Field-Coupled Devices for Nanoelectronic Integrated Circuits

Wolfgang Porod, György Csaba, and Árpád Csurgay

Center for Nano Science and Technology, Department of Electrical Engineering
University of Notre Dame, Notre Dame, Indiana 46556
Porod@nd.edu

Abstract

In this paper we review our previous work on field-coupled devices, which is motivated by the observation of Coulomb coupling between quantum dots, as well as real and artificial atoms and molecules. These types of devices and their couplings provide an interesting alternative to the more conventional wire-contacted devices for nanoelectronic integrated circuits.

1. Introduction

Nanoelectronics offers the promise of ultra-low power and ultra-high integration density. Several device structures have been proposed and realized experimentally, yet the main challenge remains the organization of these devices into new circuit architectures. For an introduction to this problem area, see the review paper [1].

Here, we investigate the idea of physical device-device interactions in the form of field coupling to provide local connectivity. In particular, we study field-coupled nanodevices in cellular nonlinear network (CNN) architectures [2, 3]. We focus here both on Coulomb-coupled molecular nanostructures and quantum-dot arrays [4-9], as well as magnetically-coupled arrays of permanent-magnet nanostructures [10,11]. We show how such field-coupled devices can be interfaced with conventional wire-contacted devices, and how both classes of devices can be modeled on the same footing within conventional circuit simulators (such s SPICE).

CNN-type architectures for nanostructures are motivated by the following considerations: On the one hand, locally-interconnected architectures appear to be natural for nanodevices where some connectivity may be provided by direct physical device-device field coupling. On the other hand, CNN arrays with sizes on the order of 1000-by-1000 (which are desirable for applications such as image processing) will require the use of nanostructures since such integration densities are beyond what can be achieved by scaling conventional CMOS devices.

2. Metal-Contacted and Field-Coupled Nanoelectronic Devices

Three ways of nanodevice interconnection have been suggested so far. Metal-contacted devices in the meso-scale range (10 to 100 nanometers), such as nano-transistors, resonant tunneling devices (RTD's), and metal-dot single-electron transistors (SET's), can be interconnected with wires. As long as each device has metal contacts, i.e. they are all embedded into a "heat bath," conventional interconnections with wires are possible. In this case, circuit dynamics obeys the conventional Kirchhoff's laws, which are a consequence of the basic conservation of charge and energy. Alternatively, nanodevices which are not metal contacted, e.g. quantum-dot arrays and artificial atoms and molecules, can be coupled by inter-device transport, or by electromagnetic (electric and/or magnetic) fields. In the case of wiring and inter-device electronic transport the flow of current generates unavoidable dissipation of energy. An alternative approach to device integration is to exploit electromagnetic field interaction between the devices, such as coupling by Coulombic or by magnetic forces. This latter approach becomes more natural as devices come closer to each other (increasing packing densities) and it also significantly reduces unwanted power dissipation.

If both metal-contacted and field-coupled devices are to be integrated into the same circuit, the physical interfaces between the two types of devices can be represented as a classical electromagnetic circuit. The boundary condition on the side of the metal-contacted devices are defined by the metal contacts (voltages and currents) and on the side of the field-coupled devices by the electric or magnetic fields generated by the nanodevice. In this paper, we will review our previous work where we have developed equivalent-circuit representations for circuits composed of both metal-contacted and field-coupled nanodevices. Thus, circuit theory techniques can be applied to build device models, to simulate and to aid the design of large-scale nanoelectronic integrated circuits.

0-7803-7215-8/01/$10.00©2001 IEEE.

3. Equivalent-Circuit Models for Field-Coupled Nanodevices

In this section, we will outline the development of equivalent-circuit models for field-coupled nanostructures. As schematically shown in Figure 1 below, the individual device (molecule) is dissipatively coupled to a heat bath, it is exposed to external forces, such as clocking circuitry, and it couples to its neighbors through electric or magnetic fields.

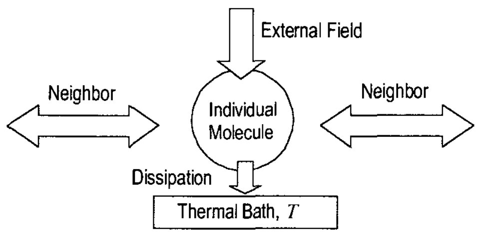


Figure 1. Schematic representation of a field-coupled nanodevice which is exposed to external fields and a heat bath, and which interacts with its neighbors through electric or magnetic fields.

3.1 Individual Nanodevices

In previous work [4], we have shown that the electronic or magnetic state at time t of any open quantum system can be described by a state-vector, the so-called coherence vector $\lambda(t)$, which represents the Hermitean density matrix of the system. For the case of a two-level system, the coherence vector has three components, which corresponds to a 2-by-2 density matrix

The electronic dynamics of such a nanostructure may be described by quantum Markovian master equations of finite-state systems. This model describes the dynamics of a device as the irreversible evolution of an open quantum system coupled to a reservoir (heat bath). This coupling to the environment introduces damping terms in the dynamical equations, which then take the general form of

$$\hbar \frac{d\lambda(t)}{dt} = \Omega\lambda(t) + R\lambda(t) + k$$

Here, Ω is the Bloch matrix of the corresponding conservative (non-dissipative) quantum system, and R and k are the damping matrix and vector, respectively. The details can be found in Ref. [4, 5].

The above resulting mixed quantum-classical equations describe the time evolution of the state of the nanodevice. The coherence vector determines the electronic evolution within the framework of a density-matrix description, and all experimentally observable quantities are related to its components. For the case of a two-state system, the third component of the vector $\lambda_3(t)$ determines the electronic charge configuration.

Notice that the above (ordinary differential) equation resemble circuit dynamics. The equations for the various components of $\lambda(t)$ can be interpreted as the state equations of a nonlinear circuit with state variables λ_1, λ_2, and λ_3. The various terms in the coupled equations can be viewed as nonlinear resistors, capacitors, inductors, and controlled sources. This is schematically shown in Figure 2 below for the case of two-state nanostructure with a 3-dimensional state vector λ.

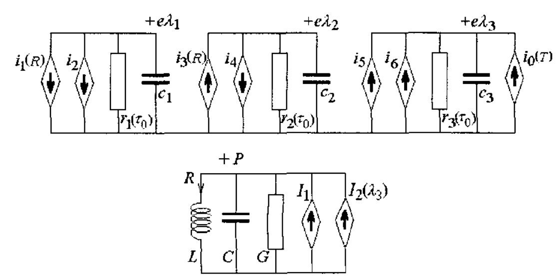


Figure 2. Equivalent-circuit representation of the mixed quantum-classical dynamics for a 2-state nanostructure with a 3-d state vector λ.

3.2 Field-Coupled Nanodevices

We assume individual device or molecules in an array are fixe in space, and that the electronic dynamics takes place inside each individual molecule (no inter-molecular charge transfer). We also assume that the molecules are far enough apart from each other that the overlap between their wave functions can be ignored. We can then identify sets of private electrons and Hamilton operators as belonging to each molecule. Intermolecular forces due to field coupling are relatively weak and their effects can be considered as perturbations.

In order to model the Coulombic interactions between individual molecules, we need to be able to describe the way in which charge is distributed inside each molecule. It is well known that Coulomb interactions between charges localized inside spheres can be specified by the interactions between multipoles (point charges, dipoles, quadrupoles, octopoles, etc.) representing the charge distribution inside the isolated sphere surrounding a molecule; this is schematically represented in Figure 3 below.

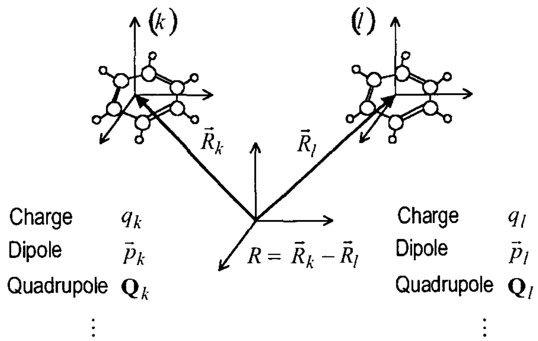


Figure 3. Schematic representation of the field coupling between individual molecules, which is modeled as multipole - multipole interactions.

In this way, the time varying Coulomb field of a molecule can be represented by multipoles at fixed positions with time-varying multipole moments. If the dynamics of the molecule with its time-varying electronic charges are known, then the potential at the site of the neighbor be determined (and thus the interaction energies).

For the equivalent circuit model, the effect of the neighbors is represented by controlled sources which are dependend upon the state variable that describes the charge configuration (λ_3 for the case of a 2-state device).

3.3 Interfaces between Field-Coupled and Metal-Contacted Nanodevices

Input to and output from an array of field-coupled nanostructures can be provided by conventional metal-contacted mircoelectronic circuitry. Voltages on metallic wires at the edge of the arrays can set the inputs which are felt by the charge configurations of those nanostructures which are close to the periphery of the array. Conversely, the internal states of the output nanodevices lead to field variations which can be detected as voltage signals on the output devices.

The time-varying electromagnetic fields generated by the metal-contacted input circuit couple to the dipoles and quadrupoles of the nearest nanodevices in the array. This relation may be represented as an equivalent circuit of the interface by solving the corresponding classical electromagnetic field problem. In the first approximation, this problem is quasi-static and the equivalent circuit is composed of ideal transformers. In general, the equivalent circuit is a linear, reciprocal reactance circuit representing the coupling between the electric field generated by the external circuit and the state-variable of the nanodevice.

At the output, the field generated by the charge configuration of the nanodevice is sensed and measured by the near-by metal contacts of the output microelectronic circuit. The coupling of the field to the voltages can again be represented as a linear, reciprocal reactance circuit, just as for the case of the input. The measurements at the output ports introduce additional non-local damping channels since the macroscopic circuitry opens up additional dissipative channels, just like a heat bath.

Figure 4 illustrates the equivalent-circuit model of the input and output of an array. As mentioned above, the input is a time-varying electric field generated by a metal contacted input circuit. Looking back from the

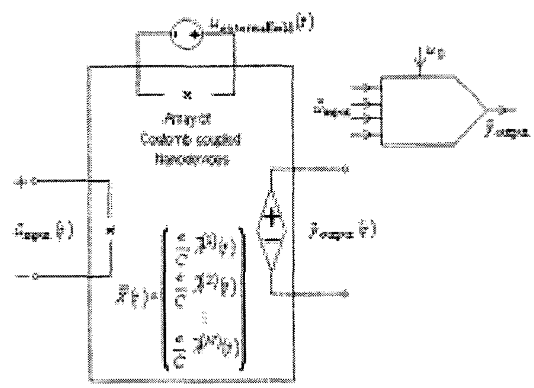


Figure 4. Schematic representation of the equivalent-circuit model for the input and output of an array of field-coupled nanodevices.

array, it can always be represented by a vector of λ_3'-s of the nanodevices (I_1, I_2,... denote the input ports)

$$\vec{u}_{\text{input}} = \left(\frac{e}{C} \lambda_3^{(I_1)}, \frac{e}{C} \lambda_3^{(I_2)}, \ldots \right).$$

The external field will be represented by an independent time-varying voltage source $\vec{u}_{\text{external field}}(t)$. The measured output is also a vector of the λ_3'-s (O_1, O_2,... denote the output ports)

$$\vec{y}_{\text{output}} = \left(\frac{e}{C} \lambda_3^{(O_1)}, \frac{e}{C} \lambda_3^{(O_2)}, \ldots \right).$$

Note that e/C, i.e. the electron's charge divided by a capacitance has voltage dimension thus the inputs and outputs are indeed virtual voltages.

3.4 Hierarchical Design

The equivalent-circuit representation of field-coupled devices and their embedding in more conventional circuitry allows for the hierarchical design of integrated circuits, using conventional circuit-simulation tools, such as SPICE. We have already used this approach to design and simulate logic circuits based on such field-coupled nanodevices [4, 5].

4. Coulomb-Coupled Quantum-Dot Cells

Based upon the emerging technology of quantum-dot fabrication and single-electron technology, the feasibility of logic devices based on single electrons confined to quantum-dot structures had been envisioned in [12]. Later, the Notre Dame group proposed a concrete scheme for computing with cells of coupled dots [6], the so-called *Quantum-Dot Cellular Automata* (QCA), which will be described in more detail below; see also the review paper contained in these proceedings [9].

4.1 Quantum-Dot Cellular Automata

The Notre Dame proposal is based on a cell which contains five quantum dots, as schematically shown in Fig. 5. The dots are shown as the circles which represent the confining electronic potential. In the ideal case, this cell is occupied by two electrons, which are schematically shown as the solid dots. The electrons are allowed to "jump" between the individual dots in a cell by the mechanism of quantum mechanical tunneling. Tunneling is possible on the nano-meter scale when there is sufficient leaking of the electronic wavefunction out of the confining potential of each dot, and the rate of these jumps may be controlled during fabrication by the physical separation between neighboring dots.

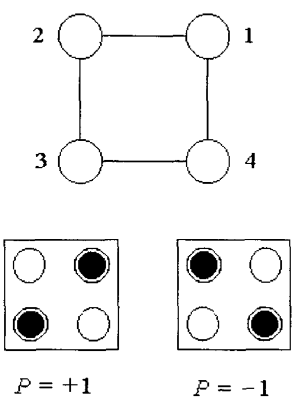
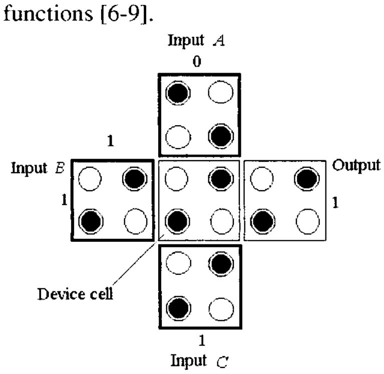


Figure 5. Schematic representation of a quantum-dot cell which is occupied by two electrons.

This quantum-dot cell represents an interesting dynamical system. The two electrons experience their mutual Coulombic repulsion, yet they are constrained to occupy the dots. If left alone, they will seek the configuration corresponding to the physical ground state of the cell. It is easy to see that the ground state of the system will be an equal superposition of the two configurations with electrons at opposite corners, as shown in Fig. 5. We may associate a "polarization" of P=+1 and P=-1 with either arrangement.

Coupling between the two cells is provided by the Coulomb interaction between the electrons in different cells. Simulations have shown that this interaction leads to a strongly bistable behavior in that the polarization in one cells induces the same polarization in the neighbor.

This bistable saturation is the basis for the application of such quantum-dot cells for computing structures. The nonlinear saturation replaces the gain in conventional circuits. Note that no power dissipation is required in this case. One can think of the saturation levels of the polarization as the "signal rails." Based upon the bistable behavior of the cell-cell coupling, the cell polarization can be used to encode binary information. The physical interactions between cells may be used to realize elementary Boolean logic functions [6-9].



Truth table

A	B	C	Out
0	0	0	0
0	0	1	0
0	1	0	0
0	1	1	1
1	0	0	0
1	0	1	1
1	1	0	1
1	1	1	1

Figure 6. Schematic of a majority logic gate built from QCA cells.

Figure 6 shows a majority logic gate, which is the basic QCA logic gate. It consists of just an intersection of lines and the "device cell" is simply the one in the center. If we view three of the neighbors as inputs (kept fixed), then the polarization of the output cell is the one which "computes" the majority votes of the inputs. Note that conventional AND and OR gates are hidden in the majority logic gate. Inspection of the majority-logic truth table reveals, that if input A is kept fixed at 0, the remaining two inputs B and C realize an AND gate. Conversely, if A is held at 1, B and C realize a binary OR gate. In other words, majority logic gates may be viewed as programmable AND and OR gates.

4.2 Quantum-Dot Cellular Neural Networks

QCA arrays can also be thought of in the framework of *Cellular Neural/Nonlinear Networks* (CNN) [2]. As described in Ref. [13], for the case of a 2-state QCA model, the equivalent circuit describing a CNN cell is composed of two linear capacitors, four nonlinear controlled sources and eight linear controlled sources representing the interactions between the cell and its eight neighbors. This network model simulates the dynamics of the polarization and the phase of the coupled cellular array. If the polarization of the driver cells at the edges of an array initially in equilibrium is changed in time, a dynamics of the polarizations and phases of the cells is launched in the whole array. This dynamics of different arrays has been studied, and a class of spatio-temporal wave-phenomena was identified and explored.

In the framework of the CNN model, ground-state computing by the Quantum Cellular Array corresponds to transients between equilibrium states. Let us assume that in an equilibrium state the configuration of the array is a binary string s. If at t=0 the polarization of a few driver cells is abruptly changed from -1 to +1 or from +1 to -1, then a transient emerges. If we wait till the new equilibrium is reached, we get a new configuration f(s) of the binary cells. We can say that the array "mapped" s to f(s). In this sense the cellular network model simulates the functions of the quantum-dot cellular automata, including QCA Logic.

4.3 Magnetically-Coupled Dots

There is a wide variety of nanosystems that might serve as "building blocks" of field-coupled QCA-type nanocomputers. In particular, nanomagnet arrays are emerging as a promising realization possibility. Due to the relatively strong interaction energy (typically few hundred kT between few–ten nm size dots), these structures might exhibit robust, room temperature operation. The feasibility of a line consisting of magnetically-coupled dots has already been proposed and experimentally verified [10].

The behavior of magnetic materials is described by the classical theory of micromagnetism. In large, (micron or bigger) size bulk materials the balance of dipolar coupling and exchange interaction between magnetic moments results in complicated domain structure, experimentally observed and theoretically calculated from the solution of the Landau – Lifshitz equations. In contrary, small (typically 1-50 nm size) magnets exhibit single – domain behavior, i.e. their state is approximately described by a single magnetization vector, and their dynamics governed by ordinary differential equations. If the dots are close to each other, these differential equations are strongly coupled.

Based on these differential equations, we have begun to construct circuit models of nanomagnet arrays and to examine the effect of geometry (dot shape, distance, etc.) on the "circuit" parameters [11]. These circuit models make the design of larger structures rather straightforward, and by using them, one can then analyze realization issues of larger systems (i.e. error tolerance, ease of design, simplest models); this work is in progress. Our goal is to show that the bistable behavior of anisotropic dots (such as magnetic pillars) can be utilized for building binary Boolean logic gates, very much like its electrical QCA counterpart.

Since large, regular matrices of nanomagnets are relatively easy to realize (unlike the irregular arrays), Boolean logic (which requires irregular geometry) probably is not the most natural way of exploiting magnetic nanocomputing. Therefore, we are examining pattern formation phenomena in nanomagnet arrays, for their application possibilities for non – Boolean computation. Our preliminary simulations so far suggest that nanomagnet arrays appear to be excellent candidates for experimentally studying, designing and utilizing complex, nonlinear phenomena in large-scale systems.

5. Summary

In this paper, we have reviewed our approach for the simulation of field-coupled devices. We have developed equivalent-circuit representations for the dynamics of arrays of field-coupled (electric and magnetic devices), as well as for their interconnection with more conventional metal-contacted devices. This approach yields circuit models, which can be implemented in a conventional circuit-simulation tool, such as SPICE. We have already demonstrated the feasibility of the co-simulation of field-coupled devices with conventional CMOS devices and single-electron transistors [14-16].

Acknowledgements. This work was supported in part by grants from the U.S. Office of Naval Research (MURI program) and the W. M. Keck Foundation.

6. References

[1] A. I. Csurgay, The Circuit Paradigm in Nano-electronics, in *Proceedings of the European Conference on Circuit Theory and Design - ECCTD'97*, pp. 240-246, Budapest, 1997.

[2] L. O. Chua and L. Yang, Cellular Neural Networks: Theory, *IEEE Trans. CAS*, .35: 1257-1272 (1998); Cellular Neural Networks: Applications, ibid. 1273-1290 (1998).

[3] CNN Software Library (Templates and Algorithms) V 7.2, Analogical and Neural Computing Laboratory, Computer and Automation Institute, Hungarian Academy of Sciences, 1998.

[4] A. I. Csurgay and W. Porod, Equivalent Circuit Representation of Arrays Composed of Coulomb-Coupled Nanoscale Devices: Modeling, Simulation, and Realizability, *International Journal of Circuit Theory and Applications*, 29: 3-35 (2001).

[5] A. I. Csurgay W. Porod, and C. S. Lent, Signal Processing with Near-Neighbor-Coupled Time-Varying Quantum-Dot Arrays, *IEEE Trans. CAS I* 47(8): 1212-1223 (2000).

[6] C. S. Lent, P. D. Tougaw, W. Porod, and G. H. Bernstein, Quantum Cellular Automata, *Nanotechnology* 4: 49-57 (1993).

[7] W. Porod, Computing with Coupled Quantum Dots: Quantum-Dot Cellular Automata and Cellular Nonlinear Networks, *Proceedings of the ECCTD'97*, 248-253 (1997).

[8] C. S. Lent and P. D. Tougaw, A device Architecture for Computing with Quantum Dots, *Proceedings of the IEEE*, 85: 541 (1997).

[9] G. L. Snider, A. O. Orlov, R. K. Kummamuru, R. Ramasubramaniam, I. Amlani, G. H. Bernstein, C. S. Lent, J. L. Merz, and W. Porod, Quantum-dot Cellular Automata: Introduction and Experimental Overview, these Proceedings.

[10] R. P. Cowburn and M. E. Welland, Room Temperature Magnetic Quantum Cellular Automata, *Science* 287: 1466 (2000).

[11] G. Csaba and W. Porod, Computing Architectures for Magnetic Dot Arrays, presented at the *First International Conference and School on Spintronics and Quantum Information Technology*, Maui, Hawaii, May 2001.

[12] D. K. Ferry and W. Porod, Interconnections and architecture for ensembles of microstructures, *Superlattices and Microstructures*: 2, 41 (1986).

[13] W. Porod, C. S. Lent, G. Toth, H. Luo, A. Csurgay, Y.-F. Huang, and R.-W. Liu, Quantum-Dot Cellular Nonlinear Networks: Computing with Locally-Connected Quantum Dot Arrays, *Proc. Int'l Symp. Circ Syst.* 745; Hong Kong, June 1997.

[14] X. Wang and W. Porod, Single-electron transistor analytic I-V model for SPICE simulations, *Superlattices and Microstructures* 28, 345 (2000).

[15] C. Gerousis, S. M. Goodnick, and W. Porod, Toward nanoelectronic cellular neural networks, *International Journal of Circuit Theory and Applications*: 28, 523-535 (2000).

[16] C. Gerousis, X. Wang, G. Toth, S. M. Goodnick, W. Porod, C. S. Lent, and A. I. Csurgay, Modeling Nanoelectronic CNN Cells: CMOS, SETs and QCAs, presented at the *2000 IEEE International Symposium on Circuits and Systems*, Geneva, Switzerland, May 2000.