Time-Domain Boundary Element Method Incorporating Strongly Nonlinear Conductivity for Application in the Modeling of 2D Devices

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***Abstract*—In this work, a time-domain surface integral equation with a strongly nonlinear Resistive Boundary Condition is formulated and approximately solved using the march on in time scheme. The discretization of the nonlinear relation between the surface current density and the electric field is approximated such that the final system of equations to be solved are linear. It is applied to solve scattering of a Gaussian plane wave by a sphere possessing a strongly nonlinear conductivity relation. This solver is developed to specifically model the effects due to the region of negative differential conductivity in the conductivity relation, which is expected in graphene superlattice structures. Numerical results demonstrate the stability and convergence of the method and the ability to enforce the constitutive relation within controllable error bounds.**

I. Introduction

Recent developments in solid state physics demand attention towards solving electromagnetic scattering problem involving nontrivial boundary condition and constitutive relation to accurately model the devices utilizing the physics. Frequency domain formulation of the integral equations along with various kind of boundary conditions have been made. However, the frequency domain analysis is usually not sufficient to capture the response of a strongly nonlinear system. Hence, time-domain methods must be considered despite their high computational requirements. Finite-Difference Time-Domain (FDTD) [1] and Time-Domain Finite Element Method (TD-FEM) are commonly used to solve time-domain scattering problems and have been shown to solve nonlinear problems but these methods suffer from the Courant-Friedrichs-Lewy (CFL) condition which limits the time step size and the need for discretization of domain larger than the object under consideration. This warrants the furthering of Time-Domain Boundary Element Method (TD-BEM) to allow the capability of modeling the nonlinear constitutive and conductivity relations of the scattering object. Modeling of imperfect conductors using time-domain integral equations have been shown in [2]. In [3], a solver for Time-Domain Electric Field Volume Integral Equation (TD-EFVIE) to consider the Kerr nonlinearity has been built using predictor-corrector (PE(CE)^m) scheme. However, the presence of the negative differential conductance (NDC) region in the characteristic would prevent its inversion required by the solver [3]. In this contribution, we formulate a method to approximately solve time-domain surface integral equation for conductivity model featuring a NDC region and demonstrate it using a simple case of scattering by a sphere.

II. Formulation

The (differentiated) time-domain electric field integral equation for an imperfect conductor reads

$$\dot{\mathscr{T}}\mathbf{j} + \hat{\mathbf{n}} \times \frac{\partial \mathbf{e}}{\partial t} = \hat{\mathbf{n}} \times \frac{\partial \mathbf{e}^{inc}}{\partial t} \tag{1}$$

where $\dot{\mathscr{T}}$ is the time derivative of the time-domain single layer operator given by,

$$\dot{\mathscr{T}}\mathbf{j} = \hat{\mathbf{n}} \times \int_S \Big[\frac{\partial^2}{\partial t^2}\frac{\mathbf{j}(\mathbf{r}', t-\frac{R}{c})}{4\pi c R} - c\nabla \frac{\nabla' \cdot \mathbf{j}(\mathbf{r}', t-\frac{R}{c})}{4\pi R}\Big] dS' \tag{2}$$

The constitutive relation used is [4]:

$$\mathbf{j} = -\overline{\overline{\sigma}} \cdot \hat{\mathbf{n}} \times (\hat{\mathbf{n}} \times \mathbf{e}) \tag{3}$$

A. Discretization

We discretize the unknown surface current density $\mathbf{j}$ and the tangential component of the electric field $\mathbf{e}_\mathrm{t}$ on the surface of the scattering object using Rao-Wilton-Glisson (RWG) basis functions [5] and in time using the shifted Lagrange bases [6] as following:

$$\mathbf{j}(\mathbf{r}, t) = \sum_{m=1}^{N_s} \sum_{l=0}^{N_t-1} J_m^{(l)} \mathbf{f}_m(\mathbf{r}) T^{(l)}(t) \tag{4}$$

and

$$\mathbf{e}_\mathrm{t}(\mathbf{r}, t) = \sum_{m=1}^{N_s} \sum_{l=0}^{N_t-1} E_m^{(l)} \mathbf{g}_m(\mathbf{r}) T^{(l)}(t) \tag{5}$$

We define the test basis function in space using the same RWG basis functions and in time using shifted delta functions. Substituting (4) and (5) in (1) and (3) and testing with the test basis functions, we get for each i:

$$\sum_{j=0}^{i} \mathbf{Z}^{(i-j)}\mathbf{J}^{(j)} + \sum_{j=0}^{i} \dot{\mathbf{G}}^{(i-j)}\mathbf{E}^{(j)} = \dot{\mathbf{E}}^{inc(i)} \tag{6}$$

$$\mathbf{G}\mathbf{J}^{(i)} = \mathbf{Q}^{(i)}\mathbf{E}^{(i)} \tag{7}$$

$\mathbf{G}$ is the Gram Matrix corresponding to the basis function $\mathbf{f_n}$, $\dot{\mathbf{G}}^{(i-j)} = \frac{\partial T^{(i-j)}(t)}{\partial t}|_{t=0} \times \mathbf{G}$ and $\mathbf{Q}^{(i)}$ is given by,

$$[\mathbf{Q}^{(i)}]_{mn} = <\mathbf{f}_m(\mathbf{r}), \overline{\overline{\sigma}}(\mathbf{r}, t_i) \cdot \mathbf{f}_n(\mathbf{r})> \tag{8}$$

B. MOT Scheme

In this work, we focus on an isotropic conductivity based on [7] which is given by:

$$\sigma(\mathbf{r},t) = a|\mathbf{e}_t(\mathbf{r},t)|^2 + b|\mathbf{e}_t(\mathbf{r},t)| + c \tag{9}$$

with $a = 1.2$, $b = -1.752$ and $c = 0.681$. The interesting aspect of this kind of conductivity behaviour is the presence of a region of NDC observed in graphene based tunelling diodes and graphene superlattice structures.

When solving (6) and (7), $\mathbf{Q}^{(i)}$ is not readily known as it depends on the tangential electric field which is an unknown itself at this stage. Assuming the time step is chosen sufficiently small, the following approximation, which amounts to a linearisation, can be used to compute the $\mathbf{Q}^{(i)}$,

$$\sigma(\mathbf{r},t_i) = \sigma(\mathbf{e}_t(\mathbf{r},t_i)) \approx \sigma(\mathbf{e}_t(\mathbf{r},t_{i-1})) \tag{10}$$

and we obtain the solution for each time step i as:

$$\begin{aligned}\mathbf{J}^{(i)} =& (\mathbf{Z}^{(0)} + \dot{\mathbf{G}}^{(0)}(\mathbf{Q}^{(i)})^{-1}\mathbf{G})^{-1} \\ & \Big(\dot{\mathbf{E}}^{inc(i)} - \sum_{j=1}^{i-1}\mathbf{Z}^{(i-j)}\mathbf{J}^{(j)} - \sum_{j=1}^{i-1}\dot{\mathbf{G}}^{(i-j)}\mathbf{E}^{(j)}\Big)\end{aligned} \tag{11}$$

and

$$\mathbf{E}^{(i)} = (\mathbf{Q}^{(i)})^{-1}\mathbf{G}\mathbf{J}^{(i)} \tag{12}$$

The convolution operations in (11) is limited in number of terms which is determined by the maximum linear dimension of the object D_{max} and the support of time basis functions L i.e. $T^{(0)}(t) = 0$ for $t > L\Delta t$. We have $\mathbf{Z}^{(i-j)} = 0$ for $(i-j) > D_{max}/(c\Delta t) + L$ and $\dot{\mathbf{G}}^{(i-j)} = 0$ for $i - j > L$. In this work, $L = 3$.

III. Results

A sphere of radius of 1.0 m with the conductivity in (9) is incident by a Gaussian pulse of a plane wave traveling along $\hat{z}$ and polarized along $\hat{x}$ with amplitude = 1.5 V/m and pulsewidth cT = 3.4 light meters. Fig. 1 shows that the solution at each time step converges to the exact current-field characteristic as the time step size is reduced. The current density at a fixed point on the sphere against time for different mesh parameters shown in the Fig. 2 demonstrates stability and convergence of the method, even in the presence of strongly nonlinear constitutive relation.

Future development is aimed at implementing excitations that more closely resemble those used in the study of these materials and the study of the surface charge's spatio-temporal behavior in 2D devices based on graphene superlattices. Of particular interest is the modelling of charge accumulation and propagation, a consequence of the type of nonlinear behaviour studied here that affects the workings of these devices and is central to their development [8].

Acknowledgement

This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (Grant agreement No. 101001847).

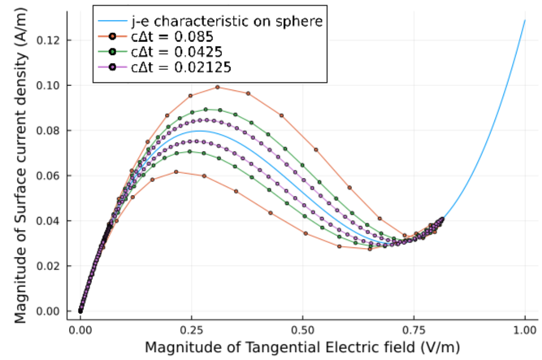

Fig. 1. The solved conductivity relation between the current and the electric field compared with the exact model for various simulation time step size shows that the solution approaches the exact model as the step size is reduced.

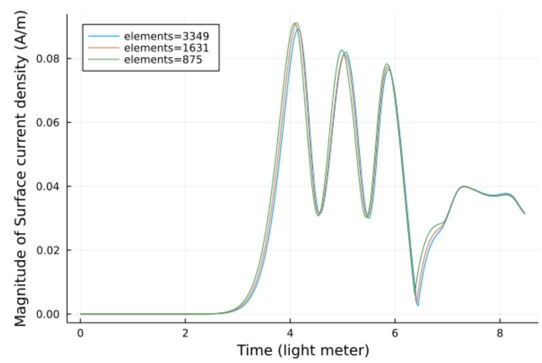

Fig. 2. Comparison of solution for different meshes also showing the induced current density response of the nonlinear conducitvity of the sphere against the incidence of a Gaussian pulse.

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