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

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Abstract: In this paper 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.

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 [14, 15], see also [12, 11, 10, 13].

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

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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 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 stable, 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 LDG methods. The LDG methods have several attractive properties [30]. 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, 24, 23]. The first a priori error estimate for the LDG method of linear convection-diffusion equations was obtained by Cockburn and Shu [14]. Later Castillo et al. [4, 5, 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 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 [31, 32, 33, 22], see also Burman, Ern and Fernández [3]. Xu and Shu [29] 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, Shu and Zhang [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. Through exploring an important relationship between the gradient and interface jump of the numerical solution with the independent numerical solution of the gradient in the LDG methods, 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 interpolation and inverse properties for the finite element spaces that will be used in the error analysis.

2.1 Basic notations

Let $I_j = (x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}})$, $j = 1, 2, \cdots, N$ be a partition of the computational domain I, $\Delta x_j = x_{j+\frac{1}{2}} - x_{j-\frac{1}{2}}$, $x_j = \frac{1}{2}\left(x_{j-\frac{1}{2}} + x_{j+\frac{1}{2}}\right)$. $h = \max\{\sup_j \Delta x_j\}$. The finite dimensional computational space is

$$V_h = V_h^k = \{z : z|_{I_j} \in P^k(I_j)\}$$

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 $V_h^k \not\subset H^1$. This is one of the main differences between the discontinuous Galerkin method and most other finite element methods. Moreover, both the mesh sizes Δx_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 notations $[u_h]_{j+\frac{1}{2}} = (u_h)^+_{j+\frac{1}{2}} - (u_h)^-_{j+\frac{1}{2}}$ 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, $0 \le t \le T$ for a fixed T. Therefore, the exact solution is always bounded.

2.2 Projection and interpolation 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,

$$\int_{I_j} (\mathcal{P}^+u(x) - u(x))v(x)dx = 0 \quad \forall v \in P^{k-1}(I_j),$$

$$and \quad \mathcal{P}^+u(x_{j-\frac{1}{2}}^+) = u(x_{j-\frac{1}{2}}),$$

$$\int_{I_j} (\mathcal{P} - u(x) - u(x))v(x)dx = 0 \quad \forall v \in P^{k-1}(I_j), \tag{2.2}$$

$$and \quad \mathcal{P}^-u(x_{j+\frac{1}{2}}^-) = u(x_{j+\frac{1}{2}}).$$

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

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

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^{∞} norm and $||\eta||_{\Gamma_h} = [\sum_{j=1}^{N}((\eta_{j+\frac{1}{2}}^+)^2 + (\eta_{j+\frac{1}{2}}^-)^2)]^{\frac{1}{2}}$. The positive constant C, solely depending on u, is independent of h. Γ_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

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

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)

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

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

where $x \in (0,1)$, with periodic boundary condition for the first equation and Dirichlet boundary condition for the potential equation: $\phi(0,t) = 0$, $\phi(1,t) = v_{bias}$. We will 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 ϕ. m_0 is the electron effective mass, k is the Boltzmann constant, e is the electron charge, μ is the mobility, T_0 is the lattice temperature, $\tau = \frac{m_0 \mu}{e}$ is the relaxation parameter, $\theta = \frac{k}{m_0} T_0$, ε 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 the equation (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 $j = 1, \cdots, N$ and v, w, r, z in V_h.

4 Semi-discrete LDG scheme and its error estimate

4.1 Semi-discrete LDG scheme

Replacing the exact solutions n, q, E and ϕ in the above equations by their numerical approximations n_h, q_h, E_h, ϕ_h in V_h^k, noticing that the numerical solutions n_h, q_h, E_h and

ϕ_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 $n_h, q_h, E_h, \phi_h \in V_h$, such that

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

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

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

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

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

The "hat" terms are the numerical fluxes. We choose the flux $\widehat{E_h n_h} = \frac{1}{2}((E_h n_h)^+ + (E_h n_h)^-)$, the alternating flux for $\hat{n}_h$ and $\hat{q}_h$, that is,

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

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

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

or

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

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

Denote $||u||_{L^\infty(0,T;L^2)} = \max_{0 \le t \le T} ||u||_{L^2(I)}$, 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 semi-discrete scheme.

Theorem 4.1:   *Let n, q be the exact solution of the problem (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). 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 $k \geq 0$, then for small enough h there holds the following error estimates

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

where the constant C depends on the final time T, k, 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 of (3.9)-(3.10), and E_h be the numerical solution of the semi-discrete LDG scheme (4.3)-(4.4). We have*

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

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 ϕ, 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:

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

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

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

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

$$\int_{I_j} (n - n_h)_t v dx + \int_{I_j} \mu(En - E_h n_h) v_x dx$$
$$-\mu(En - \widehat{E_h n_h})_{j+\frac{1}{2}} v^-_{j+\frac{1}{2}} + \mu(En - \widehat{E_h n_h})_{j-\frac{1}{2}} v^+_{j-\frac{1}{2}}$$
$$+ \int_{I_j} \sqrt{\tau\theta}(q - q_h) v_x dx - \sqrt{\tau\theta}(q - \hat{q}_h)_{j+\frac{1}{2}} v^-_{j+\frac{1}{2}} + \sqrt{\tau\theta}(q - \hat{q}_h)_{j-\frac{1}{2}} v^+_{j-\frac{1}{2}} = 0. \tag{4.12}$$

$$\int_{I_j} (q - q_h) w dx + \int_{I_j} \sqrt{\tau\theta}(n - n_h) w_x dx$$
$$-\sqrt{\tau\theta}(n - \hat{n}_h)_{j+1/2} w^-_{j+\frac{1}{2}} + \sqrt{\tau\theta}(n - \hat{n}_h)_{j-1/2} w^+_{j-\frac{1}{2}} = 0. \tag{4.13}$$

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

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

and

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

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

$$
\sum_{j=1}^{N} \int_{I_j} \xi_{n,t}\xi_n dx + \sum_{j=1}^{N} \int_{I_j} \xi_q^2 dx
$$
$$
= \sum_{j=1}^{N} \int_{I_j} \eta_{n,t}\xi_n dx + \sum_{j=1}^{N} \int_{I_j} \eta_q \xi_q dx
$$
$$
+ \sum_{j=1}^{N} \Big(\int_{I_j} \sqrt{\tau\theta}\eta_q \xi_{n,x} dx + \int_{I_j} \sqrt{\tau\theta}\eta_n \xi_{q,x} dx - \sqrt{\tau\theta}\eta^-_{q,j+\frac{1}{2}} \xi^-_{n,j+\frac{1}{2}}
$$
$$
+ \sqrt{\tau\theta}\eta^-_{q,j-\frac{1}{2}} \xi^+_{n,j-\frac{1}{2}} - \sqrt{\tau\theta}\eta^+_{n,j+\frac{1}{2}} \xi^-_{q,j+\frac{1}{2}} + \sqrt{\tau\theta}\eta^+_{n,j-\frac{1}{2}} \xi^+_{q,j-\frac{1}{2}} \Big)
$$
$$
+ \sum_{j=1}^{N} \Big(-\int_{I_j} \sqrt{\tau\theta}\xi_q \xi_{n,x} dx - \int_{I_j} \sqrt{\tau\theta}\xi_n \xi_{q,x} dx + \sqrt{\tau\theta}\xi^-_{q,j+\frac{1}{2}} \xi^-_{n,j+\frac{1}{2}}
$$
$$
- \sqrt{\tau\theta}\xi^-_{q,j-\frac{1}{2}} \xi^+_{n,j-\frac{1}{2}} + \sqrt{\tau\theta}\xi^+_{n,j+\frac{1}{2}} \xi^-_{q,j+\frac{1}{2}} - \sqrt{\tau\theta}\xi^+_{n,j-\frac{1}{2}} \xi^+_{q,j-\frac{1}{2}} \Big)
$$
$$
+ \sum_{j=1}^{N} \Big(-\int_{I_j} \mu(En - E^h n^h)\xi_{n,x} dx
$$
$$
+ \mu(En - \widehat{E^h n^h})_{j+\frac{1}{2}} \xi^-_{n,j+\frac{1}{2}} - \mu(En - \widehat{E^h n^h})_{j-\frac{1}{2}} \xi^+_{n,j-\frac{1}{2}} \Big)
$$
$$
= T_1 + T_2 + T_3 + T_4 + T_5. \tag{4.16}
$$

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

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

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

Obviously, from the projection (2.2), we have

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

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and $\eta^-_{q,j+\frac{1}{2}} = 0$, $\eta^+_{n,j+\frac{1}{2}} = 0$, then we get

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

We also have

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

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

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

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

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

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

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

For the boundary part of T_5, we have

$$
\begin{aligned}
&-\sum_{j=1}^{N}\mu(En - \tfrac{1}{2}((E_h n_h)^+ + (E_h n_h)^-))_{j-\frac{1}{2}}[\xi_n]_{j-1/2} \\
&= -\sum_{j=1}^{N}\mu(\tfrac{1}{2}E(n - (n_h)^+) + \tfrac{1}{2}(E - (E_h)^+)(n_h)^+ \\
&\quad +\tfrac{1}{2}E(n - (n_h)^-) + \tfrac{1}{2}(E - (E_h)^-)(n_h)^-)_{j-\frac{1}{2}}[\xi_n]_{j-1/2} \\
&= -\tfrac{1}{2}\sum_{j=1}^{N}\mu E_{j-\frac{1}{2}}(\xi^+_n + \xi^-_n - \eta^+_n - \eta^-_n)_{j-\frac{1}{2}}[\xi_n]_{j-1/2} \\
&\quad -\tfrac{1}{2}\sum_{j=1}^{N}\mu(E - (E_h)^+)_{j-\frac{1}{2}}(n_h)^+_{j-\frac{1}{2}}[\xi_n]_{j-1/2} - \tfrac{1}{2}\sum_{j=1}^{N}\mu(E - (E_h)^-)_{j-\frac{1}{2}}(n_h)^-_{j-\frac{1}{2}}[\xi_n]_{j-1/2}
\end{aligned}
$$

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Using the Young inequality and $||n_h||_{L^\infty} \leq C$, we get

$$-\sum_{j=1}^{N} \mu(En - \tfrac{1}{2}((E_h n_h)^+ + (E_h n_h)^-))_{j-\frac{1}{2}}[\xi_n]_{j-1/2}$$
$$\leq Ch(||\xi_n||_\Gamma^2 + ||\eta_n||_\Gamma^2 + ||E - E_h||_\Gamma^2) + \tilde{\varepsilon}h^{-1}[\xi_n]^2$$

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

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

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

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

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

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

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

To complete the proof, let us verify the reasonableness of the a-priori assumption (4.22). For $k \geq 0$, we can consider h small enough so that $Ch^{k+1} \leq \frac{1}{2}\tilde{C}h$, where C is the constant in (4.8) determined by the final time T. Then if $t^* = \sup\{t : ||n(t) - n_h(t)|| \leq \tilde{C}h\}$, 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 $t \leq t^*$, in particular $||n(t^*) - n_h(t^*)|| \leq Ch^{k+1} \leq \frac{1}{2}\tilde{C}h$. This is a contradiction if $t^* < T$. Hence $t^* \geq T$ 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 stability in the sense that the time step can be taken in any value smaller than a given constant.

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 Δt. 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, ϕ_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.

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: find the numerical solution $n_h^{m+1}, q_h^{m+1} \in V_h$, such that

$$
\begin{aligned}
(\frac{n_h^{m+1} - n_h^m}{\Delta t}, v)_{I_j} &= -(\mu E_h^m n_h^m, v_x)_{I_j} + (\mu \widehat{E_h^m n_h^m})_{j+\frac{1}{2}} v_{j+\frac{1}{2}}^- - (\mu \widehat{E_h^m n_h^m})_{j-\frac{1}{2}} v_{j-\frac{1}{2}}^+ \\
&\quad -(\sqrt{\tau \theta} q_h^{m+1}, v_x)_{I_j} + (\sqrt{\tau \theta} \hat{q}_h^{m+1})_{j+\frac{1}{2}} v_{j+\frac{1}{2}}^- - (\sqrt{\tau \theta} \hat{q}_h^{m+1})_{j-\frac{1}{2}} v_{j-\frac{1}{2}}^+, (5.1)
\end{aligned}
$$

$$
(q_h^{m+1}, w)_{I_j} = -(\sqrt{\tau \theta} n_h^{m+1}, w_x)_{I_j} + (\sqrt{\tau \theta} \hat{n}_h^{m+1})_{j+\frac{1}{2}} w_{j+\frac{1}{2}}^- - (\sqrt{\tau \theta} \hat{n}_h^{m+1})_{j-\frac{1}{2}} w_{j-\frac{1}{2}}^+ (5.2)
$$

where $j = 1, \cdots, N$ and v, w in V_h, and $(\cdot, \cdot)_j$ is the usual inner product in $L^2(I_j)$.

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

$$
-\int_{I_j} E_h^m r_x dx + (\hat{E}_h^m)_{j+\frac{1}{2}} r_{j+\frac{1}{2}}^- - (\hat{E}_h^m)_{j-\frac{1}{2}} r_{j-\frac{1}{2}}^+ = -\frac{e}{\varepsilon} \int_{I_j} (n_h^m - n_d) r dx, \qquad (5.3)
$$

$$
\int_{I_j} E_h^m z dx - \int_{I_j} \phi_h^m z_x dx + (\hat{\phi}_h^m)_{j+\frac{1}{2}} z_{j+\frac{1}{2}}^- - (\hat{\phi}_h^m)_{j-\frac{1}{2}} z_{j-\frac{1}{2}}^+ = 0, \qquad (5.4)
$$

where $j = 1, \cdots, N$ and r, z in V_h.

As in the semi-discrete case, the "hat" terms are the numerical fluxes and are still chosen as (4.5) and (4.6) (or (4.7)).

Second order scheme

Since the second and third order schemes have many terms, for simplicity of notations, we will denote

$$
H_j(E_h, n_h, v) = -(\mu E_h n_h, v_x)_{I_j} + (\mu \widehat{E_h n_h})_{j+\frac{1}{2}} v_{j+\frac{1}{2}}^- - (\mu \widehat{E_h n_h})_{j-\frac{1}{2}} v_{j-\frac{1}{2}}^+, \qquad (5.5)
$$

$$
H_j^\pm(u_h, v) = -\sqrt{\tau \theta}(u_h, v_x)_{I_j} + \sqrt{\tau \theta}(u_h^\pm)_{j+\frac{1}{2}} v_{j+\frac{1}{2}}^- - \sqrt{\tau \theta}(u_h^\pm)_{j-\frac{1}{2}} v_{j-\frac{1}{2}}^+, u = n, q. \ (5.6)
$$

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

$$
H_j(E, n, v) = -(\mu E n, v_x)_{I_j} + (\mu E n)_{j+\frac{1}{2}} v_{j+\frac{1}{2}}^- - (\mu E n)_{j-\frac{1}{2}} v_{j-\frac{1}{2}}^+,
$$

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

Using (5.5) and (5.6), the LDG scheme with the second order IMEX time-marching

scheme given in [1] is: find the numerical solution $n_h^{m+1}, q_h^{m+1} \in V_h$, such that

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

$$(\frac{n_h^{m+1} - n_h^m}{\Delta t}, v)_{I_j} = \delta H_j(E_h^m, n_h^m, v) + (1 - \delta)H_j(E_h^{m,1}, n_h^{m,1}, v)$$
$$+(1 - \gamma)H_j^-(q_h^{m,1}, v) + \gamma H_j^-(q_h^{m+1}, v), \tag{5.8}$$

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

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

The LDG scheme of the electric potential equation is: find $E_h^{m,l}, \phi_h^{m,l} \in V_h$, 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 $j = 1, \cdots, N$ and r, z in V_h, and $l = 0, 1, \quad u^{m,0} = u^m$.

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 $n_h^{m+1}, q_h^{m+1} \in V_h$, such that

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

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

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

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

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

where $j = 1, \cdots, N$ and v, w in V_h.

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

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

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

where $j = 1, \cdots, N$ and r, z in V_h, 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 $||u||_{L^\infty(0,T;L^2)} = \max\limits_{0 \le m \le M} ||u^m||_{L^2(I)}$, and $||u||_{L^2(0,T;L^2)} = (\sum\limits_{m=0}^{M} ||u^m||_{L^2(I)}^2 \Delta t)^{\frac{1}{2}}$ 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 (5.1)-(5.4). If the finite element space V_h^k is the piecewise polynomials of degree $k \ge 0$, then for small enough h, there exists a positive constant C independent of h, such that the following error estimate holds*

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

where the constant C depends on the final time T, k, 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

$$
\begin{aligned}
(\frac{n^{m+1} - n^m}{\Delta t}, v)_{I_j} =\ & -(\mu E^m n^m, v_x)_{I_j} + (\mu E^m n^m)_{j+\frac{1}{2}} v_{j+\frac{1}{2}}^- - (\mu E^m n^m)_{j-\frac{1}{2}} v_{j-\frac{1}{2}}^+ \\
& -(\sqrt{\tau\theta} q^{m+1}, v_x)_{I_j} + (\sqrt{\tau\theta} q^{m+1})_{j+\frac{1}{2}} v_{j+\frac{1}{2}}^- - (\sqrt{\tau\theta} q^{m+1})_{j-\frac{1}{2}} v_{j-\frac{1}{2}}^+ \\
& +(\frac{n^{m+1} - n^m}{\Delta t} - n_t^m, v)_{I_j} + (\sqrt{\tau\theta}(q^{m+1} - q^m), v_x)_{I_j} \\
& -\sqrt{\tau\theta}(q^{m+1} - q^m)_{j+\frac{1}{2}} v_{j+\frac{1}{2}}^- + \sqrt{\tau\theta}(q^{m+1} - q^m)_{j-\frac{1}{2}} v_{j-\frac{1}{2}}^+, \quad (5.20) \\
(q^{m+1}, w)_{I_j} =\ & -(\sqrt{\tau\theta} n^{m+1}, w_x)_{I_j} + (\sqrt{\tau\theta} n^{m+1})_{j+\frac{1}{2}} w_{j+\frac{1}{2}}^- - (\sqrt{\tau\theta} n^{m+1})_{j-\frac{1}{2}} w_{j-\frac{1}{2}}^+ (5.21)
\end{aligned}
$$

Taking the difference of (5.20) and (5.1), and the difference of (5.21) and (5.2), we have the

following error equation

$$((\frac{(n^{m+1} - n_h^{m+1}) - (n^m - n_h^m)}{\Delta t}, v)_{I_j} = -(\mu E^m n^m - \mu E_h^m n_h^m, v_x)_{I_j}$$

$$+(\mu E^m n^m - \mu \widehat{E_h^m n_h^m})_{j+\frac{1}{2}} v_{j+\frac{1}{2}}^-$$

$$-(\mu E^m n^m - \mu \widehat{E_h^m n_h^m})_{j-\frac{1}{2}} v_{j-\frac{1}{2}}^+$$

$$-\sqrt{\tau\theta}(q^{m+1} - q_h^{m+1}, v_x)_{I_j}$$

$$+\sqrt{\tau\theta}(q^{m+1} - \hat{q}_h^{m+1})_{j+\frac{1}{2}} v_{j+\frac{1}{2}}^-$$

$$-\sqrt{\tau\theta}(q^{m+1} - \hat{q}_h^{m+1})_{j-\frac{1}{2}} v_{j-\frac{1}{2}}^+$$

$$+(\frac{n^{m+1} - n^m}{\Delta t} - n_t^m, v)_{I_j} + (\sqrt{\tau\theta}q^{m+1} - q^m, v_x)_{I_j}$$

$$-\sqrt{\tau\theta}(q^{m+1} - q^m)_{j+\frac{1}{2}} v_{j+\frac{1}{2}}^- + \sqrt{\tau\theta}(q^{m+1} - q^m)_{j-\frac{1}{2}} v_{j-\frac{1}{2}}^+,$$

$$(q^{m+1} - q_h^{m+1}, w)_{I_j} = -\sqrt{\tau\theta}(n^{m+1} - n_h^{m+1}, w_x)_{I_j}$$

$$+\sqrt{\tau\theta}(n^{m+1} - \hat{n}_h^{m+1})_{j+\frac{1}{2}} w_{j+\frac{1}{2}}^-$$

$$-\sqrt{\tau\theta}(n^{m+1} - \hat{n}_h^{m+1})_{j-\frac{1}{2}} w_{j-\frac{1}{2}}^+.$$

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

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

$$= (\eta_n^{m+1} - \eta_n^m, \xi_n^{m+1}) + \Delta t(\eta_q^{m+1}, \xi_q^{m+1}) + \Delta t(\frac{n^{m+1} - n^m}{\Delta t} - n_t^m, \xi_n^{m+1})$$

$$-\Delta t(\mu E^m n^m - \mu E_h^m n_h^m, \xi_{n,x}^{m+1}) - \Delta t \sum_{j=1}^{N}(\mu E^m n^m - \mu \widehat{E_h^m n_h^m})_{j-\frac{1}{2}} [\xi_n^{m+1}]_{j-\frac{1}{2}}$$

$$-\Delta t\sqrt{\tau\theta}(\xi_q^{m+1} - \eta_q^{m+1}, \xi_{n,x}^{m+1}) - \Delta t\sqrt{\tau\theta}\sum_{j=1}^{N}((\xi_q^{m+1})^- - (\eta_q^{m+1})^-)_{j-\frac{1}{2}} [\xi_n^{m+1}]_{j-\frac{1}{2}}$$

$$+\Delta t\sqrt{\tau\theta}(q^{m+1} - q^m, \xi_{n,x}^{m+1}) + \Delta t\sqrt{\tau\theta}\sum_{j=1}^{N}((q^{m+1}) - (q^m))_{j-\frac{1}{2}} [\xi_n^{m+1}]_{j-\frac{1}{2}}$$

$$-\Delta t\sqrt{\tau\theta}(\xi_n^{m+1} - \eta_n^{m+1}, \xi_{q,x}^{m+1}) - \Delta t\sqrt{\tau\theta}\sum_{j=1}^{N}((\xi_n^{m+1})^+ - (\eta_n^{m+1})^+)_{j-\frac{1}{2}} [\xi_q^{m+1}]_{j-\frac{1}{2}}.$$

Noting that

$$(\xi_n^{m+1} - \xi_n^m, \xi_n^{m+1}) = \frac{1}{2}||\xi_n^{m+1}||^2 - \frac{1}{2}||\xi_n^m||^2 + \frac{1}{2}||\xi_n^{m+1} - \xi_n^m||^2,$$

we have

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

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

$$
T_{11} \leq \frac{1}{2}\Delta t h^{2k+2} + \frac{1}{2}\Delta t||\xi_n^{m+1}||^2. \tag{5.23}
$$

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

Noting that

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

we can get

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

Obviously, from the property (2.2), we have

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

We have also

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

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 the Young inequality, we get

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

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

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

From the above assumption, we can get $||n_h^m||_{L^\infty} \le C$. 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

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

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

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

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

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

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 $m = 1, \cdots, M-1$, then for $m = M$, we can get (5.31), that is, (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 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 second order IMEX LDG scheme (5.7)-(5.11). If the finite element space V_h^k is the*

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piecewise polynomials of degree $k \geq 0$, then for small enough h, there exists a positive constant C independent of h, such that the following error estimate holds

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

where the constant C depends on the final time T, k, 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

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

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

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

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

$$q^{m,1} = \sqrt{\tau\theta}n_x^{m,1},$$

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

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

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

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

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

$$-\int_{I_j} E^{m,l} r_x dx + E_{j+\frac{1}{2}}^{m,l} r_{j+\frac{1}{2}}^- - E_{j-\frac{1}{2}}^{m,l} r_{j-\frac{1}{2}}^+ = -\frac{e}{\varepsilon}\int_{I_j}(n^{m,l} - n_d) r dx, \tag{5.38}$$

$$\int_{I_j} E^{m,l} z dx - \int_{I_j} \phi^{m,l} z_x dx + \phi_{j+\frac{1}{2}}^{m,l} z_{j+\frac{1}{2}}^- - \phi_{j-\frac{1}{2}}^{m,l} z_{j-\frac{1}{2}}^+ = 0, \quad l = 0, 1. \tag{5.39}$$

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, that is, (5.33)-(5.35), (5.34)-(5.36) and (5.9)-(5.37), we get the following error equation

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

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

$$(\xi_q^{m,l}, w)_{I_j} = (\eta_q^{m,l}, w)_{I_j} + H_j^+(\xi_n^{m,l}, w) - H_j^+(\eta_n^{m,l}, w), \quad l = 1, 2,$$

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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

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

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

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

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

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

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

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

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

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

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

From the periodic boundary condition, we have

$$T_{22} = 0. \qquad (5.47)$$

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To estimate T_{23}, we denote $\boldsymbol{\xi}_q^T = (\xi_q^{m,1}, \xi_q^{m+1})$. Using the property of the projection (2.3), the Schwartz inequality and the Young inequality, we have

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

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

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

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

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

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

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

Then we get

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

Substituting (5.46)-(5.50) to (5.45), we get

$$||\xi_n^{m+1}||^2 - ||\xi_n^m||^2 + 2\gamma\Delta t||\xi_q^{m,1}||^2 + 2\gamma\Delta t||\xi_q^{m+1}||^2 + 2(1 - 2\gamma)\Delta t(\xi_q^{m+1}, \xi_q^{m,1})$$
$$\leq C(\Delta t)^5 + C\Delta t h^{2k+2} + C\Delta t(||\xi_n^m||^2 + ||\xi_n^{m,1}||^2 + ||\xi_n^{m+1}||^2)$$
$$+ 2\tilde{\varepsilon}\Delta t \int_I \boldsymbol{\xi}_q^T \boldsymbol{\xi}_q dx + 4\tilde{\varepsilon}\frac{C_\mu}{\sqrt{\tau\theta}}\Delta t||\xi_q^{m,1}||^2 + 8\tilde{\varepsilon}\frac{C_\mu}{\sqrt{\tau\theta}}\Delta t||\xi_q^{m+1}||^2.$$
$$(5.51)$$

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

$$||\xi_n^{m+1}||^2 - ||\xi_n^m||^2 + \frac{3}{2}\gamma\Delta t||\xi_q^{m,1}||^2 + \frac{3}{2}\gamma\Delta t||\xi_q^{m+1}||^2 + 2(1 - 2\gamma)\Delta t(\xi_q^{m+1}, \xi_q^{m,1})$$
$$\leq C(\Delta t)^5 + C\Delta t h^{2k+2} + C\Delta t(||\xi_n^m||^2 + ||\xi_n^{m,1}||^2 + ||\xi_n^{m+1}||^2) + 2\tilde{\varepsilon}\Delta t \int_I \boldsymbol{\xi}_q^T \boldsymbol{\xi}_q dx.$$
$$(5.52)$$

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If we denote the last three term of the left hand as S, that is,

$$S := \frac{3}{2}\gamma\Delta t||\xi_q^{m,1}||^2 + \frac{3}{2}\gamma\Delta t||\xi_q^{m+1}||^2 + 2(1-2\gamma)\Delta t(\xi_q^{m+1}, \xi_q^{m,1})$$
$$= \Delta t\int_I \boldsymbol{\xi}_q^T \boldsymbol{M}\boldsymbol{\xi}_q dx,$$

where

$$\boldsymbol{M} = \begin{pmatrix} \frac{3}{2}\gamma & 1-2\gamma \\ 1-2\gamma & \frac{3}{2}\gamma \end{pmatrix}.$$

It is easy to check that $\boldsymbol{M}$ is positive definite. So if we choose $\tilde{\varepsilon}$ satisfying not only $\tilde{\varepsilon}\frac{C_\mu}{\sqrt{\tau\theta}} \le \frac{1}{16}\gamma$ but also $\int_I \boldsymbol{\xi}_q^T(\boldsymbol{M} - 2\tilde{\varepsilon})\boldsymbol{\xi}_q dx \ge 0$, we can get

$$||\xi_n^{m+1}||^2 - ||\xi_n^m||^2 \le C(\Delta t)^5 + C\Delta t h^{2k+2} + C\Delta t(||\xi_n^m||^2 + ||\xi_n^{m,1}||^2 + ||\xi_n^{m+1}||^2). \quad (5.53)$$

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

$$||\xi_n^{m,1}||^2 \le C(||\xi_n^m||^2 + (\Delta t)^5 + \Delta t h^{2k+2}). \quad (5.54)$$

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

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

5.4   The error estimate of the third order IMEX LDG scheme

Theorem 5.3: *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 third order IMEX LDG scheme (5.12)-(5.18). If the finite element space V_h^k is the piecewise polynomials of degree $k \ge 0$, then for small enough h, there exists a positive constant C independent of h, such that the following error estimate holds*

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

where the constant C depends on the final time T, k, 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

$$D_1 u^m = 2u^{m,2} - 3u^{m,1}, \quad D_2 u^m = u^{m,3} - 2u^{m,2} + 2u^{m,1},$$

then introduce a series of notations

$$\begin{aligned} F_1 u^m &= u^{m,1} - u^m, & F_2 u^m &= D_1 u^m + u^m, \\ F_3 u^m &= D_2 u^m - u^{m,1}, & F_4 u^m &= 2u^{m+1} + D_1 u^m - D_2 u^m, \\ F_{41} u^m &= u^{m+1} + D_1 u^m, & F_{42} u^m &= u^{m+1} - D_2 u^m. \end{aligned}$$

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

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

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

$$\Phi_1(\boldsymbol{E}_h^m, \boldsymbol{n}_h^m, v) = \frac{1}{2}\Delta t H(E_h^m, n_h^m, v),$$

$$\Phi_2(\boldsymbol{E}_h^m, \boldsymbol{n}_h^m, v) = -\frac{5}{18}\Delta t H(E_h^m, n_h^m, v) + \frac{1}{9}\Delta t H(E_h^{m,1}, n_h^{m,1}, v),$$

$$\Phi_3(\boldsymbol{E}_h^m, \boldsymbol{n}_h^m, v) = \frac{1}{9}\Delta t H(E_h^m, n_h^m, v) - \frac{17}{18}\Delta t H(E_h^{m,1}, n_h^{m,1}, v) + \frac{1}{2}\Delta t H(E_h^{m,2}, n_h^{m,2}, v),$$

$$\Phi_4(\boldsymbol{E}_h^m, \boldsymbol{n}_h^m, v) = -\frac{7}{18}\Delta t H(E_h^m, n_h^m, v) + \frac{41}{9}\Delta t H(E_h^{m,1}, n_h^{m,1}, v) + \Delta t H(E_h^{m,2}, n_h^{m,2}, v)$$
$$-\frac{7}{2}\Delta t H(E_h^{m,3}, n_h^{m,3}, v),$$

and

$$\Psi_1(\boldsymbol{q}_h^m, v) = \frac{1}{2}\Delta t H^-(q_h^{m,1}, v),$$

$$\Psi_2(\boldsymbol{q}_h^m, v) = \frac{1}{3}\Delta t H^-(q_h^{m,1}, v) + \frac{1}{2}\Delta t H^-(D_1 q_h^m, v),$$

$$\Psi_3(\boldsymbol{q}_h^m, v) = -\frac{7}{12}\Delta t H^-(q_h^{m,1}, v) + \frac{1}{4}\Delta t H^-(D_1 q_h^m, v) + \frac{1}{2}\Delta t H^-(D_2 q_h^m, v),$$

$$\Psi_4(\boldsymbol{q}_h^m, v) = -\frac{1}{12}\Delta t H^-(q_h^{m,1}, v) - \frac{1}{4}\Delta t H^-(D_1 q_h^m, v) + \frac{1}{2}\Delta t H^-(D_2 q_h^m, v)$$
$$+\Delta t H^-(q_h^{m+1}, v).$$

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

$$\frac{n^{m,1} - n^m}{\Delta t} = \frac{1}{2}(\mu E^m n^m)_x + \frac{1}{2}\sqrt{\tau\theta}q_x^{m,1},$$

$$\frac{n^{m,2} - n^m}{\Delta t} = \frac{11}{18}(\mu E^m n^m)_x + \frac{1}{18}(\mu E^{m,1} n^{m,1})_x + \frac{1}{6}\sqrt{\tau\theta}q_x^{m,1} + \frac{1}{2}\sqrt{\tau\theta}q_x^{m,2},$$

$$\frac{n^{m,3} - n^m}{\Delta t} = \frac{5}{6}(\mu E^m n^m)_x - \frac{5}{6}(\mu E^{m,1} n^{m,1})_x + \frac{1}{2}(\mu E^{m,2} n^{m,2})_x$$
$$-\frac{1}{2}\sqrt{\tau\theta}q_x^{m,1} + \frac{1}{2}\sqrt{\tau\theta}q_x^{m,2} + \frac{1}{2}\sqrt{\tau\theta}q_x^{m,3}, \tag{5.58}$$

$$\frac{n^{m+1} - n^m}{\Delta t} = \frac{1}{4}(\mu E^m n^m)_x + \frac{7}{4}(\mu E^{m,1} n^{m,1})_x + \frac{3}{4}(\mu E^{m,2} n^{m,2})_x - \frac{7}{4}(\mu E^{m,3} n^{m,3})_x$$
$$+\frac{3}{2}\sqrt{\tau\theta}q_x^{m,1} - \frac{3}{2}\sqrt{\tau\theta}q_x^{m,2} + \frac{1}{2}\sqrt{\tau\theta}q_x^{m,3} + \frac{1}{2}\sqrt{\tau\theta}q_x^{m+1} + \frac{\zeta^m}{\Delta t},$$

$$q^{m,l} = \sqrt{\tau\theta}n_x^{m,l}, \quad l = 1, 2, 3, 4,$$

and

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

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where n^m is the exact solution n on time level m, ζ^m is the local truncation error of the third order IMEX RK method and $||\zeta^m|| \leq C(\Delta t)^4$. 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 Ψ_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

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

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

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

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

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

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

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

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

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To estimate T_Ψ, from the definition of $H^\pm$ in (5.6) 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

$$
\begin{aligned}
T_{\eta q} =\ & \frac{1}{2}(\eta_q^{m,1}, \xi_q^{m,1})\Delta t + \frac{1}{3}(D_1\eta_q^m, \xi_q^{m,1})\Delta t + \frac{1}{2}(D_1\eta_q^m, D_1\xi_q^m)\Delta t \\
& -\frac{7}{12}(D_2\eta_q^{m,1}, \xi_q^{m,1})\Delta t + \frac{1}{4}(D_2\eta_q^m, D_1\xi_q^m)\Delta t + \frac{1}{2}(D_2\eta_q^m, D_2\xi_q^m)^2\Delta t \\
& -\frac{1}{12}(\eta_q^{m+1}, \xi_q^{m,1})\Delta t - \frac{1}{4}(\eta_q^{m+1}, D_1\xi_q^m)\Delta t + \frac{1}{2}(\eta_q^{m+1}, D_2\xi_q^m)\Delta t + (\eta_q^{m+1}, \xi_q^{m+1})\Delta t,
\end{aligned}
$$

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

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

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

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

And using the Young inequality, for $\forall \tilde{\varepsilon} > 0$, we have

$$T_{\eta q} \leq \tilde{\varepsilon}\Delta t \int_I \boldsymbol{\xi}_q^T \boldsymbol{\xi}_q dx + C_{\tilde{\varepsilon}}\Delta t \sum_{l=1}^4 ||\eta_q^{m,l}||^2,$$

where $C_{\tilde{\varepsilon}}$ is a positive constant only depending on $\tilde{\varepsilon}$. Then we have

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

Finally we estimate T_Φ as follows:

$$T_\Phi = \sum_{l=1}^{4}(\Phi_l(\boldsymbol{E}^m, \boldsymbol{n}^m, v_l) - \Phi_l(\boldsymbol{E}_h^m, \boldsymbol{n}_h^m, v_l))$$

$$= \Delta t \sum_{l=1}^{4}\sum_{i=0}^{3}\delta_{li}(H(E^{m,i}, n^{m,i}, v_l) - H(E_h^{m,i}, n_h^{m,i}, v_l)).$$

Here and below we use the notations

$$v_1 = \xi_n^{m,1}, \quad v_2 = D_1\xi_n^m, \quad v_3 = D_2\xi_n^m, \quad v_4 = D_1\xi_n^{m+1}.$$

And δ_{li} are listed in the following table

	δ_{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	$-\frac{7}{2}$

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

$$H(E^{m,i}, n^{m,i}, v_l) - H(E_h^{m,i}, n_h^{m,i}, v_l)$$

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

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

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

Then we have

$$T_\Phi \le C\Delta t(\sum_{l=0}^{3}||\xi_n^{m,l}||^2 + h^{2k+2})$$

$$+\tilde{\varepsilon}\Delta t(||\xi_{n,x}^{m,1}||^2 + ||D_1\xi_{n,x}^m||^2 + ||D_2\xi_{n,x}^m||^2 + ||\xi_{n,x}^{m+1}||^2)$$

$$+\tilde{\varepsilon}\Delta t h^{-1}([\xi_n^{m,1}]^2 + [D_1\xi_n^m]^2 + [D_2\xi_n^m]^2 + [\xi_n^{m+1}]^2).$$

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

$$||v_{2,x}|| \le \frac{C_\mu}{\sqrt{\tau\theta}}(||2\xi_q^{m,2} - 3\xi_q^{m,1}|| + ||2\eta_q^{m,2} - 3\eta_q^{m,1}||)$$

$$h^{-\frac{1}{2}}[D_1\xi_n^m] \le \frac{C_\mu}{\sqrt{\tau\theta}}(||2\xi_q^{m,2} - 3\xi_q^{m,1}|| + ||2\eta_q^{m,2} - 3\eta_q^{m,1}||).$$

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

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

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

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

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

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

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

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

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

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

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:

$$n(0,t) = n_l, \quad n(1,t) = n_r \tag{6.1}$$
$$\phi(0,t) = 0, \quad \phi(1,t) = v_{bias}, \tag{6.2}$$

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

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

Or

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

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 of the problem (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 $k \geq 0$, then for small enough h there holds the following error estimates*

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

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

Proof of Theorem 6.1: 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

$$\int_{I_j} \xi_{n,t} v dx + \int_{I_j} \sqrt{\tau\theta} \xi_q v_x dx$$
$$+ \int_{I_j} \mu(En - E_h n_h) v_x dx - \mu(En - \widehat{E_h n_h})_{j+\frac{1}{2}} v_{j+\frac{1}{2}}^- + \mu(En - \widehat{E_h n_h})_{j-\frac{1}{2}} v_{j-\frac{1}{2}}^+$$
$$= \int_{I_j} \eta_{n,t} v dx + \sqrt{\tau\theta} \xi_{q,j+\frac{1}{2}}^- v_{j+\frac{1}{2}}^- - \sqrt{\tau\theta} \xi_{q,j-\frac{1}{2}}^- v_{j-\frac{1}{2}}^+,$$

$$\int_{I_j} \xi_q w dx + \int_{I_j} \sqrt{\tau\theta} \xi_n w_x dx$$
$$= \int_{I_j} \eta_q w dx + \sqrt{\tau\theta} \xi_{n,j+\frac{1}{2}}^+ w_{j+\frac{1}{2}}^- - \sqrt{\tau\theta} \xi_{n,j-\frac{1}{2}}^+ w_{j-\frac{1}{2}}^+,$$

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

$$\int_{I_1} \xi_{n,t} v dx + \int_{I_1} \sqrt{\tau\theta} \xi_q v_x dx$$
$$+ \int_{I_1} \mu(En - E_h n_h) v_x dx - \mu(En - \widehat{E_h n_h})_{\frac{3}{2}} v_{\frac{3}{2}}^- + \mu(En - \widehat{E_h n_h})_{\frac{1}{2}} v_{\frac{1}{2}}^+$$
$$= \int_{I_1} \eta_{n,t} v dx + \sqrt{\tau\theta} \xi_{q,\frac{3}{2}}^- v_{\frac{3}{2}}^- - (\sqrt{\tau\theta} \xi_{q,\frac{1}{2}}^+ v_{\frac{1}{2}}^+ - \sqrt{\tau\theta} \eta_{q,\frac{1}{2}}^+ v_{\frac{1}{2}}^+),$$

26

$$\int_{I_1} \xi_q w\, dx + \int_{I_1} \sqrt{\tau\theta}\xi_n w_x\, dx = \int_{I_1} \eta_q w\, dx + \sqrt{\tau\theta}\xi^+_{n,\frac{3}{2}} w^-_{\frac{3}{2}},$$

and

$$\int_{I_N} \xi_{n,t} v\, dx + \int_{I_N} \sqrt{\tau\theta}\xi_q v_x\, dx$$
$$+ \int_{I_N} \mu(En - E_h n_h) v_x\, dx - \mu(En - \widehat{E_h n_h})_{N+\frac{1}{2}} v^-_{N+\frac{1}{2}} + \mu(En - \widehat{E_h n_h})_{N-\frac{1}{2}} v^+_{N-\frac{1}{2}}$$
$$= \int_{I_N} \eta_{n,t} v\, dx + \sqrt{\tau\theta}\xi^-_{q,N+\frac{1}{2}} v^-_{N+\frac{1}{2}} - \sqrt{\tau\theta}\xi^-_{q,N-\frac{1}{2}} v^+_{N-\frac{1}{2}},$$

$$\int_{I_N} \xi_q w\, dx + \int_{I_N} \sqrt{\tau\theta}\xi_n w_x\, dx = \int_{I_N} \eta_q w\, dx - \sqrt{\tau\theta}\xi^+_{n,N-\frac{1}{2}} w^+_{N-\frac{1}{2}}.$$

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

$$\int_{I_j} \eta_n w_x\, dx = 0, \quad \eta^+_{n,j-\frac{1}{2}} = 0,$$

$$\int_{I_j} \eta_q v_x\, dx = 0, \quad \eta^-_{q,j+\frac{1}{2}} = 0,$$

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

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

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

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

Then (4.26) is changed to be

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

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*

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

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

Proof of Theorem 6.3: Comparing with the proof of Theorem 6.1, we have

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

Then

$$
\begin{aligned}
T_3 &= \sum_{j=1}^{N}\left(-\int_{I_j}\sqrt{\tau\theta}\xi_q\xi_{n,x}dx - \int_{I_j}\sqrt{\tau\theta}\xi_n\xi_{q,x}dx\right)\\
&\quad + \sum_{j=1}^{N}\left(\sqrt{\tau\theta}\xi^-_{q,j+\frac12}\xi^-_{n,j+\frac12} - \sqrt{\tau\theta}\xi^-_{q,j-\frac12}\xi^+_{n,j-\frac12}\right)\\
&\quad + \sqrt{\tau\theta}\xi^-_{q,\frac12}\xi^+_{n,\frac12} - \sqrt{\tau\theta}\xi^+_{q,\frac12}\xi^+_{n,\frac12} + \sqrt{\tau\theta}\eta^+_{q,\frac12}\xi^+_{n,\frac12} + c_0\sqrt{\tau\theta}[n_h]_{\frac12}\xi^+_{n,\frac12}\\
&\quad + \sum_{j=2}^{N-1}\left(\sqrt{\tau\theta}\xi^+_{n,j+\frac12}\xi^-_{q,j+\frac12} - \sqrt{\tau\theta}\xi^+_{n,j-\frac12}\xi^+_{q,j-\frac12}\right)\\
&\quad + \sqrt{\tau\theta}\xi^+_{n,\frac32}\xi^-_{q,\frac32} - \sqrt{\tau\theta}\xi^+_{n,N-\frac12}\xi^+_{q,N-\frac12}\\
&= \sqrt{\tau\theta}\eta^+_{q,\frac12}\xi^+_{n,\frac12} + c_0\sqrt{\tau\theta}[n_h]_{\frac12}\xi^+_{n,\frac12}\\
&= \sqrt{\tau\theta}\eta^+_{q,\frac12}\xi^+_{n,\frac12} + c_0\sqrt{\tau\theta}\left((n-n_h^-) - (n-n_h^+)\right)_{\frac12}\xi^+_{n,\frac12}\\
&= \sqrt{\tau\theta}\eta^+_{q,\frac12}\xi^+_{n,\frac12} - c_0\sqrt{\tau\theta}(\xi^+_{n,\frac12})^2,
\end{aligned}
$$

since $n_{\frac12} = (n_h^-)_{\frac12}$ and $\eta^+_{n,\frac12} = 0$. So

$$
\begin{aligned}
T_3 &\leq C|\eta^+_{q,\frac12}|^2 + \tilde\varepsilon|\xi^+_{n,\frac12}|^2 - c_0\sqrt{\tau\theta}|\xi^+_{n,\frac12}|^2\\
&\leq Ch^{2k+2} - (c_0\sqrt{\tau\theta} - \tilde\varepsilon)|\xi^+_{n,\frac12}|^2.
\end{aligned}
$$

Then (6.8) is changed to be

$$
\frac{1}{2}\frac{d}{dt}||\xi_n||^2 + ||\xi_q||^2 \leq C||\xi_n||^2 + Ch^{2k+2} + \tilde\varepsilon||\xi_{n,x}||^2 + \tilde\varepsilon h^{-1}[\xi_n]^2 + \tilde\varepsilon||\xi_q||^2 - (c_0\sqrt{\tau\theta} - \tilde\varepsilon)|\xi^+_{n,\frac12}|^2.
$$
(6.11)

We can choose $\tilde\varepsilon$ small enough so that $c_0\sqrt{\tau\theta} - \tilde\varepsilon \geq 0$ 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 $I_j = (x_{j-1/2}, x_{j+1/2})$,

$$
v_0^{(j)}(x) = 1, \quad v_1^{(j)}(x) = x - x_j, \quad v_2^{(j)}(x) = (x - x_j)^2 - \frac{1}{12}\Delta x_j^2, \quad \cdots.
$$

In our implementation, we use scaled Legendre polynomial basis over $[-\frac12, \frac12]$,

$$
v_0^{(j)}(\xi) = 1, \quad v_1^{(j)}(\xi) = \xi, \quad v_2^{(j)}(\xi) = \xi^2 - \frac{1}{12}, \quad \cdots.
$$

where $\xi = \frac{x-x_j}{\Delta x_j}$. The numerical solution can then be written as

$$u^h(x,t) = \sum_{l=0}^{k} u_j^{(l)}(t)v_l^{(j)}(x), \quad for \ \ x \in I_j \ \ (u = n, q).$$

We simulate the DD model with a length of $0.6\mu m$ and a doping defined by $n_d = 5 \times 10^{17} cm^{-3}$ in $[0, 0.1]$ and in $[0.5, 0.6]$ and $n_d = 2 \times 10^{15} cm^{-3}$ in $[0.15, 0.45]$, and a smooth transition in between. The lattice temperature is taken as $T_0 = 300°K$. The constants $k = 0.138 \times 10^{-4}$, $\varepsilon = 11.7 \times 8.85418$, $e = 0.1602$, $m = 0.26 \times 0.9109 \times 10^{-31} kg$, 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 $n_i = 1.4 \times 10^{10} cm^{-3}$, $\phi = \phi_0 + v_{bias}$ with the voltage drop $v_{bias} = 1.5$ at the right boundary for the potential; $T = 300°K$ at both boundaries for the temperature; and $n = 5 \times 10^{17} cm^{-3}$ at both boundaries for the concentration.

Table 7.1 and Table 7.2 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 7.1 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 Table 7.1 and Table 7.2, 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.

Table 7.1: *The time step Δt, the number of time steps nt, 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				
Δt	1.688E-5	1.2E-3	1.8E-3	2.4E-3	3.0E-3	3.6E-3
nt	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	1.482

Table 7.2: *The time step Δt, the number of time steps nt, 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				
Δt	4.22E-6	1.2E-3	1.8E-3	2.4E-3	3.0E-3	3.6E-3
nt	176081	727	480	360	298	249
t	0.7431	0.8724	0.864	0.864	0.894	0.8964
CPU time	202.3957	7.5349	5.5224	4.3680	3.4476	3.276

Figure 7.1: $[0, 0.6]$ *with 100 or 200 mesh cells, $\Delta t = 1.2E - 3$. Left: density n $(10^{12}cm^{-3})$; right: electric field E (V/um).*
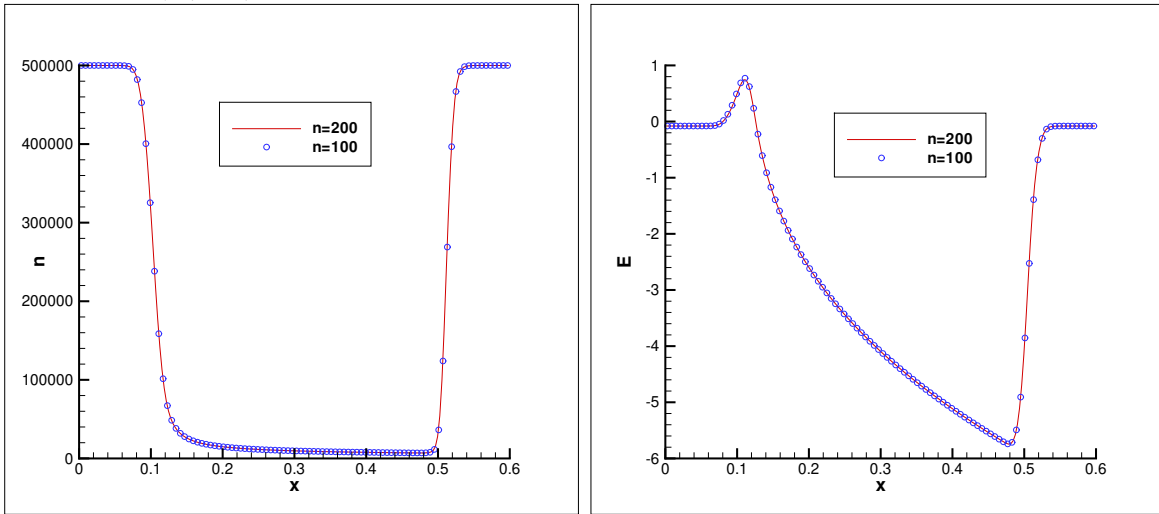
8   Concluding remarks and future work

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 Δt 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 with the independent numerical solution of 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. In future work, we plan to generalize the results to other models in semi-conductor device simulations.

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Error Analysis of the Semi-discrete Local Discontinuous Galerkin Method for Semiconductor Device Simulation Models

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Abstract: In this paper we continue our effort in [Y. Liu, C.-W. Shu, J. Comput. Electron. 3 (2004) 263 and Appl. Numer. Math. 57 (2007) 629] for developing local discontinuous Galerkin (LDG) finite element methods to discretize moment models in semiconductor device simulations. We consider drift-diffusion (DD) and high-field (HF) models of one dimensional devices, which involve not only first derivative convection terms but also second derivative diffusion terms, as well as a coupled Poisson potential equation. Error estimates are obtained for both models with smooth solutions. The main technical difficulties in the analysis include the treatment of the inter-element jump terms which arise from the discontinuous nature of the numerical method, the nonlinearity, and the coupling of the models. A simulation is also performed to validate the analysis.

Keywords: Local discontinuous Galerkin method; Error estimate; Semiconductor

1 Introduction

In our previous work [1, 2], we have developed 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 coupled to a Poisson potential equation. The convection-diffusion system is discretized by the local discontinuous Galerkin (LDG) method [3, 4, 5], see also [6, 7, 8, 9]. The potential equation for the electric field is also discretized by the LDG method. The unified discretization used to the first and higher order spatial derivatives by using the LDG method allows the full realization of the potential of this methodology in easy h-p adaptivity and parallel efficiency. The numerical results shown in [1, 2] demonstrate good resolution of the methods and an agreement with the results obtained by the ENO finite difference method [10].

The LDG methods have several attractive properties [11]. 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. They are extremely local: each cell needs to communicate only with immediate neighbors, regardless of the order of accuracy. Also, they usually have excellent provable nonlinear stability.

In this paper we continue our work in [1, 2] to give error analysis for the one dimensional drift-diffusion (DD) and high-field (HF) models of the semiconductor devices with smooth solutions. We remark that P^1 continuous finite element method solving the DD model coupled with P^0-P^1 mixed finite element method for the poisson equation is analyzed in the papers [12, 13]. For our case, the main technical difficulties in the analysis include the treatment of the inter-element jump terms which arise from the discontinuous nature of our numerical method, when coupled with the nonlinearity through the Poisson solver.

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 [14, 15, 16, 17]. The first a priori error estimate for the LDG method of linear convection-diffusion equations was obtained by Cockburn and Shu [3]. Later Castillo et al. [18, 19, 20] proved the optimal rate of convergence order $O(h^{k+1})$ for the LDG method with a particular numerical flux. Rivière and Wheeler [21] gave an optimal error estimate for the methods applied to nonlinear convection-diffusion equations for at least quadratic polynomials. Recently, Zhang and Shu presented a priori error estimates for the fully discrete Runge-Kutta DG methods with smooth solutions for scalar nonlinear conservation laws [22] and for symmetrizable systems [23]. Xu and Shu [24] provided L^2 error estimates for the semi-discrete local discontinuous Galerkin methods for nonlinear convection-diffusion equations and KdV equations with smooth solutions.

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 seems to be still unavailable. In this paper, we provide the error estimate of $O(h^{k+\frac{1}{2}})$ when P^k elements (piecewise polynomials of degree k) are used in the LDG scheme for one dimensional DD ($k \geq 1$) and HF ($k \geq 2$) models. A simulation is also performed to these two models to validate the analysis.

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 interpolation and inverse properties for the finite element spaces that will be used in the error analysis.

2.1 Basic notations

Let $I_j = (x_{j-1/2}, x_{j+1/2})$, $j = 1, 2, \cdots, N$ be a partition of the computational domain I, $\Delta x_j = x_{j+1/2} - x_{j-1/2}$, $h = \sup_j \Delta x_j$ and $x_j = \frac{1}{2}\left(x_{j-1/2} + x_{j+1/2}\right)$. The finite dimensional computational space is

$$V_h = V_h^k = \{z : z|_{I_j} \in P^k(I_j)\}$$

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 $V_h^k \not\subset H^1$. This is one of the main differences between the discontinuous Galerkin method and most other finite element methods. Moreover, both the mesh sizes Δx_j and the degree of polynomials k can be changed from element to element freely, thus allowing for easy h-p adaptivity.

We denote $(u^h)_{j+1/2}^+ = u^h(x_{j+1/2}^+)$ and $(u^h)_{j+1/2}^- = u^h(x_{j+1/2}^-)$, respectively. We use the usual notations $[u^h] = (u^h)^+ - (u^h)^-$ and $\bar{u}^h = \frac{1}{2}((u^h)^+ + (u^h)^-)$ 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, $0 \leq t \leq T$ for a fixed T. Therefore, the exact solution is always bounded.

2.2 Projection and interpolation 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 $\wp$, i.e., for each j,

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

and the special projections $\wp^\pm$ into V_h^k which satisfy, for each j,

$$\int_{I_j} (\wp^+ u(x) - u(x))v(x)dx = 0 \quad \forall v \in P^{k-1}(I_j),$$

$$and \quad \wp^+ u(x_{j-1/2}^+) = u(x_{j-1/2}),$$

$$\int_{I_j} (\wp^- u(x) - u(x))v(x)dx = 0 \quad \forall v \in P^{k-1}(I_j), \tag{2.2}$$

$$and \quad \wp^- u(x_{j+1/2}^-) = u(x_{j+1/2}).$$

From the projections mentioned above, it is easy to get (see [25])

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

where $\eta = \wp u - u$ or $\eta = \wp^\pm u - u$. The positive constant C, solely depending on u, is independent of h. Γ_h denotes the set of boundary points of all elements I_j.

2.3 Inverse properties

Finally, we list some inverse properties (see [25]) 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 a positive constant C independent of v and h, such that

$$(i) \ \ ||v_x|| \le Ch^{-1}||v||, \quad (ii) \ \ ||v||_{\Gamma_h} \le Ch^{-\frac{1}{2}}||v||, \quad (iii) \ \ ||v||_{0,\infty} \le Ch^{-\frac{d}{2}}||v||, \quad (2.4)$$

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

3 The drift-diffusion (DD) model

The drift-diffusion model is described by the following equation (we refer to [26] and the reference therein for more details)

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

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

where $x \in (0,1)$, with periodic boundary condition for the first equation and Dirichlet boundary condition for the potential equation: $\phi(0,t) = 0$, $\phi(1,t) = v_{bias}$. The second 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 ϕ. m is the electron effective mass, k is the Boltzmann constant, e is the electron charge, μ is the mobility, T_0 is the lattice temperature, $\tau = \frac{m\mu}{e}$ is the relaxation parameter, $\theta = \frac{k}{m}T_0$, ε is the dielectric permittivity, and n_d is the doping which is a given function.

3.1 Weak form and the LDG scheme

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 the equation (3.1) is rewritten as

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

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

Note that, we only rewrite equation (3.1) as a system containing first order spatial derivatives and then use the LDG method to solve it. For the Poisson equation of the electric field, we still solve it by integrating it directly or by a continuous Galerkin finite element method in this paper. This is for the convenience of the proof of the error analysis. To shorten the length of this paper, we only take the case of integrating the Poisson equation directly as an

example to perform the error analysis. We will explain briefly the case of using a continuous Galerkin finite element method to solve the Poisson equation afterwards.

Since the boundary condition of ϕ is not periodic, we treat it as following. Let $\tilde{\phi}$ be the solution of

$$\begin{cases} \tilde{\phi}_{xx} = \phi_{xx} = \frac{e}{\varepsilon}(n - n_d), \\ \\ \tilde{\phi} \ \ is \ \ periodic \ \ on \ \ the \ \ boundary, \ \ \tilde{\phi}(0,t) = 0. \end{cases}$$

We can easily check that $\phi = \tilde{\phi} + v_{bias} x$, $E = \tilde{E} - v_{bias} = -\tilde{\phi}_x - v_{bias}$. Since $\tilde{\phi}$ is periodic, we have $\tilde{E}$ is periodic, and then E is periodic.

We multiply equations (3.3)-(3.4) by test functions v, $w \in V_h^k$ respectively, and formally integrate by parts for all terms involving a spatial derivative to get

$$\int_{I_j} n_t v dx + \int_{I_j} (\mu E n + \sqrt{\tau\theta}q)v_x dx$$

$$-(\mu E n + \sqrt{\tau\theta}q)_{j+1/2}v^-_{j+1/2} + (\mu E n + \sqrt{\tau\theta}q)_{j-1/2}v^+_{j-1/2} = 0, \quad (3.5)$$

$$\int_{I_j} qw dx + \int_{I_j} \sqrt{\tau\theta}n w_x dx - \sqrt{\tau\theta}n_{j+1/2}w^-_{j+1/2} + \sqrt{\tau\theta}n_{j-1/2}w^+_{j-1/2} = 0, \quad (3.6)$$

$$E_x = -\frac{e}{\varepsilon}(n - n_d). \quad (3.7)$$

Replacing the exact solutions n, q and E in the above equations by their numerical approximations n^h, q^h in V_h^k and E^h, noticing that the numerical solutions n^h and q^h are not continuous on the cell boundaries, then replacing terms on the cell boundaries by suitable numerical fluxes, we obtain the LDG scheme:

$$\int_{I_j} (n^h)_t v dx + \int_{I_j} (\mu E^h n^h + \sqrt{\tau\theta}q^h)v_x dx$$

$$-(\mu \widehat{E^h n^h} + \sqrt{\tau\theta}\hat{q}^h)_{j+1/2}v^-_{j+1/2} + (\mu \widehat{E^h n^h} + \sqrt{\tau\theta}\hat{q}^h)_{j-1/2}v^+_{j-1/2} = 0, \quad (3.8)$$

$$\int_{I_j} q^h w dx + \int_{I_j} \sqrt{\tau\theta}n^h w_x dx - \sqrt{\tau\theta}\hat{n}^h_{j+1/2}w^-_{j+1/2} + \sqrt{\tau\theta}\hat{n}^h_{j-1/2}w^+_{j-1/2} = 0, \quad (3.9)$$

$$E^h_x = \tilde{E}^h_x = -\frac{e}{\varepsilon}(n^h - n_d), \quad (3.10)$$

$$E^h = \tilde{E}^h - v_{bias} = \int_0^x -\frac{e}{\varepsilon}(n^h - n_d)dx + E_0 - v_{bias}, \quad (3.11)$$

where $E_0 = E^h(0) = \int_0^1 (\int_0^x \frac{e}{\varepsilon}(n^h - n_d)ds)dx$. The "hat" terms are the numerical fluxes. We choose the alternate flux for $\hat{n}^h$ and $\hat{q}^h$, that is, $\hat{n}^h = (n^h)^+$, $\hat{q}^h = (q^h)^-$, and the upwind flux for $\widehat{E^h n^h}$, that is, $\widehat{E^h n^h} = \max{(E^h, 0)}(n^h)^+ + \min{(E^h, 0)}(n^h)^-$.

Notice that the auxiliary variable q^h can be locally solved from (3.9) and substituted into (3.8). 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 must be solved from a global system.

3.2 Error estimate

Theorem 3.1: Let n, q be the exact solution of the problem (3.3)-(3.4), which is sufficiently smooth with bounded derivatives. Let n^h, q^h be the numerical solution of the semi-discrete LDG scheme (3.8)-(3.9) and 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 $k \geq 1$, then for small enough h there holds the following error estimates

$$||n - n^h||_{L^\infty(0,T;L^2)} + ||q - q^h||_{L^2(0,T;L^2)} \leq Ch^{k+\frac{1}{2}} \tag{3.12}$$

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

Proof: Taking the difference of (3.5) and (3.8) and the difference of (3.6) and (3.9), we have the following error equations

$$\int_{I_j} (n - n^h)_t v \, dx + \int_{I_j} \mu(En - E^h n^h) v_x \, dx + \int_{I_j} \sqrt{\tau\theta}(q - q^h) v_x \, dx$$
$$- \mu(En - \widehat{E^h n^h})_{j+1/2} v_{j+1/2}^- + \mu(En - \widehat{E^h n^h})_{j-1/2} v_{j-1/2}^+$$
$$- \sqrt{\tau\theta}(q - \hat{q}^h)_{j+1/2} v_{j+1/2}^- + \sqrt{\tau\theta}(q - \hat{q}^h)_{j-1/2} v_{j-1/2}^+ = 0. \tag{3.13}$$

$$\int_{I_j} (q - q^h) w \, dx + \int_{I_j} \sqrt{\tau\theta}(n - n^h) w_x \, dx$$
$$- \sqrt{\tau\theta}(n - \hat{n}^h)_{j+1/2} w_{j+1/2}^- + \sqrt{\tau\theta}(n - \hat{n}^h)_{j-1/2} w_{j-1/2}^+ = 0. \tag{3.14}$$

We write the error $e_u = u - u_h$ $(u = n, q)$ as $e_u = \xi_u - \eta_u$, where $\xi_u = \wp^{(\pm)}u - u^h$, $\eta_u = \wp^{(\pm)}u - u$.

We recall that we have taken the alternate fluxes for $\hat{n}^h$ and $\hat{q}^h$, that is, $\hat{n}^h = (n^h)^+$, $\hat{q}^h = (q^h)^-$. If we choose $v = \xi_n$, $w = \xi_q$ in the error equations (3.13)-(3.14), we have

$$\int_{I_j} (\xi_n - \eta_n)_t \xi_n \, dx + \int_{I_j} \mu(En - E^h n^h) \xi_{n,x} \, dx + \int_{I_j} \sqrt{\tau\theta}(\xi_q - \eta_q) \xi_{n,x} \, dx$$
$$- \mu(En - \widehat{E^h n^h})_{j+1/2} \xi_{n,j+1/2}^- + \mu(En - \widehat{E^h n^h})_{j-1/2} \xi_{n,j-1/2}^+$$
$$- \sqrt{\tau\theta}(\xi_q - \eta_q)_{j+1/2}^- \xi_{n,j+1/2}^- + \sqrt{\tau\theta}(\xi_q - \eta_q)_{j-1/2}^- \xi_{n,j-1/2}^+ = 0, \tag{3.15}$$

and

$$\int_{I_j} (\xi_q - \eta_q) \xi_q \, dx + \int_{I_j} \sqrt{\tau\theta}(\xi_n - \eta_n) \xi_{q,x} \, dx$$
$$- \sqrt{\tau\theta}(\xi_n - \eta_n)_{j+1/2}^+ \xi_{q,j+1/2}^- + \sqrt{\tau\theta}(\xi_n - \eta_n)_{j-1/2}^+ \xi_{q,j-1/2}^+ = 0. \tag{3.16}$$

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

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

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

$$
+ \sum_{j=1}^{N}\left(\int_{I_j} \sqrt{\tau\theta}\eta_q\xi_{n,x}dx + \int_{I_j}\sqrt{\tau\theta}\eta_n\xi_{q,x}dx - \sqrt{\tau\theta}\eta_{q,j+1/2}^{-}\xi_{n,j+1/2}^{-}\right.
$$
$$
\left. + \sqrt{\tau\theta}\eta_{q,j-1/2}^{-}\xi_{n,j-1/2}^{+} - \sqrt{\tau\theta}\eta_{n,j+1/2}^{+}\xi_{q,j+1/2}^{-} + \sqrt{\tau\theta}\eta_{n,j-1/2}^{+}\xi_{q,j-1/2}^{+}\right)
$$

$$
+ \sum_{j=1}^{N}\left(-\int_{I_j}\sqrt{\tau\theta}\xi_q\xi_{n,x}dx - \int_{I_j}\sqrt{\tau\theta}\xi_n\xi_{q,x}dx + \sqrt{\tau\theta}\xi_{q,j+1/2}^{-}\xi_{n,j+1/2}^{-}\right.
$$
$$
\left. - \sqrt{\tau\theta}\xi_{q,j-1/2}^{-}\xi_{n,j-1/2}^{+} + \sqrt{\tau\theta}\xi_{n,j+1/2}^{+}\xi_{q,j+1/2}^{-} - \sqrt{\tau\theta}\xi_{n,j-1/2}^{+}\xi_{q,j-1/2}^{+}\right)
$$

$$
+ \sum_{j=1}^{N}\left(-\int_{I_j}\mu(En - E^h n^h)\xi_{n,x}dx\right.
$$
$$
\left. + \mu\widehat{(En - E^h n^h)}_{j+1/2}\xi_{n,j+1/2}^{-} - \mu\widehat{(En - E^h n^h)}_{j-1/2}\xi_{n,j-1/2}^{+}\right)
$$

$$
= T_1 + T_2 + T_3 + T_4 + T_5. \tag{3.17}
$$

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

$$
T_1 = \sum_{j=1}^{N}\int_{I_j}\eta_{n,t}\xi_n dx \le C\int_I \eta_{n,t}^2 dx + C\int_I \xi_n^2 dx \le Ch^{2k+2} + C||\xi_n||^2. \tag{3.18}
$$

$$
T_2 = \sum_{j=1}^{N}\int_{I_j}\eta_q\xi_q dx \le C\int_I \eta_q^2 dx + \tilde{\varepsilon}\int_I \xi_q^2 dx \le Ch^{2k+2} + \tilde{\varepsilon}||\xi_q||^2. \tag{3.19}
$$

Obviously, from the projection (2.2), we have

$$
T_3 = 0. \tag{3.20}
$$

We also have

$$
T_4 = \sum_{j=1}^{N}\left(-\int_{I_j}\sqrt{\tau\theta}(\xi_q\xi_n)_x dx + \sqrt{\tau\theta}\xi_{q,j+1/2}^{-}\xi_{n,j+1/2}^{-}\right.
$$
$$
\left. - \sqrt{\tau\theta}\xi_{q,j-1/2}^{-}\xi_{n,j-1/2}^{+} + \sqrt{\tau\theta}\xi_{n,j+1/2}^{+}\xi_{q,j+1/2}^{-} - \sqrt{\tau\theta}\xi_{n,j-1/2}^{+}\xi_{q,j-1/2}^{+}\right)
$$
$$
= \sum_{j=1}^{N}\left(\sqrt{\tau\theta}(\xi_q\xi_n)_{j-1/2}^{+} - \sqrt{\tau\theta}(\xi_q\xi_n)_{j+1/2}^{-} + \sqrt{\tau\theta}\xi_{q,j+1/2}^{-}\xi_{n,j+1/2}^{-}\right.
$$
$$
\left. - \sqrt{\tau\theta}\xi_{q,j-1/2}^{-}\xi_{n,j-1/2}^{+} + \sqrt{\tau\theta}\xi_{n,j+1/2}^{+}\xi_{q,j+1/2}^{-} - \sqrt{\tau\theta}\xi_{n,j-1/2}^{+}\xi_{q,j-1/2}^{+}\right)
$$
$$
= \sum_{j=1}^{N}\sqrt{\tau\theta}(\xi_{n,j+1/2}^{+}\xi_{q,j+1/2}^{-} - \xi_{n,j-1/2}^{+}\xi_{q,j-1/2}^{-}) = 0. \tag{3.21}
$$

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 (3.17), we have.

$$
\begin{aligned}
T_5 &= \sum_{j=1}^{N} (-\int_{I_j} \mu(En - E^h n^h)\xi_{n,x}dx \\
&\quad + \mu(En - \widehat{E^h n^h})_{j+1/2}\xi^{-}_{n,j+1/2} - \mu(En - \widehat{E^h n^h})_{j-1/2}\xi^{+}_{n,j-1/2}) \\
&= \sum_{j=1}^{N} \int_{I_j} \mu(E^h n^h - En)\xi_{n,x}dx - \sum_{j=1}^{N} \mu(En - \widehat{E^h n^h})_{j+1/2}[\xi_n]_{j+1/2} \\
&= \sum_{j=1}^{N} \int_{I_j} \mu E^h(n^h - n)\xi_{n,x}dx + \sum_{j=1}^{N} \int_{I_j} \mu(E^h - E)n\xi_{n,x}dx \\
&\quad + \sum_{j=1}^{N} \mu E^h_{j+1/2}(\hat{n}^h - n)_{j+1/2}[\xi_n]_{j+1/2} + \sum_{j=1}^{N} \mu(E^h - E)_{j+1/2}n_{j+1/2}[\xi_n]_{j+1/2} \\
&= \sum_{j=1}^{N} \int_{I_j} \mu E^h(\eta_n - \xi_n)\xi_{n,x}dx + \sum_{j=1}^{N} \mu E^h_{j+1/2}(\hat{\eta}_n - \hat{\xi}_n)_{j+1/2}[\xi_n]_{j+1/2} \\
&\quad + \sum_{j=1}^{N} \int_{I_j} \mu(E^h - E)n\xi_{n,x}dx + \sum_{j=1}^{N} \mu(E^h - E)_{j+1/2}n_{j+1/2}[\xi_n]_{j+1/2} \\
&= (-\sum_{j=1}^{N} \int_{I_j} \mu E^h \xi_n \xi_{n,x}dx - \sum_{j=1}^{N} \mu E^h_{j+1/2}\hat{\xi}_{n,j+1/2}[\xi_n]_{j+1/2}) \\
&\quad + \sum_{j=1}^{N} \mu E^h_{j+1/2}\hat{\eta}_{n,j+1/2}[\xi_n]_{j+1/2} + \sum_{j=1}^{N} \int_{I_j} \mu E^h \eta_n \xi_{n,x}dx
\end{aligned}
$$

$$
+ \left(\sum_{j=1}^{N} \int_{I_j} \mu(E^h - E)n\xi_{n,x}dx + \sum_{j=1}^{N} \mu((E^h - E)n[\xi_n])_{j+1/2} \right) = \sum_{i=1}^{4} T_{5i}. \tag{3.22}
$$

Next we estimate the terms T_{5i} one by one.

First we make the a-priori assumption

$$
||n - n^h|| \leq h. \tag{3.23}
$$

The a-priori assumption implies that $||n^h||_{0,\infty} \leq C$, and then $||E_0||_{0,\infty} \leq C$, $||E^h_x||_{0,\infty} \leq C$ and $||E^h||_{0,\infty} \leq C$. We will justify this a-priori assumption later. Note that the upwind flux, if $E^h < 0$, is $\widehat{E^h n^h} = E^h(n^h)^-$; otherwise, it is $\widehat{E^h n^h} = E^h(n^h)^+$. Integrating by parts, we have

$$
\begin{aligned}
T_{51} &= -\frac{1}{2} \sum_{j=1}^{N} \int_{I_j} \mu E^h(\xi_n^2)_x dx - \sum_{j=1}^{N} \mu E^h_{j+1/2}\hat{\xi}_{n,j+1/2}[\xi_n]_{j+1/2} \\
&= \frac{1}{2} \sum_{j=1}^{N} \int_{I_j} \mu E^h_x \xi_n^2 dx + \frac{1}{2} \sum_{j=1}^{N} \mu E^h_{j+1/2}[\xi_n^2]_{j+1/2} - \sum_{j=1}^{N} \mu E^h_{j+1/2}\hat{\xi}_{n,j+1/2}[\xi_n]_{j+1/2} \\
&= \frac{1}{2} \sum_{j=1}^{N} \int_{I_j} \mu E^h_x \xi_n^2 dx - \frac{1}{2} \sum_{j=1}^{N} \mu |E^h|_{j+1/2}[\xi_n]^2_{j+1/2}
\end{aligned}
$$

Using Young's inequality, we have

$$
T_{52} \leq C||\eta_n||^2_{\Gamma_h} + \tilde{\varepsilon} \sum_{j=1}^{N} \mu |E^h|_{j+1/2}[\xi_n]^2_{j+1/2},
$$

8

therefore

$$T_{51} + T_{52} \leq \frac{1}{2} \sum_{j=1}^{N} \int_{I_j} \mu E_x^h \xi_n^2 dx + C||\eta_n||_{\Gamma_h}^2 - (\frac{1}{2} - \tilde{\varepsilon}) \sum_{j=1}^{N} \mu |E^h|_{j+1/2} [\xi_n]_{j+1/2}^2$$

$$\leq C||\xi_n||^2 + Ch^{2k+1}. \tag{3.24}$$

Next, we have

$$\begin{aligned}
T_{53} &= \sum_{j=1}^{N} \int_{I_j} \mu E^h \eta_n \xi_{n,x} dx \\
&= \sum_{j=1}^{N} \int_{I_j} \mu (E^h - E_{j-1/2}^h) \eta_n \xi_{n,x} dx + \sum_{j=1}^{N} \int_{I_j} \mu E_{j-1/2}^h \eta_n \xi_{n,x} dx \\
&= \sum_{j=1}^{N} \int_{I_j} \mu (\int_{x_{j-1/2}}^{x} \frac{e}{\varepsilon}(n_d - n^h) ds) \eta_n \xi_{n,x} dx + \sum_{j=1}^{N} \int_{I_j} \mu E_{j-1/2}^h \eta_n \xi_{n,x} dx
\end{aligned}$$

From the property of the projection, the last term of the above equality is equal to zero. Noting that $\int_{x_{j-1/2}}^{x} \frac{e}{\varepsilon}(n_d - n^h) ds = O(h)$, from (2.3), (2.4) and the Schwartz inequality we have

$$T_{53} \leq Ch^{2k+2} + C||\xi_n||^2. \tag{3.25}$$

Finally, we estimate T_{54}. Integrating by parts, we have

$$\begin{aligned}
T_{54} &= \sum_{j=1}^{N} \int_{I_j} \mu (E^h - E) n \xi_{n,x} dx + \sum_{j=1}^{N} \mu (E^h - E)_{j+1/2} n_{j+1/2} [\xi_n]_{j+1/2} \\
&= -\sum_{j=1}^{N} \int_{I_j} \mu ((E^h - E)n)_x \xi_n dx - \sum_{j=1}^{N} \mu (E^h - E)_{j+1/2} n_{j+1/2} [\xi_n]_{j+1/2} \\
&\quad + \sum_{j=1}^{N} \mu (E^h - E)_{j+1/2} n_{j+1/2} [\xi_n]_{j+1/2} \\
&= \sum_{j=1}^{N} \int_{I_j} \mu ((E - E^h)n)_x \xi_n dx \\
&= \sum_{j=1}^{N} \int_{I_j} \mu (E_x - E_x^h) n \xi_n dx + \sum_{j=1}^{N} \int_{I_j} \mu (E - E^h) n_x \xi_n dx \\
&= \sum_{j=1}^{N} \frac{e\mu}{\varepsilon} \int_{I_j} (n^h - n) n \xi_n dx + \sum_{j=1}^{N} \frac{e\mu}{\varepsilon} \int_{I_j} (\int_0^x (n^h - n) ds) n_x \xi_n dx \\
&= \sum_{j=1}^{N} \frac{e\mu}{\varepsilon} \int_{I_j} (\eta_n - \xi_n) n \xi_n dx + \sum_{j=1}^{N} \frac{e\mu}{\varepsilon} \int_{I_j} (\int_0^x (\eta_n - \xi_n) ds) n_x \xi_n dx \\
&\leq C||\eta_n||^2 + C||\xi_n||^2 \\
&\quad + C \sum_{j=1}^{N} \frac{e\mu}{\varepsilon} \int_{I_j} (\int_0^x \eta_n^2 ds)^{\frac{1}{2}} n_x \xi_n dx + C \sum_{j=1}^{N} \frac{e\mu}{\varepsilon} \int_{I_j} (\int_0^x \xi_n^2 ds)^{\frac{1}{2}} n_x \xi_n dx \\
&\leq C||\eta_n||^2 + C||\xi_n||^2 \leq Ch^{2k+2} + C||\xi_n||^2
\end{aligned} \tag{3.26}$$

where C is dependent on $||n_x||_{0,\infty}$ and $||n||_{0,\infty}$.

Then substituting (3.24)-(3.26) into (3.22) we have

$$T_5 \leq Ch^{2k+1} + C||\xi_n||^2. \tag{3.27}$$

We can now substitute (3.18)-(3.21), (3.27) into (3.17) to obtain

$$\frac{d}{dt}||\xi_n||^2 + ||\xi_q||^2 \leq Ch^{2k+1} + C||\xi_n||^2. \tag{3.28}$$

Using the Gronwall's inequality, we obtain

$$||\xi_n||_{L^\infty(0,T;L^2)} + ||\xi_q||_{L^2(0,T;L^2)} \leq Ch^{k+\frac{1}{2}}. \tag{3.29}$$

From the above inequality (3.29) and the property of the projection (2.3), we get the error estimate (3.12).

To complete the proof, let us verify the a-priori assumption (3.23). For $k \geq 1$, we can consider h small enough so that $Ch^{k+\frac{1}{2}} < \frac{1}{2}h$, where C is the constant in (3.12) determined by the final time T. Then if $t^* = \sup\{t : ||n(t) - n^h(t)|| \leq h\}$, we should have $||n(t^*) - n^h(t^*)|| = h$ by continuity if t^* is finite. On the other hand, our proof implies that (3.12) holds for $t \leq t^*$, in particular $||n(t^*) - n^h(t^*)|| \leq Ch^{k+\frac{1}{2}} < \frac{1}{2}h$. This is a contradiction if $t^* < T$. Hence $t^* \geq T$ and the assumption (3.23) is correct.

Remark 3.2: If a continuous Galerkin finite element method is used to solve the Poisson equation, for example the mixed finite element method: find $(E^h, \Phi^h) \in W_h^{k+1} \times Z_h^k$ such that

$$\begin{cases} (E^h, v) - (\Phi^h, v_x) = 0, & \forall v \in W_h^{k+1} \\ (E_x^h, z) = (-\frac{e}{\varepsilon}(n^h - n_d), z) & \forall z \in Z_h^k \end{cases}$$

where $Z_h^k = \{z \in L^2(I) : z|_{I_j} \in P^k(I_j)\}$, $W_h^{k+1} = \{v \in C^0(I) : v|_{I_j} \in P^{k+1}(I_j)\}$, then we have (see [27])

$$\begin{aligned} &|\xi_E|_1 \leq C||n - n^h||, \quad ||E^h||_{0,\infty} \leq |E|_1 + C||n - n^h|| + Ch||E||_1, \\ &||E - E^h|| + |E - E^h|_1 \leq Ch^{k+1} + C||n - n^h||, \\ &||E - E^h||_{0,\infty} \leq Ch^{k+1} + C||n - n^h||. \end{aligned} \tag{3.30}$$

Here, $\xi_E = P^h E - E^h$ and $P^h E$ is the projection of E, see [27] for more details. See also the earlier work in [12, 13] for the piecewise linear case.

From (3.30) we can easily get $||E^h||_{0,\infty} \leq C$ and $||E_x^h||_{0,\infty} \leq C$. Using $E^h - E_{j-1/2}^h = O(h)$, we can estimate the term $\sum_{j=1}^{N} \int_{I_j} \mu(E^h - E_{j-1/2}^h)\eta_n \xi_{n,x} dx$ and using (3.30) we can treat the term $\sum_{j=1}^{N} \int_{I_j} \mu(E - E^h)n_x \xi_n dx$ and $\sum_{j=1}^{N} \int_{I_j} \mu(E_x - E_x^h)n\xi_n dx$ to obtain the same error estimate (3.12).

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4 The high-field (HF) model

The high-field model (see [26]) is described by the following equation, plus the Poisson electric field equation (3.2), with the periodic boundary condition

$$n_t + J_x = 0, \quad x \in (0,1) \tag{4.1}$$

where

$$J = J_{hyp} + J_{vis},$$

and

$$J_{hyp} = -\mu nE + \tau\mu(\frac{e}{\varepsilon})n(-\mu nE + \omega),$$

$$J_{vis} = -\tau(n(\theta + 2\mu^2 E^2))_x + \tau\mu E(\mu nE)_x.$$

Here $\omega = (\mu nE)|_{x=0}$ is taken to be a constant. The unknown variables are the same as in the DD model: the electron concentration n and the electric potential ϕ. Since

$$-2(nE^2)_x + E(nE)_x = -3nEE_x - E^2 n_x,$$

the equation (4.1) can be written as

$$n_t + (-\mu nE - \tau\mu^2\frac{e}{\varepsilon}n^2 E + \tau\mu\frac{e}{\varepsilon}\omega n - 3\tau\mu^2 EnE_x)_x - ((\tau\theta + \tau\mu^2 E^2)n_x)_x = 0. \tag{4.2}$$

Using $E_x = -\frac{e}{\varepsilon}(n - n_d)$, equation (4.2) can be changed to

$$n_t + \left(-\left(\frac{3\tau\mu^2 e}{\varepsilon}En_d n + \mu En - \frac{\tau\mu e\omega}{\varepsilon}n\right) + \frac{2\tau\mu^2 e}{\varepsilon}En^2\right)_x - ((\tau\theta + \tau\mu^2 E^2)n_x)_x = 0. \tag{4.3}$$

Or, by setting $C_1 = \frac{\tau\mu e}{\varepsilon}$, $C_2 = \frac{\tau\mu^2 e}{\varepsilon} = \mu C_1$, and $C_3 = \frac{\tau\mu e\omega}{\varepsilon} = \omega C_1$, we have the following HF model

$$n_t + (-(3C_2 En_d + \mu E - C_3)n + 2C_2 En^2)_x - ((\tau\theta + \tau\mu^2 E^2)n_x)_x = 0. \tag{4.4}$$

Let $q = \sqrt{\tau\theta + \tau\mu^2 E^2}\, n_x = (\sqrt{\tau\theta + \tau\mu^2 E^2}\, n)_x - (\sqrt{\tau\theta + \tau\mu^2 E^2})_x n$, we can rewrite the equation (4.4) as the following system

$$n_t + (-(3C_2 En_d + \mu E - C_3)n + 2C_2 En^2 - \sqrt{\tau\theta + \tau\mu^2 E^2}\, q)_x = 0, \tag{4.5}$$

$$q = (\sqrt{\tau\theta + \tau\mu^2 E^2}\, n)_x - (\sqrt{\tau\theta + \tau\mu^2 E^2})_x n. \tag{4.6}$$

4.1 Weak form and the LDG Scheme

We multiply equations (4.5)-(4.6) by test functions v, $w \in V_h^k$ respectively, formally integrate by parts for all terms involving a spatial derivative to get the following weak form

$$\int_{I_j} n_t v dx \quad + \int_{I_j} (3C_2 E n_d + \mu E - C_3) n v_x dx$$

$$- (3C_2 E n_d n + \mu E n - C_3 n)_{j+1/2} v_{j+1/2}^-$$

$$+ (3C_2 E n_d n + \mu E n - C_3 n)_{j-1/2} v_{j-1/2}^+$$

$$- \int_{I_j} 2C_2 E n^2 v_x dx + 2C_2 (En^2)_{j+1/2} v_{j+1/2}^- - 2C_2 (En^2)_{j-1/2} v_{j-1/2}^+$$

$$+ \int_{I_j} \sqrt{\tau\theta + \tau\mu^2 E^2} q v_x dx$$

$$- (\sqrt{\tau\theta + \tau\mu^2 E^2} q)_{j+1/2} v_{j+1/2}^- + (\sqrt{\tau\theta + \tau\mu^2 E^2} q)_{j-1/2} v_{j-1/2}^+ = 0. \qquad (4.7)$$

$$\int_{I_j} q w dx + \int_{I_j} \sqrt{\tau\theta + \tau\mu^2 E^2} n w_x dx + \int_{I_j} (\sqrt{\tau\theta + \tau\mu^2 E^2})_x n w dx$$

$$- (\sqrt{\tau\theta + \tau\mu^2 E^2} n)_{j+1/2} w_{j+1/2}^- + (\sqrt{\tau\theta + \tau\mu^2 E^2} n)_{j-1/2} w_{j-1/2}^+ = 0. \qquad (4.8)$$

Replacing the exact solutions n, q in the above equations by their numerical approximations n^h, q^h in V_h^k, noticing that the numerical solutions n^h and q^h are not continuous on the cell boundaries, then replacing terms on the cell boundaries by suitable numerical fluxes, we obtain the LDG scheme:

$$\int_{I_j} n_t^h v dx \quad + \int_{I_j} (3C_2 E^h n_d + \mu E^h - C_3) n^h v_x dx$$

$$- (3C_2 E^h n_d + \mu E^h - C_3)_{j+1/2} \hat{n}_{j+1/2}^h v_{j+1/2}^-$$

$$+ (3C_2 E^h n_d + \mu E^h - C_3)_{j-1/2} \hat{n}_{j-1/2}^h v_{j-1/2}^+$$

$$- \int_{I_j} 2C_2 E^h (n^h)^2 v_x dx + 2C_2 (E^h \widehat{(n^h)^2})_{j+1/2} v_{j+1/2}^- - 2C_2 (E^h \widehat{(n^h)^2})_{j-1/2} v_{j-1/2}^+$$

$$+ \int_{I_j} \sqrt{\tau\theta + \tau\mu^2 (E^h)^2} q^h v_x dx$$

$$- (\sqrt{\tau\theta + \tau\mu^2 (E^h)^2} \hat{q}^h)_{j+1/2} v_{j+1/2}^- + (\sqrt{\tau\theta + \tau\mu^2 (E^h)^2} \hat{q}^h)_{j-1/2} v_{j-1/2}^+ = 0. \qquad (4.9)$$

$$\int_{I_j} q^h w dx + \int_{I_j} \sqrt{\tau\theta + \tau\mu^2 (E^h)^2} n^h w_x dx + \int_{I_j} (\sqrt{\tau\theta + \tau\mu^2 (E^h)^2})_x n^h w dx$$

$$- (\sqrt{\tau\theta + \tau\mu^2 (E^h)^2} \hat{n}^h)_{j+1/2} w_{j+1/2}^- + (\sqrt{\tau\theta + \tau\mu^2 (E^h)^2} \hat{n}^h)_{j-1/2} w_{j-1/2}^+ = 0. \qquad (4.10)$$

The numerical electric field E^h is solved as before. For convenience, we denote $a^h := \sqrt{\tau\theta + \tau\mu^2(E^h)^2}$, $b^h := 3C_2 E^h n_d + \mu E^h - C_3$ in (4.9)-(4.10). The "hat" terms are the numerical fluxes. We choose the alternate flux for $a^h \hat{n}^h, a^h \hat{q}^h$, that is, $a^h \hat{n}^h = a^h (n^h)^+, a^h \hat{q}^h = a^h (q^h)^-$; the upwind flux for $b^h \hat{n}^h$, that is, if $b^h > 0$, $b^h \hat{n}^h = b^h (n^h)^+$, otherwise, $b^h \hat{n}^h = b^h (n^h)^-$; the flux $\widehat{(n^h)^2} = \frac{(n^{h-})^2 + (n^h)^-(n^h)^+ + (n^{h-})^2}{3}$ or $\widehat{(n^h)^2} = \frac{(n^{h-})^2 + (n^h)^-(n^h)^+ + (n^{h-})^2}{3} - \alpha[n^h]$ (if $E^h > 0$, $\alpha = 1$; otherwise $\alpha = -1$).

4.2 Error estimate

For convenience of notations, we denote $a := \sqrt{\tau\theta + \tau\mu^2 E^2}$, $b := 3C_2 E n_d + \mu E - C_3$ in the following analysis.

Theorem 4.1: Let n, q be the exact solution of the problem (4.5)-(4.6), which is sufficiently smooth with bounded derivatives. Let n^h, q^h be the numerical solution of the semi-discrete LDG scheme (4.9)-(4.10) and 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 $k \geq 2$, then for small enough h there holds the following error estimates

$$||n - n^h||_{L^\infty(0,T;L^2)} + ||q - q^h||_{L^2(0,T;L^2)} \leq Ch^{k+\frac{1}{2}} \tag{4.11}$$

where the constant C depends on the final time T, k, $||n||_{L^\infty(0,T;H^{k+1})}$, $||n_x||_{0,\infty}$, $||n_d||_{0,\infty}$, and the bounds on the derivatives $|a'|$ and $|b'|$.

Proof: Taking the difference of (4.7) and (4.9), and the difference of (4.8) and (4.10), we have the error equation

$\int_{I_j} (n - n^h)_t v\, dx \quad + \int_{I_j} (bn - b^h n^h) v_x\, dx$

$\qquad\qquad -((bn)_{j+1/2} - (b^h \hat{n}^h)_{j+1/2}) v_{j+1/2}^- + ((bn)_{j-1/2} - (b^h \hat{n}^h)_{j-1/2}) v_{j-1/2}^+$

$\qquad\qquad - \int_{I_j} 2C_2 (En^2 - E^h (n^h)^2) v_x\, dx$

$\qquad\qquad + 2C_2 (En^2 - E^h \widehat{(n^h)^2})_{j+1/2} v_{j+1/2}^- - 2C_2 (En^2 - E^h \widehat{(n^h)^2})_{j-1/2} v_{j-1/2}^+$

$\qquad\qquad + \int_{I_j} (aq - a^h q^h) v_x\, dx$

$\qquad\qquad -(aq - a^h \hat{q}^h)_{j+1/2} v_{j+1/2}^- + (aq - a^h \hat{q}^h)_{j-1/2} v_{j-1/2}^+ = 0. \tag{4.12}$

$\int_{I_j} (q - q^h) w\, dx + \int_{I_j} (an - a^h n^h) w_x\, dx + \int_{I_j} (a_x n - a_x^h n^h) w\, dx$

$\qquad\qquad -(an - a^h \hat{n}^h)_{j+1/2} w_{j+1/2}^- + (an - a^h \hat{n}^h)_{j-1/2} w_{j-1/2}^+ = 0. \tag{4.13}$

Taking $v = \xi_n$, $w = \xi_q$, where ξ_n, ξ_q are defined as in the proof of Theorem 3.1. Then summing (4.12) and (4.13) together, we have

$$\int_{I_j}(\xi_n - \eta_n)_t\xi_n dx + \int_{I_j}(\xi_q - \eta_q)\xi_q dx$$

$$= \left(\int_{I_j}(b^h n^h - bn)\xi_{n,x}dx + (bn - b^h\hat{n}^h)_{j+1/2}\xi^-_{n,j+1/2} - (bn - b^h\hat{n}^h)_{j-1/2}\xi^+_{n,j-1/2}\right)$$

$$+ \left(\int_{I_j} 2C_2(En^2 - E^h(n^h)^2)\xi_{n,x}dx\right.$$

$$\left. -2C_2(En^2 - E^h\widehat{(n^h)^2})_{j+1/2}\xi^-_{n,j+1/2} + 2C_2(En^2 - E^h\widehat{(n^h)^2})_{j-1/2}\xi^+_{n,j-1/2}\right)$$

$$+ \left(\int_{I_j}(a^h q^h - aq)\xi_{n,x}dx + (aq - a^h\hat{q}^h)_{j+1/2}\xi^-_{n,j+1/2} - (aq - a^h\hat{q}^h)_{j-1/2}\xi^+_{n,j-1/2}\right.$$

$$+ \int_{I_j}(a^h n^h - an)\xi_{q,x}dx + \int_{I_j}(a^h_x n^h - a_x n)\xi_q dx$$

$$\left. +(an - a^h\hat{n}^h)_{j+1/2}\xi^-_{q,j+1/2} - (an - a^h\hat{n}^h)_{j-1/2}\xi^+_{q,j-1/2}\right) = \sum_{i=1}^{3}\widetilde{T}_{ij}. \tag{4.14}$$

Summing over j, we then write the above error equation as

$$\frac{1}{2}\frac{d}{dt}||\xi_n||^2 + ||\xi_q||^2 = \sum_{j=1}^{N}\int_{I_j}\eta_{n,t}\xi_n dx + \sum_{j=1}^{N}\int_{I_j}\eta_q\xi_q dx + \sum_{i=1}^{3}\widetilde{T}_i \tag{4.15}$$

where $\widetilde{T}_i = \sum_{j=1}^{N}\widetilde{T}_{ij}$.

Next, we will estimate the right hand side of (4.15) term by term. First using the property of the projection (2.3), the Schwartz inequality, and the Young inequality, we have

$$\sum_{j=1}^{N}\int_{I_j}\eta_{n,t}\xi_n dx \leq C||\eta_{n,t}||^2 + C||\xi_n||^2 \leq Ch^{2k+2} + C||\xi_n||^2. \tag{4.16}$$

$$\sum_{j=1}^{N}\int_{I_j}\eta_q\xi_q dx \leq C||\eta_q||^2 + \tilde{\varepsilon}||\xi_q||^2 \leq Ch^{2k+2} + \tilde{\varepsilon}||\xi_q||^2. \tag{4.17}$$

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$$
\begin{aligned}
\widetilde{T}_1 &= \sum_{j=1}^{N}\int_{I_j}(b^h n^h - bn)\xi_{n,x}dx - \sum_{j=1}^{N}(bn - b^h\hat{n}^h)_{j+1/2}[\xi_n]_{j+1/2}\\
&= \sum_{j=1}^{N}\int_{I_j}b^h(n^h - n)\xi_{n,x}dx + \sum_{j=1}^{N}\int_{I_j}(b^h - b)n\xi_{n,x}dx\\
&\quad + \sum_{j=1}^{N}b^h_{j+1/2}(\hat{n}^h - n)_{j+1/2}[\xi_n]_{j+1/2} + \sum_{j=1}^{N}(b^h - b)_{j+1/2}n_{j+1/2}[\xi_n]_{j+1/2}\\
&= \sum_{j=1}^{N}\int_{I_j}b^h(\eta_n - \xi_n)\xi_{n,x}dx + \sum_{j=1}^{N}b^h_{j+1/2}(\hat{\eta}^h_n - \hat{\xi}^h_n)_{j+1/2}[\xi_n]_{j+1/2}\\
&\quad + \sum_{j=1}^{N}\int_{I_j}(b^h - b)n\xi_{n,x}dx + \sum_{j=1}^{N}(b^h - b)_{j+1/2}n_{j+1/2}[\xi_n]_{j+1/2}\\
&= \Big(-\sum_{j=1}^{N}\int_{I_j}b^h\xi_n\xi_{n,x}dx - \sum_{j=1}^{N}b^h_{j+1/2}\hat{\xi}^h_{n,j+1/2}[\xi_n]_{j+1/2}\Big)\\
&\quad + \sum_{j=1}^{N}b^h_{j+1/2}\hat{\eta}^h_{n,j+1/2}[\xi_n]_{j+1/2}\\
&\quad + \sum_{j=1}^{N}\int_{I_j}b^h\eta_n\xi_{n,x}dx\\
&\quad + \Big(\sum_{j=1}^{N}\int_{I_j}(b^h - b)n\xi_{n,x}dx + \sum_{j=1}^{N}(b^h - b)_{j+1/2}n_{j+1/2}[\xi_n]_{j+1/2}\Big)\\
&= \sum_{i=1}^{4}\widetilde{T}_{1i}. \tag{4.18}
\end{aligned}
$$

Now we estimate $\widetilde{T}_{1i}$ one by one similarly as what we have done for T_{5i} in the proof of Theorem 3.1. First,

$$
\begin{aligned}
\widetilde{T}_{11} &= -\tfrac{1}{2}\sum_{j=1}^{N}\int_{I_j}b^h(\xi_n^2)_x dx - \sum_{j=1}^{N}b^h_{j+1/2}\hat{\xi}_{n,j+1/2}[\xi_n]_{j+1/2}\\
&= \tfrac{1}{2}\sum_{j=1}^{N}\int_{I_j}b^h_x\xi_n^2 dx + \tfrac{1}{2}\sum_{j=1}^{N}b^h_{j+1/2}[\xi_n^2]_{j+1/2} - \sum_{j=1}^{N}b^h_{j+1/2}\hat{\xi}_{n,j+1/2}[\xi_n]_{j+1/2}.
\end{aligned}
$$

Since we choose the flux $b^h\hat{n}^h$ as the upwind flux, namely if $b^h < 0$, $\hat{n}^h = n^{h-}$, otherwise, $\hat{n}^h = n^{h+}$, we have

$$
\widetilde{T}_{11} = \frac{1}{2}\sum_{j=1}^{N}\int_{I_j}b^h_x\xi_n^2 dx - \frac{1}{2}\sum_{j=1}^{N}|b^h_{j+1/2}|[\xi_n]^2_{j+1/2}.
$$

We now make the same a-priori assumption (3.23) as in the proof of Theorem 3.1, which implies $||E^h_x||_{0,\infty} \leq C$ and $||E^h||_{0,\infty} \leq C$, and hence $||b^h_x||_{0,\infty} \leq C$ and $||b^h||_{0,\infty} \leq C$. Using Young's inequality,

$$
\widetilde{T}_{12} \leq C||\eta_n||^2_{\Gamma_h} + \tilde{\varepsilon}\sum_{j=1}^{N}|b^h_{j+1/2}|[\xi_n]^2_{j+1/2}.
$$

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So we have

$$\widetilde{T}_{11} + \widetilde{T}_{12} \quad \leq C||\xi_n||^2 + C||\eta_n||^2_{\Gamma_h} - \left(\frac{1}{2} - \tilde{\varepsilon}\right) \sum_{j=1}^{N} |b^h_{j+1/2}|[\xi_n]^2_{j+1/2}$$

$$\leq C||\xi_n||^2 + Ch^{2k+1} - \left(\frac{1}{2} - \tilde{\varepsilon}\right) \sum_{j=1}^{N} |b^h_{j+1/2}|[\xi_n]^2_{j+1/2}. \qquad (4.19)$$

$$\widetilde{T}_{13} \quad = \sum_{j=1}^{N} \int_{I_j} b^h \eta_n \xi_{n,x} dx$$

$$= \sum_{j=1}^{N} \int_{I_j} (b^h - b^h_{j-1/2}) \eta_n \xi_{n,x} dx + \sum_{j=1}^{N} \int_{I_j} b^h_{j-1/2} \eta_n \xi_{n,x} dx.$$

The last term of the above equality is equal to zero from the property of the projection. Also, since

$$E^h - E^h_{j-1/2} = \int_{x_{j-1/2}}^{x} \frac{e}{\varepsilon}(n_d - n^h)ds = O(h),$$

and

$$n_d - n_{d,j-1/2} = O(h),$$

we have

$$b^h - b^h_{j-1/2} = (3C_2 n_d + \mu)(E^h - E^h_{j-1/2}) + 3C_2 E^h_{j-1/2}(n_d - n_{d,j-1/2}) = O(h).$$

Using the inverse inequality, we get

$$\sum_{j=1}^{N} \int_{I_j} (b^h - b^h_{j-1/2}) \eta_n \xi_{n,x} dx \quad \leq C||\xi_n||^2 + C||\eta_n||^2$$

$$\leq C||\xi_n||^2 + Ch^{2k+2}.$$

So, we obtain

$$\widetilde{T}_{13} \leq C||\xi_n||^2 + Ch^{2k+2}. \qquad (4.20)$$

$$
\begin{aligned}
\widetilde{T}_{14} &= \sum_{j=1}^{N} \int_{I_j} (b^h - b) n \xi_{n,x} dx + \sum_{j=1}^{N} (b^h - b)_{j+1/2} n_{j+1/2} [\xi_n]_{j+1/2} \\
&= -\sum_{j=1}^{N} \int_{I_j} ((b^h - b)n)_x \xi_n dx \\
&\quad - \sum_{j=1}^{N} (b^h - b)_{j+1/2} n_{j+1/2} [\xi_n]_{j+1/2} + \sum_{j=1}^{N} (b^h - b)_{j+1/2} n_{j+1/2} [\xi_n]_{j+1/2} \\
&= -\sum_{j=1}^{N} \int_{I_j} ((b^h - b)n)_x \xi_n dx \\
&= \sum_{j=1}^{N} \int_{I_j} (b - b^h)_x n \xi_n dx + \sum_{j=1}^{N} \int_{I_j} (b - b^h) n_x \xi_n dx \\
&= \sum_{j=1}^{N} \int_{I_j} \frac{e}{\varepsilon}(3C_2 n_d + \mu)(n^h - n) n \xi_n dx + \sum_{j=1}^{N} \int_{I_j} 3C_2 (n_d)_x (E - E^h) n \xi_n dx \\
&\quad + \sum_{j=1}^{N} \int_{I_j} (3C_2 n_d + \mu)(E - E^h) n_x \xi_n dx \\
&= \sum_{j=1}^{N} \int_{I_j} \frac{e}{\varepsilon}(3C_2 n_d + \mu)(\eta_n - \xi_n) n \xi_n dx \\
&\quad + \sum_{j=1}^{N} \int_{I_j} 3C_2 (n_d)_x (\int_0^x \frac{e}{\varepsilon}(\eta_n - \xi_n) ds) n \xi_n dx \\
&\quad + \sum_{j=1}^{N} \int_{I_j} (3C_2 n_d + \mu)(\int_0^x \frac{e}{\varepsilon}(\eta_n - \xi_n) ds) n_x \xi_n dx \\
&\le C||\eta_n||^2 + C||\xi_n||^2 \le Ch^{2k+2} + C||\xi_n||^2 \tag{4.21}
\end{aligned}
$$

where C is dependent on $||n_x||_{0,\infty}$, $||n_d||_{0,\infty}$ and $||n||_{0,\infty}$.

Substituting (4.19)-(4.21) into (4.18) we have

$$
\widetilde{T}_1 \le Ch^{2k+2} + C||\xi_n||^2 - \left(\frac{1}{2} - \tilde{\varepsilon}\right) \sum_{j=1}^{N} |b_{j+1/2}^h| [\xi_n]_{j+1/2}^2. \tag{4.22}
$$

$$
\begin{aligned}
\widetilde{T}_2 &= \sum_{j=1}^{N} \int_{I_j} 2C_2 (En^2 - E^h(n^h)^2) \xi_{n,x} dx + 2C_2 \sum_{j=1}^{N} (En^2 - E^h \widehat{(n^h)^2})_{j+1/2} [\xi_n]_{j+1/2} \\
&= (2C_2 \sum_{j=1}^{N} \int_{I_j} (E - E^h) n^2 \xi_{n,x} dx + 2C_2 \sum_{j=1}^{N} (E - E^h)_{j+1/2} n_{j+1/2}^2 [\xi_n]_{j+1/2}) \\
&\quad + (2C_2 \sum_{j=1}^{N} \int_{I_j} E^h (n^2 - (n^h)^2) \xi_{n,x} dx + 2C_2 \sum_{j=1}^{N} E_{j+1/2}^h (n^2 - \widehat{(n^h)^2})_{j+1/2} [\xi_n]_{j+1/2}) \\
&= \widetilde{T}_{21} + \widetilde{T}_{22}. \tag{4.23}
\end{aligned}
$$

Integrating by parts, we get

$$
\begin{aligned}
\widetilde{T}_{21} &= -2C_2 \sum_{j=1}^{N} \int_{I_j} ((E - E^h)n^2)_x \xi_n dx - 2C_2 \sum_{j=1}^{N} (E - E^h)_{j+1/2} n_{j+1/2}^2 [\xi_n]_{j+1/2} \\
&\quad + 2C_2 \sum_{j=1}^{N} (E - E^h)_{j+1/2} n_{j+1/2}^2 [\xi_n]_{j+1/2} \\
&= -2C_2 \sum_{j=1}^{N} \int_{I_j} ((E - E^h)n^2)_x \xi_n dx \\
&= -2C_2 \sum_{j=1}^{N} \int_{I_j} (E - E^h)_x n^2 \xi_n dx - 2C_2 \sum_{j=1}^{N} \int_{I_j} (E - E^h) n_x^2 \xi_n dx
\end{aligned}
$$

We analyze the term $\widetilde{T}_{21}$ similarly as T_{54} in the proof of Theorem 3.1 to have

$$
\widetilde{T}_{21} \le Ch^{2k+2} + C||\xi_n||^2 \tag{4.24}
$$

where the constant C depends on $||n_x||_{0,\infty}$ and $||n||_{0,\infty}$.

We would like to use the following expansions to estimate $\widetilde{T}_{22}$.

$$
\begin{aligned}
n^2 - (n^h)^2 &= 2n(n - n^h) - (n - n^h)^2 \\
&= 2n(\xi_n - \eta_n) - (\xi_n - \eta_n)^2 \\
&= 2n\xi_n - 2n\eta_n - \xi_n^2 + 2\xi_n\eta_n - \eta_n^2 = \sum_{i=1}^{5} \varphi_i
\end{aligned}
$$

,

$$
n^2 - \widehat{(n^h)^2} = (n^2 - (\bar{n}^h)^2) + ((\bar{n}^h)^2 - \widehat{(n^h)^2}),
$$

$$
n^2 - (\bar{n}^h)^2 = 2n\bar{\xi}_n - 2n\bar{\eta}_n - (\bar{\xi}_n)^2 + 2\bar{\xi}_n\bar{\eta}_n - (\bar{\eta}_n)^2 = \sum_{i=1}^{5} \psi_i.
$$

Then

$$
\widetilde{T}_{22} = \sum_{i=1}^{5} X_i + \sum_{i=1}^{5} Y_i + 2C_2 \sum_{j=1}^{N} E_{j+1/2}^h ((\bar{n}^h)^2 - \widehat{(n^h)^2})_{j+1/2} [\xi_n]_{j+1/2} \tag{4.25}
$$

where

$$
X_i = 2C_2 \sum_{j=1}^{N} \int_{I_j} E^h \varphi_i \xi_{n,x} dx,
$$

$$
Y_i = 2C_2 \sum_{j=1}^{N} E_{j+1/2}^h \psi_{i,j+1/2} [\xi_n]_{j+1/2},
$$

which will be estimated term by term later.

Integrating by parts, we have

$$
\begin{aligned}
X_1 + Y_1 &= 2C_2 \sum_{j=1}^{N} \int_{I_j} E^h 2n\xi_n\xi_{n,x}dx + 2C_2 \sum_{j=1}^{N} 2E^h_{j+1/2}n_{j+1/2}\bar{\xi}_{n,j+1/2}[\xi_n]_{j+1/2} \\
&= -2C_2 \sum_{j=1}^{N} \int_{I_j} (E^h n)_x \xi_n^2 dx - 2C_2 \sum_{j=1}^{N} E^h_{j+1/2}n_{j+1/2}[\xi_n^2]_{j+1/2} \\
&\quad + 2C_2 \sum_{j=1}^{N} 2E^h_{j+1/2}n_{j+1/2}\bar{\xi}_{n,j+1/2}[\xi_n]_{j+1/2} \\
&= -2C_2 \sum_{j=1}^{N} \int_{I_j} (E^h n)_x \xi_n^2 dx
\end{aligned}
$$

$$
\leq C||\xi_n||^2 \tag{4.26}
$$

where the constant C depends on $||n_x||_{0,\infty}$.

$$
\begin{aligned}
X_2 &= -2C_2 \sum_{j=1}^{N} \int_{I_j} 2E^h n\eta_n\xi_{n,x}dx \\
&= -4C_2 \sum_{j=1}^{N} \int_{I_j} (E^h n)_{j+1/2}\eta_n\xi_{n,x}dx + 4C_2 \sum_{j=1}^{N} \int_{I_j} ((E^h n)_{j+1/2} - E^h n)\eta_n\xi_{n,x}dx.
\end{aligned}
$$

From the property of the projection, the first term of the above equality is zero. The last term

$$
4C_2 \sum_{j=1}^{N} \int_{I_j} ((E^h n)_{j+1/2} - E^h n)\eta_n\xi_{n,x}dx
$$

$$
= 4C_2 \sum_{j=1}^{N} \int_{I_j} E^h_{j+1/2}(n_{j+1/2} - n)\eta_n\xi_{n,x}dx + 4C_2 \sum_{j=1}^{N} \int_{I_j} n(E^h_{j+1/2} - E^h)\eta_n\xi_{n,x}dx.
$$

We use $n_{j+1/2} - n = O(h)$, $|E^h_{j+1/2} - E^h| = |\int_x^{x_{j+1/2}}(n^h - n_d)ds| = O(h)$, the property of the projection (2.3) and the inverse inequality (2.4) to get

$$
4C_2 \sum_{j=1}^{N} \int_{I_j} ((E^h n)_{j+1/2} - E^h n)\eta_n\xi_{n,x}dx \leq Ch^{2k+2} + C||\xi_n||^2.
$$

Here, the constant C also depends on $||n||_{0,\infty}$. Then

$$
X_2 \leq Ch^{2k+2} + C||\xi_n||^2. \tag{4.27}
$$

From (2.3) and Young's inequality, we have

$$
Y_2 = 2C_2 \sum_{j=1}^{N} (-2E^h n\bar{\eta}_n[\xi_n])_{j+1/2} \leq C||\eta_n||^2_{\Gamma_h} + \tilde{\varepsilon} \sum_{j=1}^{N} (|E^h|n[\xi_n]^2)_{j+1/2}
$$

$$\leq Ch^{2k+1} + \tilde{\varepsilon} \sum_{j=1}^{N} (|E^h| n[\xi_n]^2)_{j+1/2}. \tag{4.28}$$

Integrating by parts, we obtain

$$
\begin{aligned}
X_3 + Y_3 \ &= 2C_2 \sum_{j=1}^{N} \int_{I_j} E^h(-\xi_n^2)\xi_{n,x}dx - 2C_2 \sum_{j=1}^{N} E^h_{j+1/2}(\bar{\xi}_n)^2_{j+1/2}[\xi_n]_{j+1/2} \\[2mm]
&= -\tfrac{2C_2}{3} \sum_{j=1}^{N} \int_{I_j} E^h(\xi_n^3)_x dx - 2C_2 \sum_{j=1}^{N} E^h_{j+1/2}(\bar{\xi}_n)^2_{j+1/2}[\xi_n]_{j+1/2} \\[2mm]
&= \tfrac{2C_2}{3} \sum_{j=1}^{N} \int_{I_j} E^h_x \xi_n^3 dx + \tfrac{2C_2}{3} \sum_{j=1}^{N} E^h_{j+1/2}[\xi_n^3]_{j+1/2} - 2C_2 \sum_{j=1}^{N} E^h_{j+1/2}(\bar{\xi}_n)^2_{j+1/2}[\xi_n]_{j+1/2} \\[2mm]
&\leq C||\xi_n||_{0,\infty}||\xi_n||^2 + Ch^{-1}||\xi_n||_{0,\infty}||\xi_n||^2 \\
&\leq Ch^{-1}||\xi_n||_{0,\infty}||\xi_n||^2. \tag{4.29}
\end{aligned}
$$

Using (2.3) and (2.4) we have

$$X_4 = 2C_2 \sum_{j=1}^{N} \int_{I_j} E^h(2\xi_n\eta_n)\xi_{n,x}dx \leq Ch^{-1}||\eta_n||_{0,\infty}||\xi_n||^2 \leq C||\xi_n||^2. \tag{4.30}$$

$$Y_4 = 2C_2 \sum_{j=1}^{N} E^h_{j+1/2}(2\bar{\xi}_n\bar{\eta}_n)_{j+1/2}[\xi_n]|_{j+1/2} \leq Ch^{-1}||\eta_n||_{0,\infty}||\xi_n||^2 \leq C||\xi_n||^2. \tag{4.31}$$

$$X_5 = 2C_2 \sum_{j=1}^{N} \int_{I_j} E^h(-\eta_n^2)\xi_{n,x}dx \leq Ch^{-1}||\eta_n||_{0,\infty}(||\eta_n||^2+||\xi_n||^2) \leq Ch^{2k+2}+C||\xi_n||^2. \tag{4.32}$$

$$
\begin{aligned}
Y_5 \ &= 2C_2 \sum_{j=1}^{N} (-E^h(\bar{\eta}_n)^2)_{j+1/2}[\xi_n]_{j+1/2} \\[2mm]
&\leq Ch^{-1}||\eta_n||_{0,\infty} \sum_{j=1}^{N} h^{\frac{1}{2}}|\bar{\eta}_n|_{j+1/2} h^{\frac{1}{2}}|[\xi_n]|_{j+1/2} \\[2mm]
&\leq Ch^{-1}||\eta_n||_{0,\infty}(h||\eta_n||^2_{\Gamma_h} + ||\xi_n||^2) \\[2mm]
&\leq Ch^{2k+2} + C||\xi_n||^2. \tag{4.33}
\end{aligned}
$$

Next we estimate the last term $2C_2 \sum_{j=1}^{N} E^h_{j+1/2}((\bar{n}^h)^2 - \widehat{(n^h)^2})_{j+1/2}[\xi_n]_{j+1/2}$ of (4.25).

- If we choose $\widehat{(n^h)^2} = \frac{(n^{h+})^2 + n^{h+}n^{h-} + (n^{h-})^2}{3}$, since $[n] = 0$, we get

$$
\begin{aligned}
(\bar{n}^h)^2 - \widehat{(n^h)^2} \ &= (\tfrac{n^{h+}+n^{h-}}{2})^2 - \tfrac{(n^{h+})^2 + n^{h+}n^{h-} + (n^{h-})^2}{3} \\[2mm]
&= \tfrac{3(n^{h+})^2 + 6n^{h+}n^{h-} + 3(n^{h-})^2}{12} - \tfrac{4(n^{h+})^2 + 4n^{h+}n^{h-} + 4(n^{h-})^2}{12} \\[2mm]
&= -\tfrac{1}{12}[n^h]^2 = -\tfrac{1}{12}[\xi_n - \eta_n]^2.
\end{aligned}
$$

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Then

$$2C_2 \sum_{j=1}^{N} E^h_{j+1/2}((n^{h-})^2 - \widehat{(n^h)^2})_{j+1/2}[\xi_n]_{j+1/2}$$

$$= -\frac{C_2}{6} \sum_{j=1}^{N} E^h_{j+1/2}[\xi_n - \eta_n]^2_{j+1/2}[\xi_n]_{j+1/2}$$

$$= -\frac{C_2}{6} \sum_{j=1}^{N} E^h_{j+1/2}([\xi_n]^3_{j+1/2} - 2[\eta_n]_{j+1/2}[\xi_n]^2_{j+1/2} + [\eta_n]^2_{j+1/2}[\xi_n]_{j+1/2})$$

$$\le Ch^{-1}||\xi_n||_{0,\infty}||\xi_n||^2 + Ch^{-1}||\eta_n||_{0,\infty}||\xi_n||^2 + Ch^{-1}||\eta_n||_{0,\infty}(h||\eta_n||^2_{\Gamma_h} + ||\xi_n||^2)$$

$$\le Ch^{2k+2} + C||\xi_n||^2 + Ch^{-1}||\xi_n||_{0,\infty}||\xi_n||^2. \tag{4.34}$$

Substituting (4.26)-(4.34) to (4.25), we have

$$\widetilde{T}_{22} \le Ch^{2k+1} + C||\xi_n||^2 + Ch^{-1}||\xi_n||_{0,\infty}||\xi_n||^2 + \tilde{\varepsilon} \sum_{j=1}^{N}(|E^h|n[\xi_n]^2)_{j+1/2}. \tag{4.35}$$

And then substituting (4.24) and (4.35) to (4.23) we have

$$\widetilde{T}_2 \le Ch^{2k+1} + C||\xi_n||^2 + Ch^{-1}||\xi_n||_{0,\infty}||\xi_n||^2 + \tilde{\varepsilon} \sum_{j=1}^{N}(|E^h|n[\xi_n]^2)_{j+1/2}. \tag{4.36}$$

- If we choose $\widehat{(n^h)^2} = \frac{(n^{h+})^2 + n^{h+}n^{h-} + (n^{h-})^2}{3} - \alpha[n^h]$, since $[n] = 0$, we get

$$(\bar{n}^h)^2 - \widehat{(n^h)^2} = -\frac{1}{12}[\xi_n - \eta_n]^2 + \alpha[\eta_n - \xi_n],$$

and

$$2C_2 \sum_{j=1}^{N}(E^h\alpha[\eta_n - \xi_n][\xi_n])_{j+1/2}$$

$$= 2C_2 \sum_{j=1}^{N}(E^h\alpha[\eta_n][\xi_n])_{j+1/2} - 2C_2 \sum_{j=1}^{N}E^h_{j+1/2}\alpha[\xi_n]^2_{j+1/2}$$

$$\le C_2 \sum_{j=1}^{N}(|E^h|[\eta_n]^2)_{j+1/2} + C_2 \sum_{j=1}^{N}(|E^h|[\xi_n]^2)_{j+1/2} - 2C_2 \sum_{j=1}^{N}(|E^h|[\xi_n]^2)_{j+1/2}$$

$$= C_2 \sum_{j=1}^{N}(|E^h|[\eta_n]^2)_{j+1/2} - C_2 \sum_{j=1}^{N}(|E^h|[\xi_n]^2)_{j+1/2}$$

$$\le Ch^{2k+1} - C_2 \sum_{j=1}^{N}(|E^h|[\xi_n]^2)_{j+1/2}.$$

Then

$$\widetilde{T}_2 \le Ch^{2k+1} + C||\xi_n||^2 + Ch^{-1}||\xi_n||_{0,\infty}||\xi_n||^2$$

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$$+\tilde{\varepsilon}\sum_{j=1}^{N}(|E^h|n[\xi_n]^2)_{j+1/2} - C_2\sum_{j=1}^{N}(|E^h|[\xi_n]^2)_{j+1/2}. \tag{4.37}$$

Finally we estimate the last term $\widetilde{T}_3$ in (4.15). Since $\hat{n}^h = n^{h+}$, $\hat{q}^h = q^{h-}$, we have

$$
\begin{aligned}
\widetilde{T}_3 &= \sum_{j=1}^{N}\int_{I_j}(\sqrt{\tau\theta + \tau\mu^2(E^h)^2}q^h - \sqrt{\tau\theta + \tau\mu^2E^2}q)\xi_{n,x}dx \\
&+ \sum_{j=1}^{N}(\sqrt{\tau\theta + \tau\mu^2(E^h)^2}q^{h-} - \sqrt{\tau\theta + \tau\mu^2E^2}q)_{j+1/2}[\xi_n]_{j+1/2} \\
&+ \sum_{j=1}^{N}\int_{I_j}(\sqrt{\tau\theta + \tau\mu^2(E^h)^2}n^h - \sqrt{\tau\theta + \tau\mu^2E^2}n)\xi_{q,x}dx \\
&+ \sum_{j=1}^{N}\int_{I_j}((\sqrt{\tau\theta + \tau\mu^2(E^h)^2})_x n^h - (\sqrt{\tau\theta + \tau\mu^2E^2})_x n)\xi_q dx \\
&+ \sum_{j=1}^{N}(\sqrt{\tau\theta + \tau\mu^2(E^h)^2}n^{h+} - \sqrt{\tau\theta + \tau\mu^2E^2}n)_{j+1/2}[\xi_q]_{j+1/2} \\
&= \sum_{i=1}^{5}\widetilde{T}_{3i}. \tag{4.38}
\end{aligned}
$$

We now estimate $\widetilde{T}_{3i}$ one by one.

$$
\begin{aligned}
\widetilde{T}_{31} &= \sum_{j=1}^{N}\int_{I_j}(\sqrt{\tau\theta + \tau\mu^2(E^h)^2}q^h - \sqrt{\tau\theta + \tau\mu^2E^2}q)\xi_{n,x}dx \\
&= \sum_{j=1}^{N}\int_{I_j}\sqrt{\tau\theta + \tau\mu^2(E^h)^2}(q^h - q)\xi_{n,x}dx \\
&+ \sum_{j=1}^{N}\int_{I_j}(\sqrt{\tau\theta + \tau\mu^2(E^h)^2} - \sqrt{\tau\theta + \tau\mu^2E^2})q\xi_{n,x}dx \\
&= \sum_{j=1}^{N}\int_{I_j}\sqrt{\tau\theta + \tau\mu^2(E^h)^2}(\eta_q - \xi_q)\xi_{n,x}dx \\
&+ \sum_{j=1}^{N}\int_{I_j}(\sqrt{\tau\theta + \tau\mu^2(E^h)^2} - \sqrt{\tau\theta + \tau\mu^2E^2})q\xi_{n,x}dx \\
&= \sum_{j=1}^{N}\int_{I_j}\sqrt{\tau\theta + \tau\mu^2(E^h)^2}\eta_q\xi_{n,x}dx + (-\sum_{j=1}^{N}\int_{I_j}\sqrt{\tau\theta + \tau\mu^2(E^h)^2}\xi_q\xi_{n,x}dx) \\
&+ \sum_{j=1}^{N}\int_{I_j}(\sqrt{\tau\theta + \tau\mu^2(E^h)^2} - \sqrt{\tau\theta + \tau\mu^2E^2})q\xi_{n,x}dx = \sum_{i=1}^{3}\widetilde{T}_{31i}. \tag{4.39}
\end{aligned}
$$

Similarly,

$$\widetilde{T}_{33} = \sum_{j=1}^{N} \int_{I_j} \sqrt{\tau\theta + \tau\mu^2(E^h)^2}\eta_n\xi_{q,x}dx + (-\sum_{j=1}^{N} \int_{I_j} \sqrt{\tau\theta + \tau\mu^2(E^h)^2}\xi_n\xi_{q,x}dx)$$

$$+\sum_{j=1}^{N} \int_{I_j} (\sqrt{\tau\theta + \tau\mu^2(E^h)^2} - \sqrt{\tau\theta + \tau\mu^2 E^2})n\xi_{q,x}dx = \sum_{i=1}^{3} \widetilde{T}_{33i}. \qquad (4.40)$$

$$\begin{aligned}
\widetilde{T}_{34} &= \sum_{j=1}^{N} \int_{I_j} ((\sqrt{\tau\theta + \tau\mu^2(E^h)^2})_x n^h - (\sqrt{\tau\theta + \tau\mu^2 E^2})_x n)\xi_q dx \\
&= \sum_{j=1}^{N} \int_{I_j} (\sqrt{\tau\theta + \tau\mu^2(E^h)^2})_x (n^h - n)\xi_q dx \\
&\quad + \sum_{j=1}^{N} \int_{I_j} ((\sqrt{\tau\theta + \tau\mu^2(E^h)^2})_x - (\sqrt{\tau\theta + \tau\mu^2 E^2})_x)n\xi_q dx \\
&= \sum_{j=1}^{N} \int_{I_j} (\sqrt{\tau\theta + \tau\mu^2(E^h)^2})_x \eta_n\xi_q dx + (-\sum_{j=1}^{N} \int_{I_j} (\sqrt{\tau\theta + \tau\mu^2(E^h)^2})_x \xi_n\xi_q dx)
\end{aligned}$$

$$+\sum_{j=1}^{N} \int_{I_j} ((\sqrt{\tau\theta + \tau\mu^2(E^h)^2})_x - (\sqrt{\tau\theta + \tau\mu^2 E^2})_x)n\xi_q dx = \sum_{i=1}^{3} \widetilde{T}_{34i}. \qquad (4.41)$$

$$\begin{aligned}
\widetilde{T}_{32} &= \sum_{j=1}^{N} (\sqrt{\tau\theta + \tau\mu^2(E^h)^2}q^{h-} - \sqrt{\tau\theta + \tau\mu^2 E^2}q)_{j+1/2}[\xi_n]_{j+1/2} \\
&= \sum_{j=1}^{N} (\sqrt{\tau\theta + \tau\mu^2(E^h)^2}(q^{h-} - q))_{j+1/2}[\xi_n]_{j+1/2} \\
&\quad + \sum_{j=1}^{N} (\sqrt{\tau\theta + \tau\mu^2(E^h)^2} - \sqrt{\tau\theta + \tau\mu^2 E^2})_{j+1/2}q_{j+1/2}[\xi_n]_{j+1/2} \\
&= \sum_{j=1}^{N} (\sqrt{\tau\theta + \tau\mu^2(E^h)^2}\eta_q^-[\xi_n])_{j+1/2} + (-\sum_{j=1}^{N} (\sqrt{\tau\theta + \tau\mu^2(E^h)^2}\xi_q^-[\xi_n])_{j+1/2})
\end{aligned}$$

$$+\sum_{j=1}^{N} \int_{I_j} ((\sqrt{\tau\theta + \tau\mu^2(E^h)^2} - \sqrt{\tau\theta + \tau\mu^2 E^2})q[\xi_n])_{j+1/2} = \sum_{i=1}^{3} \widetilde{T}_{32i}. \qquad (4.42)$$

$$\widetilde{T}_{35} = \sum_{j=1}^{N} (\sqrt{\tau\theta + \tau\mu^2(E^h)^2}\eta_n^+[\xi_q])_{j+1/2} + (-\sum_{j=1}^{N} (\sqrt{\tau\theta + \tau\mu^2(E^h)^2}\xi_n^+[\xi_q])_{j+1/2})$$

$$+\sum_{j=1}^{N} ((\sqrt{\tau\theta + \tau\mu^2(E^h)^2} - \sqrt{\tau\theta + \tau\mu^2 E^2})n[\xi_q])_{j+1/2} = \sum_{i=1}^{3} \widetilde{T}_{35i}. \qquad (4.43)$$

We now estimate the terms $\widetilde{T}_{3ij}$ $(i = 1, \cdots, 5, j = 1, \cdots, 3)$ separately.

$$
\begin{aligned}
\sum_{i=1}^{5} \widetilde{T}_{3i2} &= -\sum_{j=1}^{N} \int_{I_j} \sqrt{\tau\theta + \tau\mu^2(E^h)^2}\xi_q\xi_{n,x}dx - \sum_{j=1}^{N} \int_{I_j} \sqrt{\tau\theta + \tau\mu^2(E^h)^2}\xi_n\xi_{q,x}dx \\
&\quad - \sum_{j=1}^{N} \int_{I_j} (\sqrt{\tau\theta + \tau\mu^2(E^h)^2})_x\xi_q\xi_n dx \\
&\quad - \sum_{j=1}^{N} (\sqrt{\tau\theta + \tau\mu^2(E^h)^2}\xi_q^-[\xi_n])_{j+1/2} - \sum_{j=1}^{N} (\sqrt{\tau\theta + \tau\mu^2(E^h)^2}\xi_n^+[\xi_q])_{j+1/2} \\
&= -\sum_{j=1}^{N} \int_{I_j} (\sqrt{\tau\theta + \tau\mu^2(E^h)^2}\xi_q\xi_n)_x dx \\
&\quad - \sum_{j=1}^{N} (\sqrt{\tau\theta + \tau\mu^2(E^h)^2}\xi_q^-[\xi_n])_{j+1/2} - \sum_{j=1}^{N} (\sqrt{\tau\theta + \tau\mu^2(E^h)^2}\xi_n^+[\xi_q])_{j+1/2} \\
&= -\sum_{j=1}^{N} (\sqrt{\tau\theta + \tau\mu^2(E^h)^2}\xi_q\xi_n)_{j+1/2}^- + \sum_{j=1}^{N} (\sqrt{\tau\theta + \tau\mu^2(E^h)^2}\xi_q\xi_n)_{j-1/2}^+ \\
&\quad - \sum_{j=1}^{N} (\sqrt{\tau\theta + \tau\mu^2(E^h)^2}\xi_q^-[\xi_n])_{j+1/2}
\end{aligned}
$$

$$
-\sum_{j=1}^{N} (\sqrt{\tau\theta + \tau\mu^2(E^h)^2}\xi_n^+[\xi_q])_{j+1/2} = 0. \tag{4.44}
$$

If we set $a(E^h) = a^h = \sqrt{\tau\theta + \tau\mu^2(E^h)^2}$, $a(E) = a = \sqrt{\tau\theta + \tau\mu^2 E^2}$, we have $a(E^h) - a(E^h_{j-1/2}) = a'_{E^h}(E^h - E^h_{j-1/2})$, where a'_{E^h} is the mean value. Then

$$
\begin{aligned}
\widetilde{T}_{311} &= \sum_{j=1}^{N} a(E^h)\eta_q\xi_{n,x}dx \\
&= \sum_{j=1}^{N} (a(E^h) - a(E^h_{j-1/2}))\eta_q\xi_{n,x}dx + \sum_{j=1}^{N} a(E^h_{j-1/2})\eta_q\xi_{n,x}dx \\
&= \sum_{j=1}^{N} (a'_{E^h}(E^h - E^h_{j-1/2})\eta_q\xi_{n,x}dx + \sum_{j=1}^{N} a(E^h_{j-1/2})\eta_q\xi_{n,x}dx.
\end{aligned}
$$

Similar with the estimate of T_{53}, we have

$$
\widetilde{T}_{311} \le Ch^{2k+2} + C||\xi_n||^2 \tag{4.45}
$$

where the constant C depends on the mean value $||a'_{E^h}||_{0,\infty}$.

We use Young's inequality and a similar estimate as for $\widetilde{T}_{311}$ to the term $\widetilde{T}_{331}$, obtaining

$$
\widetilde{T}_{331} \le Ch^{2k+2} + \tilde{\varepsilon}||\xi_q||^2. \tag{4.46}
$$

$$\widetilde{T}_{313} + \widetilde{T}_{323} = \sum_{j=1}^{N} \int_{I_j} (a(E^h) - a(E))q\xi_{n,x}dx + \sum_{j=1}^{N} ((a(E^h) - a(E))q[\xi_n])_{j+1/2}$$

$$= -\sum_{j=1}^{N} \int_{I_j} ((a(E^h) - a(E))q)_x \xi_n dx - \sum_{j=1}^{N} ((a(E^h) - a(E))q[\xi_n])_{j+1/2}$$

$$+ \sum_{j=1}^{N} ((a(E^h) - a(E))q[\xi_n])_{j+1/2}$$

$$= \sum_{j=1}^{N} \int_{I_j} ((a(E) - a(E^h))q)_x \xi_n dx$$

$$= \sum_{j=1}^{N} \int_{I_j} (a(E) - a(E^h))q_x \xi_n dx + \sum_{j=1}^{N} \int_{I_j} (a(E) - a(E^h))_x q\xi_n dx$$

Using $a(E) - a(E^h) = a'_E(E - E^h)$, where a'_E is the mean value, and a similar estimate as for T_{54}, we have

$$\widetilde{T}_{313} + \widetilde{T}_{323} \le Ch^{2k+2} + C||\xi_n||^2 \tag{4.47}$$

where the constant C depends on $||a'_E||_{0,\infty}$, $||q||_{0,\infty}$, and $||q_x||_{0,\infty}$.

Similarly, we have

$$\widetilde{T}_{333} + \widetilde{T}_{353} = \sum_{j=1}^{N} \int_{I_j} (a(E^h) - a(E))n\xi_{q,x}dx + \sum_{j=1}^{N} ((a(E^h) - a(E))n[\xi_q])_{j+1/2}$$

$$= \sum_{j=1}^{N} \int_{I_j} (a(E) - a(E^h))n_x \xi_q dx + \sum_{j=1}^{N} \int_{I_j} (a(E) - a(E^h))_x n\xi_q dx.$$

Since

$$a(E) - a(E^h) = a'_E(E - E^h) = \frac{e}{\varepsilon}a'_E \int_{x_{j-1/2}}^{x} (n^h - n)ds$$

$$= \frac{e}{\varepsilon}a'_E \int_{x_{j-1/2}}^{x} (\eta_n - \xi_n)ds,$$

and

$$(a(E) - a(E^h))_x = a'_E(E_x - E_x^h) = \frac{e}{\varepsilon}a'_E(n^h - n) = \frac{e}{\varepsilon}a'_E(\eta_n - \xi_n),$$

using Young inequality, we obtain

$$\widetilde{T}_{333} + \widetilde{T}_{353} = \sum_{j=1}^{N} \int_{I_j} \frac{e}{\varepsilon}a'_E (\int_{x_{j-1/2}}^{x} \eta_n ds)n_x \xi_q dx$$

$$- \sum_{j=1}^{N} \int_{I_j} \frac{e}{\varepsilon}a'_E (\int_{x_{j-1/2}}^{x} \xi_n ds)n_x \xi_q dx$$

$$+ \sum_{j=1}^{N} \int_{I_j} \frac{e}{\varepsilon}a'_E \eta_n n\xi_q dx - \sum_{j=1}^{N} \int_{I_j} \frac{e}{\varepsilon}a'_E \xi_n n\xi_q dx$$

$$\le Ch^{2k+2} + C||\xi_n||^2 + \tilde{\varepsilon}||\xi_q||^2. \tag{4.48}$$

From the property of the projection, we get

$$\widetilde{T}_{321} + \widetilde{T}_{351} = \sum_{j=1}^{N} (a(E^h)\eta_q^- [\xi_n])_{j+1/2} + \sum_{j=1}^{N} (a(E^h)\eta_n^+ [\xi_q])_{j+1/2} = 0. \tag{4.49}$$

Using (2.3) and Young's inequality, we have

$$\widetilde{T}_{341} = \sum_{j=1}^{N} \int_{I_j} a(E^h)_x \eta_n \xi_q dx \le Ch^{2k+2} + \tilde{\varepsilon} ||\xi_q||^2 \tag{4.50}$$

where the constant C depends on $||a(E^h)_x||_{0,\infty}$.

Finally, we estimate the last term $\widetilde{T}_{343}$

$$
\begin{aligned}
\widetilde{T}_{343} &= \sum_{j=1}^{N} \int_{I_j} (a(E^h) - a(E))_x n \xi_q dx \\
&= \sum_{j=1}^{N} \int_{I_j} a'_E (E_x^h - E_x) n \xi_q dx \\
&= \sum_{j=1}^{N} \int_{I_j} \frac{e}{\varepsilon} a'_E (n - n^h) n \xi_q dx \\
&= \sum_{j=1}^{N} \int_{I_j} \frac{e}{\varepsilon} a'_E (\xi_n - \eta_n) n \xi_q dx.
\end{aligned}
$$

Using Young's inequality and (2.3), we obtain

$$\widetilde{T}_{343} \le Ch^{2k+2} + C||\xi_n||^2 + \tilde{\varepsilon}||\xi_q||^2. \tag{4.51}$$

Adding all the results (4.44)-(4.51) together, we get

$$\widetilde{T}_3 \le Ch^{2k+2} + C||\xi_n||^2 + \tilde{\varepsilon}||\xi_q||^2. \tag{4.52}$$

Substituting (4.16)-(4.17), (4.22), (4.36) (or (4.37)) and (4.52) into (4.15), we get

$$\frac{1}{2}\frac{d}{dt}||\xi_n||^2 + ||\xi_q||^2 \le Ch^{2k+1} + C||\xi_n||^2 + \tilde{\varepsilon}||\xi_q||^2 + Ch^{-1}||\xi_n||_{0,\infty}||\xi_n||^2. \tag{4.53}$$

To deal with the last term of (4.53) caused by the nonlinearity of the equation we would like to make another a-priori assumption that, for small enough h, there holds

$$||\xi_n|| \le h^{\frac{3}{2}}. \tag{4.54}$$

From the above assumption and the inverse inequality, we have $||\xi_n||_{0,\infty} \le Ch$, then we get the following estimate

$$\frac{1}{2}\frac{d}{dt}||\xi_n||^2 + ||\xi_q||^2 \le Ch^{2k+1} + C||\xi_n||^2. \tag{4.55}$$

Using Gronwall's inequality, we have

$$||\xi_n||_{L^\infty(0,T;L^2)} + ||\xi_q||_{L^2(0,T;L^2)} \le Ch^{k+\frac{1}{2}}. \tag{4.56}$$

This, together with the property of the projection (2.3), yields the error estimate (4.11).

To complete the proof, let us verify the a-priori assumption (3.23) and (4.54). Since (3.23) can be deduced from (4.54) by (2.3) and the triangle inequality, we only need to verify the a-priori assumption (4.54). For $k \geq 2$, we can consider h small enough so that $Ch^{k+\frac{1}{2}} < \frac{1}{2}h^2$, where C is the constant in (4.11) determined by the final time T. Then if $t^* = \sup\{t : \|\xi_n(t)\| \leq h^{\frac{3}{2}}\}$, we should have $\|\xi_n(t^*)\| = h^{\frac{3}{2}}$ by continuity if t^* is finite. On the other hand, our proof implies that (4.11) holds for $t \leq t^*$, in particular $\|\xi_n(t^*)\| \leq Ch^{k+\frac{1}{2}} < \frac{1}{2}h^2$. This is a contradiction if $t^* < T$. Hence $t^* \geq T$ and the assumption (4.54) is correct.

Remark 4.2: The error analysis of using continuous Galerkin finite element method to solve the Poisson equation can be explained similarly as in Remark 3.2.

5 Numerical experiments for the DD and HF models

Different choices of bases for V_h^k do not alter the algorithm. We choose locally orthogonal Legendre polynomial basis over $I_j = (x_{j-1/2}, x_{j+1/2})$,

$$v_0^{(j)}(x) = 1, \quad v_1^{(j)}(x) = x - x_j, \quad v_2^{(j)}(x) = (x - x_j)^2 - \frac{1}{12}\Delta x_j^2, \quad \cdots .$$

In our implementation, we use scaled Legendre polynomial basis over $[-\frac{1}{2}, \frac{1}{2}]$,

$$v_0^{(j)}(\xi) = 1, \quad v_1^{(j)}(\xi) = \xi, \quad v_2^{(j)}(\xi) = \xi^2 - \frac{1}{12}, \quad \cdots .$$

where $\xi = \frac{x - x_j}{\Delta x_j}$. The numerical solution can then be written as

$$u^h(x, t) = \sum_{l=0}^{k} u_j^{(l)}(t) v_l^{(j)}(x), \quad for \ \ x \in I_j \ \ (u = n, q).$$

We use the third order total variation diminishing (TVD) Runge-Kutta method [28] for the time discretization, until a steady state is reached for our steady state diode test case.

We simulate the DD and HF models with a length of $0.6\mu m$ and a doping defined by $n_d = 5 \times 10^{17}cm^{-3}$ in $[0, 0.1]$ and in $[0.5, 0.6]$ and $n_d = 2 \times 10^{15}cm^{-3}$ in $[0.15, 0.45]$, and a smooth transition in between. The lattice temperature is taken as $T_0 = 300°K$. The constants $k = 0.138 \times 10^{-4}$, $\varepsilon = 11.7 \times 8.85418$, $e = 0.1602$, $m = 0.26 \times 0.9109 \times 10^{-31}kg$, and the mobility $\mu = 0.0088 \left(1 + \frac{14.2273}{1 + \frac{n_d}{143200}}\right)$ or $\mu = 0.75$, 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 $n_i = 1.4 \times 10^{10}cm^{-3}$, $\phi = \phi_0 + v_{bias}$ with the voltage drop $v_{bias} = 1.5$ at the right boundary for the potential; $T = 300°K$ at both boundaries for the temperature; and $n = 5 \times 10^{17}cm^{-3}$ at both boundaries for the concentration.

Figure 5.1 plots the simulation results of DD and HF models. The top two figures compare the simulation results for the DD model of $\mu = \mu(n_d)$ with $\mu = 0.75$. The bottom two figures compare the results of DD model with HF model, $\mu = \mu(n_d)$. The codes run
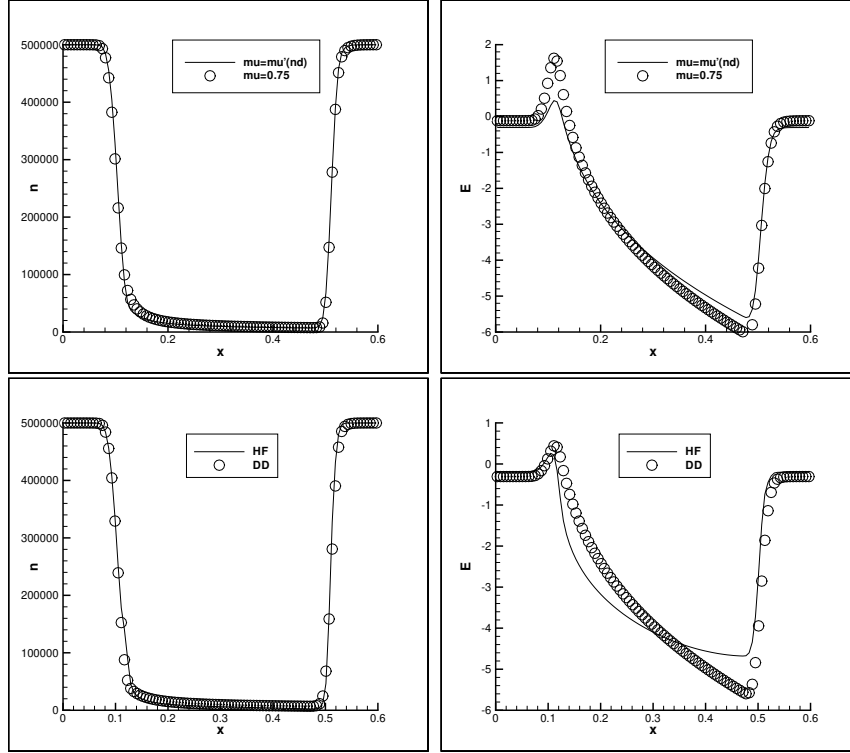
27

Figure 5.1: $[0, 0.6]$ with 100 mesh cells. Left: density n ($10^{12} cm^{-3}$); right: electric field E (V/um).

stably and 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. The numerical scheme is thus a reliable tool for the study of suitability of various moment models such as DD and HF to describe the correct physics.

6   Concluding remarks and future work

In this paper we follow up on our earlier work in [1, 2] to analyze a unified local discontinuous Galerkin (LDG) solver for moment models in semiconductor device simulations, including the DD and HF models, in which both the first derivative convection terms and the second derivative diffusion terms exist. We obtain an error estimate $O(h^{k+\frac{1}{2}})$ when P^k elements (piecewise polynomials of degree k) are used in the LDG scheme for one dimensional DD ($k \geq 1$) and HF ($k \geq 2$) models. A simulation is also performed to the two models. We use expansions and a-priori assumptions 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. The analysis in this paper is based on the smoothness of the solutions of the underlying PDEs. It is a challenge to obtain stability and convergence which require less regularity of the exact solution, which will be carried out in future work.

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