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A mass conservative characteristic finite element method with unconditional optimal convergence for semiconductor device problem

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Summary

We consider a mass conservative type method for semiconductor device problem by employing mixed finite element method (FEM) for electric potential equation, mass conservative characteristic FEM for both electron and hole density equations. The boundedness of numerical solution without certain time step restriction and optimal L^2 error estimates of full discrete scheme are proved. Numerical experiment is presented to verify the effectiveness and unconditional stability of the proposed method.

KEYWORDS:
mass conservation, unconditionally stability, optimal error estimates, semiconductor device

1 | INTRODUCTION

Here we study the semiconductor device described by the following nonlinear system [1,2]:

$$\begin{cases} \vec{u} = -\nabla\phi, \\ \nabla\cdot(\alpha\vec{u}) = q(f+p-e), \\ \dfrac{\partial e}{\partial t} - \nabla\cdot(D_e(x)\nabla e + \mu_e(x)e\vec{u}) = -R(e,p), \\ \dfrac{\partial p}{\partial t} - \nabla\cdot(D_p(x)\nabla p - \mu_p(x)p\vec{u}) = -R(e,p), \end{cases} \tag{1}$$

on polyhedral domain $\Omega \in R^d$ $(d = 2, 3)$ over time period $J = [0, T]$. Here the objective functions are the electrostatic potential ϕ, the electric field intensity $\vec{u}$, the electron density e and the hole density p. α is the dielectric permittivity, q is the electron charge constant. f is the doping profile of the device. D_i and μ_i are the diffusivity and the mobility of electrons $(i = e)$ / holes $(i = p)$. $R(e, p)$ describes the recombination and generation of carriers. The corresponding initial-boundary conditions are

$$\begin{aligned} &\vec{u}\cdot\vec{n} = D_e(x)\nabla e\cdot\vec{n} = D_p(x)\nabla p\cdot\vec{n} = 0, \quad x\in\partial\Omega, \\ &e(x,0) = e_0(x), p(x,0) = p_0(x), \quad x\in\Omega. \end{aligned} \tag{2}$$

The model reflects significant fundamental conservation laws that describe mass balance of a charged system in a material medium, and the numerical study of semiconductor device plays significant role in industrial applications which have been a key interest topic for research [1]. Some classical numerical methods have been investigated extensively in recent years, such as finite difference method (FDM) [3], upwind FDM [4], characteristics mixed FEM [5], finite volume method [6,7], discontinuous Galerkin method [8,9], two-grid method [10].

There are two key issues with numerical simulation of the model (1). On one hand, both electron and hole density equations are

[0] **Abbreviations:** ANA, anti-nuclear antibodies; APC, antigen-presenting cells; IRF, interferon regulatory factor

normally convection-dominated. As we all know, the conventional characteristic type method can obtain better approximation with nonphysical oscillations or numerical diffusion than other standard methods, unfortunately it fails to maintain mass balance. On the other hand, numerical error analyses were done roughly under some time-step condition $t = o(h^{d/2})$ in all previous works. Such time-step restriction may become more serious in practical three-dimensional computations with time-consuming. To the best of our knowledge, few work can deal with any above issue for semiconductor device problem.

In this work, we present a new mass conservative type method, where the classical mixed FEM is used to solve electrostatic potential and electric field intensity, while mass-conservation characteristic FEM as [11] to treat both electron and hole density equations. The mass-conservation characteristic FEM can keep the advantages of the traditional characteristic FEM and hold mass balance globally in some engineering simulations [12,13,14] proved that the time-step restriction is not necessary for numerical simulation of miscible displacement problem by error splitting technique, which has been rapidly applied to other equations [15,16]. The other contribution of this paper is firstly to obtain the unconditionally optimal convergence analysis for all four variables, which means that both the boundedness of numerical solution and optimal approximation are valid without any time-step condition.The rest of the paper is organized as follows. In section 2, we introduce the mass conservative characteristic finite element method and show main results. In section 3, we prove the numerical solution is bounded unconditionally and the error estimates are optimal without any time-step restriction. In section 4, numerical experiments are presented to confirm the theoretical analysis. Throughout the paper, the k and ε denote generic positive constant and a generic small positive constant respectively, which may take different values at different occurrences.

In the rest of the paper, we need the following regularity hypotheses (H) on system (1)

$$(H)\begin{cases}\vec{u} \in L^\infty(J; H^2) \cap W_2^1(J; H^2) \cap W_\infty^1(J; L^\infty),\\ \phi \in L^\infty(J; H^3),\\ e, p \in L^\infty(J; H^2) \cap W_2^1(J; H^2) \cap W_2^2(J; L^2).\end{cases}$$

2 | FULL DISCRETE SCHEME OF MASS CONSERVATIVE FEM

Let $\mathcal{T}_h$ be a shape regular finite element partition of Ω and the diameters of the elements are bounded by h. Define $M_h \subset H^1(\Omega)$ be the piecewise linear Lagrange finite element space, $V_h \subset H(\mathrm{div}; (\Omega))$ and $W_h \subset L^2(\Omega)$ be the lowest Raviart-Thomas spaces [17]. Partition the time interval $J = [0, T]$ into $0 = t^0 < t^1 < \cdots < t^N = T$ with $t^n = n\Delta t$ conveniently.

Taking $e_h^0 = I_h e_0, p_h^0 = I_h p_0$ as the Lagrangian interpolation approximation, the full-discrete mass conservative characteristic FEM of (1) is defined as follows: For $n = 1, ..., N$, find $(\vec{u}_h^n, \phi_h^n, e_h^n, p_h^n) \in V_h \times W_h \times M_h \times M_h$, such that

$$\begin{cases}(a)\ (\vec{u}_h^n, \vec{v}_h) - (\phi_h^n, \nabla \cdot \vec{v}_h) = 0,\\ (b)\ (\nabla \cdot (\alpha \vec{u}_h^n), w_h) = q(f^n + p_h^n - e_h^n, w_h),\\ (c)\ (\dfrac{e_h^n - e_h^{n-1} \circ \chi_{e_h}^n \delta_{e_h}^n}{\Delta t}, \psi_h) + (D_e \nabla e_h^n, \nabla \psi_h) = (-R(e_h^{n-1}, p_h^{n-1}), \psi_h),\\ (d)\ (\dfrac{p_h^n - p_h^{n-1} \circ \chi_{p_h}^n \delta_{p_h}^n}{\Delta t}, \psi_h) + (D_p \nabla p_h^n, \nabla \psi_h) = (-R(e_h^{n-1}, p_h^{n-1}), \psi_h),\end{cases} \tag{3}$$

for all $\vec{v}_h \in V_h, w_h \in W_h, \psi_h \in M_h$, where

$$\chi_{e_h}^n = x + \mu_e(x)\vec{u}_h^n \Delta t, \quad \chi_{p_h}^n = x - \mu_p(x)\vec{u}_h^n \Delta t, \quad \delta_{i_h}^n = \det(\partial \chi_{i_h}^n / \partial x),\ i = e,\ p.$$

We show the mass balance of discrete scheme (3) in the following lemma [12].

Lemma 1. (Mass balance) Suppose that $\{e_h^n\}_{n=1}^N$ and $\{p_h^n\}_{n=1}^N$ is the solution of (3), then it holds for $n = 1 \cdots N$

$$\int_\Omega e_h^n dx = \int_\Omega e_h^{n-1} dx + \Delta t \int_\Omega -R(e_h^{n-1}, p_h^{n-1}) dx,$$

$$\int_\Omega p_h^n dx = \int_\Omega p_h^{n-1} dx + \Delta t \int_\Omega -R(e_h^{n-1}, p_h^{n-1}) dx.$$

Now we present our main results and the proof will be given in the next section.

Theorem 1. Suppose that the model (1) has a unique solution $(\vec{u}, \phi, e, p)$ satisfying the regularity condition (H), then there exist $\tau_0 > 0$ and $h_0 > 0$ such that when $\Delta t < \tau_0, h < h_0$, the full discrete system (3) admits a unique solution $(\vec{u}_h^n, \phi_h^n, e_h^n, p_h^n) \in V_h \times W_h \times M_h \times M_h$, satisfying

$$\begin{aligned} &\max_{1\le n\le N} \|\vec{u}_h^n - \vec{u}^n\| + \max_{1\le n\le N} \|\phi_h^n - \phi^n\| \le k(\Delta t + h), \\ &\max_{1\le n\le N} \|e_h^n - e^n\| + \max_{1\le n\le N} \|p_h^n - p^n\| \le k(\Delta t + h^2). \end{aligned} \tag{4}$$

3 | UNCONDITIONAL STABILITY AND OPTIMAL ERROR ANALYSIS

To prove the unconditional stability and optimal error estimate of full discrete scheme (3), we need introduce a conservative characteristic time-discrete system as

$$\begin{cases} U^n = -\nabla \Phi^n, \\ \nabla \cdot (\alpha U^n) = q(f^n + P^{n-1} - E^{n-1}), \\ \dfrac{E^n - E^{n-1} \circ \chi_E^n \delta_E^n}{\Delta t} - \nabla \cdot (D_e \nabla E^n) = -R(E^{n-1}, P^{n-1}), \\ \dfrac{P^n - P^{n-1} \circ \chi_P^n \delta_P^n}{\Delta t} - \nabla \cdot (D_p \nabla P^n) = -R(E^{n-1}, P^{n-1}), \end{cases} \tag{5}$$

with initial condition

$$E^0(x) = e_0(x), P^0(x) = p_0(x), \tag{6}$$

where $\chi_E^n = x + \mu_e(x) U^n \Delta t,\ \chi_P^n = x - \mu_p(x) U^n \Delta t$, and $\delta_i^n = \det(\partial \chi_i^n / \partial x),\ i = E, P$.

Set $r_{\vec{u}}^n = \vec{u}^n - U^n,\ r_\phi^n = \phi^n - \Phi^n,\ r_e^n = e^n - E^n,\ r_p^n = p^n - P^n$. Denoting $d_t : d_t f^n = (f^n - f^{n-1})/\Delta t$, we will prove the following useful theorem.

Theorem 2. Under the regularity condition (H), the time-discrete system (5) exists a unique solution $(U^n, \Phi^n, E^n, P^n), n = 1, ..., N$, which satisfies

$$\|U^n\|_2 + \|\Phi^n\|_3 + \|E^n\|_2 + \|P^n\|_2 \le k, \tag{7}$$

$$\|r_{\vec{u}}^n\|_1 + \|r_\phi^n\|_2 + \|r_e^n\|_1 + \|r_p^n\|_1 \le k\Delta t. \tag{8}$$

Proof. From the semiconductor system (1) and the conservative characteristic time-discrete system (5), we can observe that the error $(r_{\vec{u}}^n, r_\phi^n, r_e^n, r_p^n)$ satisfies the following equations

$$\nabla \cdot r_{\vec{u}}^n = \nabla \cdot (-\nabla r_\phi^n) = q/\alpha(p^n - P^{n-1} - e^n + E^{n-1}), \tag{9}$$

$$\begin{aligned} &d_t r_e^n - \nabla \cdot (D_e \nabla r_e^n) \\ =& \frac{e^{n-1} \circ \chi_e^n \delta_e^n - e^{n-1} + E^{n-1} - E^{n-1} \circ \chi_E^n \delta_E^n}{\Delta t} - R_{te}^n - R(e^n, p^n) + R(E^{n-1}, P^{n-1}), \end{aligned} \tag{10}$$

$$\begin{aligned} &d_t r_p^n - \nabla \cdot (D_p \nabla r_p^n) \\ =& \frac{p^{n-1} \circ \chi_p^n \delta_p^n - p^{n-1} + P^{n-1} - P^{n-1} \circ \chi_P^n \delta_P^n}{\Delta t} - R_{tp}^n - R(e^n, p^n) + R(E^{n-1}, P^{n-1}), \end{aligned} \tag{11}$$

where $\chi_e^n = x + \mu_e(x) \vec{u}^n \Delta t,\ \chi_p^n = x - \mu_p(x) \vec{u}^n \Delta t,\ \delta_i^n = \det(\partial \chi_i^n / \partial x), (i = e,\ p)$, and

$$\begin{aligned} R_{te}^n &= \frac{\partial e}{\partial t} - \nabla \cdot (\mu_e(x) e \vec{u}) - \frac{e^n - e^{n-1} \circ \chi_e^n \delta_e^n}{\Delta t}, \\ R_{tp}^n &= \frac{\partial p}{\partial t} + \nabla \cdot (\mu_p(x) p \vec{u}) - \frac{p^n - p^{n-1} \circ \chi_p^n \delta_p^n}{\Delta t}. \end{aligned}$$

It is easy to see [11]

$$\sum_{n=1}^N \|R_{te}^n\|^2 \Delta t \le k\Delta t^2, \quad \sum_{n=1}^N \|R_{tp}^n\|^2 \Delta t \le k\Delta t^2. \tag{12}$$

Here we need to prove following estimate

$$\sum_{n=0}^m \|r_e^n\|_2^2 \Delta t \le k\Delta t^2, \quad \sum_{n=0}^m \|r_p^n\|_2^2 \Delta t \le k\Delta t^2, \tag{13}$$

by mathematical induction for $m = 0, 1..., N$.

From initial condition (6), the above inequality holds for $m = 0$. We assume (13) holds until $m = N - 1$, which implies that

$$\|E^n\|_2 + \|P^n\|_2 \le k, \quad n = 0, 1..., N - 1. \tag{14}$$

Applying the H^3 estimates of elliptic equation[18] to (5), we can obtain

$$\|\Phi^n\|_3 + \|U^n\|_2 \le k, \quad n = 1, 2, ...N. \tag{15}$$

By (9) we have

$$\|r^n_{\vec{u}}\|_1 + \|r^n_\phi\|_2 \le k(\|r^{n-1}_e\| + \|r^{n-1}_p\| + \|p^n - p^{n-1}\| + \|e^n - e^{n-1}\|). \tag{16}$$

To prove (13) for $m = N$, we multiply (10) by r^n_e to get

$$\begin{aligned}
&(d_t r^n_e, r^n_e) + (D_e \nabla r^n_e, \nabla r^n_e) \\
=&(\frac{e^{n-1} \circ \chi^n_e \delta^n_e - e^{n-1} + E^{n-1} - E^{n-1} \circ \chi^n_E \delta^n_E}{\Delta t}, r^n_e) \\
&- (R^n_{te}, r^n_e) + (R(E^{n-1}, P^{n-1}) - R(e^n, p^n), r^n_e) \\
\le& k(\|r^n_{\vec{u}}\|^2 + \|r^n_e\|^2 + \|r^{n-1}_e\|^2 + \|r^{n-1}_p\|^2 + \|R^n_{te}\|^2 + \Delta t^2) + \varepsilon \|\nabla r^n_e\|^2,
\end{aligned}$$

where the last inequality can be obtained by the same technique as[19].

Combing with (13) and (16), we multiply above inequality and sum over $1 \le n \le N$ to obtain

$$\frac{1}{2}(r^N_e, r^N_e) + \sum_{n=1}^{N} (D_e \nabla r^n_e, \nabla r^n_e)\Delta t \le k \sum_{n=1}^{N} \|r^n_e\|^2 \Delta t + \varepsilon \sum_{n=1}^{N} \|\nabla r^n_e\|^2 \Delta t + k\Delta t^2.$$

An application of the discrete Gronwall's inequality yields that

$$\max_{1\le n\le N} \|r^n_e\|^2 + \sum_{n=1}^{N} \|\nabla r^n_e\|^2 \Delta t \le k\Delta t^2, \tag{17}$$

To obtain the H^1 estimate of r^n_e, Multiplying (10) by $d_t r^n_e \Delta t$ and summing over $1 \le n \le N$, we have

$$\begin{aligned}
&\sum_{n=1}^{N} (d_t r^n_e, d_t r^n_e)\Delta t + \frac{1}{2}(D_e \nabla r^N_e, \nabla r^N_e) \\
\le& \sum_{n=1}^{N} (e^{n-1} \circ \chi^n_e \delta^n_e - e^{n-1} + E^{n-1} - E^{n-1} \circ \chi^n_E \delta^n_E, d_t r^n_e) \\
&- \sum_{n=1}^{N} (R^n_{te}, d_t r^n_e)\Delta t + \sum_{n=1}^{N} (R(E^{n-1}, P^{n-1}) - R(e^n, p^n), d_t r^n_e)\Delta t \\
\le& \varepsilon \sum_{n=1}^{N} \|d_t r^n_e\|^2 \Delta t + \varepsilon \|\nabla r^N_e\|^2 + k\Delta t^2. \\
=& I_1 + I_2 + I_3.
\end{aligned}$$

By (12) and (17) it is easy to see that

$$I_2 + I_3 \le \varepsilon \sum_{n=1}^{N} \|d_t r^n_e\|^2 \Delta t + k\Delta t^2.$$

For I_1,

$$I_1 = \sum_{n=1}^{N} (r^{n-1}_e \circ \chi^n_e \delta^n_e - r^{n-1}_e, d_t r^n_e) + \sum_{n=1}^{N} (E^{n-1} \circ \chi^n_e \delta^n_e - E^{n-1} \circ \chi^n_E \delta^n_E, d_t r^n_e) = I_{11} + I_{12}.$$

Where

$$\begin{aligned}
I_{11} =& \sum_{n=1}^{N} (\frac{r^{n-1}_e - r^{n-1}_e \circ \chi^n_e \delta^n_e}{\Delta t}, r^n_e) - \sum_{n=1}^{N} (\frac{r^{n-1}_e - r^{n-1}_e \circ \chi^n_e \delta^n_e}{\Delta t}, r^{n-1}_e) \\
=& \sum_{n=2}^{N} (d_t (r^{n-1}_e \circ \chi^n_e \delta^n_e - r^{n-1}_e), r^{n-1}_e) + (\frac{r^{N-1}_e - r^{N-1}_e \circ \chi^N_e \delta^N_e}{\Delta t}, r^N_e) \\
\le& k(\sum_{n=1}^{N} \|\nabla r^{n-1}_e\|^2 \Delta t + \sum_{n=1}^{N} \|r^{n-1}_e\|^2 \Delta t + \|r^{N-1}_e\|^2) + \varepsilon \|\nabla r^N_e\|^2 + \varepsilon \sum_{n=1}^{N} \|d_t r^{n-1}_e\|^2 \Delta t,
\end{aligned}$$

and

$$I_{12} = \sum_{n=1}^{N}(E^{n-1}\circ\chi_e^n(\delta_e^n - \delta_E^n), d_t r_e^n) + \sum_{n=1}^{N}((E^{n-1}\circ\chi_e^n - E^{n-1}\circ\chi_E^n)\delta_E^n, d_t r_e^n)$$
$$\leq k\sum_{n=1}^{N}\|r_u^n\|_1^2\Delta t + \varepsilon\sum_{n=1}^{N}\|d_t r_e^n\|^2\Delta t + k\Delta t^2.$$

Combing with (16), we obtain that

$$I_1 \leq \varepsilon\sum_{n=1}^{N}\|d_t r_e^n\|^2\Delta t + \varepsilon\|\nabla r_e^N\|^2 + k\Delta t^2.$$

So we can get the following estimate

$$\max_{1\leq n\leq N}\|\nabla r_e^n\|^2 + \sum_{n=1}^{N}\|d_t r_e^n\|^2\Delta t \leq k\Delta t^2. \tag{18}$$

With similar process to (11), we can get

$$\max_{1\leq n\leq N}\|r_p^n\|^2 + \max_{1\leq n\leq N}\|\nabla r_p^n\|^2 \leq k\Delta t^2, \tag{19}$$

then (8) follows from (16), (17) and (19). Applying H^2 estimates to (10) yields

$$\|\Delta r_e^n\| \leq k(\|d_t r_e^n\| + \|r_e^n\|_1 + \|r_{\vec{u}}^n\|_1 + \|R_{te}^n\| + \|r_e^{n-1}\| + \|r_p^{n-1}\| + \Delta t),$$

which together with (12) and (18) implies

$$\sum_{n=1}^{N}\|\Delta r_e^n\|^2\Delta t \leq k\Delta t^2.$$

It means that (13) holds for $m = N$. The proof of Theorem 2 is complete. □

Next we introduce mixed projection $(\Pi_h U, \Pi_h \Phi) \in V_h \times W_h$ as follows

$$(U^n - \Pi_h U^n, v_h) = (\Phi^n - \Pi_h\Phi^n, \nabla\cdot v_h), \quad \forall v_h \in V_h,$$
$$(\nabla\cdot\Pi_h U^n, w_h) = (q/\alpha(f^n + P^{n-1} - E^{n-1}), w_h), \quad \forall w_h \in S_h,$$

and the elliptic projection operators $Q_h : H^1 \to M_h$ to satisfy

$$(D_e\nabla E^n, \nabla\varphi_h) = (D_e\nabla Q_h E^n, \nabla\varphi_h), \quad \forall\varphi_h \in M_h,$$
$$(D_p\nabla P^n, \nabla\varphi_h) = (D_p\nabla Q_h P^n, \nabla\varphi_h), \quad \forall\varphi_h \in M_h.$$

Based on the regularity (7), the following estimates hold[16,17]

$$\begin{aligned}
&\|U^n - \Pi_h U^n\| + \|\nabla\cdot(U^n - \Pi_h U^n)\| + \|\Phi^n - \Pi_h\Phi^n\| \leq kh(\|U^n\|_2 + \|\Phi^n\|_1),\\
&\|S^n - Q_h S^n\| + h\|\nabla(S^n - Q_h S^n)\| \leq kh^2, \ S = E, P,\\
&\sum_{n=1}^{N}\|d_t(S^n - Q_h S^n)\|^2\Delta t \leq kh^4, \ S = E, P.
\end{aligned} \tag{20}$$

Let

$$\theta_{\vec{u}}^n = \vec{u}_h^n - \Pi_h U^n, \ \theta_\phi^n = \phi_h^n - \Pi_h\Phi^n, \ \theta_e^n = e_h^n - Q_h E^n, \ \theta_p^n = p_h^n - Q_h P^n,$$
$$\zeta_{\vec{u}}^n = U^n - \Pi_h U^n, \ \zeta_\phi^n = \Phi^n - \Pi_h\Phi^n, \ \zeta_e^n = E^n - Q_h E^n, \ \zeta_p^n = P^n - Q_h P^n.$$

The following Theorem shows the boundedness unconditionally of numerical solution for fully-discrete system and error with the time-discrete system.

Theorem 3. Under the regularity condition (H), there exist $\tau_0 > 0$ and $h_0 > 0$ such that when $\Delta t < \tau_0, h < h_0$,

$$\begin{aligned}
&\max_{1\leq n\leq N}\|\vec{u}_h^n\|_{0,\infty} + \max_{1\leq n\leq N}\|e_h^n\|_{0,\infty} + \max_{1\leq n\leq N}\|p_h^n\|_{0,\infty} \leq k,\\
&\|\theta_{\vec{u}}^n\|^2 + \|\theta_\phi^n\|^2 + \|\theta_e^n\|^2 + \|\theta_p^n\|^2 \leq kh^4.
\end{aligned} \tag{21}$$

Proof. From full-discrete system (3) and time-discrete system (5), we obtain

$$(\theta_{\vec{u}}^n, v_h) - (\theta_\phi^n, \nabla\cdot v_h) = 0, \tag{22}$$

$$(\nabla\cdot(\alpha\theta_{\vec{u}}^n), w_h) = (q(\theta_p^{n-1} - \zeta_p^{n-1} - \theta_e^{n-1} + \zeta_e^{n-1}), w_h), \tag{23}$$

$$
\begin{aligned}
&(d_t\theta_e^n, \varphi_h) + (D_e(x)\nabla\theta_e^n, \nabla\varphi_h)\\
=&\frac{1}{\Delta t}(E^{n-1} - E^{n-1}\circ\chi_E^n\delta_E^n - e_h^{n-1} + e_h^{n-1}\circ\chi_{e_h}^n\delta_{e_h}^n, \varphi_h)\\
&+\frac{1}{\Delta t}(\zeta_e^n - \zeta_e^{n-1}), \varphi_h) + (R(E^{n-1}, P^{n-1}) - R(e_h^{n-1}, p_h^{n-1}), \varphi_h),
\end{aligned} \tag{24}
$$

$$
\begin{aligned}
&(d_t\theta_p^n, \varphi_h) + (D_p(x)\nabla\theta_p^n, \nabla\varphi_h)\\
=&\frac{1}{\Delta t}(P^{n-1} - P^{n-1}\circ\chi_P^n\delta_P^n - p_h^{n-1} + p_h^{n-1}\circ\chi_{p_h}^n\delta_{p_h}^n, \varphi_h)\\
&+\frac{1}{\Delta t}(\zeta_p^n - \zeta_p^{n-1}), \varphi_h) + (R(E^{n-1}, P^{n-1}) - R(e_h^{n-1}, p_h^{n-1}), \varphi_h).
\end{aligned} \tag{25}
$$

Now we prove a primary estimate

$$
\|\theta_e^n\| + \|\theta_p^n\| \le kh^2, n = 0, 1, ..., N, \tag{26}
$$

by mathematical induction. It is easy to see that $\|\theta_e^0\| + \|\theta_p^0\| \le kh^2$. We assume that the inequality (26) holds until $n = N - 1$, which implies

$$
\|e_h^n\|_{0,\infty} \le \|Q_h E^n\|_{0,\infty} + \|\theta_e^n\|_{0,\infty} \le \|Q_h E^n\|_{0,\infty} + kh^{-d/2}\|\theta_e^n\| \le k, \tag{27}
$$

and $\|p_h^n\|_{0,\infty} \le k$. Using Inf-Sup condition and (22), we can obtain the estimate of $\theta_{\vec{u}}^n$ and θ_ϕ^n,

$$
\|\theta_{\vec{u}}^n\| + \|\theta_\phi^n\| \le k(\|\theta_p^{n-1}\| + \|\zeta_p^{n-1}\| + \|\theta_e^{n-1}\| + \|\zeta_e^{n-1}\| \le kh^2. \tag{28}
$$

By a similar approach as (27), we can prove that

$$
\|\vec{u}_h^n\|_{0,\infty} \le \|\Pi_h U^n\|_{0,\infty} + kh^{-d/2}h^2 \le k, \quad n = 1...N. \tag{29}
$$

Now we choose $\varphi_h = \theta_e^n$ in (24), and denote the resulting terms by L_1, L_2, L_3.

By (20) and (26), we can see that

$$
L_2 + L_3 \le k\|d_t\zeta_e^n\|^2 + k\|\theta_e^n\|^2 + kh^4, \tag{30}
$$

For L_1

$$
\begin{aligned}
L_1 =&\frac{1}{\Delta t}(E^{n-1} - e_h^{n-1} - (E^{n-1} - e_h^{n-1})\circ\chi_{e_h}^n\delta_{e_h}^n, \theta_e^n)\\
&+\frac{1}{\Delta t}(E^{n-1}\circ\chi_{e_h}^n\delta_{e_h}^n - E^{n-1}\circ\chi_E^n\delta_E^n, \theta_e^n) = L_{11} + L_{12},
\end{aligned}
$$

where

$$
L_{11} \le k\|e_h^{n-1} - E^{n-1}\|^2 + \varepsilon\|\nabla\theta_e^n\|^2 \le k\|\theta_e^{n-1}\|^2 + \varepsilon\|\nabla\theta_e^n\|^2 + kh^4.
$$

let $\overline{\theta_e^n}$ be the average value of θ_e^n on Ω, then we have

$$
\begin{aligned}
L_{12} =&\frac{1}{\Delta t}(E^{n-1}\circ\chi_{e_h}^n\delta_{e_h}^n - E^{n-1}\circ\chi_E^n\delta_E^n, \theta_e^n - \overline{\theta_e^n})\\
=&(\frac{E^{n-1}\circ\chi_{e_h}^n - E^{n-1}\circ\chi_E^n}{\Delta t}\delta_E^n, \theta_e^n - \overline{\theta_e^n}) + (\frac{E^{n-1}\circ\chi_{e_h}^n(\delta_{e_h}^n - \delta_E^n)}{\Delta t}, \theta_e^n - \overline{\theta_e^n})\\
=&L_{121} + L_{122}
\end{aligned}
$$

where

$$
L_{121} \le k\|E^{n-1}\|_{0,\infty}\|U^n - u_h^n\|\|\theta_e^n - \overline{\theta_e^n}\| \le k\|\theta_u^n\|^2 + kh^4 + \varepsilon\|\nabla\theta_e^n\|^2,
$$

and

$$
\begin{aligned}
L_{122} =&(E^{n-1}\circ\chi_{e_h}^n\nabla\cdot(\mu_e u_h^n - \mu_e U^n), \theta_e^n - \overline{\theta_e^n})\\
=&(E^{n-1}\circ\chi_{e_h}^n\mu_e\nabla\cdot(u_h^n - U^n), \theta_e^n - \overline{\theta_e^n}) + (E^{n-1}\circ\chi_{e_h}^n\nabla\mu_e(u_h^n - U^n), \theta_e^n - \overline{\theta_e^n})\\
\le&kh\|\nabla\cdot\zeta_u^n\|\|\nabla\theta_c^n\| + k\|\theta_u^n\|\|\nabla\theta_c^n\| + kh\|\zeta_u^n\|\|\nabla\theta_c^n\|\\
\le&k\|\theta_u^n\|^2 + kh^4 + \varepsilon\|\nabla\theta_c^n\|^2,
\end{aligned}
$$

Combing above inequality, we obtain

$$
\frac{1}{2}d_t(\theta_e^n, \theta_e^n) + (D_e\nabla\theta_e^n, \nabla\theta_e^n) \le k\|\theta_e^n\|^2 + \varepsilon\|\nabla\theta_e^n\|^2 + k\|d_t(Q_h E^n - E^n)\|^2 + kh^4.
$$

Multiplying Δt and summing the above estimate over n, it in turn produces by (20)

$$
\|\theta_e^N\|^2 + \sum_{n=1}^{N}\|\nabla\theta_e^n\|^2\Delta t \le k\sum_{n=1}^{N}\|\theta_e^n\|^2\Delta t + kh^4.
$$

By Gronwall's inequality, there exits $\tau_0 > 0$ such that when $\Delta t < \tau_0$,

$$\max_{1\le n\le N} \|\theta_e^n\|^2 + \sum_{n=1}^{N} \|\nabla\theta_e^n\|^2\Delta t \le kh^4.$$

Similarly we can get

$$\max_{1\le n\le N} \|\theta_p^n\|^2 + \sum_{n=1}^{N} \|\nabla\theta_p^n\|^2\Delta t \le kh^4.$$

The induction (26) is closed, thus the proof of Theorem 3 is complete. □

With the property (20), it is easy to see the error estimate (4) in Theorem 1 is optimal.

4 | NUMERICAL EXPERIMENT

In this section, we present numerical experiments to illustrate theoretical analysis and efficiency of numerical method above. For simplicity, we select the domain $\Omega = [0,1]\times[0,1]$.

***Example*4.1.** We begin with an example to verify theoretical analysis of convergence property. The analytical solution of the model (1) is known as follows

$$\begin{aligned}
&\phi(x,y,t) = \exp(t+x)\sin(t+y), \quad \vec{u}(x,y,t) = -\nabla\phi(x,y,t),\\
&e(x,y,t) = (-3t^2+1)\sin(2\pi x)\sin(2\pi y),\\
&p(x,y,t) = \exp(t)\sin(\pi x)\sin(\pi y).
\end{aligned}$$

The error estimates are listed in TABLE 1. We can see that the convergence rates for both electrostatic potential and electric field intensity are first order, for electron density and hole density are second order convergence rates which are all optimal. The one order lower approximation to $\phi, \vec{u}$ indeed not affect the accuracy of e, p.

To show the unconditional stability of full-discrete scheme, we solve the model (1) on gradually refined mesh $1/h = 10, 20, 30, 40, 50$ for each fixed $\Delta t = 0.1, 0.05, 0.025$. The corresponding numerical results are presented in FIGURE 1 . We can see that each error converges to a constant as h goes to 0, which implies that the numerical scheme (3) is unconditionally stability. Those results are all in consistent with the theoretical analysis.

TABLE 1 Error and convergence rate of Example 4.1

mesh	$\|\vec{u}-\vec{u}_h\|$	**rate**	$\|\phi-\phi_h\|$	**rate**	$\|e-e_h\|$	**rate**	$\|p-p_h\|$	**rate**
5	1.79e-3	–	1.46e-3	–	7.80e-4	–	2.12e-4	–
10	8.84e-4	1.02	7.30e-4	1.00	2.12e-4	1.88	5.42e-5	1.97
20	4.41e-4	1.01	3.65e-4	1.00	5.43e-5	1.97	1.36e-5	1.99
40	2.20e-4	1.00	1.82e-4	1.00	1.37e-5	1.99	3.43e-6	1.99

Next we give some experiments to test the performance of the mass conservative finite element method.

***Example*4.2.** In this example we just handle the electron density equations. Set $\vec{u} = (1, \tan 35°)$ and initial density as follows

$$\begin{aligned}
&e_0 = 1, \quad (x-0.25)^2 + (y-0.5)^2 \le 0.04,\\
&e_0 = 0, \quad otherwise.
\end{aligned}$$

Taking $D_e = 1e^{-5}, \mu_e = 1, R = 0, \Delta t = 0.01, h = 0.01$, the surface and contour plots at different timeare presented in FIGURE 2 and FIGURE 3 . Similar with [6], we can see that the solution has no drift-dependent bias, the method can stably keep symmetry features throughout the whole simulation.

***Example*4.3.** We consider the PN junction. Set the doping profile $f = -0.8$ in P-region $(0,0.5)\times(0.5,1)$, and $f = 0.8$ in the rest N-region. The boundary condition $e = 0.9, p = 0.1$ on $\{y = 0\}$, and $e = 0.1, p = 0.9$ on $\{y = 1, x \le 0.25\}$, and the

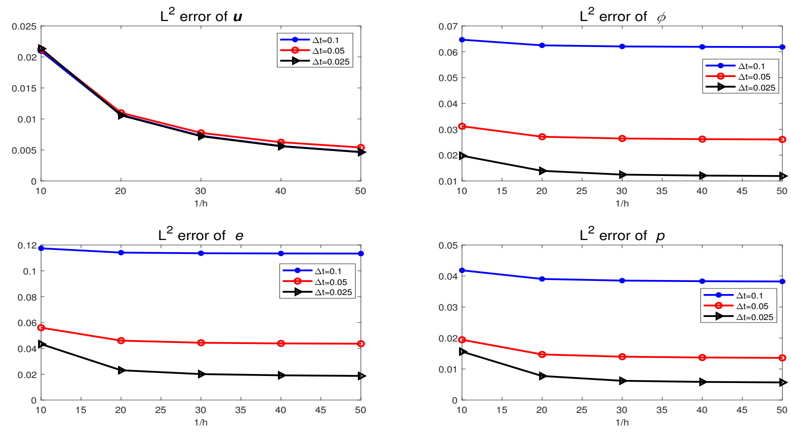

FIGURE 1 Surface plots for Example 4.1

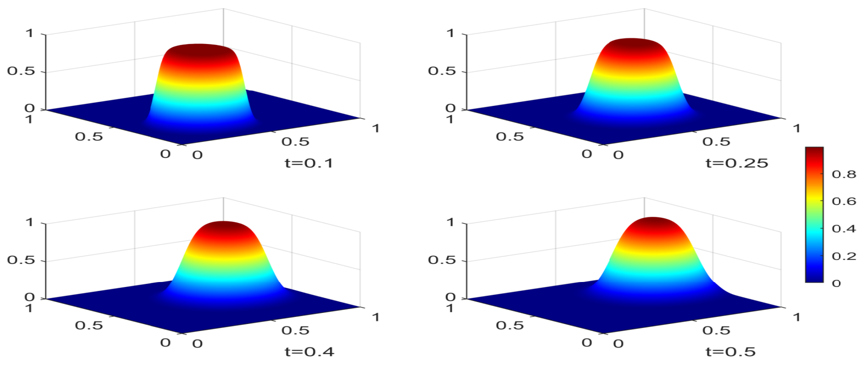

FIGURE 2 Surface plots for Example 4.2

parameters $\alpha = 0.01, D_e = D_p = \mu_e = \mu_p = 1.\Delta t = 0.001, h = 0.025$. Here we neglect the recombination and generation rate $R(e, p)$, in which case steady-state solution can be captured progressively. The density of electron and hole at different time are shown in FIGURE 4 and FIGURE 5 . These results verify the mass conservative method is efficient compared with the simulation of finite volume method[7] and HDG method[9].

5 | CONCLUSIONS

We propose the unconditional stability and optimal error estimates of a mass conservative characteristic FEM for semiconductor device problems. We prove that the numerical electron density and hole density are optimal second order accuracy with no loss of accuracy for first order approximation electrostatic potential and electric field intensity, while the estimates are obtained without time-step restriction. Numerical experiment verified the theoretical results and effectiveness of the proposed method.

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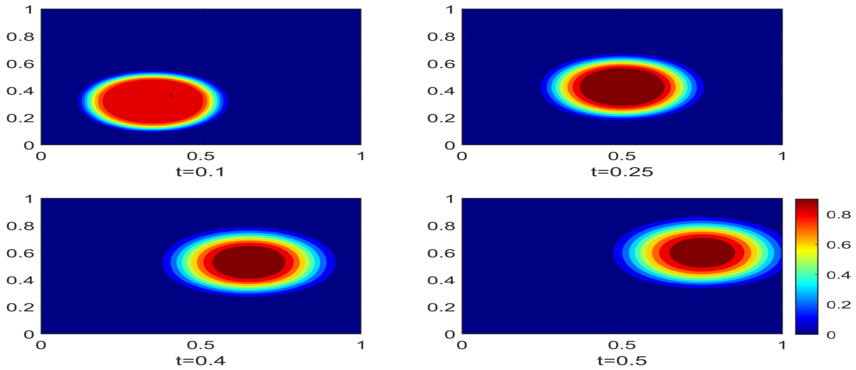

FIGURE 3 Contour plots for Example 4.2

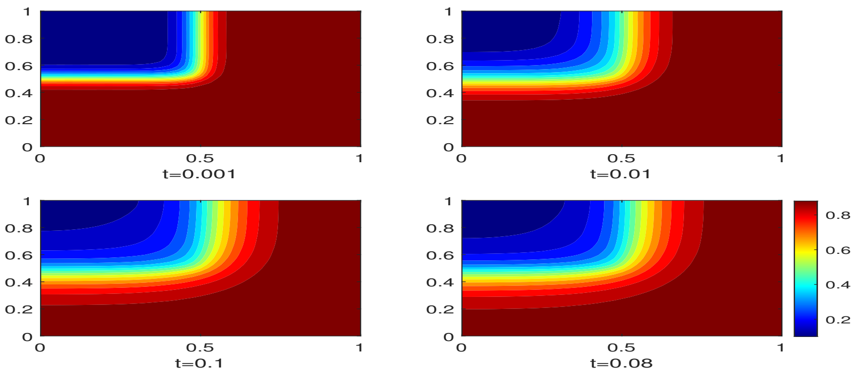

FIGURE 4 Contour plots of numerical electron density e_h for Example 4.3

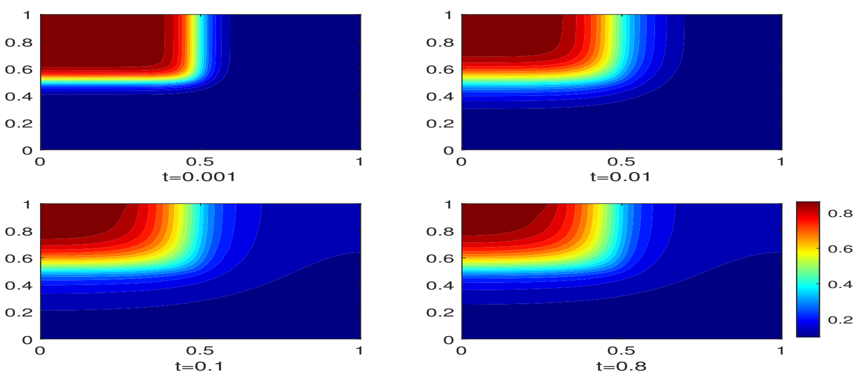

FIGURE 5 Contour plots of numerical hole density p_h for Example 4.3

Conflict of interest

The authors declare no potential conflict of interests.

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