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TQCAsim: An accurate design and essential simulation tool for ternary logic quantum-dot cellular automata

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Abstract. Having a reliable simulation tool for evaluating the performance of each design is indispensable. Designing Multiple-Valued Logic (MVL) systems helps overcome the limitations associated with binary systems. Quantum-dot Cellular Automata (QCA) is a technology that can be substituted for Complementary Metal-Oxide-Semiconductor (CMOS) in MVL designs. This paper represents an exquisite software platform for designing and simulating circuits that are restricted to Ternary QCA (TQCA). Working with TQCAsim is so convenient because it can run on both Windows or Linux-based computers. It has a tenacious simulation engine that can ensure precise results. This tool shows the results in graphical formats. Moreover, designers can easily layout their ternary QCA designs using various sets of CAD tools. In this paper, the ternary model of QCA and its energy calculation will be demonstrated. The simulation process is explained step by step. MIN, MAX, NOT, and XOR gates were simulated already by this software.

1. Introduction

The Quantum-dot Cellular Automata (QCA) is one of the new developing technologies, which is a suitable candidate for Complementary metal-oxide-semiconductor (CMOS) replacement in the future [1,2]. Logic circuit designers had proposed their designs over the past two decades [3,4]. QCA cells (semiconductor and metallic) have been fabricated and examined. The fabrication of molecular QCA was a remarkable achievement for developers because it can operate at room temperature [5,6]. Plenty of creative designs have been proposed and published in the field of Binary QCA (BQCA) logic [7–13] and ternary [14–17].

Compacting data in fewer bits is achieved by modeling systems in Multiple-Valued Logic (MVL). A significant amount of data can be transferred in MVL systems compared with binary ones [18]. MVL designs can provide faster numerical analysis and arithmetic operations, but designing and simulating these types of systems is not so easy and needs its CAD tools [19].

Every innovative concept needs a particular way of determining its functionality. The ternary QCA lacked simulation tools. This work represents a tool that is capable of simulating complex ternary QCA circuits. In this paper, the functionality of the software would be clarified step by step. TQCAsim uses a fast simulation engine that makes the computation performed in a fraction of time. In other published work, only the ternary QCA circuits have been proposed without explaining the software structure [20–22]. Section 2 presents the ternary QCA basics. Sec-

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tion 3 highlights the main functions of the simulator. Section 4 gives a benchmark for evaluating TQCAsim performance. Section 5 describes incoming plans that would make TQCAsim more thriving. At last, Section 6 concludes this paper.

2. Ternary QCA basics

The QCA is a flourishing technology that can carry out computations by Coulombic interaction, while CMOS is dependent on the electrical current [23,24]. A QCA cell is a square nanostructure with some quantum wells confining free electrons [25]. A certain number of quantum-dots have been embedded in each cell so that the mobile pair of electrons can tunnel between them. There are four quantum-dots in BQCA while only two in Ternary QCA (TQCA).

According to the Coulombic law, the two electrons will not be distributed in precarious situations among the quantum-dots, i.e., they reside furthest away from each other [25]. Figure 1 shows different modes of electrons positioning in a TQCA cell. A, B, C, D are stable modes (electrons are located at a far distance from each other due to the Coulomb repulsion effect), and the X modes are unstable.

TQCA has a polarization states that can be related to the logic values. However, there is a discrepancy between the number of polarization states in TQCA and the number of ternary logic values. There are four stable polarization states for TQCA cells (A, B, C, and D), which are equivalent to logic values −1, +1, 0, and 0, respectively (balanced ternary). So, there are two possible states (C and D) with an identic value (0). Figure 2 exhibits all four possible configurations of a TQCA cell.

The similarity between BQCA and TQCA is that

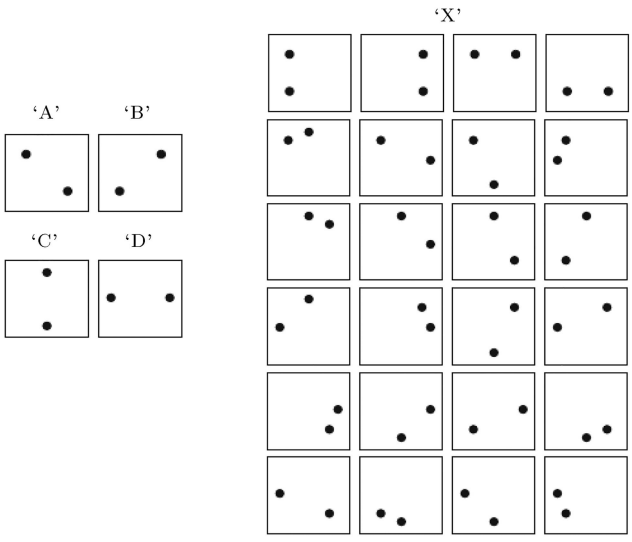


Figure 1. Different modes of electrons positioning in a TQCA cell.

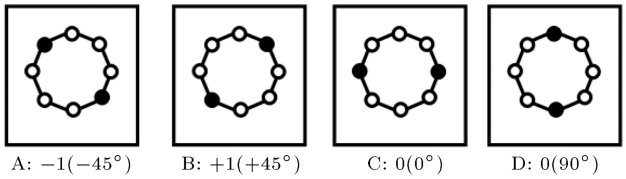


Figure 2. Four possible configurations of a TQCA cell.

states A and B in the ternary mode are the same in binary. Also, the analogy between them in the clock issue is explicit. All four phases of the clock (switch, hold, release, and relax) in TQCA are the same in BQCA. These clocks are being used to push information from inputs to the outputs by modifying the cells' tunneling energy. The whole circuit is segmented into zones. Each zone is associated with one of the four clocks in sequence [26].

2.1. Utilized TQCA cell

As mentioned in Section 1, QCA implementation is already divided into four categories: metal [27], semiconductor [28], molecular [29,30], and magnetic [31]. The other advantage of molecular QCA rather than working at room temperature is that it can be fabricated at minute dimensions. Therefore, TQCAsim is based on this type of QCA implementation. Figure 3 shows the utilized TQCA cells in this work. However, TQCAsim can scale the cell's dimensions.

2.2. Energy calculation

TQCAsim is based on calculating external electrostatic energy between neighbor cells. It computes the distance between the electron's positions in adjacent cells. It is quite noticeable that two QCA cells could be adjacent in horizontal, vertical, or even diagonal directions. Figure 4 shows the distances between electrons of two adjacent cells if both of them remain in the 'B'

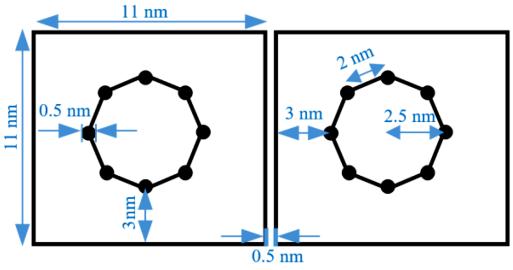


Figure 3. Utilized TQCA cells.

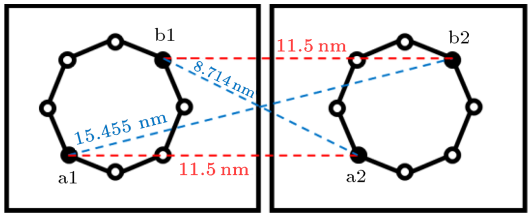


Figure 4. Distance between electrons of two adjacent cells in the 'B' polarization state.

polarization state, i.e., it was assumed that both of the input (left one) and output (right one) cells had +1 (+45) values.

Each cell affects the neighboring cells by means of external electrostatic energy. This energy can be attained from Eq. (1):

$$E_{external} = \frac{1}{4\pi\varepsilon_0\varepsilon_r}\sum_{i=0}^{m}\sum_{j=0}^{n}\frac{q_i q_j}{d_{ij}}, \quad (1)$$

where ε_0 and ε_r are vacuum and substance relative permittivity coefficients, respectively. q_i and the q_j are the charges of dots in the cell, and d_{ij} is the distance between the two. The external electrostatic energy calculation between the electrons of two adjacent cells in Figure 4 is as follows:

$$E_{e1} = E_{a1-a2} = 2.005\text{e}-20\text{J},$$

$$E_{e2} = E_{b1-b2} = 2.005\text{e}-20\text{J},$$

$$E_{e3} = E_{a1-b2} = 1.492\text{e}-20\text{J},$$

$$E_{e4} = E_{b1-a2} = 2.646\text{e}-20\text{J}. \quad (2)$$

The ultimate energy quantity would be obtained by subtracting the summation of similar named energies and the dissimilar named energies. Eq. (3) demonstrates the conclusive energy quantity for Figure 4.

$$E_t = (E_{e3} + E_{e4}) - (E_{e1} + E_{e2}) = 0.128\text{e}-20\text{J}. \quad (3)$$

All the other possible states with their final energy quantities are shown in Figure 5. The correct output state is the one with the minimum energy value among different states due to the final energy results in Figure 5. For example, if the input value is +1 (+45), the output value will be +1 (+45). Further investigations into diverse states with their energy calculation were documented [20].

3. Simulation setup

This project was written in C# under Microsoft Visual Studio. The GUI interface of TQCAsim was developed using Windows Forms. Linux users may also use this tool by installing the Windows application runtime (EXE) like Wine and .NET Framework runtime libraries. TQCAsim uses the .NET library to generate graphical models. The objective of this project is to create an easy-to-use simulation and layout tool. The latest version of the software can be found in [32].

Innovative TQCA designs were documented as proof-of-concept experiments [20–22]. The other authors have proposed ternary architectures using TQCAsim and confirmed the correct operation of our CAD tool [33,34].

Figure 6 illustrates the flowchart of the program in a general schema. In the following, the functionality of each section is explained.

3.1. Modeling scheme

A 16 × 32 cell matrix is considered to design logic circuits in the current version of the software layout environment. A TQCA circuit may consist of four different types of cells:

- Input/output cell;
- Cell with fixed polarity;
- Intermediate cell;
- Interface cell.

Each type of cell is shown with a distinct color in the layout environment, i.e., the color of each one depends on the cell's type.

At first, the kind of each cell must be determined by the user. The simulator employs a relevant icon for each cell according to its type. Then, appropriate clocks should be assigned. The software would enter the simulation phase by pressing the simulation key. It

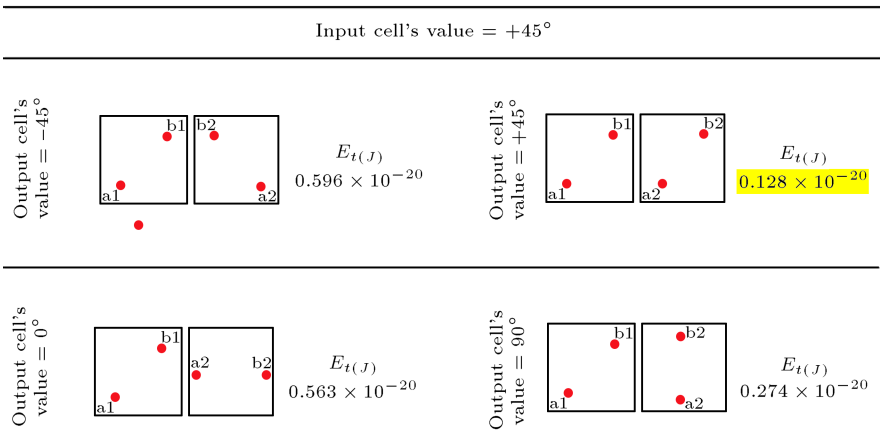


Figure 5. Energy calculation for two adjacent cells.

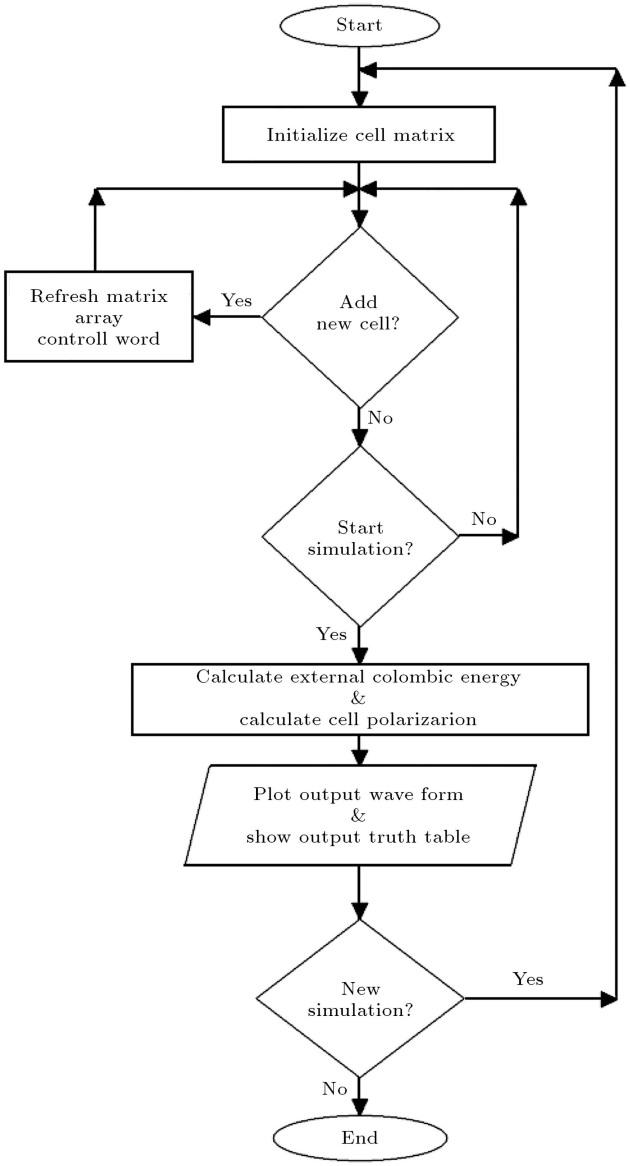


Figure 6. General flowchart of the simulator.

will consider all different possible values for inputs and will display the truth-table.

3.2. Simulation process

The polarity of the intermediate and output cells will be specified according to the energy calculations among cells at the simulation stage. The sequence of the simulation steps is listed below:

1. *Calculating the number of input/output cells and saving their coordinates in an array of global type.* The circuit's outputs should be computed and displayed in the truth-table with all possible combinations of inputs. Therefore, the number of input and output cells is counted and stored in a global-type variable in the first step of the simulation.
2. *Entering into the initializing loop of the input cells.* At this point, three values of ternary (0, −1, +1) would be replaced for each input cell. Subsequently, the output would be calculated for them. For example, for a circuit with two input cells, the simulator will calculate the output cells for nine different combinations.
3. *Determining the priority of intermediate cells based on their positions and clock's phases.* One of the most important steps is to determine the order of fixed-polarity cells' effect. As mentioned earlier, the polarity of the middle cells is affected by the cells with fixed polarity under the Coulomb interaction force. This effect is inversely related to the distance between them, i.e., the longer the distance between the cells yields less effect on each other. Therefore, the simulator considers the number of fixed-polarity cells around the surrounded cell with their distance from each other. The coordinates of the surrounded cell with its clock's phase are given as inputs to the calculator function. Therefore, numbers from 0 to 280 will be produced as a distribution priority output. Cells with fixed polarity adjacent to the target cell with one neighborhood interspace have the highest priority as Rank 5. Cells with fixed polarity adjacent to the target cell with two neighborhood interspaces are of lower priority as Rank 4 at the second round of ranking. The task of priority determination is performed for five neighborhood interspaces in the case of each cell. Figure 7 shows the priority values for one and two neighborhood interspaces. Thus, the maximum calculated priority for each cell is 280 (40 + 64 + 72 + 64 + 40 = 280).

   According to the QCA's clock principle, only cells with the same phase or −90 degrees shifted phase affect their neighbors. Therefore, the priority would be determined separately for cells with diverse clocks. The point is that cells' polarization with the same precedence will simultaneously be determined. For example, Figure 8 shows the calculated priority for a typical circuit. In this circuit, the highest priority is allotted to cell C. Cells A and B have lower priorities.

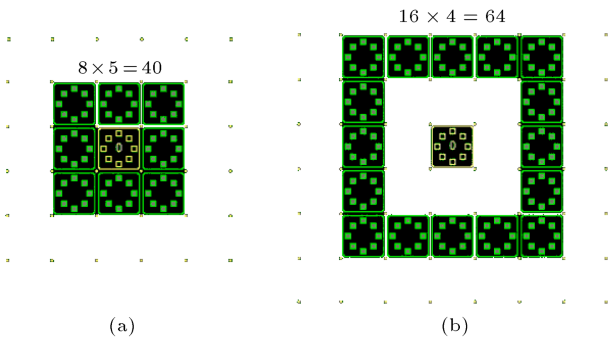
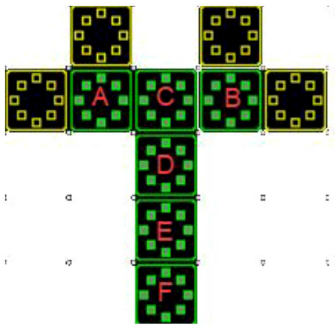


Figure 7. Priority values for (a) one and (b) two neighborhood interspaces.



$A = (5 + 5 + 4 + 3) = 17$
$B = (5 + 5 + 4 + 3) = 17$
$C = (5 + 5 + 4 + 4) = 18$
$D = (4 + 4 + 4 + 4) = 16$
$E = (4 + 4 + 3 + 3) = 14$
$F = (3 + 3 + 2 + 2) = 10$

Figure 8. Calculating priority.

4. *Specifying the intermediate cell's polarity according to its predefined priority.* The next step is to specify the polarity for intermediate cells due to their priority from the highest down to the lowest one. Cell C is the first cell whose polarity is specified in Figure 8. Then, the polarity of cells A and B would be individually and without considering the effect of each other. The polarity of cells D, E, and F remains to be considered in the next steps. Polarity is assigned to the cells according to the energy calculation, as discussed in Section 2.

3.3. Results display

The truth table of the circuit will be plotted right after the calculation hierarchy ends. Figure 9 shows a sample circuit with its truth table. This software verifies the outputs for all possible input combinations. Figure 10 shows a snapshot of the TQCAsim while displaying the result. As can be seen, the tool displays the inputs and outputs by four different clock signals. TQCAsim's team attempted to form a user interface similar to the QCADesigner [35] so that designers who had previously worked in the binary field would feel comfortable working with this software.

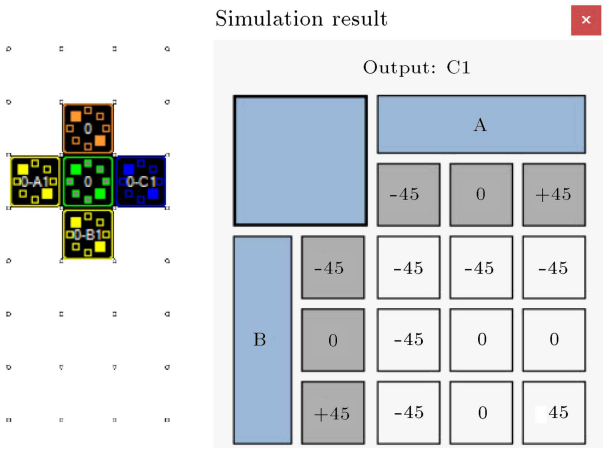


Figure 9. A sample circuit with its truth table.

4. Performance benchmark

In this section, a benchmark is given for evaluating the performance of TQCAsim. We have tested this software on two different systems. System 1 has an obsolete CPU and operating system. On the other hand, System 2 has an advanced CPU and an up-to-date operating system. In this benchmark, three primary ternary gates (NOT, AND/OR, and Majority) were simulated '10' times in a row at a specified run time. Figure 11 shows the schematics of these gates. Table 1 comprises the benchmark results.

The TQCAsim needs only 10.8 MB of free space on a drive. As can be seen from Table 1, TQCAsim has

Table 1. Benchmark results.

	CPU		Memory	Run-time	
	Threads[a]	Avg[b]	Private[c] (kB)	(sec)	
System 1					
Processor: Intel® Core™2 DUO T8300 @ 2.4GHz	6	3.22	40904	60	**Not**
Installed Memory: 4.00 GB	7	3.13	42628	105	**And/or**
Operating System: Windows 7	7	4.57	43380	135	**Majority**
System 2					
Processor: Intel® Core™ i7-9750H @ 2.6GHz	4	0.6	40432	60	**Not**
Installed Memory: 32.00 GB	5	0.28	41480	105	**And/or**
Operating System: Windows 10	6	0.57	42408	135	**Majority**

a: Threads: Number of active threads;

b: Avg: Average percent of CPU consumption by the process (60 sec);

c: Private: The amount of physical memory in use by the process that cannot be used by other processes in KB.

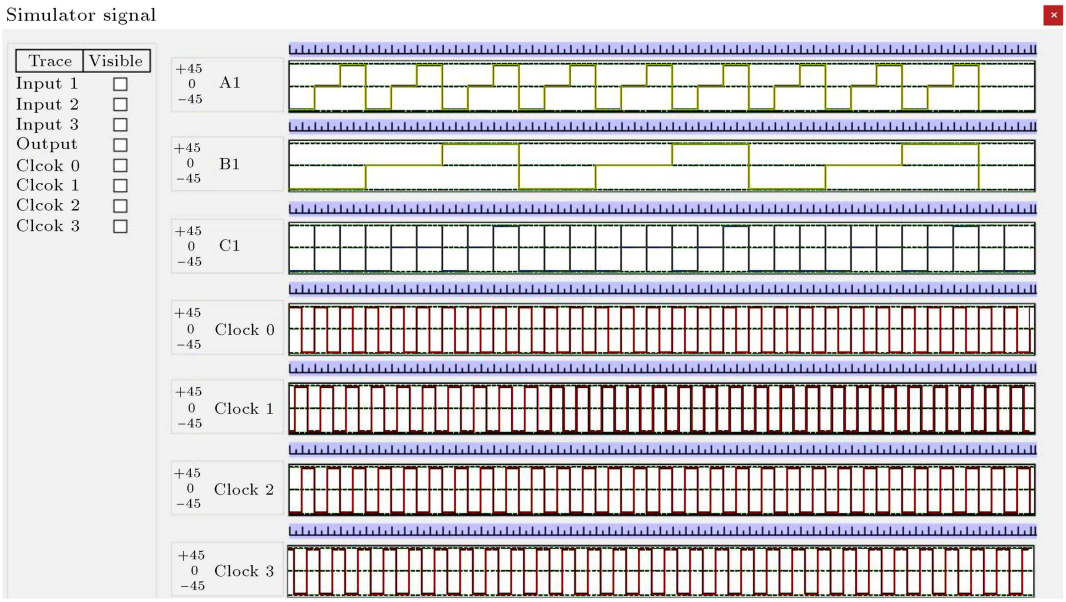


Figure 10. Simulation result of the sample circuit.

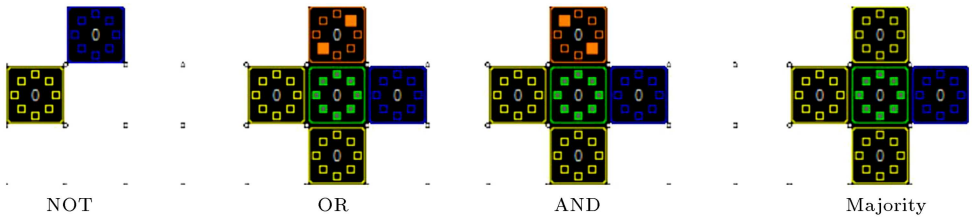


Figure 11. Primary ternary gates.

a very low CPU usage, even in an obsolete system. The amount of memory used is small enough.

5. Future work

Our QCA-team is constantly striving to offer comprehensive software for TQCA-systems designers. For this purpose, we redesigned the simulating-process and user interface for a faster and better startup in each version that seems necessary. The ability to customize layout size would appear in the next versions. Moreover, the ability to add more cell structures is under consideration. These features will allow users to simulate more intricate designs. We are trying to offer an improved tool for TQCA enthusiasts in every version of this software.

6. Conclusion

Every innovative concept needs a particular way to determine its functionality. TQCAsim is an accurate CAD tool that has been designed exclusively for ternary Quantum-dot Cellular Automata (QCA) logic designs and simulations. This tool has the ability to layout and verify any Ternary QCA (TQCA) systems. The simulation results are shown in graphical formats. Although TQCAsim is currently in its infancy, great strides are made to enhance its usability and functionality in every version of this tool.

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Biographies

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