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Self-Consistent Ion Transport Simulation in Carbon Nanotube Channels

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***Abstract*— We propose a method to self-consistently deal with polarisation effects in Monte Carlo particle simulation of charge transport. The systems of interest were membrane structures with a narrow (4-8 Å) carbon nanotube (CNT) channel in an aqueous environment. Due to computational limitations for Molecular Dynamics (MD) computations we extended the Transport Monte Carlo known from semiconductor simulations to ionic transport in water as a background medium [1]. This method has been used successfully to compute transport rates of ions in biological channels but polarization effects on protein walls cannot be easily included self-consistently, due to the complexity of the structure. Since CNTs have a regular structure, it is instead practical to include a self-consistent scheme that accounts for the charge redistribution on the channel wall when a external bias is applied or when the electrical field of a passing ion is screened out. Previous work has shown that this is necessary and the computationally efficient tight-binding (TB) approach developed there [2] is coupled to transport Monte Carlo simulation in this work.**

I. Introduction

In recent years both the fields of CNT and ion channel research have been very active. While CNTs are promising in many respects because of their mechanical and electronic properties [3], biological ion channels on the other hand have received considerable attention both because they behave like nanoscale devices and because the causes of many diseases are linked to them. This makes them very interesting to develop new applications in bioengineering so that a better understanding of the transport mechanisms is required for the development of more efficient drugs or the development of highly specific biosensors. In this respect, CNTs are useful prototypes for biomimetic applications in artificial membranes due to their simple structure [4], [5]. What makes them even more interesting is the possibility to produce functionalized CNTs which are biocompatible and selective to certain types of ions [6], [7].

II. Transport Monte Carlo for Ion Channel Simulations

Because of the vast number of degrees of freedom when an ion channel structure is fully considered including water molecules and ion charges, it is only possible to simulate transport on the nanosecond scale with MD methods on coumputers available today. This, however, is not enough to fully understand the statistical properties of biological systems. Our group has adapted its experience from semiconductor device simulations to develop implicit water transport Monte Carlo methodologies that may be applied to ion channel simulations [1]. Figure 1 shows the flow chart of this method. So far, this approach showed good aggrement with experimental data and makes it possible to simulate the transport up to microsecond or millisecon scale, yielding results with high statistical significance.

As the Poisson solver requires the permittivities of each part of the domain, in previous calculations bulk dielectric constants were used. This, of course, does not account for the fact that single molecules in the system exhibit different behavior than bulk and becomes even more problematic for pore walls realized with CNTs, where the delocalized electrons can move along the tube easily.

In order to account for this effect a quantum mechanical treatment of the electronic structure becomes necessary. As the self-consistent charge distribution on the CNT has to be recalculated frequently a fast method is required. The semi-empirical TB approach fulfills this requirement [8]. In this proof of concept, a single orbital, nearest neighbor scheme has been integrated into the Monte Carlo code 2. One of the obtained trajectories is shown in figure 3.

Various comparisons between old and new model have been performed. The average fields like showed in Fig. 4 exhibit large differences and the transport rates changed by up to 50%. Results for different biases and ion types, were qualitatively the same for CNTs of different sizes.

We identified the solution of the poisson equation as a computational bottleneck and work is in progress to parallelize this part of the code. This might allow highly precise simulations with even smaller time steps and mesh spacing. In the long term, our goal is to realize a platform for bioelectronics simulations comparable to the known tools for the design of semiconductor devices.

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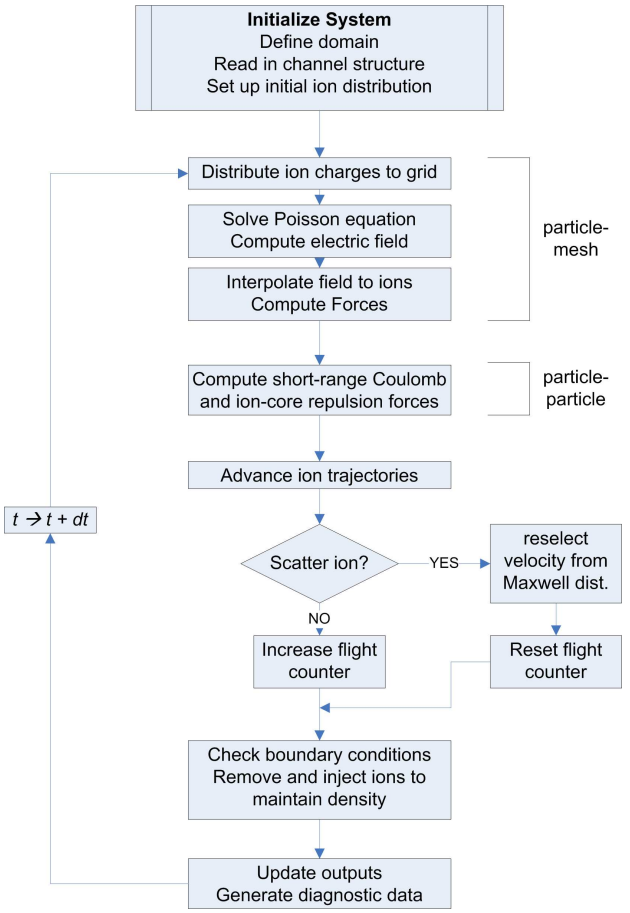

Fig. 1. Boltzman transport Monte Carlo.

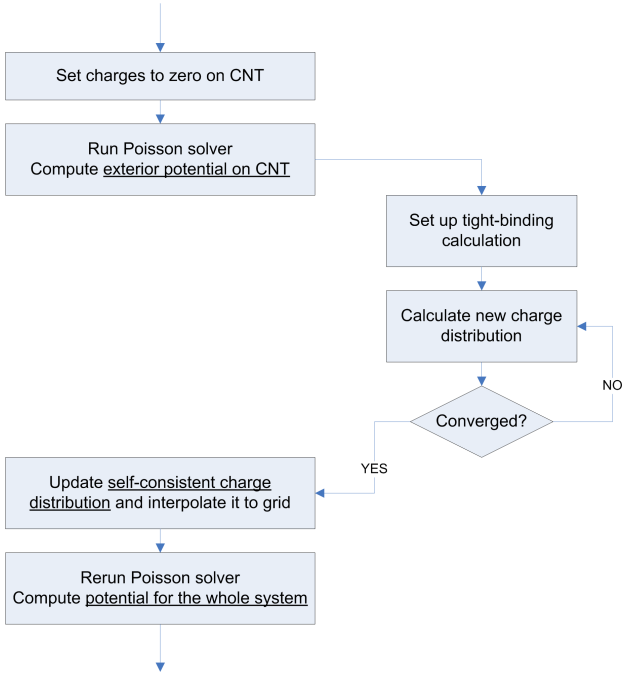

Fig. 2. Integration of the TB solver.

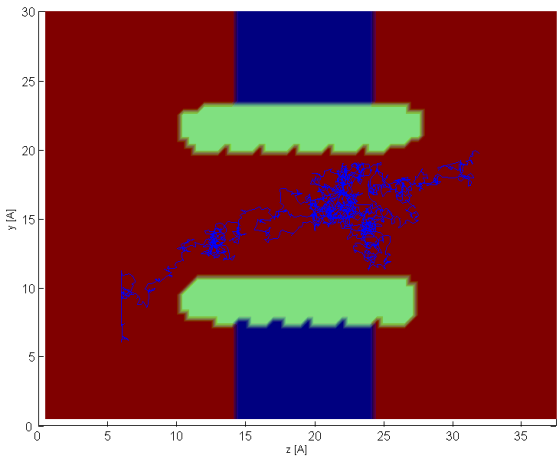

Fig. 3. Sample trajectory of a sodium ion passing through a (8,8) CNT.

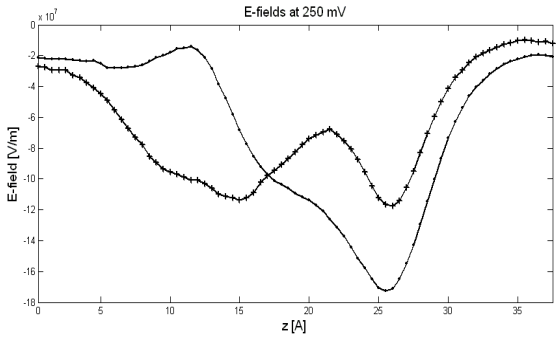

Fig. 4. Average electrical fields along the axis. Self-consistent solution is marked with (+).