Applications of the nonlinear finite difference time domain (NL-FDTD) method to pulse propagation in nonlinear media: Self-focusing and linear-nonlinear interfaces

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In an effort to meet an ever increasing demand for more accurate and realistic integrated photonics simulations, we have developed a multidimensional, nonlinear finite difference time domain (NL-FDTD) Maxwell's equations solver. The NL-FDTD approach and its application to the modeling of the interaction of an ultrashort, optical pulsed Gaussian beam with a Kerr nonlinear material will be described. Typical examples from our studies of pulsed-beam self-focusing, the scattering of a pulsed-beam from a linear-nonlinear interface, and pulsed-beam propagation in nonlinear waveguides will be discussed.

1. INTRODUCTION

With the continuing and heightened interest in linear and nonlinear semiconductor and optically integrated devices, more accurate and realistic numerical simulations of these devices and systems are in demand. Such calculations provide a test-bed in which one can investigate new basic and engineering concepts, materials, and device configurations before they are fabricated. This encourages multiple concept and design iterations that result in enhanced performances and system integrations of those devices. They also provide a framework in which one can interpret complex experimental results and suggest further diagnostics or alternate protocols. Thus the time from device conceptualization to fabrication and testing could be enormously improved with numerical simulations that incorporate more realistic models of the linear and nonlinear material responses and the actual device geometries.

To date, most of the modeling of pulse propagation in and scattering from complex linear and nonlinear media has been accomplished with one-dimensional, scalar models. These models have become quite sophisticated; they have predicted and explained many of the nonlinear as well as linear effects in present devices and systems. Unfortunately, they cannot be used to explain many observed phenomena, and expectations are that they are not adequately modeling linear and nonlinear phenomena that could lead to new effects and devices. It is felt that vector and higher-dimensional properties of Maxwell's equations that are not currently included in existing scalar models, in addition to more detailed materials models, may significantly impact the scientific and engineering results. Moreover, because they are limited to simpler geometries, current modeling capabilities are not adequate for linear/nonlinear optical-component engineering design studies.

In this paper we describe numerically obtained, multidimensional, full-wave, vector Maxwell's equations solutions to problems describing the interaction of ultrashort, pulsed beams with a nonlinear Kerr material having a finite response time. These numerical solutions
have been obtained [Ziolkowski and Judkins, 1992a, b, c, 1993a, b, c] in two space dimensions and time with a nonlinear finite difference time domain (NL-FDTD) method which combines a generalization of a standard, FDTD, full-wave, vector, linear Maxwell's equations solver with a currently used phenomenological time relaxation (Debye) model of a nonlinear Kerr material. This NL-FDTD approach has been used to obtain numerical solutions in two space dimensions and time for nonlinear self-focusing in bulk, thermal Kerr media, for normal and oblique incidence linear-nonlinear interface problems, and for the propagation of pulses in nonlinear waveguiding strutures. Although these basic geometries are straightforward, the NL-FDTD approach can readily handle more complex, realistic structures.

The NL-FDTD method is beginning to resolve several very basic physics and engineering issues concerning the behavior of the full electromagnetic field during its interaction with a nonlinear medium. The various examples of transverse electric (TE) and transverse magnetic (TM) nonlinear optics problems described by Ziolkowski and Judkins [1992a,b,c, 1993a,b,c] highlight the differences between the scalar and the vector approaches, the effects of polarization, and the effects of the finite response time of the medium. Applying the NL-FDTD approach to self-focusing problems in bulk media, (1) we have shown the existence of back reflected power from the nonlinear self-focus when the medium is responding nearly instantaneously to the applied optical field; (2) we have discovered optical vortices are formed in the trailing wakefield behind the nonlinear self-focus; and (3) we have identified that the longitudinal field component plays a significant role in limiting the self-focusing process. Applying the NL-FDTD approach to both the TM and TE nonlinear interface problems, (1) we have characterized the performance on an optical diode (linear-nonlinear interface switch) to single-cycle pulsed Gaussian beams including the appearance of a nonlinear Goos-Hänchen effect, the stimulation of stable surface modes, and the effects of a finite response time of the Kerr material; (2) we have shown definitively that the linear-nonlinear interface does not act like an optical diode for a tightly focused, single-cycle pulsed Gaussian beam; and (3) we have characterized the performance of some basic linear-nonlinear slab waveguides as optical threshold devices.

In all of these analyses we have identified the role of the longitudinal field component (which is not taken into account in the scalar models), and the resulting transverse power flows in the associated scattering-coupling processes.

The Debye model for the Kerr nonlinearity is a standard choice and has been used to investigate finite response effects in Kerr media by several groups [e.g., Mitchell and Moloney, 1990, Hayata et al., 1990, Hayata et al., 1992]. Nonetheless, we have been extended this NL-FDTD model recently [Ziolkowski and Judkins, 1993b] to materials described by a Lorentz linear dispersion model and a Raman nonlinear model. Thus the NL-FDTD model can now deal with librational effects [Reintjes, 1984] as well as many other known nonlinear behaviors.

There have been a number of groups dealing with the numerical modeling of optical wave propagation in nonlinear materials using the full-wave, vector, time-independent Maxwell's equations by Miyagi and S. Nishida [1974, 1975] and Pohl [1970] and using the vector paraxial equations by Pohl [1972], Sodha et al. [1974], Hayata and Koshiba [1988], and Hayata et al. [1990]. These efforts have provided, for instance, the modal fields present in nonlinear waveguides and the resulting propagation behavior of beams in those guides. In contrast, the NL-FDTD approach is time dependent and accounts for the complete time evolution of the system as a pulse propagates in a Kerr medium having a finite response time with no envelope approximations. In particular, it provides a complete picture of the pulse behavior during the nonlinear self-focusing process and the scattering from a linear-nonlinear interface. Note that, because of the nonlinearities, such a pulse solution cannot be obtained from any sequence of single frequency, time-independent results; it can only be obtained from a direct time integration of Maxwell's equations. Thus, these time-independent and time-
dependent modeling approaches yield additional and complementary information.

Related modeling of optical pulse propagation in nonlinear media has also been reported [Goorjian and Taflove, 1991, 1992a, 1992b; Goorjian et al., 1992a; Goorjian et al., 1992b; Goorjian et al., 1993; and Jamid and Al-Bader, 1993]. The work by Goorjian and his coworkers (to date) has emphasized modeling soliton propagation effects; they have recovered one-dimensional solitons (one space dimension and time) and solitons in two-dimensional TE guiding structures. One-dimensional nonlinear soliton propagation has also been modeled with a FDTD approach by Hile and Kath [1993]. They have shown that the one-dimensional model recovers known nonlinear Schrödinger equation results. Nonlinear guided-wave structures are also being modeled now by several groups [e.g., Ziolkowski and Judkins, 1992b, c, 1993b; Goorjian et al, 1992a; Goorjian et al., 1993; and Jamid and Al-Bader, 1993]. The interest in these nonlinear guided wave structures stems from their potential applications to integrated photonics devices and circuits. Because of the versatility of the NL-FDTD approach, all of these groups hope to be able to simulate the behavior of more complicated nonlinear guided wave structures and devices in the near future.

2. NL-FDTD APPROACH

The NL-FDTD method discussed by Ziolkowski and Judkins [1992a, b, c, 1993a, c] solves numerically Maxwell's equations

\[
\frac{\partial}{\partial t} [\mu_0 \vec{H}] = -\nabla \times \vec{E} \tag{1}
\]

\[
\frac{\partial}{\partial t} [\varepsilon_L \vec{E}] = \nabla \times \vec{H} - \frac{\partial}{\partial t} \vec{P}^{NL}, \tag{2}
\]

where the nonlinear polarization term \( \vec{P}^{NL} = \varepsilon_0 \chi^{NL} (\vec{r}, t, |\vec{E}|^2) \vec{E} \) is specified by solving simultaneously a Debye model for the third-order, nonlinear susceptibility \( \chi^{NL} \) of the Kerr medium:

\[
\frac{\partial}{\partial t} \chi^{NL} + \frac{1}{\tau} \chi^{NL} = \frac{1}{\tau} \varepsilon_2 |\vec{E}|^2. \tag{3}
\]

The nonlinear susceptibility \( \chi^{NL} \) is incorporated most simply in the FDTD approach by introducing the effective permittivity and conductivity of the Kerr medium

\[
\varepsilon_{eff} = \varepsilon_L + \varepsilon_0 \chi^{NL} \tag{4}
\]

\[
\sigma_{eff} = \varepsilon_0 \frac{\partial}{\partial t} \chi^{NL}, \tag{5}
\]

where \( \varepsilon_L \) is the linear permittivity, and by rewriting Maxwell's equations in the form

\[
\frac{\partial}{\partial t} \vec{H} = -\frac{1}{\mu_0} \nabla \times \vec{E} \tag{6}
\]

\[
\frac{\partial}{\partial t} \vec{E} = \frac{1}{\varepsilon_{eff}} \nabla \times \vec{H} - \frac{\sigma_{eff}}{\varepsilon_{eff}} \vec{E}. \tag{7}
\]

This approach models the medium as having a finite response time \( \tau \). If \( T \) represents the pulse width, then by setting \( T \gg \tau \), one obtains an instantaneous response model: \( \chi^{NL} \approx \varepsilon_2 |\vec{E}|^2 \), that is, the medium follows the pulse. On the other hand, if \( T \ll \tau \), then the finite response time effects are maximal, and the medium's response significantly lags the pulse. The NL-FDTD approach can treat both extremes. Moreover, the divergence equation associated with this system includes the nonlinear source term: \( \nabla \cdot [\varepsilon_L \vec{E}] = -\nabla \cdot \vec{P}^{NL} \), which in the TM case provides the mechanism that couples the longitudinal to the transverse electric field components.

Because of the quadratic nature of the nonlinearity in (3), the nonlinear susceptibility, hence, permittivity must be strictly positive. However, the nonlinear conductivity, which from (5) is obtained as the time derivative of the nonlinear susceptibility, can be both positive and negative. This represents both loss and gain, respectively, in the medium. In the absence of any other dispersion mechanism, one would then expect some erosion of the pulse amplitude in the pulse's leading half as it propagates in this Kerr medium. On the other hand, the conductivity changes its sign along the trailing half of the pulse. This causes growth in the pulse amplitude and a shocklike structure to form along the trail-
ing portion of the pulse. The sharpness and intensity of this shocklike structure depends on the finite response time; the structure will be more peaked the more instantaneous the medium’s response is.

In two space dimensions and time with the coordinates \((x,z,t)\) and with the choice of a TMz-polarized wave, the NL-FDTD method solves for the complete time history of each of the components \((E_z, E_z, H_y)\). The equations for a TEz-polarized wave can be obtained by reciprocity: \(E \rightarrow H\) and \(H \rightarrow -E\), and they lead to the NL-FDTD solution of the components \((E_y, H_x, H_z)\). Whereas the nonlinear source term strongly couples the transverse and longitudinal electric field components in the TM case, the corresponding magnetic field components in the TE case are driven by the transverse electric field component which exhibits the nonlinear growth. Additionally, when the linear-nonlinear interface problem is treated, Maxwell’s equations naturally provide the boundary conditions appropriate for this lossy dielectric interface. Thus the linear-nonlinear interface problem can be handled without imposing any additional constraints on the fields. Moreover, more complex structures can be added to the simulation with little difficulty, giving the NL-FDTD approach a great deal of flexibility, particularly in comparison to the scalar models.

Note that the model defined by (1)-(7) ignores any linear dispersion effects and have taken the linear permittivity to be a constant \(\varepsilon_L = \varepsilon_0\). This physically means that it is appropriate only for propagation distances shorter than the dispersion length of the material. As noted above, we have incorporated Lorentz linear dispersion and Raman nonlinearity models into the NL-FDTD approach [Ziolkowski and Judkins, 1993b]. We had investigated the nuances of a number of techniques introduced recently for modeling dispersive effects in the linear FDTD method by Luebbers et al. [1990], Kashiwa and Fukai [1990], Lee et al. [1991], and Joseph et al. [1991] and developed a stencil set that allows simultaneous solution of these models with Maxwell’s equations. In particular, we are now solving in a self-consistent manner the system of equations:

\[
\frac{\partial}{\partial t} \left[ \mu_0 \mathbf{H} \right] = -\nabla \times \mathbf{E} \quad (1')
\]

\[
\frac{\partial}{\partial t} \left[ \varepsilon_L \mathbf{E} \right] = \nabla \times \mathbf{H} - \frac{\partial}{\partial t} \mathbf{P} \quad (2')
\]

\[
\frac{\partial^2}{\partial t^2} \mathbf{P} + \Gamma_L \frac{\partial}{\partial t} \mathbf{P} + \omega_L^2 \mathbf{P}_L
\]

\[
= \varepsilon_0 \chi_0 \omega_L^2 \mathbf{E} \quad \text{Lorentz model} \quad (8)
\]

\[
\frac{\partial^2}{\partial t^2} \chi_{NL} + \Gamma_R \frac{\partial}{\partial t} \chi_{NL} + \omega_R^2 \chi_{NL}
\]

\[
= \varepsilon_R \omega_R^2 \mathbf{E}^2 \quad \text{Raman model}, \quad (9)
\]

where \(\mathbf{P} = \mathbf{P}_L + \mathbf{P}_{NL}\) and \(\mathbf{P}_{NL} = \varepsilon_0 \chi_{NL} \mathbf{E}\). Details concerning this extended NL-FDTD model will be given in several manuscripts currently under preparation. Goorjian and his coworkers have also developed a similar capability to model pulse propagation under the influence of linear and nonlinear dispersive, linear and nonlinear diffractive, and time retardation effects in the medium.

Because of the versatility of the FDTD approach, we have been able to “turn on” the dispersion effects to analyze their impact on the self-focusing and the linear-nonlinear interface reflection-transmission processes. The results we describe below have been reaffirmed by the more complex NL-FDTD model defined by (1’), (2’), (8), and (9).

The NL-FDTD results to be reported below were obtained by carefully designing and testing the numerical grid, material parameters, and the algorithm based upon (1)-(7) to insure stability, accuracy, and efficiency. The basic stencils of the NL-FDTD algorithm in both the TE and the TM polarization cases are shown in Figure 1. These standard stencils represent two staggered grids: one for the electric field components and one for the magnetic field components. These are the standard choices associated with the two-space dimensional linear FDTD algorithm. The discrete versions of the TE and the TM forms of equations (3), (6), and (7) are centered in space and time on this numerical grid. In the TM case, the electric field components \(E_z\) and \(E_z\)
Electric field components are averaged to obtain effective values at the location of the nonlinear susceptibility

Electric field is evaluated at the same location as the nonlinear susceptibility

Fig. 1. The NL-FDTD TE and TM unit cell stencils.

3. NL-FDTD RESULTS

We will specifically present NL-FDTD results obtained for the scattering of a pulsed Gaussian beam normally incident on a linear-nonlinear interface. This problem combines both the linear-nonlinear interface scattering and the nonlinear self-focusing effects. Interest in the linear-nonlinear interface problem is stimulated by the need to assess the potential of this geometry for an all-optical switch. If the pulse amplitude is below the critical value for the medium, the beam senses no interface and passes through unscathed. If the pulse amplitude is above the critical value for the medium, the beam experiences a strong reflection from the interface; and the transmitted beam experiences self-focusing.

In all of the interface problems we have considered, it has been assumed that the interface was in the far field of the source [Ziolkowski and Judkins, 1992d]. We thus used a single bipolar pulse excitation for the single-cycle cases. This initial pulse was given by the function

\[ F(t) = x (1 - x^2)^{3/2} H(1 - |x|) \]

where \( H(x) \) is Heaviside's function. A total pulse width \( T = 20.0 \) fs corresponds to an effective wavelength of 4.0 \( \mu \)m. This initial driving function has both first and second time derivatives
continuous at its endpoints, thus reducing the numerical noise initially generated in the grid. Note that the NL-FDTD approach can handle these single-cycle cases as readily as multiple-cycle cases which include pulses having an intrinsic carrier wave. Since most current optical systems deal directly with a carrier-wave type signal, the NL-FDTD approach can simulate the propagation and scattering effects associated with those systems. It can also simulate the behaviors of single-cycle optical devices and systems. The single cycle results represent behaviors that should be observed with optical systems currently under investigation and those being developed for future studies by the international optics community. However, in either case the full pulse is modeled with the NL-FDTD approach rather than only the envelope of the carrier wave, as it is with the nonlinear Schrödinger equation models. This enhanced modeling capability of the NL-FDTD approach allows one to model and distinguish the effects that arise in both the single- and multiple-cycle cases.

A variety of TE and TM cases have been considered to establish the effects of the medium response time. This is accomplished simply by varying \( r \) with respect to the input pulse width \( T \). In particular, we have run cases with \( T = 0.2r \) to \( T = 20.0 \, r \). These choices provided access to the nonlinear phenomena associated with mediums exhibiting either finite or instantaneous response times. Several grid sizes have been explored to assess the numerical stability and accuracy of the NL-FDTD approach. We found that an average spatial resolution of \( \Delta z \leq \lambda/100 \) was needed instead of the standard \( \lambda/10 \) rule-of-thumb for the wavelengths of interest, particularly in the instantaneous medium response cases. The signals steepened so quickly that this enhanced resolution was necessary to maintain the second-order accuracy of the FDTD approach. The grid size used in our linear-nonlinear interface model below was 1500 \( \times \) 2000, where \( \Delta x = \Delta z = 0.020 \, \mu m \) or 30.0 \( \mu m \) \( \times \) 40.0 \( \mu m \). This discretization provided an effective spatial resolution of \( \Delta z = \lambda/160 \) for the finite time pulse (4) that we considered. A Courant stability condition (the time step must be chosen for a two-dimensional problem with \( \Delta z = \Delta z \) so that \( \Delta t \leq \Delta z/\sqrt{2}c \) of \( \Delta t/(\Delta z/c) = 0.38 \) was selected; this means we chose \( \Delta t = 0.045 \, fs \) and \( \Delta t = 0.018 \, fs \), respectively. We found that the algorithm did not model the physics well when it was run at the linear equation Courant limit, but did for values \( \Delta t/(\Delta z/c) \leq 0.50 \). The nonlinear version of the Courant limit is not known at this time. With four unknowns and additional overhead, the corresponding total memory requirement was approximately 10.0 MWords. The time requirement is proportional to the number of unknowns and the number of time steps. This 10.0 MWord problem took approximately 510 CONVEX/240 cpu minutes to compute 7550 time steps, approximately 0.5 \( \mu s \) per unknown. In terms of the problem parameters, this corresponds to the pulse propagating 40 \( \mu m \) \( \sim \) 7 \( cT \) with a resolution of 240 cells over the spatial pulse width \( cT = 6.0 \, \mu m \). The run time would be approximately a factor of 10 less using a single processor of a CRAY YMP/8-32.

The NL-FDTD results for an above-threshold, normally incident, pulsed TM Gaussian beam, linear-nonlinear interface results are shown in Figures 2a-2d. In each part the field structure in a windowed region of the overall simulation space is represented by a contour plot of the total electric field intensity \( I = |E_x|^2 + |E_z|^2 \). The incident beam field is shown in Figure 2a. It represents a Gaussian tapered (space), bipolar (time) pulse with an initial transverse waist \( w_0 = 10.0 \, \mu m \) and a total initial pulse width \( T = 20.0 \, fs \). For the results presented below the nonlinear medium parameters were set to the nearly instantaneous-regime value \( r = 0.2 \, T \), i.e., \( T = 5.0r \), and \( e_2 = 2.0 \times 10^{-18} \, (m/V)^2 \), and we set the input electric field amplitude to \( E_0 = 9.33 \times 10^8 \, (V/m) = 2.8 \, Ecrit \) in the Kerr medium.

The interaction of the TM pulsed beam at the linear-nonlinear interface is shown in Figure 2b for a time just after the beam scatters from the interface which is located at \( z = 0 \). The reflected and transmitted pulsed beam fields are apparent. The transmitted pulsed beam begins to self-focus as it propagates into the Kerr medium as shown
in Figure 2c. The intensity pattern in the focus region is shown in Figure 2d. Figures 2c and 2d recover the well-known horn pattern in which the front (large z) portion corresponds to the linear diffraction region, and the rear (smaller z) portion incorporates the nonlinear effects.

We have found that the growth of the longitudinal electric field component causes transverse power flows and reflections from this self-focusing region [Ziolkowski and Judkins, 1992a, b, c, 1993a, b, c]. Self-focusing is restrained by these nonlongitudinal power flow mechanisms since they channel power away from the focus. By studying the Poynting's vector $\vec{S} = E_x H_y \hat{z} - E_y H_x \hat{z}$ in the instantaneous response cases, we have demonstrated the existence of nonlinear optical vortices in the wake field of the focal region [Ziolkowski and Judkins, 1993c]. Negative longitudinal power flow occurs on the horn boundary, in the region around the focus, and in the wake field of the focus. Pure reflection occurs immediately behind the region of the maximum field intensity. Part of the negative flow in the focal region feeds the focus (power must be channeled into the focal region to produce the growth in the field components there), and part is channeled into the vortices. Positive longitudinal power flow occurs everywhere else and is particularly strong immediately within the focal region, where the nonlinear field growth occurs.

These vortices can be described in terms of turbulence in the power flow of the electromagnetic field in the self-focus region. The front portion of the incident beam generates a tapered
waveguide which focuses the rest of the pulse. When the nonlinearity is nearly instantaneous and the field levels are large, the rate of the taper becomes very large. Thus the number of modes accessible to the beam increases. As the taper converts some of the field structure into these higher-order modes, nulls in the field components can develop. The presence of convective power flow is immediate and leads to the formation of the vortices. This behavior can occur whenever the power flow encounters a discontinuity in the guided-wave structure [Ziolkowski and Grant, 1986]. Vortices in nonlinear media have also been identified by several other groups [e.g., Coullet et al., 1989, Brambilla et al., 1991, Akhmanov et al., 1992, and McDonald et al., 1992]. These vortices are observed in the field patterns derived from the scalar nonlinear Schrödinger equation in planes transverse to the direction of propagation. In contrast, the vortices observed in the self-focus region are a direct result of the transverse power flow, which is intimately connected to the longitudinal field components, and are found in the planes containing the propagation axis.

Typical self-focusing results for the normal incidence problem are summarized in Figure 3 in which the waist of the energy of the pulsed beam is plotted as a function of its location along the direction of propagation. For low intensity, the beam diffracts as though it were in free space; for high intensity, some portion of the beam reflects, and the transmitted beam self-focuses in the Kerr medium. The actual reflection coefficient is substantially below the value anticipated from an equivalent monochromatic beam. This is due primarily to the fact that the pulse does not cause the medium to respond instantly; hence, much of the energy penetrates into the medium before the boundary is sufficiently reflective. The transmitted beam behaves as predicted from previously reported self-focusing beam propagation simulations.

![Figure 3. The normal incidence problem is divided into two regions: the incident region which is linear and the transmission region which is nonlinear. The linear index is continuous across the interface so that a low-intensity beam will propagate unchanged. As the intensity increases, the pulse experiences some reflection and the transmitted pulse will self-focus if the initial transmitted field amplitude is above threshold.](image-url)
4. CONCLUSIONS

Although the current NL-FDTD models are two-dimensional, we believe that the observed transverse power flow mechanisms, which remove power from the focal region, limit the self-focusing process and will prevent catastrophic focusing in three dimensions. This, in contradiction to the scalar nonlinear Schrödinger equation models, means the pulsed beam will not be focused to a point by the self-focusing process. Proof and comparisons with standard paraxial scalar models in three space dimensions await adequate computing resources.

We have completed our modeling of the scattering of an obliquely incident, focused, pulsed Gaussian beam from a linear-nonlinear interface. Our NL-FDTD calculations indicate that the anticipated switching properties of this optical diode switch are unrealizable with a tightly focused beam. These results recover the conclusions given theoretically by Tomlinson et al. [1982] and experimentally by Smith et al. [1981]. There is simply too much energy leakage into the medium from the initial pulsed beam components having wave vectors beyond critical and from the nonlinear coupling to the medium. Related nonlinear waveguide simulations, however, have recovered expected solitarylike wave emissions from a linear waveguide channel into a background nonlinear substrate. This linear-nonlinear interface class of problems has potential applications to nonlinear guided-wave couplers.

Our future efforts will include several directions. We will use the NL-FDTD model to study the interplay between the dispersive and the nonlinear effects of the medium in the presence of intense, applied optical pulsed beams. We will begin to include microscopic materials models in the NL-FDTD algorithm to study quantum effects associated with these systems. We will also be applying the NL-FDTD model to realistic device configurations; this will require modeling more complex propagation and scattering geometries.

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