

Nonlinear Lorentz Model for Explicit Integration of Optical Nonlinearity in FDTD

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Abstract—Including optical nonlinearity in FDTD software in a stable, efficient, and rigorous way can be challenging. Traditional methods address this challenge by solving an implicit form of Maxwell's equations iteratively. Reaching numerical convergence over the entire numerical space at each time step demands significant computational resources, which can be a limiting factor for the modeling of large-scale three-dimensional nonlinear optics problems (complex photonics devices, laser filamentation, ...). Recently, we proposed an explicit methodology based on a nonlinear generalization of the Lorentz dispersion model and developed example cases where it was used to account for both linear and nonlinear optical effects. An overview of this work is proposed here.

Index Terms—FDTD modeling, nonlinear materials, photonics.

I. INTRODUCTION

Including optical nonlinearity in the finite-difference time-domain (FDTD) framework is not straightforward. It is easily demonstrated with the Ampère's circuital law:

$$\nabla \times \mathbf{H} - \epsilon_0 \frac{\partial \mathbf{E}}{\partial t} = \frac{\partial \mathbf{P}}{\partial t}, \quad (1)$$

where the source term depends on a nonlinear susceptibility of the form:

$$\mathbf{P} = \epsilon_0(\chi^{(1)}\mathbf{E} + \chi^{(2)}\mathbf{E}^2 + \chi^{(3)}\mathbf{E}^3 + \dots), \quad (2)$$

Yee discretization of (1) with (2) leads to a set of coupled nonlinear equations that are implicit in the electric field vector and whose solution is nontrivial. A formal solving approach, proposed by Greene and Taflove [1], uses a recursive Newton method to obtain an approximate solution for \mathbf{E} . To ensure numerical convergence, it has to be iterated over the entire numerical space a few times per time step, at minimum. This is a rigorous way to include optical nonlinearity into FDTD, but efficient implementation for solving three-dimensional problems is inherently complex. For that reason, FDTD developers

typically rely, instead, on explicit tricks whose implementation is simpler and computationally more efficient (see, e.g., [2]). In a series of papers [3]–[5], we developed an explicit methodology based on a nonlinear generalization of the Lorentz dispersion model, providing a rigorous, flexible, efficient, and transparent approach to the nonlinear-FDTD problem.

II. THE NONLINEAR LORENTZ MODEL

Typical nonlinear optics scenarios are reasonably described by the two-level atom model (see, e.g., [6]). We have shown in [5] that when there is a negligible transition probability to the upper level (weak field, long wavelength), this quantum mechanical model can be reduced to the following second-order differential equation for the induced macroscopic polarization density \mathbf{P} :

$$\frac{d^2 \mathbf{P}}{dt^2} + \gamma \frac{d\mathbf{P}}{dt} + \omega_0^2 \mathbf{P} = \omega_0^2 \epsilon_0 (\bar{\chi}^{(1)} \mathbf{E} + \bar{\chi}^{(2)} \mathbf{E}^2 + \bar{\chi}^{(3)} \mathbf{E}^3 + \dots). \quad (3)$$

The model is parametrized by an effective damping constant γ , the transition energy $\hbar\omega_0$, and the n th-order optical susceptibility parameters $\bar{\chi}^{(n)}$ (ϵ_0 is the electric constant). The overbar indicates that the $\bar{\chi}^{(n)}$'s are assumed to be constant, i.e., they do not vary much on the electronic time-scale (see III-B for further details). As emphasized in [4], (3) can be discretized using the leapfrog method to match the Yee discretization scheme (see, e.g., [7]), resulting in a fully explicit FDTD integration of Maxwell equations. The linear and nonlinear material responses are then introduced *via* the effective susceptibility parameters $\bar{\chi}^{(n)}$, while dispersion is set by ω_0 and γ (see [5] for further development on this topic).

III. APPLICATION EXAMPLES

A. Second Harmonic Generation

We considered quasi-phase-matched (QPM) second harmonic generation (SHG) in periodically poled lithium niobate (PPLN) and compared FDTD simulations using the nonlinear Lorentz model (3) (referred to as NL-FDTD below) to a conventional theoretical model for QPM SHG (see, e.g., (2.7.10)

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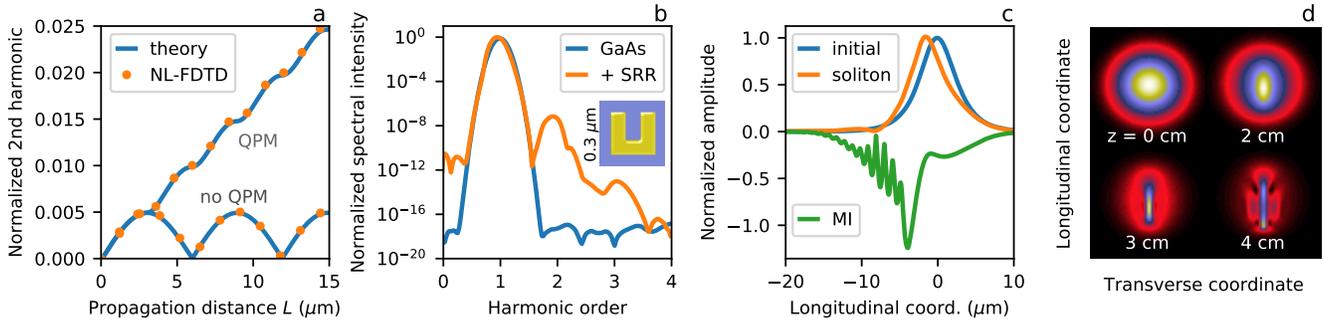


Fig. 1. Application examples of the nonlinear Lorentz model equation (3), combined with FDTD integration of Maxwell’s equations (NL-FDTD, see also [3]–[5]). In (a), NL-FDTD simulations of quasi-phase matching (QPM) in periodically poled lithium niobate show exceptional agreement with traditional theoretical models. In (b), a GaAs crystal is aligned with the polarization of the electric field to give no second harmonic (GaAs). However, SHG emerges when a gold split-ring resonator is placed on top (+ SRR, see below legend for sketch). In (c), the propagation of a sech²-shaped laser pulse in fused silica is modelled with NL-FDTD (the envelope is obtained by taking the absolute value of the Hilbert transform of the electric field). Depending on the input laser intensity, the pulse after travelling over 6 mm exhibits a solitonic behavior (compare the “soliton” and “initial” curves) or pronounced envelope distortion due to modulation instability (MI). Finally in (d), spatio-temporal structuring of a Gaussian laser pulse during self-focusing in air at propagation distance z .

and (2.7.11) in [6]). For the demonstration, we considered a plane wave moving along the axis of an infinite PPLN crystal, modelled with an homogeneous linear index and a second-order parameter $\bar{\chi}^{(2)}$ whose sign is switched periodically to achieve QPM (see [4] for details). The excellent agreement between theory and NL-FDTD in Fig. 1 (a) shows that the NL-FDTD analysis succeeds in reproducing quantitatively the dispersion, scattering, and wave mixing processes in SHG, as well as their interplay.

For rigorous modeling of three-dimensional (3D) optics in solids, it is often necessary to consider the tensorial nature of the susceptibility. This has to be added explicitly to (3). To test this procedure, we considered 3D vectorial NL-FDTD modeling of the SHG enhancement in a gallium arsenide (GaAs) substrate by a split-ring resonator (SRR) nano-antenna. The gold SRR was modelled with a Drude equation while GaAs was modelled with the nonlinear Lorentz equation that follows:

$$\frac{d^2 \mathbf{P}_{\text{GaAs}}}{dt^2} + \frac{d \mathbf{P}_{\text{GaAs}}}{dt} + \omega_0^2 \mathbf{P}_{\text{GaAs}} = \omega_0^2 \epsilon_0 \bar{\chi}^{(1)} \mathbf{E} + \epsilon_0 \bar{\chi}^{(2)} [(E_z E_z - E_y E_y) \mathbf{i} - 2 E_x E_y \mathbf{j}], \quad (4)$$

where \mathbf{i} and \mathbf{j} are unit vectors along x and y , respectively. With the electric field polarized along x , there is no second-order effect with GaAs alone [see the “GaAs” curve in Fig. 1 (b)]. Nevertheless, when the SRR is present near-field components in y and z are created, which induces SHG in GaAs [see the “+ SRR” curve in Fig. 1 (b)].

B. Raman Nonlinearity

The nonlinear Lorentz equation (3) accounts for the fast (almost instantaneous) optical response on the electronic time scale. An accurate description of the nonlinear optical processes in centrosymmetric dielectrics must also include a delayed contribution associated with stimulated molecular Raman scattering. This can be done by complementing (3) with an equation that accounts for the modification of the nonlinear susceptibility on the “slow” molecular time scale.

The complete model is then given by the following two equations [4]:

$$\frac{d^2 \mathbf{P}}{dt^2} + \gamma \frac{d \mathbf{P}}{dt} + \omega_0^2 \mathbf{P} = \omega_0^2 \epsilon_0 (\bar{\chi}^{(1)} \mathbf{E} + \alpha \bar{\chi}^{(3)} \mathbf{E}^3 + Q \mathbf{E}), \quad (5a)$$

$$\frac{d^2 Q}{dt^2} + 2\gamma_R \frac{dQ}{dt} + \omega_R^2 Q = (1 - \alpha) \bar{\chi}^{(3)} \omega_R^2 |\mathbf{E}|^2, \quad (5b)$$

where α is a parameter that defines the balance between the instantaneous (Kerr) and delayed (Raman) contributions to the third-order susceptibility. The Raman response is itself parameterized by the angular frequency and damping constants ω_R and γ_R whose values are chosen to fit a given Raman-gain spectrum. An equation like (5b) is also used for the Greene-Taflove’s implicit method [1], but here integration of both (5a) and (5b) with the leapfrog technique leads to a fully explicit nonlinear-FDTD scheme (see [4] for details). Examples of results obtained with this model are given in Figs. 1 (c-d).

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