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Extended Hydrodynamic Models and Multigrid Solver of a Silicon Diode Simulation

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Abstract. Extended hydrodynamic models for carrier transport are derived from the semiconductor Boltzmann equation with relaxation time approximation of the scattering term, by using the globally hyperbolic moment method and the moment-dependent relaxation time. Incorporating the microscopic relaxation time and the applied voltage bias, a formula is proposed to determine the relaxation time for each moment equation, which sets different relaxation rates for different moments such that higher moments damp faster. The resulting models would give more satisfactory results of macroscopic quantities of interest with a high-order convergence to those of the underlying Boltzmann equation as the involved moments increase, in comparison to the corresponding moment models using a single relaxation time. In order to simulate the steady states efficiently, a multigrid solver is developed for the derived moment models. Numerical simulations of an n^+-n-n^+ silicon diode are carried out to demonstrate the validation of the presented moment models, and the robustness and efficiency of the designed multigrid solver.

AMS subject classifications: 35L75, 35Q20, 65N55, 82D37

Key words: Boltzmann transport equation, extended hydrodynamic model, moment-dependent relaxation time, multigrid, semiconductor device simulation.

1 Introduction

Numerical simulations of carrier transport in semiconductors are of great interest in the design of modern devices. As the characteristic length of device shrinks into submicron scale regime, the famous drift-diffusion (DD) model [38] and its augmented version, such

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as the high-field model [19], become more and more inadequate to describe the important transport phenomena [22]. In such situations, one has to turn back to consider the fundamental Boltzmann transport equation (BTE), which gives a mesoscopic description of the charged particles in a semiclassical approximation. It follows, however, a great growth of the computational cost for numerical simulations based on the BTE in comparison to the DD model. This limits the widespread use of the BTE in a practical computer-aided design (CAD) of semiconductors, and nowadays to develop some appropriate macroscopic models, that describe the transport phenomena well with a significant reduction of the computational cost, is still receiving considerable attention. Following this direction, many models have been raised, such as energy-transport equations, hydrodynamic equations and high-order hydrodynamic equations, see [22] and [28] for a detailed description. One of powerful and systematic approaches to derive the macroscopic models might be employing Grad's moment method [21] with an appropriate closure ansatz for the resulting moment system. As pointed out in [22], the closure relations are crucial for the successful usage of such method. A well-posed entropy maximum closure has been proposed in [35]. Yet this closure is only of theoretical interest, for it depends on the analytical expression of the distribution function, which is unavailable in general for the system involving many moments. By imposing the derived quasi-linear moment system to satisfy the essential hyperbolicity, a new closure without any additionally empirical parameters has been presented in the context of the Boltzmann equation [7, 8] and the Wigner equation [9]. The systematic derivation makes it possible to employ the hyperbolic moment system with moments up to arbitrary order as one of promising models for the practical semiconductor device simulation. Moreover, the hyperbolic moment system is expected to converge to the underlying BTE with a high-order rate as the involved moments increase, for the Grad moment expansion can be viewed as a certain Hermite spectral discretization of the distribution function.

As a preliminary application of the hyperbolic moment method therein, the simulation of a simple n^+-n-n^+ diode, where the carrier transport can be depicted by the one dimensional BTE with the relaxation time approximation scattering term, has been carried out in [26]. It is shown that, for the diode with a channel of 400nm at the applied voltage bias lower than 0.5V, the 5th-order hyperbolic moment system is able to give the macroscopic quantities of physical interest, including current-voltage (I-V) characteristic curve, electron density, mean velocity, potential and electric field, that agree well with the reference obtained by the discrete velocity method (DVM) of the underlying BTE. However, oscillations, that may introduce numerical instability of the method, is also observed in those solutions, especially the temperature in the case the voltage bias larger than 0.5V is applied. This makes the expected convergence of the system can not be evidently verified, and restricts the application of the system to a more realistic device.

With careful and comprehensive observations, it is noticed that the scattering part of the entire moment system, derived in [26], employs the same microscopic relaxation time of the BTE scattering term. This is typically different from the usual approach of deriving hydrodynamic and extended hydrodynamic models, where a set of one single