FiPo FDTD: Computational Electrodynamics Technique Producing Both Fields and Potentials

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***Abstract*—We present the field–potential finite-difference time-domain (FiPo FDTD) algorithm, which solves 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 present the derivation and implementation of a convolutional perfectly matched layer absorbing boundary condition for this new set of equations. Potentials A and ϕ can be used as input for the single-particle electron Hamiltonian in quantum transport solvers.**

I. Introduction

To accurately model devices with tunneling or nonlinear optical properties exposed to electromagnetic fields, we need to couple quantum transport with classical electromagnetics. We need models that can accurately and efficiently calculate electromagnetic fields along with the quantum response. Choosing a quantum transport solver necessitates balancing computational expense and accuracy; the choice requires enough precision to capture the quantum nonlinear optical response from materials and devices, but fast enough to be updated on the timescales of the electromagnetic solver.

To that end, we introduce a new field–potential (FiPo) finite-difference time-domain (FDTD) algorithm using first-order $\mathbf{A}$–ϕ formulation combined with traditional $\mathbf{E}$–$\mathbf{H}$ Maxwell's equations. We further present a complex-frequency shifted form of the convolutional perfectly matched layer (CFS-CPML) medium for the termination of the FDTD domain.

II. FiPo FDTD Technique and Implementation

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

$$\begin{aligned} \partial_t \mathbf{A} &= -\mathbf{E} - \nabla\phi, \\ \epsilon^2 \mu \partial_t \phi &= -\nabla \cdot (\epsilon \mathbf{A}), \\ \epsilon \partial_t \mathbf{E} &= \nabla \times \mathbf{H} - \mathbf{J}, \\ \mu \partial_t \mathbf{H} &= -\nabla \times \mathbf{E} \end{aligned} \tag{1}$$

Figure 1 shows the order in which the fields and the potentials are updated. The center represents a single timestep for integer timestep n, with the half-step $n+1/2$ also denoted; the top and bottom are grey and represent the previous and next timesteps, respectively. Each labelled box with gives the variable being updated, as well as those neededfor the update. Arrows show the progression of updates in the order of the algorithm. ϕ is first updated from the previous $\mathbf{A}$. Next, $\mathbf{E}$ is updated from the previous $\mathbf{H}$, as well as a source $\mathbf{J}$. Moving to the half timestep, $\mathbf{A}$ is updated from $\mathbf{E}$ and ϕ, then back to $\mathbf{H}$ being updated from $\mathbf{E}$. The quantities are on a modified Yee cell [1], with collocated $\mathbf{A}$ and $\mathbf{E}$.

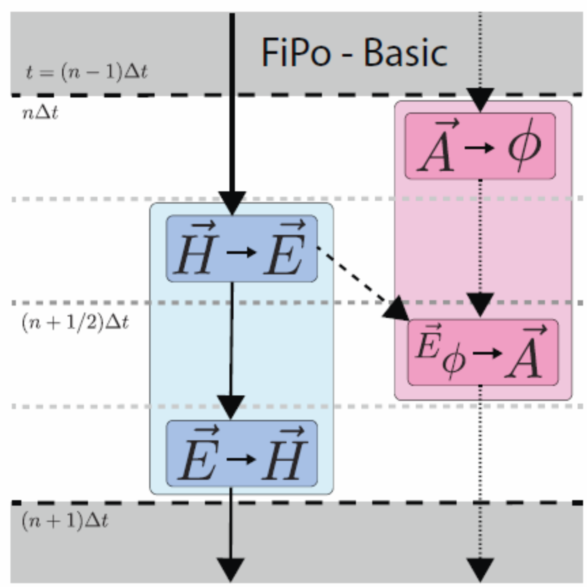

Fig. 1. Diagram of ϕ, $\mathbf{E}$, $\mathbf{A}$, and $\mathbf{H}$ updates at respective timesteps for the FiPo algorithm. Field updates are given in blue on the left, and potential updates are pink on the right. Arrows show the progression of field values through the update equations.

We derived a complex-frequency shifted form of the convolutional perfectly matched layer (CFS-CPML) for the termination of FDTD domain along the lines of Ref. [2]. The number of arrays for all relevant variables and auxiliary PML variables equals eighteen for standard FDTD in a three-dimensional domain, while it is twenty-eight for FiPo FDTD.

In Fig. 2, we show an example of a resonant cavity with and without our CPML. The source is a basic differentiated Gaussian current pulse launched from the center of the simulation domain in free space. The example allows us to visually examine the effectiveness of the PML. The snapshots are from after the pulse has hit the outer boundary. Without the PML, considerable reflection is clearly observed. In contrast, there is very little reflection for FiPo with CPML. In fact, approximately -100 dB attenuation is observed in this

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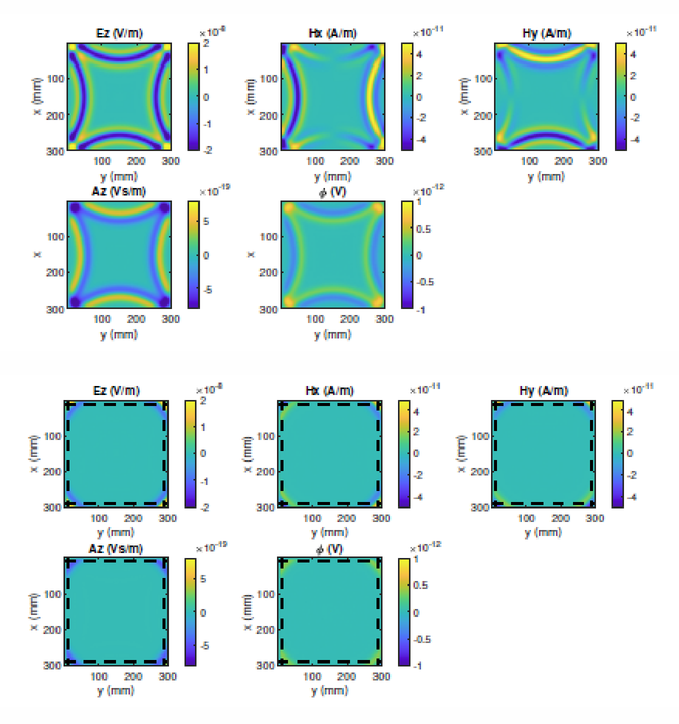

Fig. 2. Illustration of the efficiency of the PML. Various field components inside a cavity a while after the introduction of a differentiated Gaussian current pulse as a source at the center, without (top five panels) and with (bottom five panels) a PML. z-axis is normal to the plane of the figure.

particular case.

III. Conclusion

We introduced the FiPo FDTD algorithm with a complex-frequency shifted form of the convolutional perfectly matched layer medium for the termination of the FDTD domain. FiPo FDTD solves a set of first-order equations for the electric and magnetic fields, as well as the magnetic vector potential and the scalar electric potential in the Lorenz gauge. The potentials can be used as input for the single-particle electron Hamiltonian in quantum transport solvers, while the fields can be used for standard FDTD purposes with phenomenological materials parameters or coupled with semiclassical transport solvers. This versatility is an asset of FiPo when considering its contribution to future multiphysics simulations.

References

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