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Efficient Hybrid Simulation for Maxwell-Schrödinger Problems

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***Abstract*—hybrid simulation for Maxwell-Schrödinger problems is necessary to analyze electronic devices based on quantum effects, such as carbon nanotube transistors. However, the computational cost is expensive because we must solve many unknowns to satisfy two governing equations for electromagnetic fields and electrons. In this paper, we will propose a novel method to reduce computational cost by applying the length gauge.**

I. INTRODUCTION

In general, it is complicated problems to simulate electronic devices such as carbon nanotube transistors [1], because they have some characteristics based on the classical and quantum theories. One approach to solve such problems is hybrid simulation of both Maxwell's and Schrödinger's equations. Recently, some hybrid simulations have been proposed[1-3], however, those computational costs are expensive because we must solve many unknowns to satisfy two governing equations.

In this paper, a novel hybrid simulation relying on the length gauge will be proposed [4]. We will verify that the computational results are precise and cost can be reduced by using our method.

II. FORMULATION

The Maxwell's equations with the polarization current density **J** are given by

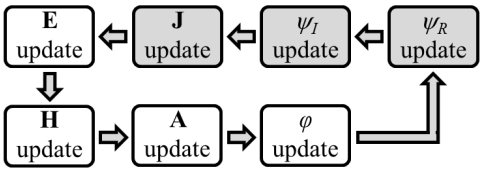
$$\nabla\times\mathbf{H}=\varepsilon_0\frac{\partial\mathbf{E}}{\partial t}+\mathbf{J}, \tag{1}$$

$$\nabla\times\mathbf{E}=-\mu_0\frac{\partial\mathbf{H}}{\partial t}, \tag{2}$$

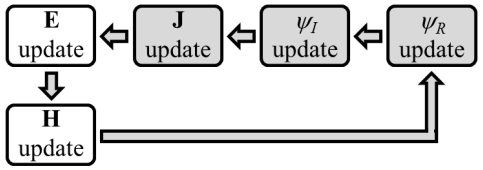
where ε_0 and μ_0 mean the permittivity and permeability in free space, respectively. We can rewrite Eqs. (1) and (2) to the following equations by selecting only time-derivative terms to the left member,

$$\frac{\partial\mathbf{E}}{\partial t}=\frac{1}{\varepsilon_0}\left(\nabla\times\mathbf{H}-\mathbf{J}\right), \tag{3}$$

$$\frac{\partial\mathbf{H}}{\partial t}=-\frac{1}{\mu_0}\nabla\times\mathbf{E}. \tag{4}$$



(a) conventional algorithm



(b) proposed algorithm

Fig. 1. Computational algorithm for hybrid simulation.

We can simulate Eqs. (3) and (4) by applying the Finite-Difference Time-Domain(: FDTD) method for the Maxwell's equations [5].

The Schrödinger's equation for an electron is given by

$$i\hbar\frac{\partial\psi}{\partial t}=\hat{H}\psi, \tag{5}$$

where $\hbar$ indicates the Planck's constant divided by 2π and $\hat{H}$ means the Hamiltonian which expresses the physical system of the problem. If an electron feels the force from only the electrostatic potential V, the Hamiltonian is given by

$$\hat{H}=-\frac{\hbar^2}{2m}\Delta+V, \tag{6}$$

where m means the mass of an electron.

We can rewrite Eq. (5) to the following equations by separating the wave function ψ to the real part ψ_R and imaginary part ψ_I :

$$\frac{\partial\psi_I}{\partial t}=\mathrm{Im}\left[-\frac{i}{\hbar}\hat{H}(\psi_R+i\psi_I)\right], \tag{7}$$

$$\frac{\partial\psi_R}{\partial t}=\mathrm{Re}\left[-\frac{i}{\hbar}\hat{H}(\psi_R+i\psi_I)\right]. \tag{8}$$

We can simulate Eqs. (7) and (8) by applying the FDTD method for the Schrödinger's equation [6].

To realize hybrid simulation in the conventional method, we must treat the Hamiltonian $\hat{H}_A$ which is given by an electron in the electromagnetic fields[1-3]:

$$\hat{H}_A = \frac{1}{2m}(-i\hbar\nabla - q\mathbf{A})^2 + q\varphi + V \,, \tag{9}$$

where q means the charge of an electron. We can simulate electrons in the electromagnetic fields by using Eq. (9).

The current density is generated when the electrons are affected by the electromagnetic fields. We evaluate it as

$$\mathbf{J} = qN\int_{-\infty}^{\infty} \psi^* \hat{\mathbf{v}} \psi d\upsilon \,, \tag{10}$$

where N and $\hat{\mathbf{v}}$ mean the electron density and velocity operator, respectively. This evaluation is appropriate when many electrons exist.

The hybrid simulation can be realized by using Eqs. (3)-(4) and (7)-(10) in the conventional method. We have indicated the algorithm in Figure 1 (a). It can be noticed that we must solve the vector potential $\mathbf{A}$ and scalar potential φ to update the wave function ψ.

We can rewrite Eq. (9) to the following new Hamiltonian $\hat{H}_L$ by applying the length gauge [4]:

$$\hat{H}_L = -\frac{\hbar^2}{2m}\Delta - q\mathbf{E}\cdot\mathbf{r} + V \,, \tag{11}$$

where $\mathbf{r}$ means the distance vector from the origin and we can notice that the vector potential $\mathbf{A}$ and scalar potential φ do not appear in the Hamiltonian.

The hybrid simulation can be realized by using Eqs. (3)-(4), (7)-(8), and (10)-(11) in our proposed method. The algorithm is indicated in Figure 1 (b). It can be noticed that we do not need to update the vector potential $\mathbf{A}$ and scalar potential φ. The computational time can be reduced by using the proposed method.

III. Computational Results

To compare the results obtained by the conventional and proposed methods, we investigate the current density in the nanoplate as shown in Figure 2. All electrons in the nanoplate are constrained by the harmonic oscillator and have the degree of freedom for the y-direction. The incident wave is a plane wave with a Gaussian window and has only E_y and H_z components. We give the ground state to all electrons as the initial condition.

Figure 3 shows the comparison of the current densities obtained by conventional and proposed hybrid simulations where the horizontal axis means time. We can confirm that both results are in an excellent agreement.

The comparison of the computational costs is indicated in Figure 4, where the horizontal axis means time steps. It is shown that the computational cost for our proposed hybrid simulation is almost half compared with the conventional one.

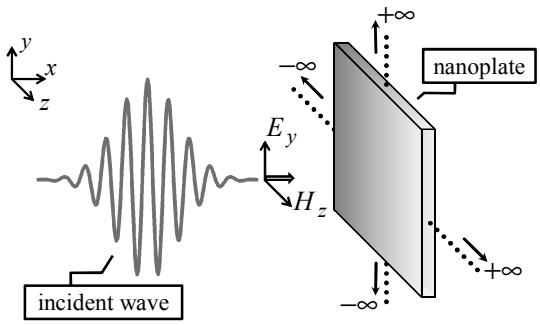


Fig. 2. Geometry and coordinate systems.

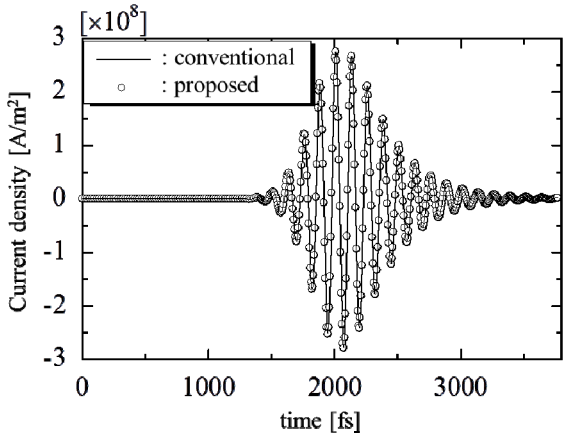


Fig. 3. Comparison of the current density in the nanoplate.

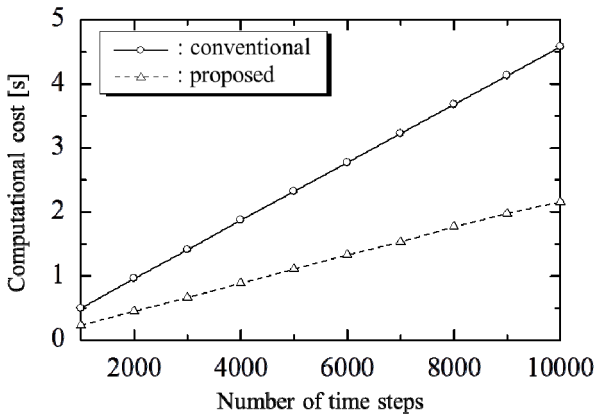


Fig. 4. Comparison of computational cost.

IV. Conclusion

We have proposed the novel hybrid simulation for Maxwell-Schrödinger problems. The proposed method relies on the length gauge and dose not require to update the vector potential $\mathbf{A}$ and scalar potential φ. We have verified that the computational cost for our proposed hybrid simulation is almost half compared with the conventional one. In addition, the results obtained by conventional and proposed methods are in an excellent agreement.

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