Statistical Algorithms for Simulation of Electron Quantum Kinetics in Semiconductors – Part I*

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Abstract. In this work we solve the Barker-Ferry equation which accounts for the quantum character of the electron-phonon interaction in semiconductors in the framework of the Monte Carlo (MC) method.
The first part of the work considers the zero electric field formulation of the equation in spherical coordinates. Different MC algorithms for solving the equation are suggested and investigated.
In the second part of the work we consider the case of an applied electric field. It is shown that the second algorithm from the first part can be successfully modified to account for the cylindrical symmetry of the task.

1 Introduction

We consider a physical model which describes a femtosecond relaxation process of optically excited carriers in an one-band semiconductor [6]. The process is described by the zero electric field form of the Barker-Ferry equation [1].

$$f(\mathbf{k},t) = \int_0^t dt' \int_0^{t'} dt'' \int d^3\mathbf{k}' \{S(\mathbf{k}',\mathbf{k},t'-t'')f(\mathbf{k}',t'') - S(\mathbf{k},\mathbf{k}',t'-t'')f(\mathbf{k},t'')\} + \phi(\mathbf{k}), \tag{1}$$

with a kernel

$$S(\mathbf{k}',\mathbf{k},t'-t'') = \frac{2V}{(2\pi)^3\hbar^2}|g_{\mathbf{k}'-\mathbf{k}}|^2 \exp(-\Gamma(\mathbf{k}',\mathbf{k})(t'-t'')) \tag{2}$$

$$\times\{(n+1)\cos(\Omega(\mathbf{k}',\mathbf{k})(t'-t'')) + n\cos(\Omega(\mathbf{k},\mathbf{k}')(t'-t''))\}$$

where $\mathbf{k}$ is the momentum, $f(\mathbf{k},t)$ is the distribution function and $\phi(\mathbf{k})$ is the positive initial condition. In the kernel (2) $\Omega(\mathbf{k}',\mathbf{k}) = (\varepsilon(\mathbf{k}') - \varepsilon(\mathbf{k}) - \hbar\omega)/\hbar$,

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where ω is the phonon frequency, $\hbar\omega$ is the phonon energy and $\varepsilon(\mathbf{k})$ is the electron energy. The coupling

$$g_{\mathbf{k}'-\mathbf{k}} = -i\left[\frac{2\pi e^2\hbar\omega}{V}\left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_s}\right)\frac{1}{(\mathbf{k}'-\mathbf{k})^2}\right]^{\frac{1}{2}}$$

applies to the Fröhlich interaction with LO phonons, which means the phonon energy $\hbar\omega$ is taken constant, (ϵ_∞) and (ϵ_s) are the optical and static dielectric constants and V is the volume. The Bose function $n = 1/(\exp[\hbar\omega/\mathcal{K}T]-1)$, where $\mathcal{K}$ is the Boltzmann constant and T is the temperature of the crystal, corresponds to an equilibrium distributed phonon bath. The damping $\Gamma(\mathbf{k}', \mathbf{k}) = \Gamma(\mathbf{k}')+\Gamma(\mathbf{k})$ is related to the finite carrier lifetime for the scattering process:

$$\Gamma(\mathbf{k}) = \int d^3\mathbf{k}' \frac{V}{2^3\pi^2\hbar}\sum_{\pm}\|g_{\mathbf{k}'-\mathbf{k}}\|^2\delta(\varepsilon(\mathbf{k}') - \varepsilon(\mathbf{k}) \pm \hbar\omega)(n + \frac{1}{2} \pm \frac{1}{2}).$$

Let us specify that the wave vectors $\mathbf{k}$, $\mathbf{k}'$ belong to a finite domain G which is sphere with radius Q. Denote with k and k' the norm of the corresponding vectors $\mathbf{k}$ and $\mathbf{k}'$. Let θ be the angle between this two vectors and the k'_z axis be oriented along $\mathbf{k}$. It holds: $d^3\mathbf{k}' = {k'}^2 \sin\theta dk' d\theta d\xi,\ \theta \in (0,\pi),\ \varphi \in (0, 2\pi)$. The functions Γ and Ω depend only on the radial variables k and k' which is denoted by $\Gamma_{k,k'}$ and $\Omega_{k,k'}$. Equation (1) in spherical coordinates becomes [5]:

$$f(k,t) = \int_0^t dt' \int_0^{t'} dt'' \int_0^Q dk' K(k,k') \times \{S_1(k,k',t',t'')f(k',t'') + S_2(k,k',t',t'')f(k,t'')\} + \phi(k), \tag{3}$$

where

$$K(k,k') = c\frac{k'}{k}\ln\left(\frac{k+k'}{|k-k'|}\right), \tag{4}$$

$$S_1(k,k',t',t'') = -S_2(k',k,t',t'') = \exp(-\Gamma_{k',k}(t'-t'')) \times \{(n+1)\cos(\Omega_{k',k}(t'-t'')) + n\cos(\Omega_{k,k'}(t'-t''))\}$$

and the constant $c = e^2\omega\left|\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_s}\right|/(\pi\hbar)$. By using the indentity $\int_0^t dt' \int_0^{t'} dt'' = \int_0^t dt'' \int_{t''}^t dt'$, equation (3) can be presented in the following form:

$$f(k,t) = \int_0^t dt'' \int_0^Q dk' K(k,k') \times [\mathcal{K}_1(k,k',t,t'')f(k',t'') + \mathcal{K}_2(k,k',t,t'')f(k,t'')] + \phi(k), \tag{5}$$

where

$$\mathcal{K}_i(k,k',t,t'') = \int_{t''}^t dt' S_i(k,k',t',t''), \quad i = 1,2. \tag{6}$$

Finally, equation (5) allows an analytical evaluation of the integrals (6), (see [2]). Thus we obtain the third integral form:

$$f(k,t) = \int_0^t dt'' \int_0^Q dk' K(k,k') \times [K_1(k,k',t,t'')f(k',t'') + K_2(k,k',t,t'')f(k,t'')] + \phi(k), \tag{7}$$

where

$$K_1(k,k',t,t'') = -K_2(k',k,t,t'') =$$
$$(n+1)L_{k',k}\left[1+\left(\frac{\Omega_{k',k}}{\Gamma_{k',k}}\sin(\Omega_{k',k}(t-t''))-\cos(\Omega_{k',k}(t-t''))\right)\exp(-\Gamma_{k',k}(t-t''))\right]$$
$$+nL_{k,k'}\left[1+\left(\frac{\Omega_{k,k'}}{\Gamma_{k,k'}}\sin(\Omega_{k,k'}(t-t''))-\cos(\Omega_{k,k'}(t-t''))\right)\exp(-\Gamma_{k,k'}(t-t''))\right]$$

and $L_{k',k} = \Gamma_{k',k}/(\Omega_{k',k}^2 + \Gamma_{k',k}^2)$.

We note that the Neumann series of the integral equation (1) converges [5] and the solution can be estimated by the MC method.

In this work three MC algorithms for solving the above three analytically equivalent integral formulations of the equation (1) are considered. They use backward time evolution of the numerical trajectories. The density function in the Markov chain for the transition $k \to k'$ is chosen to be proportional to the contribution (4). The first algorithm is called the *twice time dependent iterative* Monte Carlo (TTDIMC) algorithm and estimates equation (3). The following conditional density function, $q(t',t'') = c_1 \exp(-\Gamma_{k',k}(t'-t''))$, is used to sample time $t' \in (0,\ t)$ and $t'' \in (0,\ t')$ in the Markov chain (c_1 is a normalized constant). The second algorithm is called the *randomized iterative* Monte Carlo (RIMC) algorithm. The integral, which depend on t' in equation (5), is calculated on an each step in the Markov chain using a MC estimator. Finally, the third algorithm is called the *one time dependent iterative* Monte Carlo (OTDIMC) algorithm. It solves an one time-dimension integral form (7).

2 Monte Carlo Algorithms

The biased Monte Carlo estimator for the solution of equations (3,5,7) at the fixed point (κ_0, τ_0) is defined as follow:

$$\xi_{l_\varepsilon}[\kappa_0,\tau_0] = \phi(\kappa_0) + \sum_{j=1}^{l_\varepsilon} W_j^\alpha \phi_\alpha(\kappa_j), \tag{8}$$

where

$$W_j^\alpha = W_{j-1}^\alpha \frac{K(\kappa_{j-1},\kappa_j)\nu_\alpha(\kappa_{j-1},\kappa_j,\tau_{j-1},\tau_j)}{p_\alpha p(\kappa_{j-1},\kappa_j)q(\tau_{j-1},\tau_j)}, W_1^\alpha = 1, \alpha = 1,2,\ j = 0,1,\ldots,l_\varepsilon.$$

Here $\nu_\alpha(\kappa,\kappa',\tau,\tau') = S_\alpha(k,k',t',t'')$ in the TTDIMC algorithm; $\nu_\alpha(\kappa,\kappa',\tau,\tau')$ $= K_\alpha(k,k',t,t'')$ in the OTDIMC algorithm; and $\nu_\alpha(\kappa,\kappa',\tau,\tau')$ is a Monte Carlo

estimator of the integrals (6) in the RIMC algorithm. $p(\kappa,\kappa')$ and $q(\tau,\tau')$ are transition density functions in the Markov chain and their functional form is shown in the algorithms. p_α $(\alpha=1,2)$ are probabilities for chosing the quantities $\nu_\alpha(\kappa,\kappa',\tau,\tau')$.

Using N independent samples of the estimator (8) we obtain [7]

$$\overline{\xi}_{l_\varepsilon}[\kappa_0,\tau_0]=\frac{1}{N}\sum_{i=1}^{N}(\xi_{l_\varepsilon}[\kappa_0,\tau_0])_i\approx f(\kappa_0,\tau_0).$$

The corresponding MC algorithms for finding a solution in a fixed point (k,t) of equations (3,5,7) for one random walk is described as follow:

TTDIMC algorithm:

1. **Choose** any positive small number ε and **set** initial values $\xi=\phi(k)$, $W=1$.
2. **Sample** a value k' with a density function $p(k,k')=\overline{C}K(k,k')$ using a decomposition MC method ($\overline{C}$ is the normalized constant).
3. **Sample** the values $t'=-\log(\beta_1(\exp(-\Gamma_{k,k'}t)-1)+1)/\Gamma_{k,k'}$ and $t''=\log(\beta_2(\exp(\Gamma_{k,k'}t')-1)+1)/\Gamma_{k,k'}$, where β_1 and β_2 are uniformly distributed random variables in (0, 1).
4. **Calculate** $\nu_\alpha=S_\alpha(k,k',t',t'')$ and $p_\alpha=\frac{|\nu_\alpha|}{|\nu_1|+|\nu_2|}$, $(\alpha=1,2)$.
5. **Choose** a value β, an uniformly distributed random variable in (0, 1).
6. **If** $(p_1\le\beta)$ **then**

$$W:=W\frac{K(k,k')\nu_1}{p_1p(k,k')q(t',t'')},\ \ \xi:=\xi+W\phi(k'),\ \text{ and }\ k:=k';$$

else

$$W:=W\frac{K(k,k')\nu_2}{p_2p(k,k')q(t',t'')},\ \ \xi:=\xi+W\phi(k).$$

7. **Set** $t:=t''$ and **repeat** from step 2 until $t\le\varepsilon$.

RIMC algorithm:

1. **Choose** any positive small number ε and **set** initial values $\xi=\phi(k)$, $W=1$.
2. **Sample** a value k' as in the TTDIMC algorithm.
3. **Sample** a value t'' with a density function $q(t'')=1/t$.
4. **Sample** N_1 independent random values of t' with a density function $q_1(t')=1/(t-t'')$.
5. **Calculate**

$$\overline{\nu}_\alpha=\frac{t-t''}{N_1}\sum_{i=1}^{N_1}S_\alpha(k,k',t'_i,t''),\ \ p_\alpha=\frac{|\overline{\nu}_\alpha|}{|\overline{\nu}_1|+|\overline{\nu}_2|},\ \ \alpha=1,2.$$

6. **Choose** a value β, an uniformly distributed random variable in $(0,1)$.
7. **Do** same as steps 6 and 7 in the TTDMC algorithm.

OTDIMC algorithm:

1. **Choose** any positive small number ε and **set** initial values $\xi = \phi(k)$, $W = 1$.
2. **Sample** a value k' as in the TTDIMC algorithm.
3. **Sample** $t'' = \log(\beta_1(\exp(\Gamma_{k,k'}t) - 1) + 1)/\Gamma_{k,k'}$ with a density function $q(t, t'') = \Gamma_{k,k'} \times \exp(-\Gamma_{k,k'}(t - t''))/(1 - \exp(-\Gamma_{k,k'}))$, where β_1 is an uniformly distributed random variable in $(0, 1)$.
4. **Calculate** $\nu_\alpha = K_\alpha(k, k', t, t'')$ and $p_\alpha = \frac{|\nu_\alpha|}{|\nu_1|+|\nu_2|}$, $(\alpha = 1, 2)$.
5. **Choose** a value β, an uniformly distributed random variable in $(0, 1)$.
6. **Do** same as steps 6 and 7 in the TTDMC algorithm.

The decomposition MC method used in the second step of the algorithms is given below. The density function $p(k, k')$ can be expressed as an infinite weighted sum of other density functions [2]:

$$p(k, k') = \overline{C}K(k, k') = \sum_{i=0}^{\infty} \overline{C}_i p_i(k, k'), \quad \overline{C}_i \geq 0, \quad \sum_{i=0}^{\infty} \overline{C}_i = 1, \tag{9}$$

where

$$\overline{C}_i = \begin{cases} \frac{2}{(2i+1)(2i+3)}, & \text{when } 0 \leq k' < k \\ \frac{\frac{4k^2}{(4i^2-1)}\left(1-(\frac{k}{Q})^{2i-1}\right)}{(Q-k)\left[2k+(Q+k)\ln\left(\frac{Q+k}{Q-k}\right)\right]}, & \text{when } k < k' \leq Q \end{cases}$$

$$p_i(k, k') = \begin{cases} (2i+3)\frac{(k')^{2i+2}}{k^{2i+3}}, & \text{when } 0 \leq k' < k \\ (2i-1)\left[\frac{(Qk)^{2i-1}}{Q^{2i-1}-k^{2i-1}}\frac{1}{(k')^{2i}}\right], & \text{when } k < k' \leq Q. \end{cases}$$

Thus:

1. Sample a random integer I such that $Prob(I = i) = \overline{C}_i$.
2. Sample k' with the i-th density function $p_i(k, k')$.

This can easily be done using the inverse-transformation method.

In practice, the decomposition MC method is applied for a finite number of terms in the series (9).

The iterative MC algorithms that approximate some deterministic iterative method are characterized by two types of errors -systematic and stochastic [2,4]. Now following [4] we obtain the relation

$$E(\overline{\xi}_{l_\varepsilon}[\kappa_0, \tau_0] - f(\kappa_0, \tau_0))^2 = \frac{Var(\xi_{l_\varepsilon}[\kappa_0, \tau_0])}{N} + (f(\kappa_0, \tau_0) - E\xi_{l_\varepsilon}[\kappa_0, \tau_0])^2$$

$$\leq \frac{d_0}{N} + d_1\varepsilon^2 = \mu^2, \tag{10}$$

where μ is the desired error, d_1 is a constant and d_0 is an upper bound of the variance. Therefore, in order to obtain the error of order μ the optimal order of the quantities N and ε must be $N = O(\mu^{-2})$ and $\varepsilon = O(\mu)$. In addition, when we apply the RIMC algorithm we can take $N_1 = O(\mu^{-2})$, too. Let us note that

the choice of the density function (9) guarantees that the variance of the MC estimator is bounded (see [2]).

The computational complexity of the presented algorithms can be measured by the quantity $F = Nt_m E(l_\varepsilon)$. Here N is the number of random walks in the corresponding algorithms; $E(l_\varepsilon)$ is the mathematical expectation of the number of transitions in the Markov chain and t_m is the mean time for modeling one transition. In the case of the RIMC algorithm the quantity F must also be multiplied with the variable N_1.

According to (10) the number of the random walks and the number of transitions are connected with the stochastic and systematic errors. However the times for modeling one transition depend on the complexity of the transition density functions and the choice of the random number generator. The MC algorithms under consideration are realized using the Scalable Parallel Random Number Generator (SPRNG) Library [3]. Results for the computational cost and the accuracy of the MC solutions are obtained and compared in the next section.

3 Numerical Results

The results discussed in the following have been obtained by the iterative MC algorithms under consideration. Material parameters for $GaAs$ have been used: the electron effective mass is 0.063, the optimal phonon energy is $36meV$, the static and optical dielectric constants in the Fröhlich coupling are $\varepsilon_s = 10.92$

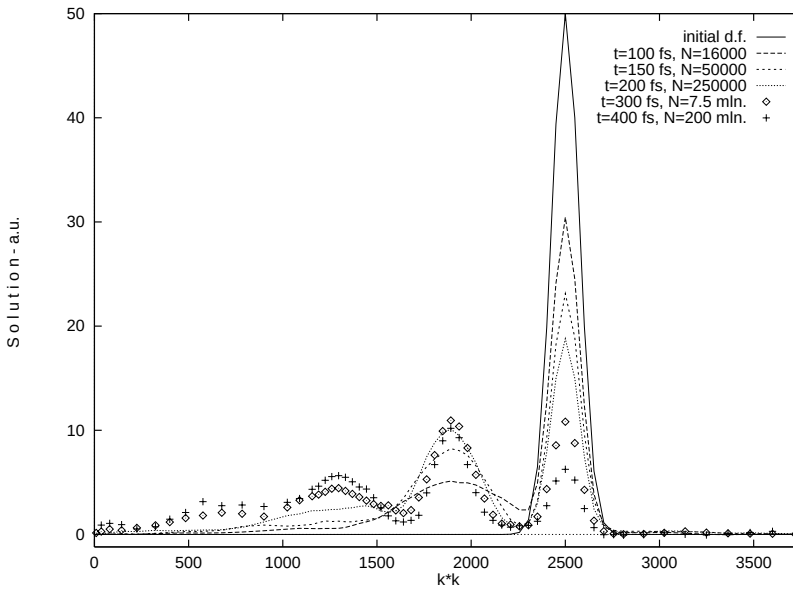

Fig. 1. The electron energy distribution $k * f(k,t)$ versus $k * k$. The drelaxation leads to a time-dependent broadening of the replicas. $\varepsilon = 0.001$.

Table 1. Comparison of the computational complexity using the iterative MC algorithms.

	t	N	$E(l_\varepsilon)$	σ_N^2	$CPUtime$
	$50fs$	10000	8.1758	0.04894	0m56.05s
TTDIMC	$100fs$	250000	9.2723	6.24605	24m7.73s
algorithm	$150fs$	6 mln.	10.2238	809.465	10h1m39.64s
	$200fs$	150 mln.	11.1173	121474.56	250h31m45.12s
	$50fs$	5000	11.8640	0.01494	17m16.57s
RIMC	$100fs$	16000	12.4894	0.1382	1h17m22.42s
algorithm	$150fs$	50000	12.9134	1.05977	4h43m46.18s
	$200fs$	250000	13.2038	8.6563	26h13m18.38s
	$50fs$	5000	11.9553	0.01575	0m41.49s
	$100fs$	16000	12.7111	0.1481	2m22.05s
OTDIMC	$150fs$	50000	13.2299	0.9982	7m43.35s
algorithm	$200fs$	250000	13.6268	6.6242	39m52.90s
	$250fs$	1.5 mln	13.9038	87.3812	2h34m57.73s
	$300fs$	7.5 mln.	14.2694	347.539	21h1m12.56s

and $\varepsilon_\infty = 12.9$. The lattice temperature is zero. The initial condition at $t = 0$ is given by a function which is Gaussian in energy, ($\phi(k) = exp(-(b_1k^2 - b_2)^2)$ $b_1 = 96$ and $b_2 = 24$), scaled in a way to ensure, that the peak value is equal to unity. The quantity presented on the y-axes in Figs. 1–2 is $k * f(k,t)$, i.e. it is proportional to the distribution function multiplied by the density of states. It is given in arbitrary units. The quantity $k * k$, given on the x-axes in units of $10^{14}/m^2$, is proportional to the electron energy.

The iterative MC algorithms were implemented in C and compiled with the "cc" compiler at optimization level "-fast". Numerical tests on Sun Ultra Enterprise 450 with 4 Ultra-SPARC, 400 MHz CPUs running Solaris were performed. Fig.1 shows the electron distribution at long evolution times using the OTDIMC algorithm. The simulation domain is between 0 and $Q = 66 \times 10^7/m$. The product $k * f(k,t)$ is calculated in 65 points.

Comparison of the electron energy distribution, which is obtained by the TTDIMC, RIMC and OTDIMC algorithms, is shown on Fig.2 for evolution times $t = 100fs$ and $t = 150fs$. We see that the MC solutions approximately coincide. Therefore, the use of the all algorithms is correct.

The results for the computational cost (CPU time for all 65 points) of the iterative MC algorithms are shown in Table 1. Here, N is the number of random walks need to obtain approximately smooth solutions using the different MC algorithms and σ_N^2 is the average estimate of the variance $Var(\xi_{l_\varepsilon}[\kappa_0, \tau_0])$ for all 65 points. We see that the efficiency of the OTDIMC algorithm is superior. In addition, the comparison of the computational cost between both TTDIMC and RIMC algorithms shows that first algorithm is more efficient for evolution times less then $150fs$ and vice versa, with the increase of the evolution time the CPU time for TTDIMC algorithm increase drastically. In order to obtain

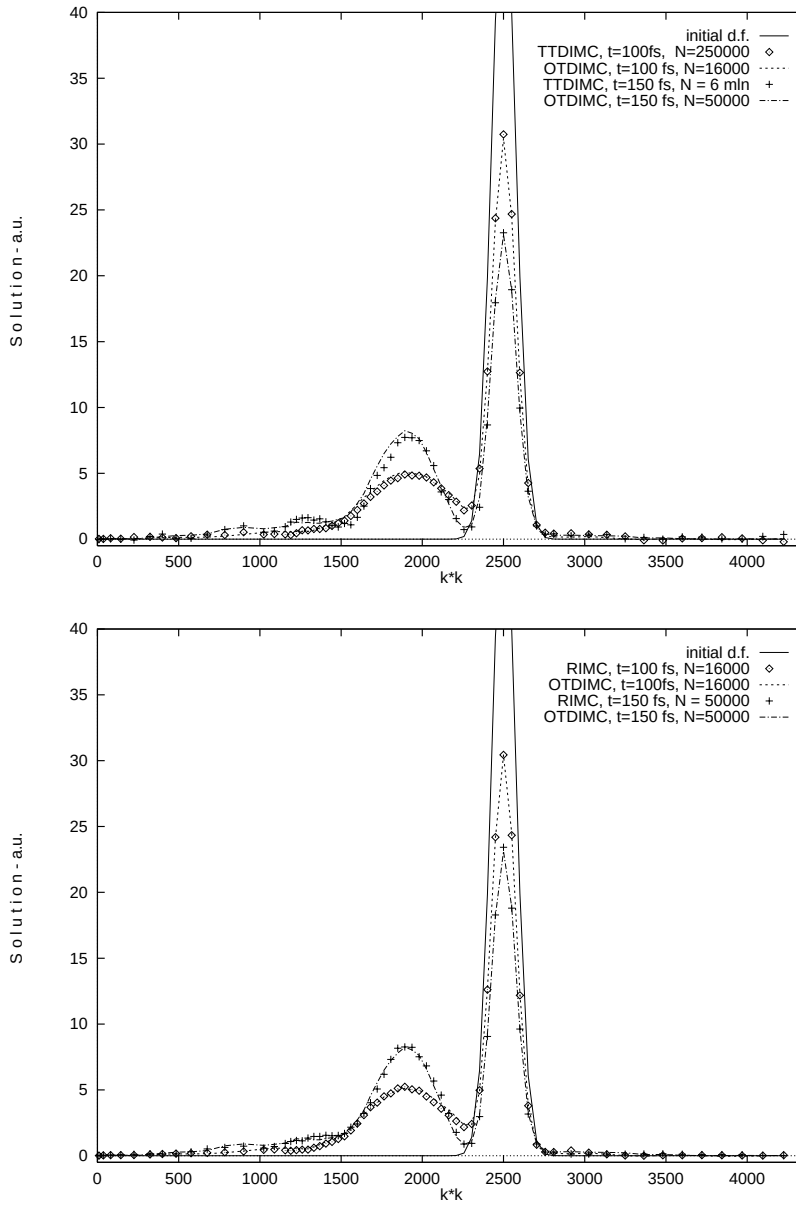

Fig. 2. Comparison of the electron energy distribution $k * f(k,t)$ versus $k * k$ obtained by the TTDIMC, RIMC and OTDIMC algorithms, $\varepsilon = 0.001$.

a good balance between both stochastics errors in the RIMC algorithm we take $N_1 = 1000$, when $t - t'' > 20fs$ and $N_1 = 100$, when $t - t'' \leq 20fs$.

The dependence of the variances, in a logarithmic scale ($\ln(\sigma_N^2)$), on the evolution time is shown on Fig. 3.

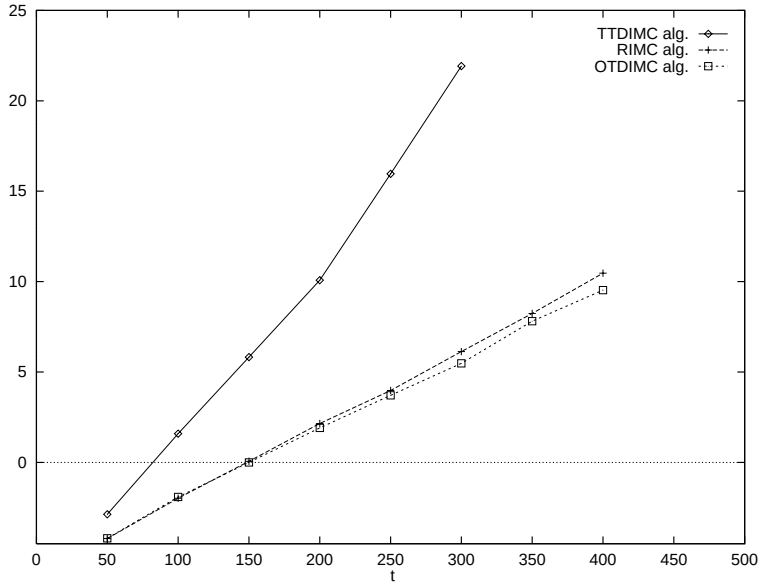

Fig. 3. Comparison of the variances, in a logarithmic scale ($\ln(\sigma_N^2)$), for $N = 500000, \varepsilon = 0.001$.

We conclude that in the case of an applied electric field the OTDIMC algorithm is not applicable because the integrals (6) are very complex and they can't be evaluated analytically. The numerical results show that the use of the TTDIMC or the RIMC algorithms depend on the evolution time for estimation of the electron distribution.

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