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Time step truncation in Direct Simulation Monte Carlo for semiconductors

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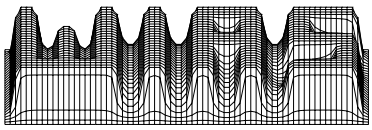

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Abstract

A homogeneous (bulk) silicon semiconductor is studied by using the Direct Simulation Monte Carlo (DSMC). Two DSMC algorithms are considered, the self scattering technique (SST) and the constant time technique (CTT). First, the results obtained by CTT are shown to converge (with vanishing time step) to the results obtained by SST. The truncation error of CTT turns out to be of first order with respect to the time step. Second, the efficiency of both algorithms is compared. It is found that SST is more efficient if a high precision (relative error less then three percent) of the results is needed.

Contents

1 Introduction.

The Direct Simulation Monte Carlo (DSMC) algorithm is a stochastic method that solves the Boltzmann equation by replacing the distribution function with a representative set of particles. In solid state physics this method has been widely investigated for describing charge transport in submicrometric semiconductors [1, 2]. The DSMC shows itself to be a very useful tool, since it permits particular physical simulations unattainable in experiments, or even investigation of nonexistent materials in order to emphasize special features of the phenomenon under study. It provides an accurate description of carrier transport phenomena because the various scattering mechanisms and band structure models are taken into account.

In contrast to the other simulation tools, like drift-diffusion or hydrodynamic models, the DSMC results are affected by discretization and stochastic errors, which influence dramatically their accuracy and efficiency .

An analysis of the stochastic error has been recently tackled in [3]. Here, in this paper, we shall draw our attention to the discretization error introduced in the free flight mechanism.

In section 2 we introduce the basics of the DSMC, and the main scattering mechanisms for silicon. In section 3 the free flight generation mechanisms, i.e. the Self Scattering and the Constant Time techniques, are treated. In section 4 we study the discretization error introduced by the Constant Time Technique, in the simulation of a homogeneous silicon semiconductor, and the efficiency of the two algorithms is compared.

2 Basic Equations.

The Monte Carlo method for evolving a solution of the Boltzmann Transport Equation (BTE) [4] consists in recreating the history evolution of electrons in time and space inside the crystal, subject to the action of external and self-consistent electric field and of the given scattering mechanisms [1, 5].

The simulation starts with one or more electrons in given initial conditions for momentum $\hbar\mathsf{k}$ and position x. During the *free flight* (i.e. the time between two collisions) the external forces are made to act according to the Newton's equations of motion in the crystal :

$$\frac{d\mathsf{x}}{dt} = \frac{1}{\hbar}\nabla_{\mathsf{k}}\varepsilon(\mathsf{k}) \tag{1}$$

$$\hbar\frac{d\mathsf{k}}{dt} = -q\mathsf{E}(t,\mathsf{x}) \tag{2}$$

where $\varepsilon(\mathsf{k})$ is the kinetic energy of the considered crystal conduction band structure measured from the band minimum, q the absolute value of the electron charge, and $\hbar$ the Planck constant divided by 2π. The electric field $\mathsf{E}(t,\mathsf{x})$ satisfies the Poisson equation

$$\Delta(\epsilon\phi) = q\Big[n(t,\mathsf{x}) - N_D(\mathsf{x}) + N_A(\mathsf{x})\Big], \tag{3}$$

$$\mathsf{E} = -\nabla_{\mathsf{x}}\phi,$$

where $\phi(t,\mathsf{x})$ is the electric potential, N_D and N_A are respectively the donor and acceptor densities (which are positive functions), ϵ the dielectric constant , and n the electron density.

In the neighborhood of the band minimum a good dispersion relation is given by the *parabolic* approximation:

$$\varepsilon(\mathsf{k}) = \frac{\hbar^2\mathsf{k}^2}{2m^\star}, \quad \mathsf{k} \in \Omega, \tag{4}$$

where $m^\star$ is the effective electron mass (which is 0.32 m_e in silicon), and k belongs to the domain Ω, called first Brillouin zone, which is a characteristic of each material. In silicon this zone is formed by six equivalent ellipsoidal valleys along the axis of the frame of reference at about 0.85 (in the units $\frac{2\pi}{a}$ where a is the lattice constant) from the zone center.

The electron group velocity $\mathsf{v} \equiv (v^1, v^2, v^3)$ is given by

$$\mathsf{v}(\mathsf{k}) = \frac{1}{\hbar}\nabla_{\mathsf{k}}\varepsilon = \frac{\hbar\mathsf{k}}{m^\star} \quad .$$

The equations (1),(2)are solved with a numerical scheme by using a time step Δt, which depends on the stability and accuracy used.

Then a scattering mechanism is chosen randomly as responsible for the end of the free flight, according to the relative probabilities of all possible scattering mechanisms. From the differential cross section of this mechanism a new k state after scattering is randomly chosen as initial state of the new free flight: after the collision the electron can remain in the same valley (intravalley scattering) or be drawn in another equivalent valley (intervalley scattering).

The main scattering mechanisms in silicon, at room temperature, are due to electron-phonon interactions (acoustic and non polar optical). Their transition probability, per unit time, from a state k to a state k' can be modeled as [1]:

$$\begin{aligned} w(\mathsf{k},\mathsf{k}') \;=\; & K_0(\mathsf{k},\mathsf{k}')\delta(\varepsilon(\mathsf{k}') - \varepsilon(\mathsf{k})) + \sum_{i=1}^{6} K_i(\mathsf{k},\mathsf{k}') \times \\ & [\delta(\varepsilon(\mathsf{k}') - \varepsilon(\mathsf{k}) + \hbar\omega_i)(\mathsf{n}_{q_i} + 1) + \delta(\varepsilon(\mathsf{k}') - \varepsilon(\mathsf{k}) - \hbar\omega_i)\mathsf{n}_{q_i}] \end{aligned} \tag{5}$$

where $\hbar\omega_i$ is a phonon energy and n_{q_i} the phonon equilibrium distribution which, according to the Bose-Einstein statistics, is given by

$$\mathsf{n}_{q_i} = \frac{1}{\exp(\hbar\omega_i/k_B T_L) - 1}.$$

where T_L is the lattice temperature. The function K_0 represents intravalley elastic scattering transition probability and it reads

$$K_0(\mathsf{k},\mathsf{k}') = \frac{k_B T_L \Xi_d^2}{4\,\pi^2 \hbar\,\rho\, v_\rho^2}, \tag{6}$$

where Ξ_d is the acoustic-phonon deformation potential, ρ the silicon mass density, v_s the sound velocity of the longitudinal acoustic mode . The inelastic scattering probability is

$$K_i(\mathsf{k},\mathsf{k}') = \frac{Z_f (D_t K_i)^2}{8\,\pi^2 \rho\,\omega_i}, \tag{7}$$

where $D_t K_i$ is the deformation potential for the i-th optical phonon, and Z_f is the number of final equivalent valleys for the considered inter-valley scattering. The electron-electron interaction is taken into account in the framework of the mean field approximation through the Poisson's equation. This is reasonable if one considers the case of low electron density, for which the short range collisions between electrons can be neglected.

3 The free flight generation.

Because the scattering process is considered *markovian*, the probability that a particle does not suffer a collision in the time interval $[0,t]$ is :

$$P(t) = exp\left[-\int_0^t w[\mathsf{k}(t')]dt'\right] \tag{8}$$

where

$$w(\mathsf{k}) = \int w(\mathsf{k},\mathsf{k}')d\mathsf{k}'$$

is the total transition probability, i.e. $w(\mathsf{k})dt'$ is the total probability that a particle with wave vector k suffers a collision in $[t', t'+dt']$.

The time t appearing in the previous formula is the free flight duration. In order to generate a stochastic free flight, one takes an uniform distribution of random numbers r and tries to solve the problem:

$$P(t) = r$$

or by taking the logarithm,

$$-\log r = \int_0^t w[\mathsf{k}(t')]dt' \quad . \tag{9}$$

This formula is used to calculate the time of flight duration t from a selected uniform random number r. The integral on the right hand side is trivial if $w[\mathsf{k}(t')]$ is constant, but in general this integral cannot be performed analytically. Since the solution of eq.(9) is of paramount importance to obtain an efficient implementation of the algorithm, some algorithms have been introduced :

1. **Self Scattering Technique (SST).**
Let be K the set of the k vectors that a particle can have during the simulation. Then we define a number Γ such as is greater then the largest scattering rate possible in the simulation, i.e.

$$\Gamma \geq max_{\mathsf{k}\in K} w(\mathsf{k}) = \frac{1}{\tau_0} \quad . \tag{10}$$

Let us introduce a fictitious scattering probability w_{ss} , called *self scattering*, such that the total scattering probability (including this process) is Γ :

$$w(\mathsf{k}) + w_{ss}(\mathsf{k}) = \Gamma \quad .$$

Whenever the self scattering is selected as the collision mechanism, nothing happens to the particle which maintains, after the scattering, the same energy and momentum it had before. If we take $w(\mathsf{k}) = \Gamma$ then eq.(9) trivially yields:

$$-\log r = \Gamma t \Rightarrow \quad t = -\frac{\log r}{\Gamma} \quad . \tag{11}$$

The self scattering is obviously a mathematical trick, with no physical meaning, which does not alter the statistical distribution of the real scattering events. The main advantage of this technique is that the programming is very simple; one disadvantage is that a lot of computer time is spent performing computations related to this scattering. Since the total scattering rate is maintained artificially high, the free flight will be much shorter than in reality: with this technique from the 70 % to 95 % of the computations might be spent just in dealing with self scattering. In order to reduce the number of self scattering , some improvements to this algorithm has proposed in [6].

If a large number of particles is simulated simultaneously (e.g. Ensemble Monte Carlo simulation), for each simulated particle a different free flight time t appears: synchronization problems arise for the evaluation of statistical indicators.

2. **Constant Time Technique (CTT) .**
The total simulation time is subdivided into tiny time intervals Δt. The probability that a particle will survive without scattering during a ballistic flight of duration Δt is given by eq. (8), i.e. (remember that $w(\mathsf{k}) = 1/\tau(\mathsf{k})$)

$$\exp\left\{-\int_t^{t+\Delta t} \frac{dt'}{\tau[\mathsf{k}(t')]}\right\} \simeq \exp\left\{-\frac{\Delta t}{\tau(\mathsf{k})}\right\} \tag{12}$$

having assumed that the time step Δt is small enough so that $\mathsf{k}(t')$ can be taken as constant during the free flight. If now $\Delta t/\tau(\mathsf{k}) \ll 1$, the probability that the particle will scatter at the end of the free-flight of duration Δt can be approximated as:

$$1 - \exp\left\{-\frac{\Delta t}{\tau(\mathsf{k})}\right\} \simeq \frac{\Delta t}{\tau(\mathsf{k})} \quad . \tag{13}$$

Therefore, for each particle the total scattering rate is evaluated at the final wavevector $\mathsf{k}(t+\Delta t)$ and we make the comparison

$$\frac{\Delta t}{\tau(\mathsf{k})} \geq < r_1 \tag{14}$$

where r_1 is a random number $\in$ [0,1]; if in eq.(14) the operator $\geq$ holds the particle suffers a scattering, otherwise no scattering occurs.

Regarding the choice of the time step Δt, it is appropriately chosen to be much smaller than the minimum total scattering time for any particle in the device. This can be estimated at the beginning of the simulation from the bias condition, lattice temperature, device dimensions and other input parameters. For submicron devices at room temperature, with few Volt bias, this time step is $\simeq 10^{-15} sec.$ which is a **severe limitation** to the total device simulation time.

In the case of an ensemble Monte Carlo device simulation, the constant time technique is the method of choice. Since the flights progress synchronously in small increments, programming becomes much easier and a number of costly checking procedures, necessary for bookkeeping when dynamics calculations are done for the whole flight, may be avoided. The technique is also very effective for vectorization, since the particles are naturally kept synchronous. The DSMC introduce an error which consists of two components the systematic error (wrong expectation) and the statistical error (fluctuating estimate of expectation). The systematic error of CTT depends on the time step, while the SST does not has any systematic error. The statistical error depends on the particle number used in the simulation. In the following we shall study these errors.

4 Simulation results.

In this paper we simulate a homogeneous (bulk) silicon semiconductor , at room temperature, in which an electric field have been frozen in the spatial direction x. The simulation was time-dependent (not space-depending) . The motion equations are solved in the time interval [0 , T_{tot}] , where T_{tot} = 50 ps, by using both CTT and SST methods.

The most relevant physical quantities in the simulations are the average drift velocity , the average energy, and the average energy-flux. At each time step

$$t_n = n\Delta t, \quad n = 1, 2, ..., int\left[\frac{T_{tot}}{\Delta t}\right]$$

these quantities are defined by the following functionals:

$$V_x(t_n) \;=\; \frac{1}{N}\sum_{part} \mathsf{v}_x(t_n) \tag{15}$$

$$W(t_n) = \frac{1}{N}\sum_{part}\varepsilon(t_n) \tag{16}$$

$$S_x(t_n) = \frac{1}{N}\sum_{part}\varepsilon(t_n)\mathsf{v}_x(t_n) \tag{17}$$

$$N = 100,000 \tag{18}$$

where N is the total particle number and the summation is extended to all the particles in the semiconductor.

As already mentioned, in our simulations the 75 % of the CPU time is spent in checking the self scattering events, and the scattering rate number is $\simeq 2\ 10^7$ for 10,000 particles.

In figures 1,2,3 we plot $V_x(t_n)$, $W(t_n)$ and $S_x(t_n)$, for an electric field of 80,000 V/cm in the time interval 0 - 5 ps, obtained by using the CTT with time step $\Delta t = 6\times10^{-15}$ sec .

For $t_n \leq 1$ ps we have the transient regime, which is characterized by a local maximum : the mean velocity overcomes (*overshoot phenomena*) the asymptotic value, that is the value attained in the stationary regime (fig. 1). This phenomena disappears for small electric field strengths. We observe that, in the stationary regime, the average velocity, energy and energy-flux are noisy.

For a fixed time step Δt, the stationary value of each functional is obtained by averaging the quantities (15), (16), (17) in the time interval 5ps - 50ps , i.e.

$$V(\Delta t) = \frac{1}{N_T}\sum_{n=1}^{N_T} V_x(t_n) \tag{19}$$

$$W(\Delta t) = \frac{1}{N_T}\sum_{n=1}^{N_T} W(t_n) \tag{20}$$

$$S(\Delta t) = \frac{1}{N_T}\sum_{n=1}^{N_T} S_x(t_n) \tag{21}$$

where N_T is the number of time steps Δt within the time interval 5ps - 50ps.

In figures 4,5,6 we plot the averaged values (19), (20), (21) as function of the time step Δt : convergence with respect to Δt is observed . In the same figures we plot, by a solid line, the value obtained by using the self-scattering technique. We observe that the values obtained by the constant time technique converge to those obtained by using the self scattering technique for $\Delta t \leq 0.1 \times 10^{-15}$ sec.

In order to understand the truncation error introduced in the CTT, we introduce the *Fractional Truncation Error* (FTE hereafter) for some functional F, as

$$E(\Delta t) = \frac{|F(\Delta t) - F_0|}{|F_0|} \tag{22}$$

where F_0 is the value obtained by using the self-scattering technique, because it does not involve any time step error. In our case we denote respectively by $E^V(\Delta t)$,$E^W(\Delta t)$ and $E^S(\Delta t)$ the fractional truncation error for mean velocity, energy and energy flux .

In figures 7,8,9 we plot the fractional truncation error E^V , E^W and E^S obtained by simulations, for an electric field 80,000 V/cm, as a function of the time step Δt. From figures 7-9 is evident that the FTE for mean velocity, energy and energy flux is an increasing function of the time step Δt. The maximum FTE for energy E^W is $\simeq$ 10 % whereas for the other functionals is $\simeq$ 6 %.

In the same figures a linear fit is shown, proving that this error is first order with respect to the time step. In figure 10 we plot, for the two algorithms, the CPU time consumed by using the same particles number. From this figure is evident that the SST is more efficient respect to the CTT, if a less relative error is needed.

But in principle the statistical error (related to the fluctuation of the estimator) must be taken into account. In order to understand this effect on the efficiency of the used method, we consider two cases. First, we take equal number of particles and we choose the CTT time step such that it has the same CPU of the SST ($\Delta t \simeq 6\times10^{-15}$ from figure 10). Then we plot the results obtained with the two algorithms in figure 11 : we see that the fluctuations are quite similar (because the same particles number is used) but there is a systematic error of $\simeq$ 4 % (evaluated with the average values). Second, we take the time step for the CTT so that the systematic error E^V is 0.5 percent (Δt= 0.6 $\times10^{-15}$ from figure 7) then we reduce the particles number (from 100,000 to 13,000) in order to have the same CPU time of the SST (i.e. $\simeq$ 4000 sec. from figure 10). We plot the velocity obtained with the two algorithms in figure 12: now the CTT has a small systematic error, but larger fluctuations ($\simeq$ 9 %) respect to the SST ($\simeq$ 3 %) . The conclusion is that the efficiency of the CTT would be similar to that of SST, if larger fluctuations of the estimator occurs. Finally we underline that similar results are obtained for other values of the electric field, and for the energy and energy flux estimators.

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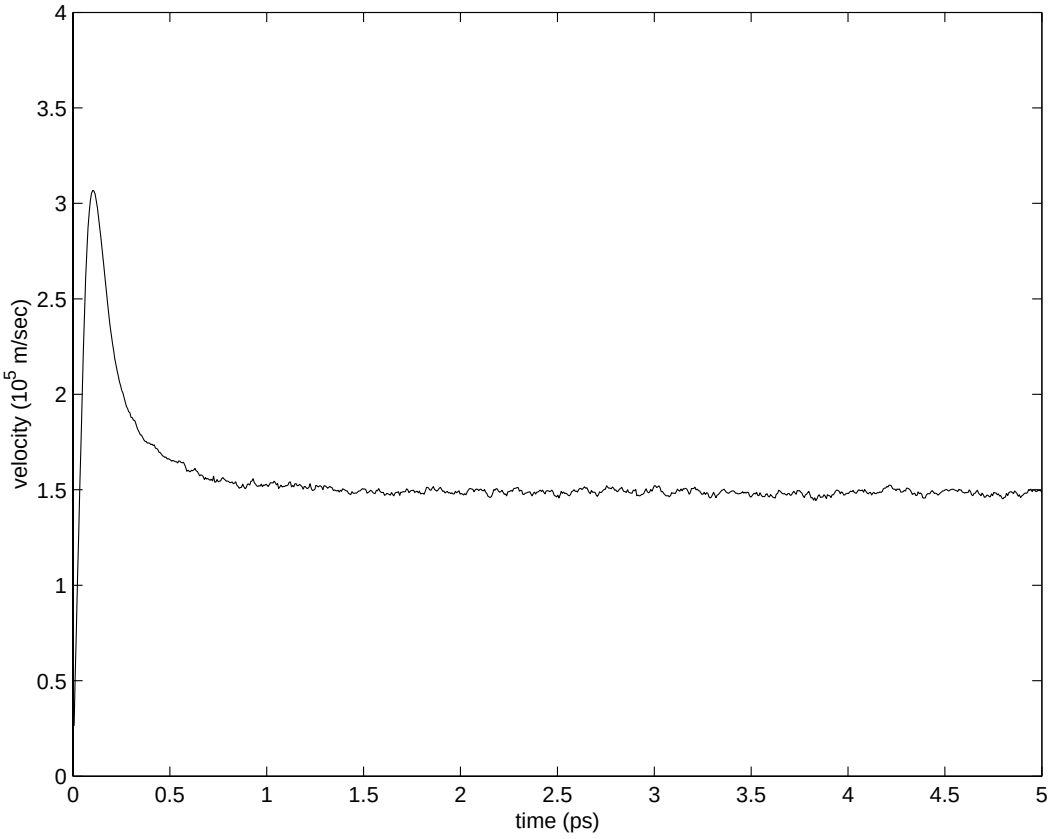

Figure 1: The velocity $V_x(t_n)$ as function of the time $t_n \in [0,5]$ for an electric field of 80,000 V/cm obtained by using the CTT with $\Delta t = 6\times10^{-15}$ sec., and 10^5 particles.

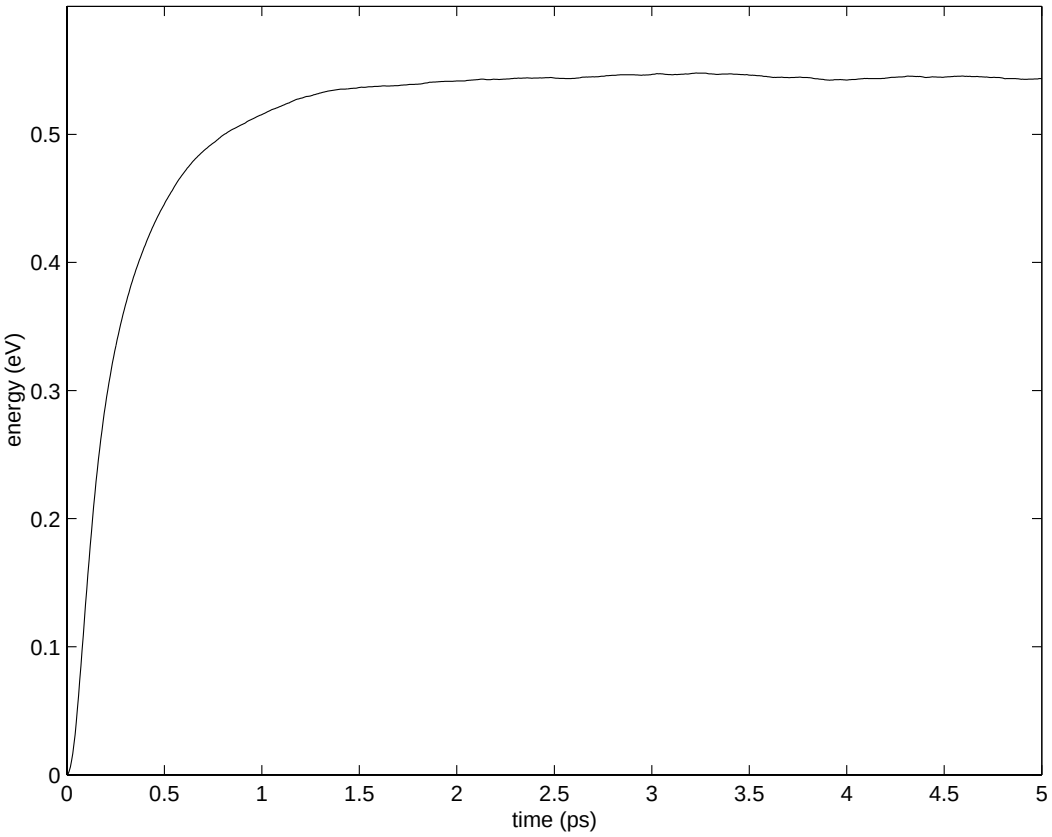

Figure 2: The energy $W(t_n)$ as function of the time $t_n \in [0,5]$ for an electric field of 80,000 V/cm obtained by using the CTT with $\Delta t = 6 \times 10^{-15}$ sec. , and 10^5 particles.

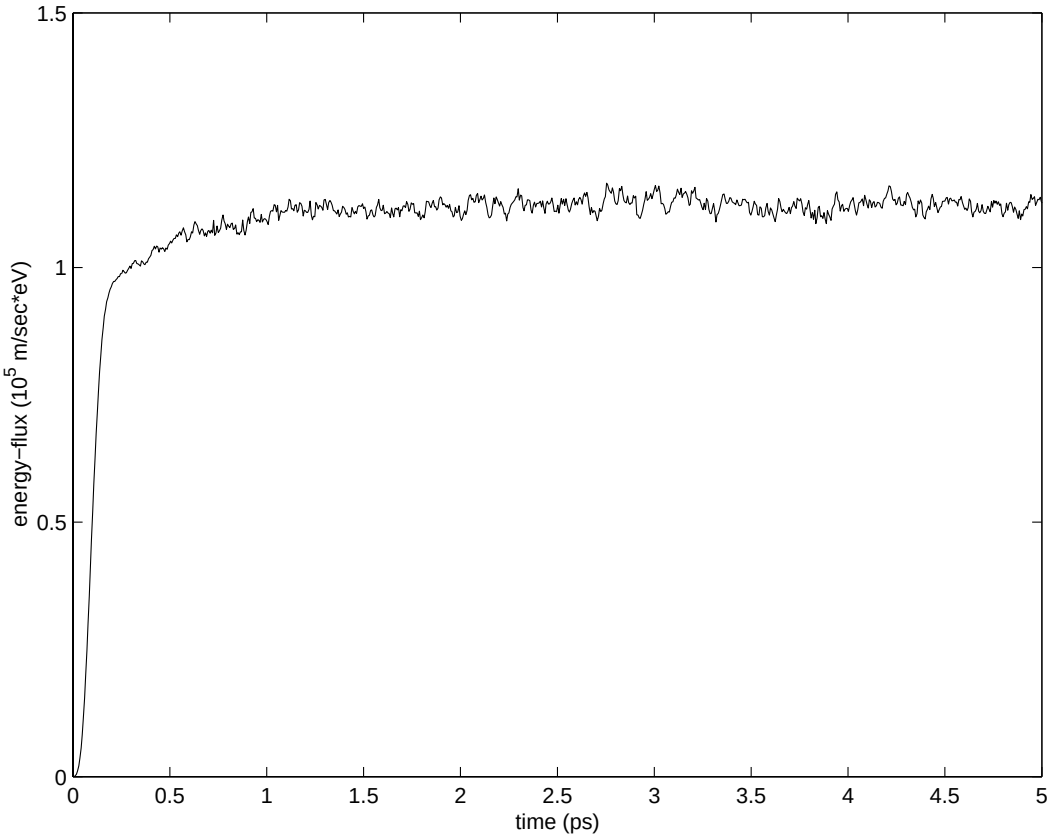

Figure 3: The energy flux $S_x(t_n)$ as function of the time $t_n \in [0,5]$ for an electric field of 80,000 V/cm obtained by using the CTT with $\Delta t = 6 \times 10^{-15}$ sec. , and 10^5 particles.

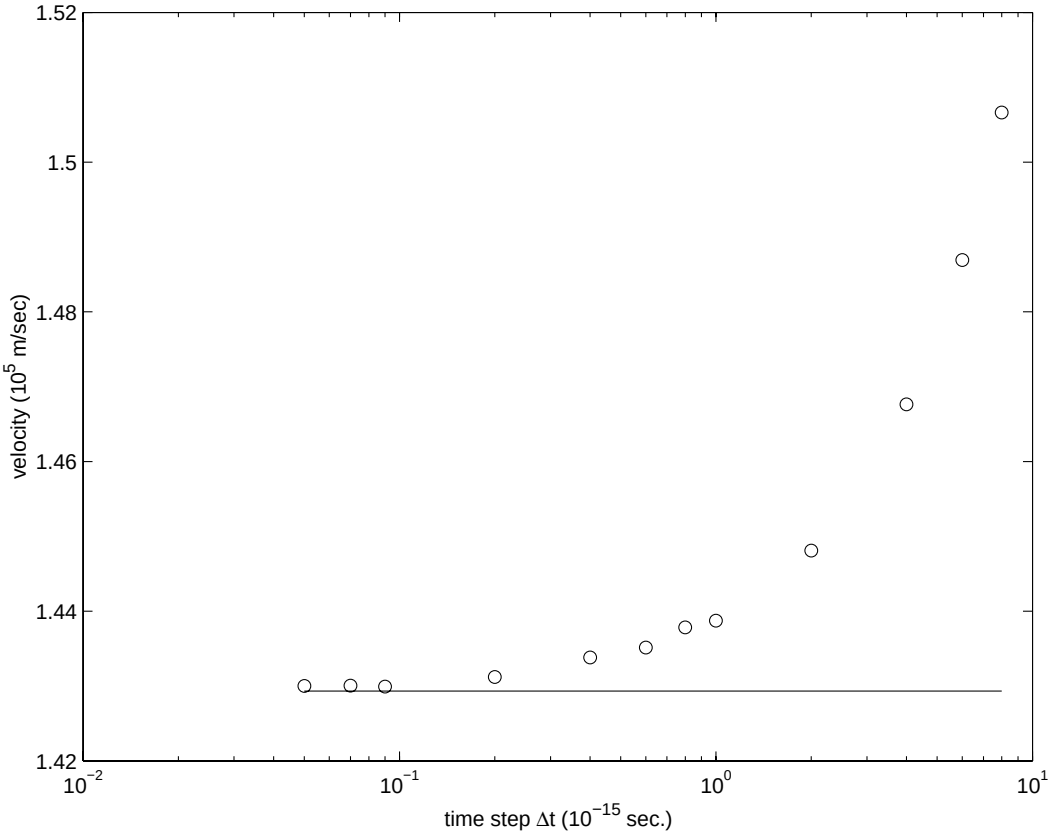

Figure 4: The mean velocity V eq.(19)obtained with CTT as function of the time step Δt obtained for an electric field of 80,000 V/cm . The solid line is the value obtained by using the SST. In both cases 10^5 particles are simulated.

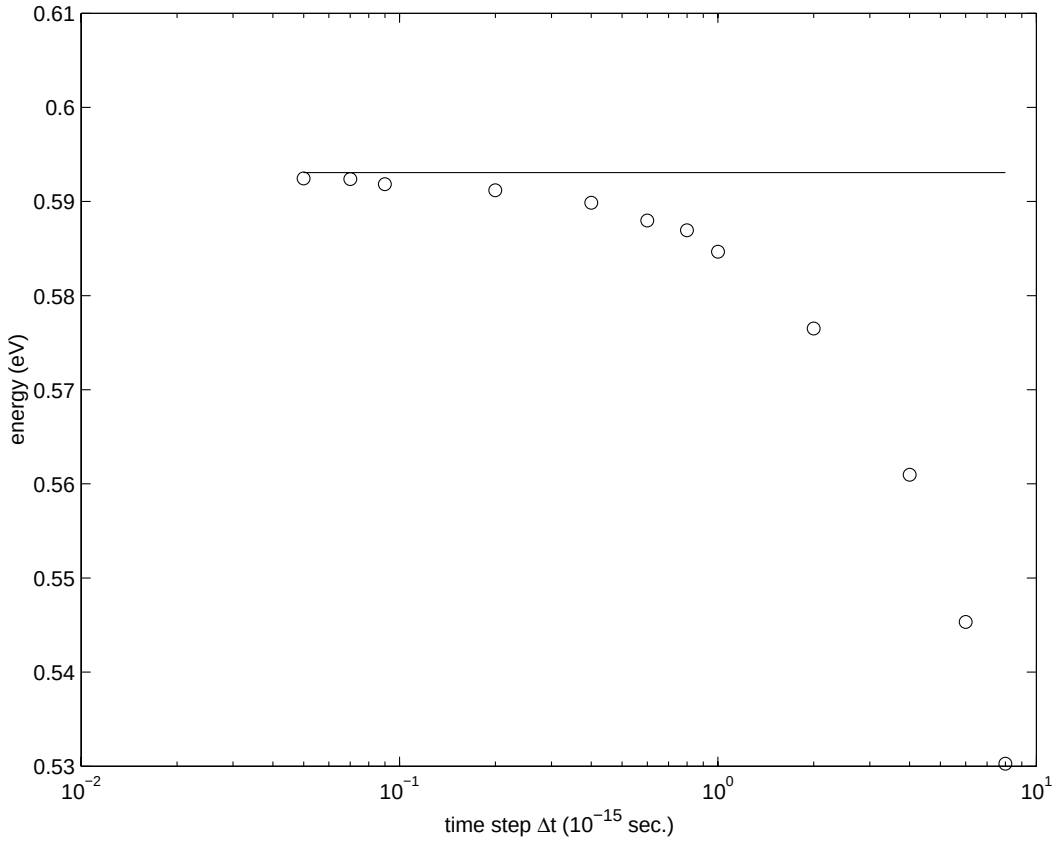

Figure 5: The mean energy W eq.(20) obtained with CTT as function of the time step Δt for an electric field of 80,000 V/cm . The solid line is the value obtained by using the SST . In both cases 10^5 particles are simulated.

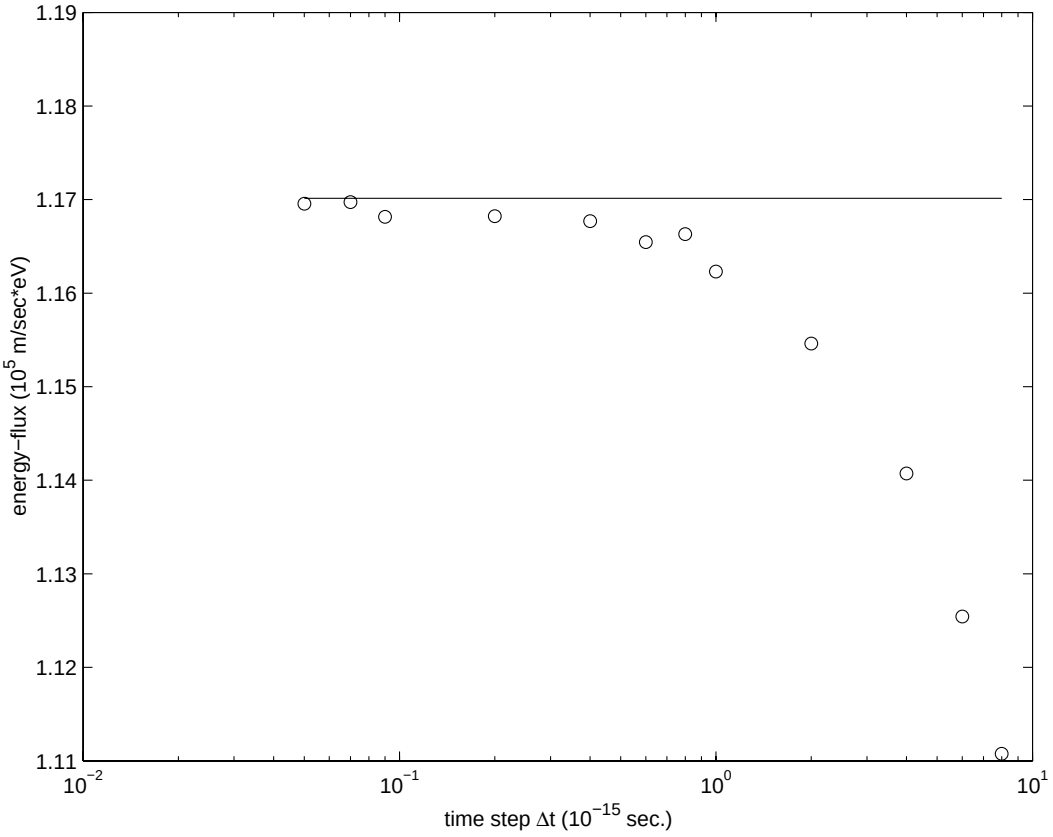

Figure 6: The mean energy flux S eq.(21)obtained with CTT as function of the time step Δt for an electric field of 80,000 V/cm . The solid line is the value obtained by using the SST .In both cases 10^5 particles are simulated.

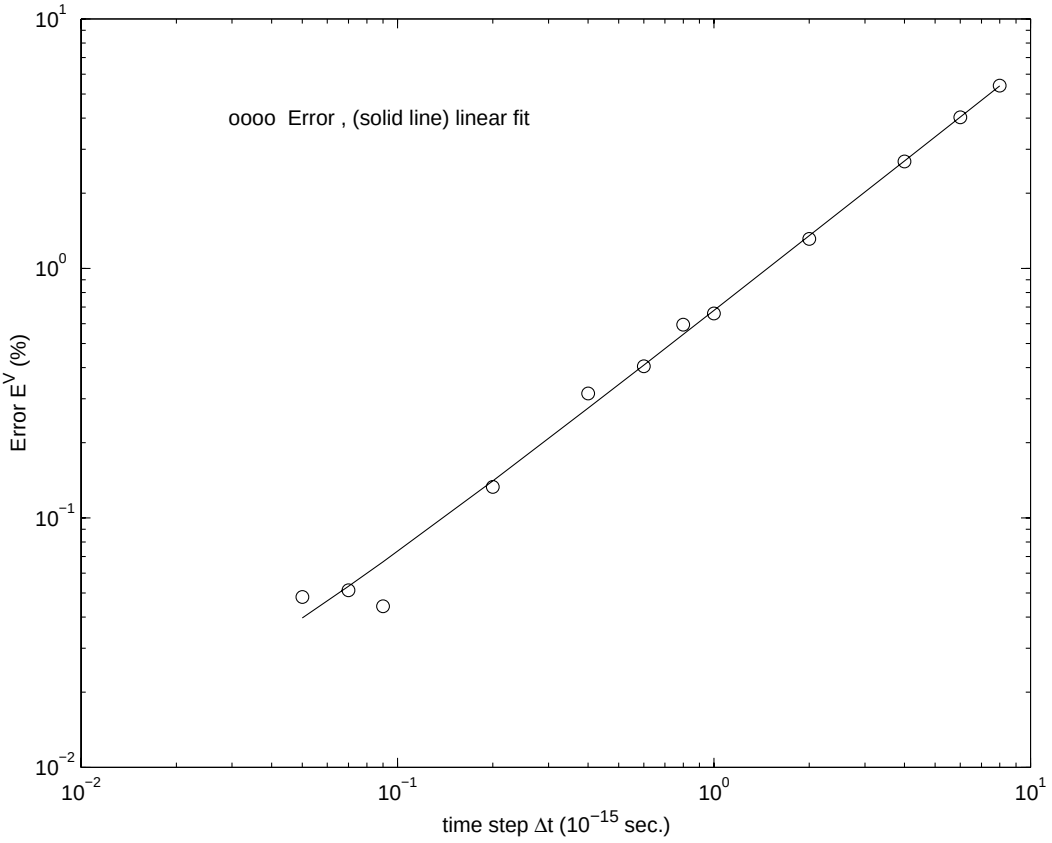

Figure 7: The fractional truncation error for the mean velocity E^V as function of the time step Δt obtained with an electric field of 80,000 V/cm, and 10^5 particles. The circles are the simulation results , the solid line is a linear fit.

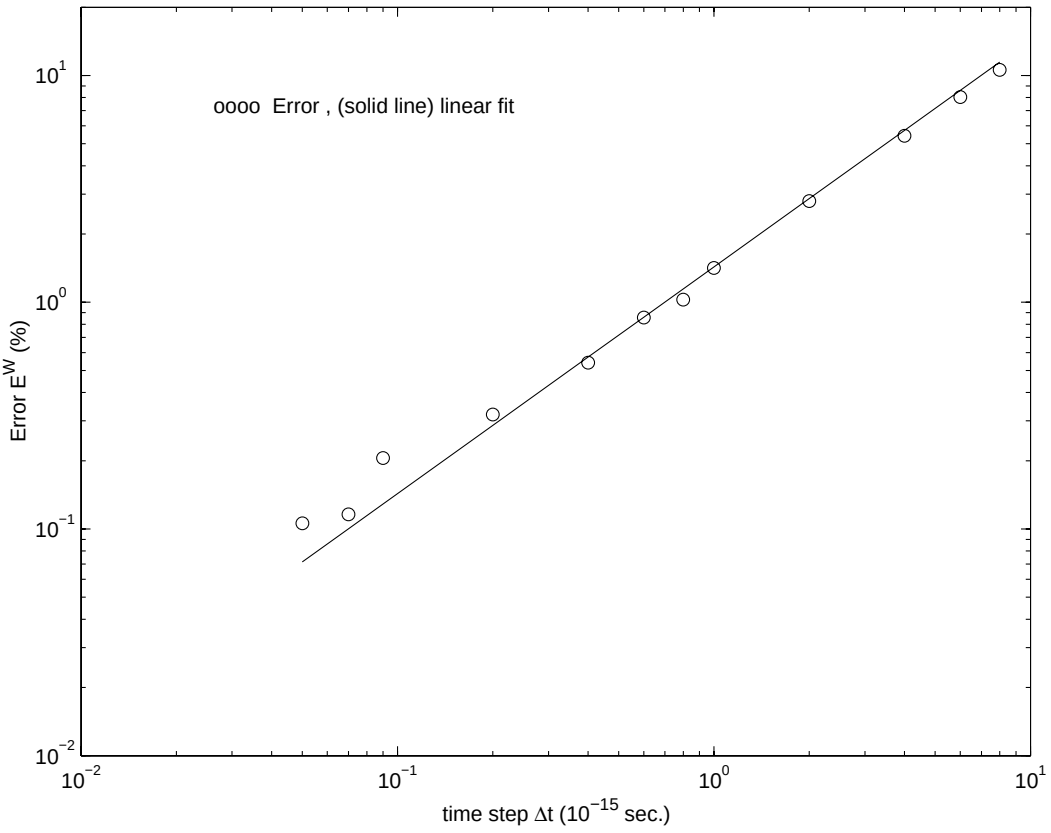

Figure 8: The fractional truncation error for the mean energy E^W as function of the time step Δt obtained with an electric field of 80,000 V/cm , and 10^5 particles. The circles are the simulation results , the solid line is a linear fit.

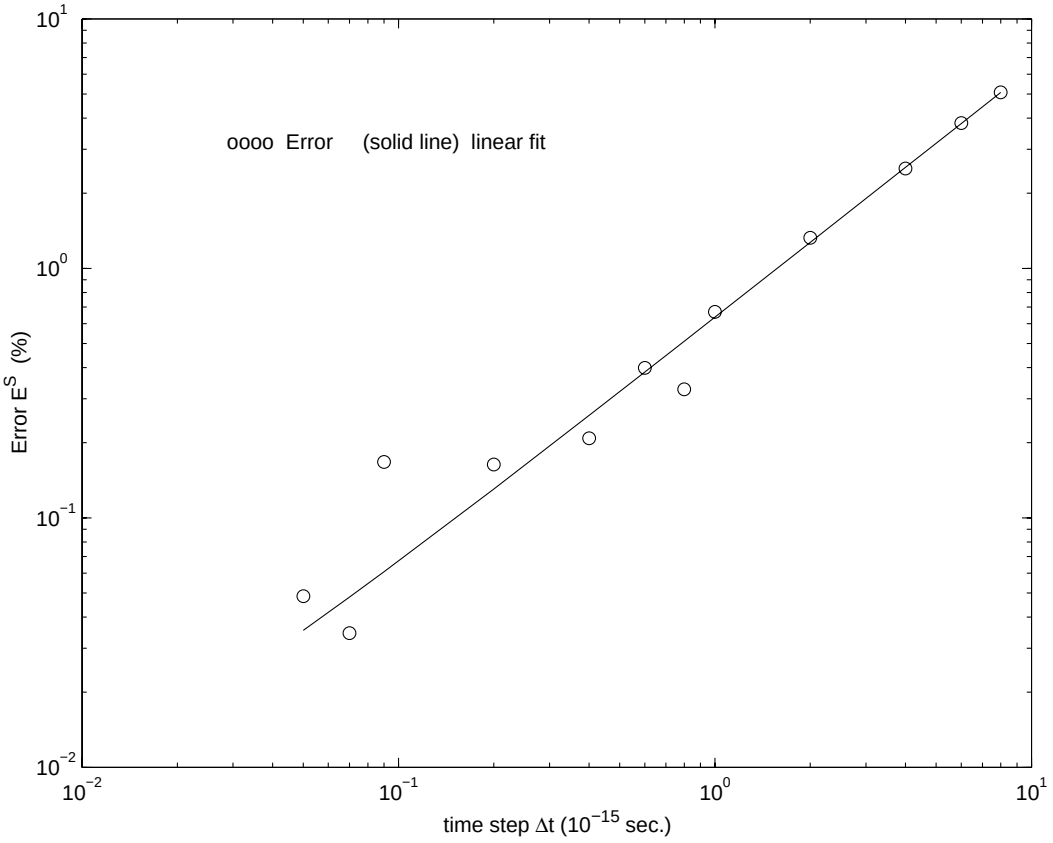

Figure 9: The fractional truncation error for the mean energy flux E^S as function of the time step Δt obtained with an electric field of 80,000 V/cm, and 10^5 particles. The circles are the simulation results , the solid line is a linear fit.

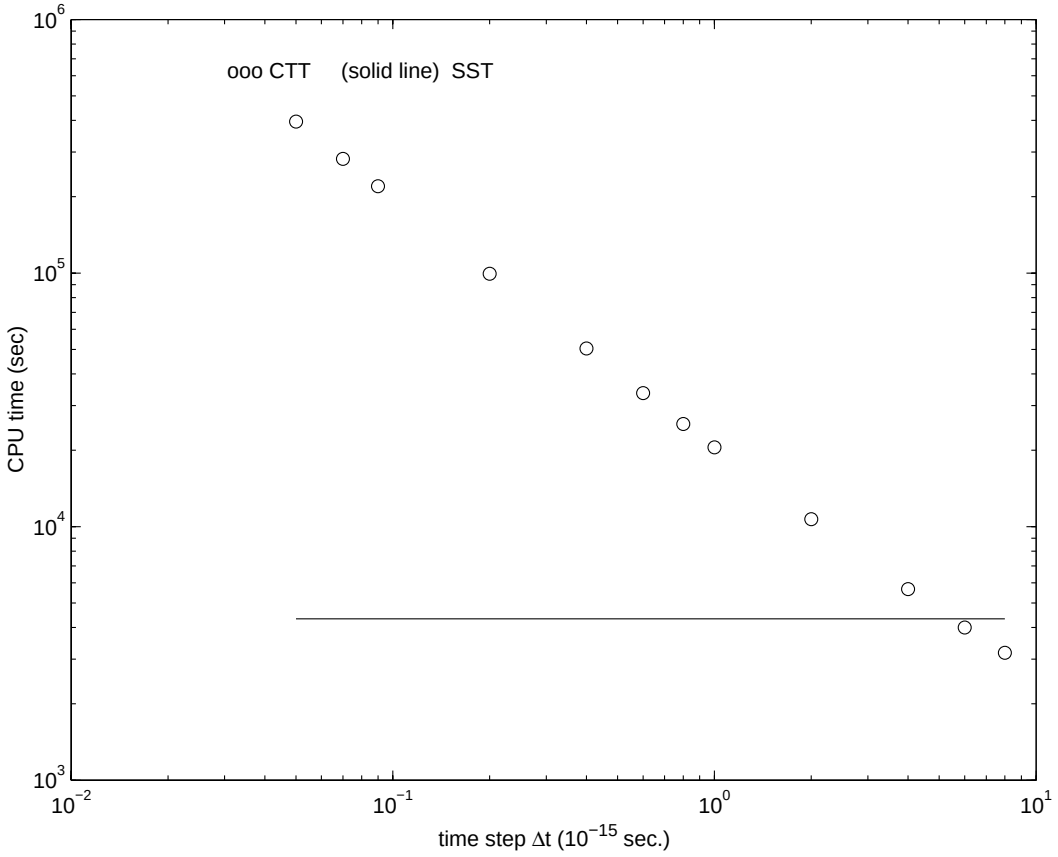

Figure 10: The CPU time consumed by the CTT (with ooo) as function of the time step Δt for an electric field of 80,000 V/cm. The solid line is the CPU time consumed by using the SST. In both cases 10^5 particles are used.

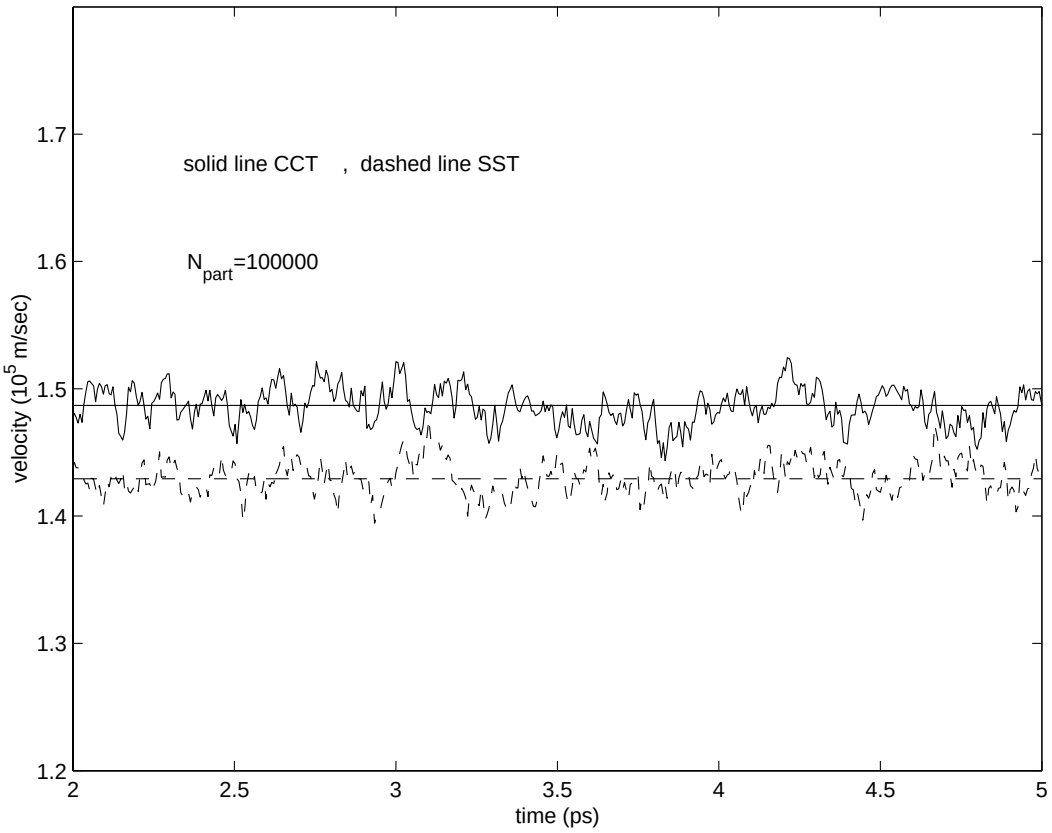

Figure 11: The velocity V as function of time obtained with the CTT (solid upper curve) and with SST (dashed lower curve) for an electric field of 80,000 V/cm, and 10^5 particles. We choose the time step Δt=6×10^{-15}sec., such that the two methods consume the same CPU . The solid straight line is the CTT mean velocity whereas the dashed straight line is the SST mean velocity.

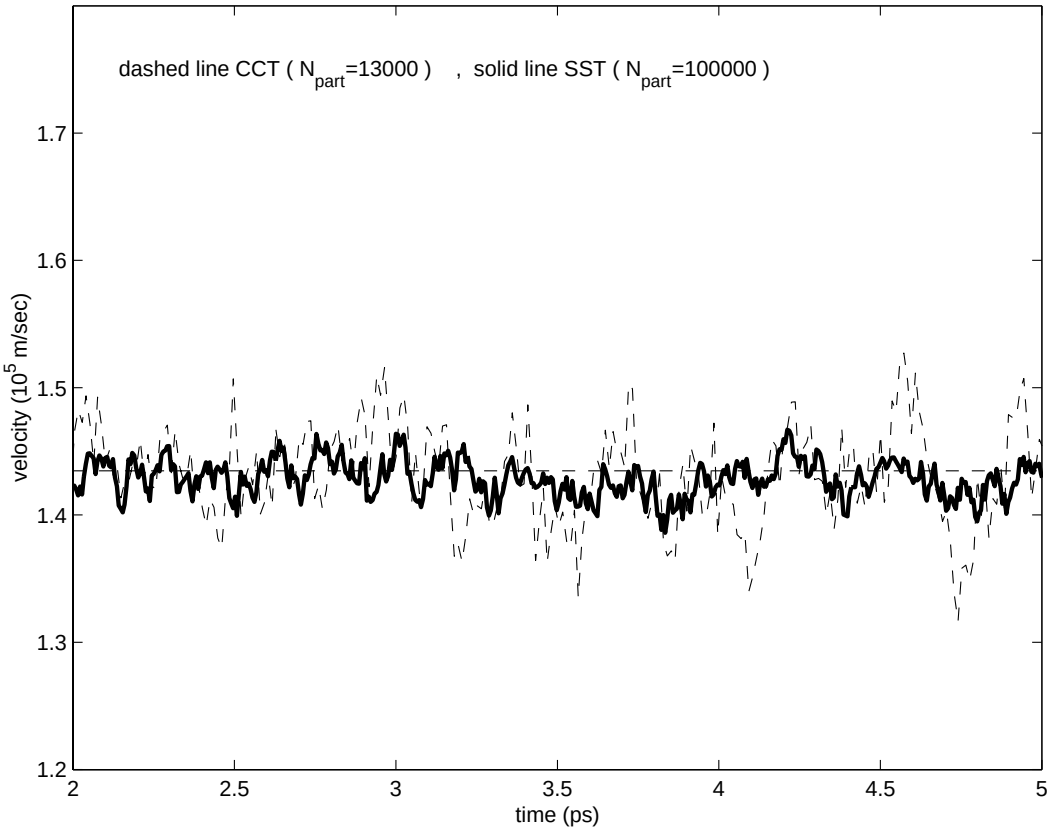

Figure 12: The velocity V as function of time obtained with the CTT (dashed line) and with SST (solid line) for an electric field of 80,000 V/cm. The time step of the CTT is chosen such that the systematic error E^V is $\simeq 0.5$ % ($\Delta t = 0.6 \times 10^{-15}$), and the particles number such that the CTT has the same CPU time of the SST ($\simeq 4000$ sec.).