Manual for QCADesigner-Energy (QD-E)

Manual version: 1.0

1 INTRODUCTION

The QCADesigner-E (QD-E) is an extension of the QCADesigner version 2.0.3 of Konrad Walus [1]. It implements the estimation of the power dissipation of QCA circuits based on the works of Timler and Lent et al. [2-4]. The extension is integrated as an additional simulation module that is based on the Coherence Vector Simulation Engine (CVSE). Further, QD-E is fully compatible to QCA designs generated with the QCADesigner version 2.0.3

This manual details the use of the additional module, its simulation options and the output. For the theoretical background, please refer to [2-4].

2 SIMULATION SETUP

In order to choose the correct simulation engine, go to **Simulation > Simulation Engine Setup…** and select **Coherence Vector (w/ Energy)**.

In order to modify the simulation options, go to **Simulation > Simulation Engine Setup…** and select **Options.** Following window in Figure 1 will appear.

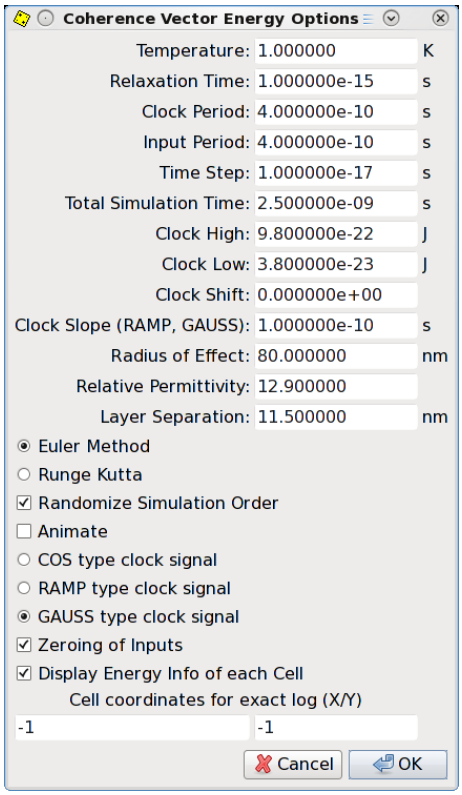

Figure 1: Simulation Options

The options are detailed in Table 1. Please note that the standard QCA cell distance is 20 nm and the standard QCA cell dimensions are 18 nm x 18 nm.

Table 1: Overview of Simulation Options

Option	Symbol	Description	Standard Value
Temperature	Temp	Operating temperature	1 K
Relaxation Time	τ	Damping factor for change of the quantum state, defines how strong the QCA cells are coupled to the environment [2]	1E-15 s
Clock Period	$T\gamma$	Period of all clock signals	10E-12 s
Input Period	Tin	Base period of the input signals. Increases by factor 2 for each input	10E-12 s
Time Step	$Tstep$	Time interval of each iteration step. The smaller the interval, the more accurate the simulation.	1E-17 s
Total Simulation Time	$Tsim$	Total simulation time	80E-12 s
Clock High	γ_H	Max. saturation energy of the clock signals	9.8E-22 J
Clock Min	γ_L	Min. saturation energy of clock signal	3.8E-23 J
Clock Shift		Adds positive or negative energy to the clock signals	0
Clock Slope (RAMP, GAUSS)	$\gamma slope$	Rise and fall time of the clock signal slopes of GAUSSIAN or RAMP shaped clock signals are chosen	1E-12 s
Radius of Effect	r_{effect}	Maximum distance between cells whose interaction is considered. The behavior of a cells depends only on cells within this radius.	80 nm
Relative Permittivity	E_r	Relative permittivity of material for QCA system	12.9*
Layer separation		Distance between QCA layers in case of multi-layer crossings	11.5 nm
Euler Method Runge Kutta	Two different algorithms used to evaluate the differential equation.		Euler
Randomize Simulation Order	When active, the order in which cells are simulated is randomized in each iteration.		ON
Animate	When active, the circuit will be animated throughout the simulation.		OFF
COS type clock signal RAMP type clock signal GAUSS type clock signal	Shape of the clock signal. COS is a cropped cosines function (similar to the standard QCADesigner)		GAUSS

	RAMP is a ramp function GAUSS is a Gaussian shaped function. The length of the slopes of RAMP and GAUSS are defined via the parameter γ_{slope}	
Zeroing of inputs	If active, polarization of inputs depends on the clock signal (see also below)	ON
Display Energy Info of each cell	The output window will contain detailed information about the energy flow of each cell	ON
Cell coordinates for exact log X/Y	Coordinates of the cell whose detailed values are logged in the file Diss.trace	-1 / -1 (OFF)

If the option **Zeroing of inputs** is enabled, the polarization of input cells follows the phase of the related clock signal and is no longer constant throughout a complete clock cycle, as shown in Figure 2. Hence, when the related clock signal of the input is in release and relax, then the input has no polarization. Consequently, if **Zeroing of inputs** is activated, it is **mandatory to verify whether the input cell and the neighboring cells are in corresponding clock zones**, i.e. all QCA cells are in the same clock zone or the neighboring cells are in the next clock zone.

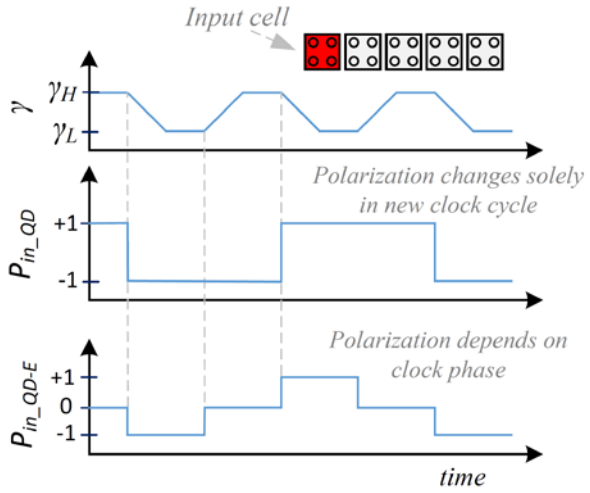

Figure 2: Zeroing of Inputs

It is possible to remove QCA cells from the energy analysis, by choosing the option **Ignore Energy Dissipation** in the **Cell Function** menu shown in Figure 3 (accessible via a Double-click on the cell). Cells that are ignored during the energy analysis are colored in purple. These cells will be simulated in a normal way and also its energy will be calculated. However, their energy dissipations and the related errors will be ignored in the final summation of all energy dissipations of all QCA cells of the design. Please not, that input cells have an energy dissipation of 0, in contrast to output cells, for which the option **Ignore Energy Dissipation** must be activated if it shall be ignored.

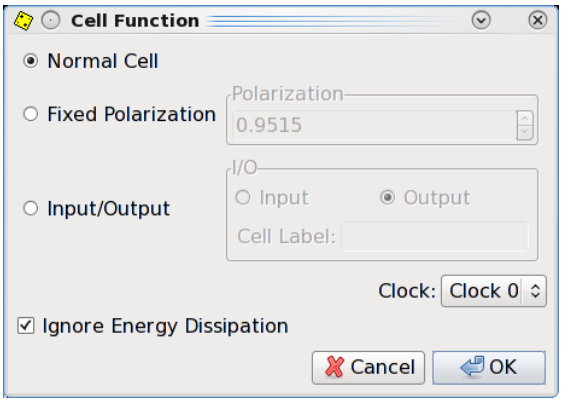

Figure 3: Cell Options (incl. Ignore Energy Dissipation)

3 SIMULATION RESULTS

At the end of each simulation, the output window of the QD-E will contain information of cells that have been ignored at the summation of the energy dissipations, with the format

Ignore for total energy/error: Layer: *L*, Cell [A_X] [A_Y] (*X* ; *Y*)

With *L* is the layer of the cell, A_X and A_Y are its 'array coordinates' (see below), and *X* and *Y* are the coordinates in the QD-E editor. The 'array coordinates' have been introduced in order to facilitate the analysis of the results. Therefore, the QCA cell at the most top-left position receives the 'array coordinates' [1][1]. The coordinates of all other cells follow from this definition assuming a virtual grid as shown in Figure 4.

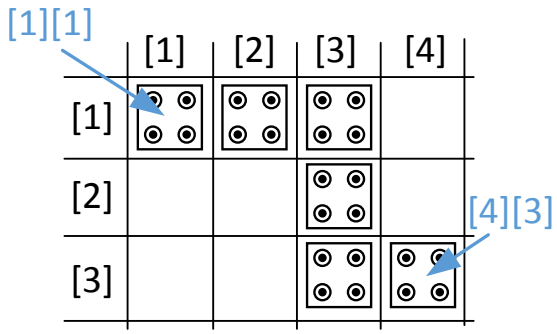

Figure 4: Array Coordinates

Further information listed in the output window of the QD-E are

E_bath_total: E_{bt1} E_{bt2} **...**
E_clk_total: E_{ct1} E_{ct2} **...**
E_Error_total: E_{Et1} E_{Et2} **...**
Sum_bath: S_b **(Er:** S_{bE}**)**
Avg_bath: A_b **(Er:** A_{bE}**)**
Sum_clk: S_c**, Avg_clk:** A_c

With E_{btx} is the sum of all energy transfers to the bath of all QCA cells separated for each clock cycle (see below are more detailed definition of 'clock cycle'), E_{ctx} is the sum of all energy transfers between QCA cells and the clock separated for each clock cycle (positive: clock receives energy, negative: clock transfers energy to the cells) and E_{Etx} is for each clock cycle the sum of all errors of the QCA cell's energy analysis. The Error follows from the assumption that the sum of all energy flows of a QCA cell is zero over a whole clock cycle, i.e. Error = E_bath - (E_clock + E_IO).

Further, S_b is the sum of all energy transfers to the bath during the whole simulation and S_{bE} is the related error. A_b and A_{bE} are the average values of the energy transfers to the bath and the error for each clock cycle. S_c is the sum of the energy transfer to/from the clock during the whole simulation, while A_c is the average energy transfer during a clock cycle.

Please note that for all above variables the cells marked with the option **Ignore Energy Dissipation** are not considered. Further, all energy values are given in eV.

If the option **Display Energy Info of each cell** was chosen, the output window of the QD-E will contain for each cell following information:

Layer: *L*, Cell [A_x] [A_y] (*X* ; *Y*), idx = I
E_bath: E_{b1} E_{b2} **…**
E_clk: E_{c1} E_{c2} **...**
E_io: E_{io1} E_{io2} **...**
E_in: E_{in1} E_{in2} **...**
E_out: E_{out1} E_{out2} **...**
E_Error: E_{E1} E_{E2} **...**
Ek[*cx*] = E_{kcx}

With I is the index of the cell and E_{bx}, E_{cx}, and E_{Ex} are the values for the energy transfers of the QCA cell with the bath and the clock and the related error, respectively, for each clock cycle. E_{iox} is the energy transfer of the QCA cells with its neighboring cells, that are located in the radius defined with via the parameter **Radius of Effect.** E_{inx} and E_{outx} relate to the energy transfer with cells located in the left side (E_{inx}) and the right side (E_{outx}) of the current QCA cell. Please note, that these values are only of interest for wires. E_{kcx} is the kink Energy E_{kink} between the current QCA cell and the neighboring cells *cx* within the radius of the parameter **Radius of Effect**. Please note that the listing contains no information about the position of the cells *cx*.

The energy values calculated in each time step are integrated over a whole period of the clock signal of the clock zone of the cell. Here, the integration interval starts and ends when the rising clock signal passes the middle value of the clock signal (see also Figure 5). The related values are listed for each cell if the option **Display Energy Info of each cell** was chosen. In case of the energy dissipation of the whole design, given per 'clock cycle', the energy dissipations of related clock phases of the clock zones are added. This is detailed in Figure 5.

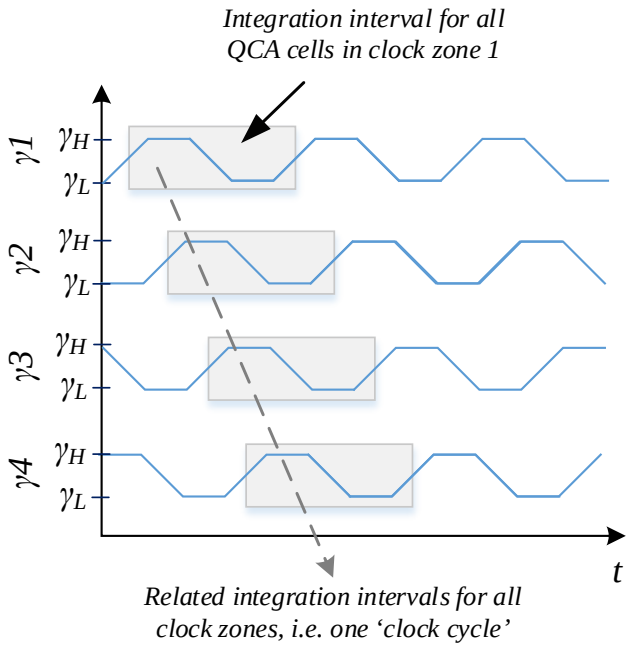

Figure 5: Integration interval for cells in the four clock zones and related integration intervals of one 'clock cycle'. γx are the clock signals of each clock zone.

If viable coordinates for the option **Cell coordinates for exact log X/Y** has been chosen, then the file diss.trace is generated in the main folder of the program. Please note that X and Y must be coordinates of the n the QD-E editor and not the array coordinates. Further, this option might increase considerably the simulation time. Each row of the file contains following values calculated for each time step:

#1 time,
#2 lambda_z // previous λ_z value
#3 lambda_z_new // new calculated λ_z value
#4 lambda_z-lambda_z_new
#5 l_ss_z // steady state value for λ_z
#6 sl_z // time_step multiplied with current $d\lambda_z$
#7 l_ss_z-lambda_z_new
#8 l_ss_x-lambda_x_new
#9 diss_bath // current value of dissipation to the bath
#10 PEk_in // Polarization * E_{kink} of left hand cells
#11 diss_in // current value of energy transfer with left hand cells
#12 diss_out // current value of energy transfer with right hand cells
#13 diss_clk // current value for energy transfer with clock
#14 clock_value // γ
#15 Pol // polarization
#16 Pol_in // polarization of left hand cells
#17 Pol_out // polarization of right hand cells
#18 PEk // Polarization * E_{kink} of all neighboring cells

Please refer to the theoretical background works for more details [2-4]. The file gnu.plot in the src folder of the project contains an exemplary script for the tool gnuplot.

4 REFERENCES

[1] K. Walus, T. J. Dysart, G. A. Jullien, and R. A. Budiman, "QCADesigner: a rapid design and Simulation tool for quantum-dot cellular automata," *IEEE Transactions on Nanotechnology,* vol. 3, pp. 26-31, 2004.

[2] J. Timler and C. S. Lent, "Power gain and dissipation in quantum-dot cellular automata," *Journal of Applied Physics,* vol. 91, pp. 823-831, Jan 15 2002.

[3] C. S. Lent, L. Mo, and L. Yuhui, "Bennett clocking of quantum-dot cellular automata and the limits to binary logic scaling," *Nanotechnology,* vol. 17, p. 4240, 2006.

[4] J. Timler and C. S. Lent, "Maxwell's demon and quantum-dot cellular automata," *Journal of Applied Physics,* vol. 94, pp. 1050-1060, 2003.