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A weak Galerkin finite element method for 1D semiconductor device simulation models

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ABSTRACT

In this paper, we study a weak Galerkin (WG) finite element method for semiconductor device simulations. We consider the one-dimensional drift–diffusion (DD) and high-field (HF) models, which involves not only first derivative convection terms but also second derivative diffusion terms, as well as a coupled Poisson potential equation. The main difficulties in the analysis include the treatment of the nonlinearity and coupling of the models. The weak Galerkin finite element method adopts piecewise polynomials of degree k for the approximations of electron concentration and electric potential in the interior of elements, and piecewise polynomials of degree $k+1$ for the discrete weak derivative space. The optimal order error estimates in a discrete H^1 norm and the standard L^2 norm are derived. Numerical experiments are presented to illustrate our theoretical analysis. Moreover, numerical schemes also work out for the discontinuous diffusion coefficient problems.

1. Introduction

In this paper, we develop a weak Galerkin finite element method to solve time dependent and steady state moment models for semiconductor device simulations. We consider the one-dimensional drift–diffusion (DD) and high-field (HF) models of the semiconductor devices with smooth solutions, which are derived from the classical Boltzmann-Poisson system that describes electron transport in semiconductor devices. In both models, the first derivative convection terms and second derivative diffusion (heat conduction) terms exist, and the convection–diffusion system is coupled with a Poisson potential equation. The main technical difficulty in the analysis is the treatment of the nonlinear coupling between the electron potential and electron concentration. Moreover, the existence of sharp discontinuous doping profiles in semiconductor devices is an another challenge [1] for numerical simulations.

The theoretical and numerical studies for semiconductor device simulations have a long history. Traditional discretization schemes, such as finite volume method [2–5] and finite element method [6,7], were applied to solve the semiconductor models. In recent years, various numerical studies for such problems appeared in the literature. The local discontinuous Galerkin (LDG) schemes for DD and HF models with the rate of convergence $O(h^{k+\frac{1}{2}})$ were proposed by Liu-Shu [8]. Later in [9], they developed a LDG scheme with optimal error estimates for DD model. In [10], Chen and Bagci derived a "decoupled" and "linearized" method for stationary drift–diffusion equations, and then discretized the resulting equations by using a LDG scheme. The discontinuous Galerkin methods (DG) solving the hydrodynamic model and high-field model of semiconductor devices were studied in [11]. Recently, a new finite volume scheme for DD model

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was proposed, which also works for the degenerate case and preserves steady-states (see [12]). Besides, the difference method [13], mixed finite element method [14,15] and virtual element method [16,17] were also applied to solve the semiconductor device simulation models.

Weak Galerkin finite element method introduced by Wang and Ye [18] is flexible in mesh generation and approximation function spaces. As it is compatible with any shape of polygonal or polyhedral meshes and discontinuous finite element functions, WG method is widely utilized to solve various types of problem [19–23]. The goal of this paper is to construct and analyze a stable and parameter-free weak Galerkin finite element method for the one-dimensional DD and HF models with smooth solutions. Our WG scheme is based on the totally discontinuous weak function and discrete weak derivative function spaces. The error estimates are established by introducing two kinds of local projection operators, Q_h and R_h. We use piecewise polynomial P_k for the approximations of electron concentration n and electric potential φ, and piecewise polynomial P_{k+1} for the discrete weak gradient. We derive the optimal order error estimates in both a discrete H^1 norm and the standard L^2 norm, respectively. Moreover, the schemes work well numerically even for models with discontinuous diffusion coefficients. The rest of paper is organized as follows. In Section 2, some notations and the definitions of weak gradients are clarified. The semi-discrete and fully discrete WG-FEM schemes for drift–diffusion and high-field models are presented in Section 3 and Section 4, respectively. The optimal order error estimates for both semi-discrete and fully discrete WG finite element schemes are proved. In Section 5, numerical experiments are performed to check the stability and accuracy of the numerical methods.

2. Preliminaries

Let $\tilde{I}$ be a subset of domain I. With a non-negative integer s, denote by $H^s(\tilde{I})$ the s-order Sobolev space on $\tilde{I}$, and let $(\cdot,\cdot)_{s,\tilde{I}}$ be the corresponding inner product. Let $\|\cdot\|_{s,\tilde{I}}$ and $|\cdot|_{s,\tilde{I}}$ represent the norm and semi-norm, respectively. When $s=0$, we denote $(\cdot,\cdot)_{\tilde{I}}$ and $\|\cdot\|_{\tilde{I}}$ to be the inner product and norm on $L^2(\tilde{I})$. When $\tilde{I}=I$, we set $\|\cdot\|_s=\|\cdot\|_{s,I}$ and $|\cdot|_s=|\cdot|_{s,I}$ for simplicity. Denote the space

$$H^l(0,T;H^s(I)):=\left\{v\in H^s(I);\ \int_0^T\sum_{1\le i\le l}\|v^{(i)}(t)\|_s^2dt<\infty\right\},$$

where $v^{(i)}(t)$ is the ith derivative of v with respect to t. The corresponding norm is defined as

$$\|v\|_{H^l(H^s(I))}:=\left(\int_0^T\sum_{1\le i\le l}\|v^{(i)}(t)\|_s^2dt\right)^{\frac{1}{2}}.$$

For simplicity, we set $I=(0,1)$ and $J=(0,T]$. Let $\mathcal{T}_h=\bigcup_{i=1}^N I_i$ with $I_i=[x_{i-\frac{1}{2}},x_{i+\frac{1}{2}}]$ for $1\le i\le N$ where

$$0=x_{\frac{1}{2}}<x_{\frac{3}{2}}<\cdots<x_{N+\frac{1}{2}}=1.$$

Define

$$h_i=x_{i+\frac{1}{2}}-x_{i-\frac{1}{2}},\ 1\le i\le N;\quad h=\max_{1\le i\le N}h_i,\quad \partial I_i=\left\{x_{i-\frac{1}{2}}\right\}\bigcup\left\{x_{i+\frac{1}{2}}\right\}.$$

The weak Galerkin method introduces a new way to define a weak function v, which allows v that takes different forms in the interior and on the boundary of the element:

$$v=\begin{cases}v_0, & \text{in } I_i^0,\\ v_b, & \text{on } \partial I_i,\end{cases}$$

where I_i^0 is the interior of element $I_i\in\mathcal{T}_h$. In the rest of the paper, we write v as $v=\{v_0,v_b\}$ in short without confusion. Denote by $P_k(I_i)$ the set of polynomials on I_i with degree no larger than k.

Before deriving the definition of weak derivative, we define the space of weak functions. Denote by $M(I_i)$ the space of weak functions on element I_i, i.e.,

$$M(I_i):=\left\{v=\{v_0,v_b\}:v_0\in L^2(I_i),|v(x_{i-\frac{1}{2}})|+|v(x_{i+\frac{1}{2}})|<\infty\right\}.$$

Denote by $M(I)$ the weak function space on $\mathcal{T}_h$ such that

$$M(I):=\mathop{\Pi}_{I_i\in\mathcal{T}_h}M(I_i).$$

The discrete weak gradient operator is defined as follows.

Definition 2.1 (*Discrete Weak Gradient*). For any $v=\{v_0,v_b\}\in M(I_i)$, a discrete weak derivative $D_wv\in P_r(I_i)$ satisfies

$$(D_wv,w)_{I_i}=-(v_0,Dw)_{I_i}+\langle v_b,w\cdot n\rangle_{\partial I_i},\quad\forall w\in P_r(I_i),$$

where $n=-1$ at $x_{i-\frac{1}{2}}$ and $n=1$ at $x_{i+\frac{1}{2}}$. Here Dw means the first order derivative of w, i.e., $Dw=w'$.

3. The drift–diffusion model

The drift–diffusion (DD) model is described as the following equations

$$n_t + (\mu\varphi_x n)_x - \tau\theta n_{xx} = 0, \tag{3.1a}$$
$$-\frac{\epsilon}{e}\varphi_{xx} + n = n_d, \tag{3.1b}$$

where $x \in I$. The corresponding boundary and initial value conditions are

$$n(0,t) = g_{n0}(t), \quad n(1,t) = g_{n1}(t), \tag{3.2a}$$
$$\varphi(0,t) = g_{\varphi 0}(t), \quad \varphi(1,t) = g_{\varphi 1}(t), \tag{3.2b}$$
$$n(x,0) = n_0(x), \quad \forall x \in I. \tag{3.2c}$$

The Poisson equation (3.1b) is the electric potential equation, and $E = -\varphi_x$ represents the electric field.

In the system of (3.1) and (3.2), the unknown variables are the electron concentration n and the electric potential φ. The parameter μ is the mobility, and $\tau = \frac{m\mu}{e}$ is the relaxation parameter, $\theta = \frac{k}{m}T_0$. Here m is the electron effective mass, e is the electron charge, k is the Boltzmann constant, T_0 is the lattice temperature, ϵ is the dielectric permittivity, and $n_d(x,t)$ is the doping which is a given function.

3.1. Weak form and discrete schemes for the DD model

First, we define the space of weak functions as follows:

$$V_n := \left\{ v \in H^1(0,T;H^1(I)) : v(0) = g_{n0}(t),\, v(1) = g_{n1}(t) \right\},$$
$$V_\varphi := \left\{ v \in H^1(0,T;H^1(I)) : v(0) = g_{\varphi 0}(t),\, v(1) = g_{\varphi 1}(t) \right\},$$
$$V_0 := \left\{ v \in H^1(0,T;H^1(I)) : v(0) = 0,\, v(1) = 0 \right\}.$$

The weak form of the DD model system (3.1)–(3.2) is:

Find $(n,\varphi) \in V_n \times V_\varphi$ such that

$$(n_t, v) - (\mu\varphi_x n, v_x) + (\tau\theta n_x, v_x) = 0, \qquad \forall\, v \in V_0, \tag{3.3a}$$
$$\frac{\epsilon}{e}(\varphi_x, w_x) + (n, w) = (n_d, w), \qquad \forall\, w \in V_0. \tag{3.3b}$$

Let $\mathcal{T}_h$ be a partition of domain I described as in Section 2. The space of discrete weak functions are denoted by

$$S_h := \left\{ v \in M(I) : v_0|_{I_i} \in P_k(I_i),\, v_b|_{\partial I_i} \in P_0(\partial I_i) \right\},$$
$$S_{h,n} := \{ v \in S_h : v_b(0) = g_{n0},\, v_b(1) = g_{n1} \},$$
$$S_{h,\varphi} := \left\{ v \in S_h : v_b(0) = g_{\varphi 0},\, v_b(1) = g_{\varphi 1} \right\},$$
$$S_{h,0} := \{ v \in S_h : v_b(0) = 0,\, v_b(1) = 0 \}.$$

The semi-discrete scheme of the DD model (3.3) is:

Find $(n_h,\varphi_h) \in S_{h,n} \times S_{h,\varphi}$ such that

$$((n_{h,0})_t, v_0) - (\mu D_w\varphi_h\, n_{h,0}, D_w v) + (\tau\theta D_w n_h, D_w v) = 0, \qquad \forall\, v \in S_{h,0}, \tag{3.4a}$$
$$\frac{\epsilon}{e}(D_w\varphi_h, D_w w) + (n_{h,0}, w_0) = (n_d, w_0), \qquad \forall\, w \in S_{h,0}. \tag{3.4b}$$

Denote by Δt the time step size and $t_m = m\Delta t\,(m = 0,1,\ldots,M)$. We utilize backward Euler method for time discretization to obtain a fully discrete WG finite element method. At time $t = t_m$, using the backward difference quotient $\bar{\partial}_t n_h^m = (n_h^m - n_h^{m-1})/\Delta t$ to approximate $n_{h,t}$ in (3.4), we can obtain the fully-discrete WG finite element scheme:

Find $(n_h^m,\varphi_h^m) \in S_{h,n} \times S_{h,\varphi}$, $m = 1,2,\ldots,M$, such that

$$(\bar{\partial}_t n_{h,0}^m, v_0) - (\mu D_w\varphi_h^m\, n_{h,0}^m, D_w v) + (\tau\theta D_w n_h^m, D_w v) = 0, \qquad \forall\, v \in S_{h,0}, \tag{3.5a}$$
$$\frac{\epsilon}{e}(D_w\varphi_h^m, D_w w) + (n_{h,0}^m, w_0) = (n_d, w_0), \qquad \forall\, w \in S_{h,0}. \tag{3.5b}$$

3.2. Error estimate for the DD model

Let $u \in H^1(I_i)$ be a smooth function on each element I_i. Denote by $Q_h u = \{Q_0 u, Q_b u\}$ the L^2-projection of u onto $P_k(I_i) \times P_0(\partial I_i)$. More precisely, the function $Q_0 u$ is defined as the L^2-projection of u in $P_k(I_i)$ and $Q_b u = \left\{ u(x_{i-\frac{1}{2}}), u(x_{i+\frac{1}{2}}) \right\}$ on ∂I_i. Furthermore, let R_h be the local L^2-projection operator onto $P_r(I_i)$. To balance the approximation accuracy between spaces S_h and $P_r(I_i)$ used to compute $D_{w,r} n_h$, we set the index $r = k+1$ in the rest of paper.

Lemma 3.1. *For $u \in H^1(I_i)$ and $r = k+1$, we have $D_w(Q_h u) = R_h(u_x)$.*

Proof. For any $q \in P_r(I_i)$, according to the definition of D_w, we have

$$\int_{I_i} D_w(Q_h u)\, q\, dx = -\int_{I_i} Q_0 u\, q_x\, dx + \langle Q_b u, q \cdot n\rangle_{\partial I_i}.$$

Since Q_0 and R_h are L^2-projection operators, the right-hand side of above equation is given by

$$\begin{aligned} -\int_{I_i} Q_0 u\, q_x\, dx + \langle Q_b u, q\cdot n\rangle_{\partial I_i} &= -\int_{I_i} u\, q_x\, dx + \langle u, q\cdot n\rangle_{\partial I_i} \\ &= \int_{I_i} u_x\, q\, dx = \int_{I_i} R_h(u_x)\, q\, dx. \end{aligned} \quad \square$$

Remark 3.1. The above identity clearly indicates that $D_{w,k+1}(Q_h u)$ is an approximation of the classical gradient of u for any $u \in H^1(I_i)$.

Lemma 3.2 (See [22]). *For any $v \in S_{h,0}$ and $r = k+1$, then $\|v_0\| \le (1+h)\|D_w v\|$.*

Next, we define a projection operator π_h for $u \in H^1(I)$, such that $\pi_h u \in H^1(I)$, and on each element $I_i = \left[x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}\right]$, one has $\pi_h u|_{I_i} \in P_{k+1}(I_i)$ and the following equations

$$\begin{aligned} &((\pi_h u)_x, q)_{I_i} = (u_x, q)_{I_i}, \quad && \forall q \in P_k(I_i), \\ &\pi_h u(x_{i-\frac{1}{2}}) = u(x_{i-\frac{1}{2}}), && i = 1, \ldots, N, \end{aligned}$$

For $u \in H^{s+1}(I_i)$ with $0 \leqslant s \leqslant k+1$, we have

$$\|u - \pi_h u\|_{I_i} + h_i \|u - \pi_h u\|_{1,I_i} \leqslant C h_i^{s+1} \|u\|_{s+1,I_i}, \quad 0 \leqslant s \leqslant k+1.$$

Lemma 3.3. *For $u \in H^1(I)$ and $v \in S_{h,0}$, then $(u_x, v_0) = -(\pi_h u, D_w v)$.*

Proof. By the definition of operator π_h, we have $(u_x, v_0) = ((\pi_h u)_x, v_0)$. Because of the definition of weak gradient on each element, it yields $((\pi_h u)_x, v_0)_{I_i} = -(\pi_h u, D_w v)_{I_i} + \langle \pi_h u \cdot n, v_b\rangle_{\partial I_i}$ Summing over the elements and noting that $v_{\frac{1}{2}} = 0$ and $v_{N+\frac{1}{2}} = 0$, proof of the lemma completes. $\square$

Lemma 3.4. *Let $n(x,t)$, $\varphi(x,t)$ be solutions of problem (3.1), then*

$$(n_t, v_0) - (\pi_h(\mu\varphi_x n), D_w v) + (\pi_h(\tau\theta n_x), D_w v) = 0, \quad \forall v \in S_{h,0} \tag{3.6a}$$

$$\frac{\varepsilon}{e}(\pi_h \varphi_x, D_w w) + (n, w_0) = (n_d, w_0), \quad \forall w \in S_{h,0} \tag{3.6b}$$

Proof. Multiplying the two equations (3.1a) and (3.1b) by v and w respectively, and integrating on domain, it yields

$$(n_t, v_0) + ((\mu\varphi_x n)_x, v_0) - (\tau\theta n_{xx}, v_0) = 0, \tag{3.7a}$$

$$-\frac{\epsilon}{e}(\varphi_{xx}, w_0) + (n, w_0) = (n_d, w_0). \tag{3.7b}$$

By Lemma 3.3, we can derive

$$\begin{aligned} &((\mu\varphi_x n)_x, v_0) = -(\pi_h(\mu\varphi_x n), D_w v), \\ &-(\tau\theta n_{xx}, v_0) = (\pi_h(\tau\theta n_x), D_w v), \\ &-\frac{\epsilon}{e}(\varphi_{xx}, w_0) = \frac{\epsilon}{e}(\pi_h\varphi_x, D_w w). \end{aligned}$$

Substituting the above identities into system (3.7), the proof of the lemma completes. $\square$

Theorem 3.1 (See [22]). *Let $n(x,t)$, $\varphi(x,t)$ and $n_h(x,t)$, $\varphi_h(x,t)$ be solutions of problem (3.1) and semi-discrete WG scheme (3.4) for DD model, respectively. Assume that the exact solution is regular such that $n, \varphi \in H^1(0,T; H^{k+2}(I))$, then*

$$\|n - n_{h,0}\|^2 + \tau\theta \int_0^T \|n_x - D_w n_h\|^2 dt \le C h^{2(k+1)} \int_0^T (\|n\|_{k+2}^2 + \|\varphi\|_{k+2}^2) dt. \tag{3.8}$$

$$\|\varphi_x - D_w\varphi_h\|^2 + \|\varphi - \varphi_h\|^2 \le C h^{2(k+1)} \left\{ \|\varphi\|_{k+2}^2 + \int_0^T (\|n\|_{k+2}^2 + \|\varphi\|_{k+2}^2) dt \right\}. \tag{3.9}$$

Theorem 3.2. *Let $n(x,t)$, $\varphi(x,t)$ and $n_h^m(x,t)$, $\varphi_h^m(x,t)$ be solutions of problem (3.1) and fully discrete WG scheme (3.5) for DD model, respectively. Assume the exact solution is regular such that $n, \varphi \in H^1(0,T;H^{k+2}(I))$, then*

$$
\begin{aligned}
&\|n^M - n_{h,0}^M\|^2 + \Delta t\,\tau\theta \sum_{i=1}^{M} \|n_x^i - D_w n_h^i\|^2 \\
&\qquad \le C\left\{\Delta t^2 \int_0^T \|n_{tt}\|^2 dt + h^{2(k+1)} \max_{1\leqslant i\leqslant M}\left(\|n^i\|_{k+2}^2 + \|\varphi^i\|_{k+2}^2\right)\right\}. \qquad (3.10)\\
&\|\varphi_x^M - D_w\varphi_h^M\|^2 + \|\varphi^M - \varphi_h^M\|^2 \\
&\qquad \le C\left\{\Delta t^2 \int_0^T \|n_{tt}\|^2 dt + h^{2(k+1)} \max_{1\leqslant i\leqslant M}\left(\|n^i\|_{k+2}^2 + \|\varphi^i\|_{k+2}^2\right)\right\}. \qquad (3.11)
\end{aligned}
$$

Proof. Subtracting (3.5) from the system (3.6), for any $v, w \in S_{h,0}$, we obtain the following error equations

$$
\begin{aligned}
&(n_t^m - \bar{\partial}_t n_{h,0}^m, v_0) - (\pi_h(\mu\varphi_x^m n^m), D_w v) + (\mu D_w\varphi_h^m\, n_{h,0}^m, D_w v) \\
&\qquad + (\pi_h(\tau\theta n_x), D_w v) - (\tau\theta D_w n_h^m, D_w v) = 0, \qquad (3.12a)\\
&\frac{\epsilon}{e}[(\pi_h\varphi_x^m, D_w w) - (D_w\varphi_h^m, D_w w)] + (n^m - n_{h,0}^m, w_0) = 0. \qquad (3.12b)
\end{aligned}
$$

For the term $(\pi_h\varphi_x^m, D_w w) - (D_w\varphi_h^m, D_w w)$ in equality (3.12b), we can derive

$$
(\pi_h\varphi_x, D_w w) - (D_w\varphi_h, D_w w) = (\pi_h\varphi_x - \varphi_x, D_w w) - (D_w Q_h\varphi - \varphi_x, D_w w) + (D_w(Q_h\varphi - \varphi_h), D_w w).
$$

Combining the above identity with (3.12b) and noting that $(n, w_0) = (Q_0 n, w_0)$, we arrive at the following equality

$$
\begin{aligned}
&\frac{\epsilon}{e}\left[(\pi_h\varphi_x^m - \varphi_x^m, D_w w) - (D_w Q_h\varphi^m - \varphi_x^m, D_w w) + (D_w(Q_h\varphi^m - \varphi_h^m), D_w w)\right] \\
&\qquad + (Q_0 n^m - n_{h,0}^m, w_0) = 0. \qquad (3.13)
\end{aligned}
$$

By a similar approach, we have

$$
\begin{aligned}
&-(\pi_h(\mu\varphi_x n), D_w v) + (\mu D_w\varphi_h\, n_{h,0}, D_w v) \\
&\quad = -(\pi_h(\mu\varphi_x n) - \mu\varphi_x n, D_w v) - (\mu\varphi_x(n - Q_0 n), D_w v) - (\mu\varphi_x(Q_0 n - n_{h,0}), D_w v) \\
&\qquad + (\mu(D_w Q_h\varphi - \varphi_x)\, n_{h,0}, D_w v) + (\mu D_w(\varphi_h - Q_h\varphi)\, n_{h,0}, D_w v). \qquad (3.14)\\
&(\pi_h(\tau\theta n_x), D_w v) - (\tau\theta D_w n_h, D_w v) \\
&\quad = (\pi_h(\tau\theta n_x) - \tau\theta n_x, D_w v) - (\tau\theta(D_w Q_h n - n_x), D_w v) + (\tau\theta D_w(Q_h n - n_h), D_w v). \qquad (3.15)
\end{aligned}
$$

For the term $n_t^m - \bar{\partial}_t n_{h,0}^m$ in error equation (3.12a), we have

$$
n_t^m - \bar{\partial}_t n_{h,0}^m = (n_t^m - \bar{\partial}_t n^m) + \bar{\partial}_t(n^m - Q_0 n^m) + \bar{\partial}_t(Q_0 n^m - n_{h,0}^m).
$$

Note that $(\bar{\partial}_t(Q_0 n^m), v_0) = (\bar{\partial}_t n^m, v_0)$, it yields

$$
(n_t^m - \bar{\partial}_t n_{h,0}^m, v_0) = (n_t^m - \bar{\partial}_t n^m, v_0) + (\bar{\partial}_t(Q_0 n^m - n_{h,0}^m), v_0). \qquad (3.16)
$$

By substituting identities (3.14) to (3.16) into (3.12a), we obtain

$$
\begin{aligned}
&(n_t^m - \bar{\partial}_t n^m, v_0) + (\bar{\partial}_t(Q_0 n^m - n_{h,0}^m), v_0) \\
&\quad - (\pi_h(\mu\varphi_x^m n^m) - \mu\varphi_x^m n^m, D_w v) - (\mu\varphi_x^m(n^m - Q_0 n^m), D_w v) - (\mu\varphi_x^m(Q_0 n^m - n_{h,0}^m), D_w v) \\
&\quad + (\mu(D_w Q_h\varphi^m - \varphi_x^m)\, n_{h,0}^m, D_w v) + (\mu D_w(\varphi_h^m - Q_h\varphi^m)\, n_{h,0}^m, D_w v) + (\pi_h(\tau\theta n_x^m) - \tau\theta n_x^m, D_w v) \\
&\quad - (\tau\theta(D_w Q_h n^m - n_x^m), D_w v) + (\tau\theta D_w(Q_h n^m - n_h^m), D_w v) = 0, \quad \forall v \in S_{h,0}. \qquad (3.17)
\end{aligned}
$$

The equalities (3.13) and (3.17) are error equations. Taking $w = Q_h\varphi^m - \varphi_h^m$ in (3.13) and utilizing Lemma 3.2, we can derive following inequality:

$$
\begin{aligned}
\frac{\epsilon}{e}\|D_w(Q_h\varphi^m - \varphi_h^m)\|^2 &= -\frac{\epsilon}{e}(\pi_h\varphi_x^m - \varphi_x^m, D_w w) + \frac{\epsilon}{e}(D_w Q_h\varphi^m - \varphi_x^m, D_w w) - (Q_0 n^m - n_{h,0}^m, w_0) \\
&\le Ch^{2(k+1)}\|\varphi^m\|_{k+2}^2 + \frac{e}{\epsilon}\|Q_0 n^m - n_{h,0}^m\|^2 + \frac{1}{2}\frac{\epsilon}{e}\|D_w(Q_h\varphi^m - \varphi_h^m)\|^2,
\end{aligned}
$$

i.e.,

$$
\frac{1}{2}\frac{\epsilon}{e}\|D_w(Q_h\varphi^m - \varphi_h^m)\|^2 \le Ch^{2(k+1)}\|\varphi^m\|_{k+2}^2 + \frac{e}{\epsilon}\|Q_0 n^m - n_{h,0}^m\|^2. \qquad (3.18)
$$

Now, we analyze the term $\|Q_0 n^m - n_{h,0}^m\|$ by letting $v = Q_h n^m - n_h^m$ in (3.17). Then

$$\begin{aligned}
&\tfrac{1}{2\Delta t}\left(\|Q_0 n^m - n_{h,0}^m\|^2 - \|Q_0 n^{m-1} - n_{h,0}^{m-1}\|^2\right) + \tau\theta\|D_w(Q_h n^m - n_h^m)\|^2\\
\le&\tfrac{1}{\Delta t}\|Q_0 n^m - n_{h,0}^m\|^2 - \tfrac{1}{\Delta t}(Q_0 n^{m-1} - n_{h,0}^{m-1}, Q_0 n^m - n_{h,0}^m) + \tau\theta\|D_w(Q_h n^m - n_h^m)\|^2\\
=&-(n_t^m - \bar{\partial}_t n^m, v_0)\\
&+(\pi_h(\mu\varphi_x^m n^m) - \mu\varphi_x^m n^m, D_w v) + (\mu\varphi_x^m(n^m - Q_0 n^m), D_w v) + (\mu\varphi_x^m(Q_0 n^m - n_{h,0}^m), D_w v)\\
&-(\mu(D_w Q_h\varphi^m - \varphi_x^m)\,n_{h,0}^m, D_w v) - (\mu D_w(\varphi_h^m - Q_h\varphi^m)\,n_{h,0}^m, D_w v) - (\pi_h(\tau\theta n_x^m) - \tau\theta n_x^m, D_w v)\\
&+(\tau\theta(D_w Q_h n^m - n_x^m), D_w v)\\
\le&C\left\{\|n_t^m - \bar{\partial}_t n^m\|^2 + h^{2(k+1)}\|n^m\|_{k+2}^2 + \|n_{h,0}^m\|_\infty^2\, h^{2(k+1)}\|\varphi^m\|_{k+2}^2 + \|Q_0 n^m - n_{h,0}^m\|^2\right.\\
&\left.+\|n_{h,0}^m\|_\infty^2\,\|D_w(\varphi_h^m - Q_h\varphi^m)\|^2\right\} + \frac{\tau\theta}{2}\|D_w(Q_h n^m - n_h^m)\|^2. \qquad (3.19)
\end{aligned}$$

We make a priori assumption

$$\|n^m - n_{h,0}^m\| \le h^{\frac{1}{2}}, \qquad (3.20)$$

which implies that $\|n_{h,0}^m\|_\infty \le C$ and $\|D_w\varphi_h^m\|_\infty \le C$. We will justify priori assumption (3.20) later. Summing the inequality (3.19) over the time step m, setting $n_h^0 = Q_h n_0$ and using the discrete Gronwall inequality and (3.20), we get

$$\begin{aligned}
&\|Q_0 n^M - n_{h,0}^M\|^2 + \Delta t\,\tau\theta\sum_{i=1}^M\|D_w(Q_h n^i - n_h^i)\|^2\\
&\le C\Delta t\left\{\sum_{i=1}^M\|n_t^i - \bar{\partial}_t n^i\|^2 + h^{2(k+1)}\sum_{i=1}^M\left(\|n^i\|_{k+2}^2 + \|\varphi^i\|_{k+2}^2\right) + \sum_{i=1}^M\|D_w(\varphi_h^i - Q_h\varphi^i)\|^2\right\}. \qquad (3.21)
\end{aligned}$$

By Taylor expansion, we have

$$\begin{aligned}
&n_t^i - \bar{\partial}_t n^i = \tfrac{1}{\Delta t}\int_{t_{i-1}}^{t_i}(t - t_{i-1})n_{tt}dt.\\
&\sum_{i=1}^M\|n_t^i - \bar{\partial}_t n^i\|^2 \le \sum_{i=1}^M\tfrac{1}{\Delta t^2}\left(\int_{t_{i-1}}^{t_i}(t - t_{i-1})^2dt\right)\cdot\left(\int_{t_{i-1}}^{t_i}\|n_{tt}\|^2dt\right) = \frac{\Delta t}{3}\int_0^T\|n_{tt}\|^2dt. \qquad (3.22)
\end{aligned}$$

It is easy to verify that

$$\Delta t\sum_{i=1}^M\|n^i\|_{k+2}^2 \le M\Delta t\max_{1\leqslant i\leqslant M}\|n^i\|_{k+2}^2 \le T\max_{1\leqslant i\leqslant M}\|n^i\|_{k+2}^2. \qquad (3.23)$$

Combining (3.21) to (3.23) leads to the following inequality:

$$\begin{aligned}
&\|Q_0 n^M - n_{h,0}^M\|^2 + \Delta t\,\tau\theta\sum_{i=1}^M\|D_w(Q_h n^i - n_h^i)\|^2\\
&\le C\left\{\Delta t^2\int_0^T\|n_{tt}\|^2dt + h^{2(k+1)}\max_{1\leqslant i\leqslant M}\left(\|n^i\|_{k+2}^2 + \|\varphi^i\|_{k+2}^2\right) + \Delta t\sum_{i=1}^M\|D_w(\varphi_h^i - Q_h\varphi^i)\|^2\right\}. \qquad (3.24)
\end{aligned}$$

Substituting (3.18) into (3.24) and utilizing the discrete Gronwall inequality, we arrive at

$$\begin{aligned}
&\|Q_0 n^M - n_{h,0}^M\|^2 + \Delta t\,\tau\theta\sum_{i=1}^M\|D_w(Q_h n^i - n_h^i)\|^2\\
&\qquad\le C\left\{\Delta t^2\int_0^T\|n_{tt}\|^2dt + h^{2(k+1)}\max_{1\leqslant i\leqslant M}\left(\|n^i\|_{k+2}^2 + \|\varphi^i\|_{k+2}^2\right)\right\}. \qquad (3.25)
\end{aligned}$$

Combining (3.25) with (3.18) and using Lemma 3.2, we have

$$\begin{aligned}
&\|D_w(Q_h\varphi^M - \varphi_h^M)\|^2 + \|Q_h\varphi^M - \varphi_h^M\|^2\\
&\qquad\le C\left\{\Delta t^2\int_0^T\|n_{tt}\|^2dt + h^{2(k+1)}\max_{1\leqslant i\leqslant M}\left(\|n^i\|_{k+2}^2 + \|\varphi^i\|_{k+2}^2\right)\right\}. \qquad (3.26)
\end{aligned}$$

By the approximation properties of operators Q_h and R_h, we have the desired estimates (3.10) and (3.11).

To complete the proof, we verify the assumption (3.20). For $m = 0$, because we choose $n_h^0 = Q_h n_0$, obviously the assumption (3.20) holds. If (3.20) holds for $m = 1, 2, \ldots, M-1$, then for $m = M$, we can get (3.10), i.e., (3.20) also holds true for $m = M$ with $k \geq 0$. □

4. The high-field model

The high-field (HF) model is described as the following equations with Dirichlet boundary condition:

$$n_t + \left((\frac{3\tau\mu^2 e}{\epsilon} n_d \varphi_x + \mu\varphi_x + \frac{\tau\mu e\omega}{\epsilon})n - \frac{2\tau\mu^2 e}{\epsilon}\varphi_x n^2 \right)_x - ((\tau\theta + \tau\mu^2\varphi_x^2)n_x)_x = 0, \tag{4.1a}$$

$$-\frac{\epsilon}{e}\varphi_{xx} + n = n_d, \tag{4.1b}$$

where $\omega = (-\mu n\varphi_x)|_{x=0}$ is taken to be a constant. The unknown variables are same as for the DD model, which are the electron concentration n and the electric potential φ.

By setting $C_1 = \frac{\tau\mu e}{\epsilon}$, $C_2 = \frac{\tau\mu^2 e}{\epsilon} = \mu C_1$, $C_3 = \frac{\tau\mu e\omega}{\epsilon} = \omega C_1$, we rewrite (4.1) as

$$n_t + \left((3C_2 n_d\varphi_x + \mu\varphi_x + C_3)n - 2C_2\varphi_x n^2\right)_x - ((\tau\theta + \tau\mu^2\varphi_x^2)n_x)_x = 0, \tag{4.2a}$$

$$-\frac{\epsilon}{e}\varphi_{xx} + n = n_d. \tag{4.2b}$$

4.1. Weak form and discrete schemes for the HF model

The weak form of the HF model is: find $(n, \varphi) \in V_n \times V_\varphi$ such that

$$(n_t, v) - \left((3C_2 n_d\varphi_x + \mu\varphi_x + C_3)n - 2C_2\varphi_x n^2, v_x\right) + ((\tau\theta + \tau\mu^2\varphi_x^2)n_x, v_x) = 0, \qquad \forall\, v \in V_0, \tag{4.3a}$$

$$\frac{\epsilon}{e}(\varphi_x, w_x) + (n, w) = (n_d, w), \qquad \forall\, w \in V_0. \tag{4.3b}$$

The semi-discrete scheme of the HF model (4.3) is:

Find $(n_h, \varphi_h) \in S_{h,n} \times S_{h,\varphi}$ such that

$$\begin{aligned}((n_{h,0})_t, v_0) &- \left((3C_2 n_d D_w\varphi_h + \mu D_w\varphi_h + C_3)\, n_{h,0} - 2C_2 D_w\varphi_h\, n_{h,0}^2, D_w v\right)\\ &+ ((\tau\theta + \tau\mu^2(D_w\varphi_h)^2)\, D_w n_h, D_w v) = 0, \quad \forall\, v \in S_{h,0},\end{aligned} \tag{4.4a}$$

$$\frac{\epsilon}{e}(D_w\varphi_h, D_w w) + (n_{h,0}, w_0) = (n_d, w_0), \qquad \forall\, w \in S_{h,0}. \tag{4.4b}$$

At $t = t_m$, using the backward difference quotient to approximate $n_{h,t}$ in (4.5), we can obtain the fully discrete WG finite element scheme for HF model:

Find $(n_h, \varphi_h) \in S_{h,n} \times S_{h,\varphi}$, $m = 1, 2, \ldots, M$ such that

$$\begin{aligned}(\bar\partial_t n_{h,0}^m, v_0) &- \left((3C_2 n_d D_w\varphi_h^m + \mu D_w\varphi_h^m + C_3)\, n_{h,0}^m - 2C_2 D_w\varphi_h^m\, (n_{h,0}^m)^2, D_w v\right)\\ &+ ((\tau\theta + \tau\mu^2(D_w\varphi_h^m)^2)\, D_w n_h^m, D_w v) = 0, \quad \forall\, v \in S_{h,0},\end{aligned} \tag{4.5a}$$

$$\frac{\epsilon}{e}(D_w\varphi_h^m, D_w w) + (n_{h,0}^m, w_0) = (n_d, w_0), \qquad \forall\, w \in S_{h,0}. \tag{4.5b}$$

4.2. Error estimate for the HF model

Lemma 4.1. *Let $n(x,t)$, $\varphi(x,t)$ be solutions of problem (4.2). Then for any $v, w \in S_{h,0}$, we obtain*

$$(n_t, v_0) - \left(\pi_h((3C_2 n_d\varphi_x + \mu\varphi_x + C_3)n - 2C_2\varphi_x n^2), D_w v\right) + (\pi_h((\tau\theta + \tau\mu^2\varphi_x^2)n_x), D_w v) = 0, \tag{4.6a}$$

$$\frac{\varepsilon}{e}\,(\pi_h\varphi_x, D_w w) + (n, w_0) = (n_d, w_0)\,. \tag{4.6b}$$

Proof. Multiplying the two equations (4.2a) and (4.2b) by v and w respectively, integrating on domain and utilizing Lemma 3.3, we can derive the lemma. □

Theorem 4.1. *Let $n(x,t)$, $\varphi(x,t)$ and $n_h(x,t)$, $\varphi_h(x,t)$ be solutions of problem (4.1) and semi-discrete WG scheme (4.4) for the HF model, respectively. Assume the exact solution is regular such that $n, \varphi \in H^1(0,T; H^{k+2}(I))$, then*

$$\|n - n_{h,0}\|^2 + \tau\theta\int_0^T \|n_x - D_w n_h\|^2 dt \leq Ch^{2(k+1)}\int_0^T (\|n\|_{k+2}^2 + \|\varphi\|_{k+2}^2)dt. \tag{4.7}$$

$$\|\varphi_x - D_w\varphi_h\|^2 + \|\varphi - \varphi_h\|^2 \leq Ch^{2(k+1)}\left\{\|\varphi\|_{k+2}^2 + \int_0^T (\|n\|_{k+2}^2 + \|\varphi\|_{k+2}^2)dt\right\}. \tag{4.8}$$

Proof. Subtracting (4.4) from the system (4.6), we obtain

$$
\begin{aligned}
&(n_t-(n_{h,0})_t, v_0)-\big(\pi_h((3C_2n_d\varphi_x+\mu\varphi_x+C_3)n-2C_2\varphi_x n^2), D_w v\big)+(\pi_h((\tau\theta+\tau\mu^2\varphi_x^2)n_x), D_w v)\\
&\quad+\big((3C_2n_dD_w\varphi_h+\mu D_w\varphi_h+C_3)\,n_{h,0}-2C_2D_w\varphi_h\, n_{h,0}^2, D_w v\big)\\
&\quad-((\tau\theta+\tau\mu^2(D_w\varphi_h)^2)D_wn_h, D_w v)=0, \qquad \forall\, v\in S_{h,0}, \qquad (4.9a)\\
&\frac{\epsilon}{e}(\varphi_x, w_{0,x})-\frac{\epsilon}{e}(D_w\varphi_h, D_w w)+(n-n_{h,0}, w_0)=0, \qquad \forall\, w\in S_{h,0}. \qquad (4.9b)
\end{aligned}
$$

Note that the equality (4.9b) can be rewritten as the following equation

$$
\begin{aligned}
&\frac{\epsilon}{e}\,((\pi_h\varphi_x-\varphi_x, D_w w)-(D_wQ_h\varphi-\varphi_x, D_w w)+(D_w(Q_h\varphi-\varphi_h), D_w w))\\
&\qquad+(Q_0n-n_{h,0}, w_0)=0. \qquad (4.10)
\end{aligned}
$$

For equality (4.9a), we have

$$
\begin{aligned}
&-\big(\pi_h((3C_2n_d\varphi_x+\mu\varphi_x+C_3)n-2C_2\varphi_x n^2), D_w v\big)\\
&\quad+\big((3C_2n_dD_w\varphi_h+\mu D_w\varphi_h+C_3)n_{h,0}-2C_2D_w\varphi_h\, n_{h,0}^2, D_w v\big)\\
&=-\big(\pi_h\left[(3C_2n_d\varphi_x+\mu\varphi_x+C_3)n-2C_2\varphi_x n^2\right]-\left[(3C_2n_d\varphi_x+\mu\varphi_x+C_3)n-2C_2\varphi_x n^2\right], D_w v\big)\\
&\quad-\big((3C_2n_d\varphi_x+\mu\varphi_x+C_3)(n-n_{h,0})-2C_2\varphi_x(n^2-n_{h,0}^2), D_w v\big)\\
&\quad-\big([3C_2n_d(\varphi_x-D_wQ_h\varphi)+\mu(\varphi_x-D_wQ_h\varphi)+C_3]\;n_{h,0}-2C_2(\varphi_x-D_wQ_h\varphi)\,n_{h,0}^2, D_w v\big)\\
&\quad-\big([3C_2n_dD_w(Q_h\varphi-\varphi_h)+\mu D_w(Q_h\varphi-\varphi_h)+C_3]\;n_{h,0}-2C_2D_w(Q_h\varphi-\varphi_h)\,n_{h,0}^2, D_w v\big). \qquad (4.11)
\end{aligned}
$$

In addition,

$$
\begin{aligned}
&((\tau\theta+\tau\mu^2\varphi_x^2)n_x, v_{0,x})-((\tau\theta+\tau\mu^2(D_w\varphi_h)^2)D_wn_h, D_w v)\\
&=(\pi_h\left[(\tau\theta+\tau\mu^2\varphi_x^2)n_x\right]-\left[(\tau\theta+\tau\mu^2\varphi_x^2)n_x\right], D_w v)+[(\tau\theta\, n_x, D_w v)-(\tau\theta\, D_wn_h, D_w v)]\\
&\quad+\left[(\tau\mu^2(\varphi_x)^2\, n_x, D_w v)-(\tau\mu^2(D_w\varphi_h)^2\, D_wn_h, D_w v)\right], \qquad (4.12)
\end{aligned}
$$

where

$$
(\tau\theta\, n_x, D_w v)-(\tau\theta\, D_wn_h, D_w v)=(\tau\theta\,(n_x-D_wQ_hn), D_w v)+(\tau\theta\, D_w(Q_hn-n_h), D_w v), \qquad (4.13)
$$

and

$$
\begin{aligned}
&(\tau\mu^2(\varphi_x)^2\, n_x, D_w v)-(\tau\mu^2(D_w\varphi_h)^2\, D_wn_h, D_w v)\\
&=(\tau\mu^2(\varphi_x-D_wQ_h\varphi)\,\varphi_xn_x, D_w v)+(\tau\mu^2D_w(Q_h\varphi-\varphi_h)\,\varphi_xn_x, D_w v)\\
&\quad+(\tau\mu^2D_w\varphi_h\,(\varphi_x-D_wQ_h\varphi)n_x, D_w v)+(\tau\mu^2D_w\varphi_h\,D_w(Q_h\varphi-\varphi_h)n_x, D_w v)\\
&\quad+(\tau\mu^2(D_w\varphi_h)^2\,(n_x-D_wQ_hn), D_w v)+(\tau\mu^2(D_w\varphi_h)^2\,D_w(Q_hn-n_h), D_w v). \qquad (4.14)
\end{aligned}
$$

By combining (4.11) to (4.14), error equation (4.9a) can be rewritten as following identity:

$$
\begin{aligned}
&(Q_0n_t-(n_{h,0})_t, v_0)\\
&\quad-\big(\pi_h\left[(3C_2n_d\varphi_x+\mu\varphi_x+C_3)n-2C_2\varphi_x n^2\right]-\left[(3C_2n_d\varphi_x+\mu\varphi_x+C_3)n-2C_2\varphi_x n^2\right], D_w v\big)\\
&\quad-\big((3C_2n_d\varphi_x+\mu\varphi_x+C_3)(n-n_{h,0})-2C_2\varphi_x(n^2-n_{h,0}^2), D_w v\big)\\
&\quad-\big([3C_2n_d(\varphi_x-D_wQ_h\varphi)+\mu(\varphi_x-D_wQ_h\varphi)+C_3]\;n_{h,0}-2C_2(\varphi_x-D_wQ_h\varphi)\,n_{h,0}^2, D_w v\big)\\
&\quad-\big([3C_2n_dD_w(Q_h\varphi-\varphi_h)+\mu D_w(Q_h\varphi-\varphi_h)+C_3]\;n_{h,0}-2C_2D_w(Q_h\varphi-\varphi_h)\,n_{h,0}^2, D_w v\big)\\
&\quad+(\pi_h\left[(\tau\theta+\tau\mu^2\varphi_x^2)n_x\right]-\left[(\tau\theta+\tau\mu^2\varphi_x^2)n_x\right], D_w v)\\
&\quad+(\tau\theta(n_x-D_wQ_hn), D_w v)+(\tau\theta D_w(Q_hn-n_h), D_w v)\\
&\quad+(\tau\mu^2(\varphi_x-D_wQ_h\varphi)\,\varphi_xn_x, D_w v)+(\tau\mu^2D_w(Q_h\varphi-\varphi_h)\,\varphi_xn_x, D_w v)\\
&\quad+(\tau\mu^2D_w\varphi_h\,(\varphi_x-D_wQ_h\varphi)n_x, D_w v)+(\tau\mu^2D_w\varphi_h\,D_w(Q_h\varphi-\varphi_h)n_x, D_w v)\\
&\quad+(\tau\mu^2(D_w\varphi_h)^2\,(n_x-D_wQ_hn), D_w v)+(\tau\mu^2(D_w\varphi_h)^2\,D_w(Q_hn-n_h), D_w v)=0. \qquad (4.15)
\end{aligned}
$$

The equalities (4.10) and (4.15) are error equations. Similar procedures as DD model, Taking $w=Q_h\varphi-\varphi_h$ in (4.10) we possess the following inequality

$$
\frac{1}{2}\frac{\epsilon}{e}\|D_w(Q_h\varphi-\varphi_h)\|^2\le Ch^{2(k+1)}\|\varphi\|_{k+2}^2+\frac{e}{\epsilon}\|Q_0n-n_{h,0}\|^2. \qquad (4.16)
$$

Next, we analyze the term $\|Q_0 n - n_{h,0}\|$ by letting $v = Q_h n - n_h$ in (4.15),

$$\begin{aligned}
&\frac{1}{2}\frac{1}{dt}\|Q_0 n - n_{h,0}\|^2 + \tau\theta\|D_w(Q_h n - n_h)\|^2 \\
&= \left(\pi_h\left[(3C_2 n_d\varphi_x + \mu\varphi_x + C_3)n - 2C_2\varphi_x n^2\right] - \left[(3C_2 n_d\varphi_x + \mu\varphi_x + C_3)n - 2C_2\varphi_x n^2\right], D_w v\right) \\
&\quad + \left((3C_2 n_d\varphi_x + \mu\varphi_x + C_3)(n - n_{h,0}) - 2C_2\varphi_x(n^2 - n_{h,0}^2), D_w v\right) \\
&\quad + \left([3C_2 n_d(\varphi_x - D_w Q_h\varphi) + \mu(\varphi_x - D_w Q_h\varphi) + C_3]\, n_{h,0} - 2C_2(\varphi_x - D_w Q_h\varphi)\, n_{h,0}^2, D_w v\right) \\
&\quad + \left([3C_2 n_d D_w(Q_h\varphi - \varphi_h) + \mu D_w(Q_h\varphi - \varphi_h) + C_3]\, n_{h,0} - 2C_2 D_w(Q_h\varphi - \varphi_h)\, n_{h,0}^2, D_w v\right) \\
&\quad - \left(\pi_h\left[(\tau\theta + \tau\mu^2\varphi_x^2)n_x\right] - \left[(\tau\theta + \tau\mu^2\varphi_x^2)n_x\right], D_w v\right) \\
&\quad - (\tau\theta(n_x - D_w Q_h n), D_w v) - (\tau\mu^2(\varphi_x - D_w Q_h\varphi)\varphi_x n_x, D_w v) \\
&\quad - (\tau\mu^2 D_w(Q_h\varphi - \varphi_h)\,\varphi_x n_x, D_w v) - (\tau\mu^2 D_w\varphi_h\,(\varphi_x - D_w Q_h\varphi)n_x, D_w v) \\
&\quad - (\tau\mu^2 D_w\varphi_h\, D_w(Q_h\varphi - \varphi_h)n_x, D_w v) - (\tau\mu^2(D_w\varphi_h)^2\,(n_x - D_w Q_h n), D_w v) \\
&\quad - (\tau\mu^2(D_w\varphi_h)^2\, D_w(Q_h n - n_h), D_w v) \\
&= \Pi_1 + \Pi_2 + \Pi_3 + \Pi_4 + \Pi_5 + \Pi_6 + \Pi_7 + \Pi_8 + \Pi_9 + \Pi_{10} + \Pi_{11} + \Pi_{12},
\end{aligned} \tag{4.17}$$

where

$$\Pi_1 \le C_{\|\varphi_x\|_\infty, \|n\|_\infty}\, h^{k+2}\|n\|_{k+2}\, \|D_w(Q_h n - n_h)\|, \tag{4.18}$$

$$\begin{aligned}
\Pi_2 &\le C_{\|\varphi_x\|_\infty, \|n\|_\infty, \|n_{h,0}\|_\infty}\, \|n - n_{h,0}\|\, \|D_w(Q_h n - n_h)\| \\
&\le C_{\|\varphi_x\|_\infty, \|n\|_\infty, \|n_{h,0}\|_\infty}\, \left(h^{k+2}\|n\|_{k+2} + \|Q_0 n - n_{h,0}\|\right)\, \|D_w(Q_h n - n_h)\|,
\end{aligned} \tag{4.19}$$

$$\Pi_3 \le C_{\|n_{h,0}\|_\infty, \|(n_{h,0})^2\|_\infty}\, h^{k+1}\|\varphi\|_{k+2}\, \|D_w(Q_h n - n_h)\|, \tag{4.20}$$

$$\Pi_4 \le C_{\|n_{h,0}\|_\infty, \|(n_{h,0})^2\|_\infty}\, \|D_w(Q_h\varphi - \varphi_h)\|\, \|D_w(Q_h n - n_h)\|, \tag{4.21}$$

$$\Pi_5 \le C_{\|\varphi_x\|_\infty}\, h^{k+1}\|n\|_{k+2}\, \|D_w(Q_h n - n_h)\|, \tag{4.22}$$

$$\Pi_6 \le C h^{k+1}\|n\|_{k+2}\, \|D_w(Q_h n - n_h)\|, \tag{4.23}$$

$$\Pi_7 \le C_{\|\varphi_x\|_\infty, \|n_x\|_\infty}\, h^{k+1}\|\varphi\|_{k+2}\, \|D_w(Q_h n - n_h)\|, \tag{4.24}$$

$$\Pi_8 \le C_{\|\varphi_x\|_\infty, \|n_x\|_\infty}\, \|D_w(Q_h\varphi - \varphi_h)\|\, \|D_w(Q_h n - n_h)\|, \tag{4.25}$$

$$\Pi_9 \le C_{\|D_w\varphi_h\|_\infty, \|n_x\|_\infty}\, h^{k+1}\|\varphi\|_{k+2}\, \|D_w(Q_h n - n_h)\|, \tag{4.26}$$

$$\Pi_{10} \le C_{\|D_w\varphi_h\|_\infty, \|n_x\|_\infty}\, \|D_w(Q_h\varphi - \varphi_h)\|\, \|D_w(Q_h n - n_h)\|, \tag{4.27}$$

$$\Pi_{11} \le C_{\|D_w\varphi_h\|_\infty}\, h^{k+1}\|n\|_{k+2}\, \|D_w(Q_h n - n_h)\|. \tag{4.28}$$

Due to the non-negativity of relaxation parameter τ, the non-positive term $-(\tau\mu^2(D_w\varphi_h)^2\, D_w(Q_h n - n_h), D_w(Q_h n - n_h))$ could be eliminated.

We make a priori assumption

$$\|n - n_{h,0}\| \le h^{\frac{1}{2}}, \tag{4.29}$$

which implies that $\|n_{h,0}\|_\infty \le C$ and $\|D_w\varphi_h\|_\infty \le C$. Because term $n_{h,0}$ is polynomial series and $\|n_{h,0}\|_\infty \le C$, the nonlinear term $\|(n_{h,0})^2\|_\infty$ is bounded by a positive constant independent of mesh size h. Combining (4.17) with inequalities (4.18)–(4.28), we can derive

$$\begin{aligned}
&\frac{1}{2}\frac{1}{dt}\|Q_0 n - n_{h,0}\|^2 + \tau\theta\|D_w(Q_h n - n_h)\|^2 \\
&\le C\left\{h^{2(k+1)}\left(\|n\|_{k+2}^2 + \|\varphi\|_{k+2}^2\right) + \|Q_0 n - n_{h,0}\|^2 + \|D_w(Q_h\varphi - \varphi_h)\|^2\right\} + \tfrac{\tau\theta}{2}\|D_w(Q_h n - n_h)\|^2,
\end{aligned}$$

i.e.,

$$\begin{aligned}
&\frac{1}{2}\frac{1}{dt}\|Q_0 n - n_{h,0}\|^2 + \frac{\tau\theta}{2}\|D_w(Q_h n - n_h)\|^2 \\
&\qquad \le C\left\{h^{2(k+1)}\left(\|n\|_{k+2}^2 + \|\varphi\|_{k+2}^2\right) + \|Q_0 n - n_{h,0}\|^2 + \|D_w(Q_h\varphi - \varphi_h)\|^2\right\},
\end{aligned} \tag{4.30}$$

where C is the constant for L^∞-norm bound for $n, n_x, n_{h,0}, \varphi_x, D_w\varphi_h$. Integrating (4.30) with respect to t, and setting $n_h(x, 0) = Q_h n(x, 0)$, we can derive the following inequality

$$\begin{aligned}
&\frac{1}{2}\|Q_0 n(T) - n_{h,0}(T)\|^2 + \frac{\tau\theta}{2}\int_0^T \|D_w(Q_h n - n_h)\|^2 dt \\
&\le C\left\{h^{2(k+1)}\int_0^T \left(\|n\|_{k+2}^2 + \|\varphi\|_{k+2}^2\right) dt + \int_0^T \|Q_0 n - n_{h,0}\|^2 dt + \int_0^T \|D_w(\varphi_h - Q_h\varphi)\|^2 dt\right\}.
\end{aligned} \tag{4.31}$$

Substituting (4.16) into (4.31), we can derive

$$\|Q_0 n - n_{h,0}\|^2 + \tau\theta \int_0^T \|D_w(Q_h n - n_h)\|^2 dt \le Ch^{2(k+1)} \int_0^T (\|n\|_{k+2}^2 + \|\varphi\|_{k+2}^2) dt. \tag{4.32}$$

By Lemma 3.2 and combining (4.32) with (4.16), we obtain

$$\frac{\epsilon}{e}\|D_w(Q_h\varphi - \varphi_h)\|^2 + \frac{\epsilon}{e}\|Q_h\varphi - \varphi_h\|^2 \le Ch^{2(k+1)} \left\{ \|\varphi\|_{k+2}^2 + \int_0^T (\|n\|_{k+2}^2 + \|\varphi\|_{k+2}^2) dt \right\}. \tag{4.33}$$

Recall the approximation property, we can complete the proof of (4.7) and (4.8).

To complete the proof, let us verify the assumption (4.29). For $k \ge 0$, we consider h is small enough so that $Ch^{k+1} < h^{\frac{1}{2}}$, where C is the constant in (4.29) determined by the final time T. Then if $t^* = sup\left\{t : \|n(t) - n_{h,0}(t)\| \le h^{\frac{1}{2}}\right\}$, we should have $\|n(t^*) - n_{h,0}(t^*)\| = h^{\frac{1}{2}}$ by continuity if t^* is finite. On the other hand, our proof implies that (4.29) holds for $t \le t^*$, in particular $\|n(t^*) - n_{h,0}(t^*)\| \le Ch^{k+1} < h^{\frac{1}{2}}$. This is a contradiction if $t^* < T$. Hence $t^* \ge T$ and the assumption (4.29) is correct. □

Theorem 4.2. *Let $n(x,t)$, $\varphi(x,t)$ and $n_h^m(x,t)$, $\varphi_h^m(x,t)$ be solutions of problem (4.1) and fully discrete WG scheme (4.5) for the HF model, respectively. Assume that the exact solution is regular such that $n, \varphi \in H^1(0,T;H^{k+2}(I))$, then*

$$\begin{aligned}
&\|n^M - n_{h,0}^M\|^2 + \Delta t\,\tau\theta \sum_{i=1}^M \|n_x^i - D_w n_h^i\|^2 \\
&\qquad \le C\left\{ \Delta t^2 \int_0^T \|n_{tt}\|^2 dt + h^{2(k+1)} \max_{1\le i\le M} \left(\|n^i\|_{k+2}^2 + \|\varphi^i\|_{k+2}^2\right)\right\}. &(4.34)\\
&\|\varphi_x^M - D_w\varphi_h^M\|^2 + \|\varphi^M - \varphi_h^M\|^2 \\
&\qquad \le C\left\{ \Delta t^2 \int_0^T \|n_{tt}\|^2 dt + h^{2(k+1)} \max_{1\le i\le M} \left(\|n^i\|_{k+2}^2 + \|\varphi^i\|_{k+2}^2\right)\right\}. &(4.35)
\end{aligned}$$

Proof. Subtracting (4.5) from the system (4.6), we obtain

$$\begin{aligned}
&(n_t^m - \bar\partial_t n_{h,0}^m, v_0) - \left(\pi_h((3C_2 n_d\varphi_x^m + \mu\varphi_x^m + C_3)n^m - 2C_2\varphi_x^m(n^m)^2), D_w v\right) \\
&\quad + \left((3C_2 n_d D_w\varphi_h^m + \mu D_w\varphi_h^m + C_3)\, n_{h,0}^m - 2C_2 D_w\varphi_h^m\,(n_{h,0}^m)^2, D_w v\right) \\
&\quad + (\pi_h((\tau\theta + \tau\mu^2(\varphi_x^m)^2)n_x^m), D_w v) - ((\tau\theta + \tau\mu^2(D_w\varphi_h^m)^2) D_w n_h^m, D_w v) = 0,\ \forall v \in S_{h,0}, &(4.36a)\\
&\frac{\epsilon}{e}(\varphi_x^m, w_{0,x}) - \frac{\epsilon}{e}(D_w\varphi_h^m, D_w w) + (Q_0 n^m - n_{h,0}^m, w_0) = 0, \qquad \forall w \in S_{h,0}. &(4.36b)
\end{aligned}$$

The equality (4.36b) can be rewritten as (3.13). Similar to the equality (4.15), for any $v \in S_{h,0}$, we have

$$\begin{aligned}
&(n_t^m - \bar\partial_t n^m, v_0) + (\bar\partial_t(Q_0 n^m - n_{h,0}^m), v_0) \\
&- \left(\pi_h\left[(3C_2 n_d\varphi_x^m + \mu\varphi_x^m + C_3)n^m - 2C_2\varphi_x^m(n^m)^2\right] - \left[(3C_2 n_d\varphi_x^m + \mu\varphi_x^m + C_3)n^m - 2C_2\varphi_x^m(n^m)^2\right], D_w v\right) \\
&- \left((3C_2 n_d\varphi_x^m + \mu\varphi_x^m + C_3)(n^m - n_{h,0}^m) - 2C_2\varphi_x^m((n^m)^2 - (n_{h,0}^m)^2), D_w v\right) \\
&- \left(\left[3C_2 n_d(\varphi_x^m - D_w Q_h\varphi^m) + \mu(\varphi_x^m - D_w Q_h\varphi^m) + C_3\right] n_{h,0}^m - 2C_2(\varphi_x^m - D_w Q_h\varphi^m)(n_{h,0}^m)^2, D_w v\right) \\
&- \left(\left[3C_2 n_d D_w(Q_h\varphi^m - \varphi_h^m) + \mu D_w(Q_h\varphi^m - \varphi_h^m) + C_3\right] n_{h,0}^m - 2C_2 D_w(Q_h\varphi^m - \varphi_h^m)(n_{h,0}^m)^2, D_w v\right) \\
&+ \left(\pi_h\left[(\tau\theta + \tau\mu^2(\varphi_x^m)^2)n_x^m\right] - \left[(\tau\theta + \tau\mu^2(\varphi_x^m)^2)n_x^m\right], D_w v\right) \\
&+ (\tau\theta(n_x^m - D_w Q_h n^m), D_w v) + (\tau\theta D_w(Q_h n^m - n_h^m), D_w v) \\
&+ (\tau\mu^2(\varphi_x^m - D_w Q_h\varphi^m)\varphi_x^m n_x^m, D_w v) + (\tau\mu^2 D_w(Q_h\varphi^m - \varphi_h^m)\varphi_x^m n_x^m, D_w v) \\
&+ (\tau\mu^2 D_w\varphi_h^m(\varphi_x^m - D_w Q_h\varphi^m)n_x^m, D_w v) + (\tau\mu^2 D_w\varphi_h^m D_w(Q_h\varphi^m - \varphi_h^m)n_x^m, D_w v) \\
&+ (\tau\mu^2(D_w\varphi_h^m)^2(n_x^m - D_w Q_h n^m), D_w v) + (\tau\mu^2(D_w\varphi_h^m)^2 D_w(Q_h n^m - n_h^m), D_w v) = 0. &(4.37)
\end{aligned}$$

The equalities (3.13) and (4.37) are error equations. Taking $w = Q_h\varphi^m - \varphi_h^m$ in (3.13), we can derive the inequality (3.18). Next, we analyze the term $\|Q_0 n^m - n_{h,0}^m\|$ by letting $v = Q_h n^m - n_h^m$ in (4.37),

$$\begin{aligned}
&\tfrac{1}{2\Delta t}\left(\|Q_0 n^m - n_{h,0}^m\|^2 - \|Q_0 n^{m-1} - n_{h,0}^{m-1}\|^2\right) + \tau\theta\|D_w(Q_h n^m - n_h^m)\|^2 \\
\le& \tfrac{1}{\Delta t}\|Q_0 n^m - n_{h,0}^m\|^2 - \tfrac{1}{\Delta t}(Q_0 n^{m-1} - n_{h,0}^{m-1}, Q_0 n^m - n_{h,0}^m) + \tau\theta\|D_w(Q_h n^m - n_h^m)\|^2 \\
=& -(n_t^m - \bar\partial_t n^m, v_0) \\
&+ \left(\pi_h\left[(3C_2 n_d\varphi_x^m + \mu\varphi_x^m + C_3)n^m - 2C_2\varphi_x^m(n^m)^2\right] - \left[(3C_2 n_d\varphi_x^m + \mu\varphi_x^m + C_3)n^m - 2C_2\varphi_x^m(n^m)^2\right], D_w v\right)
\end{aligned}$$

$$
\begin{aligned}
&+ \left((3C_2 n_d \varphi_x^m + \mu\varphi_x^m + C_3)(n^m - n_{h,0}^m) - 2C_2\varphi_x^m((n^m)^2 - (n_{h,0}^m)^2), D_w v\right)\\
&+ \left(\left[3C_2 n_d(\varphi_x^m - D_w Q_h\varphi^m) + \mu(\varphi_x^m - D_w Q_h\varphi^m) + C_3\right] n_{h,0}^m - 2C_2(\varphi_x^m - D_w Q_h\varphi^m)(n_{h,0}^m)^2, D_w v\right)\\
&+ \left(\left[3C_2 n_d D_w(Q_h\varphi^m - \varphi_h^m) + \mu D_w(Q_h\varphi^m - \varphi_h^m) + C_3\right] n_{h,0}^m - 2C_2 D_w(Q_h\varphi^m - \varphi_h^m)(n_{h,0}^m)^2, D_w v\right)\\
&- (\pi_h\left[(\tau\theta + \tau\mu^2(\varphi_x^m)^2)n_x^m\right] - \left[(\tau\theta + \tau\mu^2(\varphi_x^m)^2)n_x^m\right], D_w v)\\
&- (\tau\theta(n_x^m - D_w Q_h n^m), D_w v) - (\tau\mu^2(\varphi_x^m - D_w Q_h\varphi^m)\varphi_x^m n_x^m, D_w v)\\
&- (\tau\mu^2 D_w(Q_h\varphi^m - \varphi_h^m)\varphi_x^m n_x^m, D_w v) - (\tau\mu^2 D_w\varphi_h^m(\varphi_x^m - D_w Q_h\varphi^m)n_x^m, D_w v)\\
&- (\tau\mu^2 D_w\varphi_h^m D_w(Q_h\varphi^m - \varphi_h^m)n_x^m, D_w v) - (\tau\mu^2(D_w\varphi_h^m)^2(n_x^m - D_w Q_h n^m), D_w v)\\
&- (\tau\mu^2(D_w\varphi_h^m)^2 D_w(Q_h n^m - n_h^m), D_w v)\\
\le{}& C\Big\{\|n_t^m - \bar\partial_t n^m\|^2 + C_{\|n_{h,0}^m\|_\infty, \|(n_{h,0}^m)^2\|_\infty, \|D_w\varphi_h^m\|_\infty} h^{2(k+1)}\|\varphi^m\|_{k+2}^2 + C_{\|D_w\varphi_h^m\|_\infty} h^{2(k+1)}\|n^m\|_{k+2}^2\\
&+ C_{\|n_{h,0}^m\|_\infty}\|Q_0 n^m - n_{h,0}^m\|^2 + C_{\|n_{h,0}^m\|_\infty, \|(n_{h,0}^m)^2\|_\infty, \|D_w\varphi_h^m\|_\infty}\|D_w(Q_h\varphi^m - \varphi_h^m)\|^2\Big\}\\
&+ \tfrac{\tau\theta}{2}\|D_w(Q_h n^m - n_h^m)\|^2,
\end{aligned}
\tag{4.38}
$$

where C is the constant in the L^∞-norm bound for n^m, n_x^m and φ_x^m. Note that the non-positive term $-(\tau\mu^2(D_w\varphi_h^m)^2 D_w(Q_h n^m - n_h^m), D_w(Q_h n^m - n_h^m))$ is eliminated. We make a assumption $\|n^m - n_{h,0}^m\| \le h^{\frac{1}{2}}$ (proof is omitted due to similarity), which implies that $\|n_{h,0}^m\|_\infty \le C$ and $\|D_w\varphi_h^m\|_\infty \le C$. Because polynomial series $n_{h,0}^m$ satisfies $\|n_{h,0}^m\|_\infty \le C$, the nonlinear term $\|(n_{h,0}^m)^2\|_\infty$ is bounded by a positive constant independent of mesh size h.

Summing inequality (4.38) over the time step m and setting $n_h^0 = Q_h n_0$, we utilize the discrete Gronwall lemma and inequalities (3.22)–(3.23) to get

$$
\begin{aligned}
&\|Q_0 n^M - n_{h,0}^M\|^2 + \Delta t\,\tau\theta\sum_{i=1}^{M}\|D_w(Q_h n^i - n_h^i)\|^2\\
&\le C\Big\{\Delta t\sum_{i=1}^{M}\|n_t^i - \bar\partial_t n^i\|^2 + \Delta t\, h^{2(k+1)}\sum_{i=1}^{M}\left(\|n^i\|_{k+2}^2 + \|\varphi^i\|_{k+2}^2\right) + \Delta t\sum_{i=1}^{M}\|Q_0 n^i - n_{h,0}^i\|^2\\
&\qquad + \Delta t\sum_{i=1}^{M}\|D_w(Q_h\varphi^i - \varphi_h^i)\|^2\Big\}\\
&\le C\left\{\Delta t^2\int_0^T\|n_{tt}\|^2 dt + h^{2(k+1)}\max_{1\le i\le M}\left(\|n^i\|_{k+2}^2 + \|\varphi^i\|_{k+2}^2\right) + \sum_{i=1}^{M}\Delta t\|D_w(Q_h\varphi^i - \varphi_h^i)\|^2\right\}.
\end{aligned}
\tag{4.39}
$$

Substituting (3.18) into (4.39) and utilizing the discrete Gronwall inequality, we arrive at

$$
\begin{aligned}
&\|Q_0 n^M - n_{h,0}^M\|^2 + \Delta t\,\tau\theta\sum_{i=1}^{M}\|D_w(Q_h n^i - n_h^i)\|^2\\
&\qquad\le C\left\{\Delta t^2\int_0^T\|n_{tt}\|^2 dt + h^{2(k+1)}\max_{1\le i\le M}\left(\|n^i\|_{k+2}^2 + \|\varphi^i\|_{k+2}^2\right)\right\}.
\end{aligned}
\tag{4.40}
$$

By Lemma 3.2 and combining (4.40) with (3.18), we obtain

$$
\begin{aligned}
&\|D_w(Q_h\varphi^M - \varphi_h^M)\|^2 + \|Q_h\varphi^M - \varphi_h^M\|^2\\
&\qquad\le C\left\{\Delta t^2\int_0^T\|n_{tt}\|^2 dt + h^{2(k+1)}\max_{1\le i\le M}\left(\|n^i\|_{k+2}^2 + \|\varphi^i\|_{k+2}^2\right)\right\}.
\end{aligned}
\tag{4.41}
$$

By the approximation properties of operators Q_h and R_h, we have the desired estimate (4.34) and (4.35) . The proof of the theorem is complete. □

5. Numerical experiments

In this section, we present the numerical examples to verify our theoretical findings. We utilize backward Euler method and Newton iteration for time discretization and nonlinear terms, respectively. In our numerical experiments, we shall use piecewise uniform meshes which are constructed by equally dividing spatial domain into N subintervals.

Example 1. Let $I = [0, 1]$, $J = [0, T] = [0, 1]$. We consider the following coupled equations

$$
\begin{aligned}
&n_t + ((4\varphi_x + 1)n - 2\varphi_x n^2)_x - ((1 + \varphi_x^2)n_x)_x = g_1,\\
&-\varphi_{xx} + n = \cos x\sin t + \cos t\sin x,
\end{aligned}
$$

Table 1
Error profiles and convergence rates of Example 1.

N	$\frac{\|\varphi_x - D_w\varphi_h\|}{\|\varphi_x\|}$		$\frac{\|\varphi-\varphi_{h,0}\|}{\|\varphi\|}$		$\frac{\|n_x - D_w n_h\|}{\|n_x\|}$		$\frac{\|n-n_{h,0}\|}{\|n\|}$	
	Error	Order	Error	Order	Error	Order	Error	Order
	k = 0							
4	4.5925E−03	–	3.0875E−03	–	8.0026E−03	–	5.8079E−03	–
8	8.2621E−04	2.47	6.9826E−04	2.14	3.9589E−03	1.02	2.7804E−03	1.06
16	1.7915E−04	2.21	1.3496E−04	2.37	3.0966E−03	0.35	1.7594E−03	0.66
32	1.4471E−04	0.31	1.8882E−05	2.84	1.8685E−03	0.73	1.0039E−03	0.81
64	9.3650E−05	0.63	1.0854E−05	0.80	1.0169E−03	0.88	5.3556E−04	0.91
128	5.2483E−05	0.84	8.2263E−06	0.40	5.2934E−04	0.94	2.7644E−04	0.95
256	2.7682E−05	0.92	4.8846E−06	0.75	2.6992E−04	0.97	1.4041E−04	0.98
512	1.4204E−05	0.96	2.6397E−06	0.89	1.3628E−04	0.99	7.0759E−05	0.99
	k = 1							
4	4.6042E−04	–	2.5275E−03	–	4.8305E−03	–	4.6086E−03	–
8	1.1616E−04	1.99	6.3090E−04	2.00	1.2064E−03	2.00	1.1631E−03	1.99
16	2.9113E−05	2.00	1.5766E−04	2.00	3.0149E−04	2.00	2.9145E−04	2.00
32	7.2828E−06	2.00	3.9412E−05	2.00	7.5365E−05	2.00	7.2903E−05	2.00
64	1.8210E−06	2.00	9.8529E−06	2.00	1.8841E−05	2.00	1.8228E−05	2.00

where

$$\begin{aligned} g_1 = &-\sin t \sin x + \cos t \cos x - 8\cos t \cos x \sin t \sin x - 2\cos t \cos x^2 \sin t^2 \sin x \\ &+ 6\cos t^2 \cos x \sin t sinx^2 + \left(1 + \sin t^2 \sin x^2\right) \cos t \sin x. \end{aligned}$$

The exact solutions to this problem are

$$\begin{aligned} n(x,t) &= \cos t \sin x, \quad (x,t) \in I \times J, \\ \varphi(x,t) &= \sin t \cos x, \quad (x,t) \in I \times J. \end{aligned}$$

The errors and corresponding orders of convergence for $k = 0(\Delta t = h)$ and $k = 1(\Delta t = h^2)$ at $T = 1$ are reported in Table 1, where N is the number of elements.

It is observed that the convergence rates of relative errors in a discrete H^1 norm and the standard L^2 norm achieve $k+1$ order of accuracy. This example shows that our WG method is stable and efficient for the problem with smooth solution. In the next example, we show the performance of WG scheme for problem with discontinuous diffusion coefficient.

Example 2 (*Discontinuous Diffusion Coefficient Function*). Consider the following equation system with Dirichlet boundary condition.

$$\begin{aligned} n_t + (\varphi_x n)_x - Dn_{xx} &= \sin t\ x(x-1) + \cos t \sin t\ (1-x)(12x^2 - 9x + 1) + 2D\cos t, \\ -\varphi_{xx} + n &= -\sin t\ (6x - 4) + \cos t\ x(1-x), \end{aligned}$$

where the discontinuous diffusion coefficient function

$$D = \begin{cases} 0.026, & x \in [0, 0.5), \\ 0.1, & x \in [0.5, 1]. \end{cases}$$

The exact solutions are

$$\begin{aligned} n &= \cos t\ x(1-x), \quad (x,t) \in I \times J, \\ \varphi &= \sin t\ x(x-1)^2, \quad (x,t) \in I \times J. \end{aligned}$$

The errors and orders of convergence for $k = 0, 1$ at $T = 1$ are reported in Table 2. Clearly, it is shown that the WG finite element solution exhibits $k+1$ order convergence in the discrete H^1-norm and L^2-norm, which is consistent with Theorem 3.2.

Example 3 (*Convection-dominated Problem*). Consider the following coupled equations with Dirichlet boundary condition. The computation is carried out on the interval $I = [0, 2\pi], J = [0, 1]$.

$$\begin{aligned} n_t + (\varphi_x n)_x - Dn_{xx} &= g_2, \\ -\varphi_{xx} + n &= g_3, \end{aligned}$$

Table 2
Error profiles and convergence rates of the second example.

N	$\frac{\|\varphi_x - D_w\varphi_h\|}{\|\varphi_x\|}$		$\frac{\|\varphi-\varphi_{h,0}\|}{\|\varphi\|}$		$\frac{\|n_x - D_w n_h\|}{\|n_x\|}$		$\frac{\|n-n_{h,0}\|}{\|n\|}$	
	Error	Order	Error	Order	Error	Order	Error	Order
	k = 0							
4	6.0742E−02	–	8.2382E−02	–	1.6170E+00	–	7.7382E−01	–
8	1.3596E−02	2.16	1.8108E−02	2.19	4.1578E−01	1.96	1.9587E−01	1.98
16	3.4955E−03	1.96	3.7313E−03	2.28	1.0101E−01	2.04	4.7370E−02	2.05
32	1.5940E−03	1.13	1.5590E−03	1.26	3.1675E−02	1.67	1.7785E−02	1.41
64	8.8307E−04	0.85	9.5137E−04	0.71	1.3383E−02	1.24	9.1367E−03	0.96
128	4.7479E−04	0.90	5.3762E−04	0.82	6.5494E−03	1.03	4.8441E−03	0.92
256	2.4683E−04	0.94	2.8577E−04	0.91	3.3049E−03	0.99	2.5131E−03	0.95
	k = 1							
4	2.5469E−03	–	5.1535E−02	–	1.5702E−01	–	6.2595E−02	–
8	8.9161E−04	1.51	1.2834E−02	2.01	3.4073E−02	2.20	1.5043E−02	2.06
16	2.4747E−04	1.85	3.2002E−03	2.00	8.4472E−03	2.01	4.0781E−03	1.88
32	6.3615E−05	1.96	7.9941E−04	2.00	2.1163E−03	2.00	1.0458E−03	1.96
64	1.6017E−05	1.99	1.9981E−04	2.00	5.2951E−04	2.00	2.6320E−04	1.99

Table 3
Error profiles and convergence rates of the third example.

N	$\frac{\|\varphi_x - D_w\varphi_h\|}{\|\varphi_x\|}$		$\frac{\|\varphi-\varphi_{h,0}\|}{\|\varphi\|}$		$\frac{\|n_x - D_w n_h\|}{\|n_x\|}$		$\frac{\|n-n_{h,0}\|}{\|n\|}$	
	Error	Order	Error	Order	Error	Order	Error	Order
	k = 0							
40	4.78E−01	–	5.88E−01	–	5.28E+06	–	5.81E−02	–
80	2.43E−01	0.98	3.02E−01	0.96	1.27E+06	2.06	2.86E−02	1.02
160	1.22E−01	0.99	1.53E−01	0.98	3.18E+05	1.99	1.42E−02	1.01
240	8.14E−02	1.00	1.02E−01	0.99	1.44E+05	1.96	9.41E−03	1.01
320	6.11E−02	1.00	7.70E−02	0.99	8.15E+04	1.97	7.04E−03	1.01
360	5.43E−02	1.00	6.85E−02	0.99	6.46E+04	1.97	6.26E−03	1.01
	k = 1							
40	4.66E−01	–	5.93E−01	–	1.01E+05	–	5.84E−02	–
80	1.21E−01	1.94	1.54E−01	1.95	9.97E+04	0.02	1.54E−02	1.93
160	3.06E−02	1.98	3.88E−02	1.99	4.70E+04	1.09	3.90E−03	1.98
240	1.36E−02	1.99	1.73E−02	2.00	2.55E+04	1.51	1.74E−03	1.99
320	7.68E−03	2.00	9.72E−03	2.00	1.58E+04	1.67	9.79E−04	2.00
360	6.07E−03	2.00	7.68E−03	2.00	1.28E+04	1.74	7.74E−04	2.00

where

$$\begin{aligned} g_2 =& - sech\left(\tfrac{1}{2\sqrt{3}}(2x-t)\right)^2\left(\tfrac{1}{15\sqrt{2}} - \tfrac{1}{5\sqrt{2}}tanh\left(\tfrac{1}{2\sqrt{3}}(2x-t)\right)^2\right) \\ &+ sech\left(\tfrac{1}{2\sqrt{3}}(2x-t)\right)\left(\tfrac{D}{3\sqrt{5}} - \tfrac{2D}{3\sqrt{5}}tanh\left(\tfrac{1}{2\sqrt{3}}(2x-t)\right)^2 - \tfrac{1}{2\sqrt{15}}tanh\left(\tfrac{1}{2\sqrt{3}}(2x-t)\right)\right), \\ g_3 =& sech\left(\tfrac{1}{2\sqrt{3}}(2x-t)\right)\left(\tfrac{1}{\sqrt{5}} - \tfrac{1}{3\sqrt{10}} + \tfrac{\sqrt{2}}{3\sqrt{5}}tanh\left(\tfrac{1}{2\sqrt{3}}(2x-t)\right)^2\right), \end{aligned}$$

the diffusion coefficient function $D = 10^{-9}$. The exact solutions are

$$\begin{aligned} n &= \frac{1}{\sqrt{5}}sech\left(\frac{1}{2\sqrt{3}}(2x-t)\right), \\ \varphi &= \frac{-1}{\sqrt{10}}sech\left(\frac{1}{2\sqrt{3}}(2x-t)\right). \end{aligned}$$

From Table 3, we can observe that the WG finite element solutions exhibit the optimal order convergence with $k = 0, 1$ in norm $\frac{\|\varphi_x - D_w\varphi_h\|}{\|\varphi_x\|}$, $\frac{\|\varphi-\varphi_{h,0}\|}{\|\varphi\|}$ and $\frac{\|n-n_{h,0}\|}{\|n\|}$. The relative error $\frac{\|n_x - D_w n_h\|}{\|n_x\|}$ with $k = 1$ achieves a convergence of order $k+1$, which is in great consistency with Theorem 3.2. In addition, Table 3 shows a superconvergence of rate 2 with $k = 0$ in the discrete H^1 norm $\frac{\|n_x - D_w n_h\|}{\|n_x\|}$.

Example 4 (*Semiconductor Device Simulation*). We use the backward difference for the time discretization for this steady state diode test case. We simulate the DD model with a length of 0.6 μm and a doping defined by $n_d = 5\times 10^{17}$ cm^{-3}

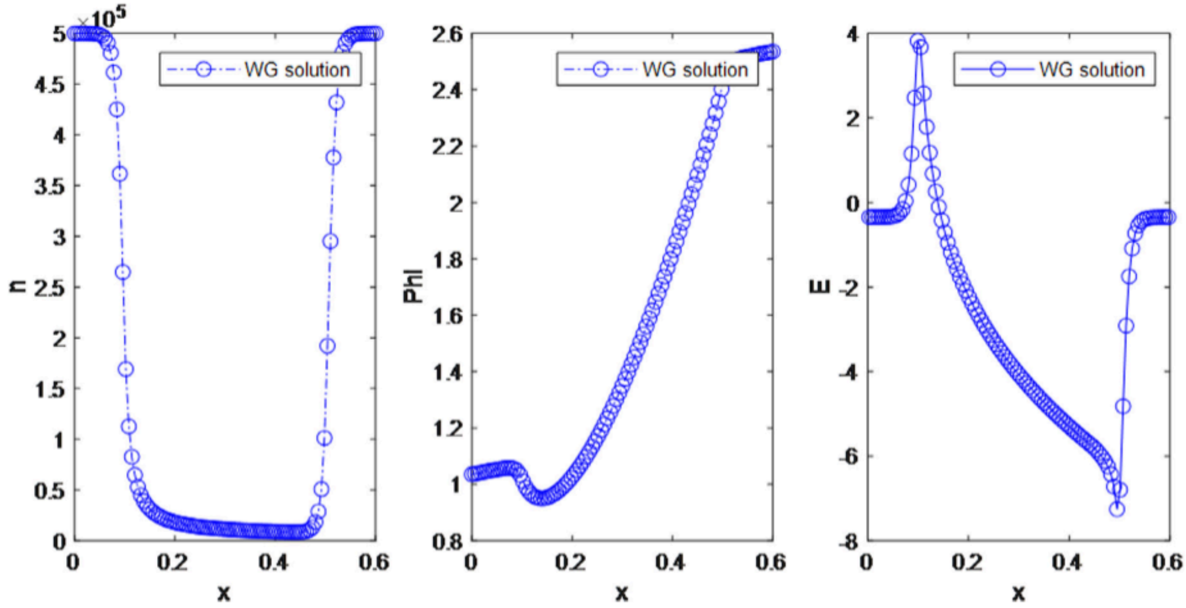

Fig. 1. $[0, 0.6]$ with 100 mesh cells for $k = 0$. Left: density $n(10^{12}\ \text{cm}^{-3})$; middle: electric potential $\phi(V)$; right: electric field $E(V/\mu\text{m})$.

in $[0, 0.1]$ and $[0.5, 0.6]$, and by $n_d = 2 \times 10^{15}\ \text{cm}^{-3}$ in $[0.15, 0.45]$ with a smooth transition in between. The lattice temperature is taken to be $T_0 = 300°$ K. The constants $k = 0.138 \times 10^{-4}$, $\epsilon = 11.7 \times 8.85418$, $e = 0.1602$, $m = 0.26 \times 0.9109 \times 10^{-31}$ kg, and the mobility $\mu = 0.0088 \left(1 + \frac{14.2273}{1+\frac{n_d}{143200}}\right)$. The boundary conditions are given as follows: $\varphi = \varphi_0 = \frac{kT}{e} \ln\left(\frac{n_d}{n_i}\right)$ at the left boundary with $n_i = 1.4 \times 10^{10}\ \text{cm}^{-3}$, $\varphi = \varphi_0 + v_{bias}$ with the voltage drop $v_{bias} = 1.5$ at the right boundary for the potential, $T = 300°$ K at both boundaries for the temperature, and $n = 5 \times 10^{17}\ \text{cm}^{-3}$ at both boundaries for the concentration. The initial condition for electron concentration is $n(x, 0) = n_0(x) = n_d(x)$.

Fig. 1 plots the simulation results of DD model. The WG algorithm works stably and produces numerically convergent results. It is confirmed that our numerical scheme is a reliable tool for the study of suitability of DD model to describe the correct physics.

6. Conclusion

In this work, we propose a weak Galerkin finite element for one-dimensional unsteady drift–diffusion and high-field semiconductor models, in which both the first derivative convection terms and the second derivative diffusion terms exist. When P_k elements are used for primal variables and P_{k+1} for the discrete weak derivative space, we derive the optimal order error estimates in both a discrete H^1 norm and the standard L^2 norm, respectively. Numerical experiments are presented to show the efficacy of the WG finite element method and confirm our theoretical analysis. In addition, our schemes also work well for solving problems with discontinuous diffusion coefficient. The stability analysis and extension of the weak Galerkin method to two dimensions will be considered in future work.

Data availability

Data will be made available on request.

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