FDTD Algorithm for Fields and Potentials with Convolutional Perfectly Matched Layer Absorbing Boundary Conditions

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Accurate simulation of light–matter interaction at the nanoscale requires self-consistent coupling at every time step between quantum transport and electrodynamics solvers. We have developed an electrodynamics solver based on the finite-difference time-domain (FDTD) method, which computes the electric field **E** and magnetic field **H,** as well as the magnetic vector potential **A** and scalar potential Φ. This field-potential (FiPo) FDTD method can take, as input, the current density **J** and charge density ρ provided by the quantum transport solver, and will output **A** and Φ, which are needed as input for the next update in the quantum-transport solver.

The FiPo FDTD algorithm employs four coupled first-order equations for **E**, **H**, **A** and Φ, where the generalized Lorenz gauge is adopted [1]. The first order of the equations simplifies the creation of absorbing boundary conditions with respect to the second-order **A**/Φ FDTD presented in [2]. We have successfully implemented a convolutional perfectly matched layer (CPML) absorbing boundary layer to absorb both fields and potentials in FiPo FDTD [3].

A FiPo FDTD simulation of electromagnetic fields arising from a differentiated Gaussian current source is illustrated for the fields just hitting the CPML (Fig. 1) and being fully in the CPML (Fig. 2); the wave appears elongated as it is absorbed, which is expected. Relative errors of the field magnitude (Fig. 3) show that the CPML is adequately absorbing all four fields. Simulations for these examples are similar to those in [2], with a differentiated Gaussian current source in z direction with a bandwidth of 6 GHz at the center of the simulation domain, relative dielectric permittivity ϵ_r of 7.73, conductivity σ of 0.273 $A^2m^{-3}kg^{-1}s^3$, α of 0.05 $A^2m^{-3}kg^{-1}s^3$, σ_{max} of 1.1*$\sigma_{optimal}$, and κ_{max} of 7.

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[2] C. J. Ryu, A. Y. Liu, W. E. I. Sha and W. C. Chew, IEEE J. Multiscale Multiphys. Comput. Tech. 1, 40 (2016).
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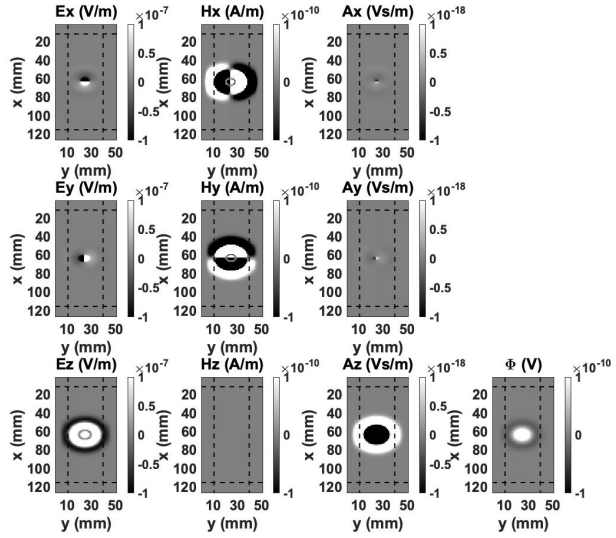

Fig.1: Snapshot of fields and potentials for FiPo FDTD at 0.32 ns.

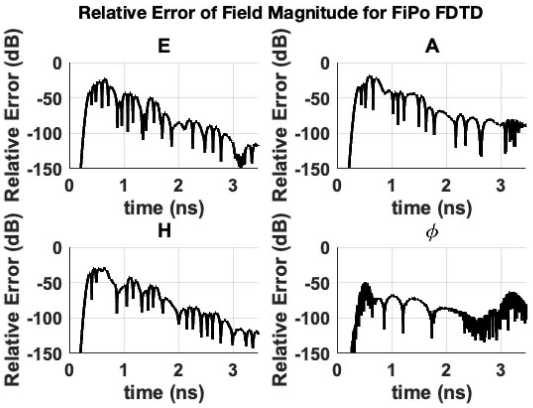

Fig.3: Relative error for magnitudes of fields with CPML implemented for E, A, H, and Φ. Reference simulation is 300x300x300 where the PML is 10 cells thick. FiPo simulation was run on a 126x51x26 grid with a PML of 10 cells.

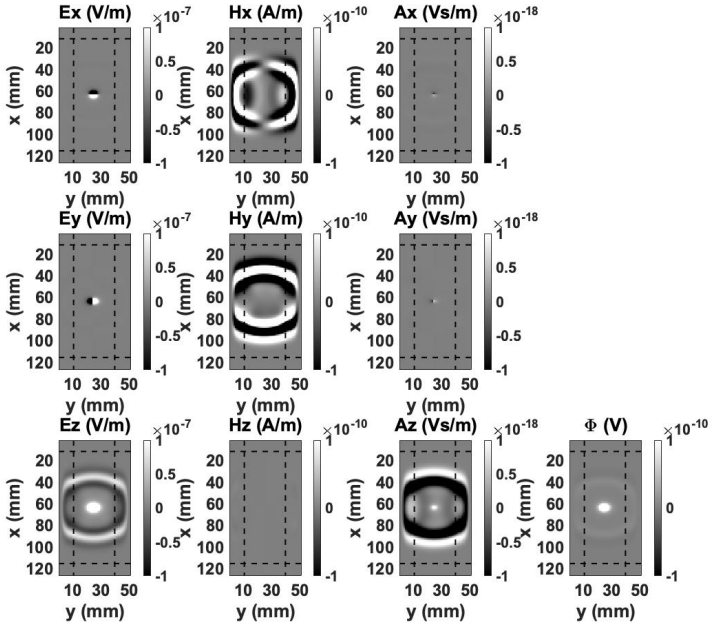

Fig.2: Snapshot of fields and potentials for FiPo FDTD at 0.49 ns.