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Proof of a simple time-step propagation scheme for Monte Carlo simulation

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Abstract

An explicit proof of a simple time-step propagation scheme is given in the framework of basic probability theory. It can be used in Monte Carlo simulations solving the Boltzmann transport equation. If the stochastically selected first scattering event occurs before a given time t_1, the particle is propagated as usual until the end of the corresponding free-flight time; otherwise, however, the propagation can be stopped in this scheme at t_1 and a new random number can be generated to decide whether the first scattering event occurs before the next specified time t_2.

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1. Introduction

Monte Carlo simulation has been established as a stochastic method for the solution of the Boltzmann transport equation [1–3] which is an integro-differential equation for the electron distribution function. Its solution can be used to compute macroscopic quantities such as the electron density or the current density. Since the Boltzmann transport equation considers the electron drift in the electric field as well as the scattering events at a microscopic level, it allows one to take physical effects occurring in deep submicron metal-oxide-semiconductor field-effect transistors (MOSFETs) into account, for example ballistic and hot-electron transport. Various algorithms have been developed to improve the computational efficiency of the Monte Carlo simulation. Among them is the self-scattering scheme of Rees [4] which uses an upper estimate Γ of the scattering rate to greatly facilitate the determination of the collisionless flight-time. In order to avoid at the same time a large number of self-scattering events involved with a global upper estimation, a variable Γ scheme is often being employed [1,5–7]. This scheme is especially useful for full-band Monte Carlo simulation where the electronic band structure is not described by an analytical

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formula, but computed by the empirical pseudopotential method and stored in a table. Here it is natural to assign a different Γ to each element of the discretized phase-space. However, for large selected free-flight times the electron will leave the original phase-space element and the flight-time is usually adjusted in order to accommodate the change of Γ [5–7]. It is the aim of this paper to show in the framework of basic probability theory that such an adjustment is not necessary, but that simply a new flight-time can be stochastically selected if the border of the original phase-space element is crossed.

2. Proof of the propagation scheme

The proof is based on the calculation of the probability that there is no scattering between the times 0 and t. This event is equivalent to the time of the first scattering, t_s, being larger than t and therefore the event will be denoted by $\{t_s \notin (0,t)\}$. At first, we decompose the time interval $(0,t)$ into two not necessarily equidistant time intervals and consider the event $\{t_s \in (0,t)\}$ that the first scattering does occur between 0 and t. The first scattering occurring between 0 and t is equivalent to the first scattering occurring between 0 and t_1 *or* the first scattering occurring between t_1 and t, where t_1 is a time somewhere between 0 and t. This leads to the union of the corresponding sets according to

$$\{t_s \in (0,t)\} = \{t_s \in (0,t_1)\} \cup \{t_s \in (t_1,t)\}. \tag{1}$$

Taking the complement of (1) and applying de Morgan's rules yields

$$\begin{aligned}\overline{\{t_s \in (0,t)\}} \equiv \{t_s \notin (0,t)\} &= \overline{(\{t_s \in (0,t_1)\} \cup \{t_s \in (t_1,t)\})} = \overline{\{t_s \in (0,t_1)\}} \cap \overline{\{t_s \in (t_1,t)\}} \\ &\equiv \{t_s \notin (0,t_1)\} \cap \{t_s \notin (t_1,t)\},\end{aligned} \tag{2}$$

i.e. we obtain for the probability that there is no scattering between the times 0 and t

$$P(\{t_s \notin (0,t)\}) = P(\{t_s \notin (0,t_1)\} \cap \{t_s \notin (t_1,t)\}). \tag{3}$$

Eq. (3) is completely general and does not refer to the Boltzmann transport equation. On the other hand, in the specific case of the Boltzmann transport equation (BE), this probability is given by [8,9]

$$P_{\mathrm{BE}}(\{t_s \notin (0,t)\}) = \exp\left(-\int_0^t S(\boldsymbol{k}(\tau))\,\mathrm{d}\tau\right), \tag{4}$$

where S is the scattering rate and $\boldsymbol{k}(\tau)$ the electron's momentum at time τ. The exponential in Eq. (4) allows a factorization according to

$$\begin{aligned}P_{\mathrm{BE}}(\{t_s \notin (0,t)\}) &= P_{\mathrm{BE}}(\{t_s \notin (0,t_1)\} \cap \{t_s \notin (t_1,t)\}) \\ &= \exp\left(-\left\{\int_0^{t_1} S(\boldsymbol{k}(\tau))\,\mathrm{d}\tau + \int_{t_1}^{t} S(\boldsymbol{k}(\tau))\,\mathrm{d}\tau\right\}\right) \\ &= \exp\left(-\int_0^{t_1} S(\boldsymbol{k}(\tau))\,\mathrm{d}\tau\right) \times \exp\left(-\int_{t_1}^{t} S(\boldsymbol{k}(\tau))\,\mathrm{d}\tau\right) \\ &= P_{\mathrm{BE}}(\{t_s \notin (0,t_1)\}) \times P_{\mathrm{BE}}(\{t_s \notin (t_1,t)\}).\end{aligned} \tag{5}$$

Since $P(A \cap B) = P(A) \times P(B)$ for stochastically independent events A and B, Eq. (5) proves that the absence of scattering in the interval (t_1,t) is independent of the absence of scattering in the interval

$(0, t_1)$. In other words, when the event that the first scattering does not occur before t_1 is realized (with the help of a random number r uniformly distributed in $[0, 1)$), the particle can be propagated until t_1 and then a new random number can be generated to decide whether scattering occurs in the next interval.

3. Consistency check

It remains to investigate the opposite event where the first scattering occurs before t_1 and the electron is propagated as usual within the self-scattering scheme according to [1]

$$t_s = -\frac{1}{\Gamma}\ln(1-r). \tag{6}$$

Here, Γ denotes an upper estimation of the scattering rate $S(\boldsymbol{k})$.

For the calculation of the probability that the first scattering occurs before t_1 we use the following equation:

$$P_{\mathrm{BE}}(\{t_s \in (0,t_1)\} \cup \{t_s \notin (0,t_1)\}) = P_{\mathrm{BE}}(\{t_s \in (0,t_1)\}) + P_{\mathrm{BE}}(\{t_s \notin (0,t_1)\}) = 1, \tag{7}$$

which follows from (i) $P(A \cup B) = P(A) + P(B)$ for $A \cap B = \emptyset$ and (ii) $P(A) + P(\bar{A}) = 1$. The probability sought-after is therefore given by

$$P_{\mathrm{BE}}(\{t_s \in (0,t_1)\}) = 1 - P_{\mathrm{BE}}(\{t_s \notin (0,t_1)\}) = 1 - \exp\left(-\int_0^{t_1} S(\boldsymbol{k}(\tau))\,\mathrm{d}\tau\right) = 1 - \exp(-\Gamma t_1), \tag{8}$$

where in the last step the self-scattering scheme has been invoked. The event that the first scattering occurs before t_1 is realized if a random number r, uniformly distributed in the interval $[0, 1)$, is smaller than the probability $P_{\mathrm{BE}}(\{t_s \in (0, t_1)\})$. Then the following equivalences hold:

$$\begin{aligned}\{t_s \in (0,t_1)\} &\Leftrightarrow r < P_{\mathrm{BE}}(\{t_s \in (0,t_1)\}) \Leftrightarrow r < 1 - \exp(-\Gamma t_1) \Leftrightarrow 1 - r > \exp(-\Gamma t_1) \\ &\Leftrightarrow -\ln(1-r) < \Gamma\, t_1 \Leftrightarrow t_s < t_1,\end{aligned} \tag{9}$$

where the definition of t_s in (6) has been used. This shows that the free-flight time is smaller than t_1 if the first scattering occurs before t_1. Finally, we note that in this scheme the computationally relatively costly logarithm in (6) needs only to be computed if the event that the first scattering occurs before t_1 is realized according to the third expression of (9).

4. Summary

The above considerations have proven in terms of basic probability theory the following propagation scheme for the Boltzmann transport equation. First, a random number is used to determine whether the first scattering occurs before a given time t_1. In this case, the particle is propagated according to the corresponding free-flight time, otherwise until t_1. Then a new, possibly different time step is defined and the procedure is repeated. The validity of this scheme has been verified by an explicit comparison with the standard Monte Carlo scheme and was used for an efficient full-band Monte Carlo device simulation [10].

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References

[1] C. Jacoboni, P. Lugli, The Monte Carlo Method for Semiconductor Device Simulation, Springer, Wien, 1989.
[2] K. Hess (Ed.), Monte Carlo Device Simulation: Full Band and Beyond, Kluwer Academic Publishers, Boston, 1991.
[3] M.V. Fischetti, S.E. Laux, Monte Carlo analysis of electron transport in small semiconductor devices including band-structure and space-charge effects, Phys. Rev. B 38 (1988) 9721–9745.
[4] H.D. Rees, Calculation of steady state distribution functions by exploiting stability, Phys. Lett. A 26 (1968) 416–417.
[5] J. Bude, R.K. Smith, Phase-space simplex Monte Carlo for semiconductor transport, Semicond. Sci. Technol. 9 (1994) 840–843.
[6] E. Sangiorgi, B. Ricco, F. Venturi, MOS^2: an efficient Monte Carlo simulator for MOS devices, IEEE Trans. Computer-Aided Des. 7 (1988) 259–271.
[7] C. Jungemann, S. Keith, M. Bartels, B. Meinerzhagen, Efficient full-band Monte Carlo simulation of silicon devices, IEICE Trans. Electron. E82-C (1999) 870–879.
[8] W. Fawcett, A.D. Boardman, S. Swain, Monte Carlo determination of electron transport properties in gallium arsenide, J. Phys. Chem. Solids 31 (1970) 1963–1990.
[9] A. Reklaitis, The calculation of electron transient response in semiconductors by the Monte Carlo technique, Phys. Lett. A 88 (1982) 367–370.
[10] F.M. Bufler, A. Schenk, W. Fichtner, Efficient Monte Carlo device modeling, IEEE Trans. Electron Devices 47 (2000) 1891–1897.