

Stochastic Galerkin Methods for the Boltzmann-Poisson system

José A. Morales Escalante⁺, Clemens Heitzinger^{*}

⁺The University of Texas at San Antonio – Departments of Mathematics and Physics & Astronomy

^{*}TU Wien – Department of Mathematics and Geoinformation

Abstract

We study uncertainty quantification for a Boltzmann-Poisson system that models electron transport in semiconductors and the physical collision mechanisms over the charges. We use the stochastic Galerkin method in order to handle the randomness associated with the problem. The main uncertainty in the Boltzmann equation concerns the initial conditions for a large number of particles, which is why the problem is formulated in terms of a probability density in phase space. The second source of uncertainty, directly related to the quantum nature of the problem, is the collision operator, as its structure in this semiclassical model comes from the quantum scattering matrices operating on the wave function associated to the electron probability density. Additional sources of uncertainty are transport, boundary data, etc. In this study we choose first the phonon energy as a random variable, since its value influences the energy jump appearing in the collision integral for electron-phonon scattering. Then we choose the lattice temperature as a random variable, since it defines the value of the collision operator terms in the case of electron-phonon scattering by being a parameter of the phonon distribution. The random variable for this case is a scalar then. Finally, we present our numerical simulations. We calculate with our stochastic Discontinuous Galerkin methods the uncertainty in kinetic moments such as density, mean energy, current, etc. associated to a possible physical temperature variation (assumed to follow a uniform distribution) in the lattice environment, as this uncertainty in the temperature is propagated into the electron PDF. Our results then let us predict in a real world problem setting the impact that possible variations in the lab conditions or limitations in the mathematical model (such as assumption of a constant phonon energy) will have over the calculated uncertainty in the behavior of electronic devices.

1 Introduction

1.1 The Deterministic Boltzmann-Poisson System

Electronic transport in semiconductors is a problem that, although definitely quantum mechanical in nature, can be approximated up to a certain point by semiclassical models featuring quantum corrections. In the semiclassical modelling, even with deterministic laws of motion, the number of electric charge

carriers $N \gg 1$ is of the order of the Avogadro number. The consequence is that a statistical model on the semiclassical scale is extremely adequate due to the large number of particles (i.e., the charge carriers, which are electrons in our problem), because it is virtually impossible to know exactly the initial conditions of positions and momentums for all the particles (on top of quantum considerations such as the Uncertainty Principle which indicate that knowing these initial conditions exactly is completely impossible). Therefore, uncertainty in the initial condition is naturally linked to the essence of the electron transport problem due to its many-carriers nature, even under a semiclassical approximation of this quantum problem, which consequently requires a statistical formulation, provided then by a particle density mechanics approach in terms of a probability density function in phase space. This probabilistic formulation is given precisely by the Boltzmann-Poisson (BP) semiclassical model for collisional electronic transport.

The Boltzmann-Poisson (BP) system for electron transport on a single conduction energy band has the form

$$\frac{\partial f}{\partial t} + \frac{1}{\hbar} \nabla_{\vec{k}} \varepsilon(\vec{k}) \cdot \nabla_{\vec{x}} f - \frac{q}{\hbar} \vec{E}(\vec{x}, t) \cdot \nabla_{\vec{k}} f = Q(f), \quad (1)$$

$$\nabla_{\vec{x}} \cdot (\epsilon \nabla_{\vec{x}} V) = q [\rho(\vec{x}, t) - N(\vec{x})], \quad \vec{E} = -\nabla_{\vec{x}} V, \quad (2)$$

with the quantum mechanical electron group velocity $\frac{1}{\hbar} \nabla_{\vec{k}} \varepsilon(\vec{k})$ and the electron density $\rho(\vec{x}, t) = \int_{\Omega_{\vec{k}}} f(\vec{x}, \vec{k}, t) d\vec{k}$. The collision integral operator $Q(f)$ describes the scattering over the electrons, where several mechanisms of quantum mechanical nature can be taken into account. In its full form, it enforces the Pauli Exclusion Principle by being given as

$$Q(f)(t, \vec{x}, \vec{k}) = \int_{\Omega_{\vec{k}'}} \left[S(\vec{k}' \rightarrow \vec{k}) f'(1 - f) - S(\vec{k} \rightarrow \vec{k}') f(1 - f') \right] d\vec{k}'. \quad (3)$$

The collision scattering term $S(\vec{k}' \rightarrow \vec{k}; \varepsilon(\vec{k}) \rightarrow \varepsilon(\vec{k}'))$ acts over f in our semiclassical model as a scattering matrix does in a quantum description over the wave function for a \vec{k} -state, i.e., representing the transition from a momentum \vec{k} to another state \vec{k}' , satisfying momentum and energy conservation principles. There's then an analogy $\langle \Psi(\vec{k}) | S | \Psi(\vec{k}') \rangle \leftrightarrow \int_{\Omega_{\vec{k}'}} S(\vec{k}' \rightarrow \vec{k}) f'(1 - f) d\vec{k}'$. It is important to mention that the specific form of $S(\vec{k}' \rightarrow \vec{k})$ can be derived from first-order time-dependent perturbation theory for the Schrödinger equation, by considering the perturbative Hamiltonian representing the scattering mechanisms under consideration. In the low density regime, however, we can relax the enforcing of the Pauli principle. In that case, the collisional integral operator can be approximated as being linear in f and therefore having the form

$$Q(f) = \int_{\Omega_{\vec{k}}} \left[S(\vec{k}', \vec{k}) f(t, \vec{x}, \vec{k}') - S(\vec{k}, \vec{k}') f(t, \vec{x}, \vec{k}) \right] d\vec{k}', \quad (4)$$

where $S(\vec{k}, \vec{k}')$ is the scattering kernel representing non-local interactions of electrons with a background density distribution. For example, in the case of silicon, one of the most important collision mechanisms are electron-phonon scatterings due to lattice vibrations of the crystal, which are modeled by acoustic (assumed

elastic) and optical (non-elastic) non-polar modes, the latter with a single frequency ω_p (assumed constant), as in

$$S(\vec{k}, \vec{k}') = (n_q + 1) K \delta(\varepsilon(\vec{k}') - \varepsilon(\vec{k}) + \hbar\omega_p) + n_q K \delta(\varepsilon(\vec{k}') - \varepsilon(\vec{k}) - \hbar\omega_p) + K_0 \delta(\varepsilon(\vec{k}') - \varepsilon(\vec{k})), \quad (5)$$

where K and K_0 are material constants for silicon. The symbol δ indicates the usual Dirac delta distribution, derived under the well-known Fermi's Golden Rule approximation in time-dependent perturbation theory [1]. The constant n_q is related to the phonon occupation factor

$$n_q(\hbar\omega_p) = \left[\exp\left(\frac{\hbar\omega_p}{K_B T_L}\right) - 1 \right]^{-1}, \quad (6)$$

where K_B is the Boltzmann constant and $T_L = 300K$ is the lattice temperature.

1.2 Main Uncertainties of the Boltzmann-Poisson Model

We can summarize the main uncertainties of the Boltzmann-Poisson model for electron transport in semiconductors as follows.

1. The initial conditions for and the large number of particles of the system, leading to a probabilistic formulation of the problem in terms of $f(\vec{x}, \vec{k}, t)$.
2. Quantum mechanical features in the Boltzmann equation, particularly in the collision operator $Q(f)$, based on a probabilistic description of the electron as a wavefunction Ψ : $\langle \Psi_{\vec{k}} | S | \Psi_{\vec{k}'} \rangle \leftrightarrow \int_{\Omega_{\vec{k}'}} S(\vec{k}' \rightarrow \vec{k}) f'(1 - f) d\vec{k}'$.
3. Uncertainty in the exact functional form of the energy band $\varepsilon(\vec{k})$. This function defines both the quantum terms of transport $\nabla_{\vec{k}} \varepsilon(\vec{k})$ and of electron-phonon scattering in silicon $\delta(\varepsilon(\vec{k}) - \varepsilon(\vec{k}') + l\hbar\omega_p)$, $l \in \{-1, 0, +1\}$, appearing in the Boltzmann equation.
4. The lattice temperature T may fluctuate, since it is related to the environmental temperature.
5. The phonon energy $\hbar\omega_p$ is often assumed to be constant, but it is known from experiments that this is not the case in general.
6. Parameters in the Poisson equation such as doping and permittivity may be uncertain. These are experimental parameters, and since they are given by measurements they are associated with measurement errors.
7. The boundary conditions that connect the domain to a stochastic environment. For example, reflection at physical boundaries might not be perfectly specular but rather have a diffusive component due to roughness in these boundaries.

In summary, uncertainty in the Boltzmann-Poisson system is crucial due to the inherent probabilistic (many particles) and quantum mechanical nature of the problem itself.

1.3 The Stochastic Boltzmann-Poisson System

Because of these reasons, we consider a stochastic Boltzmann-Poisson system of the form

$$\frac{\partial f}{\partial t} + \frac{1}{\hbar} \nabla_{\vec{k}} \varepsilon(\vec{k}, \vec{z}) \cdot \nabla_{\vec{x}} f - \frac{q}{\hbar} \vec{E}(\vec{x}, t, \vec{z}) \cdot \nabla_{\vec{k}} f = Q(f)(t, \vec{x}, \vec{k}, \vec{z}), \quad (7)$$

$$\nabla_{\vec{x}} \cdot (\epsilon \nabla_{\vec{x}} V) = q [\rho(\vec{x}, t) - N(\vec{x})], \quad \vec{E} = -\nabla_{\vec{x}} V, \quad (8)$$

with $f(t, \vec{x}, \vec{k}, \vec{z})$ being the probability density function now depending on an additional random parameter vector \vec{z} . The components of our random vector will be associated with the sources of uncertainty abovementioned, and they will be explicitly restated when we describe the stochastic Galerkin method for the Boltzmann-Poisson system.

1.4 Previous Work on Uncertainty Quantification for Boltzmann Models via Stochastic Galerkin Methods

In addition to the classical references for the stochastic Galerkin (SG) method such as Wiener's polynomial chaos [2], Ghanem and Spanos [3], Xiu and Karniadakis [4] etc., SG for Boltzmann equations in particular has recently been developed mainly by Shi Jin and his collaborators. It is a very active research area in the kinetic-theory community. The first paper that considered the use of SG for the Boltzmann equation in the context of gases was written by Hu and Jin [5]. Later on, SG was studied in the context of kinetic equations with random inputs, considering different models such as random linear and nonlinear Boltzmann equations, linear transport equations, and Vlasov-Poisson-Fokker-Planck equations. An overall view of the advances in the discipline for these equations can be found in the review paper [6], part as well of the review book [7].

More specifically, regarding SG methods for the semiconductor Boltzmann equation, the first work related to this topic was performed by Jin and Liu [8]. They consider in their model a collision operator whose scattering kernel term is bounded above and below. Although uncertainties can possibly come from the collision operator, the electric potential, initial data, or boundary data, the collision operator in this previous study of the semiconductor Boltzmann equation did not consider the more physically realistic case of Dirac delta distributions obtained by Fermi's Golden Rule for energy transitions, as the scattering kernel was assumed to be bounded. Furthermore, a possible uncertainty in the electron velocity was not considered by making the assumption of a deterministic velocity given by the parabolic energy band model. Most importantly, the numerical study in this work considered a random relaxation Maxwellian collision kernel, which does not involve energy transitions in its scattering model, in addition to random initial data in the electron density, random boundary data, a random Debye length, and random doping parameters in the Poisson equation. Therefore, the randomness of the energy band in the transport and collision terms and the uncertainty related to a collision operator that uses Dirac delta distributions due to Fermi's Golden Rule, as it is the case for electron-phonon scattering, remain as crucial topics yet to be studied for the understanding of uncertainty quantification in collisional electron transport in semiconductors via stochastic methods.

Our methodology will then be to study variables related to the electron-phonon collision operator as random in the SG method for the Boltzmann-Poisson model of electrons in semiconductors. We first choose as one of those variables the lattice temperature, as it is involved in the phonon distribution as a parameter. The dimensional cost is minimal as the temperature is a scalar.

We describe the structure of the rest of this paper as follows. In Section 2 we discuss how the SG method handles the uncertainties arising in the Boltzmann-Poisson system. Then we consider uncertainty quantification by SG first for the phonon energy being a random variable and then the lattice temperature being a random variable too. Section 3 describes the numerics of the deterministic Boltzmann-Poisson system solved by discontinuous-Galerkin (DG) methods. Then Section 4 covers in more detail the stochastic discontinuous Galerkin (SDG) method for the Boltzmann-Poisson system for the case of a random lattice temperature. In Section 5, the conclusions are drawn.

2 Stochastic Galerkin Method for the Boltzmann-Poisson System

2.1 Description of Uncertainties

The SG method handles the uncertainties in the Boltzmann-Poisson system by introducing random variables z_i , $i \in \{1, \dots, 7\}$, associated with the uncertainties as indicated below.

1. Regarding initial conditions and the large number of particles, the probabilistic formulation $f(\vec{x}, \vec{k}, t, z_1)$ with random initial conditions $f(\vec{x}, \vec{k}, 0, z_1)$ is used.
2. Regarding quantum phenomena in the collision operator $Q(f)$, the probabilistic nature of the electron wavefunction Ψ is mimicked (relaxing Pauli principle) by $\langle \Psi_{\vec{k}'} | S | \Psi_{\vec{k}} \rangle \leftrightarrow \int_{\Omega_{\vec{k}}} S(\vec{k} \rightarrow \vec{k}', z_2) f(\vec{x}, \vec{k}, t, z_2) d\vec{k}'$.
3. The uncertainty in the energy band structure is described as $\varepsilon(\vec{k}, z_3)$. This function defines both quantum terms of electron velocity $\nabla_{\vec{k}} \varepsilon(\vec{k}, z_3) / \hbar$ and of electron-phonon scattering in silicon $\delta(\varepsilon(\vec{k}, z_3) - \varepsilon(\vec{k}', z_3) + l(\hbar\omega_p + z_4))$, $l \in \{-1, 0, +1\}$.
4. The lattice temperature is written as $T + z_4$ as it may change due to fluctuations in the environment, but it is assumed to be constant in the model.
5. The phonon energy $\hbar\omega_p + z_5$ is approximated as constant in the model, but experiments show that it is nonconstant in general.
6. In the Poisson equation, the doping concentration is written as $N_D + z_6$ and the permittivity as $\epsilon + z_6$.
7. The boundary conditions are described as $f_B(\vec{x}, \vec{k}, t, z_7)|_{\partial\Omega}$, etc.

2.2 Stochastic Galerkin Method for the Boltzmann-Poisson System with the Phonon Energy as a Random Variable

In this section, we assume that the only uncertainty stems from the phonon energy model. Randomness in the phonon energy is physically relevant because it is known to be strictly speaking non-constant, and it is also a good starting point as a scalar random variable. Therefore, we replace $\hbar\omega_p$ in the deterministic equation by $\hbar\omega_p + z$. Then the phonon occupation as a function of the energy becomes

$$n_q(\hbar\omega_p, z) = \left[\exp\left(\frac{\hbar\omega_p + z}{K_B T_L}\right) - 1 \right]^{-1}. \quad (9)$$

This introduces randomness in the collision operator as well, leading to

$$\begin{aligned} S(\vec{k}, \vec{k}', z) &= [n_q(\hbar\omega_p, z) + 1] K \delta(\varepsilon(\vec{k}') - \varepsilon(\vec{k}) + \hbar\omega_p + z) \\ &+ K_0 \delta(\varepsilon(\vec{k}') - \varepsilon(\vec{k})) + n_q(\hbar\omega_p, z) K \delta(\varepsilon(\vec{k}') - \varepsilon(\vec{k}) - \hbar\omega_p - z). \end{aligned}$$

We consider two cases. First we devise a stochastic Galerkin algorithm using a distributional-derivative approximation with respect to the random variable. Then we consider the fully general case of the random variable in the collision operator without any distributional-derivative approximation in the random space. The algorithms are described in detail in the following.

2.2.1 Random Phonon Energy Using a Distributional Derivative Approximation

We consider the case $n := 1$, $P := 1$, $K := \dim(\mathcal{P}_P^n) := 2$, and approximate the density as (with $\vec{p} = \hbar\vec{k}$ being the crystal momentum)

$$f(t, \vec{x}, \vec{p}, z) \approx \sum_{k=1}^2 \alpha_k(t, \vec{x}, \vec{p}) \Psi_k(z) = \alpha(t, \vec{x}, \vec{p}) \cdot \Psi(z) = (\alpha_1, \alpha_2) \cdot (\Psi_1, \Psi_2). \quad (10)$$

Then the Boltzmann equation reads

$$\partial_t \alpha + \vec{v} \cdot \nabla_{\vec{x}} \alpha + F \cdot \nabla_{\vec{p}} \alpha = Q(\alpha), \quad (11)$$

$$Q(\alpha) = \int_{\Omega_{\vec{p}}} B(\vec{p}, \vec{p}') [M(\vec{p})\alpha(\vec{p}') - M(\vec{p}')\alpha(\vec{p})] d\vec{p}', \quad (12)$$

$$B_{ij}(\vec{p}, \vec{p}') = \int_{I_z} \sigma(\vec{p}, \vec{p}', z) \Psi_i(z) \Psi_j(z) \pi(z) dz \quad (13)$$

$$= \sigma_0(\vec{p}, \vec{p}') \delta_{ij} + \int_{I_z} \partial_z \sigma(\vec{p}, \vec{p}', z)|_{z=0} z \Psi_i(z) \Psi_j(z) \pi(z) dz, \quad (14)$$

$$\sigma(\vec{p}, \vec{p}', z) = \sigma_0(\vec{p}, \vec{p}') + \tilde{\sigma}_1(\vec{p}, \vec{p}') z = \sigma|_{z=0} + \partial_z \sigma(\vec{p}, \vec{p}', z)|_{z=0} z. \quad (15)$$

The scattering cross section is then written as

$$\sigma(\vec{p}, \vec{p}', z) = \sigma_0(\vec{p}, \vec{p}') + \tilde{\sigma}_1(\vec{p}, \vec{p}') z, \quad (16)$$

where

$$\sigma_0 = M^{-1}[K_0\delta(\varepsilon-\varepsilon')+(e^{\hbar\omega_p}-1)^{-1}K(e^{\hbar\omega_p}\delta(\varepsilon-\varepsilon'+\hbar\omega_p)+\delta(\varepsilon-\varepsilon'-\hbar\omega_p))]. \quad (17)$$

Here $\tilde{\sigma}_1(\vec{p}, \vec{p}') = \partial_z \sigma(\vec{p}, \vec{p}', z)|_{z=0}$ is a distributional derivative with respect to z , and we find

$$\begin{aligned} \tilde{\sigma}_1(\vec{p}, \vec{p}') &= M^{-1}K\partial_z \{ [1 + (e^{\hbar\omega_p+z} - 1)^{-1}]\delta(\varepsilon - \varepsilon' + \hbar\omega_p + z) \\ &\quad + (e^{\hbar\omega_p+z} - 1)^{-1}\delta(\varepsilon - \varepsilon' - \hbar\omega_p - z) \} |_{z=0}. \end{aligned}$$

Using $\delta'[\phi] = -\delta[\phi']$ and phonon distribution properties, we have

$$\begin{aligned} \tilde{\sigma}_1(\vec{p}, \vec{p}') &= M^{-1}K \{ [1 + (e^{\hbar\omega_p} - 1)^{-1}]\partial_z|_0\delta(\varepsilon - \varepsilon' + \hbar\omega_p + z) \\ &\quad + (e^{\hbar\omega_p} - 1)^{-1}\partial_z|_0\delta(\varepsilon - \varepsilon' - \hbar\omega_p - z) \\ &\quad - \frac{e^{\hbar\omega_p}}{(e^{\hbar\omega_p} - 1)^2}[\delta(\varepsilon - \varepsilon' + \hbar\omega_p) + \delta(\varepsilon - \varepsilon' - \hbar\omega_p)] \} \end{aligned}$$

and

$$\begin{aligned} B_{ij}(\vec{p}, \vec{p}') &= \sigma_0(\vec{p}, \vec{p}')\delta_{ij} + M^{-1}K \int_{I_z} dz \Psi_i(z)\Psi_j(z)\pi(z)z \cdot \\ &\quad \cdot \{ [1 + (e^{\hbar\omega_p} - 1)^{-1}]\partial_z|_0\delta(\varepsilon - \varepsilon' + \hbar\omega_p + z) \\ &\quad + (e^{\hbar\omega_p} - 1)^{-1}\partial_z|_0\delta(\varepsilon - \varepsilon' - \hbar\omega_p - z) \\ &\quad - \frac{e^{\hbar\omega_p}}{(e^{\hbar\omega_p} - 1)^2}[\delta(\varepsilon - \varepsilon' + \hbar\omega_p) + \delta(\varepsilon - \varepsilon' - \hbar\omega_p)] \} \\ &= \sigma_0(\vec{p}, \vec{p}')\delta_{ij} - M^{-1}K \cdot \\ &\quad \cdot \{ [1 + (e^{\hbar\omega_p} - 1)^{-1}]\partial_z[\Psi_i(z)\Psi_j(z)\pi(z)z]\chi|_{z=-(\varepsilon-\varepsilon'+\hbar\omega_p)} \\ &\quad + (e^{\hbar\omega_p} - 1)^{-1}\partial_z[\Psi_i(z)\Psi_j(z)\pi(z)z]\chi|_{z=+(\varepsilon-\varepsilon'-\hbar\omega_p)} \\ &\quad + \frac{e^{\hbar\omega_p}}{(e^{\hbar\omega_p} - 1)^2} \int_{I_z} dz \Psi_i(z)\Psi_j(z)\pi(z)z \sum_{\pm} \delta(\varepsilon - \varepsilon' \pm \hbar\omega_p) \} . \end{aligned}$$

If we assume the example $\pi(z) := \frac{e^{-\frac{z^2}{2}}}{\sqrt{2}}$, $\Psi_1 := 1$, and $\Psi_2 := 2z$, we obtain

$$\begin{aligned} B(\vec{p}, \vec{p}') &= \sigma_0(\vec{p}, \vec{p}')\delta_{ij} - M^{-1}K \times \\ &\quad \left\{ \left[1 + \frac{1}{e^{\hbar\omega_p} - 1} \right] \partial_z \left[\begin{pmatrix} 1 & 2z \\ 2z & 4z^2 \end{pmatrix} \pi(z)z \right] \chi|_{z=-(\varepsilon-\varepsilon'+\hbar\omega_p)} \right. \\ &\quad + (e^{\hbar\omega_p} - 1)^{-1} \partial_z \left[\begin{pmatrix} 1 & 2z \\ 2z & 4z^2 \end{pmatrix} \pi(z)z \right] \chi|_{z=+(\varepsilon-\varepsilon'-\hbar\omega_p)} \\ &\quad \left. + \frac{e^{\hbar\omega_p}}{(e^{\hbar\omega_p} - 1)^2} \sum_{\pm} \delta(\varepsilon - \varepsilon' \pm \hbar\omega_p) \begin{pmatrix} 0 & 1/2 \\ 1/2 & 0 \end{pmatrix} \right\} \\ &= \sigma_0(\vec{p}, \vec{p}')\mathcal{I} - M^{-1}K \times \\ &\quad \left\{ \frac{e^{\hbar\omega_p}}{e^{\hbar\omega_p} - 1} \begin{pmatrix} 1 - z^2 & 2z(2 - z^2) \\ 2z(2 - z^2) & 2z^2(3 - z^2) \end{pmatrix} \pi\chi|_{z=-(\varepsilon-\varepsilon'+\hbar\omega_p)} \right. \\ &\quad \left. + \frac{1}{e^{\hbar\omega_p} - 1} \begin{pmatrix} 1 - z^2 & 2z(2 - z^2) \\ 2z(2 - z^2) & 2z^2(3 - z^2) \end{pmatrix} \pi\chi|_{z=+(\varepsilon-\varepsilon'-\hbar\omega_p)} \right\} \end{aligned}$$

$$\begin{aligned}
& + \frac{e^{\hbar\omega_p}}{(e^{\hbar\omega_p} - 1)^2} \sum_{\pm} \delta(\varepsilon - \varepsilon' \pm \hbar\omega_p) \left(\begin{array}{cc} 0 & 1/2 \\ 1/2 & 0 \end{array} \right) \Big\}, \\
Q(\alpha) & = \int_{\Omega_{\vec{p}}} B(\vec{p}, \vec{p}') \left[M(\vec{p})\alpha(\vec{p}') - M(\vec{p}')\alpha(\vec{p}) \right] d\vec{p}'.
\end{aligned}$$

One could use as another example a sharper Gaussian with support mostly concentrated around the central value of zero fluctation, in order to give such a low probability to energy values $\hbar\omega_p + z < 0$ that virtually the probability density of having $z < -\hbar\omega_p$ would be numerically zero in a computational implementation.

2.2.2 Random Phonon Energy Without Approximation

Next, we consider again a random phonon energy, but now use the collision scattering term without approximation by distributional derivatives in the random space. We consider the case $n := 1$, $P := 1$, $K := \dim(\mathcal{P}_P^n) := 2$, and approximate the density again as

$$f(t, \vec{x}, \vec{p}, z) \approx \sum_{k=1}^2 \alpha_k(t, \vec{x}, \vec{p}) \Psi_k(z) = \alpha(t, \vec{x}, \vec{p}) \cdot \Psi(z) = (\alpha_1, \alpha_2) \cdot (\Psi_1, \Psi_2). \quad (18)$$

Then the Boltzmann equation reads

$$\partial_t \alpha + v \cdot \nabla_{\vec{x}} \alpha + F \cdot \nabla_{\vec{p}} \alpha = Q(\alpha), \quad (19)$$

$$Q(\alpha) = \int_{\Omega_p} B(\vec{p}, \vec{p}') [M(\vec{p})\alpha(\vec{p}') - M(\vec{p}')\alpha(\vec{p})] d\vec{p}', \quad (20)$$

$$B_{ij}(\vec{p}, \vec{p}') = \int_{I_z} \sigma(\vec{p}, \vec{p}', z) \Psi_i(z) \Psi_j(z) \pi(z) dz, \quad (21)$$

$$\sigma(\vec{p}, \vec{p}', z) = \frac{K_0 \delta(\varepsilon - \varepsilon') + K \frac{e^{\beta(\hbar\omega_p + z)} \delta(\varepsilon - \varepsilon' + \hbar\omega_p + z) + \delta(\varepsilon - \varepsilon' - \hbar\omega_p - z)}{e^{\beta(\hbar\omega_p + z)} - 1}}{M(\vec{p})} \quad (22)$$

with $\beta = (K_B T_L)^{-1}$. We then have

$$B_{ij}(\vec{p}, \vec{p}') = \frac{K_0 \delta(\varepsilon - \varepsilon') \delta_{ij} + K \int_{I_z} dz \Psi_i(z) \Psi_j(z) \pi(z) \left\{ \frac{e^{\beta(\hbar\omega_p + z)} \delta(\varepsilon - \varepsilon' + \hbar\omega_p + z) + \delta(\varepsilon - \varepsilon' - \hbar\omega_p - z)}{e^{\beta(\hbar\omega_p + z)} - 1} \right\}}{M(\vec{p})}.$$

Therefore, we find

$$B_{ij}(\vec{p}, \vec{p}') = \frac{K_0 \delta(\varepsilon - \varepsilon') \delta_{ij} + K \left(\frac{\chi(z) \Psi_i(z) \Psi_j(z) \pi(z) e^{\beta(\hbar\omega_p + z)}}{e^{\beta(\hbar\omega_p + z)} - 1} \Big|_{z=\varepsilon' - \varepsilon - \hbar\omega_p} + \frac{\chi(z) \Psi_i(z) \Psi_j(z) \pi(z)}{e^{\beta(\hbar\omega_p + z)} - 1} \Big|_{z=\varepsilon - \varepsilon' - \hbar\omega_p} \right)}{M(\vec{p})}$$

with $\chi(z)$ being the characteristic function. Furthermore, we have

$$\begin{aligned}
B & = M^{-1}(\vec{p}) K_0 \delta(\varepsilon - \varepsilon') I \\
& + \frac{\frac{K \chi(z) \pi(z)}{1 - e^{-\beta(\hbar\omega_p + z)}} \left(\begin{array}{cc} \Psi_1^2(z) & \Psi_1 \Psi_2 \\ \Psi_1 \Psi_2 & \Psi_2^2(z) \end{array} \right) \Big|_{\varepsilon' - \varepsilon - \hbar\omega_p} + \frac{K \chi(z) \pi(z)}{e^{\beta(\hbar\omega_p + z)} - 1} \left(\begin{array}{cc} \Psi_1^2(z) & \Psi_1 \Psi_2 \\ \Psi_1 \Psi_2 & \Psi_2^2(z) \end{array} \right) \Big|_{\varepsilon - \varepsilon' - \hbar\omega_p}}{M(\vec{p})}.
\end{aligned}$$

If we assume a uniform distribution $\pi(z) = N/2\beta$ for $z \in [-\beta/N, \beta/N]$ with $N > 1$, or equivalently $\pi(w) = 1/2$ by the scaling $w = Nz/\beta$ for $w \in [-1, 1]$, with the associated Legendre polynomials $\Psi_1 = 1$ and $\Psi_2(w) = w$, we obtain

$$B = M^{-1}(\vec{p})K_0\delta(\varepsilon - \varepsilon')I + \frac{\frac{K\chi(z)/2}{1-e^{-\beta(\hbar\omega_p+z)}} \left(\begin{array}{c} 1 \\ \frac{Nz}{\beta} \end{array} \right) \Big|_{z=\varepsilon'-\varepsilon-\hbar\omega_p} + \frac{K\chi(z)/2}{e^{\beta(\hbar\omega_p+z)}-1} \left(\begin{array}{c} 1 \\ \frac{Nz}{\beta} \end{array} \right) \Big|_{z=\varepsilon-\varepsilon'-\hbar\omega_p}}{M(\vec{p})},$$

$$Q(\alpha) = \int_{\Omega_{\vec{p}}} B(\vec{p}, \vec{p}') \left[M(\vec{p})\alpha(\vec{p}') - M(\vec{p}')\alpha(\vec{p}) \right] d\vec{p}'.$$

2.3 Stochastic Galerkin Method for the Boltzmann-Poisson System with the Lattice Temperature as a Random Variable

In this example, we assume that the only uncertainty in our problem stems from the lattice temperature. Randomness in the lattice temperature is motivated by physical reasons, as the temperature in the material or in its environment often fluctuates. The random variable is scalar, and randomness is introduced in the collisions, but now outside the argument of the Dirac delta distributions associated with Fermi's Golden Rule.

Therefore, the term $K_B T_L$ in the deterministic equation is replaced by $K_B T_L + z^*$, or equivalently, the term $\beta := (K_B T_L)^{-1}$ in the deterministic equation is replaced by $\beta + z$. This introduces randomness in the phonon occupation as a function the energy, yielding

$$n_q(\hbar\omega_p, z) = \left[\exp\left(\frac{\hbar\omega_p}{K_B T_L + z^*}\right) - 1 \right]^{-1} = \left[e^{(\beta+z)\hbar\omega_p} - 1 \right]^{-1}. \quad (23)$$

Additionally, randomness in the collision operator model is introduced as well. We have

$$S(\vec{k}, \vec{k}', z) = [n_q(\hbar\omega_p, z) + 1] K \delta(\varepsilon(\vec{k}') - \varepsilon(\vec{k}) + \hbar\omega_p) + K_0 \delta(\varepsilon(\vec{k}') - \varepsilon(\vec{k})) + n_q(\hbar\omega_p, z) K \delta(\varepsilon(\vec{k}') - \varepsilon(\vec{k}) - \hbar\omega_p).$$

Noticing that the randomness is just in the coefficients related to the phonon density and not inside the arguments of the delta distributions, we equivalently have

$$S(\vec{k}, \vec{k}', z) = K \frac{e^{(\beta+z)\hbar\omega_p}}{e^{(\beta+z)\hbar\omega_p} - 1} \delta(\varepsilon(\vec{k}') - \varepsilon(\vec{k}) + \hbar\omega_p) + K_0 \delta(\varepsilon(\vec{k}') - \varepsilon(\vec{k})) + K \frac{1}{e^{(\beta+z)\hbar\omega_p} - 1} \delta(\varepsilon(\vec{k}') - \varepsilon(\vec{k}) - \hbar\omega_p).$$

In particular, we consider the random temperature $T_L + z$, set $n := 1$, $P := 1$, $K := \dim(\mathcal{P}_P^n) = 2$, and approximate the density as

$$f(t, \vec{x}, \vec{p}, z) \approx \sum_{k=1}^2 \alpha_k(t, \vec{x}, \vec{p}) \Psi_k(z) = \alpha(t, \vec{x}, \vec{p}) \cdot \Psi(z) = (\alpha_1, \alpha_2) \cdot (\Psi_1, \Psi_2). \quad (24)$$

This yields the Boltzmann equation

$$\partial_t \alpha + v \cdot \nabla_{\vec{x}} \alpha + F \cdot \nabla_{\vec{p}} \alpha = Q(\alpha), \quad (25)$$

$$Q(\alpha) = \int_{\Omega_p} B(\vec{p}, \vec{p}') [M(\vec{p})\alpha(\vec{p}') - M(\vec{p}')\alpha(\vec{p})] d\vec{p}', \quad (26)$$

$$B_{ij}(\vec{p}, \vec{p}') = \int_{I_z} \sigma(\vec{p}, \vec{p}', z) \Psi_i(z) \Psi_j(z) \pi(z) dz \quad (27)$$

with the scattering cross section

$$\sigma(\vec{p}, \vec{p}', z) = \frac{1}{M(\vec{p})} \left(K_0 \delta(\varepsilon - \varepsilon') + K \frac{e^{(\beta+z)\hbar\omega_p} \delta(\varepsilon - \varepsilon' + \hbar\omega_p) + \delta(\varepsilon - \varepsilon' - \hbar\omega_p)}{e^{(\beta+z)\hbar\omega_p} - 1} \right). \quad (28)$$

Substituting σ into B_{ij} yields

$$\begin{aligned} B_{ij}(\vec{p}, \vec{p}') &= \int_{I_z} dz \Psi_i(z) \Psi_j(z) \pi(z) \frac{K_0 \delta(\varepsilon - \varepsilon') + K \frac{e^{(\beta+z)\hbar\omega_p} \delta(\varepsilon - \varepsilon' + \hbar\omega_p) + \delta(\varepsilon - \varepsilon' - \hbar\omega_p)}{e^{(\beta+z)\hbar\omega_p} - 1}}{M(\vec{p})} \\ &= M^{-1}(\vec{p}) K_0 \delta(\varepsilon - \varepsilon') \delta_{ij} + \int_{I_z} dz \Psi_i(z) \Psi_j(z) \pi(z) \frac{K \frac{e^{(\beta+z)\hbar\omega_p} \delta(\varepsilon - \varepsilon' + \hbar\omega_p) + \delta(\varepsilon - \varepsilon' - \hbar\omega_p)}{e^{(\beta+z)\hbar\omega_p} - 1}}{M(\vec{p})}. \end{aligned}$$

This expression simplifies to

$$B_{ij}(\vec{p}, \vec{p}') = \frac{K_0 \delta(\varepsilon - \varepsilon') \delta_{ij} + K \left(\delta(\varepsilon - \varepsilon' + \hbar\omega_p) \int_{I_z} \frac{dz \Psi_i \Psi_j \pi}{1 - e^{-(\beta+z)\hbar\omega_p}} + \delta(\varepsilon - \varepsilon' - \hbar\omega_p) \int_{I_z} \frac{dz \Psi_i \Psi_j \pi}{e^{(\beta+z)\hbar\omega_p} - 1} \right)}{M(\vec{p})}$$

and

$$B_{ij}(\vec{p}, \vec{p}') = M(\vec{p})^{-1} [K_0 \delta(\varepsilon - \varepsilon') \delta_{ij} + K (\delta(\varepsilon - \varepsilon' + \hbar\omega_p) C_{ij}^+ + \delta(\varepsilon - \varepsilon' - \hbar\omega_p) C_{ij}^-)]$$

with the coefficients

$$\begin{aligned} C_{ij}^- &= \int_{I_z} dz \Psi_i(z) \Psi_j(z) \pi(z) \frac{1}{e^{(\beta+z)\hbar\omega_p} - 1} = \int_{I_z} dz \Psi_i(z) \Psi_j(z) \pi(z) n_q(\hbar\omega_p, \beta + z), \\ C_{ij}^+ &= \int_{I_z} dz \Psi_i(z) \Psi_j(z) \pi(z) \left(1 + \frac{1}{e^{(\beta+z)\hbar\omega_p} - 1} \right) = \int_{I_z} dz \Psi_i \Psi_j \pi (n_q + 1) = \delta_{ij} + C_{ij}^-. \end{aligned}$$

Therefore the scattering operator becomes

$$\begin{aligned} Q(\alpha) &= \int_{\Omega_{\vec{p}}} \left(K_0 \delta(\varepsilon - \varepsilon') I_d + K \sum_{\pm} \delta(\varepsilon - \varepsilon' \pm \hbar\omega_p) C^{\pm} \right) M(\vec{p})^{-1} [M(\vec{p})\alpha(\vec{p}') - M(\vec{p}')\alpha(\vec{p})] d\vec{p}' \\ &= \int_{\Omega_{\vec{p}}} \left(\sum_{l=-1}^1 K_l \delta(\varepsilon - \varepsilon' + l\hbar\omega_p) C^l \right) M(\vec{p})^{-1} [M(\vec{p})\alpha(\vec{p}') - M(\vec{p}')\alpha(\vec{p})] d\vec{p}' \end{aligned}$$

with $K_{-1} = K = K_{+1}$ and $C_{ij}^0 = \delta_{ij}$ being the identity matrix.

It is important to note that a Gaussian distribution is not appropriate in this example, as there would arise a singularity in the integrals when the temperature (in energy units) becomes zero. We hence assume a uniform distribution $\pi(z) =$

$N/2\beta$ for $z \in [-\beta/N, \beta/N]$ with $N > 1$, or equivalently $\pi(w) = 1/2$ by the scaling $w = Nz/\beta$ for $w \in [-1, 1]$, with the associated Legendre polynomials $\Psi_1 = 1$ and $\Psi_2(w) = w$. This means that $f \approx \alpha_1 + w\alpha_2$. Therefore we find

$$C^- = \int_{-\beta/N}^{\beta/N} \frac{dz N/2\beta}{e^{(\beta+z)\hbar\omega_p} - 1} \begin{pmatrix} 1 & Nz/\beta \\ Nz/\beta & (Nz/\beta)^2 \end{pmatrix} = \frac{1}{2} \int_{-1}^1 \begin{pmatrix} 1 & w \\ w & w^2 \end{pmatrix} \frac{dw}{e^{\beta\hbar\omega_p(1+w/N)} - 1}.$$

The analytic values of these integrals are

$$\begin{aligned} \int \frac{dx}{\exp(A+Bx) - 1} &= \frac{\log(1 - e^{A+Bx})}{B} - x + ct, \\ \int \frac{xdx}{\exp(A+Bx) - 1} &= \frac{\text{Li}_2(e^{A+Bx})}{B^2} + \frac{x \log(1 - e^{A+Bx})}{B} - \frac{x^2}{2} + ct, \\ \int \frac{x^2 dx}{\exp(A+Bx) - 1} &= \frac{-2\text{Li}_3(e^{A+Bx})}{B^3} + \frac{2x\text{Li}_2(e^{A+Bx})}{B^2} + \frac{x^2 \log(1 - e^{A+Bx})}{B} - \frac{x^3}{3} + ct \end{aligned}$$

with $A = \beta\hbar\omega_p$, $B = \beta\hbar\omega_p/N$, and $\text{Li}_n(x)$ being the polylogarithm functions. Furthermore, we can evaluate these formulas to obtain C^- explicitly in the form

$$C^- = \frac{1}{2} \begin{pmatrix} \left. \frac{\log(1 - e^{A+Bx})}{B} - x \right|_{-1}^1 & \left. \frac{\text{Li}_2(e^{A+Bx})}{B^2} + \frac{x \log(1 - e^{A+Bx})}{B} \right|_{-1}^1 \\ \left. \frac{\text{Li}_2(e^{A+Bx})}{B^2} + \frac{x \log(1 - e^{A+Bx})}{B} \right|_{-1}^1 & \left. \frac{-2\text{Li}_3(e^{A+Bx})}{B^3} + \frac{2x\text{Li}_2(e^{A+Bx})}{B^2} + \frac{x^2 \log(1 - e^{A+Bx})}{B} - \frac{x^3}{3} \right|_{-1}^1 \end{pmatrix},$$

where we can omit the term $-\frac{x^2}{2}$ in the off-diagonal elements, since it will vanish when evaluating at ± 1 .

To determine concrete numbers for numerical simulations and for the evaluation of the C^- matrix, we recall that the Planck constant divided by 2π is equal to $\hbar = h/2\pi = 1.0546 \times 10^{-34} \text{ J}\cdot\text{s}$ and that the Boltzmann constant is equal to $K_B = 1.3805 \times 10^{-23} \text{ J/K}$. The mean lattice temperature is assumed to be $T_L := 300 \text{ K} = 26.85^\circ\text{C}$. Therefore, we have that $K_B T_L = 4.1415 \times 10^{-21} \text{ J} = 0.025849 \text{ eV}$, since $1 \text{ eV} = 1.60218 \times 10^{-19} \text{ J}$. Hence $\beta = (K_B T_L)^{-1} = 2.4145841 \times 10^{20} \text{ J}^{-1}$.

Moreover, the variation in the environment temperature might be of $\pm 10^\circ\text{C}$, resulting in a lattice temperature between $16.85^\circ\text{C} = 290 \text{ K}$ and $36.85^\circ\text{C} = 310 \text{ K}$. In that case $K_B T_L \in [4.00345, 4.27955] \times 10^{-21} \text{ J}$, $\beta+z \in [2.3366943, 2.4978456] \times 10^{20} \text{ J}^{-1}$, and $z \in [-0.0778898, 0.0832615] \times 10^{20} \text{ J}^{-1}$. Thus $z \in I_z$, which is $I_z \approx [-0.08057565, 0.08057565] \times 10^{20} \text{ J}^{-1}$, and therefore $\beta/N = 0.08057565 \times 10^{20} \text{ J}^{-1}$ implies $N = \frac{2.4145841 \times 10^{20} \text{ J}^{-1}}{0.08057565 \times 10^{20} \text{ J}^{-1}} = 29.9666723135$. After rounding to $N := 30$, we have $z \in [-\beta/N, \beta/N]$ with $\beta/N = 0.08048613666 \times 10^{20} \text{ J}^{-1}$. Finally, since the phonon energy is $\hbar\omega_p = 0.063 \text{ eV} = 1.0093734 \times 10^{-20} \text{ J}$, we obtain the values of the adimensional numbers $\beta\hbar\omega_p = 2.4372169626 = A$ and $\beta\hbar\omega_p/N = 0.08124056542 = B$.

Hence we find the matrices

$$\begin{aligned} C^- &= \frac{1}{2} \begin{pmatrix} 0.191825 & -0.00569012 \\ -0.00569012 & 0.0640151 \end{pmatrix} = \begin{pmatrix} 0.0959125 & -0.00284506 \\ -0.00284506 & 0.03200755 \end{pmatrix}, \\ C^+ &= \begin{pmatrix} 1.0959125 & -0.00284506 \\ -0.00284506 & 1.03200755 \end{pmatrix}, \end{aligned}$$

since $C_{ij}^+ = C_{ij}^- + \delta_{ij}$. With these matrices, the scattering operator becomes

$$Q(\alpha) = \int_{\Omega_{\vec{p}}} \left(K_0 \delta(\varepsilon - \varepsilon') I_d + K \sum_{\pm} \delta(\varepsilon - \varepsilon' \pm \hbar\omega_p) C^{\pm} \right) \frac{M\alpha' - M'\alpha}{M} d\vec{p}', \quad (29)$$

which we can write in the form

$$\begin{aligned} Q(\alpha) &= \int_{\Omega_{\vec{p}}} \left(K_0 \delta(\varepsilon - \varepsilon') + K \sum_{\pm} \delta(\varepsilon - \varepsilon' \pm \hbar\omega_p) [n_q + (1 \pm 1)/2] \right) I_d \frac{M\alpha' - M'\alpha}{M} d\vec{p}' \\ &+ \int_{\Omega_{\vec{p}}} K \left[\sum_{\pm} \delta(\varepsilon - \varepsilon' \pm \hbar\omega_p) \right] (C^- - n_q I_d) \frac{M\alpha' - M'\alpha}{M} d\vec{p}', \end{aligned}$$

since $C^+ = C^- + I_d$ and hence $C^- - n_q I_d = C^+ - (n_q + 1)I_d$.

Therefore the term in the first row is the collision operator, as originally written in the deterministic case, acting on each separate band (by means of the identity matrix) without any recombination, whereas the second term represents the recombination and diagonal terms related to the uncertainty in the temperature associated solely with inelastic integrals. Given the value of the constant $n_q = [e^{\beta\hbar\omega_p} - 1]^{-1} = 0.09577484271$, we find

$$C^- - n_q I_d = \begin{pmatrix} 0.00013765729 & -0.00284506 \\ -0.00284506 & -0.06376729271 \end{pmatrix} = C^+ - (n_q + 1)I_d.$$

3 Stochastic Galerkin Method for the Boltzmann-Poisson System Using Deterministic Discontinuous Galerkin Solvers

The numerics of deterministic solvers for the Boltzmann-Poisson system that use the discontinuous Galerkin (DG) algorithm have been studied in [9], [10] for a single PDF (one band) without randomness. We will use the deterministic DG method for two bands (representing the α vector of coefficients) to solve the stochastic Galerkin system, which contains a different kind of matrix integral collisional operator.

3.1 Discontinuous Galerkin: the Boltzmann Equation in \vec{k} -Spherical Coordinates

We perform a spherical transformation of the momentum coordinate \vec{k} taking the location of a (local) minimum of the conduction energy band as the origin. This transformation is useful (in the absence of Umklapp effects), because in low energy limits (i.e., for small potential bias) the conduction band energy scales as the square of the momentum norm, and hence the radial coordinate is an energy variable. We then have

$$\begin{aligned} \vec{k} &= \frac{\sqrt{2m^*K_B T_L}}{\hbar} \sqrt{r} \left(\mu, \sqrt{1 - \mu^2} \cos \varphi, \sqrt{1 - \mu^2} \sin \varphi \right), \\ r &\geq 0, \quad \mu \in [-1, 1], \quad \varphi \in [-\pi, \pi]. \end{aligned}$$

The variable r is proportional to the energy for small biases in the parabolic band approximation, assuming the same effective mass in all three Cartesian momentum directions. Due to this momentum coordinate transformation, we have to weight the PDF coefficients by the Jacobian of the \vec{k} -transformation, specifically for the computation of moment integrals over the \vec{k} -space. We then obtain a transformed PDF in the phase space $(\vec{x}, r, \mu, \varphi)$ given by

$$\Phi(t, \vec{x}, r, \mu, \varphi) = \frac{\sqrt{r}}{2} \alpha(t, \vec{x}, \vec{k}(r, \mu, \varphi)).$$

We also obtain a transformed Boltzmann equation in divergence form for our new PDF Φ in the $(x, y, z; r, \mu, \varphi)$ space, which reads

$$\begin{aligned} \frac{\partial \Phi}{\partial t} + \frac{\partial}{\partial x} (a_1 \Phi) + \frac{\partial}{\partial y} (a_2 \Phi) + \frac{\partial}{\partial z} (a_3 \Phi) + \\ \frac{\partial}{\partial r} (a_4 \Phi) + \frac{\partial}{\partial \mu} (a_5 \Phi) + \frac{\partial}{\partial \varphi} (a_6 \Phi) = C(\Phi), \end{aligned}$$

where the transport coefficients are, for $(a_1, a_2, a_3) \propto \nabla_{\vec{k}} \varepsilon(\vec{k})$, proportional to the \vec{k} -gradient in transformed coordinates, and the rest are given by

$$a_4 = -2 c_E \sqrt{r} \hat{e}_r \cdot \underline{\mathbf{E}} = -2 c_E \sqrt{r} \left(\mu, \sqrt{1-\mu^2} \cos \varphi, \sqrt{1-\mu^2} \sin \varphi \right) \cdot \underline{\mathbf{E}}, \quad (30)$$

$$a_5 = -c_E \frac{\sqrt{1-\mu^2}}{\sqrt{r}} \hat{e}_\mu \cdot \underline{\mathbf{E}} = -c_E \frac{\sqrt{1-\mu^2}}{\sqrt{r}} \left(\sqrt{1-\mu^2}, -\mu \cos \varphi, -\mu \sin \varphi \right) \cdot \underline{\mathbf{E}},$$

$$a_6 = -c_E \frac{1}{\sqrt{r} \sqrt{1-\mu^2}} \hat{e}_\varphi \cdot \underline{\mathbf{E}} = -c_E \frac{1}{\sqrt{r} \sqrt{1-\mu^2}} (0, -\sin \varphi, \cos \varphi) \cdot \underline{\mathbf{E}}. \quad (31)$$

Regarding the transformed linear collision operator, we write $\vec{x} = (x, y, z)$ and $\mathbf{r} = (r, \mu, \varphi)$, and obtain

$$C(\Phi)(t, \vec{x}, \mathbf{r}) = \frac{\sqrt{r}}{2} \int_{\Omega} \mathcal{S}(\mathbf{r}', \mathbf{r}) \Phi(t, \vec{x}, \mathbf{r}') d\mathbf{r}' - \Phi(t, \vec{x}, \mathbf{r}) \int_{\Omega} \mathcal{S}(\mathbf{r}, \mathbf{r}') \frac{\sqrt{r'}}{2} d\mathbf{r}',$$

showing the importance of the transformed PDF Φ . Here $\mathcal{S}(\mathbf{r}', \mathbf{r})$ represents the electron-phonon scattering for the two-band system.

We use the dimensionless Poisson equation

$$\nabla_{\vec{x}} \cdot (\epsilon_r \nabla_{\vec{x}} \Psi) = c_p [\rho(t, \vec{x}) - \mathcal{N}_D(\vec{x})], \quad (32)$$

where

$$\rho(t, \vec{x}) = \int_{\Omega} \Phi_0(t, \vec{x}, \mathbf{r}') d\mathbf{r}', \quad \mathcal{N}_D(\vec{x}) = \left(\frac{\sqrt{2} m^* K_B T_L}{\hbar} \right)^{-3} N_D(\vec{x}). \quad (33)$$

The electron density is given by the first PDF coefficient, which represents the mean of the PDF.

The discontinuous Galerkin method for the Boltzmann-Poisson system represents a dynamic extension of the Gummel iteration map. Starting with an initial condition Φ_h and given boundary conditions, the DG algorithm advances from t^n to t^{n+1} in these steps:

Step 1 Compute the charge density ρ .

Step 2 Use ρ to solve the Poisson equation (either by an integral form in 1D or by the LDG method in 2D or 3D) for the potential and electric field, and compute the transport coefficients a_i , $1 \leq i \leq 6$.

Step 3 Solve the transport part of the Boltzmann equation by DG, then use the method of lines for Φ_h (ODE system).

Step 4 Evolve the ODE system by proper time stepping from t^n to t^{n+1} (if partial time steps are necessary, as in a Runge-Kutta method, repeat steps 1 to 3 as needed).

We use a rectangular Cartesian grid in the transformed phase space. It has the form

$$\Omega_{ijkmn} = \left[x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}} \right] \times \left[y_{j-\frac{1}{2}}, y_{j+\frac{1}{2}} \right] \times \left[r_{k-\frac{1}{2}}, r_{k+\frac{1}{2}} \right] \times \left[\mu_{m-\frac{1}{2}}, \mu_{m+\frac{1}{2}} \right] \times \left[\varphi_{n-\frac{1}{2}}, \varphi_{n+\frac{1}{2}} \right]$$

with $1 \leq i \leq N_x$, $1 \leq k \leq N_r$, $1 \leq m \leq N_\mu$, and $x_{i\pm\frac{1}{2}} = x_i \pm \Delta x_i/2$, $r_{k\pm\frac{1}{2}} = r_k \pm \Delta r_k/2$, $\mu_{m\pm\frac{1}{2}} = \mu_m \pm \Delta\mu_m/2$.

The test function $\psi(x, y, r, \mu, \varphi) \in V_h$ belongs to the set of piecewise linear polynomials so that the set of all test functions is

$$V_h := V_h^l := \{v : v|_{\Omega_{ijkmn}} \in P(\Omega_{ijkmn}^l)\},$$

where the $P(\Omega_{ijkmn}^l)$ are the polynomials of degree $l \leq 1$ on Ω_{ijkmn} .

Inside the cell Ω_I , $I = (i, j, k, m, n)$, we approximate the weighted PDF Φ by a linear polynomial in V_h , i.e.,

$$\Phi_h = T_I(t) + X_I(t) \frac{(x - x_i)}{\Delta x_i/2} + Y_I(t) \frac{(y - y_j)}{\Delta y_j/2} + R_I(t) \frac{(r - r_k)}{\Delta r_k/2} + M_I(t) \frac{(\mu - \mu_m)}{\Delta \mu_m/2} + P_I \frac{(\varphi - \varphi_n)}{\Delta \varphi_n/2}. \quad (34)$$

The charge density for a piecewise linear PDF Φ is given by

$$\rho(t, x, y) = \sum_{m=1}^{N_\mu} \sum_{n=1}^{N_\varphi} \sum_{k=1}^{N_r} \left[T_{ijkmn}(t) + X_{ijkmn}(t) \frac{(x - x_i)}{\Delta x_i/2} + Y_{ijkmn}(t) \frac{(y - y_j)}{\Delta y_j/2} \right] \Delta r_k \Delta \mu_m \Delta \varphi_n.$$

In summary, the discontinuous Galerkin formulation for the vector Boltzmann equation is to find Φ_h in the piecewise polynomial space V_h such that the equation

$$\begin{aligned} & \int_K \frac{\partial \Phi_h}{\partial t} v_h d\Omega - \int_K \frac{\partial v_h}{\partial x} (a_1 \Phi_h) d\Omega - \int_K \frac{\partial v_h}{\partial y} (a_2 \Phi_h) d\Omega - \int_K \frac{\partial v_h}{\partial z} (a_3 \Phi_h) v_h d\Omega \\ & - \int_K \frac{\partial v_h}{\partial r} (a_4 \Phi_h) d\Omega - \int_K \frac{\partial v_h}{\partial \mu} (a_5 \Phi_h) d\Omega - \int_K \frac{\partial v_h}{\partial \varphi} (a_6 \Phi_h) d\Omega \\ & + F_x^+ - F_x^- + F_y^+ - F_y^- + F_z^+ - F_z^- + F_r^+ - F_r^- + F_\mu^+ - F_\mu^- + F_\varphi^+ - F_\varphi^- = \int_K C(\Phi_h) v_h d\Omega, \end{aligned}$$

where the F^\pm represent the boundary integrals, holds for any test function $v_h \in V_h$ and for each element $K = \Omega_{ijkmn}$.

4 SDG-BP: Stochastic Discontinuous Galerkin Method for the Boltzmann-Poisson System

4.1 The Symmetric Case: One-Dimensional in x , Two-Dimensional in $\vec{k}(r, \mu)$

We consider a 1D $n^+ - n - n^+$ silicon diode, rendering the problem one-dimensional in position space. The length of the diode is $L = 1 \mu\text{m}$, and the length of the n -channel in the middle is 400 nm. The doping concentration is $n^+ = 5 \cdot 10^{23}/\text{m}^3 = 5 \cdot 10^{17}/\text{cm}^3$ and $n = 2 \cdot 10^{21}/\text{m}^3 = 2 \cdot 10^{15}/\text{cm}^3$.

We consider the case with k -space azimuthal symmetry on $\varphi \in [0, 2\pi] \rightarrow \vec{k} = \vec{k}(r, \mu)$. Therefore, by the symmetry assumptions, it is only necessary to consider the radial and polar coordinates of the momentum.

The computational domain is taken as $x \in [0, 1]$, $r \in [0, r_{\max}]$, and $\mu \in [-1, 1]$. The constant r_{\max} is the cut-off such that $\Phi(t, x, r, \mu) \approx 0$ for $r \geq r_{\max}$ in the numerical experiments. For example, $r_{\max} \approx 36$ for $V_{\text{bias}} = 0.5 \text{ V}$ in a 400 nm channel.

The initial condition is $(\Phi_0, \Phi_1)(0, x, r, \mu) = (CN_D(x)e^{-\varepsilon(r)}\sqrt{r}/2, 0)$ with a constant C such that $\rho(0, x) - N_D(x) = 0$ at the initial time $t = 0$.

The boundary conditions are the following.

- In the x -space, the charge concentration is neutral at the source and drain endpoints $0 = x_{1/2}$ and $x_{N_x+1/2} = 1$. This charge neutrality condition is imposed by $\Phi(0, \vec{k}, t) = N_D(x) \frac{\Phi(x_1, \vec{k}, t)}{\rho(x_1, \vec{k}, t)}$ and $\Phi(1, \vec{k}, t) = N_D(x) \frac{\Phi(x_{N_x}, \vec{k}, t)}{\rho(x_{N_x}, \vec{k}, t)}$.
- The applied potential (bias) is $V(0, \vec{k}, t) = 0$ and $V(1, \vec{k}, t) = V_0$.
- In the (r, μ) -space, a cut-off boundary is used such that Φ vanishes at $r = r_{\max}$.
- At the ‘‘point’’ boundaries, no boundary conditions are needed and transport equals zero analytically. Hence, at the origin $r = 0$, $a_4 = 0$ holds, and likewise at the poles $\mu = \pm 1$, $a_5 = 0$ holds. Therefore the boundary integrals are analytically equal to zero at $r = 0$ and $\mu = \pm 1$.

Regarding time evolution, an RK2 Method was used in our simulations.

4.2 Numerical Results

We present the numerical results for the coefficients of the truncated PDF with a random variable. We first do so for the benchmark case of no recombination DG-BP: $-\log \alpha_0(x, r, \mu)$ (and $\alpha_1(x, r, \mu) = 0$ plotted directly) are shown for a $1 \mu\text{m}$ diode, 0.5 V bias, and $t_0 = 10.0 \text{ ps}$. In this deterministic case, the reason why there is no recombination lies in the vanishing of the first coefficient $\alpha_1 = 0$ related to random effects (Figure 2), and the zeroth coefficient α_0 contains all the information of the PDF (Figure 1).

We then consider the PDF coefficients from the simulations of the SDG-BP system with the recombination terms $-\log \alpha_0(x, r, \mu, t)$ in Figure 3 and $-\log \alpha_1(x, r, \mu, t)$ in Figure 4 for a $1 \mu\text{m}$ diode, 0.5 V bias, and $t_0 = 10.0 \text{ ps}$ as well. The variations in α_1 are located in similar regions of the phase space, while for α_0 they seem finer and more pronounced.

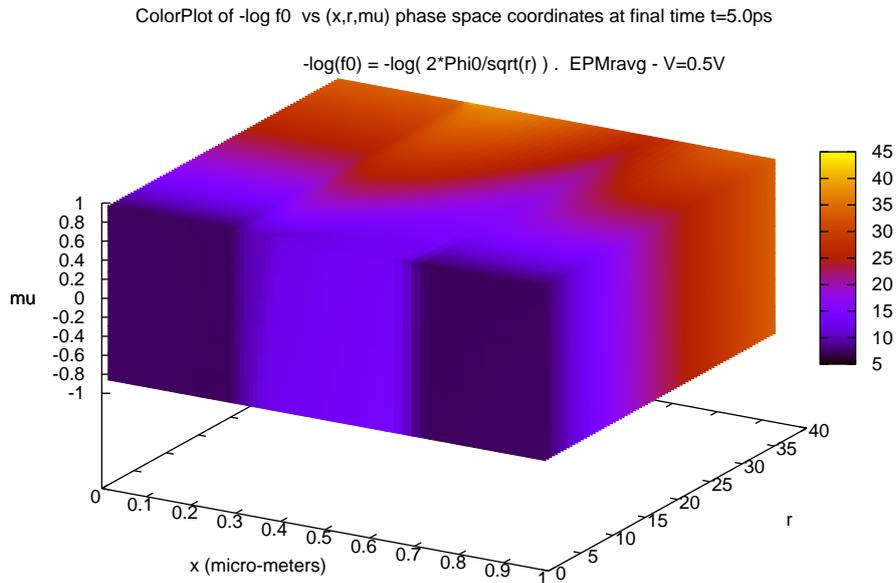


Figure 1: $-\log \alpha_0(x, r, \mu)$ for a $1 \mu\text{m}$ diode, 0.5V bias, and $t_0 = 10.0 \text{ps}$.

We also compare SDG-BP with recombination terms against SDG-BP with no recombination case by calculating the moments with Φ_0 for both. The difference is observed mainly in the prediction of the momentum (current) two orders of magnitude below the mean value of the current (Figure 11), indicating the finer resolution of the momentum by use of the stochastic Galerkin method. We also plot the expectation, variance, and standard deviation of our probability density function in the SDG-BP method, given as $E[f] = \alpha_1$, $\text{Var}[f] = \sum_{k=2}^2 \alpha_k^2 = \alpha_2^2$, and $S[f] = \sqrt{\sum_{k=2}^2 \alpha_k^2} = |\alpha_2|$, respectively.

5 Conclusions

Uncertainty quantification in the Boltzmann-Poisson system is crucial by the own probabilistic nature of the problem due to the high number of particles involved and due to its quantum mechanical features. Studying randomness in the temperature is an important leading example, both for reasons stemming from the physical nature of the problem – as the environment temperature may fluctuate – as well as related to the mathematical aspects, since the temperature is a scalar random variable that introduces randomness in the collision term and more precisely in the coefficients multiplying the Dirac delta distributions appearing in the electron-phonon collisions by the Fermi golden rule.

Our numerical results for the stochastic Galerkin method for the Boltzmann-Poisson system, assuming a random temperature in an electron-phonon collision operator, show a coefficient α_1 related to randomness, whose variations are located in similar regions of the phase space to the ones of the average term α_0 , which has no randomness but shows finer and more pronounced variations.

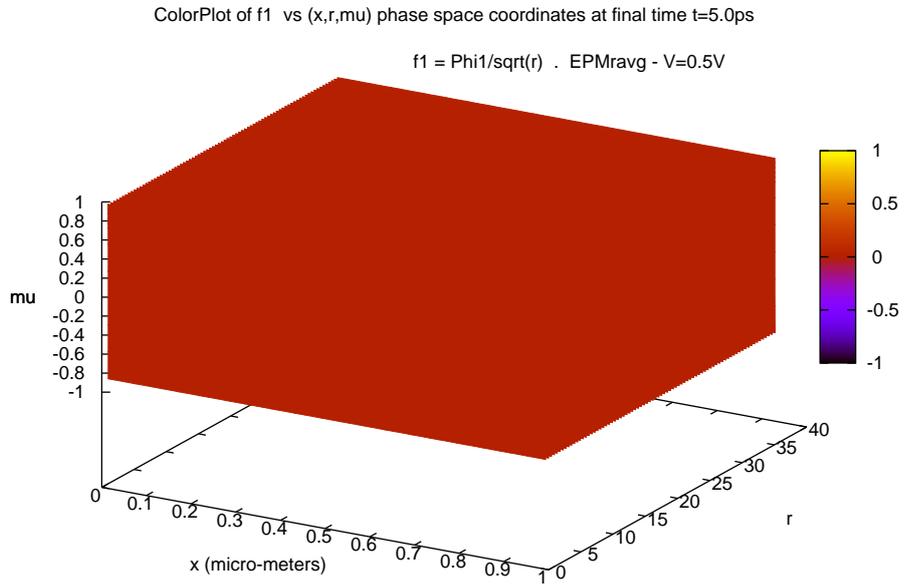


Figure 2: Coefficient $\alpha_1(x, r, \mu) = 0$ for a $1\ \mu\text{m}$ diode, $0.5\ \text{V}$ bias, and $t_0 = 10.0\ \text{ps}$.

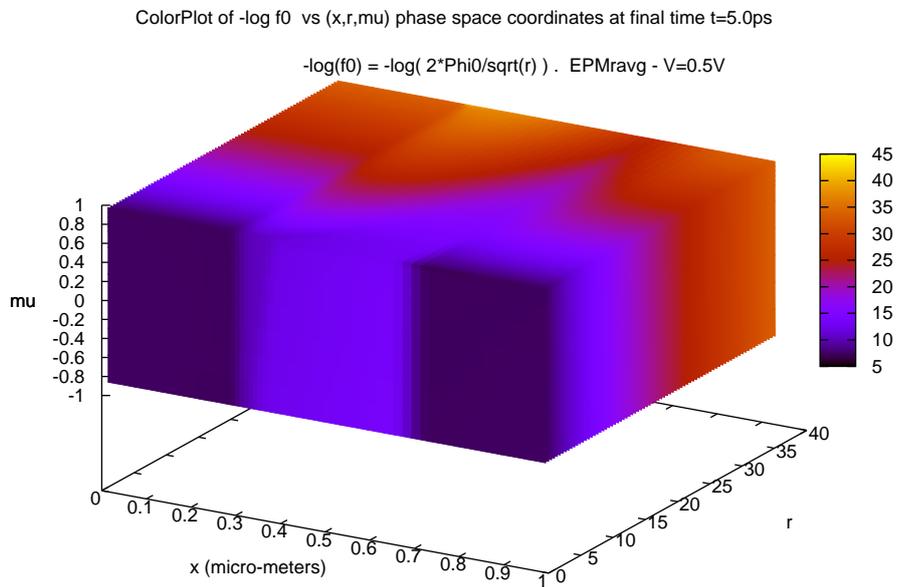


Figure 3: $-\log \alpha_0(x, r, \mu)$ for a $1\ \mu\text{m}$ diode, $0.5\ \text{V}$ bias, and $t_0 = 10.0\ \text{ps}$.

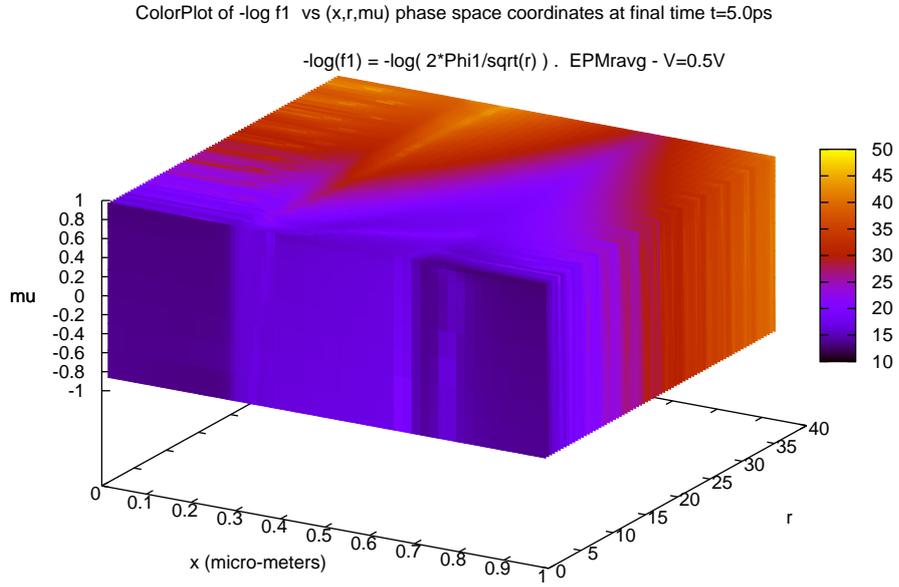


Figure 4: $-\log \alpha_1(x, r, \mu)$ for a $1\ \mu\text{m}$ diode, $0.5\ \text{V}$ bias, and $t_0 = 10.0\ \text{ps}$.

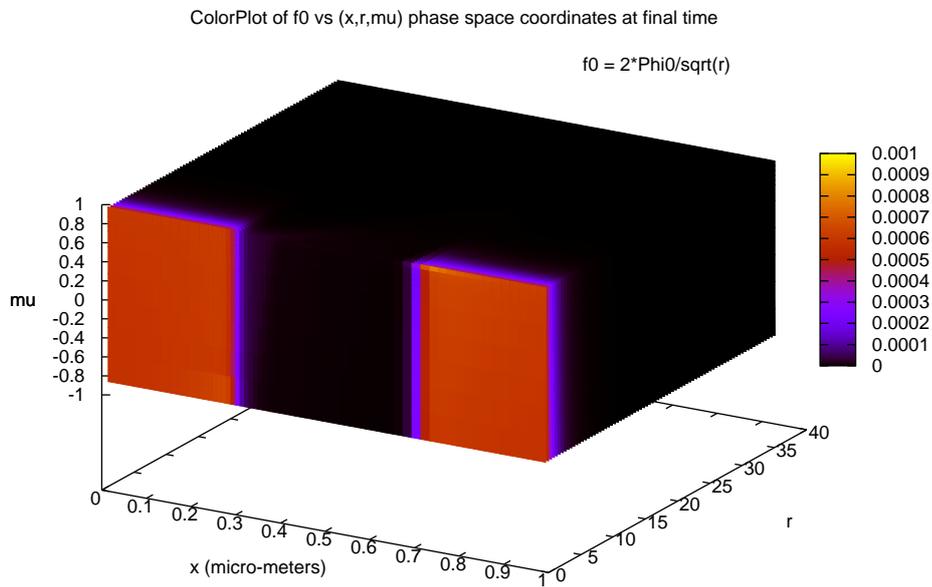


Figure 5: Coefficient $\alpha_0(x, r, \mu)$ for a $1\ \mu\text{m}$ diode, $0.5\ \text{V}$ bias, and $t_0 = 10.0\ \text{ps}$.

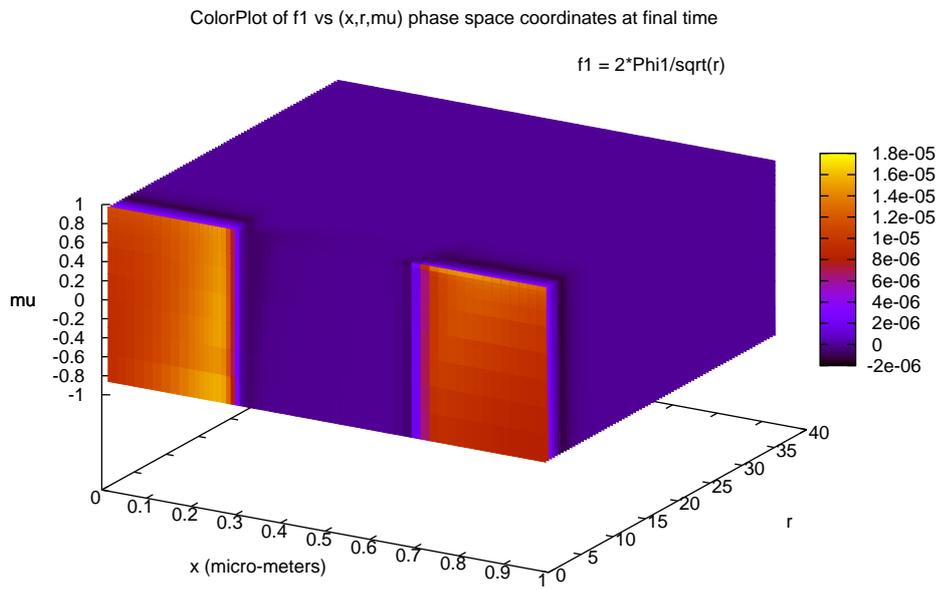


Figure 6: Coefficient $\alpha_1(x, r, \mu)$ for a $1 \mu\text{m}$ diode, 0.5 V bias, and $t_0 = 10.0 \text{ ps}$.

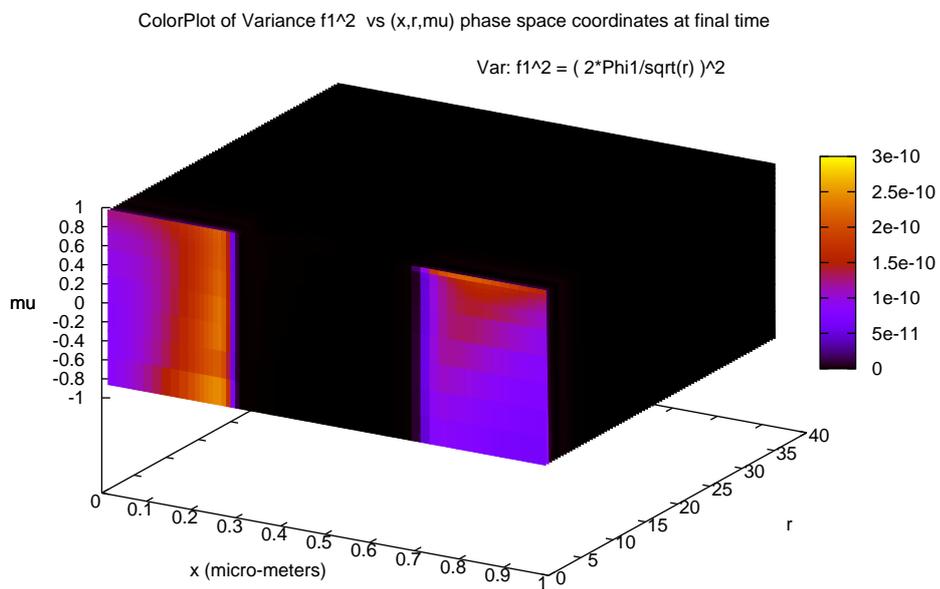


Figure 7: Variance $\text{Var}[f] = \alpha_2^2$.

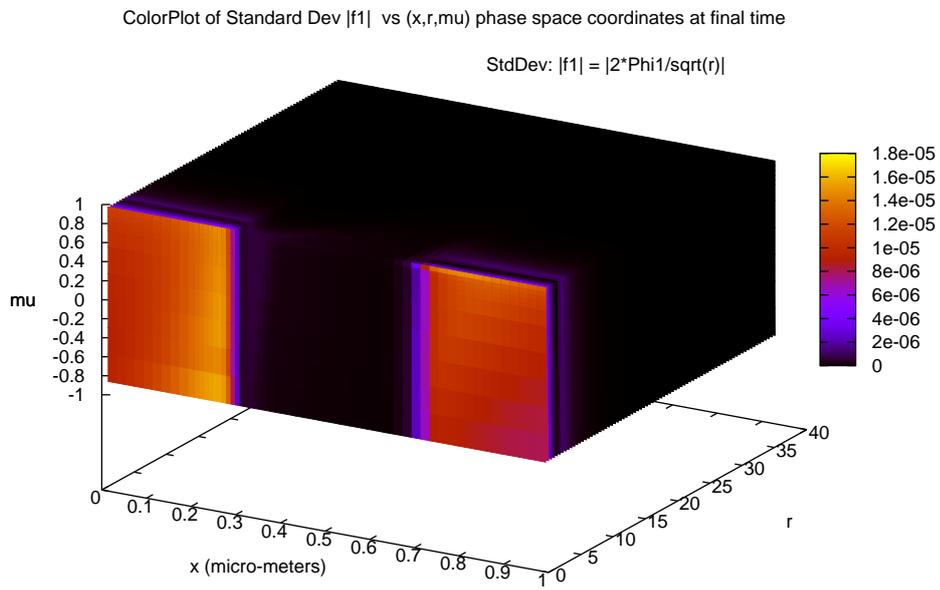


Figure 8: Standard deviation $S[f] = |\alpha_2|$.

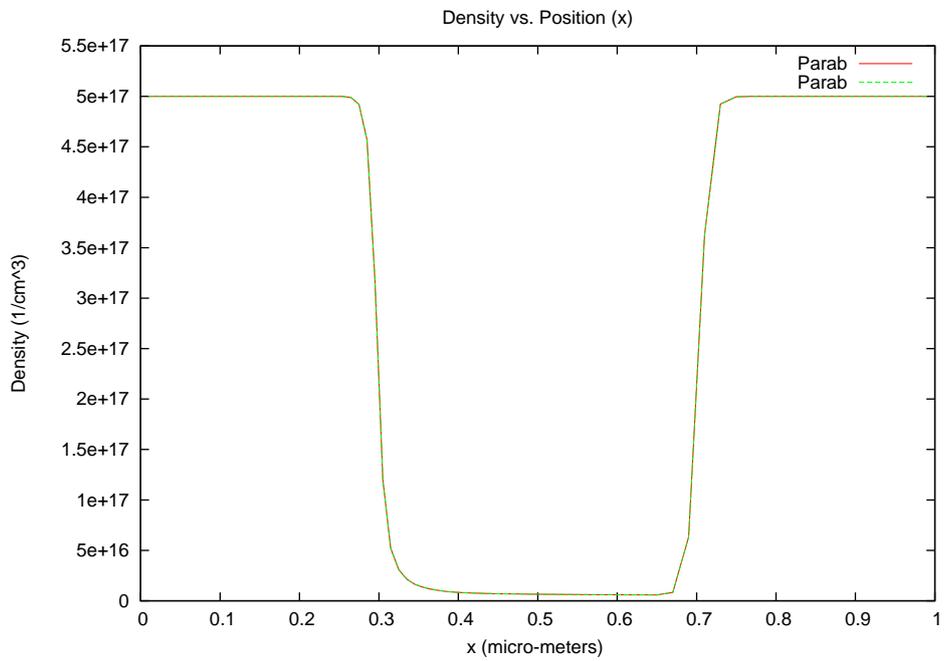


Figure 9: Density $\rho(x, t)$.

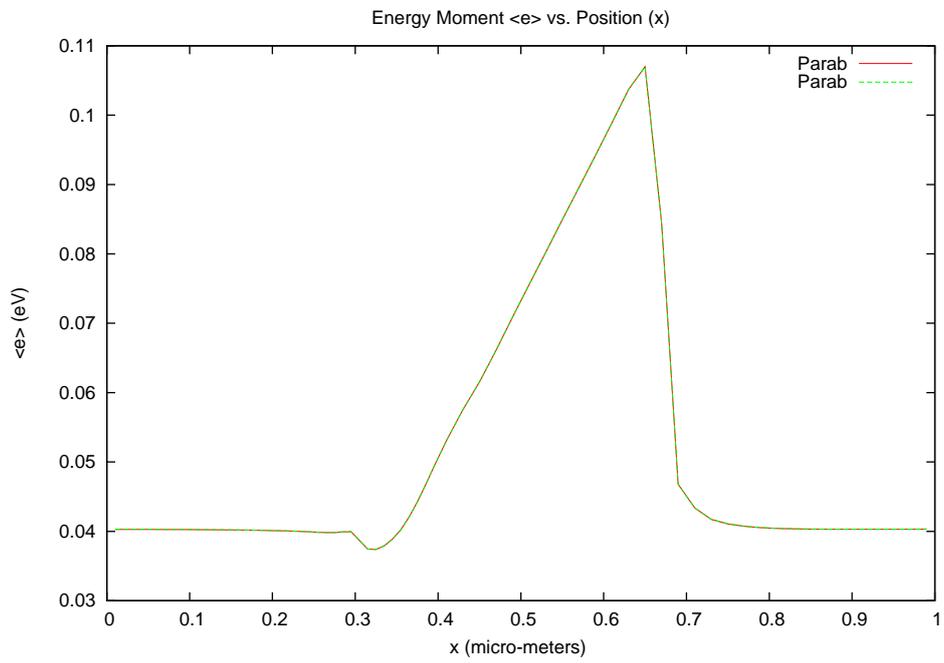


Figure 10: Energy $e(x, t)$ for a $1 \mu\text{m}$ diode, 0.5 V bias, and $t_0 = 10.0 \text{ ps}$.

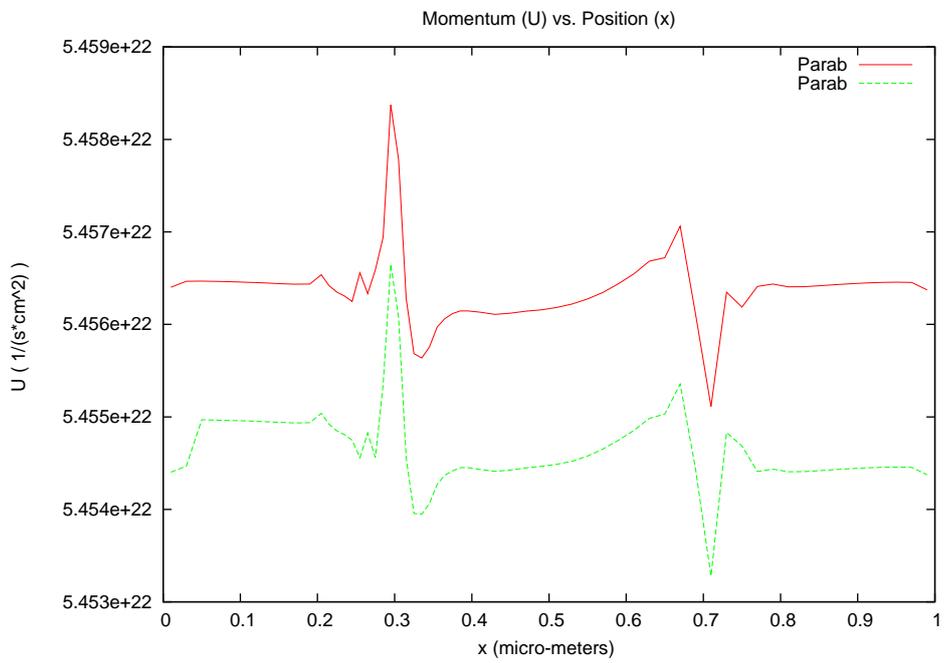


Figure 11: Momentum (current) $M(x, t)$.

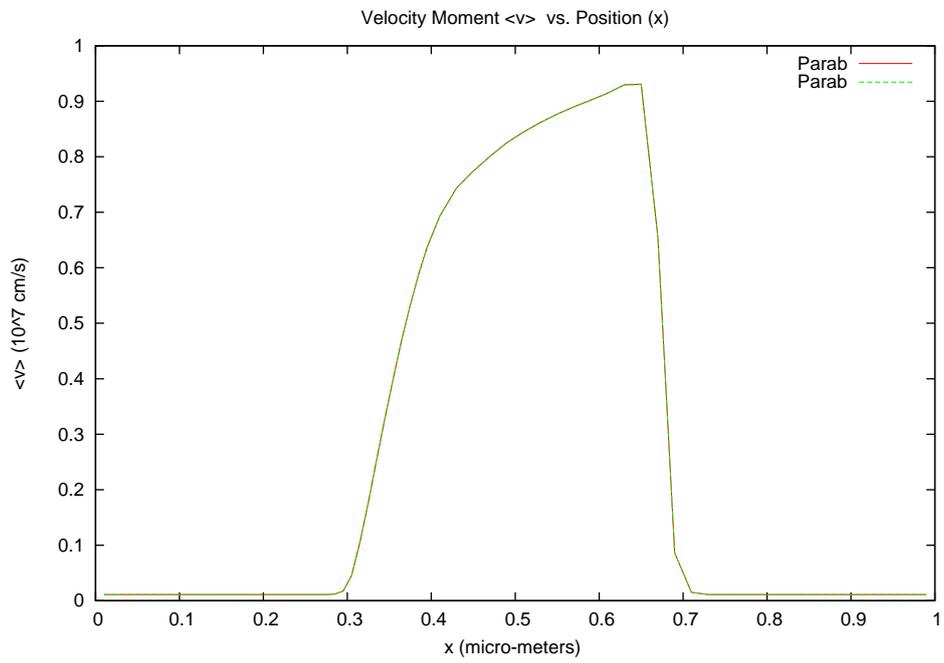


Figure 12: Velocity $v(x, t)$.

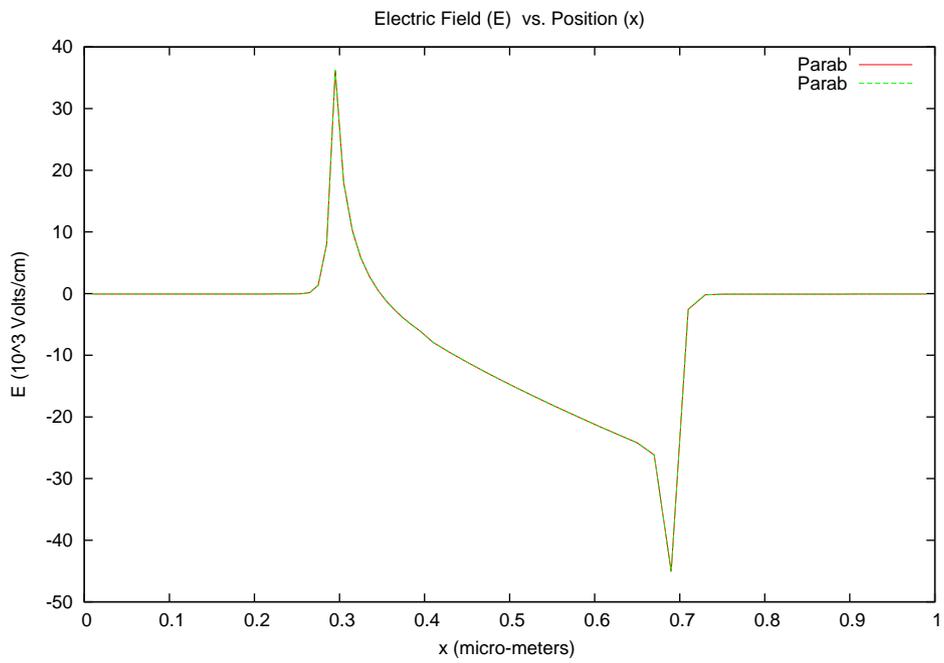


Figure 13: Electric field $E(x, t)$.

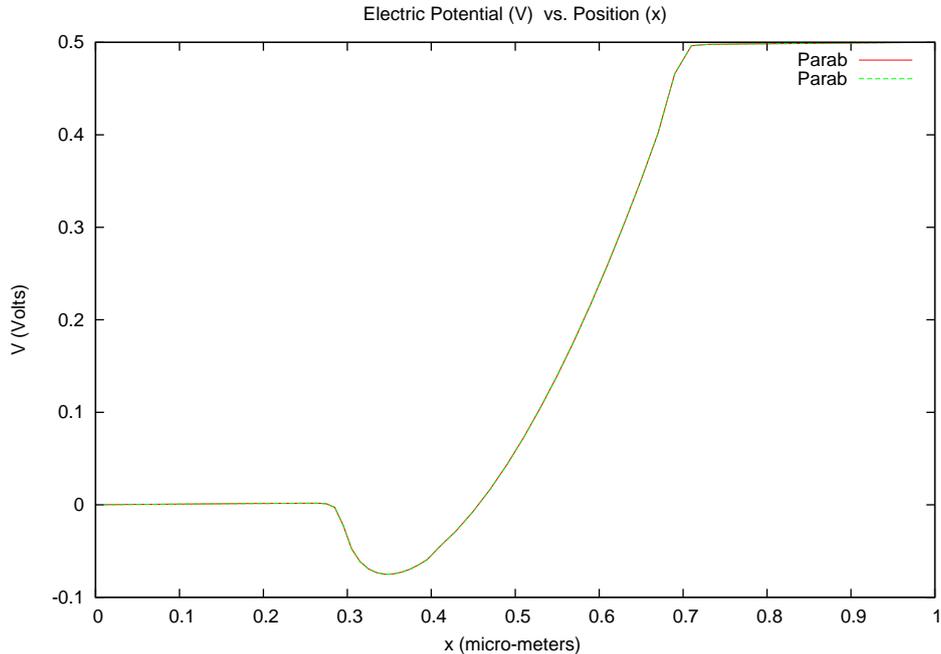


Figure 14: Potential $V(x, t)$.

Our comparison of SDG-BP with recombination terms against the no-recombination case, using the mean term α_0 in both cases to calculate the moments, shows only a difference in the moment (current) between these two cases. We have to remember that the moment is the product of density and energy, which on their own scales do not seem to exhibit a large difference between these two cases. However, the moment has a value close to a constant over the position domain when equilibrium is reached, and the difference in this mean value is observed between the two cases, although it is two orders of magnitude below the average value of the current (Figure 11). Here a truncated random expansion up to first order in z was employed, which therefore discards terms of order z^2 whose average is non-zero over the domain. This is the likely explanation for the slight difference in the momentum values between the random and deterministic simulations.

We have also devised numerical methods for quantifying uncertainty related to the phonon energy via stochastic Galerkin methods, which can be handled by the introduction of distributional derivatives with respect to the random variable. This mathematical structure departs from the usual form of the collision term in stochastic Galerkin for Boltzmann models by the need of distributional derivatives in the random space, being the first case in stochastic Galerkin methods for kinetic equations where this structure appears, and opening a new analytical treatment of randomness in the aforementioned stochastic method.

In conclusion, we have handled in this work the possible uncertainties arising in a model of electron transport in semiconductors by stochastic Galerkin, mainly related to the collision mechanisms in this paper. We calculate the propagated uncertainty in the electron probability density function due to possible uncertainties in either the phonon energy (adding a random variable given by

either a Gaussian or uniform distribution, considering first an approximate randomness to first order in the phonon energy and then the full calculation) or in the lattice temperature (assumed to vary randomly according to a uniform distribution).

Our purpose is to observe how physical variables which can either behave randomly in a real world setting (such as a varying temperature) or are known to be described approximately in our model (such as the phonon energy, which is often assumed to be constant, but really is known experimentally to be not constant) can affect physical observables such as electric current, average energy or density, since our kinetic model lets us calculate those measurable quantities by means of moments of the PDF.

Our study is useful to let us predict in real world settings the impact that uncertainties or limitations in commonly used idealized models have on the behavior of an electronic device such as a diode or a MOSFET. This study is also useful in terms of introducing uncertainties in the energy transition arguments of the collision integrals with the ultimate goal of jumping from the scalar treatment presented in this paper to the case of an energy band structure $\varepsilon(\vec{k})$, which is a scalar function of a vector variable, in future work.

We have calculated with our numerical methods the variation in kinetic moments (density, mean energy, current, etc.) associated with a physically reasonable temperature variation in the lattice environment. We have presented the algorithms to make an approximate (to first order) and exact calculation of the propagation of uncertainty of the phonon energy (bounding the error of a constant phonon energy by a uniform distribution) into the PDF which will give as well the associated uncertainty in the prediction of moments.

6 Acknowledgment

This work was supported by FWF (Austrian Science Fund) START project Y660 *PDE Models for Nanotechnology*. The first author also acknowledges start-up support from The University of Texas at San Antonio.

References

- [1] M. Lundstrom, *Fundamentals of Carrier Transport*. Cambridge University Press, 2 ed., 2000.
- [2] N. Wiener, “The homogeneous chaos,” *American Journal of Mathematics*, vol. 60, no. 4, pp. 897–936, 1938.
- [3] R. G. Ghanem and P. D. Spanos, *Stochastic Finite Elements: A Spectral Approach*. New York, NY, USA: Springer-Verlag New York, Inc., 1991.
- [4] D. Xiu and G. Karniadakis, “The Wiener–Askey polynomial chaos for stochastic differential equations,” *SIAM Journal on Scientific Computing*, vol. 24, no. 2, pp. 619–644, 2002.
- [5] J. Hu and S. Jin, “A stochastic Galerkin method for the Boltzmann equation with uncertainty,” *Journal of Computational Physics*, vol. 315, pp. 150 – 168, 2016.

- [6] J. Hu and S. Jin, *Uncertainty Quantification for Kinetic Equations*, pp. 193–229. Cham: Springer International Publishing, 2017.
- [7] S. Jin and L. Pareschi, *Uncertainty Quantification for Hyperbolic and Kinetic Equations*. Springer International Publishing, 2017.
- [8] S. Jin and L. Liu, “An asymptotic-preserving stochastic Galerkin method for the semiconductor Boltzmann equation with random inputs and diffusive scalings,” *Multiscale Modeling & Simulation*, vol. 15, no. 1, pp. 157–183, 2017.
- [9] Y. Cheng, I. M. Gamba, A. Majorana, and C.-W. Shu, “A discontinuous Galerkin solver for Boltzmann-Poisson systems in nano devices,” *Comput. Methods Appl. Mech. Engrg.*, vol. 198, no. 37-40, pp. 3130–3150, 2009.
- [10] Y. Cheng, I. Gamba, and J. Profet, “Positivity-preserving discontinuous Galerkin schemes for linear Vlasov–Boltzmann transport equations,” *Mathematics of Computation*, vol. 81, no. 277, pp. 153–190, 2011.