

Report
Numerical Simulation of Beam Propagation
including Error Convergence Analysis

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1 Introduction

Beam propagation in media is of high interest for scientists and also for industrial purposes. In this report beam propagation will be simulated, problems will be discussed. The purpose of the project is to compare numerical method and analytical solution. Convergence of used numerical method is to be shown. For the simplicity simulation of beam propagation is done in free space, linear medium, at zero angle of incidence, so to fit the scope of mini-project, later on can be extended to more sophisticated cases.

1.1 Analytical solution

To get better analytical understanding of beam propagation in space one should solve Helmholtz Equation

$$(\nabla^2 + k^2)E = 0.$$

This equation generally holds for electromagnetic wave, hence for electric and magnetic field components, for simplicity electric field E is chosen. Here k is wave number and is equal to $2\pi n/\lambda$, where λ is wavelength, n is refractive index of the medium (here it is assumed to be equal to 1). As assumption, propagation of the wave in z direction can be considered, electric field can be represented in next form

$$E(x, y, z) = u(x, y, z)e^{-ik_o z},$$

where u is complex function which describes non-plane part of the beam. Substitution of the ansatz into Helmholtz equation in cartesian coordinates and some simplifications give

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} - 2ik_o \frac{\partial u}{\partial z} + (k^2 - k_o^2)u = 0.$$

Using paraxial approximation it is easy to see that third term is smaller than others, therefore can be neglected, as result following equation is obtained.

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} - 2ik_o \frac{\partial u}{\partial z} + (k^2 - k_o^2)u = 0. \quad (1)$$

Solving this differential equation u is found, hence E can be found as well. It is assumed that $k = k_o$, solution for two dimensional case where wave propagates in z -direction and oscillates in xz plane becomes

$$E(x, z) = E_o \left(\frac{w_o}{w(z)} \right)^{\frac{1}{2}} \exp\left(\frac{x^2}{w(z)^2} \right) \exp\left(-i \left(k_o z + k_o \frac{x^2}{2R(z)} - \phi(z) \right) \right), \quad (2)$$

where $w(z)$ is beam radius, $w_o = w(0)$ is beam waist, E_o is electric field amplitude, $R(z)$ is beam curvature, ϕ is Gouy phase. Their explicit mathematical meanings can be found in the Table 1. This electric field formula later will be compared to numerical solution. From here intensity can be calculated, $I = \frac{\epsilon_o c n_o}{2} |E_z|^2$ [1]. Implementation of analytical solution can be found in Appendix A.

Beam Radius	Beam Curvature	Gouy phase
$w(z) = w_o \sqrt{1 + \left(\frac{z\lambda}{\pi w_o^2}\right)^2}$	$R = z \left[1 + \left(\frac{\pi w_o^2}{z\lambda}\right)^2\right]$	$\phi(z) = \arctan\left(\frac{z\lambda}{\pi w_o^2}\right)$

Table 1: Auxiliary formulas to equation 2.

1.2 Numerical solution

For one dimensional case Equation 1 can be rewritten in the following form

$$2ik_o \frac{\partial u}{\partial z} = \frac{\partial^2 u}{\partial x^2} + (k^2 - k_o^2)u. \quad (3)$$

To simulate light beam propagation Beam Propagation Method (BPM) is used. BMP is a discretization of differential equation (3), equation should be discretized for z-component and x-component. For beginning let's do discretization only for z component, equation will get following form.

$$2ik_o \frac{u^{l+1} - u^l}{\Delta z} = \frac{\partial^2 u^l}{\partial x^2} + (k^2 - k_o^2)u^l.$$

Superscript l denotes the order of grid points in z-direction. This finite difference scheme is known as **forward difference**. However after discretization of x-component numerical instability can be seen. There is another alternative where order of grid point is taken one step in advance, this method is called **backward difference**

$$2ik_o \frac{u^{l+1} - u^l}{\Delta z} = \frac{\partial^2 u^{l+1}}{\partial x^2} + (k^2 - k_o^2)u^{l+1}.$$

Neither this scheme shows good stability, however the combination of these two solves instability problem. These method is called **Crank-Nicolson** method

$$2ik_o \frac{u^{l+1} - u^l}{\Delta z} = (1 - \alpha) \frac{\partial^2 u^l}{\partial x^2} + (1 - \alpha)(k^2 - k_o^2)u^l + \alpha \frac{\partial^2 u^{l+1}}{\partial x^2} + \alpha(k^2 - k_o^2)u^{l+1},$$

α here shows contribution of the particular difference. Usually α is set to $1/2$, which means that forward and backward difference contribute equally. Then Crank-Nicolson scheme gets next form

$$2ik_o \frac{u^{l+1} - u^l}{\Delta z} = \frac{1}{2} \left(\frac{\partial^2 u^l}{\partial x^2} + (k^2 - k_o^2)u^l \right) + \frac{1}{2} \left(\frac{\partial^2 u^{l+1}}{\partial x^2} + (k^2 - k_o^2)u^{l+1} \right).$$

Now discretization of x-component can be performed.

$$\begin{aligned} 2ik_o \frac{u_j^{l+1} - u_j^l}{\Delta z} &= \frac{1}{2} \left(\frac{u_{j-1}^l - 2u_j^l + u_{j+1}^l}{\Delta x^2} + (k^2 - k_o^2)u_j^l \right) + \\ &\quad \frac{1}{2} \left(\frac{u_{j-1}^{l+1} - 2u_j^{l+1} + u_{j+1}^{l+1}}{\Delta x^2} + (k^2 - k_o^2)u_j^{l+1} \right) \end{aligned}$$

j subscript denotes the order of grid points in x-direction. Such discretization can be rewritten and later solved using tridiagonal matrix algorithm or so called **Thomas algorithm**

$$2ik_o \frac{u^{l+1} - u^l}{\Delta z} = \frac{1}{2} \left(L_h u^l + L_h u^{l+1} \right).$$

L_h is spacial discretization operator for one dimensional case and is numerically defined in Thomas algorithm as

$$L_h = \frac{1}{\Delta x^2} \begin{bmatrix} -2 + (k^2 - k_o^2)\Delta x^2 & 1 & 0 & \dots & 0 \\ 1 & -2 + (k^2 - k_o^2)\Delta x^2 & 1 & \dots & 0 \\ 0 & 1 & -2 + (k^2 - k_o^2)\Delta x^2 & 0 & \vdots \\ \vdots & \vdots & \vdots & \dots & \vdots \\ 0 & 0 & 0 & -2 + (k^2 - k_o^2)\Delta x^2 & \end{bmatrix}.$$

After trivial simple mathematical rearrangement previous equation can be written in the following form

$$u^{l+1} = \left(I - \frac{\Delta z}{4ik_o} L_h \right)^{-1} \left(I + \frac{\Delta z}{4ik_o} L_h \right) u^l.$$

Here I is identity matrix, which has the same size as tridiagonal matrix L . Notice that this is iterative process, in particular case is initialized at $u^{l=0}$ or $z = 0$ to Gaussian function, in another words $u(x, z = 0) = E_o \exp(-\frac{x^2}{w_o^2})$ [2, 3]. Implementation of numerical solution can be found in Appendix B.

1.2.1 Absorbing Boundary Condition

During numerical method implementation, wave approaching boundary will be reflected, this happens due to the nature of numerical algorithm. Physically this can be interpreted as a presence of mirror at the boundary. Reflection at the boundaries can be decreased or completely prevented applying grid truncation techniques. One of the most popular grid truncation techniques is introduction of absorption, such technique is called absorbing boundary condition(ABC). One such way is to add a complex part to refractive index, refractive index becomes $\tilde{n} = n + ik$. k is absorption index, it should vary gradually, slowly, since fast increase can again cause reflection. Absorption index is designed to have parabolic increase and can be expressed in following way

$$\kappa(x) = \kappa_{max} \left(\frac{x - l/2 + \delta}{\delta} \right)^2, x \in \left[\frac{l}{2}, \frac{l}{2} - \delta \right],$$

$$\kappa(x) = \kappa_{max} \left(\frac{l/2 + \delta - x}{\delta} \right)^2, x \in \left[-\frac{l}{2} + \delta, -\frac{l}{2} \right].$$

Here, κ_{max} is maximum value of absorption index to which absorption index as function of x can increase, l is the width of computational domain, in examined case will be corresponded to range of x , δ is a part of total width where absorption takes place, geometry of introduced absorption can be seen in Figure 1. It is important to notice that ABC do not change along z -direction. The function $\kappa(x)$ is show in Figure 1[2].

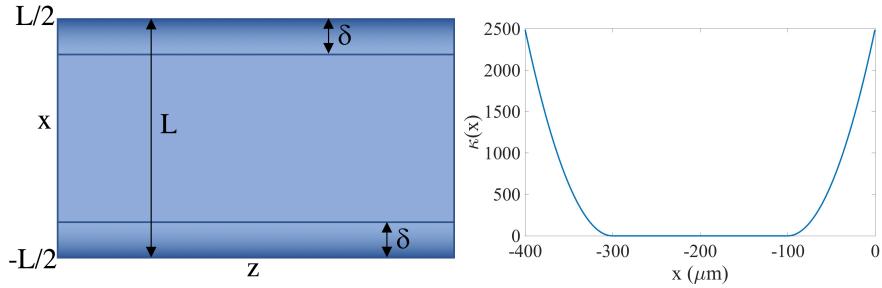


Figure 1: Absorption boundary, figure on the right shows the geometry of absorption boundary, appropriate δ can be chosen during simulation time, figure on the left shows function absorption index $\kappa(x)$ and its change along x-direction.

1.2.2 Error convergence

In order to assess the accuracy of the numerical method, error is calculated. Error is a difference between numerical and analytical electric field and can be calculated using different norms. There is a fixed relation between number of grid points and total error, if one increases the number of grid points, error is expected to decrease. If number of grid points is increased 2^n times, error should increase 2^{-n} times, n is integer number which also tells about order of error convergence.

$$\|Error\|_2 = \frac{1}{\text{Number of grid points}} \sqrt{\sum_{i=1}^n (E_z \text{ numerical} - E_z \text{ analytic})^2}$$

$$\|Error\|_\infty = (E_z \text{ numerical} - E_z \text{ analytic})_{\text{maximum}}$$

$\|Error\|_{\text{at particular point}} = \text{Error at any particular physical point is recorded}$

2 Results

Numerical algorithm and analytical solution were both implemented and compared, results can be seen in Figure 2. First row depicts Crank-Nicolson numerical method, second row shows analytical solution, first and second columns show real component of electric field and intensity of light consequently. Parameters of laser beam in considered case are: z-meshsize = x-meshsize = 1 μm , wavelength (λ) = 20 μm , waist (w_o) = 30 μm , refractive index (n_o) = 1.

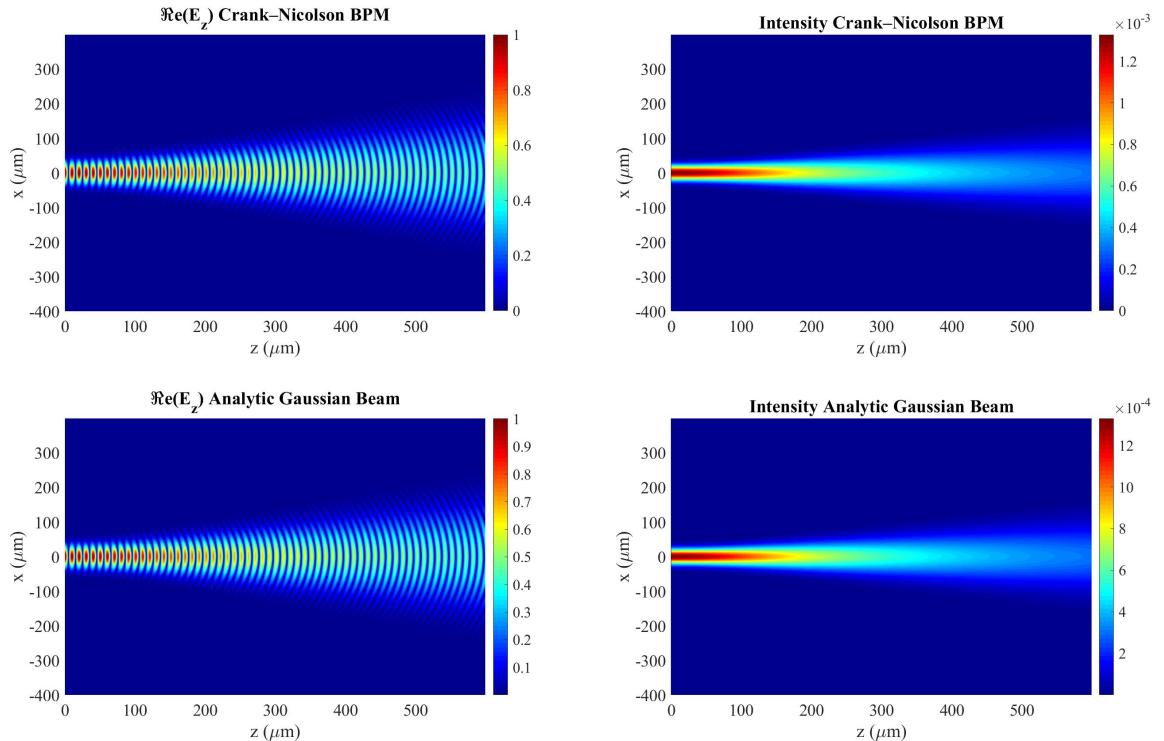


Figure 2: Comparison of Crank-Nicolson BPM and analytical solution.

2.1 Absorption Boundary Condition

In this section the results of applied ABC are shown. In Figure 3 the necessity of applying ABC can be seen. In the figure on the left no ABC is applied, as result reflection occurs on the boundary on the top and bottom. Reflection causes interference effect, which can be observed. In the figure on the right ABC is applied. Gradual absorption of electric wave can be observed, also wave doesn't reach the boundary.

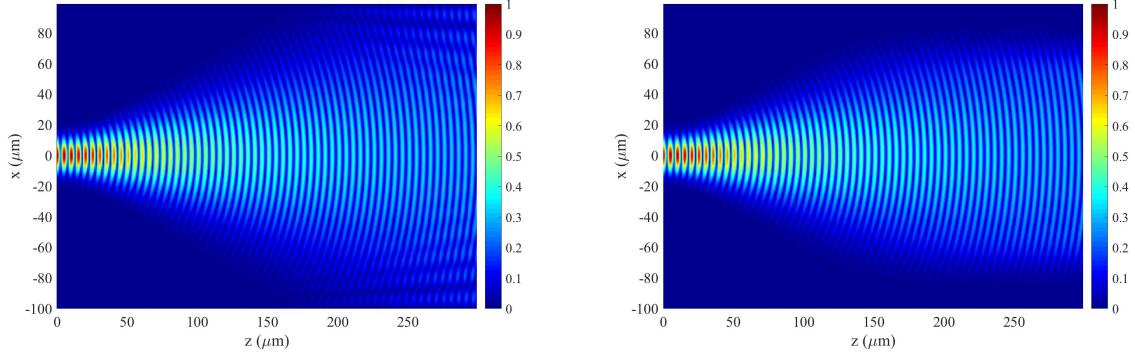
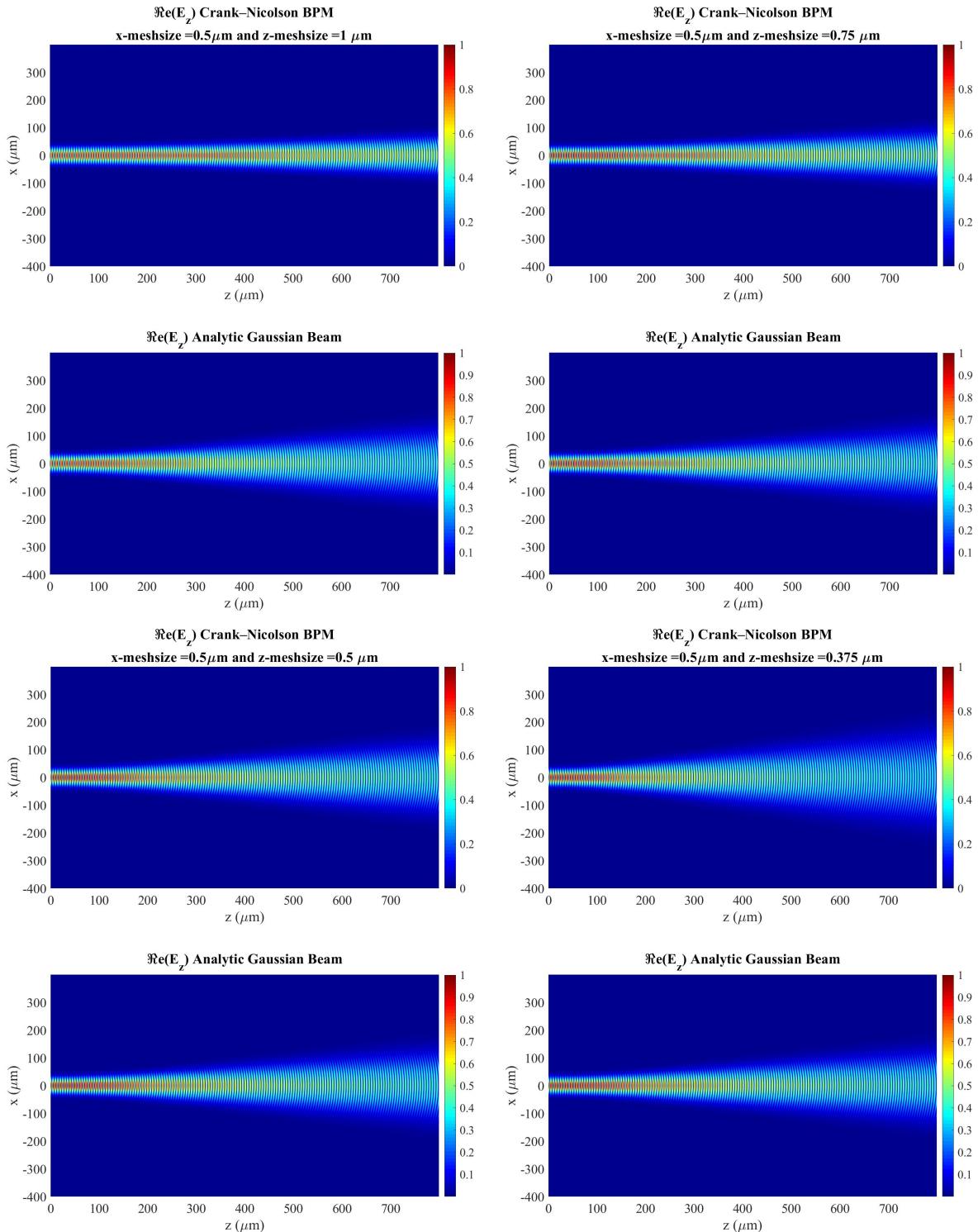


Figure 3: Propagation of electric field. On the left implementation of numerical method without ABC, on the right with ABC. Parameters used: z-meshsize = x-meshsize = $1 \mu m$, wavelength (λ) = $10 \mu m$, waist (w_o) = $10 \mu m$, refractive index (n_o) = 1. For ABC simulation $\kappa_{max} = 0.0013$, $\delta = 50 \mu m$, $l = 200 \mu m$.

2.2 X and Z direction meshsize relation

In this section research on how x-meshsize and z-meshsize relation affects simulation is made. In Figure 4 change of z-meshsize changes the result of numerical approach. At the point where z-meshsize is equal to x-meshsize numerical method has the best similarity to analytical solution. As result, one can conclude that once x-meshsize changes, z-meshsize should be changed too and furthermore z-meshsize should be set to the same value as x-meshsize. In the Figure below parameters are: x-meshsize = $0.5 \mu m$ is kept constant, wavelength (λ) = $10 \mu m$, waist (w_o) = $25 \mu m$, refractive index (n_o) = 1, z-meshsize = 1, 0.75, 0.5, 0.375, 0.25 μm .



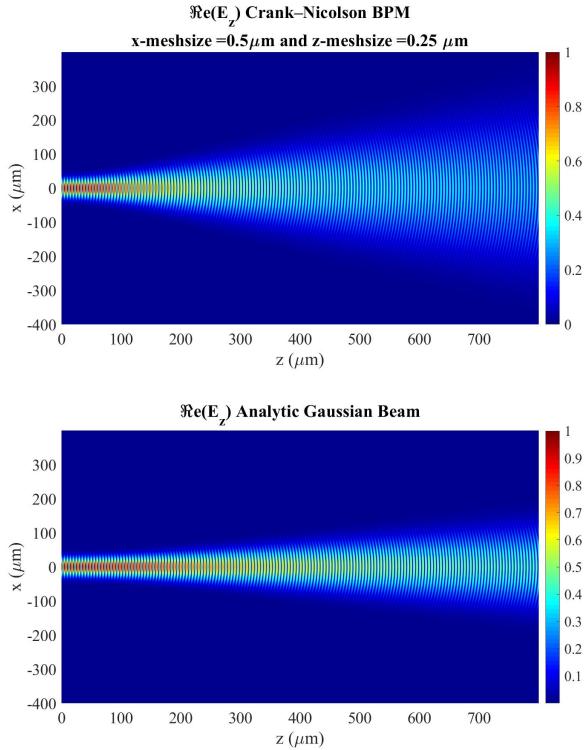


Figure 4: Numerically computed electric field at different relation of x-meshsize and y-meshsize compared to analytical solution.

2.3 Error convergence

In this section error convergence is calculated as described in section 1.2.2, plots are presented in Figure 5 and results in Table 2. From the table it is seen that if number of grid points increases twice, L_2 norm error decreases thrice, L_∞ decreases twice and so on. Also figure shows that error has steady behavior in logarithmic scale. This convergence is reached at following parameters: wavelength (λ) = 10 μm , waist (w_o) = 25 μm , refractive index (n_o) = 1, z-meshsize = x-meshsize = {2, $\sqrt{2}$, 1, $0.5\sqrt{2}$, 0.5, $0.25\sqrt{2}$, 0.25} μm .

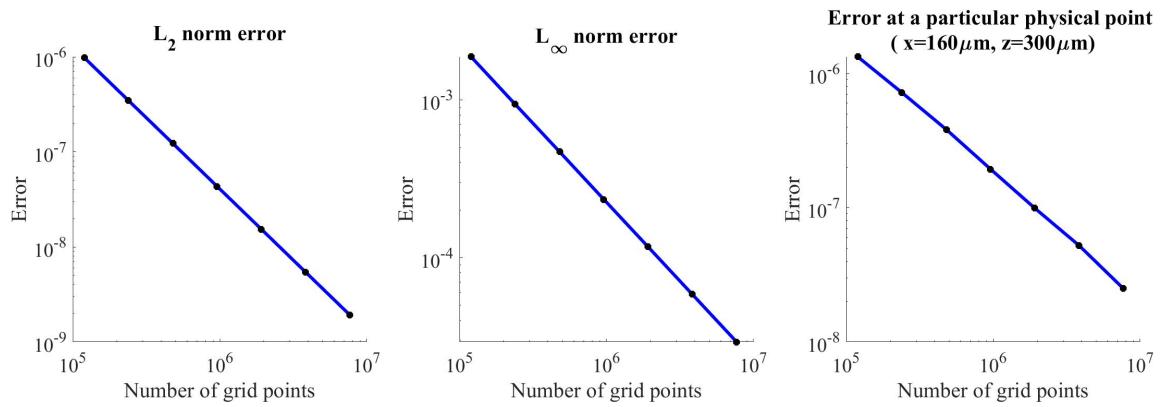


Figure 5: L_2 , L_∞ errors and error at a particular point.

Number of Grid points	1	2	4	8	16	32	64	increase 2x
L_2 norm error	1	0.3546	0.1254	0.0443	0.0156	0.0055	0.0019	decrease 3x
L_∞ norm error	1	0.5001	0.2503	0.1250	0.0625	0.0312	0.0156	decrease 2x
Error at a point	1	0.5410	0.2874	0.1457	0.0745	0.0393	0.0188	decrease 2x

Table 2: Dependence of error change on number of grid points

3 Conclusion

In this report Crank-Nicolson algorithm for BPM is used to simulate Gaussian beam propagation. Results show high resemblance between analytic solution and beam propagation method. In the case when beam propagates in the direction of upper or lower boundary, absorption boundary condition method should be used to compensate the reflection. However the ABC used here has drawbacks, extension of simulated propagation distance introduces reflections and hence interference effects. Their contribution increases as computational distance increases, in [2] another methods of ABC are described. Also in order to keep physical domain same, computational domain should be increased. Dependence of x-meshsize and z-meshsize is revealed, this relation is important for further simulation and gives good understanding on how parameters should be initialized.

References

- [1] *Chapter 2 Gaussian Beam Propagation.*
<http://www.phys.ncku.edu.tw/~cctsai/teaching/10202/gaussian>
- [2] G. L. Pedrola, *Beam Propagation Method for Design of Optical Waveguide Devices.* John Wiley & Sons, 2015.
- [3] P. D. C. Pflaum, *Script: Computational Optics SS 2017.* FAU, 2017.

Appendix A: Implementation of analytical method

```
//INITIALIZATION

// x-coordinate which specifies computational range in micrometers.
x0 = 400
// meshsize in x-direction in micrometers.
x_mesh = 1
// vector which contains x values in micrometers from -x0 to x0 with
step x_mesh.
x = from -x0 to x0 with step x_mesh.
// number of grid points in x-direction.
Nx = length(x)
// z-coordinate which specifies computational range in micrometers.
zend = 800
// meshsize in z-direction in micrometers.
z_mesh = x_mesh
// vector which contains z values in micrometers from 0 to zend with
step z_mesh.
z = from 0 to zend with step z_mesh
// number of grid points in z-direction.
Nz = length(z)
// waist in micrometers.
wo = 30
// width in micrometers.
w = 0
// curvature in micrometers.
r = 0
// Gouy phase.
gouy_phase = 0
// wavelength in micrometers.
lambda = 10
// Rayleigh length in micrometers.
zR = pi*wo^2/lambda;
// refractive index of air in vacuum.
no = 1
// spacial frequency with no.
ko = 2*pi*no/lambda
// Electric field.
E = zeros(Nx,Nz)
// Electric field amplitude.
Eo = 1
// 2 dimensional matrix with Nx*Nz size, spacial component of electric
field, 2-dimensional grid.
```

```

// CORE ALGORITHM

// Electric field.
for i from 1 to Nz
    w = wo*sqrt(1+(z(i)/zR).^2);
    r = z(i)+(zR^2/z(i));
    gouy_phase = atan(z(i)/zR);
    E(i_column) = Eo*(wo/w)^0.5.*exp(-(x^2)/w^2) ...
                  *exp(1j*(k*z(i)+k*(x^2)/(2*r)-gouy_phase))
end for

```

Appendix B: Implementation of Crank-Nicolson method

```
// INITIALIZATION

// x-coordinate which specifies computational range in micrometers.
x0 = 400
// meshsize in x-direction in micrometers.
x_mesh = 1
// vector which contains x values in micrometers from -x0 to x0 with
step x_mesh.
x = from -x0 to x0 with step x_mesh.
// number of grid points in x-direction.
Nx = length(x)

// z-coordinate which specifies computational range in micrometers.
zend = 800
// meshsize in z-direction in micrometers.
z_mesh = x_mesh
// vector which contains z values in micrometers from 0 to zend with
step z_mesh.
z = from 0 to zend with step z_mesh
// number of grid points in z-direction.
Nz = length(z)
// waist in micrometers.
wo = 30
// wavelength in micrometers.
lambda = 10
// refractive index of air in vacuum.
no = 1
// spacial frequency with no.
ko = 2*pi*no/lambda
// refractive index of medium.
n = 1
// spacial frequency with n.
k = 2*pi*n/lambda

// 2 dimensional matrix with Nx*Nz size, complete electric field, 2-dimensional
grid.
E = zeros(Nx,Nz)
// 2 dimensional matrix with Nx*Nz size, spacial component of electric
field, 2-dimensional grid.
u = zeros(Nx,Nz)
// 2 dimensional matrix with Nx*Nz size, periodic component of electric
field in z direction, 2-dimensional grid.
f = zeros(Nx,Nz)
// 2 dimensional matrix with Nx*Nx size, tridiagonal matrix or Thomas
algorithm (see section 1.2).
L = zeros(Nx,Nx)
```

```

// 2 dimensional matrix with Nx*Nx size, identity matrix used in Thomas
algorithm.
I = eye(Nx,Nx)

// set first column of u to gaussian.
u(first_column) = exp(-(x/w0)^2)

// CORE ALGORITHM

// L matrix computation.
for i from 1 to Nx
    L(i,i) = 1/x_mesh^2*(-2+(ko^2-k^2)*x_mesh^2)
    if i>1
        L(i,i-1)=1/x_mesh^2
        L(i-1,i)=1/x_mesh^2
    end if
end for

// Spacial component of electric field computation.
for i_column from 2 to Nz
    u(i_column) = MatrixInverse(I-x_mesh*L/(4*1j*ko))*...
                  (E+x_mesh*L/(4*1j*ko))*u(i_column-1)
end for

// Periodic component of electric field in z direction computation.
for i_column from 1 to Nz
    f(i_column) = exp(-1j*ko*z(i_column))
end for

// Complete Electric field.
E = Elementwise_multiplication(u,f)

```