Journal of Computational Physics 376 (2019) 634–659

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

A stochastic asymptotic-preserving scheme for the bipolar semiconductor Boltzmann-Poisson system with random inputs and diffusive scalings ☆

Liu Liu

The Institute for Computational Engineering and Sciences (ICES), University of Texas at Austin, Austin, TX 78712, USA

ARTICLE INFO

Article history:
Received 16 February 2018
Received in revised form 9 July 2018
Accepted 30 September 2018
Available online 3 October 2018

Keywords:
Bipolar Boltzmann-Poisson model
Diffusive scaling
Uncertainty quantification
Sensitivity analysis
gPC-SG method
Stochastic AP scheme

ABSTRACT

In this paper, we study the bipolar Boltzmann-Poisson model, both for the deterministic system and the system with uncertainties, with asymptotic behavior leading to the drift diffusion-Poisson system as the Knudsen number goes to zero. The random inputs can arise from collision kernels, doping profile and initial data. We adopt a generalized polynomial chaos approach based stochastic Galerkin (gPC-SG) method. Sensitivity analysis is conducted using hypocoercivity theory for both the analytical solution and the gPC solution for a simpler model that ignores the electric field, and it gives their convergence toward the global Maxwellian exponentially in time. A formal proof of the stochastic asymptotic-preserving (s-AP) property and a *uniform* spectral convergence with error decaying exponentially in time in the random space of the scheme is given. Numerical experiments are conducted to validate the accuracy, efficiency and asymptotic properties of the proposed method.

1. Introduction

Since kinetic equations are not first-principle physical equations, rather they often arise from mean field approximations of particle systems, hence there are inevitably modeling errors due to incomplete knowledge of the interaction mechanism, imprecise measurement of the initial and boundary data, forcing terms, geometry, etc. These errors can contribute uncertainties to the problems. Despite of intensive research at both theoretical and numerical levels, most researches are concerned with deterministic models and ignored uncertainties. Nevertheless, uncertainty quantification for kinetic equations, due to its importance in making reliable predications, calibrations and improvements of the kinetic models, deserves major attention from the research community.

To understand the propagation of the uncertainties and how they impact long-time behavior of the solution, sensitivity and regularity analyses are crucial, since they allow us to explore how sensitive the solution depends on random input parameters and to determine the convergence rate of the numerical methods in the parameter space. In recent years one begins to see some activities in such studies, see for examples [7,19,32,31,27,39,33]. At the numerical level, one of the popular UQ methods is the generalized polynomial chaos method in the stochastic Galerkin (referred as gPC-SG) framework [12,30,42]. Compared with the classical Monte-Carlo method, the gPC-SG approach enjoys a spectral accuracy in the random space–provided the solution is sufficiently regular in the space–while the Monte-Carlo method converges with only half-th

☆ The author is supported by the funding DOE-Simulation Center for Runaway Electron Avoidance and Mitigation, project number DE-SC0016283.
E-mail address: lliu@ices.utexas.edu.

https://doi.org/10.1016/j.jcp.2018.09.055
0021-9991/

order accuracy. As far as the non-intrusive stochastic collocation (SC) method is concerned, first the regularity analysis performed in this article is also useful for the accuracy analysis of SC methods. Second, there have been comparisons in terms of computational efficiencies between SG and SC for high dimensional problems; and there have been supporting cases the SG methods are more efficient (see for example [44]). For the problem under study, it remains an interesting question to make such a comparison for high dimensional problems, but this is out of the scope of this article and could be an interesting future project. Recent studies of gPC-SG methods for kinetic equations and their behavior in various asymptotic regimes are summarized in the review article [14].

Kinetic equations play an important role in semiconductor device modeling [34]. In such problems, the equations often have a diffusive scaling, characterized by the dimensionless Knudsen number ε, that leads asymptotically to the drift-diffusion equations as ε goes to zero. For multiscale problems in which ε can vary in several orders of magnitude, the asymptotic-preserving (AP) schemes have proven to be effective and efficient to deal with different scales in a seamless way. An AP scheme switches between a micro solver and a macro one automatically, depending on the ratio of numerical parameters (mesh size, time step, etc.) over ε [17,18,15]. Just considering the transport of electrons in the conduction band, [21] first introduced an AP scheme for the semiconductor Boltzmann equation with an anisotropic collision operator, which is able to capture the correct diffusive behavior for the underresolved numerical approximation. The scheme was further improved in [6] with better stability condition. A higher-order scheme was constructed in [8], which improved the strict parabolic stability condition to a hyperbolic one. An efficient AP scheme in the high field regime was developed in [24]. The authors in [16] further study the semiconductor Boltzmann equation with a two-scale stiff collision operators, by taking into account different effects including the interactions between electrons and the lattice defects caused by ionized impurities [3]; they design and demonstrate the efficiency and accuracy of an asymptotic-preserving scheme that leads to an energy-transport system as mean free path goes to zero at a discretized level.

For kinetic equations that contain random uncertainty, [26] first introduced the notion of stochastic AP (s-AP), which was followed recently by many works successfully handling the multiple scales for the kinetic equations with uncertainties [13, 20,2]. s-AP scheme is introduced in the SG setting. It extends the idea from the deterministic AP methods to the stochastic case, which requires that as $\varepsilon \to 0$, the SG for the microscopic model with uncertainties automatically becomes a SG approximation for the limiting macroscopic stochastic equation.

In this paper, we study the bipolar semiconductor system with random uncertainties, by taking into consideration the generation-recombination process between electrons and holes [28]. The bipolar semiconductor Boltzmann-Poisson equations will be studied, and we design and implement the gPC-SG scheme, with a formal proof of the s-AP property. In order to analyze the convergence rate of the scheme, we use the hypocoercivity theory, which was well established in deterministic kinetic theory [41,9,35,1] and recently extended to study uncertain kinetic equations in the linear case [31] and nonlinear ones [27,39,33]. By ignoring the self-consistent electric potential and using the hypocoercivity analysis done in [1,33], we obtain an exponential decay in time of the random solutions to the (deterministic) global equilibrium, and uniform spectral convergence with an exponential decay in time of the numerical error of the gPC-SG method for the underlying system with uncertainties, under suitable assumptions on the gPC polynomials and the random inputs. To our knowledge, this is the first study of AP and s-AP schemes for bipolar semiconductor Boltzmann system, in both deterministic and uncertain cases.

This paper is organized as the following. Section 2 gives an introduction of the bipolar Boltzmann-Poisson model, followed by a derivation of the limiting drift-diffusion equations. Section 3 discusses the AP scheme for the deterministic problem. A s-AP scheme in the gPC-SG framework for the bipolar model with random inputs will be studied and verified in section 4. A convergence rate analysis for both the analytical solution and the gPC solution for a simpler model (without electric field) will also be conducted in section 4. In section 5, we present several numerical examples for both the deterministic problem and the model with uncertainties, to illustrate the efficiency, accuracy and s-AP properties of the proposed scheme. Finally, the paper is concluded in section 6.

2. The bipolar semiconductor Boltzmann–Poisson system

In semiconductor devices, electrical currents originate from the transport of electrons and holes. $f_n(x, v, t)$, $f_p(x, v, t)$ represent the existence probability of an electron and a hole, respectively, at position $x \in \mathbb{R}^d$, with the velocity $v \in \mathbb{R}^d$, where d is the dimension, at time $t \geq 0$. The Boltzmann equations that give the evolution of the distribution functions for them are written by ([28,37])

$$\epsilon \partial_t f_n + (v \cdot \nabla_x f_n - E \cdot \nabla_v f_n) = \frac{1}{\epsilon} Q_n(f_n) + \epsilon I_n(f_n, f_p), \tag{2.1}$$

$$\epsilon \partial_t f_p + (\beta v \cdot \nabla_x f_p + E \cdot \nabla_v f_p) = \frac{1}{\epsilon} Q_p(f_p) + \epsilon I_p(f_n, f_p), \tag{2.2}$$

$$\gamma \, \Delta_x \Phi = n - p - C(x), \qquad E = -\nabla_x \Phi, \tag{2.3}$$

where $\beta = m_e^*/m_h^*$ is the ratio of the effective masses of electrons and holes, which we consider it a constant. $\Phi = \Phi(t, x)$ represents the electric potential, $E = E(t, x)$ is the self-consistent electric field given by the Poisson equation (2.3). γ is some scaled Debye length, $C(x)$ is the doping profile. The densities of the electron and the hole is given by