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Implicit-Explicit Runge-Kutta Schemes for the Boltzmann-Poisson System for Semiconductors

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Abstract. In this paper we develop a class of Implicit-Explicit Runge-Kutta schemes for solving the multi-scale semiconductor Boltzmann equation. The relevant scale which characterizes this kind of problems is the diffusive scaling. This means that, in the limit of zero mean free path, the system is governed by a drift-diffusion equation. Our aim is to develop a method which accurately works for the different regimes encountered in general semiconductor simulations: the kinetic, the intermediate and the diffusive one. Moreover, we want to overcome the restrictive time step conditions of standard time integration techniques when applied to the solution of this kind of phenomena without any deterioration in the accuracy. As a result, we obtain high order time and space discretization schemes which do not suffer from the usual parabolic stiffness in the diffusive limit. We show different numerical results which permit to appreciate the performances of the proposed schemes.

AMS subject classifications: 35B25, 65M06, 76R50, 82C70

Key words: IMEX-RK methods, asymptotic preserving methods, semiconductor Boltzmann equation, drift-diffusion limit.

1 Introduction

The application of kinetic theory to the modeling of semiconductor devices simulations is a long dated but still very active research field because of the richness and diversity of observed phenomena [33, 35].

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From the mathematical point of view, semiconductor devices can be accurately described by a Boltzmann equation for the distribution function of electrons [2,8,9]. When the average time between electron-phonon collisions is small, the relevant scaling is the diffusive one and in such regimes these systems can be described by macroscopic drift-diffusion equations [20, 35, 39, 40]. Unfortunately, this passage from the microscopic to the macroscopic description leads to challenging numerical difficulties.

Indeed, under the diffusive scaling, the kinetic equation contains stiff terms since both the collision rates and the characteristic speeds of the systems becomes very large. This means that classical numerical methods need time step restrictions which make their use prohibitively expensive. In these cases, it becomes attractive to use domain decomposition strategies, which are able to solve the microscopic and the macroscopic models wherever it is necessary. These approaches have been largely studied for kinetic equations both for the diffusive [4, 13, 14, 29] and for the hydrodynamic scaling [15, 16]. However, even if these methods are very efficient they are affected by some difficulties due to the fact that it is not always a simple task to define the different regions of the domain in which the use of a macroscopic model is fully justified. Thus in the recent past alternative strategies have been studied, the so-called Asymptotic Preserving (AP) schemes. They consist in solving the original kinetic model in the full domain avoiding the time step restriction caused by the presence of different stiff terms in the equations. The AP methods automatically transform the original problem in the numerical approximations of the relevant macroscopic model when the scaling parameter goes to zero [5, 7, 12, 17, 21–23, 25–28, 30, 32, 36, 37]. Recently, this approach has been considered in the framework of Implicit-Explicit (IMEX) Runge-Kutta schemes with the aim of deriving high order numerical methods which are accurate in all regimes [3, 6, 11, 18, 19, 38]. This means that such schemes are able to preserve the desired order of accuracy even in the limit when the scaling parameter tends to zero.

In this paper we develop high order schemes for the resolution of the Boltzmann-Poisson semiconductor model. In this kind of problems, since the characteristic speed of the hyperbolic part of the kinetic equation is of the order of $1/\varepsilon$ (where ε is proportional to the mean free path), the CFL condition for an explicit approach would require $\Delta t = \mathcal{O}(\varepsilon \Delta x)$. Of course, in the diffusive regime where $\varepsilon \ll \Delta x$, this would be too much restrictive since a parabolic condition $\Delta t = \mathcal{O}(\Delta x^2)$ would suffice to solve the limiting equation. This kind of difficulties has been studied in [26–28, 30, 36, 37] using different semi-implicit approaches. However, most of the previous literature on the subject, originates consistent low order explicit schemes for the limit model. Such explicit schemes clearly suffer from the usual stability restriction $\Delta t = \mathcal{O}(\Delta x^2)$. Here, on the contrary to previous approaches, we are able to guarantee for all regimes a linear time step limitation $\Delta t = \mathcal{O}(\Delta x)$, independently from ε, and high order accuracy in time and space. In order to accomplish this task, we first rewrite our system using the parity formalism then, following [6], we add and subtract the limiting diffusive flux to the convective kinetic flux. We then discretize the reformulated problem by Implicit-Explicit Runge Kutta method. As we will show this will allow to get Asymptotic Preserving high order schemes which