Dual-Potential Finite-Difference Method for Electrodynamics Within Multiphysics Solvers

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ABSTRACT

Many quantum transport simulation tools require the electric and magnetic vector potentials, rather than the electric and magnetic fields. We present a finite-difference time-domain (FDTD) technique for calculating the time-dependent potentials. The equations are first order in space and time, and separate into solenoidal and irrotational parts. The first-order nature of the equations allows us to adapt well-developed techniques for traditional FDTD with fields, such as effective absorbing boundary conditions that allow us to simulate systems in free space within a finite computational domain. We demonstrate coupling of this electrodynamics technique to a ballistic non-equilibrium Green's function transport code.

INTRODUCTION

The coupling of classical electrodynamics to quantum-mechanical charge transport is an essential process to understand for the characterization of time-dependent and high frequency optoelectronic systems. Traditionally, classical electrodynamics is formulated in terms of the electric and magnetic fields, while the key quantity in quantum charge transport, the electronic Hamiltonian, requires the gauge-dependent electric and magnetic potentials. In this work, we present a time-dependent algorithm for calculating the electric and magnetic potentials in the Coulomb gauge, with a focus on coupling to quantum transport codes.

DUAL-POTENTIAL FDTD

The finite-difference time-domain (FDTD) algorithm is a popular choice for solving Maxwell's curl equations. The algorithm marches each component of the electric and magnetic fields forward in time from initial values according to Maxwell's equations. Many problems can be accurately modeled with initial values of all fields equal to zero, and only a current density driving the time evolution, allowing one to calculate all fields using only the two curl equations. We have produced a similar set of two curl equations for the familiar magnetic vector potential,

$$\nabla \times \boldsymbol{A} = \mu_0 \epsilon_0 \frac{\partial \boldsymbol{C}}{\partial t} + \mu_0 \boldsymbol{F} \quad (1)$$

And the analogous quantity relating to the electric field, the electric vector potential,

$$\nabla \times \boldsymbol{C} = -\frac{\partial \boldsymbol{A}}{\partial t} \quad (2)$$

In (1) and (2) $\boldsymbol{A}$ is the magnetic vector potential, $\boldsymbol{C}$ is the electric vector potential, and $\boldsymbol{F}$ is a quantity analogous to current density for the potentials. In this formulation, $\boldsymbol{F}$ is related only to the solenoidal part of the actual current density. An example of a current density that makes explicit the inclusion of both a solenoidal and conservative part is shown in Fig. 1. Finally, we relate the conservative part of current density to the scalar potential, as

$$\nabla \cdot \mu_0 \boldsymbol{J} = \frac{\partial}{\partial t} \nabla^2 \phi \ (3)$$

which is equivalent to the normal continuity equation. To reduce (3) to first order in the spatial derivative, we can track ρ, which is proportional to $\nabla^2 \phi$, and solve Poisson's equation when ϕ is needed. The form of (1) and (2) is just that of Maxwell's curl equations for fields, so the advancements in the FDTD technique for fields, such as the Yee cell [1] and perfectly matched layer boundary condition [2] are easily adapted. We showcase coupling to a ballistic NEGF code (Fig. 2) by initializing a non-zero ϕ and sourcing $\boldsymbol{A}, \boldsymbol{C}$, with a tunneling current between two metallic patches in Fig. 3.

ACKNOWLEDGMENT

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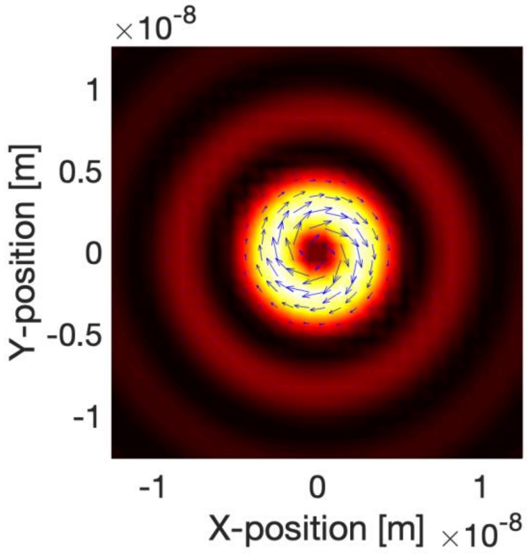

Fig. 1. Current density obtained from an electronic wavefunction for a vortex beam, with an explicitly defined angular and linear momentum. Color indicates intensity, and blue arrows indicate the solenoidal nature of the beam. The linear momentum is directed into the page.

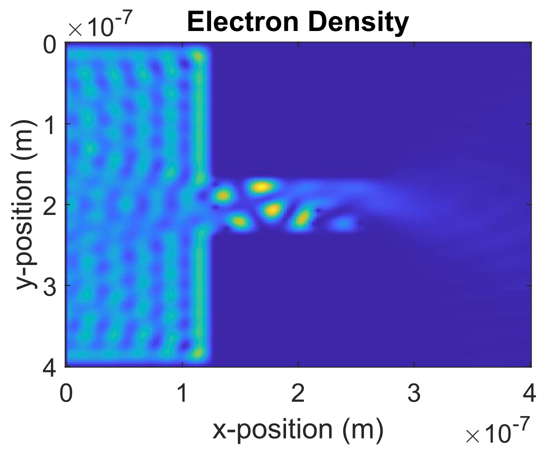

Fig. 2. Demonstration of charge transport through a narrow channel between two contacts (left: full, right: empty) with random disorder using ballistic NEGF.

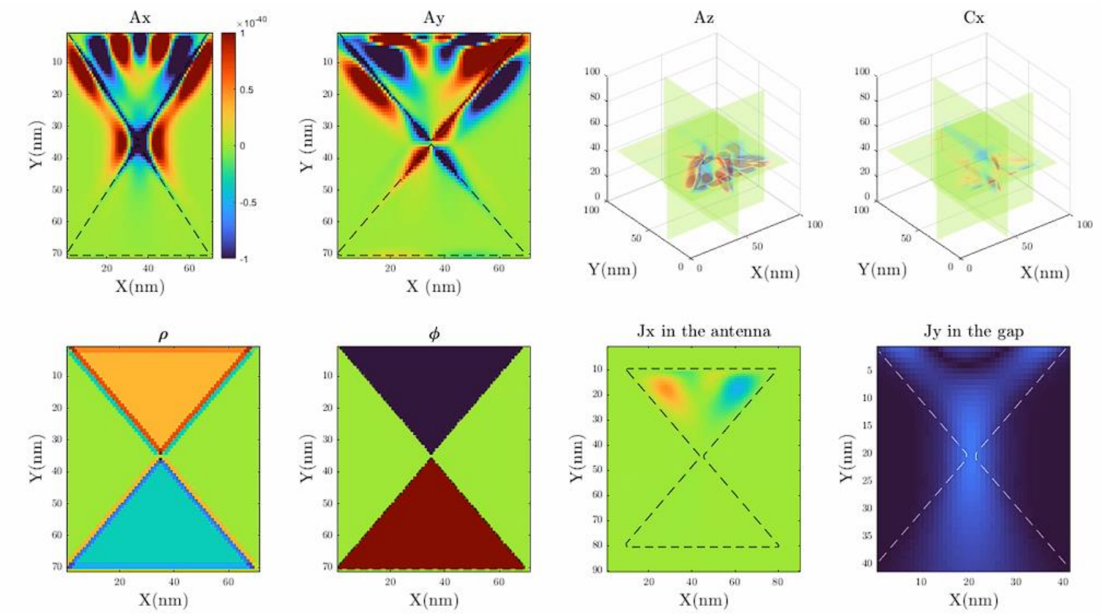

Fig. 3. Snapshot of electric and magnetic potentials sourced by two metallic patches with different initial electric potentials, and a resulting tunneling current through the small gap between the patches. Maxwell solvers on their own cannot capture phenomena such as the tunneling current and must be coupled with quantum transport solvers, as done in this work.