vec{E}$
- Homogeneous, which means that ϵ_1, μ_1, and σ do not depend on the position
- Isotropic, which means that ϵ_1, μ_1, and σ have the same values in all directions. Consequently, they will be constant values, not tensors.

- Free of charges, which means $\rho = 0$

- Non-magnetic medium, which means that $\vec{M} = 0$ and $\vec{B} = \mu_0 \vec{H}$

Using equation (1.2), we can write Maxwell's equations inside the lenses in the following way:

$$\begin{aligned} &\nabla \cdot \vec{E} = 0 \\ &\nabla \cdot \vec{B} = 0 \\ &\nabla \times \vec{E} = -\tfrac{\partial \vec{B}}{\partial t} \\ &\nabla \times \vec{B} = \epsilon_1 \mu_0 \tfrac{\partial \vec{E}}{\partial t} + \mu_0 \sigma \vec{E} \end{aligned} \tag{2.10}$$

We will suppose that ϵ_1, and σ are real, and use them to define the complex dielectric function ϵ. The index of refraction for X-rays inside the medium is given by:

$$n = 1 - \delta + i\beta$$

Where δ is the refractive decrement it is always of order $O(10^{-6})$ such that $1 - \delta$ close to one, while β is the absorption coefficient it is of order $O(10^{-9})$. So, the material of the lenses influences feebly the propagation of X-ray beams. Therefore, we can consider the field as a plane wave with the same wave number as in free space $k_0 = \frac{\omega_0}{c_0}$ and $\vec{A}_{lens}$ is the amplitude inside the lens which is slowly dependent on $\vec{r}$ and t. Hence,

$$\vec{E}(\vec{r}, t) = \vec{A}_{lens}(\vec{r}, t) \exp(i(k_0 x - \omega_0 t)) + c.c \tag{2.11}$$

We consider here a stationary wave. So,

$$\nabla \times \vec{B} = \mu_0 \left(-i\omega_0\epsilon_1 + \sigma\right) \vec{E}$$

Which can be written as:

$$\nabla \times \vec{B} = -i\mu_0\omega_0 \left(\epsilon_1 + \frac{i\sigma}{\omega_0}\right) \vec{E}$$

Now, we can define the complex dielectric function $\epsilon(\omega_0)$ as:

$$\boxed{\epsilon(\omega_0) = \epsilon_1(\omega_0) + \frac{i\sigma}{\omega_0}} \tag{2.12}$$

By the same way we can derive the wave equation for the propagation inside the lenses using equation (2.10) which gives us:

$$\boxed{\nabla^2\vec{E} - \epsilon_1\mu_0\frac{\partial^2\vec{E}}{\partial t^2} = \sigma\mu_0\frac{\partial\vec{E}}{\partial t}} \tag{2.13}$$

2.2.1 The propagation inside the lens

For the propagation inside the lenses we use the wave equation:

$$\boxed{\nabla^2\vec{E} - \epsilon_1\mu_0\frac{\partial^2\vec{E}}{\partial t^2} = \sigma\mu_0\frac{\partial\vec{E}}{\partial t}} \tag{2.14}$$

$$\left(\frac{\partial^2\vec{E}(\vec{r},t)}{\partial x^2} - \epsilon_1\mu_0\frac{\partial^2\vec{E}(\vec{r},t)}{\partial t^2}\right) - \sigma\mu_0\frac{\partial\vec{E}(\vec{r},t)}{\partial t} = -\left(\frac{\partial^2\vec{E}(\vec{r},t)}{\partial y^2} + \frac{\partial^2\vec{E}(\vec{r},t)}{\partial z^2}\right) \tag{2.15}$$

By differentiating equation (2.11), and substituting into equation (2.15) we get:

$$\left(\frac{\partial^2 \vec{A}_{lens}}{\partial x^2} + 2ik_0\frac{\partial \vec{A}_{lens}}{\partial x} - k_0^2 A\right) - \epsilon_1\mu_0\left(\frac{\partial^2 \vec{A}_{lens}}{\partial t^2} - 2i\omega_0\frac{\partial \vec{A}_{lens}}{\partial t} - \omega_0^2\vec{A}_{lens}\right) - \sigma\mu\left(\frac{\partial \vec{A}_{lens}}{\partial t} - i\omega_0\vec{A}_{lens}\right)$$

$$= -\left(\frac{\partial^2 \vec{A}_{lens}}{\partial y^2} + \frac{\partial^2 \vec{A}_{lens}}{\partial z^2}\right)$$

We shall use the same assumption as in free space, that the field inside the lenses varies progressively along x-axis only (Paraxial approximation)

$$\left|2k_0\frac{\partial \vec{A}_{lens}}{\partial x}\right| >> \left|\frac{\partial^2 \vec{A}_{lens}}{\partial x^2}\right|$$

And we are consider here a stationary wave. Hence,

$$\frac{2i\omega_0}{c_0}\frac{\partial \vec{A}_{lens}}{\partial x} - \left(\frac{\omega_0^2}{c_0^2} - \epsilon_1\mu_0\omega_0^2 - i\sigma\mu_0\omega\right)A_{lens} = -\left(\frac{\partial^2 \vec{A}_{lens}}{\partial y^2} + \frac{\partial^2 \vec{A}_{lens}}{\partial z^2}\right)$$

After some simplifications we get:

$$\frac{\partial \vec{A}_{lens}}{\partial x} + \frac{i\omega_0}{2c_0}\left(1 - \epsilon_1\mu_0 c_0^2 - \frac{i\mu_0\sigma c_0^2}{\omega_0}\right)\vec{A}_{lens} = \frac{ic_0}{2\omega_0}\left(\frac{\partial^2 \vec{A}_{lens}}{\partial y^2} + \frac{\partial^2 \vec{A}_{lens}}{\partial z^2}\right) \tag{2.16}$$

We can put $c_0^2 = 1/\epsilon_0\mu_0$

$$\frac{\partial \vec{A}_{lens}}{\partial x} + \frac{i\omega_0}{2c_0}\left(1 - \frac{\epsilon_1}{\epsilon_0} - \frac{i\sigma}{\omega_0\epsilon_0}\right)\vec{A}_{lens} = \frac{ic_0}{2\omega_0}\left(\frac{\partial^2 \vec{A}_{lens}}{\partial y^2} + \frac{\partial^2 \vec{A}_{lens}}{\partial z^2}\right)$$

Using equation (2.12) we can write the last equation in terms of the complex dielectric function as follows:

$$\frac{\partial \vec{A}_{lens}}{\partial x} + \frac{i\omega_0}{2c_0}\left(1 - \frac{\epsilon(\omega_0)}{\epsilon_0}\right)\vec{A}_{lens} = \frac{ic_0}{2\omega_0}\left(\frac{\partial^2 \vec{A}_{lens}}{\partial y^2} + \frac{\partial^2 \vec{A}_{lens}}{\partial z^2}\right) \tag{2.17}$$

Where

$$\epsilon_r = \frac{\epsilon(\omega_0)}{\epsilon_0}$$

is the relative permittivity of the medium which related to the index of refraction n with the relation

$$n = \sqrt{\epsilon_r \mu_r}$$

Where μ_r is the relative permeability and it is close to 1. Hence, we can express the index of refraction n as

$$n = \sqrt{\epsilon_r}$$

If we substitute into equation (2.17) we will get the following:

$$\frac{\partial \vec{A}_{lens}}{\partial x} + \frac{i\omega_0}{2c_0}\left(1 - n^2\right)\vec{A}_{lens} = \frac{ic_0}{2\omega_0}\left(\frac{\partial^2 \vec{A}_{lens}}{\partial y^2} + \frac{\partial^2 \vec{A}_{lens}}{\partial z^2}\right) \tag{2.18}$$

But, the index of refraction for x-rays is given by:

$$n = 1 - \delta + i\beta$$

δ and β are very small quantities so, we can neglect the term $(\delta + i\beta)^2$. Equation (2.18) takes the form:

$$\frac{\partial \vec{A}_{lens}}{\partial x} + \frac{i\omega_0}{c_0}\left(\delta - i\beta\right)\vec{A}_{lens} = \frac{ic_0}{2\omega_0}\left(\frac{\partial^2 \vec{A}_{lens}}{\partial y^2} + \frac{\partial^2 \vec{A}_{lens}}{\partial z^2}\right)$$

Which gives:

$$\frac{\partial \vec{A}_{lens}}{\partial x} + B\vec{A}_{lens} = \frac{ic_0}{2\omega_0}\left(\frac{\partial^2 \vec{A}_{lens}}{\partial y^2} + \frac{\partial^2 \vec{A}_{lens}}{\partial z^2}\right) \tag{2.19}$$

Where,

$$B = \frac{\omega_0}{c_0}(i\delta + \beta)$$

The last equation models the propagation of X-rays inside the CRLs. We can solve the equation (2.19) by two ways (for simplicity we just drop the vector notation):

- First, we can solve the equation by assuming that $A_{lens} = \exp(-Bx)A'_{lens}$ and we will have an equation similar to what we obtained in the case of free space which can be solved numerically using the FDM.

$$\frac{\partial A'_{lens}}{\partial x} = \frac{ic_0}{2\omega_0}\left(\frac{\partial^2 A'_{lens}}{\partial y^2} + \frac{\partial^2 A'_{lens}}{\partial z^2}\right) \tag{2.20}$$

$$A_{lens} = \exp(-Bx)A'_{lens}$$

- Second, we can use directly the FDM for (2.19) without any multiplication. The two methods are correct from an analytical point of view, while the second one is better in case of large systems because we will avoid the exponent that will take a lot of time. We will consider here the two approaches later in the following sections.

By the same manner as we did for equation (2.9), we need to find the dispersion relation for the equation (2.19). The following conditions must be satisfied

$$h_{lens} << \frac{w_0 h_r^2}{c_0}$$

$$h_{lens} <<< \frac{1}{\mid B \mid}$$

Where h_{lens} is the space step for the x-axis inside the lens.

3 The design of CRLs

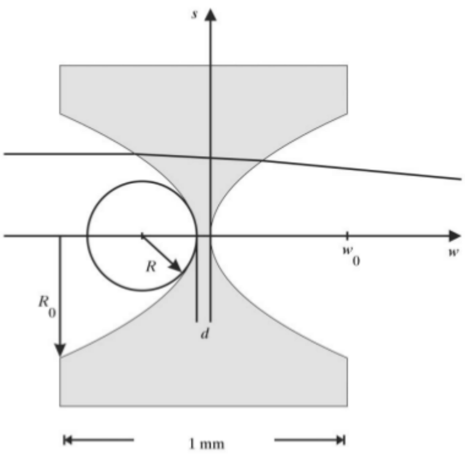


Figure 2: Single Parabolic lens from[1]

3.1 The initial conditions

In this section we will consider the initial conditions for the amplitude of the electromagnetic waves as in [1] for the undulator sources installed in the third-generation storage rings At the ESRF a high β undulator [1]. An undulator source has a finite size described by a Gaussian beam in the vertical and in the horizontal direction [1]

For the horizontal:

$$W(y) = \left(2\pi{\sigma_h}^2\right)^{\frac{-1}{2}} \exp\left(-y^2/2{\sigma_h}^2\right)$$

For the vertical:

$$W(z) = \left(2\pi{\sigma_v}^2\right)^{\frac{-1}{2}} \exp\left(-z^2/2{\sigma_h}^2\right)$$

Where $\sigma_v = 14.9\mu m$ and $\sigma_h = 297\mu m$ which is corresponding to FWHM $d_h = 700\mu m$, and $d_v = 35\mu m$ [1]

3.2 The surface of the lens

In this model we use compound refractive lenses each of them has a parabolic cross section with width(lenw)=1mm such that d is the smallest width of the lens, and R=1/r where r is the radius of curvature. Using the equation of parabola we can define the left and right surface of the lens as the following:

$$XSL(y,z) = -0.5 * R\left((y-0.5*lenw)^2 + (z-0.5*lenw)^2\right) + \left(\frac{lenw-d}{2}\right)$$

$$XSR(y,z) = 0.5 * R\left((y-0.5*lenw)^2 + (z-0.5*lenw)^2\right) + \left(\frac{lenw+d}{2}\right)$$

4 The finite-difference scheme

In this section we will find the numerical scheme for the propagation in free space and inside the CRLs. We apply the FDM to the equations (2.9) and (2.19). The FDM will transform them to a system of ODEs [19] then, we use the implicit Runge Kutta method of order two with an iteration method to solve the ODEs. As we mentioned before, for the propagation inside the lens we will consider the two ways to solve equation (2.19). If we consider the equation (2.20) which means dealing with the exponent, then we will use the same manner as in the next subsection but, for lenses. While, the second way requires solving equation (2.19) with the finite-difference method directly without exponent [18].

4.1 Free space

Let's start with equation (2.9) for the propagation in free space.

$$\frac{\partial A}{\partial x} = \frac{ic_0}{2\omega_0}\left(\frac{\partial^2 A}{\partial y^2} + \frac{\partial^2 A}{\partial z^2}\right)$$

We approximate the second derivatives in y, z direction with space step h_r using the finite difference scheme such that $y_j = jh_r$ and $z_k = kh_r$ where j, k=0,1,2,.........N and h_r is the space step in y, z. Using Taylor's expansion, we get:

$$A_{j+1,k} = A_{j,k} + h_r \left(\frac{\partial A}{\partial y}\right)_{j,k} + \frac{h_r^2}{2}\left(\frac{\partial^2 A}{\partial y^2}\right)_{j,k} + \frac{h_r^3}{6}\left(\frac{\partial^3 A}{\partial y^3}\right)_{j,k} + O(h_r^4)$$

And,

$$A_{j-1,k} = A_{j,k} - h_r \left(\frac{\partial A}{\partial y}\right)_{j,k} + \frac{h_r^2}{2}\left(\frac{\partial^2 A}{\partial y^2}\right)_{j,k} - \frac{h_r^3}{6}\left(\frac{\partial^3 A}{\partial y^3}\right)_{j,k} + O(h_r^4)$$

By adding them as we get:

$$\left(\frac{\partial^2 A}{\partial y^2}\right)_{j,k} = \frac{A_{j+1,k} - 2A_{j,k} + A_{j-1,k}}{h_r^2} + O(h_r^2)$$

By the same manner we can find the approximation to the second derivative in z direction as follows:

$$\left(\frac{\partial^2 A}{\partial z^2}\right)_{j,k} = \frac{A_{j,k+1} - 2A_{j,k} + A_{j,k-1}}{h_r^2} + O(h_r^2)$$

Equation (2.9) can be written as:

$$\frac{\partial A_{j,k}}{\partial x} = \frac{ic_0}{2\omega_0 h_r^2}\left(A_{j+1,k} + A_{j-1,k} + A_{j,k+1} + A_{j,k-1} - 4A_{j,k} + O(h_r^2)\right)$$

We can also approximate the first derivative in the left hand side using Taylor's expansion as well. We can approximate $x^n = nh_x$, where h_x is the space step in x-axis:

$$A_{j,k}^{n+1} = A_{j,k}^n + h_x \left(\frac{\partial A}{\partial x}\right)_{j,k}^n + O(h_x^2)$$

So, the forward scheme is given by:

$$\left(\frac{\partial A}{\partial x}\right)_{j,k}^{n} = \frac{A_{j,k}^{n+1} - A_{j,k}^{n}}{h_x} + O(h_x)$$

For the intermediate scheme:

$$A_{j,k}^{n+\frac{1}{2}} = A_{j,k}^{n} + \frac{h_x}{2}\left(\frac{\partial A}{\partial x}\right)_{j,k}^{n} + O(h_x^2)$$

Finally, using the midpoint scheme, equation (2.9) can be written as:

$$\frac{A_{j,k}^{n+1} - A_{j,k}^{n}}{h_x} = \frac{ic_0}{2\omega_0 h_r^2}\left(A_{j+1,k}^{n+\frac{1}{2}} + A_{j-1,k}^{n+\frac{1}{2}} + A_{j,k+1}^{n+\frac{1}{2}} + A_{j,k-1}^{n+\frac{1}{2}} - 4A_{j,k}^{n+\frac{1}{2}}\right) + O\left(h_x^2 + h_r^2\right) \quad (4.2)$$

This scheme contains unknowns $A_{j,k}^{n+1}$ and $A_{j,k}^{n+\frac{1}{2}}$. In order to calculate the intermediate quantities $A_{j,k}^{n+\frac{1}{2}}$, we apply the implicit scheme

$$2 * \frac{A_{j,k}^{n+\frac{1}{2}} - A_{j,k}^{n}}{h_x} = \frac{ic_0}{2\omega_0 h_r^2}\left(A_{j+1,k}^{n+\frac{1}{2}} + A_{j-1,k}^{n+\frac{1}{2}} + A_{j,k+1}^{n+\frac{1}{2}} + A_{j,k-1}^{n+\frac{1}{2}} - 4A_{j,k}^{n+\frac{1}{2}}\right) + O\left(h_x^2 + h_r^2\right) \quad (4.3)$$

Comparing (4.2) and (4.3), we arrive to the formula

$$A_{j,k}^{n+1} = 2A_{j,k}^{n+\frac{1}{2}} - A_{j,k}^{n} \quad (4.4)$$

The system of equations (4.2) and (4.4) or (4.3) and (4.4) gives us the implicit Runge Kutta method of the second order [19].

4.2 Inside the lens

4.2.1 Inside the lens with exponent

First, we start by the substitution $A_{lens} = \exp(-Bx)A'_{lens}$ then we will obtain the equation

$$\frac{\partial A'_{lens}}{\partial x} = \frac{ic_0}{2\omega_0}(\frac{\partial^2 A'_{lens}}{\partial y^2} + \frac{\partial^2 A'_{lens}}{\partial z^2})$$

Second, by the same way as we did in the last subsection we use the finite difference approximation to approximate the last equation.

$$2*\frac{{A'_{j,k}}^{n+\frac{1}{2}} - {A'_{j,k}}^{n}}{h_x} = \frac{ic_0}{2\omega_0 h_r^2}\left({A'_{j+1,k}}^{n+\frac{1}{2}} + {A'_{j-1,k}}^{n+\frac{1}{2}} + {A'_{j,k+1}}^{n+\frac{1}{2}} + {A'_{j,k-1}}^{n+\frac{1}{2}} - 4{A'_{j,k}}^{n+\frac{1}{2}}\right) \tag{4.5}$$

and

$${A'_{j,k}}^{n+1} = 2{A'_{j,k}}^{n+\frac{1}{2}} - {A'_{j,k}}^{n} \tag{4.6}$$

Finally, we use the substitution $A'_{lens} = \exp(Bx)A_{lens}$

The system (4.5) and (4.6) gives us the implicit Runge Kutta method of second order.

4.2.2 Inside the lens without exponent

Let's start with equation (2.19) for the propagation inside the lens. We will assume that $A_{lens} = \tilde{A}$ just for simplicity

$$\frac{\partial \tilde{A}}{\partial x} + B\tilde{A} = \frac{ic_0}{2\omega_0}\left(\frac{\partial^2 \tilde{A}}{\partial y^2} + \frac{\partial^2 \tilde{A}}{\partial z^2}\right) \tag{4.7}$$

We can use the same procedure as in the last section. For the right hand side we can use the approximation for the second derivative in y, z direction with space step h_r

$$\frac{ic_0}{2\omega_0}\left(\frac{\partial^2 \tilde{A}}{\partial y^2} + \frac{\partial^2 \tilde{A}}{\partial z^2}\right) = \frac{ic_0}{2\omega_0 h_r^2}\left(\tilde{A}^n_{j+1,k} + \tilde{A}^n_{j-1,k} + \tilde{A}^n_{j,k+1} + \tilde{A}^n_{j,k-1} - 4\tilde{A}^n_{j,k}\right) \tag{4.8}$$

Using the midpoint scheme we get:

$$\frac{\tilde{A}^{n+1}_{j,k} - \tilde{A}^{n}_{j,k}}{h_{lens}} + B\tilde{A}^{n+\frac{1}{2}}_{j,k} = \frac{ic_0}{2\omega_0 h_r^2}\left(\tilde{A}^{n+\frac{1}{2}}_{j+1,k} + \tilde{A}^{n+\frac{1}{2}}_{j-1,k} + \tilde{A}^{n+\frac{1}{2}}_{j,k+1} + \tilde{A}^{n+\frac{1}{2}}_{j,k-1} - 4\tilde{A}^{n+\frac{1}{2}}_{j,k}\right) \tag{4.9}$$

Where, h_{lens} is the space step in x direction inside the lens. This scheme contains unknowns $\tilde{A}^{n+1}_{j,k}$ and $\tilde{A}^{n+\frac{1}{2}}_{j,k}$. In order to calculate intermediate quantities $\tilde{A}^{n+\frac{1}{2}}_{j,k}$, we apply the implicit scheme

$$2 * \frac{\tilde{A}^{n+\frac{1}{2}}_{j,k} - \tilde{A}^{n}_{j,k}}{h_{lens}} + B\tilde{A}^{n+\frac{1}{2}}_{j,k} = \frac{ic_0}{2\omega_0 h_r^2}\left(\tilde{A}^{n+\frac{1}{2}}_{j+1,k} + \tilde{A}^{n+\frac{1}{2}}_{j-1,k} + \tilde{A}^{n+\frac{1}{2}}_{j,k+1} + \tilde{A}^{n+\frac{1}{2}}_{j,k-1} - 4\tilde{A}^{n+\frac{1}{2}}_{j,k}\right) \tag{4.10}$$

$$\left(1 + \frac{B * Dist}{2} + \frac{ic_0 h_{lens}}{\omega_0 h_r^2}\right)\tilde{A}^{n+\frac{1}{2}}_{j,k} = \tilde{A}^{n}_{j,k} + \frac{ic_0 h_{lens}}{4\omega_0 h_r^2}\left(\tilde{A}^{n+\frac{1}{2}}_{j+1,k} + \tilde{A}^{n+\frac{1}{2}}_{j-1,k} + \tilde{A}^{n+\frac{1}{2}}_{j,k-1} + \tilde{A}^{n+\frac{1}{2}}_{j,k+1}\right) \tag{4.11}$$

Where, Dist is the distance between two points inside the lens that needs to be defined according to the shape of our parabolic lens.
Comparing (4.10) and (4.9), we arrive to simple formula

$$\tilde{A}^{n+1}_{j,k} = 2\tilde{A}^{n+\frac{1}{2}}_{j,k} - \tilde{A}^{n}_{j,k} \tag{4.12}$$

The system of equations (4.9) and (4.12) or (4.10) and (4.12) gives us the implicit Runge Kutta method of the second order [18].

5 The numerical scheme

5.1 Implicit Runge Kutta inside the lens

5.1.1 Inside the lens without exponent

We consider here the Equations (4.11) and (4.12).

First step

$$\tilde{A}_{j,k}^{n+\frac{1}{2}(0)} = \frac{\tilde{A}_{j,k}^{n} + \frac{ic_0 h_{lens}}{4\omega_0 h_r^2}(\tilde{A}_{j+1,k}^{n} + \tilde{A}_{j-1,k}^{n} + A_{j,k+1}^{n} + \tilde{A}_{j,k-1}^{n})}{\left(1 + \frac{B*Dist}{2} + \frac{ic_0 h_{lens}}{\omega_0 h_r^2}\right)}$$

Second step we need to run it for several times

$$\tilde{A}_{j,k}^{n+\frac{1}{2}(m+1)} = \frac{\tilde{A}_{j,k}^{n} + \frac{ic_0 h_{lens}}{4\omega_0 h_r^2}(\tilde{A}_{j+1,k}^{n(m)} + \tilde{A}_{j-1,k}^{n(m)} + \tilde{A}_{j,k+1}^{n(m)} + \tilde{A}_{j,k-1}^{n(m)})}{\left(1 + \frac{B*Dist}{2} + \frac{ic_0 h_{lens}}{\omega_0 h_r^2}\right)}$$

Last step

$$\tilde{A}_{j,k}^{n+1} = 2\tilde{A}_{j,k}^{n+\frac{1}{2}(m)} - \tilde{A}_{j,k}^{n}$$

In calculation it's enough to take m = 4.

5.1.2 Inside the Lens with exponent

We will consider the equation (2.20) inside the lens with the same procedure as in (4.2) and (4.4) except for the exponent. For simplicity we write A' instead of A'_{lens}

First step

$$A'_{lens} = \exp(B * Dist)A_{lens}$$

$$A_{j,k}^{\prime n+\frac{1}{2}(0)} = \frac{A_{j,k}^{\prime n} + \frac{ic_0 h_{lens}}{4\omega_0 h_r^2}(A_{j+1,k}^{\prime n} + A_{j-1,k}^{\prime n} + A_{j,k+1}^{\prime n} + A_{j,k-1}^{\prime n})}{1 + \frac{ic_0 h_{lens}}{\omega_0 h_r^2}}$$

The second step we need to run it for several times

$$A'^{n+\frac{1}{2}(m+1)}_{j,k} = \frac{A'^{n}_{j,k} + \frac{ic_0 h_{lens}}{4\omega_0 h_r^2}(A'^{n(m)}_{j+1,k} + A'^{n(m)}_{j-1,k} + A'^{n(m)}_{j,k+1} + A'^{n(m)}_{j,k-1})}{1 + \frac{ic_0 h_{lens}}{\omega_0 h_r^2}}$$

Third step

$$A'^{n+1}_{j,k} = 2A'^{n+\frac{1}{2}(m)}_{j,k} - A'^{n}_{,j,k} \tag{5.1}$$

Last step

$$A_{lens} = \exp(-B * Dist)A'_{lens} \tag{5.2}$$

In calculation, it's enough to take m= 4.

5.2 Implicit Runge Kutta in vacuum

In this part we consider the equations (4.2) and (4.4)

First step

$$A^{n+\frac{1}{2}(0)}_{j,k} = \frac{A^{n}_{j,k} + \frac{ic_0 h_x}{4\omega_0 h_r^2}(A^{n}_{j+1,k} + A^{n}_{j-1,k} + A^{n}_{j,k+1} + A^{n}_{j,k-1})}{1 + \frac{ic_0 h_x}{\omega_0 h_r^2}}$$

The second step we need to run it for several times

$$A^{n+\frac{1}{2}(m+1)}_{j,k} = \frac{A^{n}_{j,k} + \frac{ic_0 h_x}{4\omega_0 h_r^2}(A^{n(m)}_{j+1,k} + A^{n(m)}_{j-1,k} + A^{n(m)}_{j,k+1} + A^{n(m)}_{j,k-1})}{1 + \frac{ic_0 h_x}{\omega_0 h_r^2}}$$

Last step

$$A^{n+1}_{j,k} = 2A^{n+\frac{1}{2}(m)}_{j,k} - A^{n}_{j,k}$$

In calculation, it's enough to take m = 4.

6 The stability and the error

6.1 The stability of the scheme

In this section we investigate the stability of the implicit scheme by using the Von Neumann stability method (also known as Fourier stability analysis). We will define the stability as it's in [15]. The stability of numerical schemes is related to the numerical error. A finite difference scheme is stable if the errors made in one step do not cause the errors to increase as the computations are continued [15]

Let's start with the scheme,

$$A_{j,k}^{n+\frac{1}{2}} = A_{j,k}^{n} + \frac{ic_0 h_x}{4\omega_0 h_r^2}\left(A_{j+1,k}^{n+\frac{1}{2}} + A_{j-1,k}^{n+\frac{1}{2}} + A_{j,k+1}^{n+\frac{1}{2}} + A_{j,k-1}^{n+\frac{1}{2}} - 4A_{j,k}^{n+\frac{1}{2}}\right) + O\left(h_x^2 + h_r^2\right) \quad (6.1)$$

Which can be written as the following,

$$A_{j,k}^{n} = (1+4q)\, A_{j,k}^{n+\frac{1}{2}} - q\left(A_{j+1,k}^{n+\frac{1}{2}} + A_{j-1,k}^{n+\frac{1}{2}} + A_{j,k+1}^{n+\frac{1}{2}} + A_{j,k-1}^{n+\frac{1}{2}}\right) \quad (6.2)$$

Where

$$q = \frac{ic_0 h_x}{4\omega_0 h_r^2}$$

And the solution $A_{j,k}^{n}$ of the discrete equation approximates the analytical solution $A(x, y, z)$ of the PDE on the grid. Now we define the round-off error $\epsilon_{j,k}^{n} as$:

$$\epsilon_{j,k}^{n} = N_{j,k}^{n} - A_{j,k}^{n} \quad (6.3)$$

Where $N_{j,k}^{n}$ is the numerical solution. Since the exact solution $A_{j,k}^{n}$ must satisfy the discrete equation, the error $\epsilon_{j,k}^{n}$ must also satisfy the discrete equation. So,

$$\epsilon_{j,k}^{n} = (1+4q)\,\epsilon_{j,k}^{n+\frac{1}{2}} - q\left(\epsilon_{j+1,k}^{n+\frac{1}{2}} + \epsilon_{j-1,k}^{n+\frac{1}{2}} + \epsilon_{j,k+1}^{n+\frac{1}{2}} + \epsilon_{j,k-1}^{n+\frac{1}{2}}\right) \tag{6.4}$$

We now substitute $\epsilon_{j,k}^{n} = \epsilon^{n} e^{ijk\theta}$. After some simplifications the last equation becomes:

$$\epsilon^{n} = \epsilon^{n+\frac{1}{2}}\left(1+4q-q\left(e^{ij\theta}+e^{-ij\theta}+e^{ik\theta}+e^{-ik\theta}\right)\right) \tag{6.5}$$

Consider

$$f(\theta) = \left(1+4q-q\left(e^{ij\theta}+e^{-ij\theta}+e^{ik\theta}+e^{-ik\theta}\right)\right)$$

using Euler's relation we can see that

$$f(\theta) = (1+4q-q\,(2\cos(j\theta)+2\cos(k\theta))) \tag{6.6}$$

Put

$$\cos(j\theta) = 1-2\sin^{2}(j\theta/2)$$

And

$$\cos(k\theta) = 1-2\sin^{2}(k\theta/2)$$

We can reach

$$f(\theta) = \left(1+2q\left(\sin^{2}(j\theta/2)+\sin^{2}(k\theta/2)\right)\right) (6.7)$$

$$\epsilon^{n} = \epsilon^{n+\frac{1}{2}} f(\theta) \tag{6.8}$$

We now define the amplification factor $g(\theta) = \frac{\epsilon^{n+\frac{1}{2}}}{\epsilon^{n}}$ so, it's clear that

$$g(\theta) = \frac{1}{f(\theta)} \tag{6.9}$$

The condition for stability is given by:

$$|g(\theta)| \leq 1 \tag{6.10}$$

$$\left| \frac{1}{1 + 2q\left(\sin^2(j\theta/2) + \sin^2(k\theta/2)\right)} \right| \leq 1 \tag{6.11}$$

Which is true for all the values of θ since $1 + 2q\left(\sin^2(j\theta/2) + \sin^2(k\theta/2) \geq 1\right.$

We can conclude that the implicit scheme is unconditionally stable

6.2 The Runge rule for the estimation of the error

Suppose that we need to calculate some physical value Z, we apply the approximate finite-difference calculations. Let the symbol Z_h is a result of our finite-difference calculations, and R is the error of the calculations such that

$$R = C * h^n + O(h^{n+1})$$

where C is a constant and n is the order of approximation error. The problem is that we do not know the constant C. Runge suggested the method to estimate the error of the calculations.

- We can write:

$$Z = Z_h + Ch^n + O(h^{n+1})$$

- And

$$Z = Z_{2h} + C * (2h)^n + O(h^{n+1})$$

Where Z_{2h} is the approximate calculations done with the step $2h$.

- We can estimate the error within the main order

$$R = Ch^n + O(h^{n+1}) = \frac{Z_h - Z_{2h}}{2^n - 1} + O(h^{n+1})$$

We apply the second order schemes. So, $n = 2$, and

$$R = \frac{Z_h - Z_{2h}}{3} + O(h^3)$$

We are interested in the spot size, and the focal distance. So, let Z be the size of our focal spot or the focal distance. We have steps h_r, h_x, h_{lens} in our calculations which means that we need to investigate all the corresponding errors [19].

6.3 The estimation of the spot size using FWHM

We will use the definition of the FWHM as in [16], and [17]. Full width at half maximum (FWHM) is an expression of the extent of a function, given by the difference between the two extreme values of the independent variable at which the dependent variable is equal to half of its maximum value [16]. The technical term Full-Width Half-Maximum, or FWHM, is used to describe a measurement of the width of an object in a picture [17].

In our case we will obtain the FWHM using σ (the Standard deviation):

$$\sigma = \sqrt{\frac{\sum_{j,k} |A_{jk}|^2 \left(y_j^2 + z_k^2\right)}{\sum_{j,k} |A_{jk}|^2}}$$

or

$$\sigma_y = \sqrt{\frac{\sum_j |A_j|^2 y_j^2}{\sum_j |A_j|^2}}$$

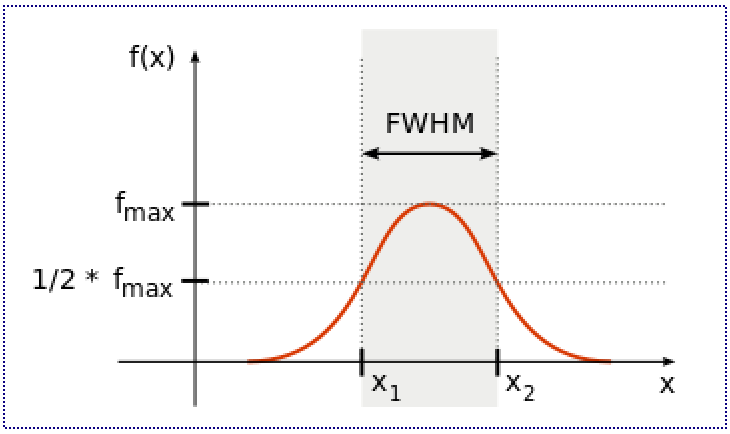


Figure 3: FWHM for Gaussian curve from [16]

or

$$\sigma_z = \sqrt{\frac{\sum_k |A_k|^2 z_k^2}{\sum_k |A_k|^2}}$$

Because the points are distributed with Gaussian distribution , it will be easy to calculate FWHM through the dispersion σ:

$$\frac{1}{2} = \exp\left(-\left(\frac{FWHM}{2*\sigma}\right)^2\right)$$

Therefore

$$FWHM = 2 * \sqrt{2\ln(2)} * \sigma$$

7 The numerical results

In this part we will discuss our numerical results. The initial conditions are Gaussian beams with FWHM=700μm in the horizontal direction, and FWHM= 35μm in the vertical direction. If we need to consider the same initial conditions, we need to conider them over a space bigger than the space for the CRLs. We use here lenses of 1mm in each direction. The results showed that we need to consider the initial conditions over 8mm with the same number of points. So, we will consider the propagation from the source to the CRLs according to the bigger space, then we do the resizing before the lenses. We consider here two cases, the first case using the data from [1], and the second case with energy 15Kev with different number of lenses to perform the 2-d simulation.

7.1 33 AL lenses with energy 15Kev

The first case we consider the data from [1]. We need to choose h_x, and h_r the space steps in x, y, and z directions respectively correctly, and try to find the suitable number of points for our mesh. The dispersion relation governs the relation between the space steps in each direction $h_x << \frac{\omega_0 {h_r}^2}{c_0}$. In order to choose the number of points in y, z direction we need to calculate $0.001/h_r$ this relation will give us the number of points in the horizontal and vertical direction. h_x here is used as the space step in x-axis to identify the place of the detector. For instance, if the focal plane at 1.298m from the CRLs it means that we need $1.298/h_x$ points in x-axis while, h_{lens} is used as the space step inside the lens and it should satisfy the conditions in the dispersion relation for equation (2.20). For the propagation before the CRLs, we use the data for the bigger space. By the same way we can compute the space step in x-axis before the lenses from the relation $h'_x << \frac{\omega_0 {h'_r}^2}{c_0}$. In this simulation, we consider only the one dimensional case, we will see in the following subsections that we need to consider more than 50000 points in each direction which can not be done using the personal computer.

- Number of AL lenses =33
- Radius of curvature=0.2mm
- Energy=15Kev
- $\delta = 2.414 \times 10^{-6}$

- $\beta = 1.299 \times 10^{-8}$
- Gaussian beam for the initial condition in the horizontal direction has FWHM=700μm with sigma=279μm
- Gaussian beam for the initial condition in the vertical direction has FWHM=35μm with sigma=14.9μm
- The distance from the source to the CRLs is 63m

7.1.1 The error of the space steps

In this part we need to choose correctly the space steps in each direction. So, we need to define a suitable value for the constant in the relation h_x =constant$\times\frac{\omega_0}{c_0}h_r^2$. Using the values for 15 Kev, I mean $\omega = 2 \times \pi \times 3.627E18$ constant ≤ 1. We can find this constant only empirically such that the error associated with h_x be negligible. In our case we use 33 lenses it means that we need to consider more points in each direction to get the accurate results. We started here with 40000 points because for 20000 points the plot has some error Fig(4). We fix the space step inside the lens $h_{lens} = 0.000001$ which will satisfy the condition from the dispersion relation in equation (2.20) we will consider the choice of h_{lens} in detail later after fixing the space steps h_x and h_r. We measure the spot size at 1.298m from the lenses as in [1] so that we can compare the results.

The choice of h_x

Let's start first to choose the best value for the constant in the relation

$$h_x = constant \times \frac{\omega_0}{c_0}h_r^2$$

that will give us the best choice for the space step h_x. We fixed here the number of points to be 40000, which means that we fixed the space step h_r. We tried here with

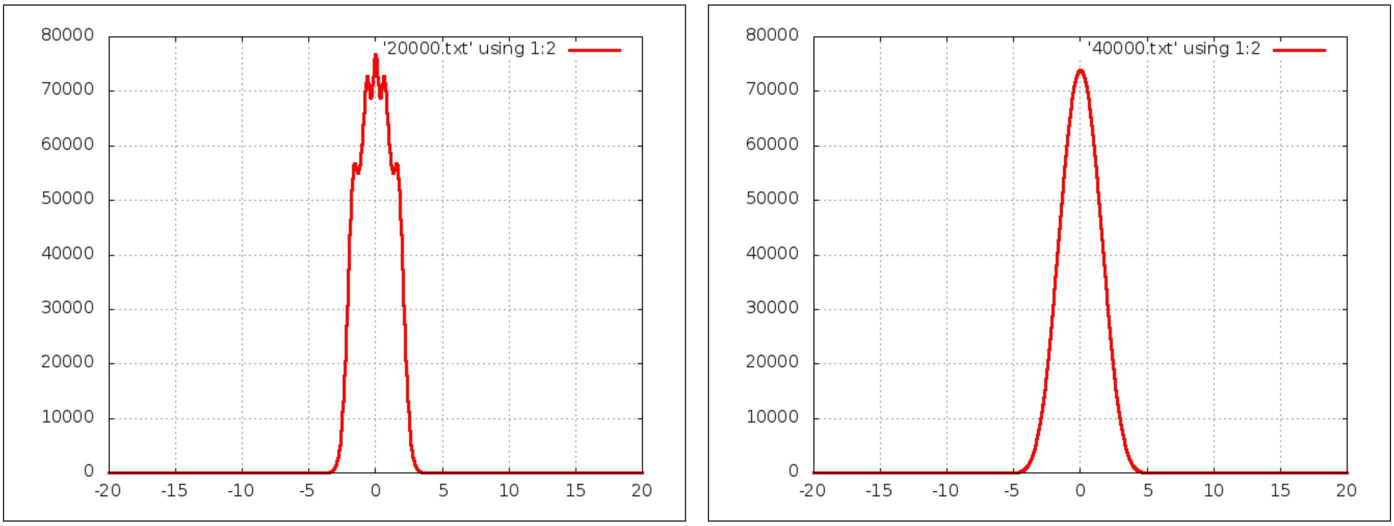


Figure 4: Results for 2000, and 40000 points

Number of points	const	h_r	h_x	focal distance	FWHM
40000	0.131645688	0.000000025	0.00000625	1.2580312m	3.25μm
40000	0.065822844	0.000000025	0.000003125	1.2539093m	3.55μm
40000	0.032911422	0.000000025	0.000001562	1.2528818m	3.65μm

Table 1: The choice of h_x

some values for the constant, the results showed that the best choice for the constant is 0.032911422 which gives us small error in the FWHM, and in the focal distance Table(1). We can go further by choosing a smaller value for the constant which means smaller value for h_x that will give us smaller error. But, in this case we need more points for the propagation after the CRLs for example, if we choose the constant to be 0.016455711 that gives us space step $h_x = 0.000000781$, and we need 1661440 points in x-axis to reach the detector at 1.298m. So, it's enough to consider the value 0.032911422 for the constant.

The error of choosing h_x

In order to compute the error we will use the Runge rule. We can assume that Z_h=3.55 and Z_{2h}=3.65 for the spot size. The error can be written as

$$R = \frac{Z_h - Z_{2h}}{3} = 0.033333333$$

which is small if we compare it to the FWHM= 3.65. We can do the same for the focal distance f if Z_h=1.2539093, Z_{2h}=1.2528818, then

$$R = \frac{Z_h - Z_{2h}}{3} = 0.0003425$$

which is very small if you compare it to 1.2528818. From the last investigations we can say that the best choice for the constant in the relation

$$h_x = constant \times \frac{\omega_0}{c_0} h_r^2$$

is 0.032911422 which is equivalent to $h_x = 0.000001562$.

7.1.2 The space step inside the lens

Now, after getting the best choice for $h_x = 0.000001562$ which is corresponding to the constant 0.032911422 in the relation

$$h_x = constant \times \frac{\omega_0}{c_0} h_r^2$$

We need to choose the space step inside the lens h_{lens} that will give us small error according to Runge rule for the spot size, and for the focal distance. We fix here the number of points to be 40000 which means that $h_r = 0.000000025$. We have seen from the

h_{lens}	focal distance	FWHM
0.000001	1.2528818m	3.65μm
0.0000005	1.2492204m	3.90μm
0.00000025	1.2483004m	3.95μm
0.000000125	1.2480707m	3.95μm

Table 2: The choice of h_{lens}

dispersion relation for the propagation inside the lens that the following conditions have to be satisfied

$$h_{lens} << \frac{w_0 h_r^2}{c_0}$$

And

$$h_{lens} <<< \frac{1}{\mid B \mid}$$

$\frac{1}{|B|} = 5.4533 * 10^{-6}$. Table(2) gives us different values for h_{lens} with the corresponding spot size, and focal distance. As you can see that the best choice for h_{lens} is 0.000000125 that will give us small error according to (Runge rule).

7.1.3 The choice of h_r

Now, we will try to find the best choice for the space step in y, and z direction h_r I mean to find the suitable number of points in y, and z direction we do that by changing the number of points and try to prove that the results don't depend on the number of points. We fixed here the space step inside the lens $h_{lens} = 0.000000125$, and the best choice for the constant to obtain h_x from the relation

$$h_x = constant \times \frac{\omega_0}{c_0} h_r^2$$

which is equivalent to 0.000001562 for 40000 points, and 0.000001 for 50000 Table(3). Due to the large number of lenses, we need to consider more points we started with 40000 points, and checked 50000 points. The results for 40000, and 50000 points are very close

Number of points	constant	h_r	h_x	focal distance	FWHM
40000	0.032911422	0.000000025	0.000001562	1.2480707m	3.95μm
50000	0.032911422	0.00000002	0.000001	1.2470340m	3.92μm

Table 3: The choice of h_r

for the focal distance, and for the FWHM. We could take more points which means smaller h_r, and h_x. But, we use here the implicit Runge Kutta method of the second order it means that we need to take 80000 points as the next step after 40000 not 50000. Because of the limitations in the computer we will consider only 50000 points. We can say that as a starting point, it's enough to consider 50000 points. In the future we must try with more points using supercomputers, and also for the 2-d case. In other words, the suitable choice of h_r will be 0.00000002.

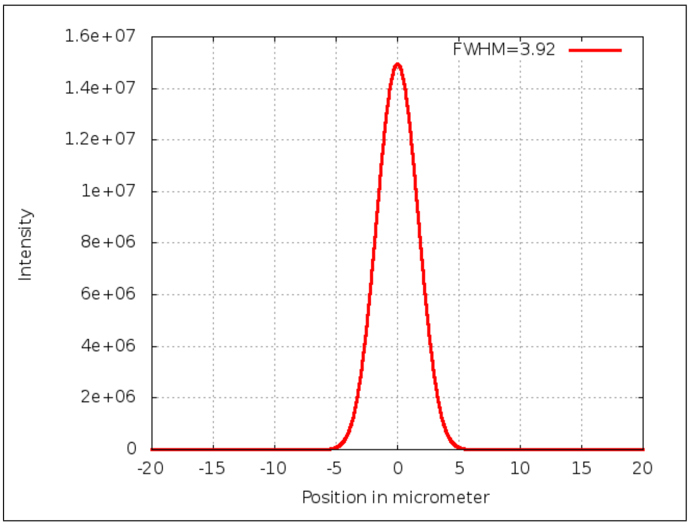
8 Comparing the results

Results for ideal lenses

We have obtained the best choice for the space steps h_x, h_{lens} and h_r which corresponding to using 50000 points. Our results give focal distance f=1.2470340m, and FWHM= 3.92μm at 1.298m from the CRLs Figure(5). We considered ideal lenses without any defects that's the main reason for having smaller FWHM than the experimental data. We considered only the 1-dim case for the horizontal direction while in the experimental data you will see the horizontal, and vertical results Figure(6). In the following comparison, we used all the data in [1] with the smallest width of the lens d=16μm, while in the previous plots we used 100μm it's just to compare the results with the experimental data. Table(4) gives us the comparison between our results, and the experimental data. The results show that we have a good agreement with the experimental data for the focal distance, and for the intensity at the focal plane, while in case of the FWHM we have a smaller FWHM. We believe that is perhaps because of the ideal CRLs that we use, and the fixed frequency.

Item	focal distance	Detector	FWHM(Horizontal scale)
Our results(perfect lenses)	1.2470340m	1.298m	3.92μm
Experimental data	1.2553036m	1.298$\pm$0.04m	14.0μm

Table 4: Comparing the Results



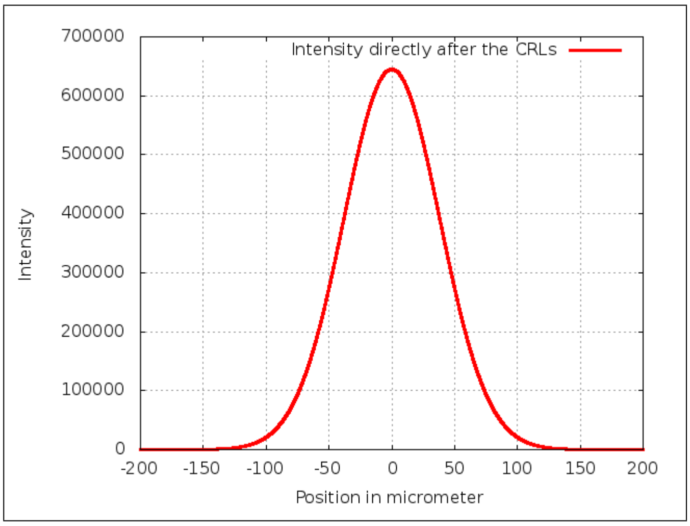


Figure 5: Results for focusing hard X-rays with 33 perfect Al CRLs directly after the lenses, and at 1.298m from the lenses

9 Two dimensional simulation

In this section we perform simulation for the 2-dimensional case. We obtained from the last section that we need to consider more than 50000 points in each direction in order to get the accurate results, which makes it difficult to make 2-d simulation for the first case using the P.C. In this section, we just wanted to test the program for getting results in 2-d. We perform simulations here with few number of lenses up to 15 lenses made of AL. We use the same parameters as in the first case but, we considered here the initial condition to be one everywhere. Figure(7), and Figure(8) give us the results directly after the lenses. When we increase the number of lenses, the maximum value of the intensity

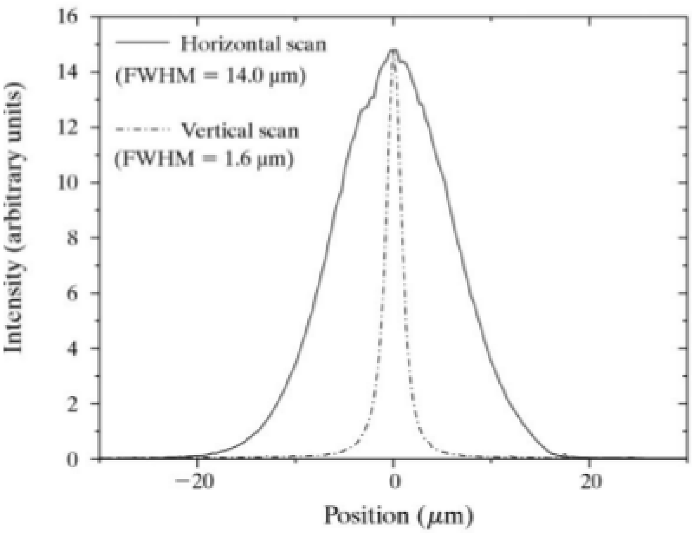


Figure 6: Experimental data for the horizontal and vertical direction [1]

decreases that's because the absorption will increase with the number of lenses.

10 Conclusion

We presented here a new numerical method based on the finite-difference method to focus X-rays using the CRLs. We solve the wave equation inside, and outside the lenses using the FDM, and implicit Runge Kutta method of second order with iterative method. The program written in FORTRAN to compute the focal distance, and the spot size. We considered here two cases with the same shape of the lenses as in [1]. The first case we considered 33 AL lenses with 15Kev, we have good agreement with the experimental data for the focal distance, for the intensity at the focal plane while in case of the FWHM we have a smaller FWHM. We believe that is perhaps because of the ideal CRLs that we use, and the fixed frequency. The results showed that we need to use more than 50000 points in each direction that forced us to perform only one dimensional simulation. For the same number of lenses time of calculation increase 16 times when quantity of points in each

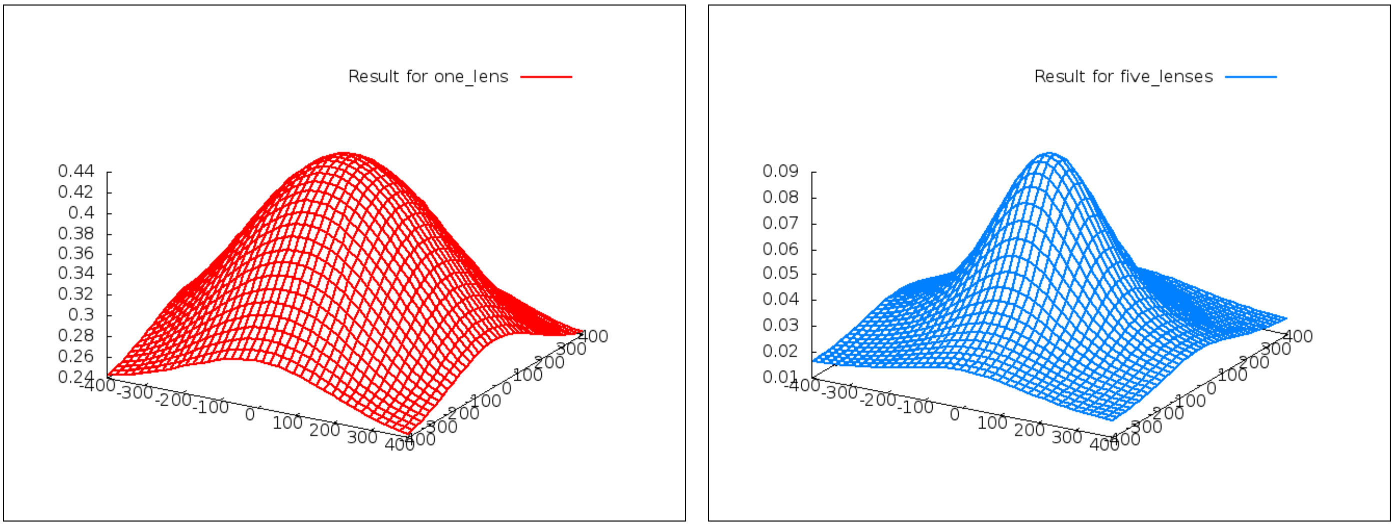


Figure 7: Two dimensional results for 1 lens, and 5 lenses

direction increases two times, that's because of the condition $h_x << \frac{\omega_0 {h_r}^2}{c_0}$. It means that if we compare a system of 100×100 points with system of 1000×1000 for such number of lenses we need to do 10000 times more operation than in the first case. The maximum quantity of complex points which could be calculated nowadays on a personal computer is about 5000 × 5000 to 10000× 10000. So, the program should properly optimized and paralyzed to perform the 2-d simulation using the supercomputer. In the second case, we tested the program for a small number of lenses up to 15 lenses made of AL. In the future, we will try to add some defects to the lenses, and check the influence of the defects on the spot size, and on the focal distance.

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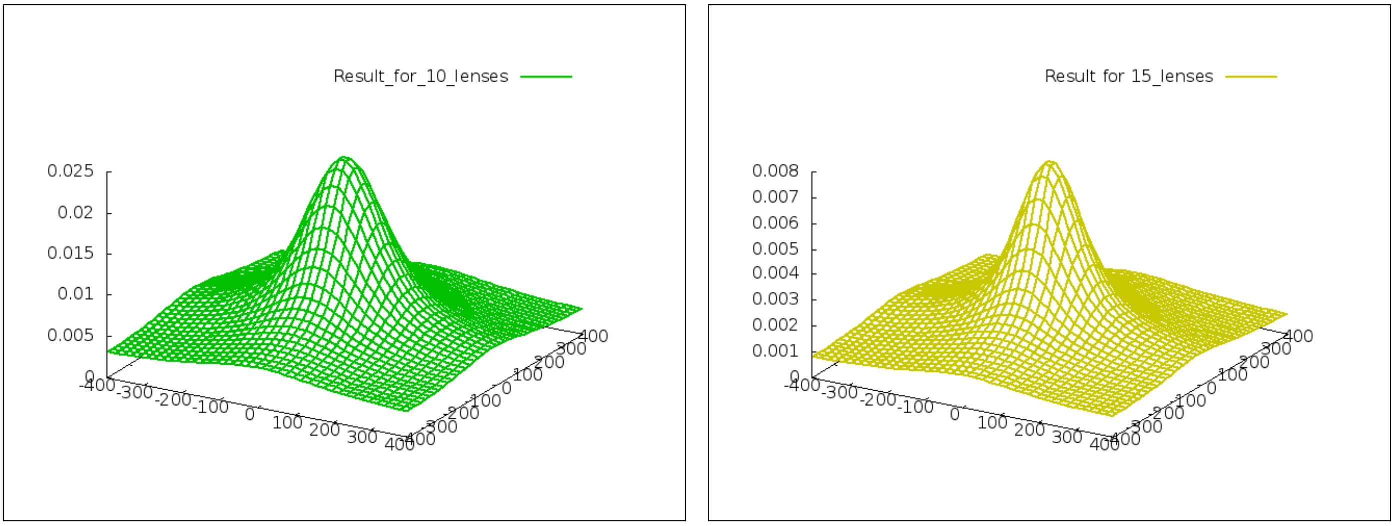

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