A Provably Stable and Simple FDTD Formulation for Electromagnetic Modeling of Graphene Sheets

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A new finite-difference time-domain (FDTD) formulation for modeling Graphene is proposed, in which Graphene is modeled as a resistive sheet with a frequency-dependent conductivity. The formulation is first developed in the context of the vector wave finite-element time-domain (FETD) and then reduced to the FDTD based on the equivalence between these two techniques. The obtained formulation is easy-to-implement and does not alter the original FDTD update equations. It can be applied to an existing FDTD code by simply adding a correction term to the appropriate variables. One of the main contributions of the paper is analyzing the stability of the proposed formulation, which has not been done previously.

***Index Terms*— Finite difference methods; Finite element analysis; boundary conditions.**

I. INTRODUCTION

Invented in 2004, Graphene is often called a revolutionary material of the 21st century. Due to its outstanding electrical and mechanical properties, Graphene has recently gained significant interest among scientists. Many Graphene based applications have been introduced in recent years and the need for a time domain simulation tool for studying Graphene based devices has emerged.

In electromagnetic fields Graphene acts like a thin surface with conductivity that depends on chemical doping or external fields [1]. Up to now, three approaches have been used to model Graphene in FDTD methods which are: 1) regular FDTD method with very fine field discretization in Graphene layer [2-3], 2) sub-cell FDTD approach [4] and 3) Graphene as a surface boundary condition (SBC) in FDTD [5]. Since Graphene is very thin (one atomic thick layer) the first approach will be very expensive requiring a lot of memory and time, which makes it a poor option in practice. In spite of the merits of the other two approaches, they share at least two major drawbacks: 1) they require different update equations in the vicinity of the Graphene sheet, which makes the programming difficult; 2) the effect of the modified equations on the stability of the underlying FDTD has not been analytically studied. In this paper, Graphene is considered as a resistive sheet, as in [5]; however, the formulation is inspired by the FETD method based on the wave equation [6]. The formulation is then reduced to the FDTD method by evaluating FETD integrals using the trapezoidal rule. The proposed FDTD formulation can be implemented with minimal modification on an existing FDTD code. In addition, because of the equivalence between FDTD and FETD, the stability of the proposed FDTD method including arbitrary-oriented layers of Graphene, unlike the widely-used von Neumann technique in FDTD (in which an unbounded and homogeneous domain is assumed) can be analyzed by finding the location of the eigenvalues in the FETD formulation.

II. FORMULATION

A. Graphene conductivity model

Graphene has a frequency-dependent complex-valued conductivity. The macroscopic Graphene conductivity model is used in the FDTD method, which consists of two terms: inter-band conductivity and intraband conductivity. The Graphene surface conductivity (in units of [S]) is given by the Kubo formula in an integral form. The simplified Kubo formula for intraband conductivity term is [7]:

$$\sigma_{intra}(\omega,\mu_c,\gamma,T)=\frac{\alpha}{\omega-j2\gamma} \qquad (1)$$

in which $\alpha=\frac{je^2k_BT}{\pi\hbar^2}\left(\frac{\mu_c}{k_BT}+2ln\left(e^{(-\mu_c/k_BT)}+1\right)\right)$, ω is the angular frequency in radians and γ is the scattering rate in s^{-1}. Also, μ_c is the chemical potential in eV, which can be controlled by chemical doping or by applying a bias voltage, T is the temperature in Kelvin, e is the electron charge, $\hbar$ is the reduced Planck's constant, and k_B is the Boltzmann constant. The reason why just intraband conductivity has been introduced here is because in microwave frequencies, in which we are interested here, the interband term can be neglected.

B. Modeling of Graphene in FETD

Fig. 1 shows a 2-D rectangular grid in which the electric field unknowns {e} are assumed to be represented by edges. Graphene can be considered as a resistive sheet on which we have

$$\sigma_{intra}E=\hat{n}\times H \qquad (2)$$

Such a condition can be incorporated into the FETD formulation as [6]

$$[T]\frac{d^2\{e\}}{dt^2}+\sigma_{intra}[G]\frac{d\{e\}}{dt}+[S]\{e\}=\{0\} \quad (3)$$

Where $\{e\}=[e_1,e_2,\dots e_N]^T$ and $[T],[G],[S]$ are square matrices given by:

$$T_{ij} = \int \epsilon W_i^{(1)} . W_j^{(1)} \, d\Omega \qquad (4)$$

$$S_{ij} = \int \mu^{-1} \nabla \times W_i^1 . \nabla \times W_j^{(1)} \, d\Omega \qquad (5)$$

$$G_{ij} = \int_{Graphene} \hat{n} \times W_i^{(1)} . \hat{n} \times W_j^{(1)} ds \qquad (6)$$

in which $W^{(1)}$ represents the Whitney 1-form element. Eq. (3) can be transformed into the mixed FETD formulation in which both electric $\{e\}$ and magnetic fields $\{b\}$ are being updated together similar to the FDTD, as

$$\begin{cases} [T]\dfrac{\partial\{e\}}{\partial t} = [C]^T[T_f]\{b\} - \{J\} \\ \dfrac{\partial\{b\}}{\partial t} = -[C]\{e\} \end{cases} \qquad (7)$$

Where $\frac{\partial\{J\}}{\partial t} = (\sigma_{intra}(t)[G]) * \partial\{e\}/\partial t$, $[C]$ is the discrete curl operator, and

$$T_{f,ij} = \int W_i^{(2)} . W_j^{(2)} \, d\Omega \qquad (8)$$

in which $W^{(2)}$ represents the Whitney 2-form element. In order to obtain the FDTD equations from (7), the trapezoidal integration has to be employed to evaluate integrals, which makes $[T], [T_f]$, and $[G]$ fully diagonal. It should be noted that only those unknowns on which the Graphene sheet lie have non-zero contribution in $[G]$. Having discretized (7) in time using desired method, update equations identical to the fully-discretized FDTD can be obtained in which the electric field update equation for those unknown resided on the Graphene sheet have an additional term $\{J\}$. In case of an explicit FDTD, e.g., the standard leap-frog FDTD, J can be updated separately and applied as a correction term after the standard update process is performed, which greatly simplifies implementation. Needless to mention the update equation for the magnetic field is not changed in this approach.

III. Results

In order to validate the proposed formulation, we conducted a simple numerical example: calculating reflection and transmission coefficients of an infinitely long Graphene sheet. The problem was solved in 1-D and the plane-wave had a Blackman-Harris pulse shape. The parameters of the Graphene are as in [7] and the exact solutions were calculated by $T = 2/(2 + \eta_0\sigma_{gr})$ and $\Gamma = T - 1$, in which η_0 is free space impedance and σ_{gr} is Graphene conductivity.

Fig. 2 shows comparison of the numerical and analytical results of transmission and reflection coefficients in which we can observe our method is in an excellent agreement with the analytical results. Relative error between the analytical results and the proposed method is less than %0.02 in the considered frequency range. Our numerical studies showed that the formulation is stable for time steps smaller than the stability limit of the FDTD technique.

IV. Conclusion

A new FDTD formulation based on the equivalence between the FETD and the FDTD on a Cartesian grid has been proposed. The formulation can be easily embedded in an existing FDTD code.

Detailed formulation and more numerical examples will be presented in the conference and the long version of the paper. Moreover, we will include the stability condition of (3), which has similar stability condition as the corresponding FDTD formulation.

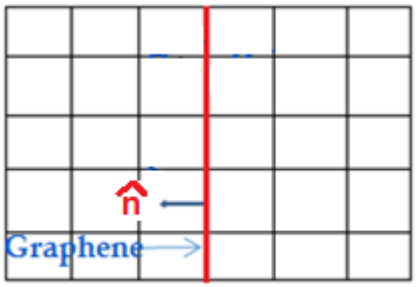

Fig.1. Graphene sheet placed in a 2-D rectangular grid.

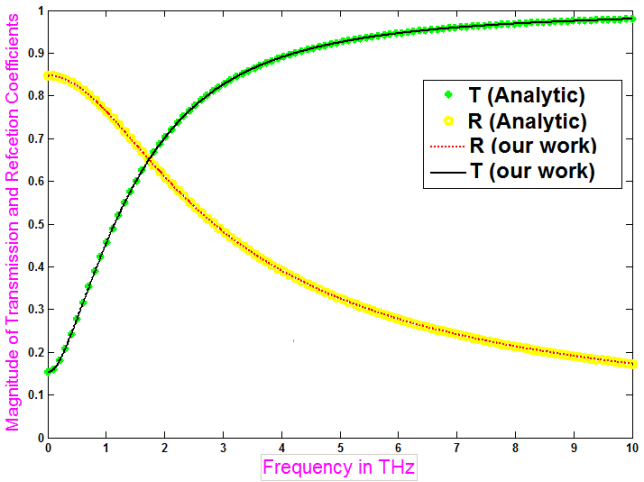

Fig.3. Comparison between transmission and reflection coefficients of our numerical method and analytical results for Graphene; T=300K, τ=0.5ps, μc=0.5ev.

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