R describes the contribution from Raman- scattering and the term \( A \) \( P \) is the spatial linear polarisation contributions by Lorentz- and Drude-poles. There are two possibilities of how to solve this equation, both have their own advantages and shall be described next. It can be shown that for positive third order susceptibilities \( \chi^3 > 0 \) there are up to three different possible solutions from which it is hard to determine which one is correct. The solution of the positive case \( \chi^3 > 0 \) is given by

\[
P^{(1)} = \left( \frac{q}{2} + \sqrt{\frac{q^2}{4} - 2k} \right)^{\frac{1}{3}}
\]

where the constants are defined as

\[
K = \frac{\rho}{c},
p = \frac{2k\rho}{\omega^2},
q = \frac{2k\rho}{\omega^2},
D = \frac{\rho}{\omega^2}.
\]

This solution has two advantages compared with the approach of \([1]\):

- allows splitting up of polarisation updates contributing an additive constant to the standard update
- does not require a computationally expensive iteration

Hence, a better overall performance in speed and accuracy can be expected.

For the negative case \( \chi^3 < 0 \), we solve the cubic update equation \((1.3)\) for \( I \) by performing a fixed-point iteration as the problem is hard-conditioned for other methods such as the Newton or the secant method. As it will be shown below, a criterion for the fixed-point iteration under which it converges to the correct solution can be derived analytically. The advantage of the fixed-point iteration is that it finds the correct solution regardless if the update field component lies on the material border where other field components at the same grid point have other update equations. For the analytical solution on a material border, the adjoining field update equations have to be known requiring many additional parameters to be stored in memory. Thus, it is most efficient to solve the update equation \((1.3)\) for \( I \) on material borders and regions with negative susceptibility \( \chi^3 < 0 \) by applying the fixed-point iteration while at material interiors with positive third order susceptibility \( \chi^3 > 0 \) the analytical solution is used. This new algorithm is hence particularly efficient in voluminous materials with positive third order susceptibility \( \chi^3 > 0 \).

**STABILITY OF THE FDTD UPDATE**

In this section, the stability and phase error of our new algorithm will be derived. The used methodology is presented in \([2]\) and \([3]\). As a result, a stability condition is found which determines how to chose the spatial and the temporal sampling.

The phase error of the algorithm describes how much faster or slower a numerical wave front is compared with the physical wave front. While stability depends on complex dependencies between the material parameters and the spatial and temporal grid resolution, the phase error solely depends on the spatial grid resolution and it disappears if the spatial grid resolution tends to infinity. The algorithm’s accuracy also depends on the temporal resolution, i.e. on the size of the time-step because only in the lines where the time-step tends to 0, the numerical dispersion relation becomes equal to the physical dispersion relation of the simulated material. First, the numerical dispersion relation which in fact represents the phase error of the algorithm is derived. Assuming that each unknown in the system is represented as a plane wave of the form \( e^{i(k_\parallel x - \omega t)} \), the temporal derivatives in the time-domain are replaced with multiplications of -io in the frequency domain and the spatial derivative is replaced with ik. With respect to the discretized space, -io is replaced with -\( \Omega \) and ik with k where \((x,y,z)\) and \(a,b,c\) are the unit vectors in x,y,z respectively.

\[
\Omega = \frac{2}{\lambda} \sin \left( \frac{\omega}{2} \right) \frac{\lambda}{2},
\]

\[
K = 2 \left( \sin \left( \frac{\omega}{2} \right) \frac{\lambda}{2} + \sin \left( \frac{\omega}{2} \right) \frac{\lambda}{2} \right)
\]

Clearly, as the spatial size and the cell size tend to 0, the above expressions reduce to their analytical counterparts. Applying the above expressions as described to the present problem and solving the resulting system, the numerical dispersion relation for the Kerr-effect is found to be

\[
\epsilon_{non} = \epsilon_{Re} + \chi^3 I
\]

Which is similar to the standard Yee-algorithm dispersion with an intensity dependent permittivity. Solving the numerical dispersion relation

\[
K = \frac{\chi^2}{\epsilon_{Re}} \Omega^2
\]

for \( \omega \) in one dimension yields

\[
\omega = \Delta \frac{1}{2} \sqrt{\frac{2}{\sin^2 \left( \frac{\Omega}{2} \right)}} \epsilon_{Re} \chi^3 I
\]

As a consequence, \( \Omega \) becomes imaginary if \( \chi^3 > 1 \). Using the maximal value that \( \chi^3 \) can reach, the following stability condition is found

\[
S \leq \sqrt{\epsilon_{Re} + \chi^3 I}
\]

As expected, this condition depends on the field intensity and it seems that stability is increased with increasing intensity as the Courant-number \( S \) is not limited by \( \epsilon \) but by the intensity. For low intensities, the Courant-condition of the standard FDTD algorithm applies. It is important to be aware that this condition only ensures stability of the FDTD-algorithm itself. Solving the update equation for the Kerr-effect requires to solve a non-linear equation. This has to be done either by the Newton-method used in \([1]\) or by applying a fixed-point iteration. If these iterations converge depends on the intensity of the applied field as shown later in this section. As a consequence, the above condition does not ensure stability of the entire algorithm, but it needs to be satisfied. To determine the minimal grid sampling number \( N_2 \), the numerical phase vector \( k \) which is given by

\[
k = \frac{1}{2} \frac{\Omega}{\Delta} \sin \left( \frac{\Omega}{2} \right) \epsilon_{Re} \chi^3 I
\]

has to be analysed. If \( S \gtrless 1 \), then \( \Omega \) becomes imaginary which results in an exponential exponential decay of the wave. This is the case if the grid sampling number \( N_2 \) is too small, i.e. it is required that

\[
N_2 \geq \frac{\pi S}{\sin^2 \left( \frac{\Omega}{2} \right) \epsilon_{Re} \chi^3 I}
\]

As the intensity is increased, the sampling number \( N_2 \) has to be increased as well.

The verification of the simulated physics of the nonlinear algorithm is done by reproducing the qualitative behavior of the nonlinearity (e.g. soliton propagation figure 3) by comparison with other numerical results (see figures 4 & 5). \([4]\) suggested a very interesting approach to test the accuracy of numerical models of the third order nonlinearity: a comparison of the numerical results with the analytical solution for four-wave mixing (FWM). FWM is a process which solely depends on the third order nonlinearity and therefore the accuracy analysis is not affected by inaccuracies of dispersion models (as required for soliton simulation). FWM describes how a pump and a signal wave of frequency \( \omega_0 \) and \( \omega_1 \), respectively are converted to a frequency \( \omega_1 - \omega_0 \) and \( \omega_1 + \omega_0 \), which is parametrically amplified. An output power spectrum after a pump (at 192 THz) and a signal (at 195 THz) were generated. A slab of length 50µm with \( \chi^3 = 10^{-18} \) of Kerr-material is shown in figure 1. The new algorithm applies. It is important to be aware that this condition only ensures stability of the entire algorithm, but it needs to be satisfied. To determine the minimal grid sampling number \( N_2 \), the numerical phase vector \( k \) which is given by

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As the intensity is increased, the sampling number \( N_2 \) has to be increased as well.
a function of pump power is shown. It is found that the FDTD results asymptotically converge to the analytical solution as pump power is decreased. Generally, the FDTD method shows a smaller conversion efficiency than the analytical solution, which can be explained by the fact that pump and signal depletion in the analytical formulation are ignored (an effect that grows with increasing field intensities). Moreover, the so-called small-signal condition used in the analytical derivation is not valid anymore for strong beam intensities. Overall, high accuracy for the new FDTD formulation of the third order susceptibility can be assessed.

Figure 1: Electric field power spectrum after pump (at 195 THz) and signal (at 205 THz) wave traversed a slab of length 50\,m with $\chi^{(3)} = 10^{-18}$. The new generated frequencies due to FWM (at 190 THz; 186 THz; ...) are clearly visible.

Figure 2: Signal conversion efficiency in a nonlinear Kerr-medium as a function of pump power. The solid line is the analytical solution, the dotted line results from our new FDTD scheme. For high pump powers, pump and signal depletion is observed giving rise to a strong deviation from the analytical solution.

CONVERGENCE OF THE FIXED-POINT ITERATION

The convergence of the fixed point iteration which is needed to solve for the Kerr-effect is proven by using Banach’s fixed point theorem. For simplicity, the third-order susceptibility $\chi^{(3)}$ shall be written without the susceptibility index, i.e., $\chi$ instead of $\chi^{(3)}$, for the rest of this section. Banach’s fixed point theorem is applied for $f^{(4pi)}$ which has been defined in equation (3.3). To this end, it has first to be shown that the first derivative of $f^{(4pi)}$ is limited for all $p^{(n)}$ at least within an interval $D$:

$$f^{(4pi)}(x^{n+1}) = \frac{-2\mu_0 c}{(x + c^{n+1})^2}$$

(3.1)

Apparently, the supremum of $|f^{(4pi)}|$ is found where $p^{(n)} = 0$ and is given by

$$S = \sup_{x^{n+1}} |f^{(4pi)}(x^{n+1})| = \frac{2\mu_0 c}{b^2}$$

(3.2)

Next, it has to be shown that the above supremum $S$ is smaller than 1 such that $f^{(4pi)}$ is Lipschitz-continuous with a Lipschitz-constant $L \leq 1$ and consequently, $f^{(4pi)}$ is a contraction on the interval $D$ and the fixed-point iteration will be convergent on $D$. The condition for $f^{(4pi)}$ to be a contraction on $D$ can be written as

$$a^{2}c^{2} \leq \frac{1}{2} b^{2}$$

(3.3)

As long as this condition holds the fixed-point iteration will converge. Thus, using a smaller Courant-number increases the physical accuracy has been investigated by simulating FWM assessing high accuracy for low intensities. For intensities sufficiently lower than the characteristic Convergence-Intensity (3.5) it has been shown analytically that the applied fixed-point iteration converges to the correct value. Furthermore, the stability analysis of the new FDTD scheme revealed that the algorithm is stable under the Courant-stability condition of the standard FDTD scheme.

The performed benchmarks such as soliton simulation and the simulation of a nonlinear PC showed excellent agreement between the findings of other nonlinear FDTD schemes and the one presented here.

REFERENCES


CONCLUSIONS

A novel algorithm that tremendously increases the efficiency of the FDTD method applied to materials with third-order nonlinear susceptibility has been developed and applied to various benchmarks. The core advantage of the approach being that it allows parallelisation of the algorithm and its computational efficiency, particularly for materials with positive third order susceptibility. The three dimensional algorithm was successfully implemented into the fully featured FDTD EM platform SEMCAD X.

Physical accuracy has been investigated by simulating FWM assessing high accuracy for low intensities. For intensities sufficiently lower than the characteristic Convergence-Intensity (3.5) it has been shown analytically that the applied fixed-point iteration converges to the correct value. Furthermore, the stability analysis of the new FDTD scheme revealed that the algorithm is stable under the Courant-stability condition of the standard FDTD scheme.