

# A Higher-Order Accurate FDTD Solution to Scalar SHG Problems

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**Abstract-** A higher-order accurate FDTD simulation algorithm for the solution of the phase-dependent SHG problem is presented. This algorithm approximates the spatial derivatives in the propagation direction using 4<sup>th</sup> order FD schemes. It has been shown that this scheme guarantees the convergence of the solution using significantly less computation time and less memory requirement as compared to 2<sup>nd</sup> order schemes

## 1. INTRODUCTION

Higher order FDTD schemes allow the modeling of electromagnetic wave interaction in structures that have very long electrical lengths without jeopardizing the limit on phase error accumulation set by standard 2<sup>nd</sup> order methods. These higher order schemes become even more attractive in problems involving nonlinear interactions. For example, in a second harmonic generation (SHG) problem, the energy coupling between the propagating input optical beam and the generated beam is a strong function of the phase shift between the two waves. Failing to accurately estimate the phase of the waves at any given distance along the propagation direction results in errors in the calculation of both coherence length and the amount of coupled energy. Several researchers have attempted the FDTD solution of wave propagation in both linear as well as nonlinear optical structures using higher order methods to overcome the limitations of 2<sup>nd</sup> order explicit schemes [1]-[3].

In this paper, the FDTD-SHG solution reported in [4] is revisited. The second order accurate approximations of the spatial derivatives are replaced by 4<sup>th</sup> order accurate schemes. Such a scheme has not been yet discussed in literature in the context of the nonlinear wave equation representing SHG.

## 2. FORMULATIONS

A time-domain formulation of the SHG problem in nonlinear optical waveguides with has been proposed in [4]. The equations representing the propagating waves are derived using a nonlinear wave equation such that the problem is reduced to an equivalent scalar problem. This new formulation of the SHG problem offers great advantages over both the classical BPM technique and other frequency-domain methods. While it completely accounts for the wave-medium interactions, it avoids the limitations associated with conventional asymptotic behavior and paraxial propagation. On the other hand, it provides an efficient method for the time-domain characterization of nonlinear optical structures by focusing on such quantities as beam intensity, nonlinear depletion and phase shift, characteristic lengths, etc., in which detailed analysis of the field components is not necessary. For a 2D SHG problem, the proposed time-domain algorithm solves for only two fields; the fundamental field and the second harmonic field. In addition, the algorithm is capable of incorporating different matching techniques in the SHG process including quasi-phase matching and it can simulate CW second-order nonlinear effects as well as operations with short time-varying envelopes. The SHG model equations are given by:

$$\nabla^2 E^f = \mu_o \epsilon_o n_f^2 \frac{\partial^2 E^f}{\partial t^2} + 2\mu_o \epsilon_o \chi^{(2)} \left\langle E^f \frac{\partial^2 E^s}{\partial t^2} + E^s \frac{\partial^2 E^f}{\partial t^2} + 2 \frac{\partial E^f}{\partial t} \frac{\partial E^s}{\partial t} \right\rangle \quad (1)$$

$$\nabla^2 E^s = \mu_o \epsilon_o n_s^2 \frac{\partial^2 E^s}{\partial t^2} + 2\mu_o \epsilon_o \chi^{(2)} \left\langle E^f \frac{\partial^2 E^f}{\partial t^2} + \frac{\partial E^f}{\partial t} \frac{\partial E^f}{\partial t} \right\rangle \quad (2)$$

where  $E^f$  and  $E^s$  are the fundamental and the second harmonic fields, respectively,  $n$  is the material refractive index and  $\chi^{(2)}$  is the dispersionless nonlinear susceptibility. The second order FD approximation of the laplacian is systematically used in many wave propagation problems. Provided that the spatial step size in the propagation direction is made a small fraction of the shortest wavelength, the amount of numerical dispersion of a 2<sup>nd</sup> order scheme is generally acceptable. It will be interesting to investigate this general criterion when the simulation involves phase-dependent interactions between coexisting waves, such as the case of a SHG problem. Using the 4<sup>th</sup> order scheme, which is proposed to replace the 2<sup>nd</sup> order scheme, the spatial derivative of the fundamental wave, for example, in the propagation direction will be given by:

$$\frac{\partial^2 E^f}{\partial y^2} \cong \frac{1}{12(\Delta y)^2} \left[ -E^f(i, j-2) + 16E^f(i, j-1) - 30E^f(i, j) + 16E^f(i, j+1) - E^f(i, j+2) \right] \quad (3)$$

### 3. SOLUTION METHOD AND NUMERICAL RESULTS

To study the effectiveness of the proposed 4<sup>th</sup> order method, a symmetric AlGaAs-based dielectric slab waveguide is considered. It consists of a 0.44- $\mu\text{m}$  thick guiding layer sandwiched between two 3- $\mu\text{m}$  thick AIAs layers. The excitation field is a CW signal at a fundamental wavelength of  $\lambda_f = 1.064 \mu\text{m}$ . The transverse profile of the excitation corresponds to the first guided mode at the given operating frequency. For the sake of comparison, both 2<sup>nd</sup> and 4<sup>th</sup> order schemes were considered. No matching technique is used such that the level of coupling between the input and the generated waves depends entirely on the phase shift between them. This phase shift is defined by the effective refractive indices of the two coexisting guided modes. The coherence length is given by  $L_c = \lambda_f / 2(n_s - n_f)$ , where  $n$  is the effective refractive index. Because of the nature of the problem, propagation occurs in only one direction. Several numerical experiments have shown that negligible gain in accuracy is achieved by applying the 4<sup>th</sup> order scheme to the transverse direction. Figures 1 to 3 summarize the effectiveness of the 4<sup>th</sup> order scheme in speeding up convergence. In the figures, the grid factor is defined as the ratio of the wavelength to the spatial step size. For this particular problem, a grid factor of 80 in the 4<sup>th</sup> order scheme is sufficient to ensure low levels of numerical dispersion. By applying the 4<sup>th</sup> order scheme to the spatial derivatives in the propagation direction only, an overall increase of 11% in computation time per time step is expected, but no additional memory resources are necessary. As shown in figure 4, this additional computation time is insignificant if compared to the savings made by relaxing the spatial step and hence the time step. For the same error tolerance, the 4<sup>th</sup> order scheme uses spatial steps with more than double the size required by the 2<sup>nd</sup> order scheme.

### 4. CONCLUSIONS

A 4<sup>th</sup> order accurate FDTD simulation algorithm for the solution of the phase-dependent SHG problem has been presented. This algorithm guarantees the convergence of the solution using significantly less computation time and less memory requirement as compared to 2<sup>nd</sup> order schemes.

## ACKNOWLEDGEMENT

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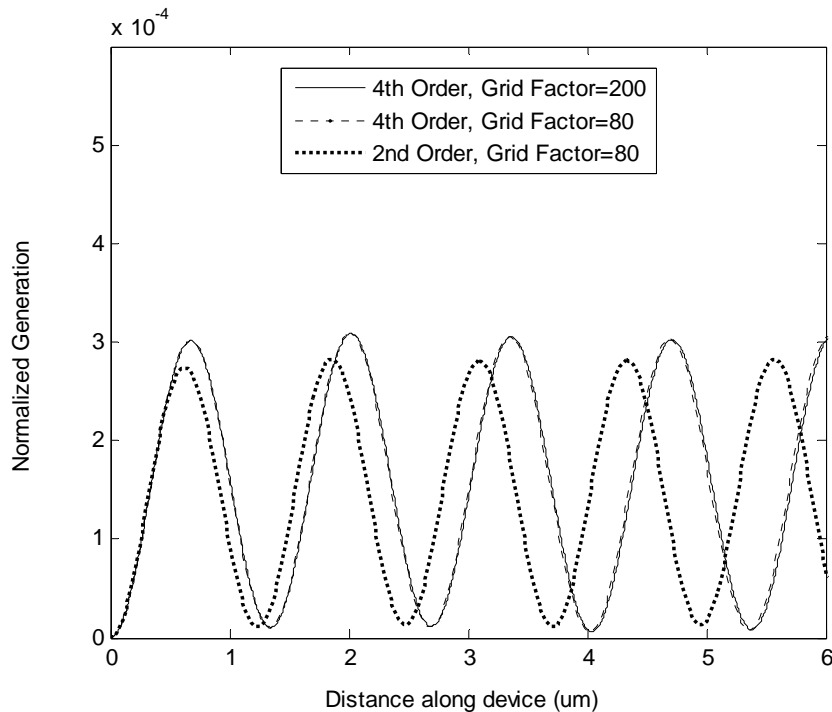


Figure 1. SHG results for 2<sup>nd</sup> and 4<sup>th</sup> order FDTD schemes

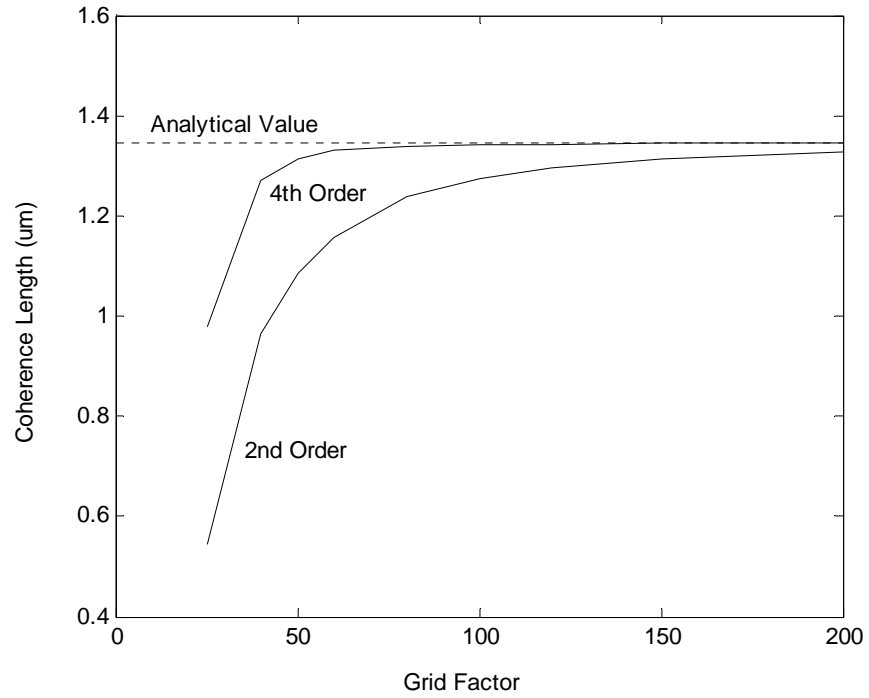


Figure 2. Coherence length vs. Grid factor using 4<sup>th</sup> order (solid) and 2<sup>nd</sup> order (dashed) schemes

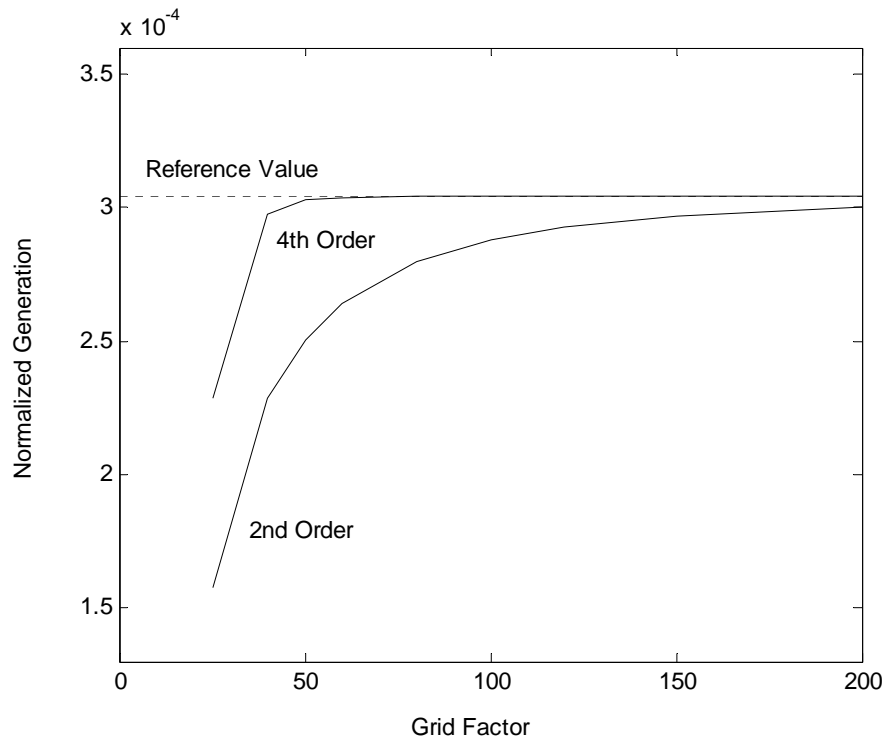


Figure 3. Peak value of second harmonic power vs. Grid factor using 4<sup>th</sup> order (solid) and 2<sup>nd</sup> order (dashed) schemes

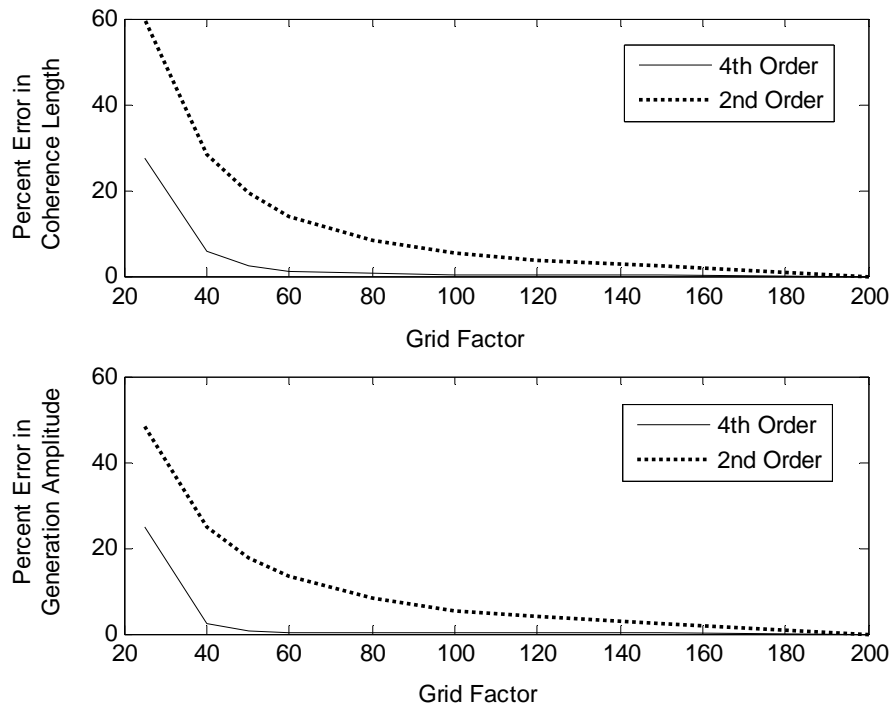


Figure 4. Error analysis for 4<sup>th</sup> order (solid) and 2<sup>nd</sup> order (dashed) schemes