FiPo FDTD Algorithm: Modeling Electric and Magnetic Fields with Potentials A and ϕ for Quantum Transport Solvers

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Abstract

We present the FiPo FDTD algorithm, which can solve a set of first-order equations for the electric and magnetic fields (**E** and **H**), as well as the magnetic vector potential **A** and the scalar electric potential ϕ in the Lorenz gauge. We also provide the derivation and implementation of a state-of-the-art convolutional perfectly matched layer absorbing boundary condition for this new set of equations. Knowing that potentials **A** and ϕ can be utilized as input for the single-particle electron Hamiltonian in quantum transport solvers, we demonstrate that by initializing **A** and ϕ we can extract information about electric and magnetic fields (**E** and **H**). The FiPo FDTD algorithm can provide a balance between computational expense and accuracy and has significant potential applications in various fields such as optics, photonics, and quantum transport.

Introduction

Computational electromagnetics has traditionally focused on the Lorenz gauge to model electromagnetic fields for quantum transport applications. However, the decoupled second-order wave equations for the magnetic vector potential **A** and the scalar electric potential ϕ in this gauge pose significant challenges when it comes to boundary conditions and sourcing. Instead of pursuing the decoupled second-order equations, we propose a new algorithm that utilizes first-order field-potential (FiPo) hybrid algorithm, which utilizes the **A**–ϕ formulation combined with traditional **E**–**H** Maxwell's equations. It can be solved using the finite-difference time-domain (FDTD) technique on a staggered spatial grid and using the leapfrog method [1]. This model can accurately and efficiently calculate both electromagnetic fields and quantum transport response in devices with tunneling or nonlinear optical properties. We also present a complex-frequency shifted form of the convolutional perfectly matched layer (CFS- CPML) medium to terminate the FDTD domain.

Hybrid Field and Potential Technique: FiPo Hybrid

The FiPo equations are derived from Maxwell's equations and the Lorenz gauge. The full set of equations reads:

$$\varepsilon \partial t \boldsymbol{E} = \nabla \times \boldsymbol{H} - \boldsymbol{J}, \tag{1a}$$

$$\mu \partial t \boldsymbol{H} = -\nabla \times \boldsymbol{E}, \tag{1b}$$

$$\partial t \boldsymbol{A} = -\boldsymbol{E} - \nabla \phi, \tag{1c}$$

$$\varepsilon 2 \mu \partial t \phi = -\nabla \cdot (\varepsilon \boldsymbol{A}), \tag{1d}$$

They are updated in the order shown in Figure 1.

Furthermore, we present a complex-frequency shifted form of the convolutional perfectly matched layer (CFS–CPML) for the termination of the finite-difference time-domain (FDTD) simulation region, based on the approach described in reference [2]. In the standard FDTD method, the number of arrays required for relevant variables and auxiliary PML variables is eighteen in a three-dimensional domain, while the proposed FiPo FDTD method requires twenty-eight arrays for the same purpose and this number is much higher for traditional second-order potential wave equation approach. The effectiveness of our CFS–CPML is demonstrated by the low reflection error of -100dB for FiPo Hybrid, as shown in Figure 2.

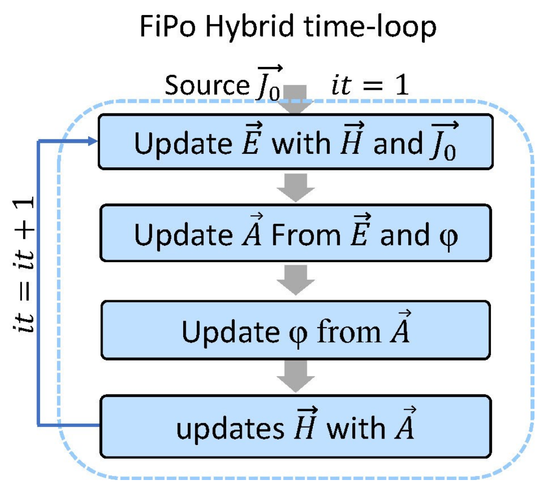

Fig. 1. Flowchart of the $\boldsymbol{\phi}$, **E**, **A**, and **H** time-stepping loop for the FiPo Hybrid algorithm. Field and potential updates are consecutive. Arrows show the progression of field or potential values through the update equations.

Additionally, we provide an example showcasing the capabilities of using a combination of **A** and ϕ to initialize the simulation (Fig. 3). This technique can be coupled with a quantum solver to use the potentials as an input for FDTD or export the potentials to the quantum solver, enabling a better understanding of the light–matter interaction in quantum effects such as tunneling.

Conclusion

In conclusion, we have presented the FiPo FDTD algorithm with a new convolutional perfectly matched layer medium that can efficiently terminate the FDTD domain. By utilizing a set of first-order equations for the electric and magnetic fields, along with the magnetic vector potential and scalar electric potential in the Lorenz gauge, we have demonstrated the potential for coupling with quantum transport solvers. The ability to use the potentials as input for the single-particle electron Hamiltonian, and the fields for standard FDTD purposes with phenomenological materials parameters or coupled with semiclassical transport solvers, makes FiPo a versatile tool for future multiphysics simulations.

References

[1] A. Taflove and S. C. Hagness, *Computational electrodynamics: the finite- difference time-domain method*, 3rd ed. Norwood: Artech House, (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, **27**, 334 (2000).

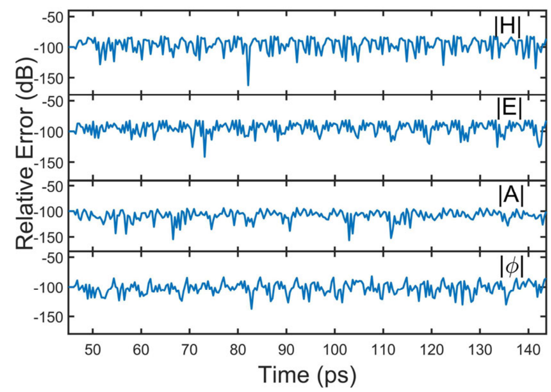

Fig. 2. Relative reflection error for the magnitudes of fields and potentials with CPML implemented for **H**, **E**, **A**, and $\boldsymbol{\phi}$. Reference simulation is $300 \times 300 \times 300$ where the PML is 10 cells thick. FiPo simulation was run on a $100 \times 100 \times 100$ grid with a PML of 10 cells.

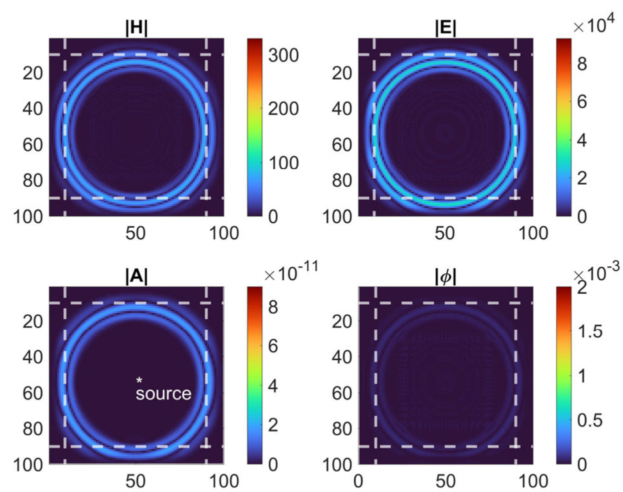

Fig. 3. Visualization of fields and potentials amplitude showing axial x-y cross-section of a 3D simulation domain, sourced by a first derivative of a Gaussian wave packet vector potential (A) at the center and enclosed by an active CPML region, demonstrating the algorithm's vector-potential-sourcing capabilities. FiPo simulation was run on a $100 \times 100 \times 100$ grid with a PML of 10 cells, *z*-axis is normal to the plane of the figure.