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Interference and diffraction analysis of holographic gratings using the Finite-Difference Time-Domain method

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Abstract
The Finite-Difference Time-Domain method (FDTD) is based on a time-marching algorithm that has proven accurate in predicting microwave scattering from complicated objects. In this work the method is applied at optical wavelengths, more concretely the method is applied to rigorously analyze holographic gratings for the near-field distribution. It is well known that diffraction gratings with feature sizes comparable to the wavelength of light must be treated electromagnetically, because the scalar diffraction theories, including Fourier and Fresnel approximations, no longer apply. The FDTD method permits to analyze the electromagnetic field distribution in function of time and space. In optical wavelengths the simulation of wide areas implies more memory and time processing. For that reason, some add-ons are included in order to correctly calculate the far field distribution obtained from the numerical near-field values computed in the simulation region. As a consequence the total grid simulation size can be reduced improving the performance of the simulation, in terms of memory usage and time processing. Values in the near-field region are computed due to the illumination of the grating by means of a plane wave with different angle of incidence. In addition, we compare the results obtained by the FDTD method to those obtained using the Kogelnik’s theoretical expressions applied to diffraction gratings. As it will be seen in this work there is good agreement between numerical and analytical values, thus validating our FDTD implementation.

Keywords: Holographic grating, FDTD, Interference, Diffraction

1. Introduction

The Finite-Difference Time-Domain method (FDTD) [1, 2] is based on a time-marching algorithm that has proven accurate in predicting microwave scattering from complicated objects for instance. The FDTD method solves the differential Maxwell equations, substituting the time and spatial derivates with central-difference approximation providing the transient electromagnetic field and wide band frequency analysis via a single simulation.

In the last decades diffractive optical elements have been used in many applications such lenses and mirrors manufacturing [3, 4], broadband communications [5], optical computation [6] or information storage [7]. Because of the small sizes of this optical elements, rigorous electromagnetic computational methods are needed to obtain their diffraction performance. There are several numerical methods applied to solve electromagnetic problems such as the finite-element method [8] or the boundary-element method which require the solution of a large system of equations.

In this work a improved implementation of the FDTD method has been applied to rigorously analyze holographic volume gratings for the near-field distribution. This optimization is based on using the advanced vectorial instructions of the CPU. Concretely, it has been used optimized code according to the detected processor which is going to do the processing. An optimal version of the Single Instruction Multiple Data (SIMD) has been used to reduce the time costs of the FDTD method. A reformulation of the algorithm and memory management are necessary in order to achieve performance improvements.
Other techniques for reducing time processing and memory requirements are based on minimizing the area to be simulated. For that purpose, some add-ons have been included in our algorithm such as: Near Field to Far Field propagation (NF/FF), Perfectly Matched Layers (PML) and Total Field Scattered Field formulation (TF/SF). All those formalisms are necessary for simulating optical devices such as diffraction gratings that usually are excited by a laser. More concretely, with the FDTD method have been studied different parameters such as diffraction and transmission efficiencies of volume holographic gratings.

In Section 2 the elemental theory related with the FDTD method is introduced, including boundary conditions and far field transformation. For simplicity TM polarization has been considered in all of the experiments (electric field parallel to the z-axis, and magnetic field in the xy plane). In many applications an infinitely large one-dimensional structure in the z direction can be assumed, which is illuminated by a TM plane wave. In such a case, the solutions of Maxwell’s curl equations can be reduced to the two-dimensional problem. In this section basic concepts related with diffraction holographic gratings are explained. Therefore, special considerations predicting the performance of gratings and other optical devices are detailed also. The analytical closed form expressions from Kogelnik works are enumerated. During decades researchers in the field of Holography have used the analytical expressions deduced by Kogelnik [9] to estimate the theoretical predictions of phase and amplitude, transmission and reflection volume holograms. Although this theory assumes that only two orders propagate inside the hologram the curves obtained are quite good enough for validating our numerical algorithm.

Section 3 shows the optimization basis of the code. The comparison of the typical FDTD loop is done with the SIMD version. All gratings simulated in Section 4 are studied in two dimensions. All values obtained via FDTD algorithm are compared with those obtained by means of the analytical expressions deduced by Kogelnik [9, 10] to estimate the theoretical predictions of phase and amplitude, transmission and reflections volume holograms.

2. Theory

In this section it is detailed the basis of the FDTD method applied to solve the electromagnetic fields. More concretely, this method is applied at optical wavelengths. Moreover, some basical equations related with analytical analysis of the volume diffraction gratings are introduced.

2.1. Finite Difference Time Domain Method

Light propagation is described by means of Maxwell’s time-dependent curl equations in Gaussian Units[11, 12]:

\[
\begin{align*}
\frac{\partial \tilde{D}}{\partial t} &= \frac{1}{\sqrt{\epsilon_0 \mu_0}} \left( \nabla \times \tilde{H} - \sigma \tilde{E} \right), \\
\tilde{D}(\omega) &= \epsilon_\ast(\omega) \cdot \tilde{E}, \\
\frac{\partial \tilde{H}}{\partial t} &= -\frac{1}{\sqrt{\epsilon_0 \mu_0}} \nabla \times \tilde{E} - \frac{\sigma_m}{\mu_0} \tilde{H},
\end{align*}
\]

where \(\epsilon_0\) is the electrical permittivity in farads per meter, \(\epsilon_\ast\) is the medium’s relative complex permittivity constant, \(\mu_0\) is the magnetic permeability in henrys per meter, \(\sigma_m\) is an equivalent magnetic resistivity in ohms per meter and \(\sigma\) is the electric conductivity in siemens per meter. The flux density is denoted by \(\tilde{D}\) and both \(\tilde{D}\) and \(\tilde{E}\) are normalized respect to the vacuum impedance \(\eta_0\).

The FDTD algorithm used here is based on the Yee[13] lattice as depicted in Fig. 1.a). The electrical field components \(\tilde{E}\) and the magnetical field components \(\tilde{H}\) are centered in a three-dimensional cell so that every \(\tilde{E}\) component is surrounded by four circulating \(\tilde{H}\) components, and every \(\tilde{H}\) component is surrounded by four circulating \(\tilde{E}\) components [14, 15].

To solve Maxwell’s curl equations in two dimensions for TM polarization, Eqs.(1-3) are discretized by using central-difference expressions for both the time and the space derivatives. For two dimensions, the Yee cell is still useful and an xy plane containing \(\tilde{H}\) fields is only necessary, as can be seen in Figure 1. The Eqs.(1-3) are reduced to the following taking into account nonmagnetic and lossless medium:
Here, $\Delta x$ and $\Delta y$ are respectively, the lattice space increments in the \( x \) and \( y \) coordinate directions, and \( i \) and \( j \) are integers that denote the position of sample points in the \( x \) and \( y \) directions, respectively. The time increment is represented by $\Delta t$ and is related with the integer \( n \) to localize a determined observation interval. At the material boundaries the continuity conditions for the electric and magnetic fields are satisfied implicitly within the accuracy of the numerical discretization. In the time domain a leapfrog algorithm is applied [14]. The electric and magnetic fields are calculated alternately in intervals of $\frac{1}{2}\Delta t$. The time step has an upper bound to ensure the numerical stability of the algorithm [11, 14, 16]. This is summarized by the well-known “Courant Condition”:

$$\Delta t \leq \frac{\Delta}{\sqrt{\mu_0}}$$

where \( p \) is the dimension of the simulation and $\Delta = \Delta x = \Delta y$.

In order to simulate unbounded free space, absorbing boundary conditions are included in the region in which the optical device is totally enclosed. Usually, in calculating the \( E \) field, we need to know the surrounding \( H \) values. At the edge of the grid the values at one side are unknown and arbitrary assumed as null. As a consequence, reflected waves would go inward in order to keep the boundary conditions mentioned previously. This phenomenon causes an unpredictable field pattern in the simulation region. The perfectly matched layer absorbing boundary conditions proposed by Berenger [17], which have been found to be effective and to cause only slight reflection error, are used in our study. Although, in this work, a slight deviation from the Berenger method [18] will be made by introducing fictitious conductivities associated with \( D \) and \( H \), instead of \( E \) and \( H \). The basic idea of this formalism is to create a medium that is lossy and minimize the amount of reflection between free air and the PML region. The effect of this is to create a nonphysical absorbing medium adjacent to the outer FDTD mesh boundary that has a wave impedance independent of the angle of incidence and frequency of the outgoing scattered waves. There have been numerous approaches to this problem [14, 16, 19].
On the other hand, it is necessary a method for illuminate the simulation with a light source. A typical laser of 633nm emits a coherent plane wave. For this reason, a formalism (TF/SF) has been implemented in order to simulate a light illumination behavior similar to a laser. It is supposed a TM plane wave, whose incidence is assumed to be from air to medium and whose propagation in the FDTD region is determined by using the time-marching algorithm. It is introduced along the connecting boundary by using a total field/scattered field algorithm [11, 14, 16], where \((E, H)_{\text{Total}} = (E, H)_{\text{inc}} + (E, H)_{\text{scat}}\). An arbitrary angle of incidence has been taken into account. With this add-on the simulation region is divided into two new regions: the total field region and the scattered field region. In the first one, the plane wave source interacts with the medium under study. Whereas, in the scattered region the incident wave is suppressed and the perturbation produced by the element into the total region travels to the outer region. This phenomena permits for instance analyze diffracted and transmitted orders of a diffraction grating without interference produced by the source.

Nevertheless, in many cases a wider area of simulation is needed to observe diffraction patterns or similar. To increase the simulation region produces an exponential increase of the time costs of the simulation and memory allocation. Therefore, many authors have been working on the solution of this problem. The Near Field to Far Field propagation permits to propagate the numerical near field values to a far field. In the time domain, the Schelkunoff equivalence principle has been used by many authors in different works [20]-[24] for three dimensional transient calculations evaluating the time-domain integral expresion (TDIE) of the fields. Nevertheless the evaluation of the TDIE in two dimensions is not straightforward. Luebbers et al [25] proposed a mixed frequency/time-domain algorithm which involves two Fourier transformations to obtain the time-domain response. In this work an approach based on the equivalence principle has been implemented to calculate, in the time domain, the transient far-field response of a two-dimensional structure by directly evaluating a two-dimensional form of the TDIE [26]. The procedure, leads to an easily implementable algorithm consisting of the numerical evaluation of a two-dimensional integral. This algorithm can be implemented in a marching-on-in-time procedure simultaneously with the FDTD advancing algorithm.

2.2. Basic Volume gratings theory

A hologram can be treated as a photographic film with a spatial varying transmittance. The interference pattern consists of planes running almost parallel to the surface of the recording material. With a thick recording medium, the hologram is made up of layers corresponding to a periodic variation of the transmittance or refractive index. If the two interfering wavefronts are incident on the recording medium from the same side, these layers are approximately perpendicular to its surface, and the hologram produces an image by transmission. However, it is also possible to have the two interfering wavefronts incident on the recording medium from opposite sides, in which case the interference surfaces run approximately parallel to the surface of the recording medium. In this case, the reconstructed image is produced by the light reflected from the hologram [27]. In both cases (an scheme of these diffraction gratings is illustrated in Figure 2), the diffracted amplitude is a maximum only when the angle of incidence is equal to the Bragg angle \(\theta_B\), satisfying the Bragg condition

\[
\cos(\psi - \theta_B) = \frac{K}{2n_0k_0},
\]

where \(n_0\) is the average refractive index of the recording medium, and \(k_0 = \frac{2\pi}{\lambda}\). The grating vector \(K\) defines the normal of the interference surfaces of the recording medium. This vector is of length \(K = \frac{2\pi}{\Lambda}\), where \(\Lambda\) is the grating period and makes an angle \(\psi\) with the \(y\) angle. It is well known the relationship between the refractive index and the dielectric permittivity of the form \(n = \sqrt{\epsilon_r}\).

First, we consider a lossless volume transmission phase grating of thickness \(d\) with the grating planes running normal to its surface. If we assume that the refractive index varies sinusoidally with amplitude \(n_1\) about a mean value \(n_0\), the diffraction efficiency of the grating at the Bragg angle is \(\theta_B\) is:

\[
\eta_T^B = \sin^2(\Phi),
\]

where \(\Phi = \pi n_1 d / \lambda \cos \theta_B\) is known as the modulation parameter. At the output of the grating, and for arbitrary angle of incidence the output angle of the different orders are defined as follows

\[
\Lambda(\sin \theta_m - \sin \theta_B) = m\lambda,
\]
Figure 2: Volume transmission and reflection gratings and their associated vector diagrams for Bragg incidence [10, 27].

where $\theta_m$ is the angle formed by the direction vector of the diffracted order between the normal output of the grating. On the other hand, the diffraction efficiency of a volume reflection phase grating at the Bragg angle is given by the relation

$$\eta^R_B = \tanh^2(\Phi).$$

(11)

3. Implementation of the FDTD algorithm for SIMD instructions

The use of SIMD instructions in general purpose processors was promoted by Intel in 1999 due to the increasing PC volume market. This required a balanced platform for 3D graphics performance in order to scale from arcade consoles to workstation applications. The Single Instruction Multiple Data (SIMD) belongs to the parallel computation model. This is the most cost-effective way of accelerating floating-point performance in general purpose processors. The use of the Intel’s SIMD instructions permits a theoretical full x4 performance gain (full 4-wide SIMD operation can also be done every clock cycle) for single precision data, although 2x is the typical gain on real applications due to other factors such as memory access and other tasks [28]. In the Figure 3 can be seen the difference between the typical ALU instruction commonly used by compilers and SIMD instructions available in Streaming SIMD Extensions (SSE) at Intel’s processors.

Figure 3: a) Adding diagram of a typical ALU. b) Adding diagram of a SIMD instruction of SSE CPU.

In order to be effective during the computation, the pointers in memory of the array to be used by SIMD instruction must be aligned. For that reason, the allocation of the memory for an array with $N$ rows and $M$ columns has been modified. In our implementation of the FDTD method, all matrix has been stored as a single aligned column vector. In the Figure 4 can be seen leap frog algorithm flow chart which summarizes steps to be implemented in a FDTD algorithm. For instance, the $\hat{D}_z$ field is calculated from the previous values stored in memory of the inner $\hat{D}_z$ and the magnetic fields. The $\mathbf{C}$ matrix (or
1-D array for optimized version of the algorithm) is a data structure that defines the medium: dielectric constant, space and time resolution [11, 14].

Figure 4: The leap frog algorithm is shown at the left. The classical implementation of the component in \( z \) direction for displacement vector and the optimized implementation are showed. The variables which name starts with “p” indicates that is a pointer to an one-dimensional array. The variables prefixed with “curl” are temporal one-dimensional arrays needed to store auxiliary data.

5. Results

In this work different gratings have been studied (transmission and reflection) with the FDTD method. In the Figure 5 are shown different time steps of the simulation of a volume transmission grating excited by a plane wave satisfying Bragg condition. It can be seen how the diffracted order becomes more perceptible as soon as the steady state is reached. Concretely, the diffraction efficiency is not so high due to the values fixed in this simulation. In the Figure 5 is detailed where the grating is placed in the simulation. Also, in the Figure 5.c) the sampling plane where the near field values are propagated to far field are represented concretely. As can be seen, the near field values are chosen near the output of the grating. The far field values obtained from the propagation are used to compute the irradiance pattern \( I \) which is defined as \( I \propto |E|^2 \). These irradiance patterns are illustrated in the Figure 6 for reflection and transmission volume diffraction gratings.
**Figure 5:** Sequence of the simulation of a volume transmission grating with parameters: $n_0=1.63$, $n_1=0.025$, $\Lambda=0.83\ \mu\text{m}$, $d=10\ \mu\text{m}$). a) $\Delta t = 400$. b) $\Delta t = 1000$. c) $\Delta t = 1400$. d) $\Delta t = 1800$.

Furthermore, a more exhaustive analysis of the diffraction efficiency of both gratings: transmission and reflection has been obtained. For that purpose the thickness of gratings has been modified in order to study the relationship between $\eta_B$ and $d$. The curves obtained are compared with the analytical values obtained from Eq.(9) and (11). In both cases the parameters defining the gratings are $n_0 = 1.63$, $n_1 = 0.025$, $\Lambda = 0.83\ \mu\text{m}$ and $\lambda = 633\ \text{nm}$. The time and spatial resolution are defined in order to minimize the inner numerical error of the method [14] and avoiding instabilities as $\Delta x = \lambda/10$ and $\Delta t = \Delta x/(2c_0)$, with $c_0$ being the light speed. In Figure 6.a) the results due to the use of SIMD instructions in the implementation of the algorithm are represented. Notice that all simulations have been realized with the Intel Core2 Quad Processor Q6600 (4 cores, 2.4 GHz and 8 MB L2). The size of L2 memory is the parameter that produces a decreasing in the performance. If the matrix size becomes greater, it is possible that whole L2 memory becomes unable of storing all data needed for the computation.

Although performance results showed by the Figure 6 are refereed only to one thread or single processor.
7. Conclusions

In this work the FDTD has been applied with succesfully results to volume diffraction gratings. Also, an optimized version of the typical FDTD loop has been presented. This improvement is based on using the SIMD instructions available in the general purpouse Intel’s processors. The adoption of these instructions in the FDTD code implies different changes in the way of storing the data inside the memory in order to be effective. These changes, basically are focused on aligning the data consecutively in memory in order to be loaded into the processor correctly. Hence, performance of the FDTD method by using the SIMD extension has been proved to be greater than the heavily optimized classical FDTD loop. As illustrated in the Figure 6.b) it has been obtained a 3x gain when working on L2 cache limits and a 2x Gain beyond L2 cache limits. On the other hand, the accuracy of the simulations of volume diffraction gratings are good enough, since the analytical and numerical values are quite similar. Notice that Kogelnik’s closed expressions assumes infinite plane wavefronts as well as a slow energy interchange. Also the zero-order and Bragg-diffracted waves propagate within the grating. However, even if the first of these assumptions is satisfied, the existence of higher-order diffracted waves in phase gratings cannot be ignored, even for refractive index modulation greater than 0.005. Currently, the authors are working in parallel computation applied to FDTD. And more optical elements and paremeters of the diffraction gratings are being studied such as angular efficiency and wavelength selectivity.
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References


