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A FULLY DISCRETE ULTRA-WEAK DISCONTINUOUS GALERKIN METHOD FOR SOLVING THE DRIFT-DIFFUSION MODEL OF SEMICONDUCTOR DEVICES

XINYU DING, FUZHENG GAO*, AND YUNXIAN LIU*

Abstract. In this paper, we study an ultra-weak discontinuous Galerkin (UWDG) method for spatial discretization to solve the drift-diffusion (DD) model of one-dimensional semiconductor devices. Optimal error estimates are obtained using a special projection for both the semi-discrete and fully discrete UWDG schemes with smooth solutions. In the fully discrete UWDG scheme, we use an explicit third-order total variation diminishing Runge-Kutta method, which ensures stability under general temporal-spatial conditions. Numerical simulations are also performed to verify the analysis.

Key words. Drift-diffusion model, ultra-weak discontinuous Galerkin method, Runge-Kutta, error estimates.

1. Introduction

In this paper, we develop a UWDG method in space for solving the DD model of one-dimensional semiconductor devices, which is coupled with an explicit total variation diminishing Rung-Kutta (TVDRK) time-marching algorithm. Thereafter, we refer to the method as RK-UWDG. The DD model[2] is described by the following equations

$$n_t - \nabla \cdot (\mu E n) = \tau\theta\Delta n, \tag{1}$$

$$\Delta\phi = \frac{e}{\epsilon}(n - n_d), \tag{2}$$

$$E = -\nabla\phi, \tag{3}$$

where the unknown variables are the electron concentration n and the electric potential ϕ. (1) is the electron concentration equation and (2) is the electric potential equation. E represents the electric field.

The DD model is derived from the classical Boltzmann-Poisson system [1] that describes electron transport in semiconductor devices. Many numerical methods have been applied to solve the DD model, such as finite volume method [14, 15, 16], finite element method [17, 18] and also some other types of numerical methods [19]. In [3, 4], Squeff et al. analyzed the P^1 continuous finite element method for solving the DD model coupled with $P^0 - P^1$ mixed finite element method for the poisson equation. Liu and Shu[5] used a local discontinuous Galerkin (LDG) method to solve the DD model and gave suboptimal error estimates and numerical simulations. Later in [6], Liu developed the LDG method for the DD model with the optimal error estimates. Here, we present a RK-UWDG to solve the DD model of one-dimensional semiconductor devices.

The first dicontinuous Galerkin (DG) method was introduced by Reed and Hill[20] within the context of neutron linear transport in 1973. Subsequently, Cockburn

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*Corresponding author.

and Shu et al. developed the RKDG method for the hyperbolic conservation laws, which employs the DG method in space coupled with an explicit TVDRK time-marching[21, 22, 23, 24]. In 1998, Cockburn and Shu[26] proposed the LDG method as an extension to general convection-diffusion problems of the numerical scheme for the compressible Navier-Stokes equation. This method rewrites the equation into a first-order system, then apply the DG method on the system.

Meanwhile, the UWDG method was first proposed in [7], unlike the LDG method, it does not need to introduce any auxiliary variables. The principle of the UWDG method is to use integration by parts repeatedly and to move all the spatial derivatives from the trial function to the test function in the weak formulations. Cheng and Shu[8] proposed the UWDG method for general time-dependent problems with higher order spatial derivatives in 2008. In 2013, Bona et al. proposed a UWDG method for the generalised KdV equation with error estimation in [9]. Chen and Cheng[10] applied the UWDG method to the nonlinear Schrödinger equation and used a special projection to obtain optimal error estimates in 2019. In 2022, Wang and Xu applied the UWDG method to the convection diffusion equation in [11]. The UWDG method has the advantages of the classic DG method. Firstly, it can be easily designed for any order of accuracy that can be locally determined in each cell (p-adaptivity). Secondly, it can be used on arbitrary triangulations, even those with hanging nodes (h-adaptivity). Thirdly, it is extremely local in data communications. The evolution of the solution in each cell needs to communicate only with the immediate neighbors, regardless of the order of accuracy (parallel implementations). Furthermore, it is more compact than the LDG scheme and is simpler in formulation and coding.

In this work, we will first present the optimal error estimate of the semi-discrete UWDG scheme for solving one-dimensional drift-diffusion model with periodic boundary condition. The main technique is a special projection to be defined following from [11]. The projection can eliminate the projection errors involved in the diffusion part, but not eliminate the projection errors involved in the nonlinearity part. To avoid losing accuracy, we use a priori assumption to obtain optimal error estimate for the semi-discrete UWDG scheme. In practice, the DD model of semiconductor devices is described with Dirichlet boundary condition, so we also perform the error estimate of UWDG method with Dirichlet types. Furthermore, the error estimate for the third-order fully discrete explicit TVD RK-UWDG format will be analysed. The interaction of different intermediate time layers in the explicit TVDRK method renders the theoretical analysis of full discretisation considerably more challenging than that of semi-discretisation.

The organization of the paper is as follows. In Section 2, we present the discrete format of the UWDG method for solving the one-dimensional DD model. In Section 3, we describe the corresponding projection. Optimal L^2 error estimation of the semi-discrete UWDG scheme is derived in Section 4. In Section 5, we obtain the error estimate of the UWDG scheme for the DD model with Dirichlet boundary conditions. In Section 6, we present a fully discrete third-order RK-UWDG format and derive optimal L^2 error estimate. Simulation results are presented in Section 7. Concluding remarks and a plan for future work are given in Section 8.

2. The DD model and the semi-discrete UWDG scheme

In this section, we consider the following DD model

$$n_t - (\mu E n)_x - \tau\theta n_{xx} = 0, \tag{4}$$