A Fast and Stable Poisson-Schrödinger Solver for the Analysis of Carbon Nanotube Transistors

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Carbon nanotube field-effect transistors have been studied in recent years as a potential alternative to CMOS devices because of their capability of ballistic transport. In order to account properly for ballistic transport we solve the coupled Poisson and Schrödinger equations for the analysis of these devices. Conventionally the coupled Schrödinger-Poisson equation is solved iteratively with appropriate numerical damping. Convergence problems of this coupled equation system are quite well known. We show that these problems occur due to inappropriate energy discretization for evaluating the carrier concentration. By using an adaptive integration method the simulation time is reduced and most of the simulations converge in a few iterations. Based on this approach we investigated the behavior of carbon nanotube field effect transistors.

Exceptional electronic and mechanical properties together with nanoscale diameter make carbon nanotubes (CNTs) candidates for nanoscale field effect transistors (FETs). In short devices (less than 100 nm) the carrier transport is nearly ballistic [1, 2]. The contact between metal and CNT can be of ohmic [1] or Schottky type [3]. In this work we focus on p-type ohmic contact CNTFETs which theoretically [4] and experimentally [2] show better performance than Schottky type devices. In a p-type ohmic contact device holes see no barrier while the barrier height for electrons is $\mathrm{E_g}$. By changing the gate voltage the transmission probability of holes through the device is modulated and as a result the total current changes [1]. In order to account for ballistic transport we solve the coupled Poisson and Schrödinger equations.

$$-\frac{\hbar^2}{2\mathrm{m}^*}\frac{\partial^2\Psi_s}{\partial x^2}+(U-E)\Psi_s=0 \qquad (1)$$

$$\nabla^2\epsilon\phi=-\mathrm{q}(p-n) \qquad (2)$$

$$n_s=\frac{4}{2\pi}\int f_s|\Psi_s|^2dk_s=\int\frac{\sqrt{2\mathrm{m}^*}}{\pi\hbar\sqrt{E_s}}f_s|\Psi_s|^2dE_\mathrm{s} \qquad (3)$$

$$I_d=\frac{4\mathrm{q}}{\mathrm{h}}\int[f_s(E)-f_d(E)]TC(E)dE \qquad (4)$$

The Schrödinger equation (1) is solved on the surface of the CNT and, since we neglected the azimuthal variation of potential on the surface of the CNT, which is a good approximation by considering the small diameter of the CNT, (1) is limited just to one dimension. In (2) $n=n_s+n_d$ and $p=p_s+p_d$, where $n_{s,d}$ and $p_{s,d}$ represent the contributions of the source and drain to the electron and hole concentrations calculated with (3). Carriers were taken into account by means of a sheet charge distributed uniformly over the surface of the CNT [5]. The drain current is calculated using the Landauer-Büttiker formula (4).

Conventionally the coupled Schrödinger and Poisson equations are solved iteratively, by using appropriate numerical damping. If a too high damping factor is selected the simulations may oscillate and will not converge. Using a too low damping factor will also result in long simulation time. We show that by appropriate evaluation of the carrier concentration this problem can be avoided. The integration in (3) is performed in an energy interval. In the simplest way the interval is divided into equidistant steps. By using this method narrow resonances at some energies may be missed or may not be evaluated correctly. In successive iterations the potential profile changes and so does the the position of the resonances. It is possible that a resonance point locates very near to one of the energy grid points. In this case the carrier concentration suddenly changes and as a result the simulation oscillates and will not converge. To avoid this problem the accuracy of the integration should be independent of the location of resonances. By using an adaptive method the integration in (3) can be evaluated with a desirable accuracy. In this work an adaptive Simpson quadrature [6, 7] with Romberg extrapolation [7] is used. Fig. 1-a shows the CPU time demand on an IBM-RS6000 for the same simulation using adaptive integration and non-adaptive integration with 5×10^4 and 10^5 points. By increasing data points in a non-adaptive method the simulation becomes more stable. For all these simulations an adaptive damping factor was used [8]. By using an adaptive integration method only 9×10^2 points are required and it converges very fast. It is also possible to make the simulations faster and more stable by providing the derivate of the carrier concentration with respect to the electrostatic potential for the Poisson solver [9, 10]. As shown in Fig. 1-b by including the derivate, the stability of the simulations increases and the simulation time is decreased. By including the derivative for most of the simulations no damping is required ($\alpha=1$), however, in very rare cases a weak damping $\alpha\geq0.5$ is beneficial. It is of importance to use the adaptive integration for calculating the carrier concentration (3) rather than the current (4). Fig. 1-c shows that if the adaptive integration is performed for the current the simulation will oscillate. In order to acquire stable simulations it is necessary to calculate the carrier concentration accurately, especially in the presence of narrow resonances. With our method very narrow resonances are properly resolved. For the potential profile shown in Fig. 2-a the transmission probability of carries is shown in Fig. 2-b. As seen in Fig. 2-c, the width of the first resonance is only a few $\mathrm{n\,eV}$. While such narrow resonances are resolved the total number of energy points required for this simulation is only about 3×10^3. We applied this methodology to investigate the behavior of a CNTFET. For a fair comparison with experimental results, we used the same material and geometrical parameters as reported in [2], see Fig. 3-a. As shown in Fig. 3-b and Fig. 3-c, an excellent agreement between simulation and experimental results is achieved.

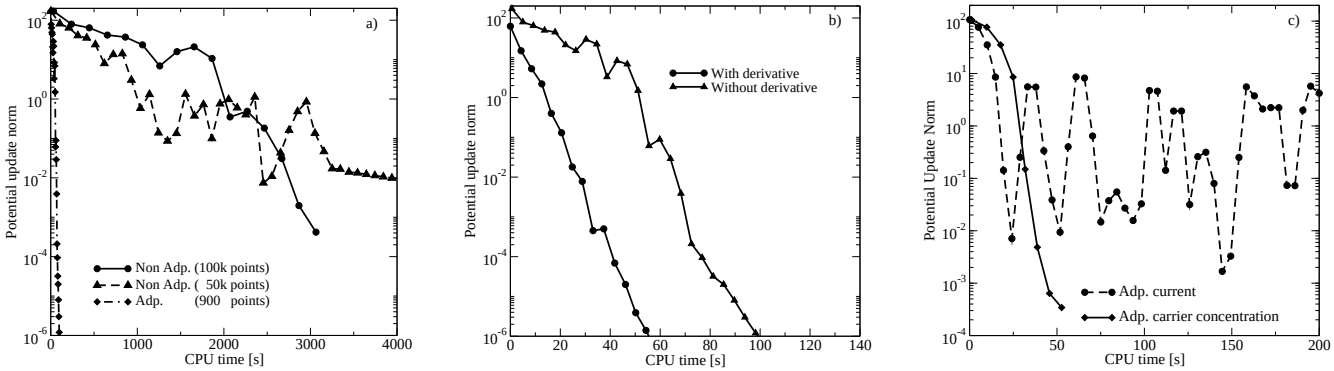

Figure 1: Comparison of CPU time demand on an IBM-RS6000 for different integration methods. The norm of the potential update is considered to be a measure of convergence. a) Shows the results for adaptive and non-adaptive integration (adaptive damping). b) Shows the result for adaptive integration with and without including the derivative of the carrier concentration versus potential (adaptive damping). c) Shows the results for adaptive integration for carrier concentration and current (without damping).

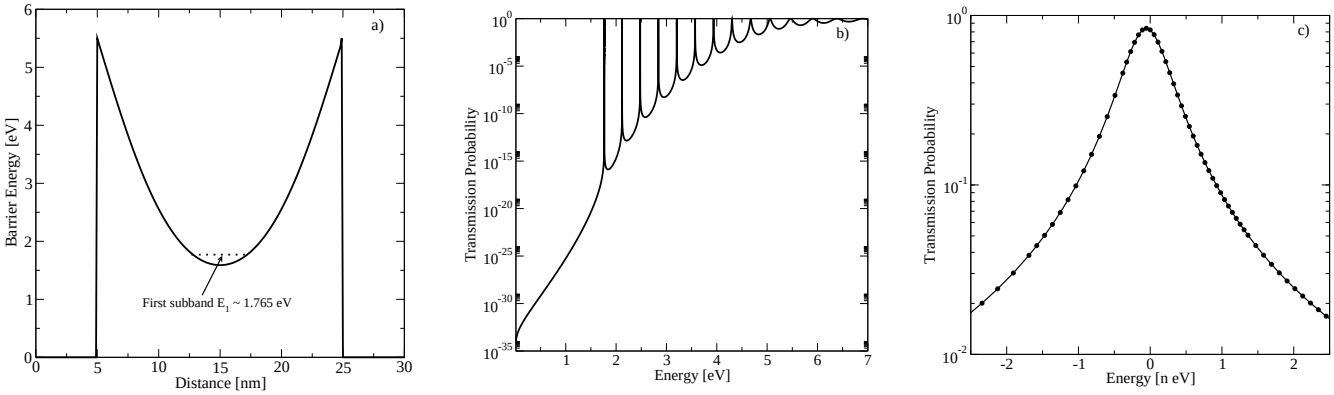

Figure 2: The resolution of the adaptive integration method. a) Potential profi le. b) Transmission probability of carriers through the barrier. c) The width of the fi rst resonance is only a few n eV. The location of the fi rst peak is shifted to zero energy.

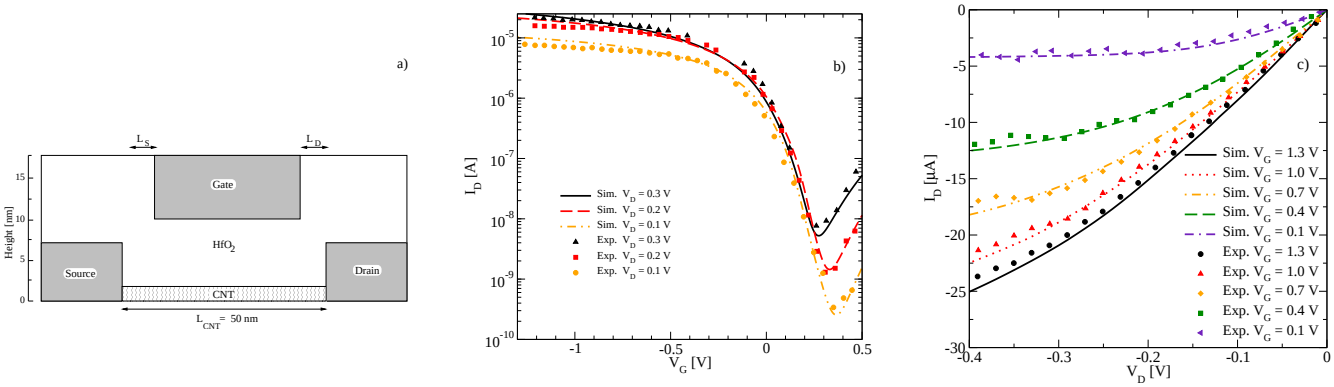

Figure 3: a) Two dimensional cross section of the device. Comparison of the experimental and simulation results for the b) Transfer characteristics and c) Output characteristics.

ACKNOWLEDGMENTS

This work was partly supported by the European Commission, contract No. 506844 (NoE SINANO), and the National Program for Tera-level Nano-devices of the Korean Ministry of Science and Technology.

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