Numerical Validations of a Nonlinear PML Scheme for Absorption of Nonlinear Electromagnetic Waves

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***Abstract*— There have been several algorithms which extend the finite-difference time-domain (FDTD) solution of Maxwell's equations to nonlinear electromagnetic problems. Relative to other methods, FDTD achieves robustness by directly solving for the fundamental quantities, electric field E, and magnetic field H in space and time, rather than performing asymptotic analyses or assuming paraxial propagation and nonphysical envelope functions. As a result, the FDTD method is almost completely general and can account for any type of electromagnetic problems. As in linear cases, for a practical simulation, nonlinear FDTD modeling also requires the development of absorbing boundary conditions (ABC's) to effectively absorb the nonlinear electromagnetic waves for open nonlinear structures. In this paper, based on the Berenger's perfectly matched layer (PML), a nonlinear PML (nPML) absorbing scheme is presented and then implemented in the transmission-line matrix (TLM)-based FDTD method. Numerical results are given to demonstrate the effectiveness of the nPML proposed.**

***Index Terms*— Absorbing boundary, absorption, FDTD, nonlinear PML, TLM.**

I. Introduction

Due to the potential applications such as all-optical signal processing [1]–[3], properties of electromagnetic waves in nonlinear media have received increasing attention [1]–[10], [14], [15]. Since finding analytical solutions for nonlinear waves without certain approximations is difficult, numerical techniques, both in frequency domain [3]–[7] and in time domain [1], [8]–[10], [14], [15], have to be employed. Among the numerical techniques of time domain are various versions of finite-difference time-domain (FDTD) schemes [1], [8], [14], [15]. One of these techniques is the transmission-line matrix (TLM)-based FDTD method that combines features of both FDTD and TLM methods [16]. The method can account for very general electromagnetic problems and allows the direct use of field quantities and direct implementation of anisotropics for simulation and modeling of electromagnetic problems. Like the FDTD of Yee's scheme, the TLM-based FDTD has been successfully applied to the nonlinear electromagnetic-wave problems [14].

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In order to apply the above mentioned FDTD methods to open nonlinear structures (e.g., transmission-line structures), an appropriate absorbing boundary condition (ABC) is required to truncate an infinite computational domain for a practical simulation. Similar to the conventional ABC, the requirement for the nonlinear ABC is that it is able to effectively absorb nonlinear electromagnetic waves impinging on it.

Since the initial work by Berenger [12], the perfectly matched layer (PML) has been demonstrated in many cases to be the most effective ABC for linear electromagnetic-wave propagation [1], [13]. Standard PML's consist of lossy layers with both electric and magnetic conductivities [12]. By deliberately splitting the field quantities in Maxwell's equations and appropriately selecting loss parameters in PML regions, zero reflections between the PML layer and vacuum and between the PML layers themselves are achieved regardless of incident angles and frequencies, while the waves inside the PML region are attenuated as they propagate. When such an attenuation is made large enough with a sufficient number of the PML layers, the overall reflections from a PML absorbing boundary become extremely small, being several orders of magnitude lower than those achievable by other absorbing conditions developed thus far. Various numerical experiments have validated this claim.

Further studies and enhancements of the PML scheme have been recently reported. The so-called modified PML (MPML) is one of them [17]. In MPML, extra parameters for permittivity and permeability are introduced to enhance the absorption of the evanescent energy, but without affecting the absorption performance for propagation modes. The result is a further reduction of distance between the PML boundary and scatters, leading to the saving of central processing unit (CPU) time and memory.

In spite of all these developments, to the best knowledge of the authors, all the PML schemes reported thus far are applicable only to linear electromagnetic waves (where constitutive parameters are independent of field intensities); they cannot be directly applied to nonlinear open structures without modifications. In this paper, we present a nonlinear PML (nPML) scheme for the absorption of nonlinear electromagnetic waves. It is based on the MPML with the differences being that permittivity and permeability are now changed with time and, therefore, need to be updated at every time step of

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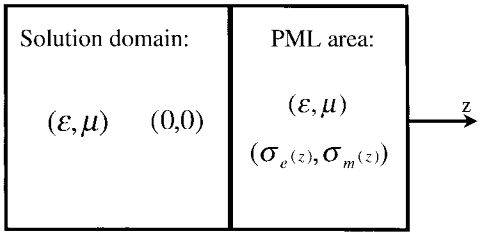


Fig. 1. The PML geometry.

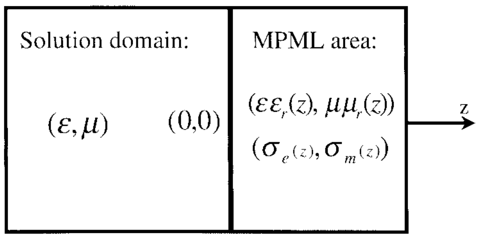


Fig. 2. The MPML geometry.

an FDTD simulation. The nPML scheme is implemented in the TLM-based FDTD scheme [16] developed in our research group. Numerical results confirm the effectiveness of nPML. Implementations of the nPML in other FDTD schemes such as Yee's scheme [1] can be done in the same way and should be straightforward. Note that the authors have presented the original form of the nPML scheme in [7]. However, in this paper, the nPML scheme is further enhanced by introducing the iterative technique into the nPML operations, in addition to the extensive numerical experiments, including soliton propagation.

II. The nPML Scheme

In the PML scheme developed thus far, the relationships between field component (E, H) and flux density (D, B) are linear. In other words, the constitutive parameters (μ, ε) of a medium are constantly independent of the field intensities. Therefore, the PML can absorb only linear electromagnetic waves. The formulation of such a PML first involves the splitting of the Maxwell's equations, and then the introductions of both electric and magnetic conductivity, as shown Fig. 1, where a PML is placed in the z-direction. As a result, the electromagnetic wave traveling in the z-direction will be attenuated very quickly without reflections in the PML region and thus absorbed.

To ensure zero reflections between layers, including the interface between the solution domain and the PML, the following matching condition must be satisfied [12]:

$$\frac{\sigma_e}{\varepsilon} = \frac{\sigma_m}{\mu}. \tag{1}$$

However, in the MPML, the extra relative dielectric constants $\varepsilon_r(z)$ and $\mu_r(z)$ are introduced and varied in the MPML region (see Fig. 2). The result is that absorption of evanescent energy is improved, while the absorption for propagation modes remains the same. The dielectric constant ε_r in the first layer at the interface between the solution domain and MPML region is chosen to be the same as the dielectric constant of the solution domain. It then gradually changes to bigger values along the direction to the end layer of the MPML. Reference [17] gives the details about the selection of the appropriate $\varepsilon(z)$ and $\mu(z)$. The relationship between E and D is not constant any more, but dependent on locations.

Again, to ensure the zero reflections, the following matching conditions must be met [17]:

$$\frac{\sigma_e}{\varepsilon} = \frac{\sigma_m}{\mu} \quad \varepsilon_r(z) = \mu_r(z) \tag{2}$$

which allows the determinations of other quantities, σ_e, σ_m, $\varepsilon_r(z)$, and $\mu_r(z)$.

Note that in (1) and (2), ε and μ are the permittivity and permeability of the linear background medium. They are not necessarily the vacuum permittivity and permeability.

Now, let us consider the situation of a nonlinear wave. For a nonlinear electromagnetic wave, the relationships between the field components (E, H) and flux densities (D, B) are no longer linear. That is, permittivity and permeability of a medium are not constants. In other words, they become not only location-dependent, but also dependent on the field intensity and, therefore, time. As a result, to enable a PML to absorb such nonlinear waves in a time-domain scheme, permittivity and permeability of a PML need to be changed with time or numerically to be updated at each time step.

In a nonlinear medium, E fields can be expressed in terms of electric flux densities plus terms related to linear and nonlinear polarizations. For simplicity, consider a one-dimensional (1-D) case where we can have

$$E_x = \frac{1}{\varepsilon_0 \varepsilon_\infty}(D_x - P_L - P_K - P_R). \tag{3}$$

Here, ε_∞ is the relative permittivity of a nonlinear medium when the operating frequency goes to infinity, P_L is the linear polarization term, P_K is the nonlinear polarization term corresponding to the so-called "Kerr effect," and P_R is another nonlinear polarization term due to the Raman scattering. Equation (3) can be numerically realized in an FDTD formulation with a recursive formula using Z-transform [9].

If the E and D are found at each time, the equivalent permittivity ε for the PML operations can be calculated as

$$\varepsilon = D/E. \tag{4}$$

Substituting it into the matching conditions (2), one can obtain the other parameters in the matching conditions for PML and then perform PML operations.

However, in an actual simulation, (4) asks for up-to-date ε, which is a function of the up-to-date electric field E. This E has to be updated at the current time step via the PML-split FDTD equations. Therefore, one needs to solve (2)–(4) and the split-PML FDTD equations simultaneously (instead of solving them separately) in order to obtain ε. One of the techniques is to use the iterative method. That is, first give an initial guessed value for ε, substitute it into (3) and the split-PML FDTD formulations to obtain the new E and D, and compute the second iteration value for ε with (4). Then, substitute this second value to (3) and the PML FDTD formulations, and compute the third value for ε with (4). Repeat the process until ε converges to a stable value. In our case, we use D/E on the PML layer left (which has been calculated) to the current PML layer as the first guess for ε and proceed with the iterations. However, numerical experience shows that in the cases we simulated, a single iteration is sufficient to give very good absorption of a nonlinear wave. This may be due to the fact that an FDTD mesh has to be made fine enough so that either linear or nonlinear waves have small spatial variations across two neighboring cells (otherwise, simulation results will not be correct because of the possible large numerical dispersion). As the result, the equivalent permittivity indicated by (4) will not be changed much between two neighboring cells (or two layers in our case), and the equivalent permittivity of the layer left to the current layer can be a very good guess for the equivalent permittivity of the current layer, leading to the fast convergence. In consequence, the nPML computation count does not increase in comparison with the linear PML. A specific example will be given in Section III.

As a summary, the nPML computation procedure for each time step can be described as follows.

1) Perform the regular nonlinear FDTD calculations in the solution domain.
2) Obtain ε at the solution-domain layer which interface with the nPML, and then use this value as the dielectric constant of the first layer of the nPML region.
3) Find all the other nPML parameters required for the first nPML layer based on the matching conditions (2) (in the same way as that for the linear MPML). Perform the nPML computation for the first layer using the above-mentioned iterative method.
4) Record the ratio of D to E of the first nPML layer and use it for the second nPML layer computation, again using the iterative method. Once done, record D/E of the second nPML layer.
5) Use D/E of the second nPML layer for the third nPML layer and repeat the similar computation steps for third, fourth, ..., until the last nPML layers. For each nPML layer, D/E of the previous layer is used as its guessed ε value.
6) Go back to 1) for next time step computation.

The above scheme has been implemented in the TLM-based FDTD method developed in our group. A three-dimensional (3-D) code is written and used to validate the proposed nPML, as described in the following sections. For comparison reasons, a simple 1-D nonlinear wave, temporal soliton, and spatial soliton, which had been studied before, were computed.

III. nPML Absorption of 1-D Nonlinear Waves

Consider a 1-D Kerr-type material that assumes an instantaneous nonlinear response. The nonlinearity here is modeled by the following very simple relation [1], [3]:

$$D = \varepsilon E \tag{5}$$

with $\varepsilon = n^2\varepsilon_0 = (n_0 + n_2|E|^2)^2\varepsilon_0$.

Here, n_0 is the linear part of the refractive index while n_2 is the nonlinear coefficient for Kerr-nonlinearity. n_0 is dimensionless and n_2 has units of m^2/V^2. Generally, the nonlinear term of (5) is very small compared to n_0 [1], [3]. Therefore, relative dielectric constant of the nonlinear medium can be obtained approximately as [1], [3]

$$\varepsilon \approx (n_0^2 + 2n_0n_2|E|^2)\varepsilon_0. \tag{6}$$

Assume that the nPML region is from layer 1 to layer m with layer 0 being in the problem domain. As discussed before, we then have

$$\varepsilon(z_{n+1})(\approx n_0^2 + 2n_0n_2|E(z_n)|^2)\varepsilon_0 \tag{7}$$

as the first guess of ε for layer $n+1$ $(n = 0, 1, 2, \cdots, m-1)$ at each FDTD time step. Since it is related to the instantaneous electric-field intensity, it varies with time.

The matching condition, which dictates the relationships among the electric conductivity, magnetic conductivity, permittivity, and permeability, remains the same as (2). In our simulation, 16 PML layers were used and $\sigma_{\max}$ was chosen to be 44640 s/m. The other PML parameters were taken the same as those in [17].

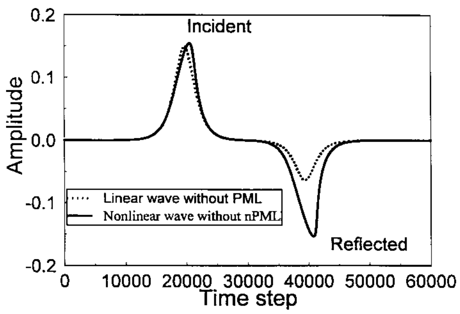
To further reduce the reflections, instead of placing perfect conducting wall as a termination for the last nPML layer, a resistance wall with $E/H =$ the wave impedance of the last cell [14] is employed. This should dissipate some of the wave energy incident on it, thus decreasing the magnitude of the waves reflected from the nPML termination.

The 3-D TLM-based FDTD with nPML is used to simulate the 1-D problem [14]. A spatially distributed symmetric pulse was excited at the initial time $t = 0$. The nonlinear parameters for the nonlinear medium were taken as the same as [15]. To ensure that the nonlinear wave is indeed excited, a reference simulation with the linear medium of the same dimensions, initial excitation, and grids was also run. Fig. 3(a) shows the simulation results of the linear and nonlinear media terminated with the same resistance wall without PML and nPML.

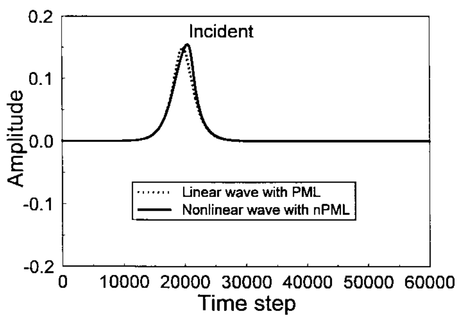
As can be seen, both linear and nonlinear waves are indeed excited. They behave differently, especially for the reflected waves. For the linear waves, both incident and reflected waves are spatially symmetrical because the initial spatial excitation is symmetrical. However, for the nonlinear waves, both forward and reflected waves become spatially asymmetrical. They are tilted toward the propagation direction. More significantly, magnitude of the nonlinear reflected wave is much larger than that of the linear reflected wave. This indicates that the waves, both linear and nonlinear, react differently to the same boundary, thus confirming that a nonlinear wave was excited.

Once existence of the nonlinear wave was confirmed, 16-layer PML's and nPML's were then inserted between the solutions domain and the resistance wall in both linear and nonlinear cases, respectively. Fig. 3(b) shows the simulation results.

As can be seen, both reflected linear and nonlinear waves become invisible and, therefore, can be assumed having been absorbed effectively. We conclude that the nPML works very well in absorbing the nonlinear waves.



(a)



(b)

Fig. 3. (a) Simulation results for linear and nonlinear waves without PML's. (b) Simulation results for linear and nonlinear waves with PML's.

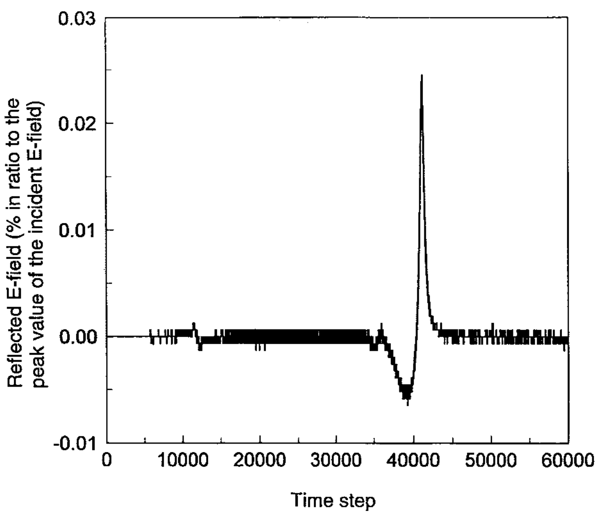
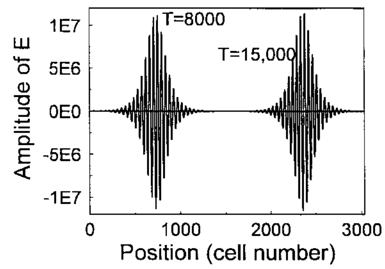


Fig. 4. The nonlinear wave reflected from the nPML recorded at a fixed spatial point.

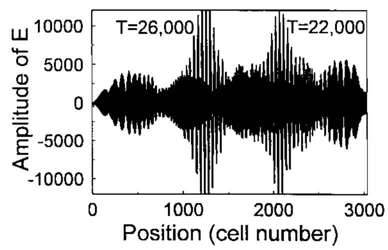
For a quantitative description of the nPML absorption, Fig. 4 shows the magnitude of the nonlinear wave reflected, recorded at a fixed spatial point in the solution domain. Values on the vertical axis were normalized to the peak value of the incident wave and are shown in percentage. It can be seen that the amplitude of the reflected nonlinear wave is very small in comparison with the incident wave. The reflection magnitude in reference to the peak of the incident wave is less than -72 dB in time domain. It shows that the nPML does absorb the nonlinear wave very effectively.

IV. nPML Absorption of Solitons

In this section, soliton propagation in one- and two-dimensional cases is simulated with nPML. Solitons were chosen for our testing for two reasons: soliton propagation involves not only nonlinearity, but also temporal or spatial dispersion. As a result, the effectiveness of the nPML can be evaluated in a wider scope. Secondly, solitons are the most interesting nonlinear phenomena, which have been studied theoretically and later proven experimentally. They have been tested for long-haul error-free data transmission [18].



(a)



(b)

Fig. 5. (a) Soliton recorded at two different time instants: 8000th and 15 000th time steps. (b) The reflected waves after the soliton impinges on the nPML.

A. 1-D Temporal Soliton

The TLM-based FDTD has been successfully applied to simulate 1-D soliton in Kerr-type nonlinear media and the results has been verified with the results from other techniques [14]. By terminating the nPML at both ends of the computation domain, the effects of the nPML can be evaluated. In the simulation, the soliton was assumed to be switched on at $t = 0$ in Type-RN Corning glass [1]. The nonlinear parameters are $n_0 = 2.46$ and $n_2 = 1.25 \times 10^{-18}$ m^2/W. When the initial pulse is given with sufficient strength, nonlinear effects will be large enough to cancel the dispersive effects of the medium, forming a soliton (i.e., a pulse whose temporal shape will not change as it propagates). The incident field in our case was a pulse with a center frequency of 137 THz modulated by a hyperbolic secant envelope function with a characteristic time constant of 14.6 f/s [9]. The FDTD cell size was 52.8 nm. The size of the computation domain was 3032 cells terminated at both ends with the nPML. Every nPML region had 16 layers with $\sigma_{\max}$ being 94000 S/m and $\sigma = \sigma_{\max}(\rho/\delta)^2$.

Fig. 5(a) shows an incident solitary pulse with amplitude of about 1.2×10^7 V/m at two different times corresponding to 8000 and 14 000 time steps. The pulse had to be made strong enough such as to engage the nonlinear behaviors in the pulse dispersion, and thus induce the soliton propagation.

Fig. 5(b) shows the reflected pulse at 22 000 and 26 000 time steps due to the terminated nPML's. The maximum amplitude

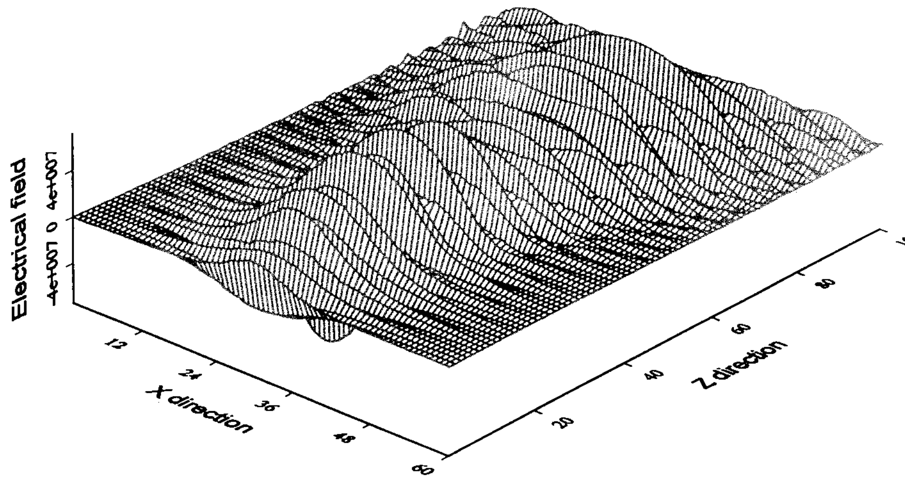


Fig. 6. Wave spreading in the linear medium (recorded at the 7800th time step).

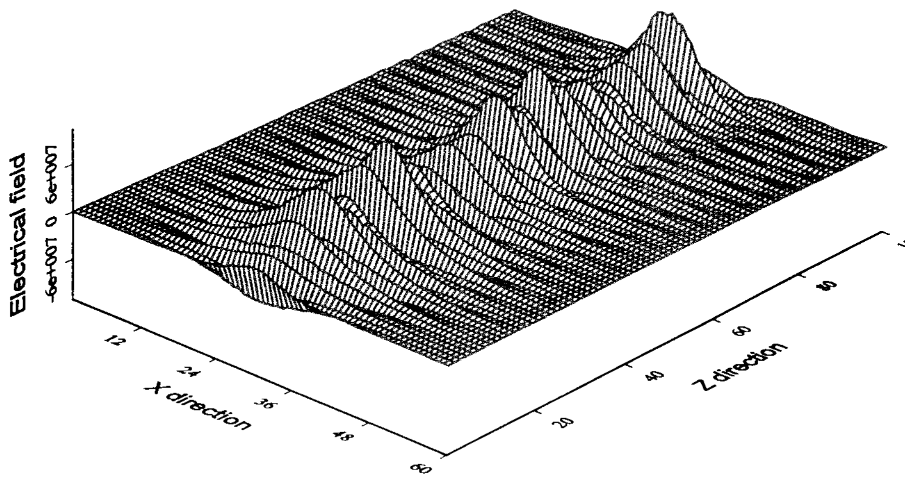


Fig. 7. Spatial soliton recorded at the 7800th time step.

of the reflected waves is about 12 500 V/m. However, when it is compared with the maximum of the incident wave, about 1.2×10^7 V/m, the reflected wave is only 0.1% of the incident wave. This corresponds to absorption of about −60 dB. Again, the nonlinear electromagnetic wave was found to be absorbed very well by the nPML.

B. Two-Dimensional Spatial Soliton

Two-dimensional spatial-soliton propagation was simulated in this case. In a linear medium, when a spatial pulse is propagating in a two-dimensional plane, the pulse will spread, due to linear diffraction, in the direction transverse to the intended propagation direction. However, if the medium is replaced by a nonlinear medium, the transverse spreading of the pulse can be completely cancelled by the transverse-beamwidth sharpening effect of self-focusing due to nonlinearity, provided that the pulse is initially given sufficient strength. Consequently, the pulse will propagate without changing its spatial shape, forming a spatial soliton. FDTD calculations were made for such propagation. The initial excitation for a single beam is of a hyperbolic-secant transverse profile with an intensity beamwidth of 1.3 μm and a carrier frequency of 2.31×10^{14} Hz ($\lambda = 1.3$ μm). The beam was assumed to be switched on at $t = 0$ in Type-RN Corning glass again [1] and the nonlinear parameters were $n_0 = 2.46$ and $n_2 = 1.25 \times 10^{-18}$ m^2/W. The two-dimensional case was successfully simulated in [1] using the conventional FDTD of Yee's scheme.

To ensure that the spatial soliton can be indeed excited in the FDTD grid, a parallel reference simulation for the same medium, but without the nonlinearity terms (i.e., $n_2 = 0$), was also run. Thus, the pulse propagation in this linear medium should present traverse spreading (due to the linear diffraction) and comparisons between the results for linear and nonlinear media can be made.

Assuming that the z-direction is the propagation, Fig. 6 shows the pulse propagation in the linear medium, while Fig. 7 shows the spatial-soliton propagation in the nonlinear medium. The initial excitation pulses were exactly the same in the two cases. As can be seen, the pulse in the linear medium indeed spread (in the x-direction in this case) as it propagates, while the pulse in the nonlinear medium does not. This indicated that the nonlinear medium was correctly simulated and a spatial soliton was induced.

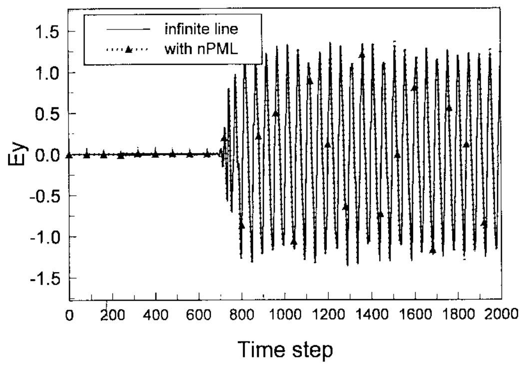


Fig. 8. Variations of the E_y-component of the spatial soliton with time.

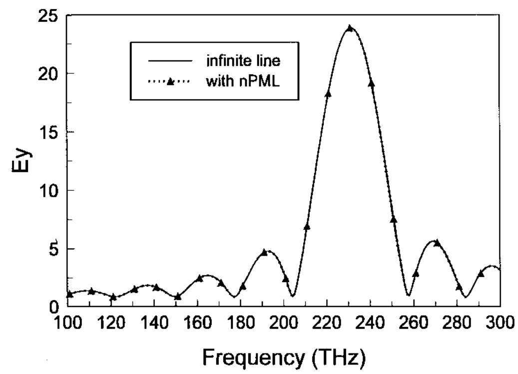


Fig. 9. Fourier transform of E_y.

Once the induction of the spatial soliton was confirmed, we proceeded to measure the nPML absorption of the spatial soliton. To be able to measure the absorption numerically, we ran two simulations: one with a longer computation domain (serve as a benchmark solution) and the other with a shorter computation domain with nPML terminated in both ends along the z-direction. In doing so, the absorption effect of the nPML can be evaluated by comparing the results from the two simulations.

The longer computation domain is with $300\Delta l$ (in x) $\times$ $1800\Delta l$ (in z) while the shorter one (which has the nPML terminations) is with $300\Delta l$ (in x) $\times$ $170\Delta l$ (in z). In both cases, the FDTD cell size Δl is 52.8 nm in both x- and z-directions, and the z-direction is the propagation direction. The excitation was set at $z = 50\Delta l$. An observation point was selected at $z = 150\Delta l$. For the longer domain simulation with the number of iterations being selected as 2000, the field recorded at the observation point can be considered as an incident wave. The reason is that the wave reflected from the terminations does not reach the observation point under 2000 iterations. We, therefore, can treat the longer domain case as the infinite long case and its solution as a benchmark solution for comparisons. The nPML chosen for the shorter domain simulation again had a thickness of 16 nPML layers with $\sigma_{\max}$ being 94 000 S/m and $\sigma = \sigma_{\max}(\rho/\delta)^2$.

Fig. 8 shows the output electric field E_y in time, recorded at $z = 50\Delta l$ for the two different cases. The differences between the two results are not visible, in spite of the fact that in both cases, as expected, the electric fields E_y oscillates in time.

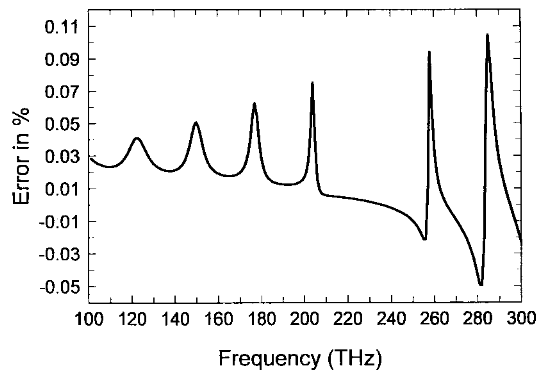


Fig. 10. Relative errors of the E_y simulated with nPML in frequency domain.

Fig. 9 gives comparison of the electric fields E_y in the frequency domain between the two cases. A peak is shown at the frequency of 2.31 $\times$ 10^{14} Hz ($\lambda = 1.3$ μm) which is, as expected, the carrier frequency of the excitation. The ripples beside the peak can be considered as the result of truncation of the time in simulation. It can be now seen that, in frequency domain, the differences between the longer domain case and the nPML case are also very small, even in the ripple region. Fig. 10 shows the relative errors. As can be seen, the difference is less than 0.1%, which corresponds to -60 dB of absorption. The nPML is again proven to work very well in absorbing the nonlinear electromagnetic waves.

V. CONCLUSION

In this paper, an nPML scheme is presented for effective absorption of nonlinear electromagnetic waves propagating in a nonlinear medium. The nPML is established by varying the permittivity and permeability of the nPML's in accordance with nonlinearity of a nonlinear medium. In the subsequent numerical experiments, nonlinear waves, especially solitons (which involve both nonlinear and dispersive effects of a medium), were successfully simulated with the nPML terminations. As a result, effectiveness of the nPML was demonstrated. FDTD schemes can now be applied to nonlinear open structures, and application scope of FDTD methods are further expanded. Although the proposed nPML was implemented in the TLM-based FDTD, it should also be easily implemented in other FDTD schemes such as Yee's scheme.

It is noted that at the time of this paper's revision, a further-improved PML scheme, the PML-D scheme, was reported in [19] for an effective general absorption of propagating and evanescent waves. The authors believe that the nPML scheme proposed in this paper can be implemented with the PML-D scheme for the effective absorption of both propagating and evanescent *nonlinear* waves.

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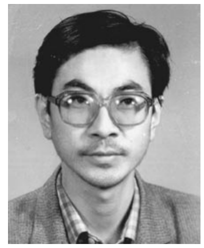

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