An FDTD Algorithm for Simulation of EM Waves Propagation in Laser with Static and Dynamic Gain Models

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Abstract—**This paper presents methods of simulating gain media in the finite difference time-domain (FDTD) algorithm utilizing a generalized polarization formulation. The gain can be static or dynamic. For static gain, Lorentzian and non-Lorentzian models are presented and tested. For the dynamic gain, rate equations for two-level and four-level models are incorporated in the FDTD scheme. The simulation results conform with the expected behavior of wave amplification and dynamic population inversion.**

Keywords—FDTD; Gain Medium; laser; Static Gain; Dynamic Gain; Two-level System; Four-level system

I. Introduction

The finite difference time domain (FDTD) method is very popular among electromagnetic numerical methods. It directly solves Maxwell's equations in the time domain over a given space. This feature makes it a convenient tool for researchers to design and estimate response of structures and devices. The beauty of this method is its ability to incorporate material properties in space and time. Gain, as a material property was first implemented in the FDTD method by R. Hawkins, et al [1], where they applied a very old technique that was used to study antennas by taking gain as negative loss added to Maxwell's equation. To be able to simulate lasers, the medium of propagation has to be modeled as a gain medium. Gain can be modeled as static or dynamic gain. Static gain modeling provides an easy way of laser simulation in FDTD, however an important feature like saturation has to be forced to the model. With dynamic gain model, Saturation comes automatically from the interaction of different variables solved during the simulation. Laser operation in gain medium was modeled by S. Hagness in [2], where a non-Lorentzian gain model with saturation was assumed. Also, Nagra et al [3] developed their own algorithm to account for both static and dynamic gain. They used the rate equation to simulate the propagation of light in lasing medium. This model was later extended to simulate propagation in lasing material with more and more specifications added to it [4, 5].

In this paper, the general algorithm in [6], previously developed to simulate dispersion, is extended to take into account gain. Here we simulate the propagation of light in various gain models. We started by implementing it on simple gain first. Then Lorentzian and non-Lrentzian dispersive gains are implemented using the general algorithm. Derivation and simple test are presented here. The dynamic gain model, which is more accurate than the static gain is implemented using the general algorithm. The rate equation is one of the ways to explain the laser physics. Using the rate equation, we implemented dynamic gain in the general algorithm. Based on two-level and four-level systems propagation of light in laser is simulated. Derivation and test that shows agreement with theory are provided.

II. The General Algorithm

The main idea behind the general algorithm in [6] is to separate calculations of Maxwell's equations into layers. In each layer, variables are solved independently. In the first layer, the electric flux density, D, is evaluated. In the second layer, the electric field, E, is evaluated utilizing available time samples of polarization, P. In the third layer, polarization is evaluated using updated samples of E and previous values of P. This will limit the calculation effort as accounting for dispersion needs only be done in the third layer. If there is a nonlinearity like second harmonic or third harmonic another layer of calculation is added to the FDTD loop as shown in [7]. For fast material response, the static gain model is not accurate for laser simulation. Instead, dynamic gain models are more accurate and sophisticated and can incorporate quantum physics. In this paper, we show that by adding a single layer of calculations, the dynamic gain of a laser can be simulated. This approach is simpler than other approaches reported in the literature.

III. Static Gain

The propagation of an EM wave in a simple gain material will be considered first. This problem has also been worked out in [1] where gain can be introduced in FDTD as a negative loss. Here, the problem is reformulated to fit the general algorithm. In the first layer, the magnetic flux density B and electric flux density D are calculated using the following material independent equations.

$$\nabla \times E = -\frac{\partial B}{\partial t} \quad (1)$$

$$\nabla \times H = -\frac{\partial D}{\partial t} \quad (2)$$

In the second layer, electric and magnetic fields are evaluated using the following equations.

$$H = \frac{B}{\mu} \quad (3)$$

$$E = \frac{D}{\varepsilon} \quad (4)$$

For gain media, equation 4 should be modified and another layer of calculations is needed. Equation 2 is rewritten in the frequency domain as .

$$\nabla \times H = j\omega\varepsilon(\omega)E(\omega) + \sigma(\omega)E(\omega) \quad (5)$$

We redefine $D(\omega)$ to be equal to

$$D(\omega) = \varepsilon(\omega)E(\omega) + \frac{\sigma(\omega)}{j\omega}E(\omega) \quad (6)$$

So, permittivity of material with gain or loss is given by

$$\varepsilon(\omega) = \varepsilon(\omega) \pm \frac{\sigma(\omega)}{j\omega} \quad (7)$$

This is the permittivity of material in general, where the imaginary part of the permittivity is positive for loss and negative for gain. In the general algorithm format [6], one can write

$$P = \frac{\sigma}{j\omega}E \quad (8)$$

This implies

$$j\omega P = \sigma E \quad (9)$$

Discretizing gives

$$\frac{P^n - P^{n-1}}{\Delta t} = \sigma E^{n-1} \quad (10)$$

Solving for polarization we get

$$P^n = P^{n-1} + \Delta t\sigma E^{n-1} \quad (11)$$

So, the constants are

$$C_1 = 1,\ C_2 = 0 \text{ and } C_3 = \Delta t\sigma \quad (12)$$

A 1-D simulation test of a wave propagating in material with constant gain of 2, the wave is found to grow inside the gain material as shown in figure 1.

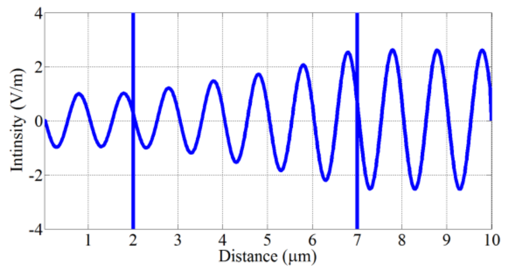

Figure 1: A wave traveling in a medium with constant gain. The general algorithm with negative conductivity is used for simple gain. The gain medium is between 2μm and 7μm.

For a gain model described by a Lorentzian, similar derivation can be followed. If the permittivity of such material is given by

$$\varepsilon(\omega) = \varepsilon_o - \frac{\alpha}{\omega_0^2 + j\gamma\omega - \omega^2} \quad (13)$$

Then, the constants for the general algorithm are

$$C_1 = \frac{4-2\omega_0^2\Delta t^2}{2+\gamma\Delta t},\ C_2 = \frac{\gamma\Delta t - 2}{2+\gamma\Delta t} \text{ and } C_3 = \frac{-2\Delta t^2\alpha}{2+\gamma\Delta t} \quad (14)$$

The simulation results are shown in figure 2, which show agreement with the expected amplification.

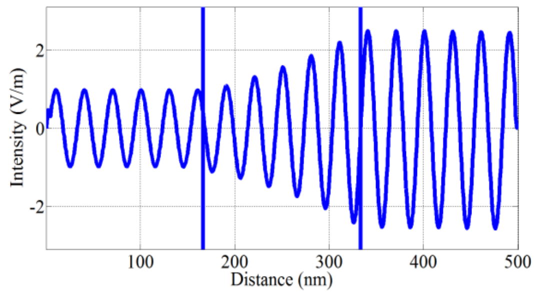

Figure 2: Propagation in a lorentzian gain medium . The gain medium is between 166 nm and 333 nm.

An example of a non-Lorentzian gain model is the one presented by S. Hagness [2] which is a decaying cosine function in time, of the form

$$\sigma(t) = \frac{\sigma_0}{T_2}\cos(\omega_0 t)\, e^{-\frac{t}{T_2}}u(t) \quad (15)$$

This conductivity function can be written in the frequency domain as

$$\sigma(\omega) = \frac{\sigma_0(1+j\omega T_2)}{(1+\omega_0^2T_2^2)+2j\omega T_2+\omega^2T_2^2} \quad (16)$$

To account for saturation, a saturation factor is added to the function, as

$$\sigma(\omega) = \frac{1}{1+\frac{I}{I_s}}\left[\frac{\sigma_0(1+j\omega T_2)}{(1+\omega_0^2T_2^2)+2j\omega T_2+\omega^2T_2^2}\right] \quad (17)$$

where I_s is the saturation factor. The permittivity function in equation 7 can now be rewritten as

$$\varepsilon(\omega) = \varepsilon_o + \frac{\frac{\sigma_0}{j\omega}+\sigma_0T_2}{(1+\omega_0^2T_2^2)+2j\omega T_2+\omega^2T_2^2} \quad (18)$$

This is a multi-pole dispersion relation that can be treated as shown in [8].

For small signals, saturation is neglected. A simulation of the propagation of a Gaussian pulse in such medium is shown in figure 3a. When the saturation term is added to the model the amplification reaches certain value then it's clamped as shown in figure 3b.

IV. Dynamic Gain

For the simulation of dynamic gain, quantum physics of lasers need to be incorporated in the simulation. The polarization in a laser can be written as [9]

$$\frac{d^2P(t)}{dt} + \Delta\omega_a\frac{dP(t)}{dt} + \omega_a^2P(t) = \kappa\Delta N(t)E(t) \quad (19)$$

This equation is called the quantum polarization equation of motion which is derived from the classical electron oscillator. ω_a is oscillator frequency and is related to the band gap of the material. ΔN is the population

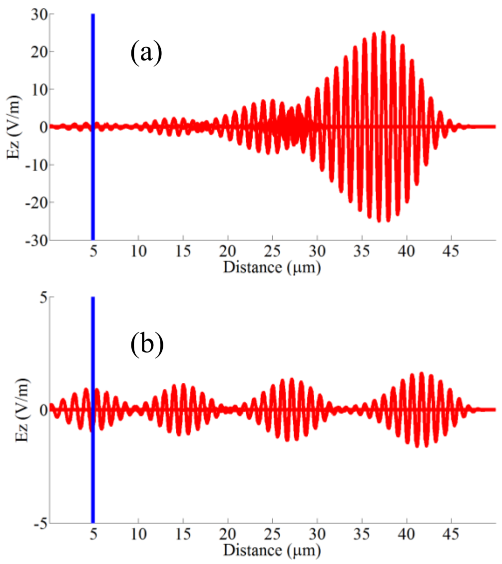

Figure 3: Propagation of an EM wave propagating in a gain medium. Gain medium starts at 5 μm.(a) without saturation, (b) with saturation.

difference. This equation connects quantum physics to Maxwell's equations. To simulate propagation in dynamic gain media using the general algorithm, another layer of calculation is added to the FDTD algorithm. This calculation layer is to find the population difference. This idea was first introduced in [3]. The polarization can be treated as found in[6]. From there, the general algorithm constants are

$$C_1 = \frac{4 - 2\omega_a^2 \Delta t^2}{\Delta\omega_a \Delta t + 2} \quad (20)$$

$$C_2 = \frac{\Delta\omega_a \Delta t - 2}{\Delta\omega_a \Delta t + 2} \quad (21)$$

$$C_3 = \frac{2\Delta t^2 \kappa}{\Delta\omega_a \Delta t + 2} \quad (22)$$

And the update will be

$$P^n = C_1 P^{n-1} + C_2 P^{n-2} + C_3 \Delta N^{n-1} E^{n-1} \quad (23)$$

Finding the population differenceΔN, requires another layer of calculation. For two-level system, calculating ΔN requires the solution of two rate equations and in the four-level system it requires four rate equations to be solved.

A. Two-Level System

In the two-level system, atoms in the gain material have only two energy levels. At the beginning, number of atoms, N_2, at the excited state, E_2, are less than number of atoms N_1 in the ground state E_1. At this condition, any wave or photon applied to the material will be absorbed. As a result, the material can be considered as a lossy material. To change a material into gain material, population inversion should be reached. This can be done either by electrical pumping or by high energy optical pumping. Once the material is in population inversion, any photon propagating in the material will stimulate the

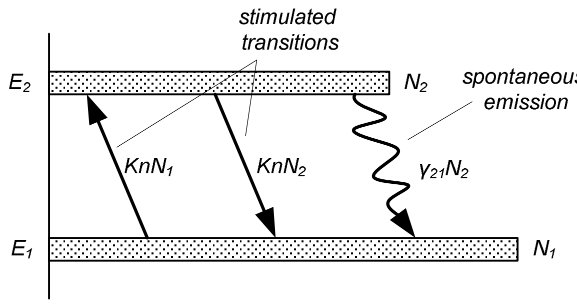

Figure 4: The Two-level system. Atoms at the ground state are more than atoms at the excited state, therefore, photons will be absorbed.

transition from the excited state to ground state, emitting another photon in the process. A Simple diagram is given in figure 4. The population difference $\Delta N(t)$ is derived from rate equation of $N_1$and N_2, as

$$\frac{d\Delta N(t)}{dt} = -\frac{2}{\hbar\omega_a} E(t) \cdot \frac{dP(t)}{dt} - \frac{\Delta N(t) - \Delta N_0}{\tau_{21}} \quad (24)$$

By discretizing around (n-1)

$$\frac{\Delta N^n - \Delta N^{n-1}}{\Delta t} = -\frac{2}{\hbar\omega_a} E^n \cdot \frac{P^n - P^{n-1}}{\Delta t} - \frac{\Delta N^n - \Delta N_0}{\tau_{21}} \quad (25)$$

$$\Delta N^n = -\frac{\tau_{21}}{\Delta t + \tau_{21}} \Delta N^{n-1} + \frac{2\Delta t \Delta N_0}{\Delta t + \tau_{21}} - \frac{4E^n (P^n - P^{n-1})}{(\Delta t + \tau_{21})\hbar\omega_a} \quad (26)$$

From equation 26, we can see that, current value of ΔN can be calculated from current and previous values ΔN, E and P. In summary, the procedure can be as shown in the flowchart of figure 5. Each calculation layer depends on the previous layer. To test the algorithm, the case given in [5] is simulated. As shown in figure 6, the Gaussian pulse is attenuated as it propagates in the medium.

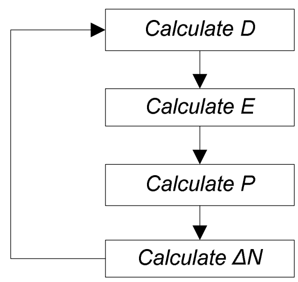

Figure 5: Schematic diagram of the FDTD loop. Each calculation layer depends on the previous layer which makes the solution easier to handle

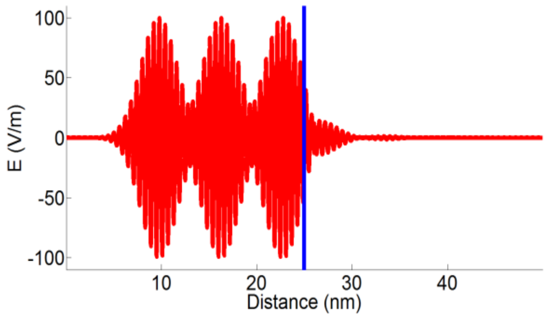

Figure 6: five snapshots of a Gaussian pulse propagating in air impinging on a medium modeled by the two-level system. As the pulse gets inside the medium, it gets absorbed.

When the magnitude of the input field is low, it has no effect on the gain and the material will act like a static gain material. If the magnitude is increased to high values then ΔN gets smaller and the gain becomes smaller causing the saturation. For very high magnitudes, ΔN will oscillate until it reaches equilibrium. These results, agree well with theoretical behavior given by L. Coldren [10] (see figure 7).

B. Four-Level System:

As shown in figure 8, in this system, atoms have four energy levels, E_0, E_1, E_2 and E_3. Populations of these level respectively are N_0,N_1,N_2, and N_3. Atoms in the ground state are pumped optically or electrically. Pumping will populate the level of energy E_3. Lasing happens if the pumping is high enough to cause population inversion between E_2 and E_1. For the four-level system, the ground state E_0 is assumed to have constant population all the time. Therefore, we have three rate equations for the rest of the energy levels. The rate equations for the three levels are given below

$$\frac{dN_3(t)}{dt} = \mathrm{W}_p(t) - \frac{\mathrm{N}_3(t)}{\tau_3} \quad (27)$$

$$\frac{dN_2(t)}{dt} = \frac{\mathrm{N}_3(t)}{\tau_{32}} + \frac{1}{\hbar\omega_a}E(t)\frac{dP(t)}{dt} - \frac{N_2(t)}{\tau_2} \quad (28)$$

$$\frac{dN_1(t)}{dt} = \frac{\mathrm{N}_3(t)}{\tau_{31}} + \frac{1}{\hbar\omega_a}E(t)\frac{dP(t)}{dt} - \frac{N_2(t)}{\tau_{21}} - \frac{N_1(t)}{t_1} \quad (29)$$

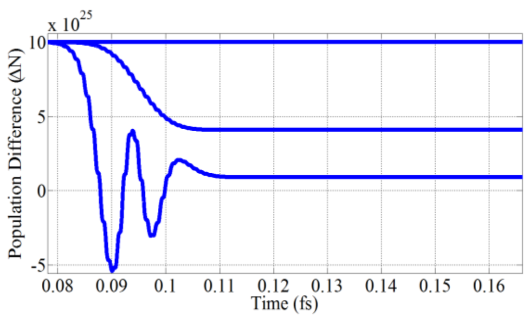

Figure 7: Effect of magnitude of applied signal on population difference and saturation. Small magnitude have no effect on population difference. High magnitude reduces population difference and very high signal makes it oscillate and saturation is reached.

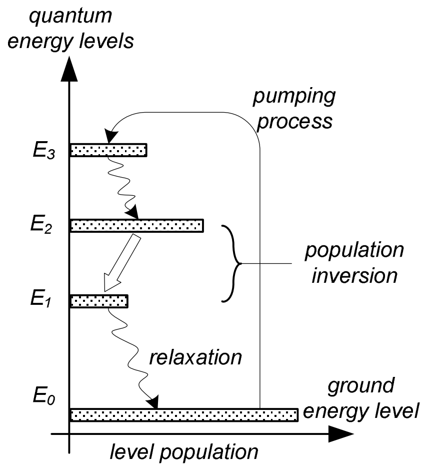

Figure 8: A four-level laser pumping system

For these equations, one can start solving for N_3. Having N_3,N_2 can be calculated. Having N_2, N_1 can be calculated. Such a scheme is perfect for the general algorithm. We applied this scheme in the calculation and added a layer of calculation to the FDTD algorithm to take care of the rate equations. We test our algorithm using same parameters in [3]. A Gaussian pulse is propagated inside the gain medium. The Gaussian pulse gets amplified in the gain medium (see figure 9). To measure the amplification in frequency domain, the pulse is recoded at two points that are at a distance of one wavelength (λ) apart. Recoded values are transformed to frequency domain. Taking the ratio of the two pulses in frequency domain shows amplification around 1×10^{14} Hz, which complies with the transition frequency used in the simulation, $\omega = (E_2 - E_1)/\hbar$.

The main advantage of this algorithm over reported ones in the literature, is the ability of modeling a gain material and dispersive maerial in the same manners. Layers of

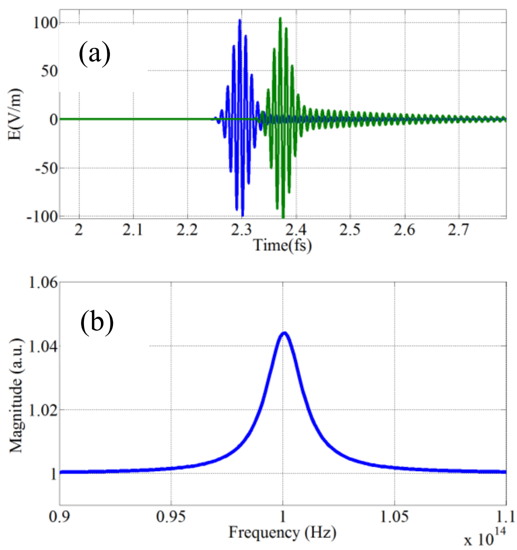

Figure 9: Amplification of a Gaussian pulse. (a) the pulse is recorded after one wavelength of propagation in the gain medium. (b) Frequency domain ratio of the two pulses which shows amplification around transition frequency.

calculations will be apply only in dispersive areas. This means the whole device can be treated with the same algorithm. Also, because polarizations and electric fields are not coupled in the simulation at one instant of time, any number of polarizations each having different energy levels can be included. This is very important if we want to have absorption and emission at the same point in the calcualtion domain.

V. Conclusion

In conclusion, we have implemented the general algorithm to simulate the propagation of EM waves in laser which was modeled as gain material. We presented the derivation for static and dynamic gain models used in the literature. For static model, Simple, Lorentzian and non-Lorentzian gain models were tested. For dynamic gain, the two level and the four-level systems are derived and tested. The simulation shows agreement with theory. This work is platform for full laser simulation as it has shown the ability of the general algorithm to simulate both static and dynamic models. Even though, only 1D derivation is presented, extending it to 2D and 3D is straight forward.

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