RECENT DEVELOPMENTS IN FDTD-RELATED SCHEMES

FOR TIME-DOMAIN ANALYSIS OF

FREQUENCY CONVERSION IN NONLINEAR OPTICAL STRUCTURES

Tae-Woo Lee[(1)] and Susan C. Hagness[(2)]

[(1)] University of Wisconsin-Madison, Electrical and Computer Engineering,
1415 Engineering Drive, Madison, WI, 53706, USA
Email: tae-woo@cae.wisc.edu

[(2)] As (1) above, but E-mail: hagness@engr.wisc.edu

Abstract: The numerical dispersion inherent in the finite-difference time-domain (FDTD) method is problematic in modeling phase-sensitive nonlinear frequency conversion processes such as second-harmonic generation. Rather than resorting to extremely fine FDTD grids to overcome this difficulty, we propose a pseudo-spectral time-domain method with fourth-order accuracy in time (PSTD-4) for solving Maxwell's equations in nonlinear media. Due to its drastically reduced numerical dispersion error, PSTD-4 offers high levels of accuracy with coarser grid resolutions and larger time steps compared to PSTD-2 and FDTD. Accordingly, preliminary results suggest that PSTD-4 is significantly more computationally efficient for modeling frequency conversion in nonlinear optical structures.

Significant progress has been made over the last decade in finite-difference time-domain (FDTD) algorithms for modeling electromagnetic wave interactions with nonlinear optical materials [1]. These modeling capabilities have been successfully applied to a variety of second- and third-order nonlinear phenomena, including optical switching in nonlinear photonic bandgap structures, temporal and spatial soliton propagation, self-focusing of optical beams, pulse propagation through nonlinear corrugated waveguides, and pulse-selective behavior in nonlinear Fabry-Perot cavities. However, the numerical phase velocity error associated with FDTD remains problematic in accurately modeling phase-sensitive nonlinear frequency conversion processes such as second-harmonic generation [2].

The implications of numerical phase velocity errors in simulations of nonlinear frequency conversion processes can be clearly seen with a simple example. Consider the case of two waves oscillating at the fundamental and second harmonic frequencies. If these interacting optical waves propagate with the same phase velocities through a second-order nonlinear material, they will be perfectly phase matched and the coherence length (that is, the maximum distance over which second-harmonic generation is efficient) will be infinite. If these interacting optical waves propagate with different phase velocities, a phase mismatch will arise and the second-harmonic-generation efficiency will be reduced. In an FDTD simulation of a bulk nonlinear material exhibiting no material dispersion, the waves will experience a phase mismatch due to numerical dispersion. Consequently, the FDTD simulation will erroneously predict a finite coherence length. Likewise, when modeling wave propagation in an environment where physical (i.e. material or waveguide) dispersion is present, the actual phase mismatch will be perturbed by the presence of numerical dispersion, resulting in inaccurate estimates of the physical coherence length and frequency conversion efficiency. To overcome these problems, the standard FDTD method requires an extremely fine grid resolution, which significantly increases the computational burden.

In this paper, we present a computationally efficient solution to this problem based on the pseudo spectral time-domain (PSTD) method [3]. In contrast to the standard FDTD method which relies on second-order-accurate centered differences to approximate spatial derivatives, the PSTD method uses Fourier transforms which ideally provide infinite-order accuracy in space for grid-sampling densities of two or more points per wavelength. Hence, numerical phase velocity errors arise only from the central difference approximations used for the time derivatives. We propose a PSTD scheme with fourth-order accuracy in time, which we denote as PSTD-4, for solving Maxwell's equations for a second-order nonlinear material. For comparison purposes, we also adapt the existing PSTD-2 scheme, which uses Yee-type second-order-accurate leapfrog time-stepping, for modeling nonlinear optical materials. While the PSTD-4 algorithm requires additional FFT subroutine calls for each field update and therefore more CPU time per time step than PSTD-2, its exceptionally high accuracy permits the use of a much larger time step than that which would be required by PSTD-2 to achieve the same level of accuracy, thereby offering a significant reduction in the comp utational burden involved in accurately modeling nonlinear frequency conversion processes.

We illustrate this claim with the following 1-D example. Specifically, we compare FDTD, PSTD-2, and PSTD-4 in modeling second-harmonic generation in a homogeneous grid comprised of a nondispersive second-order nonlinear material. Assuming a fixed stability factor, the FDTD grid cell size required for achieving accuracy comparable to the PSTD-4 method is approximately 14 times smaller than that used in the PSTD-4 simulation. In the PSTD-2 model, the time step required for achieving comparable accuracy is approximately 10 times smaller than that used in PSTD-4, assuming that the same grid resolution is used in both schemes. The total number of time steps required to achieve less than 1.5 % error over a 300 micron propagation distance are 168,000 for FDTD, 188,400 for PSTD-2, and 18,840 for PSTD-4. CPU run times per time step on a SUN Ultra80 workstation are 16.5 ms, 4.9 ms, and 7.0 ms for FDTD, PSTD-2, and PSTD-4, respectively. Therefore in this example, PSTD-4 is 7 times faster than PSTD-2 and 21 times faster than FDTD in overall CPU time.

Acknowledgments: This work was supported by the National Science Foundation Presidential Early Career Award for Science and Engineers ECS-9985004.

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