Hybrid FDTD modeling of a two-level atomic system

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Abstract—**The new concept of coupling rate equations, describing the evolution of a two-level atomic system, with rigorous electromagnetic simulations undertaken with a finite-difference time-domain method is presented. The proposed procedure allows updating electromagnetic fields and population densities with different time-scales, which leads to the significant reduction of computational effort of the analysis of absorbing materials.**

Index Terms—**FDTD method, rate equations, two-level atomic system.**

I. INTRODUTION

The evolution of a two-level atomic system exposed to an incident electromagnetic wave can be solved rigorously with a full-wave finite-difference time-domain (FDTD) method [1], where rate equations are coupled with curl Maxwell equations, and the material is represented as a time-varying Lorentz dispersive model [2]. However, if the characteristic time of the investigated atomic system is much longer than the period of the wave, the Lorentz model is evolving very slowly and the simulation become prohibitively long. Therefore, the goal of this paper is to introduce a hybrid algorithm, where rate equations are decoupled from an FDTD analysis. The evolution of the system in computed iteratively with a population density updated with rate equations after consecutive FDTD simulations, where the current state of the atomic system is represented with a time-invariant Lorentz model. As it will be shown, FDTD simulation time can be orders of magnitude shorter than the step of such a hybrid algorithm. Consequently, the method allows taking the advantage of the versatile FDTD method with substantially reduced computational effort of the whole analysis.

II. HYBRID FDTD ALGORITHM

The rate equation describing the evolution of the population difference, ΔN, in a two-level atomic system can be given as follows [2]:

$$\frac{d\Delta N(t)}{dt} = -\frac{2}{E_a}\vec{E}(t)\vec{J}(t) - \frac{\Delta N(t) - \Delta N_{eq}}{\tau_{21}}, \qquad (1)$$

where E_a stands for the transition energy, τ_{21} is the characteristic lifetime of atoms in the upper level, and ΔN_{eq} represents the population difference in thermal equilibrium.

Electrodynamics of the system, represented in (1) by the electric field E and current density J, is coupled with atomic populations by the following equation [2]:

$$\frac{d\vec{J}(t)}{dt} + \Delta\omega_a \vec{J}(t) + \omega_a^2 \int \vec{J}(t)\,dt = \sigma\,\Delta N(t)\,\vec{E}(t), \qquad (2)$$

where ω_a is a resonant frequency directly related to E_a, $\Delta\omega_a$ stands for a resonant linewidth, and σ represents a coupling strength.

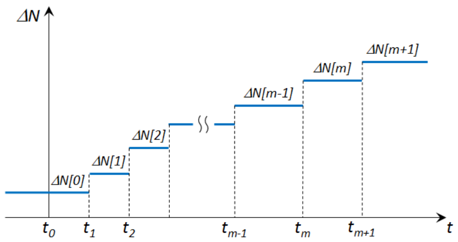

Figure 1. Discretized evolution of a population difference ΔN.

The integration and, subsequently, discretization of (1), according to the scheme shown in Fig. 1, leads to the following update formula of the population density:

$$\Delta N_{m+1} = \Delta N_0 + \Delta N_{eq}\frac{t_{m+1}}{\tau_{21}} - \frac{2}{E_a} w_{loss}(t_{m+1}) - \frac{1}{\tau_{21}} M_{m+1}, \qquad (3)$$

where

$$M_{m+1} = M_m + \frac{1}{\tau_{21}}\Delta N_m (t_{m+1} - t_m) \qquad (4)$$

is an auxiliary equation accumulating the evolution of ΔN from the beginning of the simulation, while

$$w_{loss}(t_{m+1}) = w_{loss}(t_m) + \int_{t_m}^{t_{m+1}} \vec{E}(t)\vec{J}(t)dt = w_{loss}(t_m) + \int_{t_m}^{t_{m+1}} p(t)dt \qquad (5)$$

is the update equation of the total volumetric density of energy gain/loss, which is responsible in (3) for the coupling between (1) and (2).

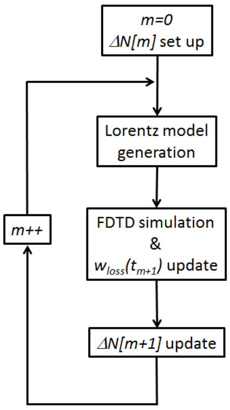

Figure 2. Hybrid algorithm with FDTD simulations preceded by the update of a Lorentz model representing the current state of a 2-level atomic system.

Consequently, the evolution of the system can be solved with a hybrid approach depicted in Fig. 2, where each FDTD simulation is executed for a given Lorentz dispersive model representing (2) to calculate the average volumetric density of power gain/loss, *p(t)*, as in (5). Subsequently, the population difference, ΔN, can be updated with (3) and a new Lorentz model can be computed for the next turn of the hybrid simulation. It should be emphasized that the duration of the FDTD simulation does not have to be equal to the global time-step, $\Delta T_m = (t_{m+1}-t_m)$, of the hybrid algorithm. Assuming that the incident wave is driven with a monochromatic signal of frequency f_a, only a few periods of the signal are needed to reach a steady state in the scenario. Consequently, if ΔT_m is much longer than the period of the wave, the update of (5) can be approximated by:

$$w_{loss}(t_{m+1}) = w_{loss}(t_m) + \frac{\Delta T_m}{2}\left[p_{\max} + p_{\min}\right], \qquad (6)$$

where p_{min} (p_{max}) denotes the time-minimum (time-maximum) of the total volumetric density of power gain/loss determined in the steady-state during an FDTD simulation.

III. Computational Results

The example investigated in this paper is the same as in [2], where the following settings have been applied: f_a = 500THz, Δf_a = 50THz, τ_{21} = 20ns, σ = 22.78×10^{-12} C^{2}kg^{-1}, $\Delta N_0 = \Delta N_{eq}$ = 10^{26} m^{-3}. It can be noticed that τ_{21} is 7 orders of magnitude longer than the period of the excited wave, $1/f_a$, so the proposed hybrid algorithm can be examined. Figure 3 shows the evolution of ΔN in one of FDTD cells computed rigorously, as in [2], for the incident electric field amplitude of 2.5×10^7 V/m, and Fig. 4 shows the discrepancy between ΔN shown in Fig. 3 and that computed with the hybrid FDTD algorithm proposed in this paper.

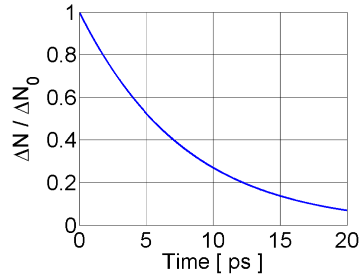

Figure 3. The evolution of the population difference, ΔN, computed rigorously with FDTD for an incident electric field amplitude of 2.5×10^7 V/m.

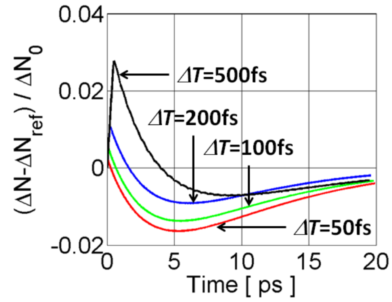

Figure 4. Inaccuracy of the hybrid algorithm for various time steps applied in the computational loop shown in Fig. 3.

The results shown in Fig. 4 imply that a good agreement has been achieved. Each FDTD simulation is continued for 20 periods of the driving signal, that is, 40fs, while the time steps of the hybrid algorithm can be well over 500fs. It means that the speed-up of the analysis is more than 12.5 in the considered example.

IV. Conclusion

It has been shown that the evolution of a two-level atomic system exposed to an electromagnetic wave can be solved in a hybrid approach, where relatively short FDTD simulations allow updating the population density of the system at a much longer time scale than a single cycle of the wave. As a result, a significant speed-up can be achieved with a negligible impact on the accuracy of the analysis.

Acknowledgment

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