SCIENCE CHINA
Mathematics

• ARTICLES •

January 2016 Vol. 59 No. 1: 115–140
doi: 10.1007/s11425-015-5055-8

# Analysis of the local discontinuous Galerkin method for the drift-diffusion model of semiconductor devices

LIU YunXian[1] & SHU Chi-Wang[2,*]

[1] *School of Mathematics, Shandong University, Jinan* 250100*, China;*
[2] *Division of Applied Mathematics, Brown University, Providence, RI* 02912*, USA*
*Email: yxliu@sdu.edu.cn, shu@dam.brown.edu*

Received January 21, 2015; accepted June 5, 2015; published online July 28, 2015

**Abstract** We consider the drift-diffusion (DD) model of one dimensional semiconductor devices, which is a system involving not only first derivative convection terms but also second derivative diffusion terms and a coupled Poisson potential equation. Optimal error estimates are obtained for both the semi-discrete and fully discrete local discontinuous Galerkin (LDG) schemes with smooth solutions. In the fully discrete scheme, we couple the implicit-explicit (IMEX) time discretization with the LDG spatial discretization, in order to allow larger time steps and to save computational cost. The main technical difficulty in the analysis is to treat the inter-element jump terms which arise from the discontinuous nature of the numerical method and the nonlinearity and coupling of the models. A simulation is also performed to validate the analysis.

**Keywords** local discontinuous Galerkin method, semi-discrete, implicit-explicit scheme, error estimate, semiconductor

**MSC(2010)** 65M12, 65M15, 65M60

**Citation:** Liu Y X, Shu C-W. Analysis of the local discontinuous Galerkin method for the drift-diffusion model of semiconductor devices. Sci China Math, 2016, 59: 115–140, doi: 10.1007/s11425-015-5055-8

## 1 Introduction

In a previous work [21], we have analyzed a local discontinuous Galerkin (LDG) finite element method to solve time dependent and steady state moment models for semiconductor device simulations, in which both the first derivative convection terms and second derivative diffusion (heat conduction) terms exist and the convection-diffusion system is discretized by the local discontinuous Galerkin (LDG) method [13, 15], see also [10–12, 14].

In the work [21], we have only used the LDG method to discretize the electron concentration equation. For the electric potential equation, we still used the continuous methods to avoid having discontinuities of two independent solution variables on cell boundaries, which is difficult to analyze. Also, we only obtained the suboptimal error estimates $O(h^{k+\frac{1}{2}})$ when $P^k$ elements (piecewise polynomials of degree $k$) are used in the LDG scheme because of the nonlinear coupling of the electron concentration and the electric field.

In this paper, we will give error estimates of the semi-discrete LDG scheme and implicit-explicit (IMEX) time discretization coupled with the LDG scheme (see [27,28]) for smooth solutions. Unlike in [21], in this paper the potential equation is also discretized by the LDG method. This unified discretization by using the LDG method allows the full realization of the potential of this methodology in easy $h$-$p$ adaptivity

*Corresponding author

 

and parallel efficiency. The numerical results shown in [19, 20] already demonstrated good performance of such unified LDG discretization for the moment models, comparable with the results obtained by the ENO finite difference method [16]. However, as far as we know, an error estimate for such unified methods has not been available until now. In the fully discrete scheme, we couple the LDG scheme with the IMEX Runge-Kutta time discretization up to third order accuracy. We treat the nonlinear coupled term explicitly and the diffusion term implicitly. With this treatment, we show that the IMEX LDG schemes are unconditionally convergent, in the sense that the time step $\Delta t$ does not need to be related to the spatial mesh size $h$ when both of them go to zero, even though the nonlinear coupled term is treated explicitly. This greatly improves the computational efficiency of the scheme by allowing us to use larger time steps.

We now briefly review the background of the LDG methods. The LDG methods have several attractive properties [31]. They can be easily designed for any order of accuracy. In fact, the order of accuracy can be locally determined in each cell, which allows for efficient $p$ adaptivity. They can be used on arbitrary triangulations, even those with hanging nodes, which allows for efficient $h$ adaptivity. The methods have excellent parallel efficiency, since they are extremely local in the sense that each cell needs to communicate only with its immediate neighbors, regardless of the order of accuracy. Also, the methods have excellent provable nonlinear stability.

For the DG method solving smooth solutions of linear conservation laws, optimal a priori error estimates $O(h^{k+1})$ for tensor product and certain other special meshes, and $O(h^{k+\frac{1}{2}})$ for other cases, have been given in [9, 17, 18, 23, 24]. The first a priori error estimate for the LDG method of linear convection-diffusion equations was obtained by Cockburn and Shu [13]. Later, Castillo et al. [4–6] proved the optimal rate of convergence order $O(h^{k+1})$ for the LDG method with a particular numerical flux. Rivière and Wheeler [25] gave an optimal error estimate for the methods applied to nonlinear convection-diffusion equations for at least quadratic polynomials. Zhang and Shu [22, 32–34] presented a priori error estimates for the fully discrete Runge-Kutta DG methods with smooth solutions for scalar nonlinear conservation laws and for symmetrizable systems, see also Burman et al. [3]. Xu and Shu [30] provided $L^2$ error estimates for the semi-discrete local discontinuous Galerkin methods for nonlinear convection-diffusion equations and KdV equations with smooth solutions. Wang et al. [27, 28] obtained optimal error estimates of the LDG methods with IMEX time marching for linear and nonlinear convection-diffusion problems.

Although there have been many theoretical analysis of the LDG method, such analysis for semiconductor device moment models which involve a coupling to a Poisson potential equation, by a unified LDG method to both the concentration equation and the potential equation, still seems to be unavailable. The main difficulty is how to treat the inter-element discontinuities of two independent solution variables (one from the concentration equation and the other from the potential equation) on cell boundaries. Notice that, in an LDG method, the solution and its spatial gradient are approximated by two independent polynomials. Through exploring an important relationship between the gradient and interface jump of the numerical solution polynomial with the independent polynomial numerical solution for the gradient in the LDG methods, which is stated in Lemma 4.3, we obtain in this paper optimal error estimates for both the semi-discrete LDG scheme and the IMEX LDG scheme.

The organization of the paper is as follows. In Section 2, we list some preliminaries. In Section 3, we describe the drift-diffusion (DD) model and give its weak form. The semi-discrete LDG scheme for the DD model with periodic boundary condition and its error estimate are given in Section 4. Section 5 contains several IMEX LDG schemes for the DD model with periodic boundary condition and their error estimates. In Section 6, we obtain the error estimates of the LDG scheme for the DD model with Dirichlet boundary conditions. Simulation results are presented in Section 7. Concluding remarks and a plan for future work are given in Section 8.

## 2 Preliminaries

In this section, we introduce some notations and definitions to be used later in the paper and also present some auxiliary results.

First, we will give some basic notations of the finite element space. Then we define some projections and present certain projection and inverse properties for the finite element spaces that will be used in the error analysis.

## 2.1 Basic notation

Let $I_j = (x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}})$, $j = 1, 2, \dots, N$ be a partition of the computational domain $I$,

$$\Delta x_j = x_{j+\frac{1}{2}} - x_{j-\frac{1}{2}}, \quad x_j = \frac{1}{2}(x_{j-\frac{1}{2}} + x_{j+\frac{1}{2}}), \quad h = \max\Big\{\sup_j \Delta x_j\Big\}.$$

The finite-dimensional computational space is $V_h^k = \{z : z|_{I_j} \in P^k(I_j)\}$ where $P^k(I_j)$ denotes the set of polynomials of degree up to $k$ defined on $I_j$. Both the numerical solution and the test functions will come from this space $V_h^k$.

Note that in $V_h^k$, the functions are allowed to have jumps at the interfaces $x_{j+1/2}$, hence $V_h^k \not\subseteq H^1$. This is one of the main differences between the discontinuous Galerkin method and most other finite element methods. Moreover, both the mesh sizes $\Delta x_j$ and the degree of polynomials $k$ can be changed from element to element freely, thus allowing for easy $h$-$p$ adaptivity.

We denote $(u_h)^+_{j+\frac{1}{2}} = u_h(x^+_{j+\frac{1}{2}})$ and $(u_h)^-_{j+\frac{1}{2}} = u_h(x^-_{j+\frac{1}{2}})$ , respectively. We use the usual notation $[u_h]_{j+\frac{1}{2}} = (u_h)^+_{j+\frac{1}{2}} - (u_h)^-_{j+\frac{1}{2}}$ and $(\bar{u}_h)_{j+\frac{1}{2}} = \frac{1}{2}((u_h)^+_{j+\frac{1}{2}} + (u_h)^-_{j+\frac{1}{2}})$ to denote the jump and the mean of the function $u_h$ at each element boundary point, respectively.

We will denote by $C$ a generic positive constant independent of $h$, which may depend on the exact solution of the partial differential equations (PDEs) considered in this paper. We also denote by $\tilde{\varepsilon}$ a generic small positive constant. $C$ and $\tilde{\varepsilon}$ may take a different value in each occurrence. For problems considered in this paper, the exact solution is assumed to be smooth. Also, $0 \leqslant t \leqslant T$ for a fixed $T$. Therefore, the exact solution is always bounded.

## 2.2 Projection properties

In what follows, we will consider the standard $L^2$-projection of a function $u$ with $k+1$ continuous derivatives into space $V_h^k$, denoted by $\mathcal{P}$, i.e., for each $j$,

$$\int_{I_j} (\mathcal{P}u(x) - u(x))v(x)dx = 0, \quad \forall\, v \in P^k(I_j), \tag{2.1}$$

and the special projections $\mathcal{P}^\pm$ into $V_h^k$ which satisfy, for each $j$,

$$\begin{aligned}
&\int_{I_j} (\mathcal{P}^+u(x) - u(x))v(x)dx = 0, \quad \forall\, v \in P^{k-1}(I_j), \quad \text{and} \quad \mathcal{P}^+u(x^+_{j-\frac{1}{2}}) = u(x_{j-\frac{1}{2}}),\\
&\int_{I_j} (\mathcal{P}^-u(x) - u(x))v(x)dx = 0, \quad \forall\, v \in P^{k-1}(I_j), \quad \text{and} \quad \mathcal{P}^-u(x^-_{j+\frac{1}{2}}) = u(x_{j+\frac{1}{2}}).
\end{aligned} \tag{2.2}$$

From the projections mentioned above, it is easy to get (see [8])

$$\|\eta\| + h\|\eta\|_{0,\infty} + h^{\frac{1}{2}}\|\eta\|_{\Gamma_h} + |\eta(x_0)| \leqslant Ch^{k+1}, \tag{2.3}$$

where $\eta = \mathcal{P}u - u$ or $\eta = \mathcal{P}^\pm u - u$, $\|\cdot\|$ refers to the usual $L^2$ norm, $\|\cdot\|_{0,\infty}$ refers to the $L^\infty$ norm, $\|\eta\|_{\Gamma_h} = [\sum_{j=1}^N ((\eta^+_{j+\frac{1}{2}})^2 + (\eta^-_{j+\frac{1}{2}})^2)]^{\frac{1}{2}}$, and $x_0$ is a fixed point in the computational domain $I$ (e.g. one of the boundary points). The positive constant $C$, solely depending on $u$ and its derivatives, is independent of $h$. $\Gamma_h$ denotes the set of boundary points of all elements $I_j$.

### 2.3 Inverse properties

Finally, we list some inverse properties (see [8]) of the finite element space $V_h^k$ that will be used in our error analysis. For any $v \in V_h^k$, there exists positive constants $C_i$ independent of $v$ and $h$, such that

$$\text{(i)}\ \ \|v_x\| \leqslant C_1 h^{-1}\|v\|, \quad \text{(ii)}\ \ \|v\|_{\Gamma_h} \leqslant C_2 h^{-\frac{1}{2}}\|v\|, \quad \text{(iii)}\ \ \|v\|_{0,\infty} \leqslant C_3 h^{-\frac{d}{2}}\|v\|, \tag{2.4}$$

where $d$ is the spatial dimension. In our case $d = 1$.

## 3 The drift-diffusion (DD) model and the weak form

### 3.1 The DD model

The drift-diffusion model is described by the following equation (we refer to [7] and the reference therein for more details)

$$n_t - (\mu E n)_x = \tau\theta n_{xx}, \tag{3.1}$$

$$\phi_{xx} = \frac{e}{\varepsilon}(n - n_d), \tag{3.2}$$

where $x \in (0,1)$, with periodic boundary condition for the first equation and Dirichlet boundary condition for the potential equation: $\phi(0,t) = 0$, $\phi(1,t) = v_{\text{bias}}$. We will also consider Dirichlet boundary condition for the first equation in Section 6. The Poisson equation (3.2) is the electric potential equation, $E = -\phi_x$ represents the electric field.

In the system (3.1)–(3.2), the unknown variables are the electron concentration $n$ and the electric potential $\phi$. $m_0$ is the electron effective mass, $k$ is the Boltzmann constant, $e$ is the electron charge, $\mu$ is the mobility, $T_0$ is the lattice temperature, $\tau = \frac{m_0\mu}{e}$ is the relaxation parameter, $\theta = \frac{k}{m_0}T_0$, $\varepsilon$ is the dielectric permittivity, and $n_d$ is the doping which is a given function.

### 3.2 Weak form

The starting point of the LDG method is the introduction of an auxiliary variable to rewrite the PDE (3.1) containing higher order spatial derivatives as a larger system containing only first order spatial derivatives.

Let $q = \sqrt{\tau\theta}\, n_x$, thus (3.1) is rewritten as

$$n_t - (\mu E n)_x - \sqrt{\tau\theta}\, q_x = 0, \tag{3.3}$$

$$q - \sqrt{\tau\theta}\, n_x = 0, \tag{3.4}$$

$$E_x = -\frac{e}{\varepsilon}(n - n_d), \tag{3.5}$$

$$E = -\phi_x. \tag{3.6}$$

We multiply equations (3.3)–(3.6) by test functions $v, w, r, z \in V_h^k$, respectively, and formally integrate by parts for all terms involving a spatial derivative to get

$$\int_{I_j} n_t v dx + \int_{I_j} (\mu E n + \sqrt{\tau\theta} q) v_x dx - (\mu E n + \sqrt{\tau\theta} q)_{j+\frac{1}{2}} v^-_{j+\frac{1}{2}} + (\mu E n + \sqrt{\tau\theta} q)_{j-\frac{1}{2}} v^+_{j-\frac{1}{2}} = 0, \tag{3.7}$$

$$\int_{I_j} q w dx + \int_{I_j} \sqrt{\tau\theta} n w_x dx - \sqrt{\tau\theta} n_{j+\frac{1}{2}} w^-_{j+\frac{1}{2}} + \sqrt{\tau\theta} n_{j-\frac{1}{2}} w^+_{j-\frac{1}{2}} = 0, \tag{3.8}$$

$$-\int_{I_j} E r_x dx + E_{j+\frac{1}{2}} r^-_{j+\frac{1}{2}} - E_{j-\frac{1}{2}} r^+_{j-\frac{1}{2}} = -\frac{e}{\varepsilon}\int_{I_j} (n - n_d) r dx, \tag{3.9}$$

$$\int_{I_j} E z dx - \int_{I_j} \phi z_x dx + \phi_{j+\frac{1}{2}} z^-_{j+\frac{1}{2}} - \phi_{j-\frac{1}{2}} z^+_{j-\frac{1}{2}} = 0, \tag{3.10}$$

where $j = 1, \ldots, N$ and $v, w, r, z$ in $V_h^k$.

# 4 Semi-discrete LDG scheme and its error estimate

## 4.1 Semi-discrete LDG scheme

Replacing the exact solutions $n$, $q$, $E$ and $\phi$ in the above equations by their numerical approximations $n_h$, $q_h$, $E_h$, $\phi_h$ in $V_h^k$, noticing that the numerical solutions $n_h$, $q_h$, $E_h$ and $\phi_h$ are not continuous on the cell boundaries, then replacing terms on the cell boundaries by suitable numerical fluxes, we obtain the semi-discrete LDG scheme: For any $t>0$, find the numerical solution $n_h, q_h, E_h, \phi_h \in V_h^k$, such that

$$\begin{aligned}&\int_{I_j}(n_h)_t v dx + \int_{I_j}(\mu E_h n_h + \sqrt{\tau\theta} q_h) v_x dx \\ &\quad -(\mu\widehat{E_h n_h} + \sqrt{\tau\theta}\hat{q}_h)_{j+\frac{1}{2}} v^-_{j+\frac{1}{2}} + (\mu\widehat{E_h n_h} + \sqrt{\tau\theta}\hat{q}_h)_{j-\frac{1}{2}} v^+_{j-\frac{1}{2}} = 0, \end{aligned} \tag{4.1}$$

$$\int_{I_j} q_h w dx + \int_{I_j}\sqrt{\tau\theta} n_h w_x dx - \sqrt{\tau\theta}(\hat{n}_h)_{j+\frac{1}{2}} w^-_{j+\frac{1}{2}} + \sqrt{\tau\theta}(\hat{n}_h)_{j-\frac{1}{2}} w^+_{j-\frac{1}{2}} = 0, \tag{4.2}$$

$$-\int_{I_j} E_h r_x dx + (\hat{E}_h)_{j+\frac{1}{2}} r^-_{j+\frac{1}{2}} - (\hat{E}_h)_{j-\frac{1}{2}} r^+_{j-\frac{1}{2}} = -\frac{e}{\varepsilon}\int_{I_j}(n_h - n_d) r dx, \tag{4.3}$$

$$\int_{I_j} E_h z dx - \int_{I_j}\phi_h z_x dx + (\hat{\phi}_h)_{j+\frac{1}{2}} z^-_{j+\frac{1}{2}} - (\hat{\phi}_h)_{j-\frac{1}{2}} z^+_{j-\frac{1}{2}} = 0, \tag{4.4}$$

where $j = 1, \dots, N$ and $v, w, r, z$ in $V_h^k$.

The "hat" terms are the numerical fluxes. We choose the flux $\widehat{E_h n_h} = \frac{1}{2}((E_h n_h)^+ + (E_h n_h)^-)$ (we can also choose an upwind flux here, the analysis in later section can go through as well), the alternating flux for $\hat{n}_h$ and $\hat{q}_h$, i.e.,

$$\hat{n}_h = (n_h)^+, \quad \hat{q}_h = (q_h)^- \quad \text{or} \quad \hat{n}_h = (n_h)^-, \quad \hat{q}_h = (q_h)^+, \tag{4.5}$$

and the alternating flux for $\hat{\phi}_h$ and $\hat{E}_h$, with an adjustment at one of the boundaries to take care of the Dirichlet boundary condition, namely

$$\begin{aligned}&(\hat{\phi}_h)_{\frac{1}{2}} = (\phi_h^-)_{\frac{1}{2}} = 0, \quad (\hat{\phi}_h)_{j-\frac{1}{2}} = (\phi_h^+)_{j-\frac{1}{2}}, \quad j = 2, \dots, N, \quad (\hat{\phi}_h)_{N+\frac{1}{2}} = (\phi_h^+)_{N+\frac{1}{2}} = v_{\text{bias}}, \\ &(\hat{E}_h)_{\frac{1}{2}} = (E_h^+)_{\frac{1}{2}} + c_0[\phi]_{\frac{1}{2}}, \quad (\hat{E}_h)_{j-\frac{1}{2}} = (E_h^-)_{j-\frac{1}{2}} + c_0[\phi]_{j-\frac{1}{2}}, \quad j = 2, \dots, N+1,\end{aligned} \tag{4.6}$$

or

$$\begin{aligned}&(\hat{\phi}_h)_{\frac{1}{2}} = (\phi_h^-)_{\frac{1}{2}} = 0, \quad (\hat{\phi}_h)_{j-\frac{1}{2}} = (\phi_h^-)_{j-\frac{1}{2}}, \quad j = 2, \dots, N, \quad (\hat{\phi}_h)_{N+\frac{1}{2}} = (\phi_h^+)_{N+\frac{1}{2}} = v_{\text{bias}}, \\ &(\hat{E}_h)_{j-\frac{1}{2}} = (E_h^+)_{j-\frac{1}{2}} + c_0[\phi]_{j-\frac{1}{2}}, \quad j = 1, \dots, N, \quad (\hat{E}_h)_{N+\frac{1}{2}} = (E_h^-)_{N+\frac{1}{2}} + c_0[\phi]_{N+\frac{1}{2}},\end{aligned} \tag{4.7}$$

where $c_0 > 0$ is an arbitrary positive constant. We take $c_0 = 1$ in our numerical experiments.

Notice that the auxiliary variable $q_h$ or $E_h$ can be locally solved from (4.2) or (4.4) and substituted into (4.1) or (4.3). This is the reason the method is called the "local" discontinuous Galerkin method and this also distinguishes LDG from the classical mixed finite element methods, where the auxiliary variable $q_h$ or $E_h$ must be solved from a global system.

## 4.2 Error estimate

We denote $\|u\|_{L^\infty(0,T;L^2)} = \max_{0\leqslant t\leqslant T}\|u\|_{L^2(I)}$, and $\|u\|_{L^2(0,T;L^2)} = (\int_0^T \|u\|^2_{L^2(I)} dt)^{\frac{1}{2}}$ in the following analysis of the semi-discrete scheme.

**Theorem 4.1.** *Let $n, q$ be the exact solution to* (3.7)–(3.10)*, which is sufficiently smooth with bounded derivatives. Let $n_h, q_h$ be the numerical solution to the semi-discrete LDG scheme* (4.1)–(4.4)*. Denote the corresponding numerical error by $e_u = u - u_h$ $(u = n, q)$. If the finite element space $V_h^k$ is the piecewise polynomials of degree $k \geqslant 0$, then for small enough $h$ there holds the following error estimates*:

$$\|n - n_h\|_{L^\infty(0,T;L^2)} + \|q - q_h\|_{L^2(0,T;L^2)} \leqslant Ch^{k+1}, \tag{4.8}$$

*where the constant $C$ depends on the final time $T$, $k$, $C_\mu$ (see Lemma 4.3), the inverse constant $C_2$, $\|n\|_{L^\infty(0,T;H^{k+1})}$, $\|n_x\|_{L^\infty}$ and $\|E\|_{L^\infty}$.*

Before the proof of the theorem, we give two lemmas first.

**Lemma 4.2.** *Let $E$ be the exact solution of the problem to (3.9)–(3.10), and $E_h$ be the numerical solution to the semi-discrete LDG scheme (4.3)–(4.4). We have*

$$\|E - E_h\| \leqslant C(h^{k+1} + \|n - n_h\|). \tag{4.9}$$

For a detailed proof of this lemma for the case of periodic boundary condition, we refer to [2]. For our case with Dirichlet boundary condition for $\phi$, the result can be proved along a similar line and is hence omitted.

We recall that we have taken the alternating fluxes for $\hat{n}_h$ and $\hat{q}_h$, that is, $\hat{n}_h = (n_h)^+$, $\hat{q}_h = (q_h)^-$. We write the error $e_u = u - u_h$ $(u = n, q)$ as $e_u = \xi_u - \eta_u$, where $\xi_n = \mathcal{P}^+ n - n_h$, $\eta_n = \mathcal{P}^+ n - n$; $\xi_q = \mathcal{P}^- q - q_h$, $\eta_q = \mathcal{P}^- q - q$. Then we state the second lemma:

**Lemma 4.3.**

$$\|\xi_{n,x}\| \leqslant \frac{C_\mu}{\sqrt{\tau\theta}}(\|\xi_q\| + \|\eta_q\|), \tag{4.10}$$

$$|\sqrt{h^{-1}}[\xi_n]| \leqslant \frac{C_\mu}{\sqrt{\tau\theta}}(\|\xi_q\| + \|\eta_q\|). \tag{4.11}$$

For a detailed proof of this lemma we refer to [27].

*Proof.* Taking the difference of (3.7) and (4.1) and the difference of (3.8) and (4.2), we have the following error equations:

$$\begin{aligned}
&\int_{I_j} (n - n_h)_t v dx + \int_{I_j} \mu(En - E_h n_h) v_x dx \\
&\quad - \mu(En - \widehat{E_h n_h})_{j+\frac{1}{2}} v^-_{j+\frac{1}{2}} + \mu(En - \widehat{E_h n_h})_{j-\frac{1}{2}} v^+_{j-\frac{1}{2}} \\
&\quad + \int_{I_j} \sqrt{\tau\theta}(q - q_h) v_x dx - \sqrt{\tau\theta}(q - \hat{q}_h)_{j+\frac{1}{2}} v^-_{j+\frac{1}{2}} + \sqrt{\tau\theta}(q - \hat{q}_h)_{j-\frac{1}{2}} v^+_{j-\frac{1}{2}} = 0, \qquad (4.12)\\
&\int_{I_j} (q - q_h) w dx + \int_{I_j} \sqrt{\tau\theta}(n - n_h) w_x dx \\
&\quad - \sqrt{\tau\theta}(n - \hat{n}_h)_{j+1/2} w^-_{j+\frac{1}{2}} + \sqrt{\tau\theta}(n - \hat{n}_h)_{j-1/2} w^+_{j-\frac{1}{2}} = 0. \qquad (4.13)
\end{aligned}$$

If we choose $v = \xi_n$, $w = \xi_q$ in the error equations (4.12)–(4.13), we have

$$\begin{aligned}
&\int_{I_j} (\xi_n - \eta_n)_t \xi_n dx + \int_{I_j} \mu(En - E_h n_h) \xi_{n,x} dx \\
&\quad - \mu(En - \widehat{E_h n_h})_{j+\frac{1}{2}} \xi^-_{n,j+\frac{1}{2}} + \mu(En - \widehat{E_h n_h})_{j-\frac{1}{2}} \xi^+_{n,j-\frac{1}{2}} \\
&\quad + \int_{I_j} \sqrt{\tau\theta}(\xi_q - \eta_q) \xi_{n,x} dx - \sqrt{\tau\theta}(\xi_q - \eta_q)^-_{j+\frac{1}{2}} \xi^-_{n,j+\frac{1}{2}} + \sqrt{\tau\theta}(\xi_q - \eta_q)^-_{j-\frac{1}{2}} \xi^+_{n,j-\frac{1}{2}} = 0, \qquad (4.14)
\end{aligned}$$

and

$$\begin{aligned}
&\int_{I_j} (\xi_q - \eta_q) \xi_q dx + \int_{I_j} \sqrt{\tau\theta}(\xi_n - \eta_n) \xi_{q,x} dx \\
&\quad - \sqrt{\tau\theta}(\xi_n - \eta_n)^+_{j+\frac{1}{2}} \xi^-_{q,j+\frac{1}{2}} + \sqrt{\tau\theta}(\xi_n - \eta_n)^+_{j-\frac{1}{2}} \xi^+_{q,j-\frac{1}{2}} = 0. \qquad (4.15)
\end{aligned}$$

Summing the above two equations, and summing over $j$, we have

$$\sum_{j=1}^{N} \int_{I_j} \xi_{n,t} \xi_n dx + \sum_{j=1}^{N} \int_{I_j} \xi_q^2 dx$$

$$
\begin{aligned}
&= \sum_{j=1}^{N} \int_{I_j} \eta_{n,t}\xi_n dx + \sum_{j=1}^{N} \int_{I_j} \eta_q \xi_q dx \\
&\quad + \sum_{j=1}^{N} \bigg( \int_{I_j} \sqrt{\tau\theta}\eta_q \xi_{n,x} dx + \int_{I_j} \sqrt{\tau\theta}\eta_n \xi_{q,x} dx - \sqrt{\tau\theta}\eta^-_{q,j+\frac12}\xi^-_{n,j+\frac12} \\
&\quad + \sqrt{\tau\theta}\eta^-_{q,j-\frac12}\xi^+_{n,j-\frac12} - \sqrt{\tau\theta}\eta^+_{n,j+\frac12}\xi^-_{q,j+\frac12} + \sqrt{\tau\theta}\eta^+_{n,j-\frac12}\xi^+_{q,j-\frac12} \bigg) \\
&\quad + \sum_{j=1}^{N} \bigg( - \int_{I_j} \sqrt{\tau\theta}\xi_q \xi_{n,x} dx - \int_{I_j} \sqrt{\tau\theta}\xi_n \xi_{q,x} dx + \sqrt{\tau\theta}\xi^-_{q,j+\frac12}\xi^-_{n,j+\frac12} \\
&\quad - \sqrt{\tau\theta}\xi^-_{q,j-\frac12}\xi^+_{n,j-\frac12} + \sqrt{\tau\theta}\xi^+_{n,j+\frac12}\xi^-_{q,j+\frac12} - \sqrt{\tau\theta}\xi^+_{n,j-\frac12}\xi^+_{q,j-\frac12} \bigg) \\
&\quad + \sum_{j=1}^{N} \bigg( - \int_{I_j} \mu(En - E^h n^h)\xi_{n,x} dx + \mu(En - \widehat{E^h n^h})_{j+\frac12}\xi^-_{n,j+\frac12} \\
&\quad - \mu(En - \widehat{E^h n^h})_{j-\frac12}\xi^+_{n,j-\frac12} \bigg) \\
&=: T_1 + T_2 + T_3 + T_4 + T_5.
\end{aligned} \tag{4.16}
$$

Next, we estimate $T_i$ term by term. From the property (2.3) of the projection and the Schwartz inequality, we can get

$$
T_1 = \sum_{j=1}^{N} \int_{I_j} \eta_{n,t}\xi_n dx \leqslant C \int_I \eta^2_{n,t} dx + C \int_I \xi^2_n dx \leqslant Ch^{2k+2} + C\|\xi_n\|^2, \tag{4.17}
$$

$$
T_2 = \sum_{j=1}^{N} \int_{I_j} \eta_q \xi_q dx \leqslant C \int_I \eta^2_q dx + \tilde{\varepsilon} \int_I \xi^2_q dx \leqslant Ch^{2k+2} + \tilde{\varepsilon}\|\xi_q\|^2. \tag{4.18}
$$

Obviously, from the projection (2.2), we have

$$
\int_{I_j} \eta_n v dx = 0, \quad \int_{I_j} \eta_q v dx = 0, \quad \forall\, v \in P^{k-1}(I_j),
$$

and $\eta^-_{q,j+\frac12} = 0$, $\eta^+_{n,j+\frac12} = 0$, then we get

$$
T_3 = 0. \tag{4.19}
$$

We also have

$$
\begin{aligned}
T_4 &= \sum_{j=1}^{N} \bigg( - \int_{I_j} \sqrt{\tau\theta}(\xi_q\xi_n)_x dx + \sqrt{\tau\theta}\xi^-_{q,j+\frac12}\xi^-_{n,j+\frac12} \\
&\quad - \sqrt{\tau\theta}\xi^-_{q,j-\frac12}\xi^+_{n,j-\frac12} + \sqrt{\tau\theta}\xi^+_{n,j+\frac12}\xi^-_{q,j+\frac12} - \sqrt{\tau\theta}\xi^+_{n,j-\frac12}\xi^+_{q,j-\frac12} \bigg) \\
&= \sum_{j=1}^{N} (\sqrt{\tau\theta}(\xi_q\xi_n)^+_{j-\frac12} - \sqrt{\tau\theta}(\xi_q\xi_n)^-_{j+\frac12} + \sqrt{\tau\theta}\xi^-_{q,j+\frac12}\xi^-_{n,j+\frac12} \\
&\quad - \sqrt{\tau\theta}\xi^-_{q,j-\frac12}\xi^+_{n,j-\frac12} + \sqrt{\tau\theta}\xi^+_{n,j+\frac12}\xi^-_{q,j+\frac12} - \sqrt{\tau\theta}\xi^+_{n,j-\frac12}\xi^+_{q,j-\frac12}) \\
&= \sum_{j=1}^{N} \sqrt{\tau\theta}(\xi^+_{n,j+1/2}\xi^-_{q,j+1/2} - \xi^+_{n,j-1/2}\xi^-_{q,j-1/2}) \\
&= 0.
\end{aligned} \tag{4.20}
$$

The above estimate of $T_4$ used the periodic boundary condition for $n$, $n_h$, $q$ and $q_h$. About the last term $T_5$ of (4.16), since we have chosen $\widehat{E_h n_h} = \frac{1}{2}((E_h n_h)^+ + (E_h n_h)^-)$, we have

$$T_5 = -\int_I \mu(En - E_h n_h)\xi_{n,x} dx - \sum_{j=1}^{N} \mu\left(En - \frac{1}{2}((E_h n_h)^+ + (E_h n_h)^-)\right)_{j-\frac{1}{2}} [\xi_n]_{j-1/2} \tag{4.21}$$

For the integral part of $T_5$, we treat it as following:

$$-\int_I \mu(En - E_h n_h)\xi_{n,x} dx = -\int_I \mu E(n - n_h)\xi_{n,x} dx - \int_I \mu(E - E_h) n_h \xi_{n,x} dx.$$

For the time being, we make the a-priori assumption

$$\|n - n_h\| \leqslant \tilde{C} h. \tag{4.22}$$

We will verify the reasonableness of this a-priori assumption later. The a-priori assumption implies that $\|n_h\|_{L^\infty} \leqslant C$. With Young's inequality, (2.3), and Lemma 4.2, we have

$$\int_I \mu(En - E_h n_h)\xi_{n,x} dx \leqslant C\|\xi_n\|^2 + Ch^{2k+2} + \tilde{\varepsilon}\|\xi_{n,x}\|^2. \tag{4.23}$$

For the boundary part of $T_5$, we have

$$\begin{aligned}
&-\sum_{j=1}^{N} \mu\left(En - \frac{1}{2}((E_h n_h)^+ + (E_h n_h)^-)\right)_{j-\frac{1}{2}} [\xi_n]_{j-1/2} \\
&\quad = -\sum_{j=1}^{N} \mu\left(\frac{1}{2}E(n - (n_h)^+) + \frac{1}{2}(E - (E_h)^+)(n_h)^+\right. \\
&\qquad \left. + \frac{1}{2}E(n - (n_h)^-) + \frac{1}{2}(E - (E_h)^-)(n_h)^-\right)_{j-\frac{1}{2}} [\xi_n]_{j-1/2} \\
&\quad = -\frac{1}{2}\sum_{j=1}^{N} \mu E_{j-\frac{1}{2}} (\xi_n^+ + \xi_n^- - \eta_n^+ - \eta_n^-)_{j-\frac{1}{2}} [\xi_n]_{j-1/2} \\
&\qquad - \frac{1}{2}\sum_{j=1}^{N} \mu(E - (E_h)^+)_{j-\frac{1}{2}} (n_h)^+_{j-\frac{1}{2}} [\xi_n]_{j-1/2} \\
&\qquad - \frac{1}{2}\sum_{j=1}^{N} \mu(E - (E_h)^-)_{j-\frac{1}{2}} (n_h)^-_{j-\frac{1}{2}} [\xi_n]_{j-1/2}.
\end{aligned}$$

Using Young's inequality and $\|n_h\|_{L^\infty} \leqslant C$, we get

$$\begin{aligned}
&-\sum_{j=1}^{N} \mu\left(En - \frac{1}{2}((E_h n_h)^+ + (E_h n_h)^-)\right)_{j-\frac{1}{2}} [\xi_n]_{j-1/2} \\
&\qquad \leqslant Ch(\|\xi_n\|_\Gamma^2 + \|\eta_n\|_\Gamma^2 + \|E - E_h\|_\Gamma^2) + \tilde{\varepsilon} h^{-1} [\xi_n]^2.
\end{aligned}$$

Then from the inverse inequality (2.4), together with (4.9), we can obtain

$$-\sum_{j=1}^{N} \mu\left(En - \frac{1}{2}((E_h n_h)^+ + (E_h n_h)^-)\right)_{j-\frac{1}{2}} [\xi_n]_{j-1/2} \leqslant C(h^{2k+2} + \|\xi_n\|^2) + \tilde{\varepsilon} h^{-1} [\xi_n]^2. \tag{4.24}$$

Substituting (4.23) and (4.24) into (4.21), we have

$$T_5 \leqslant C\|\xi_n\|^2 + Ch^{2k+2} + \tilde{\varepsilon}\|\xi_{n,x}\|^2 + \tilde{\varepsilon} h^{-1} [\xi_n]^2. \tag{4.25}$$

Then substituting (4.17)–(4.20) and (4.25) into (4.16), we get

$$\frac{1}{2}\frac{d}{dt}\|\xi_n\|^2 + \|\xi_q\|^2 \leqslant C\|\xi_n\|^2 + Ch^{2k+2} + \tilde{\varepsilon}\|\xi_{n,x}\|^2 + \tilde{\varepsilon}h^{-1}[\xi_n]^2 + \tilde{\varepsilon}\|\xi_q\|^2. \tag{4.26}$$

Using Lemma 4.3, together with the property of the projection and Gronwall's inequality, we can obtain the theorem.

To complete the proof, let us verify the reasonableness of the a-priori assumption (4.22). For $k \geqslant 0$, we can consider $h$ small enough so that $Ch^{k+1} \leqslant \frac{1}{2}\tilde{C}h$, where $C$ is the constant in (4.8) determined by the final time $T$. Then if $t^* = \sup\{t : \|n(t) - n_h(t)\| \leqslant \tilde{C}h\}$, we should have $\|n(t^*) - n_h(t^*)\| = \tilde{C}h$ by continuity if $t^*$ is finite. On the other hand, our proof implies that (4.8) holds for $t \leqslant t^*$, in particular $\|n(t^*) - n_h(t^*)\| \leqslant Ch^{k+1} \leqslant \frac{1}{2}\tilde{C}h$. This is a contradiction if $t^* < T$. Hence $t^* \geqslant T$ and the assumption (4.22) is then valid. □

## 5 IMEX Runge-Kutta fully discrete LDG schemes and their error estimates

In this section, we would like to consider the LDG spatial discretization coupled with three specific IMEX Runge-Kutta schemes up to third order which are presented in [1, 27]. The idea is to treat the linear diffusion part implicitly and to treat the nonlinear, coupled drift term explicitly, in order to save computational cost, while still aiming for unconditional convergence in the sense that the time step and the spatial mesh size do not need to be related when both of them go to zero.

### 5.1 Fully discrete schemes

Let $\{t^m = m\Delta t\}_{m=0}^M$ be the uniform partition of the time interval $[0, T]$, with time step $\Delta t$. The time step could actually change from step to step, but in this paper we take the time step as a constant for simplicity. Given $n_h^m$, hence $q_h^m, E_h^m, \phi_h^m$, we would like to find the numerical solution at the next level $t^{m+1}$, maybe through several intermediate stages $t^{m,l}$, by the following IMEX RK methods.

For simplicity of notation, we will denote

$$H_j(E_h, n_h, v) = -(\mu E_h n_h, v_x)_{I_j} + (\widehat{\mu E_h n_h})_{j+\frac{1}{2}} v^-_{j+\frac{1}{2}} - (\widehat{\mu E_h n_h})_{j-\frac{1}{2}} v^+_{j-\frac{1}{2}}, \tag{5.1}$$

$$H_j^{\pm}(u_h, v) = -\sqrt{\tau\theta}(u_h, v_x)_{I_j} + \sqrt{\tau\theta}(u_h^{\pm})_{j+\frac{1}{2}} v^-_{j+\frac{1}{2}} - \sqrt{\tau\theta}(u_h^{\pm})_{j-\frac{1}{2}} v^+_{j-\frac{1}{2}}, \quad u = n, q, \tag{5.2}$$

where $j = 1, \ldots, N$ and $(\cdot,\cdot)_{I_j}$ is the usual inner product in $L^2(I_j)$.

Obviously, for smooth $E, n, u$, we have

$$H_j(E, n, v) = -(\mu E n, v_x)_{I_j} + (\mu E n)_{j+\frac{1}{2}} v^-_{j+\frac{1}{2}} - (\mu E n)_{j-\frac{1}{2}} v^+_{j-\frac{1}{2}},$$
$$H_j^{\pm}(u, v) = -\sqrt{\tau\theta}(u, v_x)_{I_j} + \sqrt{\tau\theta} u_{j+\frac{1}{2}} v^-_{j+\frac{1}{2}} - \sqrt{\tau\theta} u_{j-\frac{1}{2}} v^+_{j-\frac{1}{2}}.$$

**First order scheme.** The LDG scheme with the first order IMEX time-marching scheme, where the coupled nonlinear part of the concentration equation is treated by the forward Euler method and the diffusion part is treated by the backward Euler method, is given in the following form using the notation in (5.1) and (5.2): Find the numerical solution $n_h^{m+1}, q_h^{m+1} \in V_h^k$, such that

$$\left(\frac{n_h^{m+1} - n_h^m}{\Delta t}, v\right)_{I_j} = H_j(E_h^m, n_h^m, v) + H_j^-(q_h^{m+1}, v), \tag{5.3}$$

$$(q_h^{m+1}, w)_{I_j} = H_j^+(n_h^{m+1}, w), \tag{5.4}$$

where $j = 1, \ldots, N$ and $v, w$ in $V_h^k$.

The LDG scheme of the electric potential equation is: Find $E_h^m, \phi_h^m \in V_h^k$, such that

$$-\int_{I_j} E_h^m r_x dx + (\hat{E}_h^m)_{j+\frac{1}{2}} r^-_{j+\frac{1}{2}} - (\hat{E}_h^m)_{j-\frac{1}{2}} r^+_{j-\frac{1}{2}} = -\frac{e}{\varepsilon}\int_{I_j} (n_h^m - n_d) r dx, \tag{5.5}$$

$$\int_{I_j} E_h^m z dx - \int_{I_j} \phi_h^m z_x dx + (\hat{\phi}_h^m)_{j+\frac{1}{2}} z^-_{j+\frac{1}{2}} - (\hat{\phi}_h^m)_{j-\frac{1}{2}} z^+_{j-\frac{1}{2}} = 0, \tag{5.6}$$

where $j = 1, \ldots, N$ and $r, z$ in $V_h^k$.

As in the semi-discrete case, the "hat" terms are the numerical fluxes and are still chosen as (4.6) or (4.7).

**Second order scheme.** Using (5.1) and (5.2), the LDG scheme with the second order IMEX time-marching scheme given in [1] is: Find the numerical solution $n_h^{m+1}, q_h^{m+1} \in V_h^k$, such that

$$\left(\frac{n_h^{m,1} - n_h^m}{\Delta t}, v\right)_{I_j} = \gamma H_j(E_h^m, n_h^m, v) + \gamma H_j^-(q_h^{m,1}, v), \tag{5.7}$$

$$\begin{aligned}\left(\frac{n_h^{m+1} - n_h^m}{\Delta t}, v\right)_{I_j} &= \delta H_j(E_h^m, n_h^m, v) + (1-\delta) H_j(E_h^{m,1}, n_h^{m,1}, v) \\ &\quad + (1-\gamma) H_j^-(q_h^{m,1}, v) + \gamma H_j^-(q_h^{m+1}, v),\end{aligned} \tag{5.8}$$

$$(q_h^{m,l}, w)_{I_j} = H_j^+(n_h^{m,l}, w), \quad l = 1, 2, \quad q_h^{m,2} = q_h^{m+1}, \tag{5.9}$$

where $j = 1, \ldots, N$ and $v, w$ in $V_h^k$, and $\gamma = 1 - \frac{\sqrt{2}}{2}$, $\delta = 1 - \frac{1}{2\gamma}$.

The LDG scheme of the electric potential equation is: Find $E_h^{m,l}, \phi_h^{m,l} \in V_h^k$, such that

$$-\int_{I_j} E_h^{m,l} r_x dx + (\hat{E}_h^{m,l})_{j+\frac{1}{2}} r^-_{j+\frac{1}{2}} - (\hat{E}_h^{m,l})_{j-\frac{1}{2}} r^+_{j-\frac{1}{2}} = -\frac{e}{\varepsilon} \int_{I_j} (n_h^{m,l} - n_d) r dx, \tag{5.10}$$

$$\int_{I_j} E_h^{m,l} z dx - \int_{I_j} \phi_h^{m,l} z_x dx + (\hat{\phi}_h^{m,l})_{j+\frac{1}{2}} z^-_{j+\frac{1}{2}} - (\hat{\phi}_h^{m,l})_{j-\frac{1}{2}} z^+_{j-\frac{1}{2}} = 0, \tag{5.11}$$

where $j = 1, \ldots, N$ and $r, z$ in $V_h^k$, and $l = 0, 1$, $u^{m,0} = u^m$.

The "hat" terms for the numerical flux are chosen as before.

**Third order scheme.** The LDG scheme with the third order IMEX time-marching scheme given in [1] is: Find the numerical solution $n_h^{m+1}, q_h^{m+1} \in V_h^k$, such that

$$\left(\frac{n_h^{m,1} - n_h^m}{\Delta t}, v\right)_{I_j} = \frac{1}{2} H_j(E_h^m, n_h^m, v) + \frac{1}{2} H_j^-(q_h^{m,1}, v), \tag{5.12}$$

$$\begin{aligned}\left(\frac{n_h^{m,2} - n_h^m}{\Delta t}, v\right)_{I_j} &= \frac{11}{18} H_j(E_h^m, n_h^m, v) + \frac{1}{18} H_j(E_h^{m,1}, n_h^{m,1}, v) \\ &\quad + \frac{1}{6} H_j^-(q_h^{m,1}, v) + \frac{1}{2} H_j^-(q_h^{m,2}, v),\end{aligned} \tag{5.13}$$

$$\begin{aligned}\left(\frac{n_h^{m,3} - n_h^m}{\Delta t}, v\right)_{I_j} &= \frac{5}{6} H_j(E_h^m, n_h^m, v) - \frac{5}{6} H_j(E_h^{m,1}, n_h^{m,1}, v) + \frac{1}{2} H_j(E_h^{m,2}, n_h^{m,2}, v) \\ &\quad - \frac{1}{2} H_j^-(q_h^{m,1}, v) + \frac{1}{2} H_j^-(q_h^{m,2}, v) + \frac{1}{2} H_j^-(q_h^{m,3}, v),\end{aligned} \tag{5.14}$$

$$\begin{aligned}\left(\frac{n_h^{m+1} - n_h^m}{\Delta t}, v\right)_{I_j} &= \frac{1}{4} H_j(E_h^m, n_h^m, v) + \frac{7}{4} H_j(E_h^{m,1}, n_h^{m,1}, v) \\ &\quad + \frac{3}{4} H_j(E_h^{m,2}, n_h^{m,2}, v) - \frac{7}{4} H_j(E_h^{m,3}, n_h^{m,3}, v) \\ &\quad + \frac{3}{2} H_j^-(q_h^{m,1}, v) - \frac{3}{2} H_j^-(q_h^{m,2}, v) \\ &\quad + \frac{1}{2} H_j^-(q_h^{m,3}, v) + \frac{1}{2} H_j^-(q_h^{m+1}, v),\end{aligned} \tag{5.15}$$

$$(q_h^{m,l}, w)_{I_j} = H_j^+(n_h^{m,l}, w), \quad l = 1, 2, 3, 4, \quad q_h^{m,4} = q_h^{m+1}, \tag{5.16}$$

where $j = 1, \ldots, N$ and $v, w$ in $V_h^k$.

The LDG scheme of the electric potential equation is: Find $E_h^{m,l}, \phi_h^{m,l} \in V_h^k$, such that

$$-\int_{I_j} E_h^{m,l} r_x dx + (\hat{E}_h^{m,l})_{j+\frac{1}{2}} r^-_{j+\frac{1}{2}} - (\hat{E}_h^{m,l})_{j-\frac{1}{2}} r^+_{j-\frac{1}{2}} = -\frac{e}{\varepsilon}\int_{I_j}(n_h^{m,l} - n_d) r dx, \tag{5.17}$$

$$\int_{I_j} E_h^{m,l} z dx - \int_{I_j} \phi_h^{m,l} z_x dx + (\hat{\phi}_h^{m,l})_{j+\frac{1}{2}} z^-_{j+\frac{1}{2}} - (\hat{\phi}_h^{m,l})_{j-\frac{1}{2}} z^+_{j-\frac{1}{2}} = 0, \tag{5.18}$$

where $j = 1, \dots, N$ and $r, z$ in $V_h^k$, and $l = 0, 1, 2, 3$, $u^{m,0} = u^m$.

The "hat" terms for the numerical flux are chosen as before.

### 5.2 The error estimate of the first order IMEX LDG scheme

Denote $\|u\|_{L^\infty(0,T;L^2)} = \max_{0 \leqslant m \leqslant M} \|u^m\|_{L^2(I)}$, and $\|u\|_{L^2(0,T;L^2)} = (\sum_{m=0}^M \|u^m\|^2_{L^2(I)} \Delta t)^{\frac{1}{2}}$ in the following analysis of fully-discrete schemes.

**Theorem 5.1.** *Let $n^m, q^m$ be the exact solution of the problem* (3.7)–(3.10) *at time level $m$, which is sufficiently smooth with bounded derivatives. Let $n_h^m, q_h^m$ be the numerical solution of the first order IMEX LDG scheme* (5.3)–(5.6). *If the finite element space $V_h^k$ is the piecewise polynomials of degree $k \geqslant 0$, then for small enough $h$, there exists a positive constant $C$ independent of $h$, such that the following error estimate holds*:

$$\|n - n_h\|_{L^\infty(0,T;L^2)} + \|q - q_h\|_{L^2(0,T;L^2)} \leqslant C(h^{k+1} + \Delta t), \tag{5.19}$$

*where the constant $C$ depends on the final time $T$, $k$, $C_\mu$, the inverse constant $C_2$, $\|n\|_{L^\infty(0,T;H^{k+1})}$, $\|n_x\|_{L^\infty}$ and $\|E\|_{L^\infty}$.*

*Proof.* To get the error equation of the first order IMEX LDG scheme, we first rewrite (3.7) and (3.8) at time level $m$ or $m+1$ as the following:

$$\begin{aligned}\left(\frac{n^{m+1}-n^m}{\Delta t}, v\right)_{I_j} &= -(\mu E^m n^m, v_x)_{I_j} + (\mu E^m n^m)_{j+\frac{1}{2}} v^-_{j+\frac{1}{2}} - (\mu E^m n^m)_{j-\frac{1}{2}} v^+_{j-\frac{1}{2}} \\ &\quad - (\sqrt{\tau\theta} q^{m+1}, v_x)_{I_j} + (\sqrt{\tau\theta} q^{m+1})_{j+\frac{1}{2}} v^-_{j+\frac{1}{2}} - (\sqrt{\tau\theta} q^{m+1})_{j-\frac{1}{2}} v^+_{j-\frac{1}{2}} \\ &\quad + \left(\frac{n^{m+1}-n^m}{\Delta t} - n_t^m, v\right)_{I_j} + (\sqrt{\tau\theta}(q^{m+1} - q^m), v_x)_{I_j} \\ &\quad - \sqrt{\tau\theta}(q^{m+1} - q^m)_{j+\frac{1}{2}} v^-_{j+\frac{1}{2}} + \sqrt{\tau\theta}(q^{m+1} - q^m)_{j-\frac{1}{2}} v^+_{j-\frac{1}{2}},\end{aligned} \tag{5.20}$$

$$(q^{m+1}, w)_{I_j} = -(\sqrt{\tau\theta} n^{m+1}, w_x)_{I_j} + (\sqrt{\tau\theta} n^{m+1})_{j+\frac{1}{2}} w^-_{j+\frac{1}{2}} - (\sqrt{\tau\theta} n^{m+1})_{j-\frac{1}{2}} w^+_{j-\frac{1}{2}}. \tag{5.21}$$

Taking the difference of (5.20) and (5.3), and the difference of (5.21) and (5.4), we have the following error equation:

$$\begin{aligned}\left(\frac{(n^{m+1}-n_h^{m+1}) - (n^m - n_h^m)}{\Delta t}, v\right)_{I_j} &= -(\mu E^m n^m - \mu E_h^m n_h^m, v_x)_{I_j} + (\mu E^m n^m - \mu \widehat{E_h^m n_h^m})_{j+\frac{1}{2}} v^-_{j+\frac{1}{2}} \\ &\quad - (\mu E^m n^m - \mu \widehat{E_h^m n_h^m})_{j-\frac{1}{2}} v^+_{j-\frac{1}{2}} - \sqrt{\tau\theta}(q^{m+1} - q_h^{m+1}, v_x)_{I_j} \\ &\quad + \sqrt{\tau\theta}(q^{m+1} - \hat{q}_h^{m+1})_{j+\frac{1}{2}} v^-_{j+\frac{1}{2}} - \sqrt{\tau\theta}(q^{m+1} - \hat{q}_h^{m+1})_{j-\frac{1}{2}} v^+_{j-\frac{1}{2}} \\ &\quad + \left(\frac{n^{m+1}-n^m}{\Delta t} - n_t^m, v\right)_{I_j} + (\sqrt{\tau\theta} q^{m+1} - q^m, v_x)_{I_j} \\ &\quad - \sqrt{\tau\theta}(q^{m+1} - q^m)_{j+\frac{1}{2}} v^-_{j+\frac{1}{2}} + \sqrt{\tau\theta}(q^{m+1} - q^m)_{j-\frac{1}{2}} v^+_{j-\frac{1}{2}},\end{aligned}$$

$$\begin{aligned}(q^{m+1} - q_h^{m+1}, w)_{I_j} &= -\sqrt{\tau\theta}(n^{m+1} - n_h^{m+1}, w_x)_{I_j} + \sqrt{\tau\theta}(n^{m+1} - \hat{n}_h^{m+1})_{j+\frac{1}{2}} w^-_{j+\frac{1}{2}} \\ &\quad - \sqrt{\tau\theta}(n^{m+1} - \hat{n}_h^{m+1})_{j-\frac{1}{2}} w^+_{j-\frac{1}{2}}.\end{aligned}$$

Choosing $v = \xi_n^{m+1}, w = \xi_q^{m+1}$, summing the above two equalities and summing $j$ over $I$, we get

$$(\xi_n^{m+1} - \xi_n^m, \xi_n^{m+1}) + \Delta t(\xi_q^{m+1}, \xi_q^{m+1})$$

$$
\begin{aligned}
&= (\eta_n^{m+1} - \eta_n^m, \xi_n^{m+1}) + \Delta t(\eta_q^{m+1}, \xi_q^{m+1}) + \Delta t\left(\frac{n^{m+1} - n^m}{\Delta t} - n_t^m, \xi_n^{m+1}\right) \\
&\quad - \Delta t(\mu E^m n^m - \mu E_h^m n_h^m, \xi_{n,x}^{m+1}) - \Delta t \sum_{j=1}^N (\mu E^m n^m - \mu \widehat{E_h^m n_h^m})_{j-\frac12} [\xi_n^{m+1}]_{j-\frac12} \\
&\quad - \Delta t\sqrt{\tau\theta}(\xi_q^{m+1} - \eta_q^{m+1}, \xi_{n,x}^{m+1}) - \Delta t\sqrt{\tau\theta} \sum_{j=1}^N ((\xi_q^{m+1})^- - (\eta_q^{m+1})^-)_{j-\frac12} [\xi_n^{m+1}]_{j-\frac12} \\
&\quad + \Delta t\sqrt{\tau\theta}(q^{m+1} - q^m, \xi_{n,x}^{m+1}) + \Delta t\sqrt{\tau\theta} \sum_{j=1}^N ((q^{m+1}) - (q^m))_{j-\frac12} [\xi_n^{m+1}]_{j-\frac12} \\
&\quad - \Delta t\sqrt{\tau\theta}(\xi_n^{m+1} - \eta_n^{m+1}, \xi_{q,x}^{m+1}) - \Delta t\sqrt{\tau\theta} \sum_{j=1}^N ((\xi_n^{m+1})^+ - (\eta_n^{m+1})^+)_{j-\frac12} [\xi_q^{m+1}]_{j-\frac12}.
\end{aligned}
$$

Noting that $(\xi_n^{m+1} - \xi_n^m, \xi_n^{m+1}) = \frac12\|\xi_n^{m+1}\|^2 - \frac12\|\xi_n^m\|^2 + \frac12\|\xi_n^{m+1} - \xi_n^m\|^2$, we have

$$
\begin{aligned}
&\frac12\|\xi_n^{m+1}\|^2 - \frac12\|\xi_n^m\|^2 + \frac12\|\xi_n^{m+1} - \xi_n^m\|^2 + \Delta t\|\xi_q^{m+1}\|^2 \\
&\leqslant (\eta_n^{m+1} - \eta_n^m, \xi_n^{m+1}) + \Delta t(\eta_q^{m+1}, \xi_q^{m+1}) + \Delta t\left(\frac{n^{m+1} - n^m}{\Delta t} - n_t^m, \xi_n^{m+1}\right) \\
&\quad + \Bigg(\Delta t\sqrt{\tau\theta}(\eta_q^{m+1}, \xi_{n,x}^{m+1}) + \Delta t\sqrt{\tau\theta}(\eta_n^{m+1}, \xi_{q,x}^{m+1}) \\
&\quad + \Delta t\sqrt{\tau\theta} \sum_{j=1}^N (\eta_q^{m+1})_{j-\frac12}^- [\xi_n^{m+1}]_{j-\frac12} + \Delta t\sqrt{\tau\theta} \sum_{j=1}^N (\eta_n^{m+1})_{j-\frac12}^+ [\xi_q^{m+1}]_{j-\frac12}\Bigg) \\
&\quad + \Bigg( - \Delta t\sqrt{\tau\theta}(\xi_q^{m+1}, \xi_{n,x}^{m+1}) - \Delta t\sqrt{\tau\theta}(\xi_n^{m+1}, \xi_{q,x}^{m+1}) \\
&\quad - \Delta t\sqrt{\tau\theta} \sum_{j=1}^N (\xi_n^{m+1})_{j-\frac12}^+ [\xi_q^{m+1}]_{j-\frac12} - \Delta t\sqrt{\tau\theta} \sum_{j=1}^N (\xi_q^{m+1})_{j-\frac12}^- [\xi_n^{m+1}]_{j-\frac12}\Bigg) \\
&\quad + \Bigg(\Delta t\sqrt{\tau\theta}(q^{m+1} - q^m, \xi_{n,x}^{m+1}) - \Delta t\sqrt{\tau\theta} \sum_{j=1}^N (q^{m+1} - q^m)_{j-\frac12} [\xi_n^{m+1}]_{j-\frac12}\Bigg) \\
&\quad + \Bigg( - \Delta t(\mu E^m n^m - \mu E_h^m n_h^m, \xi_{n,x}^{m+1}) - \Delta t \sum_{j=1}^N (\mu E^m n^m - \mu \widehat{E_h^m n_h^m})_{j-\frac12} [\xi_n^{m+1}]_{j-\frac12}\Bigg) \\
&=: \sum_{i=1}^7 T_{1i}.
\end{aligned} \tag{5.22}
$$

Now, we estimate $T_{1i}$ term by term. From (2.3) of the projection, and Schwartz's inequality or Young's inequality, we have

$$
T_{11} \leqslant \frac12 \Delta t h^{2k+2} + \frac12 \Delta t\|\xi_n^{m+1}\|^2, \tag{5.23}
$$

$$
T_{12} \leqslant C\Delta t h^{2k+2} + \tilde{\varepsilon}\Delta t\|\xi_q^{m+1}\|^2. \tag{5.24}
$$

Noting that

$$
\frac{n^{m+1} - n^m}{\Delta t} - n_t^m = O(\Delta t),
$$

we can get

$$
T_{13} \leqslant \frac12 (\Delta t)^3 + \frac12 \Delta t\|\xi_n^{m+1}\|^2. \tag{5.25}
$$

Obviously, from (2.2), we have

$$
T_{14} = 0. \tag{5.26}
$$

We have also

$$\begin{aligned}T_{15}&=-\Delta t\sqrt{\tau\theta}\sum_{j=1}^{N}\left(\int_{I_j}(\xi_q^{m+1}\xi_n^{m+1})_x dx+(\xi_n^{m+1})^+_{j-\frac{1}{2}}[\xi_q^{m+1}]_{j-\frac{1}{2}}+(\xi_q^{m+1})^-_{j-\frac{1}{2}}[\xi_n^{m+1}]_{j-\frac{1}{2}}\right)\\&=-\Delta t\sqrt{\tau\theta}\sum_{j=1}^{N}((\xi_n^{m+1})^+_{j+\frac{1}{2}}(\xi_q^{m+1})^-_{j+\frac{1}{2}}-(\xi_n^{m+1})^+_{j-\frac{1}{2}}(\xi_q^{m+1})^-_{j-\frac{1}{2}})\\&=0.\end{aligned}\tag{5.27}$$

The above estimate of $T_{15}$ used the periodic boundary condition for $n$, $n_h$, $q$ and $q_h$.

Noting that $q^{m+1}-q^m=O(\Delta t)$, using Young's inequality, we get

$$T_{16}\leqslant C(\Delta t)^3+\tilde{\varepsilon}\Delta t\|\xi_{n,x}^{m+1}\|^2+C(\Delta t)^3h+\tilde{\varepsilon}h^{-1}\Delta t[\xi_n^{m+1}]^2.\tag{5.28}$$

About the last term $T_{17}$, we need the a-priori assumption similarly to (4.22),

$$\|n^m-n_h^m\|\leqslant\tilde{C}h.\tag{5.29}$$

From the above assumption, we can get $\|n_h^m\|_{L^\infty}\leqslant C$. Then we estimate $T_{17}$ similarly as $T_5$ of the semi-discrete scheme, using $E_h^m n_h^m$, $\xi_{n,x}^{m+1}$ and $[\xi_n^{m+1}]$ instead of $E_h n_h$, $\xi_{n,x}$ and $[\xi_n]$, respectively to obtain

$$T_{17}\leqslant C\Delta t\|\xi_n^m\|^2+C\Delta t h^{2k+2}+\tilde{\varepsilon}\Delta t\|\xi_{n,x}^{m+1}\|^2+\tilde{\varepsilon}h^{-1}\Delta t[\xi_n^{m+1}]^2.\tag{5.30}$$

Substituting (5.23)–(5.30) to (5.22), we have

$$\begin{aligned}&\frac{1}{2}\|\xi_n^{m+1}\|^2-\frac{1}{2}\|\xi_n^m\|^2+\frac{1}{2}\|\xi_n^{m+1}-\xi_n^m\|^2+\Delta t\|\xi_q^{m+1}\|^2\\&\quad\leqslant C\Delta t h^{2k+2}+C\Delta t(\|\xi_n^{m+1}\|^2+\|\xi_n^m\|^2)+\tilde{\varepsilon}\Delta t\|\xi_q^{m+1}\|^2\\&\qquad+(\Delta t)^3+\tilde{\varepsilon}\Delta t\|\xi_{n,x}^{m+1}\|^2+C(\Delta t)^3h+\tilde{\varepsilon}h^{-1}\Delta t[\xi_n^{m+1}]^2.\end{aligned}$$

Summing the above inequality over the time step $m$, using the discrete Gronwall inequality and Lemma 4.3, we get

$$\|\xi_n^M\|^2+\Delta t\sum_{m=0}^{M}\|\xi_q^m\|^2\leqslant\|\xi_n^0\|^2+Ch^{2k+2}+C(\Delta t)^2.\tag{5.31}$$

To complete the proof, let us verify the a-priori assumption (5.29). For $m=0$, we choose $n_h^0$ as the projection of $n^0$, so obviously, the assumption (5.29) holds. If (5.29) holds for $m=1,\dots,M-1$, then for $m=M$, we can get (5.31), i.e., (5.29) holds also for $m=M$. □

### 5.3 The error estimate of the second order IMEX LDG scheme

**Theorem 5.2.** *Let $n^m,q^m$ be the exact solution to* (3.7)–(3.10) *at time level $m$, which is sufficiently smooth with bounded derivatives. Let $n_h^m,q_h^m$ be the numerical solution to the second order IMEX LDG scheme* (5.7)–(5.11). *If the finite element space $V_h^k$ is the piecewise polynomials of degree $k\geqslant 0$, then for small enough $h$, there exists a positive constant $C$ independent of $h$, such that the following error estimate holds*

$$\|n-n_h\|_{L^\infty(0,T;L^2)}\leqslant C(h^{k+1}+(\Delta t)^2),\tag{5.32}$$

*where the constant $C$ depends on the final time $T$, $k$, $C_\mu$, the inverse constant $C_2$, $\|n\|_{L^\infty(0,T;H^{k+1})}$, $\|n_x\|_{L^\infty}$ and $\|E\|_{L^\infty}$.*

*Proof.* First, we rewrite the scheme (5.7)–(5.8) as the following

$$(n_h^{m,1}-n_h^m,v)_{I_j}=\gamma\Delta tH_j(E_h^m,n_h^m,v)+\gamma\Delta tH_j^-(q_h^{m,1},v), \tag{5.33}$$

$$(n_h^{m+1}-n_h^{m,1},v)_{I_j}=(\delta-\gamma)\Delta tH_j(E_h^m,n_h^m,v)+(1-\delta)\Delta tH_j(E_h^{m,1},n_h^{m,1},v)\\ +(1-2\gamma)\Delta tH_j^-(q_h^{m,1},v)+\gamma\Delta tH_j^-(q_h^{m+1},v), \tag{5.34}$$

To get the error equation, we need to define $n^{m,1},q^{m,1}$,

$$\frac{n^{m,1}-n^m}{\Delta t}=\gamma(\mu E^mn^m))x+\gamma\sqrt{\tau\theta}q_x^{m,1},\quad q^{m,1}=\sqrt{\tau\theta}n_x^{m,1},$$

where $n^m$ is the exact solution $n$ at the $m$-th time level. Then we get the weak forms

$$(n^{m,1}-n^m,v)_{I_j}=\gamma\Delta tH_j(E^m,n^m,v)+\gamma\Delta tH_j^-(q^{m,1},v), \tag{5.35}$$

$$(n^{m+1}-n^{m,1},v)_{I_j}=(\delta-\gamma)\Delta tH_j(E^m,n^m,v)+(1-\delta)\Delta tH_j(E^{m,1},n^{m,1},v)\\ +(1-2\gamma)\Delta tH_j^-(q^{m,1},v)+\gamma\Delta tH_j^-(q^{m+1},v)+(\zeta^m,v), \tag{5.36}$$

$$(q^{m,l},w)_{I_j}=H_j^+(n^{m,l},w),\quad l=1,2, \tag{5.37}$$

where $\zeta^m$ is the truncation error and $\|\zeta^m\|\leqslant C(\Delta t)^3$. The weak forms of the electric potential equation are

$$-\int_{I_j}E^{m,l}r_xdx+E^{m,l}_{j+\frac12}r^-_{j+\frac12}-E^{m,l}_{j-\frac12}r^+_{j-\frac12}=-\frac{e}{\varepsilon}\int_{I_j}(n^{m,l}-n_d)rdx, \tag{5.38}$$

$$\int_{I_j}E^{m,l}zdx-\int_{I_j}\phi^{m,l}z_xdx+\phi^{m,l}_{j+\frac12}z^-_{j+\frac12}-\phi^{m,l}_{j-\frac12}z^+_{j-\frac12}=0,\quad l=0,1. \tag{5.39}$$

Denote $e_u^{m,l}=u^{m,l}-u_h^{m,l}=\xi_u^{m,l}-\eta_u^{m,l},u=n,q$. Here, $\xi_n,\eta_n,\xi_q,\eta_q$ are the same as before.

Subtracting the above weak forms of the electron concentration equation from those second order IMEX LDG scheme of the electron concentration equation, i.e., (5.33)–(5.35), (5.34)–(5.36) and (5.9)–(5.37), we get the following error equation

$$\begin{aligned}(\xi_n^{m,1}-\xi_n^m,v)_{I_j}&=\gamma\Delta t(H_j(E^m,n^m,v)-H_j(E_h^m,n_h^m,v))\\&\quad+(\eta_n^{m,1}-\eta_n^m,v)_{I_j}+\gamma\Delta tH_j^-(\xi_q^{m,1},v)-\gamma\Delta tH_j^-(\eta_q^{m,1},v),\\(\xi_n^{m+1}-\xi_n^{m,1},v)_{I_j}&=(\delta-\gamma)\Delta t(H_j(E^m,n^m,v)-H_j(E_h^m,n_h^m,v))\\&\quad+(1-\delta)\Delta t(H_j(E^{m,1},n^{m,1},v)-H_j(E_h^{m,1},n_h^{m,1},v))\\&\quad+(1-2\gamma)\Delta tH_j^-(\xi_q^{m,1},v)-(1-2\gamma)\Delta tH_j^-(\eta_q^{m,1},v)\\&\quad+\gamma\Delta tH_j^-(\xi_q^{m+1},v)-\gamma\Delta tH_j^-(\eta_q^{m+1},v)+(\eta_n^{m+1}-\eta_n^{m,1},v)_{I_j}+(\zeta^m,v)_{I_j},\\(\xi_q^{m,l},w)_{I_j}&=(\eta_q^{m,l},w)_{I_j}+H_j^+(\xi_n^{m,l},w)-H_j^+(\eta_n^{m,l},w),\quad l=1,2.\end{aligned}$$

Noting that $H_j^-(\eta_q^{m,l},v)=0$ and $H_j^+(\eta_n^{m,l},w)=0$ from the projection, taking $v=\xi_n^{m,1},\xi_n^{m+1}$, $w=\xi_q^{m,1},\xi_q^{m+1}$ in the above equalities, we get

$$(\xi_n^{m,1}-\xi_n^m,\xi_n^{m,1})_{I_j}=\gamma\Delta t(H_j(E^m,n^m,\xi_n^{m,1})-H_j(E_h^m,n_h^m,\xi_n^{m,1}))\\ +(\eta_n^{m,1}-\eta_n^m,\xi_n^{m,1})_{I_j}+\gamma\Delta tH_j^-(\xi_q^{m,1},\xi_n^{m,1}), \tag{5.40}$$

$$(\xi_n^{m+1}-\xi_n^{m,1},\xi_n^{m+1})_{I_j}=(\delta-\gamma)\Delta t(H_j(E^m,n^m,\xi_n^{m+1})-H_j(E_h^m,n_h^m,\xi_n^{m+1}))\\ +(1-\delta)\Delta t(H_j(E^{m,1},n^{m,1},\xi_n^{m+1})-H_j(E_h^{m,1},n_h^{m,1},\xi_n^{m+1}))\\ +(1-2\gamma)\Delta tH_j^-(\xi_q^{m,1},\xi_n^{m+1})+\gamma\Delta tH_j^-(\xi_q^{m+1},\xi_n^{m+1})\\ +(\eta_n^{m+1}-\eta_n^{m,1},\xi_n^{m+1})_{I_j}+(\zeta^m,\xi_n^{m+1})_{I_j}, \tag{5.41}$$

$$(\xi_q^{m,1},\xi_q^{m,1})_{I_j}=(\eta_q^{m,1},\xi_q^{m,1})_{I_j}+H_j^+(\xi_n^{m,1},\xi_q^{m,1}), \tag{5.42}$$

$$(\xi_q^{m+1},\xi_q^{m+1})_{I_j}=(\eta_q^{m+1},\xi_q^{m+1})_{I_j}+H_j^+(\xi_n^{m+1},\xi_q^{m+1}). \tag{5.43}$$

If we choose $w = \xi_q^{m,1}$ instead of $w = \xi_q^{m+1}$ in (5.43), we get

$$(\xi_q^{m+1}, \xi_q^{m,1})_{I_j} = (\eta_q^{m+1}, \xi_q^{m,1})_{I_j} + H_j^+(\xi_n^{m+1}, \xi_q^{m,1}). \tag{5.44}$$

Taking (5.42) $\times\ \gamma\Delta t +$ (5.43) $\times\ \gamma\Delta t +$ (5.44) $\times\ (1-2\gamma)\Delta t$, then summing them together with (5.40) and (5.41), and summing $j$ over $I$, we have

$$\begin{aligned}
&\frac{1}{2}\|\xi_n^{m+1}\|^2 - \frac{1}{2}\|\xi_n^m\|^2 + \frac{1}{2}\|\xi_n^{m+1} - \xi_n^{m,1}\|^2 + \frac{1}{2}\|\xi_n^{m,1} - \xi_n^m\|^2 \\
&\quad + \gamma\Delta t\|\xi_q^{m,1}\|^2 + \gamma\Delta t\|\xi_q^{m+1}\|^2 + (1-2\gamma)\Delta t(\xi_q^{m+1}, \xi_q^{m,1}) \\
&\quad = ((\eta_n^{m,1} - \eta_n^m, \xi_n^{m,1}) + (\eta_n^{m+1} - \eta_n^{m,1}, \xi_n^{m+1})) \\
&\qquad + (\gamma\Delta t H^-(\xi_q^{m,1}, \xi_n^{m,1}) + (1-2\gamma)\Delta t H^-(\xi_q^{m,1}, \xi_n^{m+1}) + \gamma\Delta t H^-(\xi_q^{m+1}, \xi_n^{m+1}) \\
&\qquad + \gamma\Delta t H^+(\xi_n^{m,1}, \xi_q^{m,1}) + (1-2\gamma)\Delta t H^+(\xi_n^{m+1}, \xi_q^{m,1}) + \gamma\Delta t H^+(\xi_n^{m+1}, \xi_q^{m+1})) \\
&\qquad + ((\zeta^m, \xi_n^{m+1}) + \gamma\Delta t(\eta_q^{m,1}, \xi_q^{m,1}) + \gamma\Delta t(\eta_q^{m+1}, \xi_q^{m+1}) + (1-2\gamma)\Delta t(\eta_q^{m+1}, \xi_q^{m,1})) \\
&\qquad + (\gamma\Delta t(H(E^m, n^m, \xi_n^{m,1}) - H(E_h^m, n_h^m, \xi_n^{m,1})) \\
&\qquad + (\delta-\gamma)\Delta t(H(E^m, n^m, \xi_n^{m+1}) - H(E_h^m, n_h^m, \xi_n^{m+1})) \\
&\qquad + (1-\delta)\Delta t(H(E^{m,1}, n^{m,1}, \xi_n^{m+1}) - H(E_h^{m,1}, n_h^{m,1}, \xi_n^{m+1}))) \\
&\quad =: \sum_{i=1}^{4} T_{2i}.
\end{aligned} \tag{5.45}$$

Next, we estimate the term $T_{2i}$ one by one. Obviously, from the property of the projection (2.3) and the Schwartz inequality, we can get

$$T_{21} \leqslant C\Delta t h^{2k+2} + C\Delta t(\|\xi_n^{m,1}\|^2 + \|\xi_n^{m+1}\|^2). \tag{5.46}$$

From the periodic boundary condition, we have

$$T_{22} = 0. \tag{5.47}$$

To estimate $T_{23}$, we denote $\boldsymbol{\xi}_q^{\mathrm{T}} = (\xi_q^{m,1}, \xi_q^{m+1})$. Using the property of the projection (2.3), Schwartz's inequality and Young's inequality, we have

$$T_{23} = C(\Delta t)^5 + C\Delta t\|\xi_n^{m+1}\|^2 + C\Delta t h^{2k+2} + \tilde{\varepsilon}\Delta t\int_I \boldsymbol{\xi}_q^{\mathrm{T}}\boldsymbol{\xi}_q dx. \tag{5.48}$$

Similarly as the estimation of the term $T_{17}$ in the first order IMEX LDG scheme, we have

$$\begin{aligned}
&\gamma\Delta t(H_j(E^m, n^m, \xi_n^{m,1}) - H_j(E_h^m, n_h^m, \xi_n^{m,1})) \\
&\quad \leqslant C\Delta t(h^{2k+2} + \|\xi_n^m\|^2) + \tilde{\varepsilon}(\Delta t\|\xi_{n,x}^{m,1}\|^2 + \Delta t h^{-1}[\xi_n^{m,1}]^2). \\
&(\delta-\gamma)\Delta t(H_j(E^m, n^m, \xi_n^{m+1}) - H_j(E_h^m, n_h^m, \xi_n^{m+1})) \\
&\quad \leqslant C\Delta t(h^{2k+2} + \|\xi_n^m\|^2) + \tilde{\varepsilon}(\Delta t\|\xi_{n,x}^{m+1}\|^2 + \Delta t h^{-1}[\xi_n^{m+1}]^2). \\
&(1-\delta)\Delta t(H_j(E^{m,1}, n^{m,1}, \xi_n^{m+1}) - H_j(E_h^{m,1}, n_h^{m,1}, \xi_n^{m+1})) \\
&\quad \leqslant C\Delta t(h^{2k+2} + \|\xi_n^{m,1}\|^2) + \tilde{\varepsilon}(\Delta t\|\xi_{n,x}^{m+1}\|^2 + \Delta t h^{-1}[\xi_n^{m+1}]^2).
\end{aligned}$$

Noting that for both pairs of $(\xi_n^{m,l}, \xi_q^{m,l}), l = 1, 2$, we have the similar result as Lemma 4.3,

$$\begin{aligned}
\|\xi_{n,x}^{m,l}\| &\leqslant \frac{C_\mu}{\sqrt{\tau\theta}}(\|\xi_q^{m,l}\| + \|\eta_q^{m,l}\|) \\
h^{-\frac{1}{2}}[\xi_n^{m,l}] &\leqslant \frac{C_\mu}{\sqrt{\tau\theta}}(\|\xi_q^{m,l}\| + \|\eta_q^{m,l}\|).
\end{aligned} \tag{5.49}$$

Then we get

$$T_{24} \leqslant C\Delta t(h^{2k+2} + \|\xi_n^m\|^2 + \|\xi_n^{m,1}\|^2) + 2\tilde{\varepsilon}\frac{C_\mu}{\sqrt{\tau\theta}}\Delta t\|\xi_q^{m,1}\|^2 + 4\tilde{\varepsilon}\frac{C_\mu}{\sqrt{\tau\theta}}\Delta t\|\xi_q^{m+1}\|^2. \tag{5.50}$$

Substituting (5.46)–(5.48) and (5.50) to (5.45), we get

$$\begin{aligned}&\|\xi_n^{m+1}\|^2-\|\xi_n^m\|^2+2\gamma\Delta t\|\xi_q^{m,1}\|^2+2\gamma\Delta t\|\xi_q^{m+1}\|^2+2(1-2\gamma)\Delta t(\xi_q^{m+1},\xi_q^{m,1})\\&\quad\leqslant C(\Delta t)^5+C\Delta th^{2k+2}+C\Delta t(\|\xi_n^m\|^2+\|\xi_n^{m,1}\|^2+\|\xi_n^{m+1}\|^2)\\&\qquad+2\tilde\varepsilon\Delta t\int_I\boldsymbol{\xi}_q^{\mathrm T}\boldsymbol{\xi}_qdx+4\tilde\varepsilon\frac{C_\mu}{\sqrt{\tau\theta}}\Delta t\|\xi_q^{m,1}\|^2+8\tilde\varepsilon\frac{C_\mu}{\sqrt{\tau\theta}}\Delta t\|\xi_q^{m+1}\|^2.\end{aligned}\tag{5.51}$$

We can choose $\tilde\varepsilon$ small enough that $\tilde\varepsilon\frac{C_\mu}{\sqrt{\tau\theta}}\leqslant\frac{1}{16}\gamma$, so we have

$$\begin{aligned}&\|\xi_n^{m+1}\|^2-\|\xi_n^m\|^2+\frac32\gamma\Delta t\|\xi_q^{m,1}\|^2+\frac32\gamma\Delta t\|\xi_q^{m+1}\|^2+2(1-2\gamma)\Delta t(\xi_q^{m+1},\xi_q^{m,1})\\&\quad\leqslant C(\Delta t)^5+C\Delta th^{2k+2}+C\Delta t(\|\xi_n^m\|^2+\|\xi_n^{m,1}\|^2+\|\xi_n^{m+1}\|^2)+2\tilde\varepsilon\Delta t\int_I\boldsymbol{\xi}_q^{\mathrm T}\boldsymbol{\xi}_qdx.\end{aligned}\tag{5.52}$$

If we denote the last three term of the left hand as $S$, i.e.,

$$\begin{aligned}S&:=\frac32\gamma\Delta t\|\xi_q^{m,1}\|^2+\frac32\gamma\Delta t\|\xi_q^{m+1}\|^2+2(1-2\gamma)\Delta t(\xi_q^{m+1},\xi_q^{m,1})\\&=\Delta t\int_I\boldsymbol{\xi}_q^{\mathrm T}\boldsymbol{M}\boldsymbol{\xi}_qdx,\end{aligned}$$

where

$$\boldsymbol{M}=\begin{pmatrix}\frac32\gamma & 1-2\gamma\\ 1-2\gamma & \frac32\gamma\end{pmatrix}.$$

It is easy to check that $\boldsymbol{M}$ is positive definite. So if we choose $\tilde\varepsilon$ satisfying not only $\tilde\varepsilon\frac{C_\mu}{\sqrt{\tau\theta}}\leqslant\frac{1}{16}\gamma$ but also $\int_I\boldsymbol{\xi}_q^{\mathrm T}(\boldsymbol{M}-2\tilde\varepsilon)\boldsymbol{\xi}_qdx\geqslant0$, we can get

$$\|\xi_n^{m+1}\|^2-\|\xi_n^m\|^2\leqslant C(\Delta t)^5+C\Delta th^{2k+2}+C\Delta t(\|\xi_n^m\|^2+\|\xi_n^{m,1}\|^2+\|\xi_n^{m+1}\|^2).\tag{5.53}$$

The estimate for the stage values $\|\xi_n^{m,1}\|$ can be obtained along the similar argument as the result of (5.53), so we omit the details and only state it in the following inequality:

$$\|\xi_n^{m,1}\|^2\leqslant C(\|\xi_n^m\|^2+(\Delta t)^5+\Delta th^{2k+2}).\tag{5.54}$$

Combining (5.54) to (5.53), summing $t$ over $(0,T)$ and using the discrete Gronwall inequality, we obtain

$$\|\xi_n\|_{L^\infty(0,T;L^2(I))}\leqslant C(\Delta t)^2+Ch^{k+1}.\tag{5.55}$$

This completes the proof. □

### 5.4 The error estimate of the third order IMEX LDG scheme

**Theorem 5.3.** *Let $n^m,q^m$ be the exact solution to* (3.7)–(3.10) *at time level $m$, which is sufficiently smooth with bounded derivatives. Let $n_h^m,q_h^m$ be the numerical solution to the third order IMEX LDG scheme* (5.12)–(5.18). *If the finite element space $V_h^k$ is the piecewise polynomials of degree $k\geqslant0$, then for small enough $h$, there exists a positive constant $C$ independent of $h$, such that the following error estimate holds*:

$$\|n-n_h\|_{L^\infty(0,T;L^2)}\leqslant C(h^{k+1}+(\Delta t)^3),\tag{5.56}$$

*where the constant $C$ depends on the final time $T$, $k$, $C_\mu$, the inverse constant $C_2$, $\|n\|_{L^\infty(0,T;H^{k+1})}$, $\|n_x\|_{L^\infty}$ and $\|E\|_{L^\infty}$.*

*Proof.* For the convenience of analysis, we would like to denote

$$D_1u^m=2u^{m,2}-3u^{m,1},\quad D_2u^m=u^{m,3}-2u^{m,2}+2u^{m,1},$$

then introduce a series of notation

$$F_1u^m = u^{m,1} - u^m, \quad F_2u^m = D_1u^m + u^m,$$
$$F_3u^m = D_2u^m - u^{m,1}, \quad F_4u^m = 2u^{m+1} + D_1u^m - D_2u^m,$$
$$F_{41}u^m = u^{m+1} + D_1u^m, \quad F_{42}u^m = u^{m+1} - D_2u^m.$$

We sum $j$ over $I$ and rewrite the scheme (5.12)–(5.15) into the following compact form:

$$\begin{cases}(F_l n_h^m, v) = \Phi_l(\boldsymbol{E}_h^m, \boldsymbol{n}_h^m, v) + \Psi_l(\boldsymbol{q}_h^m, v), \quad l = 1,2,3,4,\\ (q_h^{m,l}, w) = H^+(n_h^{m,l}, v), \quad l = 1,2,3,4,\end{cases} \tag{5.57}$$

where $\boldsymbol{n}_h^m = (n_h^m, n_h^{m,1}, n_h^{m,2}, n_h^{m,3})$, $\boldsymbol{q}_h^m = (q_h^{m,1}, q_h^{m,2}, q_h^{m,3}, q_h^{m+1})$, and

$$\begin{aligned}
\Phi_1(\boldsymbol{E}_h^m, \boldsymbol{n}_h^m, v) &= \frac{1}{2}\Delta t H(E_h^m, n_h^m, v),\\
\Phi_2(\boldsymbol{E}_h^m, \boldsymbol{n}_h^m, v) &= -\frac{5}{18}\Delta t H(E_h^m, n_h^m, v) + \frac{1}{9}\Delta t H(E_h^{m,1}, n_h^{m,1}, v),\\
\Phi_3(\boldsymbol{E}_h^m, \boldsymbol{n}_h^m, v) &= \frac{1}{9}\Delta t H(E_h^m, n_h^m, v) - \frac{17}{18}\Delta t H(E_h^{m,1}, n_h^{m,1}, v) + \frac{1}{2}\Delta t H(E_h^{m,2}, n_h^{m,2}, v),\\
\Phi_4(\boldsymbol{E}_h^m, \boldsymbol{n}_h^m, v) &= -\frac{7}{18}\Delta t H(E_h^m, n_h^m, v) + \frac{41}{9}\Delta t H(E_h^{m,1}, n_h^{m,1}, v) + \Delta t H(E_h^{m,2}, n_h^{m,2}, v)\\
&\quad - \frac{7}{2}\Delta t H(E_h^{m,3}, n_h^{m,3}, v),
\end{aligned}$$

and

$$\begin{aligned}
\Psi_1(\boldsymbol{q}_h^m, v) &= \frac{1}{2}\Delta t H^-(q_h^{m,1}, v),\\
\Psi_2(\boldsymbol{q}_h^m, v) &= \frac{1}{3}\Delta t H^-(q_h^{m,1}, v) + \frac{1}{2}\Delta t H^-(D_1 q_h^m, v),\\
\Psi_3(\boldsymbol{q}_h^m, v) &= -\frac{7}{12}\Delta t H^-(q_h^{m,1}, v) + \frac{1}{4}\Delta t H^-(D_1 q_h^m, v) + \frac{1}{2}\Delta t H^-(D_2 q_h^m, v),\\
\Psi_4(\boldsymbol{q}_h^m, v) &= -\frac{1}{12}\Delta t H^-(q_h^{m,1}, v) - \frac{1}{4}\Delta t H^-(D_1 q_h^m, v) + \frac{1}{2}\Delta t H^-(D_2 q_h^m, v)\\
&\quad + \Delta t H^-(q_h^{m+1}, v).
\end{aligned}$$

To get the error equation, we need to define $n^{m,l}, q^{m,l}, E^{m,l}, \phi^{m,l}$ as the following:

$$\begin{aligned}
\frac{n^{m,1} - n^m}{\Delta t} &= \frac{1}{2}(\mu E^m n^m)_x + \frac{1}{2}\sqrt{\tau\theta} q_x^{m,1},\\
\frac{n^{m,2} - n^m}{\Delta t} &= \frac{11}{18}(\mu E^m n^m)_x + \frac{1}{18}(\mu E^{m,1} n^{m,1})_x + \frac{1}{6}\sqrt{\tau\theta} q_x^{m,1} + \frac{1}{2}\sqrt{\tau\theta} q_x^{m,2},\\
\frac{n^{m,3} - n^m}{\Delta t} &= \frac{5}{6}(\mu E^m n^m)_x - \frac{5}{6}(\mu E^{m,1} n^{m,1})_x + \frac{1}{2}(\mu E^{m,2} n^{m,2})_x\\
&\quad - \frac{1}{2}\sqrt{\tau\theta} q_x^{m,1} + \frac{1}{2}\sqrt{\tau\theta} q_x^{m,2} + \frac{1}{2}\sqrt{\tau\theta} q_x^{m,3},\\
\frac{n^{m+1} - n^m}{\Delta t} &= \frac{1}{4}(\mu E^m n^m)_x + \frac{7}{4}(\mu E^{m,1} n^{m,1})_x + \frac{3}{4}(\mu E^{m,2} n^{m,2})_x - \frac{7}{4}(\mu E^{m,3} n^{m,3})_x\\
&\quad + \frac{3}{2}\sqrt{\tau\theta} q_x^{m,1} - \frac{3}{2}\sqrt{\tau\theta} q_x^{m,2} + \frac{1}{2}\sqrt{\tau\theta} q_x^{m,3} + \frac{1}{2}\sqrt{\tau\theta} q_x^{m+1} + \frac{\zeta^m}{\Delta t},\\
q^{m,l} &= \sqrt{\tau\theta} n_x^{m,l}, \quad l = 1,2,3,4,
\end{aligned} \tag{5.58}$$

and

$$E^{m,l} = -\phi_x^{m,l}, \quad E_x^{m,l} = -\frac{e}{\varepsilon}(n^{m,l} - n_d), \quad l = 0,1,2,3, \tag{5.59}$$

where $n^m$ is the exact solution $n$ on time level $m$, $\zeta^m$ is the local truncation error of the third order IMEX RK method and $\|\zeta^m\| \leqslant C(\Delta t)^4$. Then we get the weak forms of the concentration equation,

$$\begin{cases}(F_l n^m, v) = \Phi_l(\boldsymbol{E}^m, \boldsymbol{n}^m, v) + \Psi_l(\boldsymbol{q}^m, v) + \delta_l(\zeta^m, v), \\ (q^{m,l}, w) = H^+(n^{m,l}), w), \quad l = 1, 2, 3, 4.\end{cases} \tag{5.60}$$

Here, $\boldsymbol{n}^m = (n^m, n^{m,1}, n^{m,2}, n^{m,3})$, $\boldsymbol{q}^m = (q^{m,1}, q^{m,2}, q^{m,3}, q^{m+1})$, and $\delta_l = 0$ if $l = 1, 2, 3$, $\delta_4 = 1$. Now, we get the error equation

$$\begin{cases}(F_l \xi_n^m, v) = \Phi_l(\boldsymbol{E}^m, \boldsymbol{n}^m, v) - \Phi_l(\boldsymbol{E}_h^m, \boldsymbol{n}_h^m, v) + \Psi_l(\boldsymbol{\xi}_q^m, v) + (F_l \eta_n^m + \delta_l \zeta^m, v), \\ (\xi_q^{m,l}, w) = H^+(\xi_n^{m,l}, w) + (\eta_q^{m,l}, w), \quad l = 1, 2, 3, 4,\end{cases} \tag{5.61}$$

since the projection error related terms in $\Psi_l$ and $H^+$ vanish by the property of the projection (2.3). Taking $v = \xi_n^{m,1}, D_1\xi_n^m, D_2\xi_n^m, \xi_n^{m+1}$ in (5.61), and writing $F_4\xi_n^m = F_{41}\xi_n^m + F_{42}\xi_n^m$, we have

$$\begin{aligned}&\frac{1}{2}\|\xi_n^{m,1}\|^2 + \frac{1}{2}\|F_1\xi_n^m\|^2 - \frac{1}{2}\|\xi_n^m\|^2 \\ &\quad = \Phi_1(\boldsymbol{E}^m, \boldsymbol{n}^m, \xi_n^{m,1}) - \Phi_1(\boldsymbol{E}_h^m, \boldsymbol{n}_h^m, \xi_n^{m,1}) + \Psi_1(\boldsymbol{\xi}_q^m, \xi_n^{m,1}) + (F_1\eta_n^m, \xi_n^{m,1}),\end{aligned} \tag{5.62}$$

$$\begin{aligned}&\frac{1}{2}\|D_1\xi_n^m\|^2 + \frac{1}{2}\|F_2\xi_n^m\|^2 - \frac{1}{2}\|\xi_n^m\|^2 \\ &\quad = \Phi_2(\boldsymbol{E}^m, \boldsymbol{n}^m, D_1\xi_n^m) - \Phi_2(\boldsymbol{E}_h^m, \boldsymbol{n}_h^m, D_1\xi_n^m) + \Psi_2(\boldsymbol{\xi}_q^m, D_1\xi_n^m) + (F_2\eta_n^m, D_1\xi_n^m),\end{aligned} \tag{5.63}$$

$$\begin{aligned}&\frac{1}{2}\|D_2\xi_n^m\|^2 + \frac{1}{2}\|F_3\xi_n^m\|^2 - \frac{1}{2}\|\xi_n^{m,1}\|^2 \\ &\quad = \Phi_3(\boldsymbol{E}^m, \boldsymbol{n}^m, D_2\xi_n^m) - \Phi_3(\boldsymbol{E}_h^m, \boldsymbol{n}_h^m, D_2\xi_n^m) + \Psi_3(\boldsymbol{\xi}_q^m, D_2\xi_n^m) + (F_3\eta_n^m, D_2\xi_n^m),\end{aligned} \tag{5.64}$$

$$\begin{aligned}&\|\xi_n^{m+1}\|^2 + \frac{1}{2}\|F_{41}\xi_n^m\|^2 + \frac{1}{2}\|F_{42}\xi_n^m\|^2 - \frac{1}{2}\|D_1\xi_n^m\|^2 - \frac{1}{2}\|D_2\xi_n^m\|^2 \\ &\quad = \Phi_4(\boldsymbol{E}^m, \boldsymbol{n}^m, \xi_n^{m+1}) - \Phi_4(\boldsymbol{E}_h^m, \boldsymbol{n}_h^m, \xi_n^{m+1}) \\ &\qquad + \Psi_4(\boldsymbol{\xi}_q^m, \xi_n^{m+1}) + (F_4\eta_n^m, \xi_n^{m+1}) + (O(\Delta t)^4, \xi_n^{m+1}).\end{aligned} \tag{5.65}$$

Adding them together, we have

$$\|\xi_n^{m+1}\|^2 - \|\xi_n^m\|^2 + S = T_\Phi + T_\Psi + T_\eta, \tag{5.66}$$

where $S = \frac{1}{2}\|F_1\xi_n^m\|^2 + \frac{1}{2}\|F_2\xi_n^m\|^2 + \frac{1}{2}\|F_3\xi_n^m\|^2 + \frac{1}{2}\|F_{41}\xi_n^m\|^2 + \frac{1}{2}\|F_{42}\xi_n^m\|^2$, and

$$\begin{aligned}T_\Phi &= \Phi_1(\boldsymbol{E}^m, \boldsymbol{n}^m, \xi_n^{m,1}) - \Phi_1(\boldsymbol{E}_h^m, \boldsymbol{n}_h^m, \xi_n^{m,1}) + \Phi_2(\boldsymbol{E}^m, \boldsymbol{n}^m, D_1\xi_n^m) - \Phi_2(\boldsymbol{E}_h^m, \boldsymbol{n}_h^m, D_1\xi_n^m) \\ &\quad + \Phi_3(\boldsymbol{E}^m, \boldsymbol{n}^m, D_2\xi_n^m) - \Phi_3(\boldsymbol{E}_h^m, \boldsymbol{n}_h^m, D_2\xi_n^m) + \Phi_4(\boldsymbol{E}^m, \boldsymbol{n}^m, \xi_n^{m+1}) - \Phi_4(\boldsymbol{E}_h^m, \boldsymbol{n}_h^m, \xi_n^{m+1}), \\ T_\Psi &= \Psi_1(\boldsymbol{\xi}_q^m, \xi_n^{m,1}) + \Psi_2(\boldsymbol{\xi}_q^m, D_1\xi_n^m) + \Psi_3(\boldsymbol{\xi}_q^m, D_2\xi_n^m) + \Psi_4(\boldsymbol{\xi}_q^m, \xi_n^{m+1}), \\ T_\eta &= (F_1\eta_n^m, \xi_n^{m,1}) + (F_2\eta_n^m, D_1\xi_n^m) + (F_3\eta_n^m, D_2\xi_n^m) + (F_4\eta_n^m, \xi_n^{m+1}) + (O(\Delta t)^4, \xi_n^{m+1}).\end{aligned}$$

Easily from Schwarz's inequality and the property of the projection, we can get

$$T_\eta \leqslant C\Delta t \sum_{l=1}^{4} \|\xi_n^{m,l}\|^2 + C\Delta t h^{2k+2} + C(\Delta t)^7. \tag{5.67}$$

To estimate $T_\Psi$, from the definition of $H^\pm$ in (5.2) and the error equation (5.61), we first have

$$H^-(\xi_q, \xi_n) = -H^+(\xi_n, \xi_q) = -\|\xi_q\|^2 + (\eta_q, \xi_q), \tag{5.68}$$

and

$$H^-(\xi_q^1, \xi_n^2) = -H^+(\xi_n^2, \xi_q^1) = -(\xi_q^2, \xi_q^1) + (\eta_q^2, \xi_q^1). \tag{5.69}$$

Then we have $T_\Psi = T_{\eta q} + T_{\xi q}$, where

$$T_{\eta q} = \frac{1}{2}(\eta_q^{m,1}, \xi_q^{m,1})\Delta t + \frac{1}{3}(D_1\eta_q^m, \xi_q^{m,1})\Delta t + \frac{1}{2}(D_1\eta_q^m, D_1\xi_q^m)\Delta t$$

$$
\begin{aligned}
&-\frac{7}{12}(D_2\eta_q^{m,1},\xi_q^{m,1})\Delta t+\frac{1}{4}(D_2\eta_q^{m},D_1\xi_q^{m})\Delta t+\frac{1}{2}(D_2\eta_q^{m},D_2\xi_q^{m})^2\Delta t\\
&-\frac{1}{12}(\eta_q^{m+1},\xi_q^{m,1})\Delta t-\frac{1}{4}(\eta_q^{m+1},D_1\xi_q^{m})\Delta t+\frac{1}{2}(\eta_q^{m+1},D_2\xi_q^{m})\Delta t+(\eta_q^{m+1},\xi_q^{m+1})\Delta t,
\end{aligned}
$$

$$
\begin{aligned}
T_{\xi q}=&-\frac{1}{2}\|\xi_q^{m,1}\|^2\Delta t-\frac{1}{3}(D_1\xi_q^{m},\xi_q^{m,1})\Delta t-\frac{1}{2}\|D_1\xi_q^{m}\|^2\Delta t\\
&+\frac{7}{12}(D_2\xi_q^{m,1},\xi_q^{m,1})\Delta t-\frac{1}{4}(D_2\xi_q^{m,1},D_1\xi_q^{m})\Delta t-\frac{1}{2}\|D_2\xi_q^{m}\|^2\Delta t\\
&+\frac{1}{12}(\xi_q^{m+1},\xi_q^{m,1})\Delta t+\frac{1}{4}(\xi_q^{m+1},D_1\xi_q^{m})\Delta t-\frac{1}{2}(\xi_q^{m+1},D_2\xi_q^{m})\Delta t-\|\xi_q^{m+1}\|^2\Delta t\\
=&-\Delta t\int_I \boldsymbol{\xi}_q^{\mathrm{T}}\boldsymbol{M}\boldsymbol{\xi}_q dx,
\end{aligned}
$$

here, $\boldsymbol{\xi}_q^{\mathrm{T}}=(\xi_q^{m,1},D_1\xi_q^{m},D_2\xi_q^{m},\xi_q^{m+1})$, and

$$
\boldsymbol{M}=\begin{pmatrix}
\frac{1}{2} & \frac{1}{6} & -\frac{7}{24} & -\frac{1}{24}\\
\frac{1}{6} & \frac{1}{2} & -\frac{1}{8} & -\frac{1}{8}\\
-\frac{7}{24} & \frac{1}{8} & -\frac{1}{2} & \frac{1}{4}\\
-\frac{1}{24} & -\frac{1}{8} & \frac{1}{4} & 1
\end{pmatrix}.
$$

It can be verified that $\boldsymbol{M}$ is positive definite by verifying the principle minor determinants of $\boldsymbol{M}$ are all positive, so $T_{\xi q}\leqslant 0$.

And using Young's inequality, for $\forall\,\tilde{\varepsilon}>0$, we have $T_{\eta q}\leqslant\tilde{\varepsilon}\Delta t\int_I\boldsymbol{\xi}_q^{\mathrm{T}}\boldsymbol{\xi}_q dx+C_{\tilde{\varepsilon}}\Delta t\sum_{l=1}^{4}\|\eta_q^{m,l}\|^2$, where $C_{\tilde{\varepsilon}}$ is a positive constant only depending on $\tilde{\varepsilon}$. Then we have

$$
T_{\Psi}\leqslant-\Delta t\int_I\boldsymbol{\xi}_q^{\mathrm{T}}(\boldsymbol{M}-\tilde{\varepsilon}\boldsymbol{I})\boldsymbol{\xi}_q dx+C_{\tilde{\varepsilon}}\Delta t h^{2k+2}. \tag{5.70}
$$

Finally, we estimate $T_{\Phi}$ as follows:

$$
\begin{aligned}
T_{\Phi}&=\sum_{l=1}^{4}(\Phi_l(\boldsymbol{E}^m,\boldsymbol{n}^m,v_l)-\Phi_l(\boldsymbol{E}_h^m,\boldsymbol{n}_h^m,v_l))\\
&=\Delta t\sum_{l=1}^{4}\sum_{i=0}^{3}\delta_{li}(H(E^{m,i},n^{m,i},v_l)-H(E_h^{m,i},n_h^{m,i},v_l)).
\end{aligned}
$$

Here and below we use the notation $v_1=\xi_n^{m,1}$, $v_2=D_1\xi_n^{m}$, $v_3=D_2\xi_n^{m}$, $v_4=D_1\xi_n^{m+1}$, and $\delta_{li}$ are listed in Table 1.

For each $H(E^{m,i},n^{m,i},v_l)-H(E_h^{m,i},n_h^{m,i},v_l)$ in $T_{\Phi}$, from the definition of $H$, we have

$$
\begin{aligned}
&H(E^{m,i},n^{m,i},v_l)-H(E_h^{m,i},n_h^{m,i},v_l)\\
&\quad=-(\mu E^{m,i}n^{m,i}-\mu E_h^{m,i}n_h^{m,i},v_{l,x})-\sum_{j=1}^{M}(\mu E^{m,i}n^{m,i}-\mu\widehat{E_h^{m,i}n_h^{m,i}})_{j-\frac{1}{2}}[v_l]_{j-\frac{1}{2}}.
\end{aligned}
$$

**Table 1** The value of $\delta_{li}$

| | $\delta_{li}$ | | | |
|---|---|---|---|---|
| $li$ | 0 | 1 | 2 | 3 |
| 1 | $\frac{1}{2}$ | 0 | 0 | 0 |
| 2 | $-\frac{5}{18}$ | $\frac{1}{9}$ | 0 | 0 |
| 3 | $\frac{1}{9}$ | $-\frac{17}{18}$ | $\frac{1}{2}$ | 0 |
| 4 | $-\frac{7}{18}$ | $\frac{41}{9}$ | 1 | $-\frac{7}{2}$ |

Similar analysis as the term $T_{17}$ in the first order IMEX LDG scheme, we get

$$|H(E^{m,i},n^{m,i},v_l)-H(E_h^{m,i},n_h^{m,i},v_l)|\leqslant C\bigg(\sum_{i=0}^{3}\|\xi_n^{m,i}\|^2+h^{2k+2}\bigg)+\tilde{\varepsilon}(\|v_{l,x}\|^2+h^{-1}[v_l]^2). \tag{5.71}$$

Then we have

$$\begin{aligned}T_\Phi\leqslant{}& C\Delta t(\sum_{l=0}^{3}\|\xi_n^{m,l}\|^2+h^{2k+2})+\tilde{\varepsilon}\Delta t(\|\xi_{n,x}^{m,1}\|^2+\|D_1\xi_{n,x}^{m}\|^2+\|D_2\xi_{n,x}^{m}\|^2+\|\xi_{n,x}^{m+1}\|^2)\\&+\tilde{\varepsilon}\Delta t h^{-1}([\xi_n^{m,1}]^2+[D_1\xi_n^m]^2+[D_2\xi_n^m]^2+[\xi_n^{m+1}]^2).\end{aligned}$$

Noting that for any pair of $(\xi_n^{m,l},\xi_q^{m,l}), l=1,2,3,4$, we have the similar result as (5.49). Moreover, by the linear structure of (5.61), (5.49) also holds for any linear combination of any pairs of $(\xi_n^{m,l},\xi_q^{m,l})$. For example, for $v_2=D_1\xi_n^m=2\xi_n^{m,2}-3\xi_n^{m,1}$, we have

$$\begin{aligned}\|v_{2,x}\|&\leqslant\frac{C_\mu}{\sqrt{\tau\theta}}(\|2\xi_q^{m,2}-3\xi_q^{m,1}\|+\|2\eta_q^{m,2}-3\eta_q^{m,1}\|),\\h^{-\frac{1}{2}}[D_1\xi_n^m]&\leqslant\frac{C_\mu}{\sqrt{\tau\theta}}(\|2\xi_q^{m,2}-3\xi_q^{m,1}\|+\|2\eta_q^{m,2}-3\eta_q^{m,1}\|).\end{aligned}$$

Hence, from (5.49) ($l=1,2,3,4$), the above inequalities and the property of the projection (2.3), we have

$$T_\Phi\leqslant C\Delta t\bigg(\sum_{l=0}^{3}\|\xi_n^{m,l}\|^2+h^{2k+2}\bigg)+\tilde{\varepsilon}\Delta t\int_I\boldsymbol{\xi}_q^{\mathrm{T}}\boldsymbol{\xi}_q dx. \tag{5.72}$$

Substituting (5.67), (5.70) and (5.72) into (5.66), we obtain

$$\|\xi_n^{m+1}\|^2-\|\xi_n^m\|^2+S\leqslant C\Delta t\bigg(\sum_{l=0}^{4}\|\xi_n^{m,l}\|^2+h^{2k+2}\bigg)+C(\Delta t)^7-\Delta t\int_I\boldsymbol{\xi}_q^{\mathrm{T}}(\boldsymbol{M}-2\tilde{\varepsilon}\boldsymbol{I})\boldsymbol{\xi}_q dx.$$

We can choose $\tilde{\varepsilon}$ small enough, so that $\int_I\boldsymbol{\xi}_q^{\mathrm{T}}(\boldsymbol{M}-2\tilde{\varepsilon}\boldsymbol{I})\boldsymbol{\xi}_q dx\geqslant 0$. Then we get

$$\|\xi_n^{m+1}\|^2-\|\xi_n^m\|^2\leqslant C\Delta t\sum_{l=0}^{4}\|\xi_n^{m,l}\|^2+C\Delta t h^{2k+2}+C(\Delta t)^7. \tag{5.73}$$

Similar argument as the result of (5.73), we can get

$$\|\xi_n^{m,l}\|^2\leqslant C(\|\xi_n^m\|^2+\Delta t h^{2k+2}+(\Delta t)^7),\quad l=1,2,3. \tag{5.74}$$

Combining the above two inequalities (5.73) and (5.74), using the discrete Gronwall inequality, we can obtain

$$\|\xi_n\|_{L^\infty(0,T;L^2(I))}\leqslant C(\Delta t)^3+Ch^{k+1}. \tag{5.75}$$

This completes the proof. □

## 6 Error estimates of the LDG method with Dirichlet boundary conditions

We have used periodic boundary condition for the concentration equation in the previous sections to simplify the analysis. In practice, the boundary condition of the models of semiconductor devices is usually Dirichlet. In this section, we discuss the error estimates of LDG method with Dirichlet boundary conditions. We only give the detailed analysis for the semi-discrete scheme, as the analysis for the fully-discrete schemes follows the same lines but is more tedious.

The Dirichlet boundary condition is

$$n(0,t) = n_l, \quad n(1,t) = n_r \tag{6.1}$$

$$\phi(0,t) = 0, \quad \phi(1,t) = v_{\text{bias}}. \tag{6.2}$$

The semi-discrete LDG scheme is the same as (4.1)–(4.4), except that the fluxes $\hat{n}_h$ and $\hat{q}_h$ should be changed at one of the boundaries to take care of the Dirichlet boundary condition. We choose the flux for $\hat{n}_h$ and $\hat{q}_h$ similarly to (4.6) or (4.7) as the following because of the Dirichlet boundary condition:

$$\begin{aligned}&(\hat{n}_h)_{\frac{1}{2}} = (n_h^-)_{\frac{1}{2}} = n_l, \quad (\hat{n}_h)_{j-\frac{1}{2}} = (n_h^+)_{j-\frac{1}{2}}, \quad j = 2,\dots,N, \quad (\hat{n}_h)_{N+\frac{1}{2}} = (n_h^+)_{N+\frac{1}{2}} = n_r,\\ &(\hat{q}_h)_{\frac{1}{2}} = (q_h^+)_{\frac{1}{2}}, \quad (\hat{q}_h)_{j-\frac{1}{2}} = (q_h^-)_{j-\frac{1}{2}}, \quad j = 2,\dots,N+1.\end{aligned} \tag{6.3}$$

Or

$$\begin{aligned}&(\hat{n}_h)_{\frac{1}{2}} = (n_h^-)_{\frac{1}{2}} = n_l, \quad (\hat{n}_h)_{j-\frac{1}{2}} = (n_h^-)_{j-\frac{1}{2}}, \quad j = 2,\dots,N, \quad (\hat{n}_h)_{N+\frac{1}{2}} = (n_h^+)_{N+\frac{1}{2}} = n_r,\\ &(\hat{q}_h)_{j-\frac{1}{2}} = (q_h^+)_{j-\frac{1}{2}}, \quad j = 1,\dots,N, \quad (\hat{q}_h)_{N+\frac{1}{2}} = (q_h^-)_{N+\frac{1}{2}}.\end{aligned} \tag{6.4}$$

The fluxes $\hat{E}_h$ and $\hat{\phi}_h$ are the same as before. Then we get the following error estimate.

**Theorem 6.1.** *Let $n, q$ be the exact solution to* (3.7)–(3.10)*, which is sufficiently smooth with bounded derivatives. Let $n_h, q_h$ be the numerical solution of the semi-discrete LDG scheme* (4.1)–(4.4)*, and choose the fluxes of $\hat{n}_h, \hat{q}_h$ as* (6.3) *or* (6.4)*. Denote the corresponding numerical error by $e_u = u - u_h$ $(u = n, q)$. If the finite element space $V_h^k$ is the piecewise polynomials of degree $k \geqslant 0$, then for small enough $h$ there holds the following error estimates*

$$\|n - n_h\|_{L^\infty(0,T;L^2)} + \|q - q_h\|_{L^2(0,T;L^2)} \leqslant Ch^{k+\frac{1}{2}}, \tag{6.5}$$

*where the constant $C$ depends on the final time $T$, $k$, $C_\mu$, the inverse constant $C_2$, $\|n\|_{L^\infty(0,T;W_\infty^{k+1})}$, $\|n_x\|_{L^\infty}$ and $\|E\|_{L^\infty}$.*

*Proof.* Taking the difference of (3.7) and (4.1) and the difference of (3.8) and (4.2), we get the same error equations (4.12) and (4.13). Taking the flux (6.3) for example, we have

$$\begin{aligned}&\int_{I_j} \xi_{n,t} v dx + \int_{I_j} \sqrt{\tau\theta}\xi_q v_x dx + \int_{I_j} \mu(En - E_h n_h) v_x dx\\ &\quad - \mu(\widehat{En - E_h n_h})_{j+\frac{1}{2}} v_{j+\frac{1}{2}}^- + \mu(\widehat{En - E_h n_h})_{j-\frac{1}{2}} v_{j-\frac{1}{2}}^+\\ &\quad = \int_{I_j} \eta_{n,t} v dx + \sqrt{\tau\theta}\xi_{q,j+\frac{1}{2}}^- v_{j+\frac{1}{2}}^- - \sqrt{\tau\theta}\xi_{q,j-\frac{1}{2}}^- v_{j-\frac{1}{2}}^+,\\ &\int_{I_j} \xi_q w dx + \int_{I_j} \sqrt{\tau\theta}\xi_n w_x dx = \int_{I_j} \eta_q w dx + \sqrt{\tau\theta}\xi_{n,j+\frac{1}{2}}^+ w_{j+\frac{1}{2}}^- - \sqrt{\tau\theta}\xi_{n,j-\frac{1}{2}}^+ w_{j-\frac{1}{2}}^+,\end{aligned}$$

for $j = 2,\dots,N-1$, and

$$\begin{aligned}&\int_{I_1} \xi_{n,t} v dx + \int_{I_1} \sqrt{\tau\theta}\xi_q v_x dx\\ &\quad + \int_{I_1} \mu(En - E_h n_h) v_x dx - \mu(\widehat{En - E_h n_h})_{\frac{3}{2}} v_{\frac{3}{2}}^- + \mu(\widehat{En - E_h n_h})_{\frac{1}{2}} v_{\frac{1}{2}}^+\\ &\quad = \int_{I_1} \eta_{n,t} v dx + \sqrt{\tau\theta}\xi_{q,\frac{3}{2}}^- v_{\frac{3}{2}}^- - (\sqrt{\tau\theta}\xi_{q,\frac{1}{2}}^+ v_{\frac{1}{2}}^+ - \sqrt{\tau\theta}\eta_{q,\frac{1}{2}}^+ v_{\frac{1}{2}}^+),\\ &\int_{I_1} \xi_q w dx + \int_{I_1} \sqrt{\tau\theta}\xi_n w_x dx = \int_{I_1} \eta_q w dx + \sqrt{\tau\theta}\xi_{n,\frac{3}{2}}^+ w_{\frac{3}{2}}^-,\end{aligned}$$

and

$$\int_{I_N} \xi_{n,t} v dx + \int_{I_N} \sqrt{\tau\theta}\xi_q v_x dx$$

$$
\begin{aligned}
&+\int_{I_N}\mu(En-E_hn_h)v_xdx-\mu(En-\widehat{E_hn_h})_{N+\frac{1}{2}}v^-_{N+\frac{1}{2}}+\mu(En-\widehat{E_hn_h})_{N-\frac{1}{2}}v^+_{N-\frac{1}{2}}\\
&=\int_{I_N}\eta_{n,t}vdx+\sqrt{\tau\theta}\xi^-_{q,N+\frac{1}{2}}v^-_{N+\frac{1}{2}}-\sqrt{\tau\theta}\xi^-_{q,N-\frac{1}{2}}v^+_{N-\frac{1}{2}},\\
&\int_{I_N}\xi_qwdx+\int_{I_N}\sqrt{\tau\theta}\xi_nw_xdx=\int_{I_N}\eta_qwdx-\sqrt{\tau\theta}\xi^+_{n,N-\frac{1}{2}}w^+_{N-\frac{1}{2}}.
\end{aligned}
$$

We get the above equalities for $j=1,\dots,N$ by using the projection

$$
\begin{aligned}
&\int_{I_j}\eta_nw_xdx=0,\quad \eta^+_{n,j-\frac{1}{2}}=0,\\
&\int_{I_j}\eta_qv_xdx=0,\quad \eta^-_{q,j+\frac{1}{2}}=0,
\end{aligned}
$$

and $(n-\hat{n}_h)_{\frac{1}{2}}=0$, $(n-\hat{n}_h)_{N+\frac{1}{2}}=0$.

Still choosing $v=\xi_n$, $w=\xi_q$ and summing $j$ from 1 to $N$, we get

$$
\begin{aligned}
\sum_{j=1}^N\int_{I_j}\xi_{n,t}\xi_ndx+\sum_{j=1}^N\int_{I_j}\xi_q^2dx&=\sum_{j=1}^N\int_{I_j}\eta_{n,t}\xi_ndx+\sum_{j=1}^N\int_{I_j}\eta_q\xi_qdx\\
&\quad+\sum_{j=1}^N\bigg(-\int_{I_j}\sqrt{\tau\theta}\xi_q\xi_{n,x}dx-\int_{I_j}\sqrt{\tau\theta}\xi_n\xi_{q,x}dx\bigg)\\
&\quad+\sum_{j=1}^N(\sqrt{\tau\theta}\xi^-_{q,j+\frac{1}{2}}\xi^-_{n,j+\frac{1}{2}}-\sqrt{\tau\theta}\xi^-_{q,j-\frac{1}{2}}\xi^+_{n,j-\frac{1}{2}})\\
&\quad+\sqrt{\tau\theta}\xi^-_{q,\frac{1}{2}}\xi^+_{n,\frac{1}{2}}-\sqrt{\tau\theta}\xi^+_{q,\frac{1}{2}}\xi^+_{n,\frac{1}{2}}+\sqrt{\tau\theta}\eta^+_{q,\frac{1}{2}}\xi^+_{n,\frac{1}{2}}\\
&\quad+\sum_{j=2}^{N-1}(\sqrt{\tau\theta}\xi^+_{n,j+\frac{1}{2}}\xi^-_{q,j+\frac{1}{2}}-\sqrt{\tau\theta}\xi^+_{n,j-\frac{1}{2}}\xi^+_{q,j-\frac{1}{2}})\\
&\quad+\sqrt{\tau\theta}\xi^+_{n,\frac{3}{2}}\xi^-_{q,\frac{3}{2}}-\sqrt{\tau\theta}\xi^+_{n,N-\frac{1}{2}}\xi^+_{q,N-\frac{1}{2}}\\
&\quad+\sum_{j=1}^N\bigg(-\int_{I_j}\mu(En-E^hn^h)\xi_{n,x}dx\\
&\quad+\mu(En-\widehat{E^hn^h})_{j+\frac{1}{2}}\xi^-_{n,j+\frac{1}{2}}-\mu(En-\widehat{E^hn^h})_{j-\frac{1}{2}}\xi^+_{n,j-\frac{1}{2}}\bigg)\\
&=:T_1+T_2+T_3+T_4.
\end{aligned}
\tag{6.6}
$$

We analyze $T_1,T_2$ and $T_4$ as before. For $T_3$, after a trivial deduction, we have

$$
T_3=\sqrt{\tau\theta}\eta^+_{q,\frac{1}{2}}\xi^+_{n,\frac{1}{2}}\leqslant Ch^{-1}|\eta^+_{q,\frac{1}{2}}|^2+Ch|\xi^+_{n,\frac{1}{2}}|^2\leqslant Ch^{2k+1}+C\|\xi_n\|^2. \tag{6.7}
$$

Then (4.26) is changed to be

$$
\frac{1}{2}\frac{d}{dt}\|\xi_n\|^2+\|\xi_q\|^2\leqslant C\|\xi_n\|^2+Ch^{2k+1}+\tilde{\varepsilon}\|\xi_{n,x}\|^2+\tilde{\varepsilon}h^{-1}[\xi_n]^2+\tilde{\varepsilon}\|\xi_q\|^2. \tag{6.8}
$$

Using Lemma 4.3, together with the property of the projection and the Gronwall inequality, we can obtain the theorem. □

**Remark 6.2.** If we choose the flux at the boundary as

$$
(\hat{q}_h)_{\frac{1}{2}}=(q_h^+)_{\frac{1}{2}}+c_0[n_h]_{\frac{1}{2}}. \tag{6.9}
$$

we can obtain the following optimal error estimate.

**Theorem 6.3.** *Replace the flux $(\hat{q}_h)_{\frac{1}{2}}$ in (6.3) by (6.9) in Theorem 6.1, we have the following optimal error estimates:*

$$\|n-n_h\|_{L^\infty(0,T;L^2)}+\|q-q_h\|_{L^2(0,T;L^2)}\leqslant Ch^{k+1}, \tag{6.10}$$

*where the constant $C$ depends on the final time $T$, $k$, $C_\mu$, the inverse constant $C_2$, $\|n\|_{L^\infty(0,T;W^{k+1}_\infty)}$, $\|n_x\|_{L^\infty}$ and $\|E\|_{L^\infty}$.*

*Proof.* Comparing with the proof of Theorem 6.1, we have

$$\begin{aligned}&\int_{I_1}\xi_{n,t}vdx+\int_{I_1}\sqrt{\tau\theta}\xi_q v_x dx+\int_{I_1}\mu(En-E_hn_h)v_xdx\\&\quad-\mu(En-\widehat{E_hn_h})_{\frac{3}{2}}v^-_{\frac{3}{2}}+\mu(En-\widehat{E_hn_h})_{\frac{1}{2}}v^+_{\frac{1}{2}}\\&\qquad=\int_{I_1}\eta_{n,t}vdx+\sqrt{\tau\theta}\xi^-_{q,\frac{3}{2}}v^-_{\frac{3}{2}}-(\sqrt{\tau\theta}\xi^+_{q,\frac{1}{2}}v^+_{\frac{1}{2}}-\sqrt{\tau\theta}\eta^+_{q,\frac{1}{2}}v^+_{\frac{1}{2}}-c_0\sqrt{\tau\theta}[n_h]_{\frac{1}{2}}v^+_{\frac{1}{2}}).\end{aligned}$$

Then

$$\begin{aligned}T_3&=\sum_{j=1}^N\bigg(-\int_{I_j}\sqrt{\tau\theta}\xi_q\xi_{n,x}dx-\int_{I_j}\sqrt{\tau\theta}\xi_n\xi_{q,x}dx\bigg)\\&\quad+\sum_{j=1}^N(\sqrt{\tau\theta}\xi^-_{q,j+\frac{1}{2}}\xi^-_{n,j+\frac{1}{2}}-\sqrt{\tau\theta}\xi^-_{q,j-\frac{1}{2}}\xi^+_{n,j-\frac{1}{2}})\\&\quad+\sqrt{\tau\theta}\xi^-_{q,\frac{1}{2}}\xi^+_{n,\frac{1}{2}}-\sqrt{\tau\theta}\xi^+_{q,\frac{1}{2}}\xi^+_{n,\frac{1}{2}}+\sqrt{\tau\theta}\eta^+_{q,\frac{1}{2}}\xi^+_{n,\frac{1}{2}}+c_0\sqrt{\tau\theta}[n_h]_{\frac{1}{2}}\xi^+_{n,\frac{1}{2}}\\&\quad+\sum_{j=2}^{N-1}(\sqrt{\tau\theta}\xi^+_{n,j+\frac{1}{2}}\xi^-_{q,j+\frac{1}{2}}-\sqrt{\tau\theta}\xi^+_{n,j-\frac{1}{2}}\xi^+_{q,j-\frac{1}{2}})\\&\quad+\sqrt{\tau\theta}\xi^+_{n,\frac{3}{2}}\xi^-_{q,\frac{3}{2}}-\sqrt{\tau\theta}\xi^+_{n,N-\frac{1}{2}}\xi^+_{q,N-\frac{1}{2}}\\&=\sqrt{\tau\theta}\eta^+_{q,\frac{1}{2}}\xi^+_{n,\frac{1}{2}}+c_0\sqrt{\tau\theta}[n_h]_{\frac{1}{2}}\xi^+_{n,\frac{1}{2}}\\&=\sqrt{\tau\theta}\eta^+_{q,\frac{1}{2}}\xi^+_{n,\frac{1}{2}}+c_0\sqrt{\tau\theta}((n-n_h^-)-(n-n_h^+))_{\frac{1}{2}}\xi^+_{n,\frac{1}{2}}\\&=\sqrt{\tau\theta}\eta^+_{q,\frac{1}{2}}\xi^+_{n,\frac{1}{2}}-c_0\sqrt{\tau\theta}(\xi^+_{n,\frac{1}{2}})^2,\end{aligned}$$

since $n_{\frac{1}{2}}=(n_h^-)_{\frac{1}{2}}$ and $\eta^+_{n,\frac{1}{2}}=0$. So

$$T_3\leqslant C|\eta^+_{q,\frac{1}{2}}|^2+\tilde{\varepsilon}|\xi^+_{n,\frac{1}{2}}|^2-c_0\sqrt{\tau\theta}|\xi^+_{n,\frac{1}{2}}|^2\leqslant Ch^{2k+2}-(c_0\sqrt{\tau\theta}-\tilde{\varepsilon})|\xi^+_{n,\frac{1}{2}}|^2.$$

Then (6.8) is changed to be

$$\frac{1}{2}\frac{d}{dt}\|\xi_n\|^2+\|\xi_q\|^2\leqslant C\|\xi_n\|^2+Ch^{2k+2}+\tilde{\varepsilon}\|\xi_{n,x}\|^2+\tilde{\varepsilon}h^{-1}[\xi_n]^2+\tilde{\varepsilon}\|\xi_q\|^2-(c_0\sqrt{\tau\theta}-\tilde{\varepsilon})|\xi^+_{n,\frac{1}{2}}|^2. \tag{6.11}$$

We can choose $\tilde{\varepsilon}$ small enough so that $c_0\sqrt{\tau\theta}-\tilde{\varepsilon}\geqslant 0$ to get the optimal error result in Theorem 6.3. □

## 7 Numerical simulation

In this section, we show the simulation results of the third order IMEX LDG scheme, until a steady state is reached for our steady state diode test case. We also show the results by the third order explicit total variation diminishing (TVD) Runge-Kutta time discretization [26] for comparison. Since different choices of bases for $V_h^k$ do not alter the algorithm, we choose locally orthogonal Legendre polynomial basis over $I_j=(x_{j-1/2},x_{j+1/2})$, $v_0^{(j)}(x)=1$, $v_1^{(j)}(x)=x-x_j$, $v_2^{(j)}(x)=(x-x_j)^2-\frac{1}{12}\Delta x_j^2,\dots$ In our implementation, we use scaled Legendre polynomial basis over $[-\frac{1}{2},\frac{1}{2}]$, $v_0^{(j)}(\xi)=1$, $v_1^{(j)}(\xi)=\xi$, $v_2^{(j)}(\xi)=\xi^2-\frac{1}{12},\dots,$

**Table 2** The time step $\Delta t$, the number of time steps $n_{steps}$, the time $t$, and the CPU time to reach the steady state for third order RK LDG and third order IMEX LDG methods with 100 mesh cells in $[0, 0.6]$

| | Third order EX-RK | Third order IMEX | | | | |
|---|---|---|---|---|---|---|
| $\Delta t$ | 1.688e−5 | 1.2e−3 | 1.8e−3 | 2.4e−3 | 3.0e−3 | 3.6e−3 |
| $n_{\text{steps}}$ | 44063 | 711 | 476 | 356 | 286 | 239 |
| $t$ | 0.7436 | 0.8532 | 0.8568 | 0.8544 | 0.8580 | 0.8604 |
| CPU time | 58.8904 | 4.6332 | 3.4008 | 2.5272 | 2.0592 | 1.4820 |

**Table 3** The time step $\Delta t$, the number of time steps $n_{steps}$, the time $t$, and the CPU time to reach the steady state for third order RK LDG and third order IMEX LDG methods with 200 mesh cells in $[0, 0.6]$

| | Third order EX-RK | Third order IMEX | | | | |
|---|---|---|---|---|---|---|
| $\Delta t$ | 4.22e−6 | 1.2e−3 | 1.8e−3 | 2.4e−3 | 3.0e−3 | 3.6e−3 |
| $n_{\text{steps}}$ | 176081 | 727 | 480 | 360 | 298 | 249 |
| $t$ | 0.7431 | 0.8724 | 0.8640 | 0.8640 | 0.8940 | 0.8964 |
| CPU time | 202.3957 | 7.5349 | 5.5224 | 4.3680 | 3.4476 | 3.2760 |

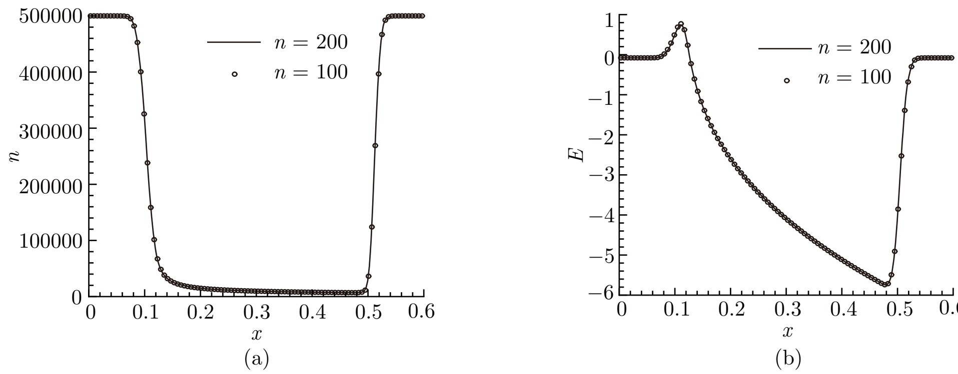


**Figure 1** $[0, 0.6]$ with 100 or 200 mesh cells, $\Delta t = 1.2E-3$. (a) density $n$ ($10^{12}cm^{-3}$); (b) electric field $E$ (V/um)

where $\xi = \frac{x-x_j}{\Delta x_j}$. The numerical solution can then be written as $u^h(x,t) = \sum_{l=0}^{k} u_j^{(l)}(t)v_l^{(j)}(x)$, for $x \in I_j$ $(u = n, q)$.

We simulate the DD model with a length of $0.6\mu m$ and a doping defined by $n_d = 5\times10^{17}cm^{-3}$ in $[0, 0.1]$ and in $[0.5, 0.6]$ and $n_d = 2 \times 10^{15}\text{cm}^{-3}$ in $[0.15, 0.45]$, and a smooth transition in between. The lattice temperature is taken as $T_0 = 300°K$. The constants $k = 0.138 \times 10^{-4}$, $\varepsilon = 11.7 \times 8.85418$, $e = 0.1602$, $m = 0.26\times0.9109\times10^{-31}\text{kg}$, and the mobility $\mu = 0.75$, in our units. The boundary conditions are given as follows: $\phi = \phi_0 = \frac{kT}{e}\ln(\frac{n_d}{n_i})$ at the left boundary, with $n_i = 1.4 \times 10^{10}\text{cm}^{-3}$, $\phi = \phi_0 + v_{\text{bias}}$ with the voltage drop $v_{\text{bias}} = 1.5$ 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.

Tables 2 and 3 show the time step, the number of time steps, the time, and the CPU time on the steady state for third order RK LDG and third order IMEX LDG methods when we use 100 mesh cells and 200 mesh cells in $[0, 0.6]$, respectively. Figure 1 plots the simulation results of DD model with 100 and 200 mesh cells in $[0, 0.6]$.

The numerical simulations show that the scheme is stable regardless of the choice of $h$ (100 or 200 mesh cells in $[0, 0.6]$). The codes produce numerically convergent results during mesh refinement (mesh refinement results not shown to save space), as can be anticipated from the theoretical results shown in this paper.

From Tables 2 and 3, we can see that using the third order IMEX LDG scheme, we can use much larger time step and hence save in CPU time significantly. The IMEX scheme is thus a reliable and efficient tool for the study of suitability of models such as DD to describe the correct physics.

## 8 Concluding remarks and future work

In this paper, we study a unified local discontinuous Galerkin (LDG) spatial discretization to the drift-diffusion (DD) model for semi-conductor device simulations, both in semi-discrete form and in fully discrete form by the implicit-explicit (IMEX) Runge-Kutta time discretization. Optimal a priori $L^2$ error estimates are obtained in both cases. The IMEX method uses implicit time discretization only for the linear diffusion term and treat the nonlinear drift term coupled with the potential equation explicitly, yet the method is still shown to be unconditionally stable and convergent for smooth solutions in the sense that the time step $\Delta t$ only needs to be smaller than a fixed constant. The proof relies on an important relationship between the gradient and interface jump of the numerical solution polynomial with the independent polynomial numerical solution for the gradient in the LDG methods, which was first obtained in [27], and also a careful study on different stages of the IMEX discretization and the coupling between the potential equation and the concentration equation. Comparing with the results in [21], this paper uses semi-discrete and fully-discrete unified LDG method to approximate the DD model with periodic or Dirichlet boundary condition and obtain optimal error estimate, while [21] used only semi-discrete semi-LDG (the concentration equation was approximated by an LDG method, but the potential equation was approximated by a continuous method) to approximate the DD model with periodic boundary condition and obtained sub-optimal error estimate. Comparing with the results in [28], this paper treats a model including a nonlinear coupling term of the concentration and the electric field with Dirichlet boundary condition, while [28] treated an uncoupled nonlinear equation with periodic boundary condition. Numerical results are provided to verify the efficiency of the IMEX time discretization. There is in principle no difficulty in generalizing the proof to higher order IMEX methods, especially to higher order multi-step IMEX methods. The proof can also be easily extended to fully explicit Runge-Kutta methods, under the standard time step restriction $\Delta t = O(h^2)$, see [29] for such results for linear convection-diffusion equations without coupling to the potential equation. In future work, we plan to generalize the results to other models in semi-conductor device simulations.

**Acknowledgements** This work was supported by National Natural Science Foundation of China (Grant No. 11471194), Department of Energy of USA (Grant No. DE-FG02-08ER25863) and National Science Foundation of USA (Grant No. DMS-1418750).

### References

1 Ascher U M, Ruuth S J, Spiteri R J. Implicit-explicit Runge-Kutta methods for time-dependent partial differential equations. Appl Numer Math, 1997, 25: 151–167

2 Ayuso B, Carrillo J A, Shu C-W. Discontinuous Galerkin methods for the one-dimensional Vlasov-Poisson system. Kinet Relat Models, 2011, 4: 955–989

3 Burman E, Ern A, Fernández M A. Explicit Runge-Kutta schemes and finite elements with symmetric stabilization for first-order linear PDE systems. SIAM J Numer Anal, 2010, 48: 2019–2042

4 Castillo P. An optimal error estimate for the local discontinuous Galerkin method. In: Cockburn B, Karniadakis G, Shu C-W, eds. Discontinuous Galerkin Methods: Theory, Computation and Application. Lecture Notes in Computational Science and Egnineering, vol. 11. Berlin: Springer, 2000, 285–290

5 Castillo P, Cockburn B, Perugia I, et al. An a priori error analysis of the local discontinuous Galerkin method for elliptic problems. SIAM J Numer Anal, 2000, 38: 676–706

6 Castillo P, Cockburn B, Schötzau D, et al. Optimal a priori error estimates for the hp-version of the LDG method for convection diffusion problems. Math Comp, 2002, 71: 455–478

7 Cercignani C, Gamba I M, Jerome J W, et al. Device benchmark comparisons via kinetic, hydrodynamic, and high-field models. Comput Methods Appl Mech Engrg, 2000, 181: 381–392

8 Ciarlet P. The Finite Element Method for Elliptic Problem. Amsterdam-New York: NorthHolland, 1978

9 Cockburn B, Dong B, Guzman J. Optimal convergence of the original discontinuous Galerkin method for the transport-reaction equation on special meshes. SIAM J Numer Anal, 2008, 48: 1250–1265

10 Cockburn B, Hou S, Shu C-W. The Runge-Kutta local projection discontinuous Galerkin finite element method for conservation laws IV: The multidimensional case. Math Comp, 1990, 54: 545–581

11 Cockburn B, Lin S-Y, Shu C-W. TVB Runge-Kutta local projection discontinuous Galerkin finite element method for conservation laws III: One-dimensional systems. J Comput Phys, 1989, 84: 90–113

12 Cockburn B, Shu C-W. TVB Runge-Kutta local projection discontinuous Galerkin finite element method for conservation laws II: General Framework. Math Comp, 1989, 52: 411–435

13 Cockburn B, Shu C-W. The local discontinuous Galerkin method for time-dependent convection-diffusion systems. SIAM J Numer Anal, 1998, 35: 2440–2463

14 Cockburn B, Shu C-W. The Runge-Kutta discontinuous Galerkin method for conservation Laws $V$-Multidimensional systems. J Comput Phys, 1998, 141: 199–224

15 Cockburn B, Shu C-W. Runge-Kutta Discontinuous Galerkin methods for convection-dominated problems. J Sci Comput, 2002, 16: 173–261

16 Jerome J, Shu C-W. Energy models for one-carrier transport in semiconductor devices. In: Coughran W, Cole J, Lloyd P, et al., eds. IMA Volumes in Mathematics and Its Applications, vol. 59. Berlin: Springer-Verlag, 1994, 185–207

17 Johnson C, Pitkäranta J. An analysis of the discontinuous Galerkin method for a scalar hyperbolic equation. Math Comp, 1986, 46: 1–26

18 Lesaint P, Raviart P A. On a finite element method for solving the neutron transport equation. In: de Boor C, ed. Mathematical Aspects of Finite Elements in Partial Differential Equations. New York: Academic Press, 1974, 89–145

19 Liu Y, Shu C-W. Local discontinuous Galerkin methods for moment models in device simulations: Formulation and one dimensional results. J Comput Electronics, 2004, 3: 263–267

20 Liu Y, Shu C-W. Local discontinuous Galerkin methods for moment models in device simulations: Performance assessment and two-dimensional results. Appl Numer Math, 2007, 57: 629–645

21 Liu Y, Shu C-W. Error analysis of the semi-discrete local discontinuous Galerkin method for semiconductor device simulation models. Sci China Math, 2010, 53: 3255–3278

22 Luo J, Shu C-W, Zhang Q. A priori error estimates to smooth solutions of the third order Runge-Kutta discontinuous Galerkin method for symmetrizable systems of conservation laws. Math Modelling Num Anal, in press, 2015

23 Meng X, Shu C-W, Wu B. Optimal error estimates for discontinuous Galerkin methods based on upwind-biased fluxes for linear hyperbolic equations. Math Comp, in press, 2015

24 Richter G R. An optimal-order error estimate for the discontinuous Galerkin method. Math Comp, 1988, 50: 75–88

25 Rivière B, Wheeler M F. A discontinuous Galerkin methods applied to nonlinear parabolic equations. In: Cockburn B, Karniadakis G, Shu C-W, eds. Discontinuous Galerkin Methods: Theory, Computation and Application, vol. 11. Lecture Notes in Computational Science and Egnineering. Berlin: Springer, 2000, 231–244

26 Shu C-W, Osher S. Efficient implementation of essentially non-oscillatory shock-capturing schemes. J Comput Phys, 1988, 77: 439–471

27 Wang H, Shu C-W, Zhang Q. Stability and error estimates of local discontinuous Galerkin methods with implicit-explicit time-marching for advection-diffusion problems. SIAM J Numer Anal, 2015, 53: 206–227

28 Wang H, Shu C-W, Zhang Q. Stability analysis and error estimates of local discontinuous Galerkin methods with implicit-explicit time-marching for nonlinear convection-diffusion problems. Appl Math Comp, 2015, doi:10.1016/j.amc.2015.02.067

29 Wang H, Zhang Q. Error estimate on a fully discrete local discontinuous Galerkin method for linear convection-diffusion problem. J Comput Math, 2013, 31: 283–307

30 Xu Y, Shu C-W. Error estimates of the semi-discrete local discontinuous Galerkin method for nonlinear convection-diffusion and KdV equations. Comput Methods Appl Mech Engrg, 2007, 196: 3805–3822

31 Xu Y, Shu C-W. Local discontinuous Galerkin methods for high-order time-dependent partial differential equations. Comm Comput Phys, 2010, 7: 1–46

32 Zhang Q, Shu C-W. Error estimates to smooth solutions of Runge-Kutta discontinuous Galerkin methods for scalar conservation laws. SIAM J Numer Anal, 2004, 42: 641–666

33 Zhang Q, Shu C-W. Error estimates to smooth solutions of Runge-Kutta discontinuous Galerkin methods for symmetrizable systems of conservation laws. SIAM J Numer Anal, 2006, 44: 1703–1720

34 Zhang Q, Shu C-W. Stability analysis and a priori error estimates to the third order explicit Runge-Kutta discontinuous Galerkin method for scalar conservation laws. SIAM J Numer Anal, 2010, 48: 1038–1063