# PSTD Modeling of Nonlinear Electrodynamics

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Frequency conversion processes in nonlinear materials are extremely sensitive to the phase velocities of interacting electromagnetic waves. In order to accurately model such problems using FDTD, extremely fine grid resolutions are required to minimize the effects of numerical dispersion. We have recently shown that PSTD methods with second-order (PSTD-2) and fourth-order (PSTD-4) accuracy in time offer significant improvements in computational efficiency and accuracy for modeling electromagnetic wave interactions in frequency-independent $c^{(2)}$ nonlinear optical materials (T. W. Lee and S. C. Hagness, *IEEE Antennas and Propagation Society International Symposium*, vol. 3, pp. 232-235, San Antonio, TX, June 2002). However, accurate simulations require not only minimizing numerical dispersion, but also incorporating the material dispersion characteristics inherent in optical media.

In this paper, we present an algorithm extension of our previous work. Specifically, we incorporate the physics of material dispersion into the nonlinear PSTD-4 method using an auxiliary differential equation (ADE) technique. The dispersion model used in this study is that of a Lorentz medium. The ADE approach offers the ability the model the linear susceptibility of the Lorentz dispersion and the instantaneous nonlinear susceptibility. The ADE approach used here differs from previous techniques (for example, see P. M. Goorjian, A. Taflove, R. M. Joseph, and S C. Hagness, *IEEE J. Quantum Electronics*, 28: 2416-2442, 1992) in that it is developed for PSTD rather than FDTD and is applied to a second-order nonlinearity rather than a third-order nonlinearity. Also, it does not require iteratively solving a nonlinear constitutive relation.

In this talk, the computational features of the PSTD-4 algorithm will be discussed. The accuracy and computational efficiency are evaluated by modeling second harmonic generation in a simple nonlinear waveguide with a quasi-phase matched grating. The results show that even though a second-order-accurate time discretization is applied in the ADE approach, PSTD-4 still provides accurate results with a relatively large time step compare to PSTD-2. In some cases, it is found that the stability limit becomes sensitive to the choice of Lorentz dispersion parameters. This sensitivity is impacted by how the central differencing is implemented in the ADE.

In addition, we will present a few application examples illustrating the use of the PSTD-4 algorithm for modeling frequency conversion processes in nonlinear dispersive media. The first-principles modeling tool developed in this study can help provide invaluable insights about the complex wave phenomena inherent in photonic nonlinear-micro/nanostructures such as nonlinear photonic crystals.