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DEVELOPMENT OF SOFTWARE FOR INTERFERENCE AND OPTICAL DIFFRACTION ANALYSIS BASED ON FDTD

Jorge Francés[1], Manuel Perez-Molina[1], Elena Fernandez[2], Cristian Neipp[1]
jfmonllor@ua.es manuelpm@ua.es elena.fernandez@ua.es cristian@dfists.ua.es

[1]Departamento de Física, Ingeniería de Sistemas y Teoría de la Señal
Escuela Politécnica Superior
Universidad de Alicante
Ctra San Vicente del Raspeig S/N CP:03690
Alicante (España)

[2]Departamento de Óptica, Farmacología y Anatomía
Escuela Universitaria de Óptica y Optometría
Universidad de Alicante
Ctra San Vicente del Raspeig S/N CP:03690
Alicante (España)

Abstract. The Finite-Difference Time-Domain method has been applied to microwaves with successfully results. This method has not frequently been applied in optical engineering due to the disadvantages due to optical wavelengths. In this work, FDTD method has been used for simulating elemental optical systems. Interference and diffraction of light is an elementary topic in optics. The aim of this work is to develop an accurate simulation software of optical systems avoiding the problems in laboratories and the expensive price of optical instrumentation.

In this work, four elementary systems have been implemented: one thin slit, two thin slit known as the Young's experiment, an array of seven thin slits and finally a circular aperture. In real laboratory, a coherent light source would illuminate these systems and diffraction pattern of bright and dark bands could be analyzed on a screen.

The FDTD method solves the differential Maxwell equations, substituting the time and spatial derivates with central-difference approximation. In order to achieve successfully results with FDTD method, absorbing boundary conditions (ABC), total and scattered field (TF-SF) formulation and near-to-far field propagation have been implemented. These techniques have permitted to calculate the wave field outside the simulation grid (in a screen far away slits), reducing the simulation area to the slits plane. The numerical results calculated with FDTD method are contrasted with analytical results obtaining quite similar curves.

The use of this software in practical laboratory seasons in optical degrees can provide to student the possibility of simulating many optical systems based on thin slits. Irradiance distribution can be evaluated with successfully results in different planes far away of grid simulation without performance detriment.

1 INTRODUCTION. In education, visual experiments are important for improving student knowledge. In optic's area, laboratory sessions have an important role. Frequently, in this type of sessions, students have to use different instruments such as laser, analyzers, detectors, etc…. All these instruments usually are very expensive and in many cases are no correctly handled. In this work a software has been developed in order to simulate many optical experiments such as Young's double slit experiment, diffraction gratings and circular slit. These experiments are focused on demonstrating interference and the wave nature of light. The light diffracts from these slits and illuminates a viewing screen at a large distance compared to the slits separation. The software based in Finite-difference Time-Domain Method (FDTD) is a direct solution method for Maxwell's time-dependent curl equations. With this method, the electromagnetic fields can be calculated as a function of time and space, providing the students the possibility to analyze how the light diffracts from the slits or other type of experiments related to electromagnetic wave propagation. Using the software in the first years of optical or physics degrees may give the students the opportunity of evaluating many experiments related to optical systems with an easy and accurate software, and without using expensive instrumentation. This software is structured in an API based on MATLAB that modifies C++ libraries. These source files are compiled in UNIX based operative systems. Plots of the result and values are shown by a MATLAB interface taking the values from the results files obtained via C++ processing. The helpful interface and the accurate results make this software an attractive and useful complement for students education.

2 THEORY. In this section, The theory under the FDTD method is explained. This method is based on volumetric sampling of the unknown near-field distribution ($\vec{E}$ and $\vec{H}$) within and surrounding the structure of interest, and over a period of time. The sampling in space is at sub λ_0 resolution set by the user to properly sample, in the Nyquist sense, the highest near-field spatial frequencies thought to be important in the physics of the problem. Typically, 10 to 20 samples per wavelength are needed. The sampling in time is selected to ensure numerical stability of the algorithm as could be seen in (12). Due to the fact that optical wavelengths are in the range of nanometers, wide nets must be processed to obtain wave fields in a screen far away from the optical source. In order to simulate the experiments with low time cost processing, different formulation have been added to the FDTD method that solves many problems related with this type of formalism.

1.1 FDTD basic formulation. Yee [3] introduced the notation for space points and functions of space and time in a rectangular lattice as

$$(i, j, k) = (i\Delta x, j\Delta y, k\Delta z). \tag{1}$$

Here, Δx, Δy and Δz are respectively, the lattice space increments in the x, y and z coordinate directions, and i, j and k are integers. Further, we denote any function u of space and time evaluated at a discrete point in the grid and at a discrete point in time as

$$u(i\Delta x, j\Delta y, k\Delta z) = u\big|_{i,j,k}^{n}, \tag{2}$$

Where Δt is the time increment, assumed uniform over the observation interval, and n is an integer.

Yee used centered finite-difference (central-difference) expressions for the space and time derivates. The first partial derivate of u in the x-direction, evaluated at the fixed time $t_n = n\Delta t$, and the time partial derivate of u, evaluated at the fixed space (i, j, k) can be expressed as follows

$$\frac{\partial u}{\partial x}(i\Delta x, j\Delta y, k\Delta z) = \frac{u\big|_{i+1/2,j,k}^{n} - u\big|_{i-1/2,j,k}^{n}}{\Delta x} + O[(\Delta x)^2], \tag{3}$$

$$\frac{\partial u}{\partial t}(i\Delta x, j\Delta y, k\Delta z) = \frac{u\big|_{i,j,k}^{n+1/2} - u\big|_{i,j,k}^{n-1/2}}{\Delta t} + O[(\Delta t)^2]. \tag{4}$$

The $n+1/2$ notation is used to interleave $\vec{E}$ and $\vec{H}$ components in time at intervals $1/2\Delta t$ for purposes of implementing a leapfrog algorithm. The time-dependent Maxwell's curl equations in free space are

$$\frac{\partial \vec{D}}{\partial t} = \frac{1}{\sqrt{\varepsilon_0 \mu_0}} \nabla \times \vec{H}, \tag{5}$$

$$\vec{D} = \varepsilon_r \vec{E}, \tag{6}$$

$$\frac{\partial \vec{H}}{\partial t} = -\frac{1}{\sqrt{\varepsilon_0 \mu_0}} \nabla \times \vec{E}. \tag{7}$$

Where $\vec{D}$ is the electric flux density, μ_0 is the magnetic permeability in henrys per meter and ε_0 is the electric permittivity in farads per meter. The ideas showed above (3,4) can be applied to obtain a numerical approximation of Maxwell's curl equations in three dimensions. We will use only the z-component of $\vec{D}$ and the x-component $\vec{H}$ field as examples. From (5) and (7) we can obtain the following expressions:

$$\frac{\partial D_z}{\partial t} = \frac{1}{\sqrt{\varepsilon_0 \mu_0}} \left(\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} \right), \tag{8}$$

$$\frac{\partial H_x}{\partial t} = \frac{1}{\sqrt{\varepsilon_0 \mu_0}} \left(\frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial y} \right). \tag{9}$$

The first step is to take the finite difference approximations to (8) and (9):

$$D_z\Big|_{i,j,k+1/2}^{n+1/2} = D_z\Big|_{i,j,k+1/2}^{n-1/2} + \frac{\Delta t}{\Delta x \sqrt{\varepsilon_0 \mu_0}} \begin{pmatrix} H_y\Big|_{i+1/2,j,k+1/2}^{n} - H_y\Big|_{i-1/2,j,k+1/2}^{n} \\ -H_x\Big|_{i,j+1/2,k+1/2}^{n} + H_x\Big|_{i,j-1/2,k+1/2}^{n} \end{pmatrix}, \tag{10}$$

$$H_x\Big|_{i,j+1/2,k+1/2}^{n+1/2} = H_x\Big|_{i,j+1/2,k+1/2}^{n-1/2} + \frac{\Delta t}{\Delta x \sqrt{\varepsilon_0 \mu_0}} \begin{pmatrix} E_y\Big|_{i,j+1/2,k+1}^{n} - E_y\Big|_{i,j+1/2,k}^{n} \\ -E_z\Big|_{i,j+1,k+1/2}^{n} + E_z\Big|_{i,j,k+1/2}^{n} \end{pmatrix}. \tag{11}$$

Note that the $\vec{E}$ and $\vec{H}$ fields are assumed interleaved around a cell whose origin is at the location (i, j, k). A cubic cell is assumed $(\Delta x = \Delta y = \Delta z)$. Every $\vec{E}$ field is located ½ cell width from the origin in the direction of its orientation; every $\vec{H}$ field is offset ½ cell in each direction except that of its orientation.

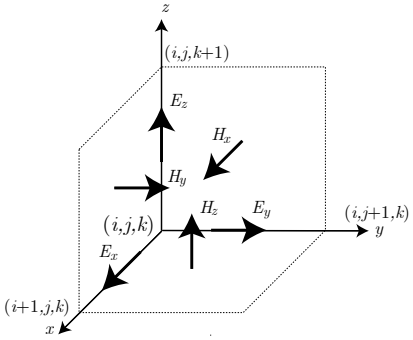

Figure 1. The Yee cell.

Since the stability analysis is discussed with rigor in [1], we can determine the time step easily taking into account that a wave propagating in free space cannot go faster than speed of light. To propagate a distance of one cell requires a minimum time of $\Delta t = \Delta x / c_0$. In two-dimensional simulation, we have to allow for the propagation in the diagonal direction, which brings the time requirement to $\Delta t = \Delta x / \sqrt{2} c_0$. Obviously, three-dimensional simulation requires $\Delta t = \Delta x / \sqrt{3} c_0$. This is summarized by the well-known "Courant Condition":

$$\Delta t \le \frac{\Delta x}{\sqrt{p} \cdot c_0}, \tag{12}$$

where p is the dimension of simulation. Unless otherwise specified, we will determine Δt for simplicity by

$$\Delta t \le \frac{\Delta x}{2 \cdot c_0}. \tag{13}$$

1.2 Boundary conditions. Clearly, no computer can store an unlimited amount of data, and therefore, the field computation domain must be limited in size. Suppose we are simulating a wave generated from a point source propagating in free space. As the wave propagates outwards, it will eventually come to the edges of the allowable space, which is dictated by how the matrices have been dimensioned in the program. If nothing is done to address this, unpredictable reflections would be generated in the boundaries and would go back inward. This phenomenon is produced because wave fields outside our simulation region are unknown and their values are arbitrary assumed as null. Boundary condition permits all outward-propagating numerical wave to exit from our finite grid almost as if the simulation were performed on a computational domain of infinite extent. In the process, the boundary condition must suppress

spurious reflections of the outgoing numerical waves to an acceptable level. There have been many approaches to this problem and depending upon their theoretical basis, outer grid boundary conditions of this type have been called either radiation boundary conditions (RBCs) or absorbing boundary conditions (ABCs). One of the most flexible and efficient ABCs is the perfectly matched layer (PML) developed by Berenger [4].

This method is based in the addition of layers conforming a new medium that is lossy and with null reflection. The amount of reflection is dicated by the intrinsic impedances of two media with $\eta = \sqrt{\mu/\varepsilon}$. A media with ε and μ complex can model lossy properties, because the imaginary part represents the part that causes decay.

In this work, we will work in TM mode, but all analysis could be made for TE mode and both cases simultaneously. To implement the PML, ficticious dielectric constants and permeabilites $\varepsilon^*_{F_z}$, $\mu^*_{F_x}$ and $\mu^*_{F_y}$ are added in (5-7)

$$j\omega D_z \varepsilon^*_{F_z}(x)\varepsilon^*_{F_z}(y)\varepsilon^*_{F_z}(z) = \frac{1}{\sqrt{\varepsilon_0\mu_0}}\left(\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y}\right), \tag{14}$$

$$j\omega H_x \mu^*_{F_x}(x)\mu^*_{F_x}(y)\mu^*_{F_x}(z) = -\frac{1}{\sqrt{\varepsilon_0\mu_0}}\frac{\partial E_z}{\partial y}. \tag{15}$$

$$j\omega Hy \mu^*_{F_y}(x)\mu^*_{F_y}(y)\mu^*_{F_y}(z) = \frac{1}{\sqrt{\varepsilon_0\mu_0}}\frac{\partial E_z}{\partial x}. \tag{16}$$

The value $\varepsilon^*_{F_z}$ is associated with the flux density $\vec{D}$, and are completely fictitious, these constants implement the PML and have nothing to do with the real ε^*_r which specifies the medium. Due to the fact that the reflection coefficient must be unity, we will assume that each of these is a complex constant of the form

$$\varepsilon^*_{F_m} = \varepsilon_{F_m} + \frac{\sigma_{D_m}}{j\omega\varepsilon_0} = 1 + \frac{\sigma_D}{j\omega\varepsilon_0} \quad \text{for } m = x, y \text{ or } z, \tag{17}$$

$$\mu^*_{F_m} = \mu_{F_m} + \frac{\sigma_{H_m}}{j\omega\varepsilon_0} = 1 + \frac{\sigma_D}{j\omega\varepsilon_0} \quad \text{for } m = x, y \text{ or } z. \tag{18}$$

Figure 2 shows the $\vec{E}$ field emanating from a point for different time slots. Notice that absorption in boundaries is achieved without reflections.

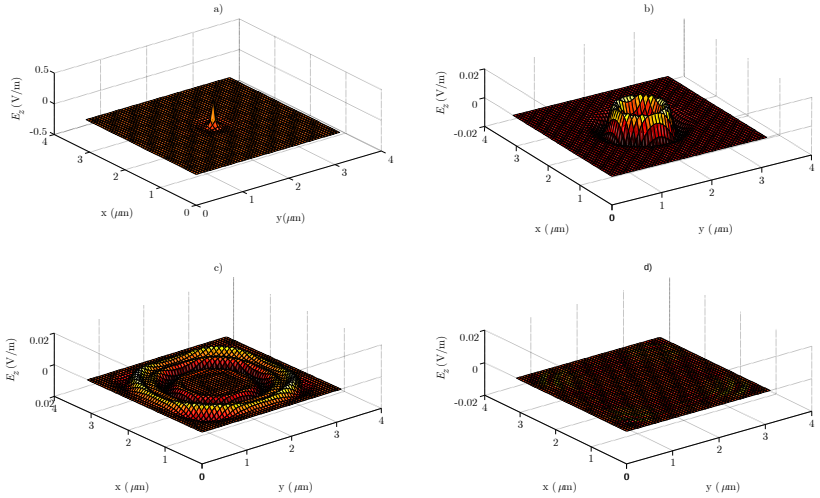

Figure 2: Radiation from a point source in an FDTD program with several-point PML. a) $t = 40\Delta t$, b) $t = 80\Delta t$, c) $t = 150\Delta t$ and d) $t = 200\Delta t$

1.3 Total-Field and Scattered-Field formulation. The simulation of plane waves is often of interest in computational electromagnetics. This formulation is the result of continued attempts

to create a compact wave source for use in simulations of sinusoidal steady-state illumination [2],[5] and [6]. This approach is based firmly on the linearity of Maxwell's equations and the decomposition of the electric and magnetic fields as

$$\vec{E}_{\text{tot}} = \vec{E}_{\text{tot}} + \vec{E}_{\text{scat}}, \tag{19}$$

$$\vec{H}_{\text{tot}} = \vec{H}_{\text{tot}} + \vec{H}_{\text{scat}}. \tag{20}$$

Here $\vec{E}_{\text{inc}}$ and $\vec{H}_{\text{inc}}$ are the values of the incident wave fields, which are assumed to be known at all space points of the FDTD grid at all time steps. These are field values that would exist in vacuum, that is, if there were no materials of any sort in the modelling space. $\vec{E}_{\text{scat}}$ and $\vec{H}_{\text{scat}}$ are the values of the scattered wave fields, which are initially unknown. These are the fields that result from the interaction of the incident wave with any materials in the grid. In order to simulate a plane wave in a 3D FDTD program, the problem space will be divided up into two regions, the *total field* and the *scattered field* region. One benefit applying this formulation is that the propagating wave should not interact with the absorbing boundary conditions. Figure 4 illustrates how this is accomplished. In the three-dimensional field every point in the problem space is either in the total field region or it is not. Therefore, if a point is in the total field but it uses points outside to calculate the spatial derivates when updating its value, it must be modified. The incident array contains the needed values to make these modifications. The connecting conditions are a set of equations that are applied in the interface between *total field* and *scattered field* and confines incident plane waves into *total field*. These equations are defined in the six planes showed in figure 3.There are several places that must be modified (table 1).

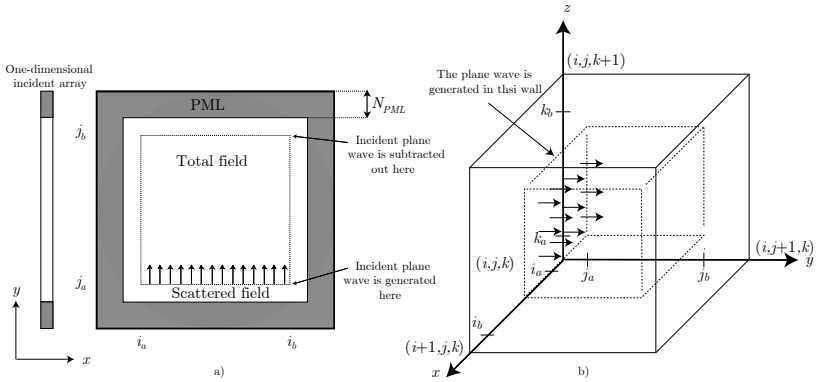

Figure 3: a)Total field/Scattered field of the two-dimensional problem space. b) Total field/Scatterd field in 3D.

The D_z value at $j = j_a$ or $j = j_b$	The D_y value at $k = k_a$ or $k = k_b$
$D_z\big\|_{i,jb,k} = D_z\big\|_{i,jb,k} - \frac{c_0\Delta t}{\Delta x} H_{x\_inc}\big\|_{jb+1/2}$	$D_y\big\|_{i,j+1/2,ka} = D_y\big\|_{i,j+1/2,ka} - \frac{c_0\Delta t}{\Delta x} H_{x\_inc}\big\|_{j}$
$D_z\big\|_{i,ja,k} = D_z\big\|_{i,ja,k} + \frac{c_0\Delta t}{\Delta x} H_{x\_inc}\big\|_{ja-1/2}$	$D_y\big\|_{i,j+1/2,kb+1} = D_y\big\|_{i,j+1/2,kb+1} + \frac{c_0\Delta t}{\Delta x} H_{x\_inc}\big\|_{j}$
The H_x value at $j = j_a$ or $j = j_b$	**The H_y value at $i = i_a$ or $i = i_b$**
$H_x\big\|_{i,ja-1/2,k} = H_x\big\|_{i,ja-1/2,k} + \frac{c_0\Delta t}{\Delta x} E_{z\_inc}\big\|_{ja}$	$H_y\big\|_{ib+1/2,j,k} = H_y\big\|_{ib+1/2,j,k} + \frac{c_0\Delta t}{\Delta x} E_{z\_inc}\big\|_{j}$
$H_x\big\|_{i,jb+1/2,k} = H_x\big\|_{i,jb+1/2,k} - \frac{c_0\Delta t}{\Delta x} E_{z\_inc}\big\|_{jb}$	$H_y\big\|_{ia-1/2,j,k} = H_y\big\|_{ia-1/2,j,k} - \frac{c_0\Delta t}{\Delta x} E_{z\_inc}\big\|_{j}$

Table 1: Connecting conditions for 3D simulation.

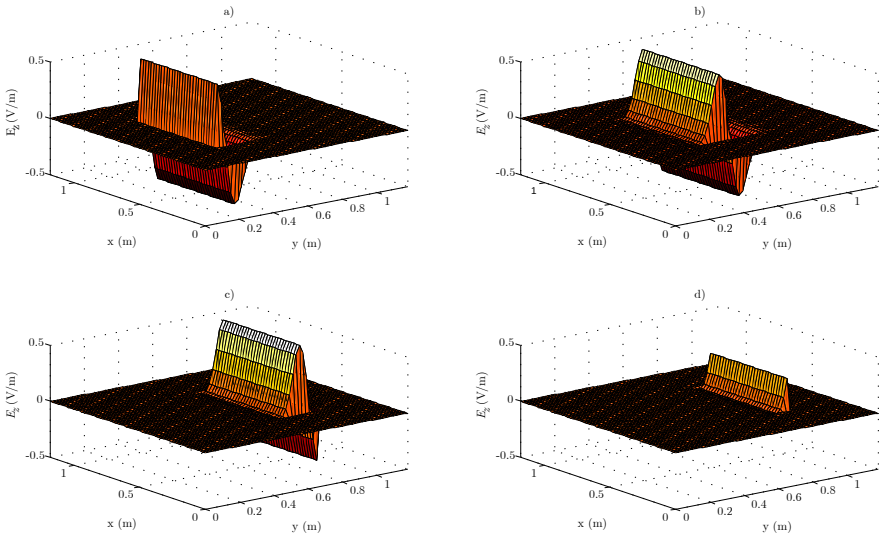

Figure 4: Simulation of a plane wave pulse propagating in free space. The incident pulse is generate at one end and subtracted out the other end.

1.4 Time-domain near-to-far-field transformation. The method involves setting up time-dimensioned arrays for the far-field vector potentials. Each array element is determined by a conducting a recursive (running) sum of contributions from the time-domain electric and magnetic current sources just computed via FDTD on S'. These contributions are delayed in time according to the propagation delay between a source element on S' and the far-field observation point. In our problem, this formulation give us the possibility of minimize the simulation cell to the illumination area, calculating the diffraction pattern on the screen via NF/FF transformation.

We begin with the vector potential [1]-[2]:

$$\vec{A}(r) = \frac{1}{4\pi} \iint_{S'} \vec{J}_S(r') \frac{e^{-j\vec{k}\vec{R}}}{R} dS', \qquad (21)$$

where $R = |\vec{r} - \vec{r}'|$, $\vec{J}_S(r')$ is the current source and $e^{-j\vec{k}\vec{R}} / R$ is the Green's function.

Developing this expression and carrying out different mathematical operations [2], we can obtain the following expression, which is introduced in the algorithm FDTD:

$$E_z\Big|_{i,j,k}^{n} = \frac{1}{\pi} \sum_{i'} \sum_{j'} \frac{r_x}{R_{\Delta x}} \left[\frac{E_z\Big|_{i',j',k'}^{n-2R_{\Delta x}} - E_z\Big|_{i',j',k'}^{n-1-2R_{\Delta x}}}{\Delta t} + \frac{E_z\Big|_{i',j',k'}^{n-2R_{\Delta x}}}{2R_{\Delta x}} \right] \qquad (22)$$

where the distance $R_{\Delta x}$ is defined as an integer, $R_{\Delta x} \cong R / \Delta x$.

The accuracy of the method is verified by using an FDTD program that calculates the $\vec{E}$ field at three external points via eq. (22). A rectangular aperture is simulated and different points inside grid simulation are selected. Field values obtained directly via FDTD method and via NF/FF transformation are compared in figure. Clearly, the agreement is quite good.

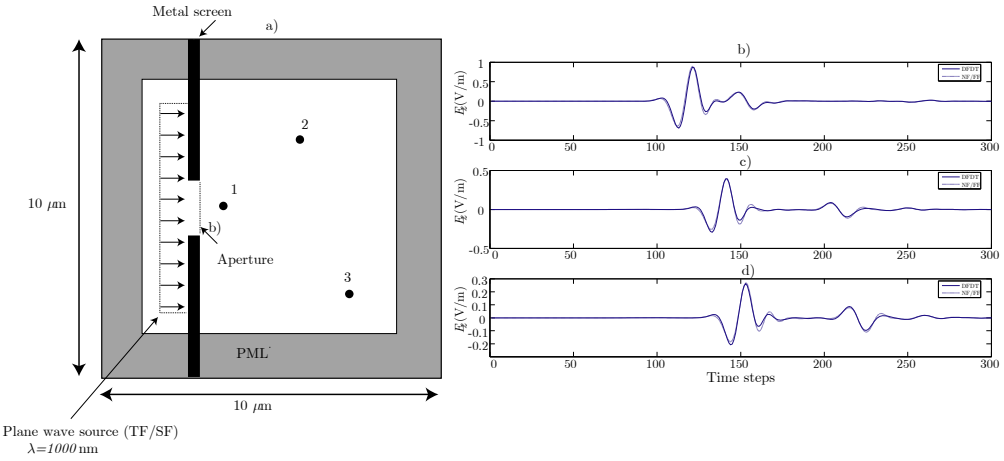

Figure 5: a) Diagram of the problem, the time domain fields at points 1, 2 and 3 are calculated via eq. (22). The accuracy is verified by comparison with the time domain data calculated directly by the FDTD progam in points 1 a), 2 b) and 3, d).

3 RESULTS. Optical simple systems have been chosen for the study of the diffraction in Fraunhofer's region. These systems are shown in Figure 6. The variable parameters such as wavelength and spatial period are fixed as $\lambda = 633$ nm and $\Delta x = \lambda/10$. The plane on which we calculate the diffraction pattern must be placed at a distance from the slits that must satisfy Fraunhofer's far field condition $F = a^2/L\lambda \ll 1$. Where a is the width of the slit and L is the distance between far field observation point (screen) and the plane slits. Distance L has been established for all the simulations as $4000\,\Delta x$. The distant observation points have been obtained by means of the near-field to far-field transformation along x-coordinate at $z = 4000\Delta x$. The irradiance patterns are shown in figure 7. The results of simulations are compared with analytical values. These expressions are well known and resumed in table 2.

	1 slit	**2 slits**	**N slits**	**Circular aperture**
$I(\theta)$	$I(0)\left(\frac{\sin\beta}{\beta}\right)^2$	$4I(0)\left(\frac{\sin\beta}{\beta}\right)^2\cos^2\alpha$	$\frac{I(0)}{N^2}\left(\frac{\sin\beta}{\beta}\right)^2\left(\frac{\sin N\alpha}{\alpha}\right)^2$	$I(0)\left[\frac{2J_1(ka\sin\theta)}{ka\sin\theta}\right]^2$

Table 2: Analytical irradiance expresions for the unique slit, two slits, N slits and circular aperture [7].

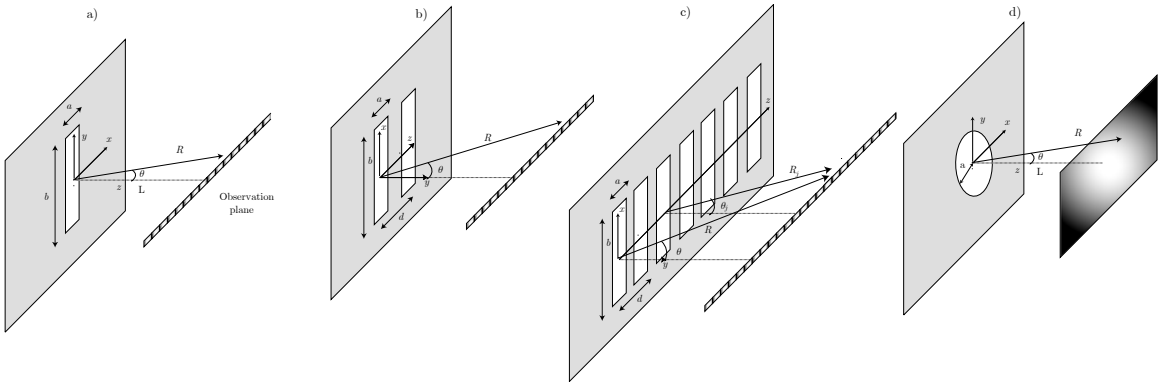

Figure 6: Diagram of different experiments simulated. a) unique slit. b) Double slit (Young's experiment). c) N slits (with N=7). d) Circular aperture.

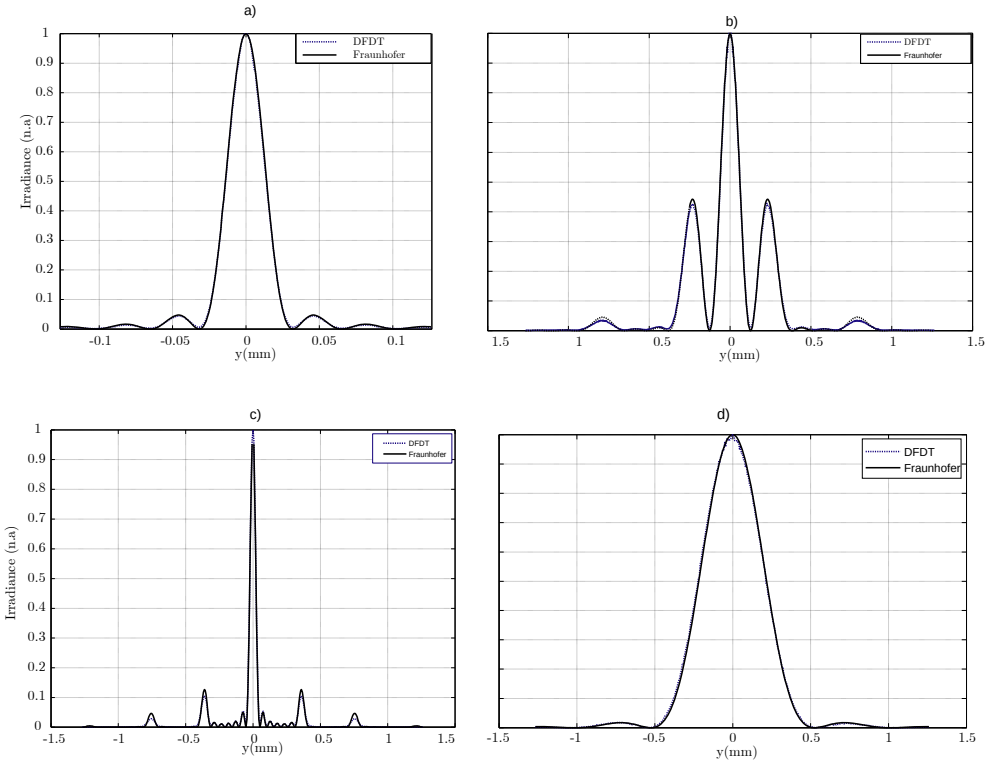

Figure 7: Comparative between numerical results and analytical values. a) unique slit with $a = 80\Delta x$. Simulation of 100x100x80 cells. b) Double slit (Young's experiment) with $a = 50\Delta x$ and $d = 100\Delta x$. Simulation of 120x100x80 cells c) N slits (with N=7) with $a = 50\Delta x$ and $d = 100\Delta x$. Simulation of 650x100x80 cells. d) Circular aperture with $a = 30\Delta x$. Simulation of 120x120x80 cells.

5 CONCLUSIONS

In this work, software for optical simulation systems has been developed. More precisely, it has been applied to study diffraction and interference of light waves in Fraunhofer's region. The software is based on the FDTD method, which has been detailed in this work. Different formulations related with this method have been included to permit simulate correctly this type of applications. Software is focused on helping students in laboratory sessions related with optical or physics degrees in which expensive and difficult experiments can be introduced in a proper manner with this software.

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