Stability Issues in Self-Consistent Monte Carlo-Poisson Simulations

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Abstract

This paper investigates the time stability of self-consistent Monte Carlo-Non Linear Poisson simulations (MC-NLP). A simplified analytical stability theory has been developed and verified by means of extensive simulations. The properties of the MC-NLP scheme are compared to those of Monte Carlo-Linear Poisson (MC-LP) scheme. The influence of statistics collection and charge assignment algorithms is also analyzed.

1. Introduction

Self-consistent Monte Carlo-Poisson simulation is typically based on the linear form of Poisson equation (LP). As recently demonstrated [1], this approach can lead to instability, hence to unphysical results, unless the time step between successive Poisson solutions (Δt) is appropriately chosen. Stability forces to choose very small Δt, resulting in long CPU times.

In principle, the non linear formulation of the Poisson equation (NLP), in which charge concentration is expressed as an exponential function of potential and pseudopotentials, helps to alleviate these problems due to the damped sensitivity of potential to charge fluctuations, typical of Monte Carlo simulation [2]. In the following, the time stability of coupled Monte Carlo-Non Linear Poisson simulation will be studied in detail by means of an analytical theory and extensive simulations.

2. Analytical theory of MC-NLP time stability

Following the guide example of [1], we first derived a linearized analytical theory of MC-NLP stability for a uniformly doped semiconductor at zero applied field. All relevant quantities (concentration n, field E, velocity u) are the sum of a steady state value and a perturbation ($A = A_{DC} + \tilde{A}(x,t)$). The perturbation is expressed as $\tilde{A}(x,t) = \tilde{A}e^{ikx}e^{-i\omega t}$ where $k = \frac{2\pi}{\lambda}$, λ being the perturbation wavelength. In addition we have $n_{DC} = N_D$, $E_{DC} = 0$, $u_{DC} = 0$. The system is described by the first two moments of the Boltzmann equation and by the non linear form of the Poisson equation. Neglecting space discretization and assuming a

constant effective mass m^*, these equations can be easily linearized and discretized in the time domain. In particular, the discretized non linear Poisson equation reads:

$$ikE_n = -\frac{q}{\epsilon_s}\left[n - \frac{n_{DC}}{ikV_T}(E_n - E_{n-1})\right], \quad (1)$$

where q is the electron charge, ϵ_s the semiconductor dielectric constant, V_T the thermal voltage, and $E_n = E(t_n)$ is the perturbation field. The system of equations can be solved exactly between t_n and $t_n + \Delta t$ under a constant perturbation field E_n, thus obtaining a third order characteristic equation in the quantity $z = e^{-i\omega\Delta t}$

$$z^3 + z^2\left[\left(\frac{\alpha - (1-\delta)}{\eta^2} - \beta\right)\gamma - (1+\delta)\right] + z\left[\delta - \frac{\alpha\delta - (1-\delta)}{\eta^2}\gamma + \beta\gamma(1+\delta)\right] - \beta\gamma\delta = 0, \quad (2)$$

where $\nu_c = q/\mu_0 m^*$ is the scattering rate (related to low field mobility μ_0), $\omega_p = \sqrt{q^2 n_{DC}/\epsilon_s m^*}$ is the plasma frequency, $\eta = \nu_c/\omega_p$, $\alpha = \nu_c\Delta t$, $\delta = e^{-\alpha}$, L_D is the Debye length, $\beta = (\lambda/L_D)^2$, $\gamma = 1/(1+\beta)$. The main differences between Eq.(2) and the corresponding one for MC-LP [1] are: 1) the equation is cubical in z (instead of being quadratic) since the NLP equation (1) depends on the field at the previous iteration; 2) the perturbation wavelength λ (i.e. β) never cancels out. Fig.1 compares the stability domain ($|z| < 1$) of MC-NLP to that of MC-LP for a few values of β. Since β can be assumed to have an uniform spectrum, the instability domain of MC-NLP appears to be larger than that of MC-LP.

3. Simulations

The above analysis is based on a linear approximation neglecting space discretization and the non linear dependence of scattering rates on energy. To verify its accuracy, we employed a simplified 1D MC code featuring one parabolic band, optical and acoustic phonon scattering and periodic boundary conditions. Transport parameters were tuned to reproduce drift velocity [3] and mean kinetic energy [4] in the low field regime. For self-consistent simulations we employed a uniform grid with spacing equal to the Debye length. First, particles are placed uniformly in space with Maxwellian energy distribution; then, their motion is simulated according to the total scattering rate, until the Monte Carlo iteration ends. Finally, the charge is assigned to each grid node, and the Poisson equation is solved.

Fig.2 reports simulation results of a uniformly doped bar for different values of ν_c/ω_p and $\omega_p\Delta t$. It shows that while the analytical theory is reasonably accurate in predicting the stability of the simulation conditions (filled symbols), unpredicted stable solutions (open symbol) can be obtained in the proximity of the limit $\beta \to 0$, representing the boundary of the region stable for any β. Fig.3 shows the time evolution of mean kinetic energy (W) for parameters corresponding to MC-NLP instability. Notice that identifying stable simulations is not always as simple as Fig.3 may suggest. As an example, Fig.4 shows W for a few simulations featuring large $\omega_p\Delta t$. The one performed with MC-NLP is apparently stable, while the MC-LP ones are clearly unstable. However, the electrostatic field energy increases continuously for both schemes (Fig.5). Thus, both simulations are actually unstable [1].

The stability domains of Fig.1 imply severe restrictions on the choice of Δt for both MC-LP and MC-NLP, with significant increase of the CPU time spent for solving Poisson equation. To explore ways of relaxing these tight constraints, we investigated different methods for collecting statistics: Before Scattering (BS) and Ensemble Monte Carlo (EMC) [5] to collect data; Nearest Grid Point (NGP) and Cloud in Cell (CIC) [6] to assign charge to the grid. EMC advances particles synchronously and collects statistics at the end of each iteration, while BS moves particles asynchronously and collects statistic just before each scattering. NGP assigns the whole charge of a particle to the nearest mesh point, while CIC spreads the charge over the cell and assigns it to its vertices according to their distance from the particle. Fig.6 shows results obtained using MC-LP, short time step and two extreme configurations: BS+NGP and EMC+CIC. As can be seen, EMC+CIC provides stable solutions for $\omega_p\Delta t$

twice as large as that of BS+NGP. Eq.(2) cannot predict this result because it neglects space discretization.

To further investigate the properties of MC-NLP, we simulated a 1-D $n^+ - n - n^+$ diode ($N_D = 10^{18} - 10^{17} - 10^{18}$) with different methods. We compared the average device current obtained with the configuration featuring the largest stability domain (EMC+CIC+LP+ short Δt) to that one computed using (BS+NGP+NLP+long Δt), as in [2]. Fig.7 and Fig.8 show the corresponding results as a function of the simulation time for the same total CPU time. Although parameters are such that the MC-NLP simulation should be unstable, the NLP algorithm damps oscillations within limits only slightly larger than those of LP, while it still provides the same average current ($\simeq 1.8mA/\mu m^2$). On the other hand, MC-NLP does not reproduce the details of the initial velocity overshoot due to the long Δt, but collects enough statistics for comparable standard deviation in less CPU time and memory occupation than MC-LP, thus providing a significant performance advantage.

4. Conclusion

We have analyzed the performance trade-offs of different self-consistent Monte Carlo-Poisson solution schemes, showing that: a) EMC+CIC+LP provides the largest stability domain and reproduces time dependent physical effects at the expenses of very large CPU and memory requirements; b) BS+NGP+NLP has a smaller convergence domain, but the uncertainty on terminal currents and other physical quantities is often acceptable even in unstable conditions. Hence, with respect to LP solution schemes much larger time steps or less particles can be chosen, with a significant reduction of CPU and memory requirements.

References

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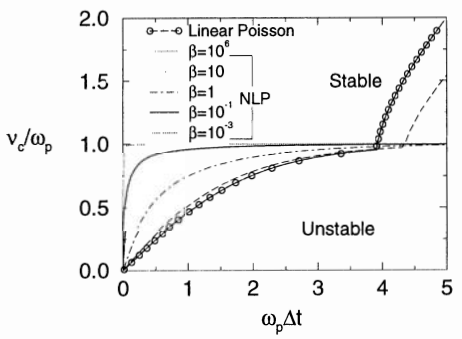

Fig.1 Stability regions as a function of collisionality ν_c/ω_p and normalized time step $\omega_p \Delta t$ for linear Poisson [1] and non linear Poisson (NLP) with different normalized perturbation wavelength $\beta = (\lambda/L_D)^2$.

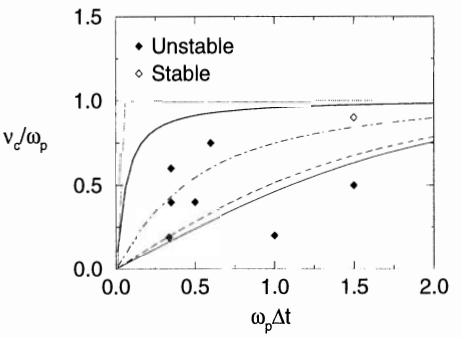

Fig.2 Numerical stability of MC-NLP as a function of collisionality ν_c/ω_p and normalized time step $\omega_p \Delta t$. Lines represent the analytic thresholds from Fig.1. Markers represent simulation results: open for stable, filled for unstable.

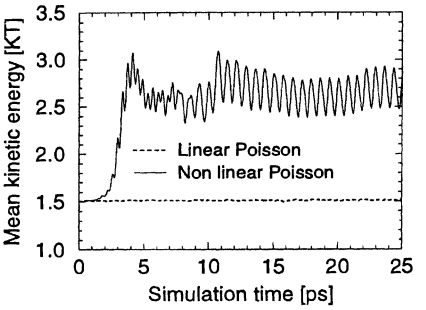

Fig.3 Mean kinetic energy in KT units as a function of the simulation time with $\nu_c/\omega_p = 0.2$ and $\omega_p \Delta t = 0.35$. As expected from Fig.1, the MC-NLP solution is unstable.

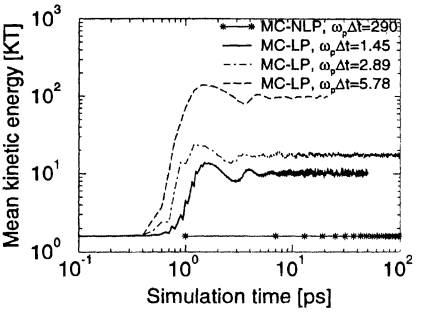

Fig.4 Mean kinetic energy in KT units as a function of the simulation time for a few simulations of a uniformly doped bar featuring large $\omega_p \Delta t$.

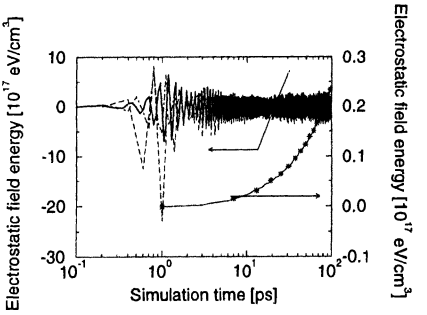

Fig.5 Electrostatic field energy as a function of the simulation time for the same simulations and using the same symbols of Fig.4.

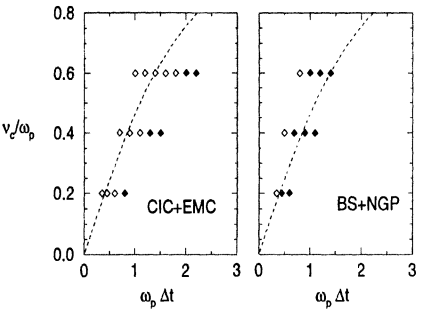

Fig.6 Numerical stability of MC-LP as a function of collisionality ν_c/ω_p and normalized time step $\omega_p \Delta t$ for two differents methods of computing statistics. Dashed line is the analytic stability threshold. Markers represent results of simulations: open for stable, filled for unstable.

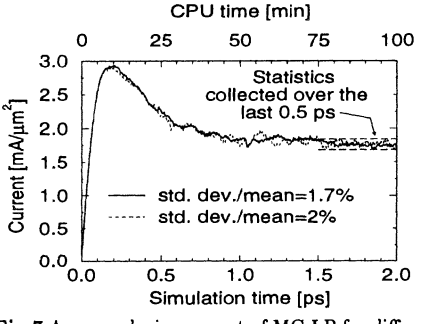

Fig.7 Average device current of MC-LP for different number of simulated particles . Solid line: 2×10^5 part.; dashed: 1×10^5 part. The ratio (standard deviation/mean value) is computed over the data of the last $0.5ps$ of simulation. $\Delta t = 0.002ps$. The CPU scale refers to the 2×10^5 particles case.

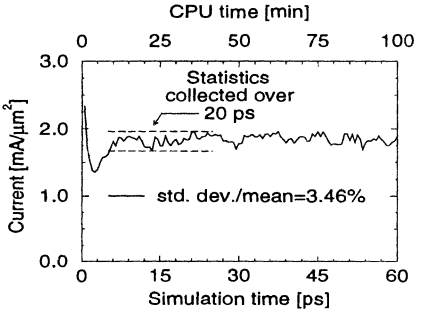

Fig.8 Average device current of MC-NLP. The ratio (standard deviation/mean value) is computed over the data of $20ps$. $\Delta t = 0.5ps$. The number of simulated particles is 5×10^4.