# Computing with Magnetic Field in Carbon Nanotube Tissues

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***Abstract*—We suggest a novel Computation-in-Materio paradigm whereby the change of magnetic field is used to manipulate the conductance of carbon nanotubes in order to achieve computations. The underlying physics is described followed by a proof of concept scenario in which a one–dimensional cellular automaton is built in carbon nanotube tissue and driven by magnetic field. Preliminary results are presented for the simulation of such architecture evolving according to basic rule 110. Also, some directions for the future work are given.**

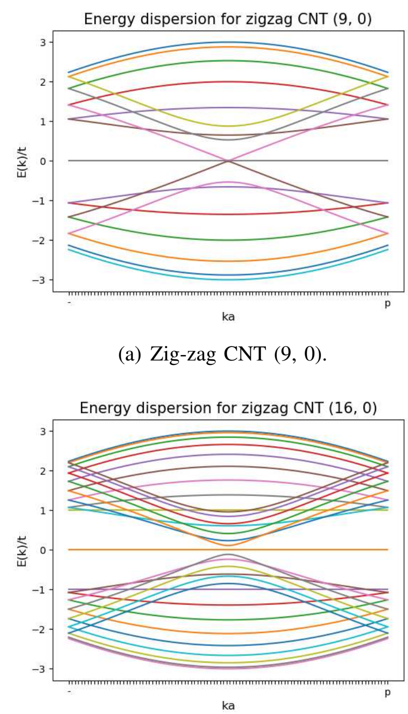
***Index Terms*—computation-in-materio, carbon nanotubes, Aharonov-Bohm effect, cellular automata**

## I. Introduction

Novel computing substrates and novel computing paradigms are gaining attention as a possible way to address the challenges faced by the semiconductor industry. For some time, nanomaterials have been in focus due to their favourable properties regarding miniaturisation and power consumption, to name a few.

We look into carbon nanotubes (CNT) and the ways in which their conductivity can be manipulated in order to achieve computations. Previously, Evolution-in-Materio approach was applied to randomly dispersed CNTs in a polymer substrate and promising results were achieved for a number of computational tasks [1]. In this report we present our ongoing research into a novel approach to using CNT-based tissue for computations. In particular, magnetic field is used to manipulate the conductivity of CNT. It is the main goal of this short paper to introduce such paradigm for computations. To demonstrate its viability, a model of a simple computational architecture in a form of a one–dimensional cellular automaton (CA) which is built in CNT tissue is simulated to evolve according to the basic rule 110.

Section II presents the physics of quantum transport in CNTs which provides the basis for our approach. It is followed by Section III which describes a model of a CNT-based computing cell and the way it is used in a CA. In Section IV the results of our preliminary simulation runs are presented. Finally, Section V presents a brief discussion of the suggested approach as well as some directions for future work.




(a) Zig-zag CNT (9, 0).

(b) Zig-zag CNT (16, 0).

Fig. 1. Energy dispersion relations for CNTs of different chirality illustrated by examples of a metallic (a) and a semiconducting (b) profile.

## II. Conductance of Carbon Nanotubes

Conductance of CNTs is primarily determined by their geometry: the diameter and chirality. Therefore it is given at the time of their production. Interestingly, dependent on chirality, their character can be semiconducting or metallic [2]. Figure 1 shows the energy bands for the example of a metallic and a semiconducting nanotube. The plots were generated according to the equations based on the tight-binding method [2]:

$$E_q^a(n) = \pm t\sqrt{1 \pm 4\cos\frac{q\pi}{n}\cos\frac{ka}{2} + 4\cos^2\frac{ka}{2}} \qquad (1)$$

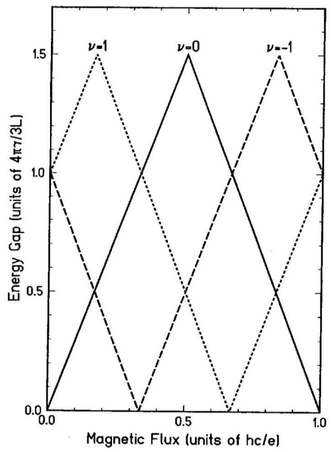



Fig. 2. Energy gap versus magnetic flux passing through the tube cross section for $\nu = 0$ (metallic CN) and $\nu = \pm 1$ (semiconducting CN). (Taken over from [5])

$$E_q^z(n) = \pm t \sqrt{1 + 4\cos\frac{\sqrt{3}ka}{2}\cos\frac{q\pi}{n} + 4\cos^2\frac{q\pi}{n}} \qquad (2)$$

where $k$ is a wave vector, $a$ unit vector of the CNT lattice, $q$ unit of electric charge, $n$ index of energy subband and $t$ transfer integral. The equations stand for the armchair and zig-zag CNT geometry as denoted by superscripts $a$ and $z$ respectively.

However, this property can be changed when CNT is affected by magnetic field. Dependent on the strength and the direction of the magnetic field relative to the axis of CNT, a metallic CNT can become semiconducting and vice versa in the extreme case.

When the magnetic field is parallel to CNT axis, a shift is noted in the phase of the complex wave function which describes the charge particle moving in the corresponding electromagnetic potential. This quantum mechanical phenomenon is known as Aharonov-Bohm effect (AB effect) [3]. Theoretical findings of its existence in CNTs were confirmed experimentally by optical spectroscopy [2], [4]. Dependent on the strength of the magnetic field, the band gap of a CNT (in Figure 1 it is the distance at the mid-point of the plot between the lowest in the upper half and the highest energy band of the lower part) changes its width and in certain cases turns semiconducting CNTs into metallic and the other way round. Figure 2, taken from [5], illustrates this change.

## III. Model and Simulation Approach

There are few assumptions we make for the model used in simulations to demonstrate computations in CNT tissue guided by the changes of magnetic field. CNT-based tissue consists of cells where each cell contains one CNT and a local source of magnetic field. The CNT is in a form of a CNT FET transistor. The local magnetic field affects only the CNT in the same cell. The schematic view of the assumed cell is shown in Figure 3.

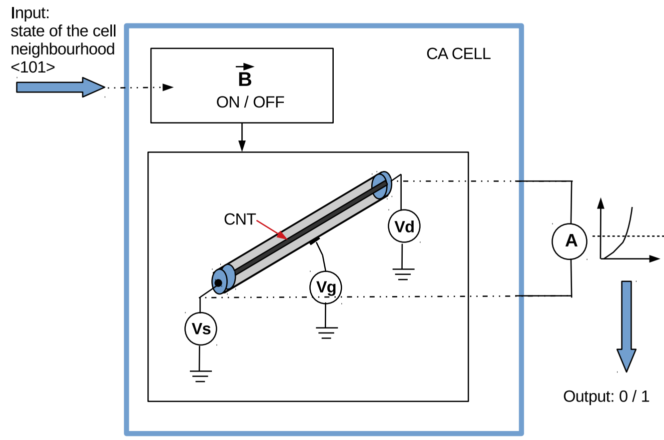
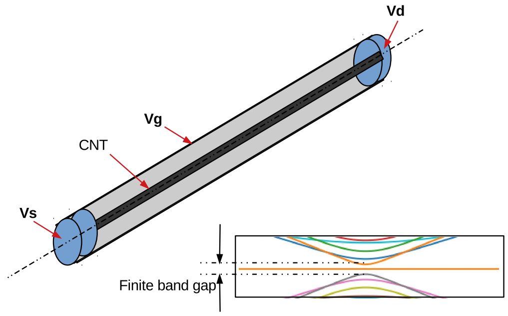



Fig. 3. Schematic view of the CA cell based on the CNT.

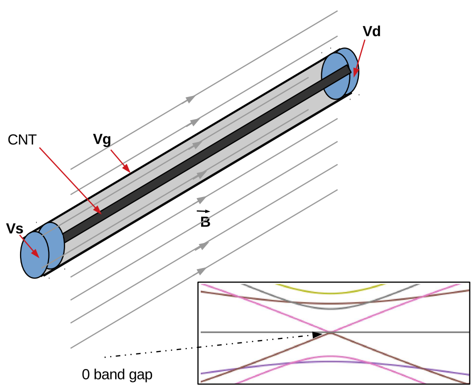
Magnetic field is assumed to be parallel to the CNT axis thereby making AB effect be the physical phenomenon responsible for the change of the CNT conductance. Further, it is assumed that the type of change of the magnetic field is binary, i.e., it is either present or not. In this way the control mechanism for the magnetic field source within the cell can be realised as a simple switch which turns the magnetic field source on and off. It is further assumed that the character of the CNT is semiconducting in the absence of the magnetic field, i.e., that it is characterised by some finite band gap see Figure 4(a). This character is assumed to change to become metallic when the magnetic field source within the cell is switched on. This is due to the band gap effectively shrinking as a consequence of AB effect see Figure 4(b). The state of the cell is determined based on the value of the DC current flowing through the CNT, which is in essence Landauer current, where certain threshold is set to determine whether the response is 1 or 0 as shown schematically in Figure 3.

The computational architecture considered is one–dimensional CA as shown in Figure 5 which is assumed to evolve in time according to a certain basic rule. The CA cells are assumed to be of a kind described at the beginning of this section. For each time step of the CA evolution, the character of the CNT per cell is determined based on the state of the cell neighbourhood. The following sequence can be identified per cell per each time step:

1) the presence or the absence of the magnetic field is determined based on the state of the neighbourhood and the applied CA rule
2) the value of the CNT band gap is determined based on the presence or the absence of the magnetic field; accordingly, the electrical character of the CNT is metallic or semiconducting




(a) CNT with semiconducting response.




(b) CNT with metallic response.

Fig. 4. Illustration of the CNT within the CA cell: (a) with no magnetic field and (b) with the magnetic field which changes the band gap and thereby the character of the cell reponse.

3) the current which flows along the CNT is determined via simulations of the electrical transport in CNT which account for the size of the CNT band gap

## IV. Simulation Results

At this place we present the results of the preliminary simulation runs where one–dimensional CA of 16 cells is let to evolve in time according to the 110 rule [6] which is shown to be Turing complete [7]. Electrical transport in CNTs is simulated by a well-known Schrödinger-Poisson (SP) solver as in [8]–[10].

The following assumptions were made for the simulation of the transport in CNT, see [10] for explanation of concrete values:

- all CNTs are of the same chirality, i.e., (16, 0)
- the size of the band gap is 0.62 $[eV]$ in the absence of magnetic field and 0.001 $[eV]$ when magnetic field is present
- all CNTs are of the same dimensions: the diameter $0.63[nm]$ (follows from the chirality), the length $20[nm]$

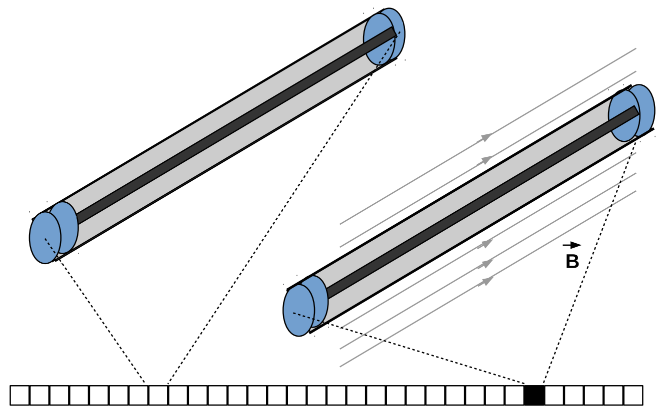
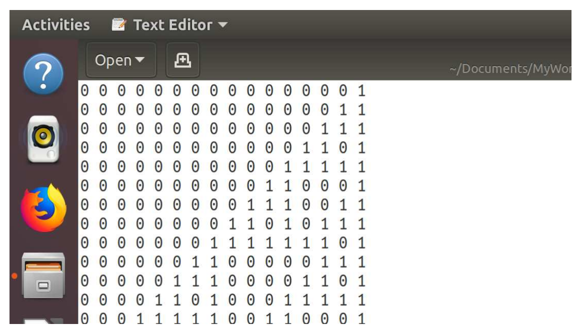
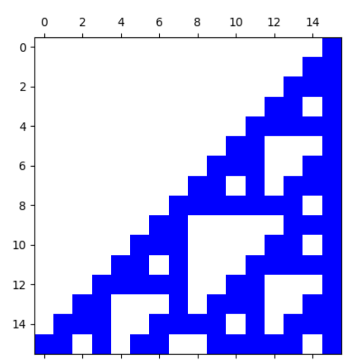



Fig. 5. 1D cellular automaton and illustration of two states of the cell. When there is no magnetic field, response of the cell will correspond to a semiconducting CNT; when magnetic field is present, the response will be different and correspond to the metallic CNT.




(a) Screenshot of the file generated for the simulation of 16-cell CA for 16 steps.




(b) Plot of the CA test run for the first 16 steps.

Fig. 6. The results of the simulation run for the 1D CA of 16 cells, 16 steps of time-evolution guided by the rule 110.

- the size of the slots used for the scattering matrix approach within Schrödinger equation numerical solution is $0.1[nm]$
- the insulator thickness $2[nm]$, and dielectric constant 25
- the work function of the electrodes $4.5[eV]$
- voltages on the electrodes of the CNT FET transistor, which drive the current flow, were chosen based on the results in [10] and are of the following values: source $0[V]$, drain $0.4[V]$, gate $0.5[V]$

The threshold for distinguishing between the currents corresponding to states 1 and 0 was determined based on the test runs for the CNT FET with and without magnetic field applied.

The results for the first 16 time steps are give in Figure 6. States of the cells where the Landauer current was above the established threshold is recorded as 1 and those below the threshold as 0. The presence or absence of the magnetic field for a specific cell for the next step is determined based on the states of the neighbouring cells according to the 110 rule [6]. Due to long simulation times on a PC, only 10 iterations per cell were used during which convergence was not achieved. However, in all cases, the Landauer currents measured for the cells with magnetic field applied were, on average, orders of magnitude larger than the Landauer currents measured for the cells with no magnetic field applied. Therefore, we find the approach promissing.

## V. Discussion and Future Work

In this brief report, a novel way of computing in-materio has been presented. Suggested computational tissue is based on CNTs and suggested way of achieving computations is the manipulation of the CNT conductivity by changing the magnetic field to which they are exposed. As a proof of concept, a simple example of an architecture is considered where CNTs are placed in an ordered arrangement, i.e., a CA built in a CNT tissue and driven by the presence / absence of the magnetic field per each cell. Also simple was the assumed magnetic field - it was parallel to the CNT axis and it was simply either present or not. By bringing in varieties into these two simplifications, new research directions are planned for future work, to name a few:

- examine unorganised arrangement of CNTs, similar to those used within Nascence project [1] and run Evolution-in-Materio scenario driven by varying magnetic field
- examine the case where CNTs are of different dimensions and chiralities
- examine the case where actual values of the magnetic field take on a range of values
- examine various directions of the magnetic field relative to the CNT axis: conductivity may be changed but also the underlying physical phenomena may be of a different kind

The results presented in this brief report are based on prototype runs of the simulator. Before addressing mentioned research topics, it is the aim to further improve simulation results in order to bring them closer to a real life CNT FET operation. Also, it would be interesting to look into the realisation of the mechanisms which would drive magnetic fields per cell based on the given rule. In conclusion, although the results are only preliminary, we find them valuable and encouraging for further investigation into this novel in-materio computation paradigm.

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