Dual-Potential Finite-Difference Technique for Computational Electrodynamics

Samuel Belling, Laleh Avazpour, Michelle King, and Irena Knezevic
Department of Electrical and Computer Engineering
University of Wisconsin-Madison, Madison, WI 53706, USA
swbelling@wisc.edu

***Abstract*—We present a finite-difference time-domain (FDTD) technique suitable for coupling with quantum-transport solvers. We derive first-order equations for the electric and magnetic vector potentials and the electric scalar potential which, upon the adoption of the Coulomb gauge, decouple into solenoidal and irrotational equation sets and are sourced by the solenoidal and irrotational parts of the current density, respectively. The solenoidal electric and magnetic vector potentials obey equations analogous to the normal curl equations for the electric and magnetic fields, a fact we exploit to develop an effective absorbing boundary layer used to simulate unbounded regions in a way identical to standard FDTD. We demonstrate coupling to a simple quantum transport technique known as the Usuki transfer matrix technique.**

I. Introduction

Time-dependent and high-frequency processes in nanoscale electronic, optical, and optoelectronic systems are characterized by the interplay between the quantum-mechanical nature of charge carrier transport and full-wave electrodynamics. Quantum transport is centered around the electronic Hamiltonian and thus requires electrodynamics formulated in terms of the gauge-dependent potentials rather than the gauge-independent electric and magnetic fields. Unfortunately, computational-electrodynamics techniques with potentials are rare, and are not usually formulated with coupling to quantum transport in mind.

In this paper, we showcase our recent work on the development of a dual-potential (DuPo) finite-difference time-domain (FDTD) technique for computational electrodynamics with potentials that is suitable for coupling with quantum transport.

II. Dual-Potential FDTD Technique

The standard finite-difference time-domain (FDTD) algorithm [1] is a popular technique for solving time-dependent Maxwell curl equations. At its core is a system of first-order update equations that march each component of the electric and magnetic fields forward in time. We produce a similar set of first-order equations for the potentials, which allows us to adopt the FDTD framework and associated computational advances.

The vector magnetic potential ($\mathbf{A}$) and scalar electric potential (ϕ) are well known and relate to the magnetic flux density and electric field intensity as

$$\mathbf{B} = \nabla \times \mathbf{A}, \quad \mathbf{E} = -\frac{\partial \mathbf{A}}{\partial t} + \nabla\phi. \tag{1}$$

However, it is also true that the electric field will admit the Helmholz decomposition, which introduces the electric vector potential $\mathbf{C}$ and another scalar potential ψ:

$$\mathbf{E} = \nabla \times \mathbf{C} + \nabla\psi. \tag{2}$$

It can be shown that $\psi = \phi$ and

$$\nabla \times \mathbf{C} = -\frac{\partial \mathbf{A}}{\partial t}, \tag{3}$$

which looks very similar to Faraday's law. If we insert the Helmholz decomposition of $\mathbf{E}$ into Ampere's law, we obtain

$$\nabla \times \nabla \times \mathbf{A} = \mu_0 \mathbf{J} + \mu_0 \varepsilon_0 \frac{\partial}{\partial t}[\nabla \times \mathbf{C} + \nabla\phi]. \tag{4}$$

We now introduce a quantity $\mathbf{F}$ that satisfies $\nabla \times \mathbf{F} = \mathbf{J}_{rot}$ (the solenoidal part of current density). After some manipulation, we arrive at one of our final equations,

$$\nabla \times \mathbf{A} = \mu_0 \varepsilon_0 \frac{\partial \mathbf{C}}{\partial t} + \mu_0 \mathbf{F} \tag{5}$$

which looks very similar to Ampere's law. Finally, we can arrive at our last equation in a number of ways, including taking the divergence of Eq. (4), which results in,

$$\nabla \cdot \mu_0 \mathbf{J} = \frac{\partial}{\partial t} \nabla^2 \phi, \tag{6}$$

which is equivalent to the normal continuity equation. We have assumed the Coulomb gauge for each of the following quantities: $\mathbf{A}$, $\mathbf{C}$, and $\mathbf{F}$. Equations (3), (5), and (6) are used for our FDTD technique. The two curl equations for $\mathbf{A}$ and $\mathbf{C}$ depend only on $\mathbf{F}$ (related to the solenoidal part of the current density). Also note that the continuity equation is uncoupled from the curl equations and only depends on the irrotational part of the current density.

Typically, we expect to be given a current and/or charge density, and not $\mathbf{F}$. Unfortunately, it is difficult to solve the "inverse curl" problem, $\nabla \times \mathbf{F} = \mathbf{J_{rot}}$. Instead, define a quantity $\nabla \times \mathbf{J} = \mathbf{U}$, so that (given $\nabla \cdot \mathbf{F} = 0$) we get $\nabla \times \nabla \times \mathbf{F} = \nabla^2 \mathbf{F} = \mathbf{U}$. This equation amounts to three Poisson's equations, which are easily solved using the successive over-relaxation algorithm or a similar technique.

III. Numerical Implementation

The main benefit of the dual-potential equations is that the two curl equations for $\mathbf{A}$ and $\mathbf{C}$ are of the exact same

978-1-6654-7899-1/22/$31.00 ©2022 IEEE

form as the two curl equations for electric and magnetic fields (Faraday's and Ampere's laws), which allows us to adopt the advances in the FDTD technique for fields when dealing with the potentials **A** and **C**. We utilize the Yee cell [1] to stagger **A** and **C** in an exactly analogous way to **E** and **H** (put **A** where **E** would go, and put **C** where **H** would go). All finite differences are calculated using the central difference scheme. With our equations from above and the central difference method, we can calculate the time evolution of **A** and **C** in a self-consistent loop.

A key advance in FDTD that seek to take advantage of is the perfectly matched layer (PML) boundary condition. This boundary condition allows one to simulate radiation into free space from a finite region. Fortunately, a lot of thought has already been put into developing good PMLs for fields, resulting in the convolutional PML (CPML) that we will be using here [2]. Since our curl equations look just like those for fields, we can utilize the CPML formulations that have been developed already with appropriate variable substitutions. The details of the CPML formulation can be found in [2], [3], but the end result is a set of coefficients and auxilliary variables that modify the update equations (3) and (5). The coefficients include the parameters of the fictitious PML absorbing material such as permittivity, permeability, and conductivity.

IV. Results

For the purpose of demonstrating coupling, we connect the DuPo FDTD code to a simple Usuki transfer matrix quantum transport solver [4]. The transfer matrix method is equivalent to a nonequilibrium Green's function approach with no scattering, so it is useful for testing coupling with very simple quantum systems. Our system of choice is a nanotriangle antenna, which can demonstrate quantum tunneling if the gap between the two metallic triangles is small enough ($\leq$ 1 nm) [5]. This phenomenon cannot be captured by standalone Maxwell's solvers.

We initialize the simulation with a current source that has both nonzero curl and nonzero divergence, while initializing all other quantities to zero. We expect that, after some time, there will be a nonzero difference in ϕ between the two sides of the antenna, leading to a tunneling current. We show in Fig. 1 that, indeed, eventually there is a ϕ difference between the two sides and we have a nonzero tunneling current.

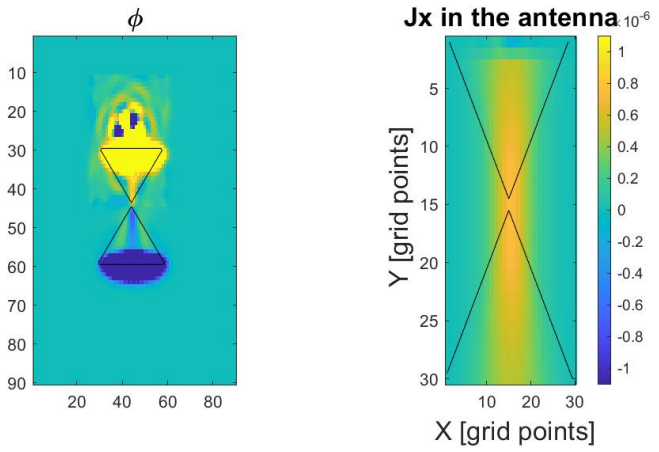

Fig. 1. (Preliminary results) A difference in ϕ between the two sides of the antenna (left panel) results in a tunneling current density (right panel). Note that ϕ is not uniform throughout the triangle material because the time constant (permittivity divided by conductivity) is much larger than the simulation time in this particular simulation.

V. Conclusion

We presented our recent work on the development of a dual-potential finite-difference time-domain technique for computational electrodynamics with potentials that is suitable for coupling with quantum transport. We derived first-order equations for the electric and magnetic vector potentials and the electric scalar potential which, upon the adoption of the Coulomb gauge, decouple into two equation sets that are independently sourced by the solenoidal and irrotational parts of the current density. The solenoidal electric and magnetic vector potentials satisfy equations amenable to standard FDTD. We demonstrated the utility of dual-potential FDTD by coupling it to a simple quantum transport technique known as the Usuki transfer matrix technique and obtaining preliminary results for a nanoantenna in the receiver mode. More details will be presented at the conference.

References

[1] A. Taflove and S. C. Hagness, *Computational electrodynamics: the finite-difference time-domain method*. Norwood: Artech House, 3rd ed., 2005.

[2] J. A. Roden and S. D. Gedney, "Convolution pml (cpml): An efficient fdtd implementation of the cfs–pml for arbitrary media," *Microwave and Optical Technology Letters*, vol. 27, no. 5, pp. 334–339, 2000.

[3] J. A. Roden and S. D. Gedney, "Convolution PML (CPML): An efficient FDTD implementation of the CFS-PML for arbitrary media," *Microwave and Optical Technology Letters*, vol. 27, no. 5, pp. 334–339, 2000.

[4] T. Usuki, M. Saito, M. Takatsu, R. A. Kiehl, and N. Yokoyama, "Numerical analysis of ballistic-electron transport in magnetic fields by using a quantum point contact and a quantum wire," *Phys. Rev. B*, vol. 52, pp. 8244–8255, Sep 1995.

[5] K. J. Savage, M. M. Hawkeye, R. Esteban, A. G. Borisov, J. Aizpurua, and J. J. Baumberg, "Revealing the quantum regime in tunnelling plasmonics," *Nature*, vol. 491, p. 574, nov 2012.