

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].

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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 $I_j = (x_{j-1/2}, x_{j+1/2})$, $j = 1, 2, \dots, N$ 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 $x_j = \frac{1}{2}(x_{j-1/2} + x_{j+1/2})$. 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 $V_h^k \not\subseteq H^1$. This is one of the main differences between the discontinuous Galerkin method and most other finite element methods. Moreover, both the mesh sizes 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 ,

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

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

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

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

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

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

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

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)

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

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

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

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

$$q - \sqrt{\tau\theta} n_x = 0. \quad (3.4)$$

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

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

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

$$\begin{aligned} \int_{I_j} n_t v dx + \int_{I_j} (\mu E n + \sqrt{\tau\theta} q) v_x dx \\ - (\mu E n + \sqrt{\tau\theta} q)_{j+1/2} v_{j+1/2}^- + (\mu E n + \sqrt{\tau\theta} q)_{j-1/2} v_{j-1/2}^+ = 0, \end{aligned} \quad (3.5)$$

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

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

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:

$$\begin{aligned} \int_{I_j} (n^h)_t v dx + \int_{I_j} (\mu E^h n^h + \sqrt{\tau\theta} q^h) v_x dx \\ - (\mu \widehat{E^h n^h} + \sqrt{\tau\theta} \hat{q}^h)_{j+1/2} v_{j+1/2}^- + (\mu \widehat{E^h n^h} + \sqrt{\tau\theta} \hat{q}^h)_{j-1/2} v_{j-1/2}^+ = 0, \end{aligned} \quad (3.8)$$

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

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

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

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

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

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

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

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

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

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

and

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

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

$$\begin{aligned}
& \sum_{j=1}^N \int_{I_j} \xi_{n,t} \xi_n dx + \sum_{j=1}^N \int_{I_j} \xi_q^2 dx \\
= & \sum_{j=1}^N \int_{I_j} \eta_{n,t} \xi_n dx + \sum_{j=1}^N \int_{I_j} \eta_q \xi_q dx \\
+ & \sum_{j=1}^N \left(\int_{I_j} \sqrt{\tau\theta} \eta_q \xi_{n,x} dx + \int_{I_j} \sqrt{\tau\theta} \eta_n \xi_{q,x} dx - \sqrt{\tau\theta} \eta_{q,j+1/2}^- \xi_{n,j+1/2}^- \right. \\
& \left. + \sqrt{\tau\theta} \eta_{q,j-1/2}^- \xi_{n,j-1/2}^+ - \sqrt{\tau\theta} \eta_{n,j+1/2}^+ \xi_{q,j+1/2}^- + \sqrt{\tau\theta} \eta_{n,j-1/2}^+ \xi_{q,j-1/2}^+ \right) \\
+ & \sum_{j=1}^N \left(- \int_{I_j} \sqrt{\tau\theta} \xi_q \xi_{n,x} dx - \int_{I_j} \sqrt{\tau\theta} \xi_n \xi_{q,x} dx + \sqrt{\tau\theta} \xi_{q,j+1/2}^- \xi_{n,j+1/2}^- \right. \\
& \left. - \sqrt{\tau\theta} \xi_{q,j-1/2}^- \xi_{n,j-1/2}^+ + \sqrt{\tau\theta} \xi_{n,j+1/2}^+ \xi_{q,j+1/2}^- - \sqrt{\tau\theta} \xi_{n,j-1/2}^+ \xi_{q,j-1/2}^+ \right) \\
+ & \sum_{j=1}^N \left(- \int_{I_j} \mu(E_n - E^h n^h) \xi_{n,x} dx \right. \\
& \left. + \mu(E_n - \widehat{E^h n^h})_{j+1/2} \xi_{n,j+1/2}^- - \mu(E_n - \widehat{E^h n^h})_{j-1/2} \xi_{n,j-1/2}^+ \right) \\
= & T_1 + T_2 + T_3 + T_4 + T_5. \tag{3.17}
\end{aligned}$$

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

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

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

Obviously, from the projection (2.2), we have

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

We also have

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

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 (3.17), we have.

$$\begin{aligned}
T_5 &= \sum_{j=1}^N \left(- \int_{I_j} \mu(E^n - E^h n^h) \xi_{n,x} dx \right. \\
&\quad \left. + \mu(E^n - \widehat{E^h n^h})_{j+1/2} \xi_{n,j+1/2}^- - \mu(E^n - \widehat{E^h n^h})_{j-1/2} \xi_{n,j-1/2}^+ \right) \\
&= \sum_{j=1}^N \int_{I_j} \mu(E^h n^h - E^n) \xi_{n,x} dx - \sum_{j=1}^N \mu(E^n - \widehat{E^h n^h})_{j+1/2} [\xi_n]_{j+1/2} \\
&= \sum_{j=1}^N \int_{I_j} \mu E^h (n^h - n) \xi_{n,x} dx + \sum_{j=1}^N \int_{I_j} \mu(E^h - E) n \xi_{n,x} dx \\
&\quad + \sum_{j=1}^N \mu E_{j+1/2}^h (\hat{n}^h - n)_{j+1/2} [\xi_n]_{j+1/2} + \sum_{j=1}^N \mu(E^h - E)_{j+1/2} n_{j+1/2} [\xi_n]_{j+1/2} \\
&= \sum_{j=1}^N \int_{I_j} \mu E^h (\eta_n - \xi_n) \xi_{n,x} dx + \sum_{j=1}^N \mu E_{j+1/2}^h (\hat{\eta}_n - \hat{\xi}_n)_{j+1/2} [\xi_n]_{j+1/2} \\
&\quad + \sum_{j=1}^N \int_{I_j} \mu(E^h - E) n \xi_{n,x} dx + \sum_{j=1}^N \mu(E^h - E)_{j+1/2} n_{j+1/2} [\xi_n]_{j+1/2} \\
&= \left(- \sum_{j=1}^N \int_{I_j} \mu E^h \xi_n \xi_{n,x} dx - \sum_{j=1}^N \mu E_{j+1/2}^h \hat{\xi}_{n,j+1/2} [\xi_n]_{j+1/2} \right) \\
&\quad + \sum_{j=1}^N \mu E_{j+1/2}^h \hat{\eta}_{n,j+1/2} [\xi_n]_{j+1/2} + \sum_{j=1}^N \int_{I_j} \mu E^h \eta_n \xi_{n,x} dx \\
&\quad + \left(\sum_{j=1}^N \int_{I_j} \mu(E^h - E) n \xi_{n,x} dx + \sum_{j=1}^N \mu((E^h - E)n)_{j+1/2} [\xi_n]_{j+1/2} \right) = \sum_{i=1}^4 T_{5i}. \tag{3.22}
\end{aligned}$$

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 $\|E_0\|_{0,\infty} \leq C$, $\|E_x^h\|_{0,\infty} \leq C$ 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

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

Using Young's inequality, we have

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

therefore

$$\begin{aligned}
T_{51} + T_{52} &\leq \frac{1}{2} \sum_{j=1}^N \int_{I_j} \mu E_x^h \xi_n^2 dx + C \|\eta_n\|_{\Gamma_h}^2 - \left(\frac{1}{2} - \tilde{\varepsilon}\right) \sum_{j=1}^N \mu |E^h|_{j+1/2} [\xi_n]_{j+1/2}^2 \\
&\leq C \|\xi_n\|^2 + Ch^{2k+1}.
\end{aligned} \tag{3.24}$$

Next, we have

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

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

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

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

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

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

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

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

Using the Gronwall's inequality, we obtain

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

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])

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

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).

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

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

where

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

and

$$\begin{aligned} J_{hyp} &= -\mu n E + \tau \mu \left(\frac{e}{\varepsilon}\right) n (-\mu n E + \omega), \\ J_{vis} &= -\tau (n(\theta + 2\mu^2 E^2))_x + \tau \mu E (\mu n E)_x. \end{aligned}$$

Here $\omega = (\mu n E)|_{x=0}$ 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

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

the equation (4.1) can be written as

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

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

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

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

$$n_t + (-(3C_2 E n_d + \mu E - C_3) n + 2C_2 E n^2)_x - ((\tau \theta + \tau \mu^2 E^2) n_x)_x = 0. \quad (4.4)$$

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

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

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

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

$$\begin{aligned}
& \int_{I_j} n_t v dx + \int_{I_j} (3C_2 E n_d + \mu E - C_3) n v_x dx \\
& - (3C_2 E n_d n + \mu E n - C_3 n)_{j+1/2} v_{j+1/2}^- \\
& + (3C_2 E n_d n + \mu E n - C_3 n)_{j-1/2} v_{j-1/2}^+ \\
& - \int_{I_j} 2C_2 E n^2 v_x dx + 2C_2 (E n^2)_{j+1/2} v_{j+1/2}^- - 2C_2 (E n^2)_{j-1/2} v_{j-1/2}^+ \\
& + \int_{I_j} \sqrt{\tau\theta + \tau\mu^2 E^2} q v_x dx \\
& - (\sqrt{\tau\theta + \tau\mu^2 E^2} q)_{j+1/2} v_{j+1/2}^- + (\sqrt{\tau\theta + \tau\mu^2 E^2} q)_{j-1/2} v_{j-1/2}^+ = 0. \tag{4.7}
\end{aligned}$$

$$\begin{aligned}
& \int_{I_j} q w dx + \int_{I_j} \sqrt{\tau\theta + \tau\mu^2 E^2} n w_x dx + \int_{I_j} (\sqrt{\tau\theta + \tau\mu^2 E^2})_x n w dx \\
& - (\sqrt{\tau\theta + \tau\mu^2 E^2} n)_{j+1/2} w_{j+1/2}^- + (\sqrt{\tau\theta + \tau\mu^2 E^2} n)_{j-1/2} w_{j-1/2}^+ = 0. \tag{4.8}
\end{aligned}$$

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:

$$\begin{aligned}
& \int_{I_j} n_t^h v dx + \int_{I_j} (3C_2 E^h n_d + \mu E^h - C_3) n^h v_x dx \\
& - (3C_2 E^h n_d + \mu E^h - C_3)_{j+1/2} \hat{n}_{j+1/2}^h v_{j+1/2}^- \\
& + (3C_2 E^h n_d + \mu E^h - C_3)_{j-1/2} \hat{n}_{j-1/2}^h v_{j-1/2}^+ \\
& - \int_{I_j} 2C_2 E^h (n^h)^2 v_x dx + 2C_2 (E^h (\widehat{(n^h)^2}))_{j+1/2} v_{j+1/2}^- - 2C_2 (E^h (\widehat{(n^h)^2}))_{j-1/2} v_{j-1/2}^+ \\
& + \int_{I_j} \sqrt{\tau\theta + \tau\mu^2 (E^h)^2} q^h v_x dx \\
& - (\sqrt{\tau\theta + \tau\mu^2 (E^h)^2} \hat{q}^h)_{j+1/2} v_{j+1/2}^- + (\sqrt{\tau\theta + \tau\mu^2 (E^h)^2} \hat{q}^h)_{j-1/2} v_{j-1/2}^+ = 0. \tag{4.9}
\end{aligned}$$

$$\begin{aligned}
& \int_{I_j} q^h w dx + \int_{I_j} \sqrt{\tau\theta + \tau\mu^2 (E^h)^2} n^h w_x dx + \int_{I_j} (\sqrt{\tau\theta + \tau\mu^2 (E^h)^2})_x n^h w dx \\
& - (\sqrt{\tau\theta + \tau\mu^2 (E^h)^2} \hat{n}^h)_{j+1/2} w_{j+1/2}^- + (\sqrt{\tau\theta + \tau\mu^2 (E^h)^2} \hat{n}^h)_{j-1/2} w_{j-1/2}^+ = 0. \tag{4.10}
\end{aligned}$$

The numerical electric field E^h is solved as before. For convenience, we denote $a^h := \sqrt{\tau\theta + \tau\mu^2(E^h)^2}$, $b^h := 3C_2E^hn_d + \mu E^h - C_3$ 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 $a := \sqrt{\tau\theta + \tau\mu^2E^2}$, $b := 3C_2En_d + \mu E - C_3$ 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

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

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

$$\begin{aligned} & \int_{I_j} (n - n^h)_t v dx + \int_{I_j} (bn - b^h n^h) v_x dx \\ & - ((bn)_{j+1/2} - (b^h \hat{n}^h)_{j+1/2}) v_{j+1/2}^- + ((bn)_{j-1/2} - (b^h \hat{n}^h)_{j-1/2}) v_{j-1/2}^+ \\ & - \int_{I_j} 2C_2(E n^2 - E^h (n^h)^2) v_x dx \\ & + 2C_2(E n^2 - E^h \widehat{(n^h)^2})_{j+1/2} v_{j+1/2}^- - 2C_2(E n^2 - E^h \widehat{(n^h)^2})_{j-1/2} v_{j-1/2}^+ \\ & + \int_{I_j} (aq - a^h q^h) v_x dx \\ & - (aq - a^h \hat{q}^h)_{j+1/2} v_{j+1/2}^- + (aq - a^h \hat{q}^h)_{j-1/2} v_{j-1/2}^+ = 0. \end{aligned} \quad (4.12)$$

$$\begin{aligned} & \int_{I_j} (q - q^h) w dx + \int_{I_j} (an - a^h n^h) w_x dx + \int_{I_j} (a_x n - a_x^h n^h) w dx \\ & - (an - a^h \hat{n}^h)_{j+1/2} w_{j+1/2}^- + (an - a^h \hat{n}^h)_{j-1/2} w_{j-1/2}^+ = 0. \end{aligned} \quad (4.13)$$

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

$$\begin{aligned}
& \int_{I_j} (\xi_n - \eta_n)_t \xi_n dx + \int_{I_j} (\xi_q - \eta_q) \xi_q dx \\
&= \left(\int_{I_j} (b^h n^h - bn) \xi_{n,x} dx + (bn - b^h \hat{n}^h)_{j+1/2} \xi_{n,j+1/2}^- - (bn - b^h \hat{n}^h)_{j-1/2} \xi_{n,j-1/2}^+ \right) \\
&+ \left(\int_{I_j} 2C_2 (En^2 - E^h(n^h)^2) \xi_{n,x} dx \right. \\
&\quad \left. - 2C_2 (En^2 - E^h(\widehat{n^h})^2)_{j+1/2} \xi_{n,j+1/2}^- + 2C_2 (En^2 - E^h(\widehat{n^h})^2)_{j-1/2} \xi_{n,j-1/2}^+ \right) \\
&+ \left(\int_{I_j} (a^h q^h - aq) \xi_{n,x} dx + (aq - a^h \hat{q}^h)_{j+1/2} \xi_{n,j+1/2}^- - (aq - a^h \hat{q}^h)_{j-1/2} \xi_{n,j-1/2}^+ \right) \\
&\quad + \int_{I_j} (a^h n^h - an) \xi_{q,x} dx + \int_{I_j} (a_x^h n^h - a_x n) \xi_q dx \\
&\quad + (an - a^h \hat{n}^h)_{j+1/2} \xi_{q,j+1/2}^- - (an - a^h \hat{n}^h)_{j-1/2} \xi_{q,j-1/2}^+ = \sum_{i=1}^3 \tilde{T}_{ij}. \tag{4.14}
\end{aligned}$$

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

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

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

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

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

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

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

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

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

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

$$\tilde{T}_{11} = \frac{1}{2} \sum_{j=1}^N \int_{I_j} b_x^h \xi_n^2 dx - \frac{1}{2} \sum_{j=1}^N |b_{j+1/2}^h| [\xi_n]_{j+1/2}^2.$$

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

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

So we have

$$\begin{aligned}
\tilde{T}_{11} + \tilde{T}_{12} &\leq C\|\xi_n\|^2 + C\|\eta_n\|_{\Gamma_h}^2 - \left(\frac{1}{2} - \tilde{\varepsilon}\right) \sum_{j=1}^N |b_{j+1/2}^h| [\xi_n]_{j+1/2}^2 \\
&\leq C\|\xi_n\|^2 + Ch^{2k+1} - \left(\frac{1}{2} - \tilde{\varepsilon}\right) \sum_{j=1}^N |b_{j+1/2}^h| [\xi_n]_{j+1/2}^2.
\end{aligned} \tag{4.19}$$

$$\begin{aligned}
\tilde{T}_{13} &= \sum_{j=1}^N \int_{I_j} b^h \eta_n \xi_{n,x} dx \\
&= \sum_{j=1}^N \int_{I_j} (b^h - b_{j-1/2}^h) \eta_n \xi_{n,x} dx + \sum_{j=1}^N \int_{I_j} b_{j-1/2}^h \eta_n \xi_{n,x} dx.
\end{aligned}$$

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

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

and

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

we have

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

Using the inverse inequality, we get

$$\begin{aligned}
\sum_{j=1}^N \int_{I_j} (b^h - b_{j-1/2}^h) \eta_n \xi_{n,x} dx &\leq C\|\xi_n\|^2 + C\|\eta_n\|^2 \\
&\leq C\|\xi_n\|^2 + Ch^{2k+2}.
\end{aligned}$$

So, we obtain

$$\tilde{T}_{13} \leq C\|\xi_n\|^2 + Ch^{2k+2}. \tag{4.20}$$

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

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

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

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

Integrating by parts, we get

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

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

$$\tilde{T}_{21} \leq Ch^{2k+2} + C\|\xi_n\|^2 \quad (4.24)$$

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

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

$$\begin{aligned}
n^2 - (n^h)^2 &= 2n(n - n^h) - (n - n^h)^2 \\
&= 2n(\xi_n - \eta_n) - (\xi_n - \eta_n)^2, \\
&= 2n\xi_n - 2n\eta_n - \xi_n^2 + 2\xi_n\eta_n - \eta_n^2 = \sum_{i=1}^5 \varphi_i \\
n^2 - \widehat{(n^h)^2} &= (n^2 - (\bar{n}^h)^2) + ((\bar{n}^h)^2 - \widehat{(n^h)^2}), \\
n^2 - (\bar{n}^h)^2 &= 2n\bar{\xi}_n - 2n\bar{\eta}_n - (\bar{\xi}_n)^2 + 2\bar{\xi}_n\bar{\eta}_n - (\bar{\eta}_n)^2 = \sum_{i=1}^5 \psi_i.
\end{aligned}$$

Then

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

where

$$\begin{aligned}
X_i &= 2C_2 \sum_{j=1}^N \int_{I_j} E^h \varphi_i \xi_{n,x} dx, \\
Y_i &= 2C_2 \sum_{j=1}^N E_{j+1/2}^h \psi_{i,j+1/2} [\xi_n]_{j+1/2},
\end{aligned}$$

which will be estimated term by term later.

Integrating by parts, we have

$$\begin{aligned}
X_1 + Y_1 &= 2C_2 \sum_{j=1}^N \int_{I_j} E^h 2n \xi_n \xi_{n,x} dx + 2C_2 \sum_{j=1}^N 2E_{j+1/2}^h n_{j+1/2} \bar{\xi}_{n,j+1/2} [\xi_n]_{j+1/2} \\
&= -2C_2 \sum_{j=1}^N \int_{I_j} (E^h n)_x \xi_n^2 dx - 2C_2 \sum_{j=1}^N E_{j+1/2}^h n_{j+1/2} [\xi_n^2]_{j+1/2} \\
&\quad + 2C_2 \sum_{j=1}^N 2E_{j+1/2}^h n_{j+1/2} \bar{\xi}_{n,j+1/2} [\xi_n]_{j+1/2} \\
&= -2C_2 \sum_{j=1}^N \int_{I_j} (E^h n)_x \xi_n^2 dx \\
&\leq C \|\xi_n\|^2
\end{aligned} \tag{4.26}$$

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

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

We use $n_{j+1/2} - n = O(h)$, $|E_{j+1/2}^h - E^h| = |\int_x^{x_{j+1/2}} (n^h - n_d) ds| = O(h)$, 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

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

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

Integrating by parts, we obtain

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

Using (2.3) and (2.4) we have

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

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

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

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

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

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

Then

$$\begin{aligned}
& 2C_2 \sum_{j=1}^N E_{j+1/2}^h ((n^{h^-})^2 - \widehat{(n^h)^2})_{j+1/2} [\xi_n]_{j+1/2} \\
&= -\frac{C_2}{6} \sum_{j=1}^N E_{j+1/2}^h [\xi_n - \eta_n]_{j+1/2}^2 [\xi_n]_{j+1/2} \\
&= -\frac{C_2}{6} \sum_{j=1}^N E_{j+1/2}^h ([\xi_n]_{j+1/2}^3 - 2[\eta_n]_{j+1/2} [\xi_n]_{j+1/2}^2 + [\eta_n]_{j+1/2}^2 [\xi_n]_{j+1/2}) \\
&\leq Ch^{-1} \|\xi_n\|_{0,\infty} \|\xi_n\|^2 + Ch^{-1} \|\eta_n\|_{0,\infty} \|\xi_n\|^2 + Ch^{-1} \|\eta_n\|_{0,\infty} (h \|\eta_n\|_{\Gamma_h}^2 + \|\xi_n\|^2) \\
&\leq Ch^{2k+2} + C \|\xi_n\|^2 + Ch^{-1} \|\xi_n\|_{0,\infty} \|\xi_n\|^2. \tag{4.34}
\end{aligned}$$

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

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

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

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

- 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

$$\begin{aligned}
& 2C_2 \sum_{j=1}^N (E^h \alpha[\eta_n - \xi_n][\xi_n])_{j+1/2} \\
&= 2C_2 \sum_{j=1}^N (E^h \alpha[\eta_n][\xi_n])_{j+1/2} - 2C_2 \sum_{j=1}^N E_{j+1/2}^h \alpha[\xi_n]_{j+1/2}^2 \\
&\leq C_2 \sum_{j=1}^N (|E^h|[\eta_n]^2)_{j+1/2} + C_2 \sum_{j=1}^N (|E^h|[\xi_n]^2)_{j+1/2} - 2C_2 \sum_{j=1}^N (|E^h|[\xi_n]^2)_{j+1/2} \\
&= C_2 \sum_{j=1}^N (|E^h|[\eta_n]^2)_{j+1/2} - C_2 \sum_{j=1}^N (|E^h|[\xi_n]^2)_{j+1/2} \\
&\leq Ch^{2k+1} - C_2 \sum_{j=1}^N (|E^h|[\xi_n]^2)_{j+1/2}.
\end{aligned}$$

Then

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

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

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

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

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

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

Similarly,

$$\begin{aligned}
\tilde{T}_{33} &= \sum_{j=1}^N \int_{I_j} \sqrt{\tau\theta + \tau\mu^2(E^h)^2} \eta_n \xi_{q,x} dx + \left(- \sum_{j=1}^N \int_{I_j} \sqrt{\tau\theta + \tau\mu^2(E^h)^2} \xi_n \xi_{q,x} dx \right) \\
&\quad + \sum_{j=1}^N \int_{I_j} (\sqrt{\tau\theta + \tau\mu^2(E^h)^2} - \sqrt{\tau\theta + \tau\mu^2 E^2}) n \xi_{q,x} dx = \sum_{i=1}^3 \tilde{T}_{33i}. \tag{4.40}
\end{aligned}$$

$$\begin{aligned}
\tilde{T}_{34} &= \sum_{j=1}^N \int_{I_j} ((\sqrt{\tau\theta + \tau\mu^2(E^h)^2})_x n^h - (\sqrt{\tau\theta + \tau\mu^2 E^2})_x n) \xi_q dx \\
&= \sum_{j=1}^N \int_{I_j} (\sqrt{\tau\theta + \tau\mu^2(E^h)^2})_x (n^h - n) \xi_q dx \\
&\quad + \sum_{j=1}^N \int_{I_j} ((\sqrt{\tau\theta + \tau\mu^2(E^h)^2})_x - (\sqrt{\tau\theta + \tau\mu^2 E^2})_x) n \xi_q dx \\
&= \sum_{j=1}^N \int_{I_j} (\sqrt{\tau\theta + \tau\mu^2(E^h)^2})_x \eta_n \xi_q dx + \left(- \sum_{j=1}^N \int_{I_j} (\sqrt{\tau\theta + \tau\mu^2(E^h)^2})_x \xi_n \xi_q dx \right) \\
&\quad + \sum_{j=1}^N \int_{I_j} ((\sqrt{\tau\theta + \tau\mu^2(E^h)^2})_x - (\sqrt{\tau\theta + \tau\mu^2 E^2})_x) n \xi_q dx = \sum_{i=1}^3 \tilde{T}_{34i}. \tag{4.41}
\end{aligned}$$

$$\begin{aligned}
\tilde{T}_{32} &= \sum_{j=1}^N (\sqrt{\tau\theta + \tau\mu^2(E^h)^2} q^{h^-} - \sqrt{\tau\theta + \tau\mu^2 E^2} q)_{j+1/2} [\xi_n]_{j+1/2} \\
&= \sum_{j=1}^N (\sqrt{\tau\theta + \tau\mu^2(E^h)^2} (q^{h^-} - q))_{j+1/2} [\xi_n]_{j+1/2} \\
&\quad + \sum_{j=1}^N (\sqrt{\tau\theta + \tau\mu^2(E^h)^2} - \sqrt{\tau\theta + \tau\mu^2 E^2})_{j+1/2} q_{j+1/2} [\xi_n]_{j+1/2} \\
&= \sum_{j=1}^N (\sqrt{\tau\theta + \tau\mu^2(E^h)^2} \eta_q^- [\xi_n])_{j+1/2} + \left(- \sum_{j=1}^N (\sqrt{\tau\theta + \tau\mu^2(E^h)^2} \xi_q^- [\xi_n])_{j+1/2} \right) \\
&\quad + \sum_{j=1}^N \int_{I_j} ((\sqrt{\tau\theta + \tau\mu^2(E^h)^2} - \sqrt{\tau\theta + \tau\mu^2 E^2}) q [\xi_n])_{j+1/2} = \sum_{i=1}^3 \tilde{T}_{32i}. \tag{4.42}
\end{aligned}$$

$$\begin{aligned}
\tilde{T}_{35} &= \sum_{j=1}^N (\sqrt{\tau\theta + \tau\mu^2(E^h)^2} \eta_n^+ [\xi_q])_{j+1/2} + \left(- \sum_{j=1}^N (\sqrt{\tau\theta + \tau\mu^2(E^h)^2} \xi_n^+ [\xi_q])_{j+1/2} \right) \\
&\quad + \sum_{j=1}^N ((\sqrt{\tau\theta + \tau\mu^2(E^h)^2} - \sqrt{\tau\theta + \tau\mu^2 E^2}) n [\xi_q])_{j+1/2} = \sum_{i=1}^3 \tilde{T}_{35i}. \tag{4.43}
\end{aligned}$$

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

$$\begin{aligned}
\sum_{i=1}^5 \tilde{T}_{3i2} &= - \sum_{j=1}^N \int_{I_j} \sqrt{\tau\theta + \tau\mu^2(E^h)^2} \xi_q \xi_{n,x} dx - \sum_{j=1}^N \int_{I_j} \sqrt{\tau\theta + \tau\mu^2(E^h)^2} \xi_n \xi_{q,x} dx \\
&\quad - \sum_{j=1}^N \int_{I_j} (\sqrt{\tau\theta + \tau\mu^2(E^h)^2})_x \xi_q \xi_n dx \\
&\quad - \sum_{j=1}^N (\sqrt{\tau\theta + \tau\mu^2(E^h)^2} \xi_q^- [\xi_n])_{j+1/2} - \sum_{j=1}^N (\sqrt{\tau\theta + \tau\mu^2(E^h)^2} \xi_n^+ [\xi_q])_{j+1/2} \\
&= - \sum_{j=1}^N \int_{I_j} (\sqrt{\tau\theta + \tau\mu^2(E^h)^2} \xi_q \xi_n)_x dx \\
&\quad - \sum_{j=1}^N (\sqrt{\tau\theta + \tau\mu^2(E^h)^2} \xi_q^- [\xi_n])_{j+1/2} - \sum_{j=1}^N (\sqrt{\tau\theta + \tau\mu^2(E^h)^2} \xi_n^+ [\xi_q])_{j+1/2} \\
&= - \sum_{j=1}^N (\sqrt{\tau\theta + \tau\mu^2(E^h)^2} \xi_q \xi_n)_{j+1/2}^- + \sum_{j=1}^N (\sqrt{\tau\theta + \tau\mu^2(E^h)^2} \xi_q \xi_n)_{j-1/2}^+ \\
&\quad - \sum_{j=1}^N (\sqrt{\tau\theta + \tau\mu^2(E^h)^2} \xi_q^- [\xi_n])_{j+1/2} \\
&\quad - \sum_{j=1}^N (\sqrt{\tau\theta + \tau\mu^2(E^h)^2} \xi_n^+ [\xi_q])_{j+1/2} = 0. \tag{4.44}
\end{aligned}$$

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 $a(E^h) - a(E_{j-1/2}^h) = a'_{E^h}(E^h - E_{j-1/2}^h)$, where a'_{E^h} is the mean value. Then

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

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

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

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 \tilde{T}_{311} to the term \tilde{T}_{331} , obtaining

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

$$\begin{aligned}
\tilde{T}_{313} + \tilde{T}_{323} &= \sum_{j=1}^N \int_{I_j} (a(E^h) - a(E))q\xi_{n,x}dx + \sum_{j=1}^N ((a(E^h) - a(E))q[\xi_n])_{j+1/2} \\
&= - \sum_{j=1}^N \int_{I_j} ((a(E^h) - a(E))q)_x \xi_n dx - \sum_{j=1}^N ((a(E^h) - a(E))q[\xi_n])_{j+1/2} \\
&\quad + \sum_{j=1}^N ((a(E^h) - a(E))q[\xi_n])_{j+1/2} \\
&= \sum_{j=1}^N \int_{I_j} ((a(E) - a(E^h))q)_x \xi_n dx \\
&= \sum_{j=1}^N \int_{I_j} (a(E) - a(E^h))q_x \xi_n dx + \sum_{j=1}^N \int_{I_j} (a(E) - a(E^h))_x q \xi_n dx
\end{aligned}$$

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

$$\tilde{T}_{313} + \tilde{T}_{323} \leq Ch^{2k+2} + C\|\xi_n\|^2 \quad (4.47)$$

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

Similarly, we have

$$\begin{aligned}
\tilde{T}_{333} + \tilde{T}_{353} &= \sum_{j=1}^N \int_{I_j} (a(E^h) - a(E))n\xi_{q,x}dx + \sum_{j=1}^N ((a(E^h) - a(E))n[\xi_q])_{j+1/2} \\
&= \sum_{j=1}^N \int_{I_j} (a(E) - a(E^h))n_x \xi_q dx + \sum_{j=1}^N \int_{I_j} (a(E) - a(E^h))_x n \xi_q dx.
\end{aligned}$$

Since

$$\begin{aligned}
a(E) - a(E^h) &= a'_E(E - E^h) = \frac{e}{\varepsilon} a'_E \int_{x_{j-1/2}}^x (n^h - n) ds \\
&= \frac{e}{\varepsilon} a'_E \int_{x_{j-1/2}}^x (\eta_n - \xi_n) ds,
\end{aligned}$$

and

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

using Young inequality, we obtain

$$\begin{aligned}
\tilde{T}_{333} + \tilde{T}_{353} &= \sum_{j=1}^N \int_{I_j} \frac{e}{\varepsilon} a'_E (\int_{x_{j-1/2}}^x \eta_n ds) n_x \xi_q dx \\
&\quad - \sum_{j=1}^N \int_{I_j} \frac{e}{\varepsilon} a'_E (\int_{x_{j-1/2}}^x \xi_n ds) n_x \xi_q dx \\
&\quad + \sum_{j=1}^N \int_{I_j} \frac{e}{\varepsilon} a'_E \eta_n n \xi_q dx - \sum_{j=1}^N \int_{I_j} \frac{e}{\varepsilon} a'_E \xi_n n \xi_q dx \\
&\leq Ch^{2k+2} + C\|\xi_n\|^2 + \tilde{\varepsilon}\|\xi_q\|^2.
\end{aligned} \quad (4.48)$$

From the property of the projection, we get

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

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

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

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

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

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

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

$$\tilde{T}_{343} \leq Ch^{2k+2} + C\|\xi_n\|^2 + \tilde{\varepsilon}\|\xi_q\|^2. \quad (4.51)$$

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

$$\tilde{T}_3 \leq Ch^{2k+2} + C\|\xi_n\|^2 + \tilde{\varepsilon}\|\xi_q\|^2. \quad (4.52)$$

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

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

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

$$\|\xi_n\| \leq h^{\frac{3}{2}}. \quad (4.54)$$

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

$$\frac{1}{2} \frac{d}{dt} \|\xi_n\|^2 + \|\xi_q\|^2 \leq Ch^{2k+1} + C\|\xi_n\|^2. \quad (4.55)$$

Using Gronwall's inequality, we have

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

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 $I_j = (x_{j-1/2}, x_{j+1/2})$,

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

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

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

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

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

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 $T_0 = 300^\circ K$. 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: $\phi = \phi_0 = \frac{kT}{e} \ln\left(\frac{n_d}{n_i}\right)$ 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; $T = 300^\circ K$ 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

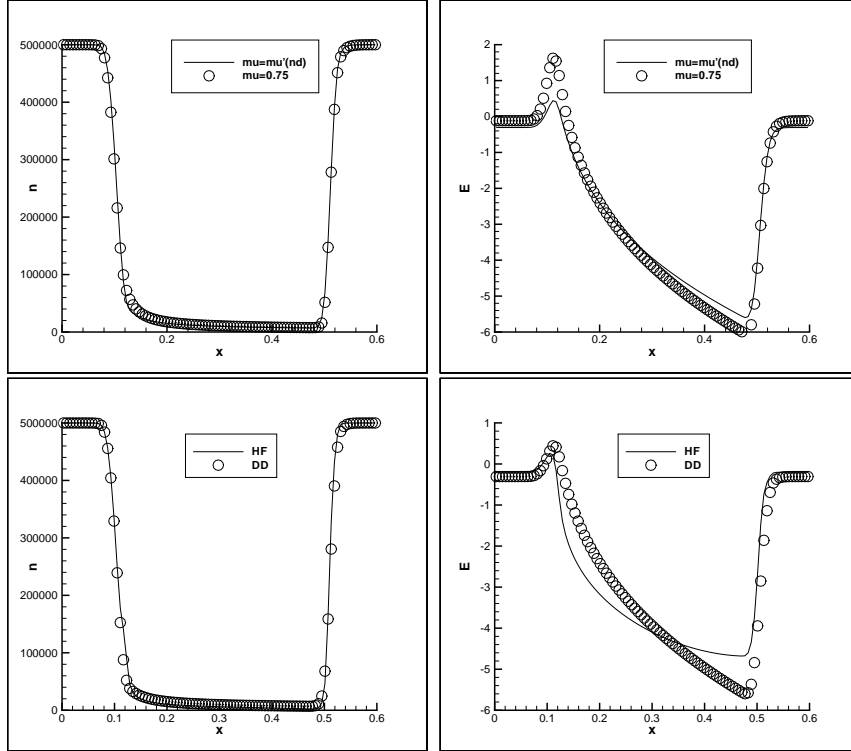


Figure 5.1: $[0, 0.6]$ with 100 mesh cells. Left: density n (10^{12}cm^{-3}); right: electric field E (V/um).

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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