Automata noise
in diffusion cellular-automata models*

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Abstract. Two new cellular-automata models of the diffusion process are proposed. They are based on integer states of cells instead of Boolean ones in the known models: asynchronous naive diffusion by Toffolli and block-synchronous Margolus diffusion. Computing experiments have been carried out with these models; they demonstrate a good correlation with this physical phenomenon. A dependence of a maximum state value of the multi-particle model on the averaging radius of the Boolean one with equal automaton noise level is obtained. The main advantages of the proposed models are (i) low automata noise and (ii) variable diffusion rate.

1. Introduction

Following the common practice, the diffusion process is represented by the differential equation. Usually, computers solve this equation because its analytical solution cannot be obtained. But computers operating with real numbers accumulate round-off errors. In addition, complicated boundary conditions cause certain difficulties.

Since the end of the last century cellular automata have been used for the diffusion process simulation. One of them is an asynchronous cellular automaton of naive diffusion, proposed by Tomasso Toffolli [1]. Another one is a block-synchronous cellular automaton that was offered by Norman Margolus [1]. Both of them operate over the Boolean alphabet, therefore no round-off errors are available.

A noise is aperiodic oscillating of a certain physical quantity. A noise which is caused by the influence of discrete nature of cellular automata, we call the automaton noise.

In this paper, an attempt to eliminate the problem of noise in Boolean-valued cellular-automata simulation is undertaken. For each of the referred Boolean models an analog, which operates over integers, is proposed. Computer experiments with the proposed models are executed, their behavior is investigated, and a dependence of a maximum state value of the multi-particle model on the averaging radius of the Boolean one with an equal automaton noise level is obtained.

2. Main definitions

2.1. Boolean models. A 2D cellular automaton of diffusion has the cellular array $W = \{w_{ij} : i \in [1, I], j \in [1, J]\}$; $|W| = I \cdot J$ being the cardinality of the array. The cells $w_{ij} \in W$ are arranged in the Cartesian plane according to Figure 1. Each cell $w_{ij} \in W$ has a state $s(w_{ij}) \in \{0, 1\}$. A value

i $\diagdown$ j	1	2	3	4	5
1	w_{11}	w_{12}	w_{13}	w_{14}	w_{15}
2	w_{21}	w_{22}	w_{23}	w_{24}	w_{25}
3	w_{31}	w_{32}	w_{33}	w_{34}	w_{35}
4	w_{41}	w_{42}	w_{43}	w_{44}	w_{45}
5	w_{51}	w_{52}	w_{53}	w_{54}	w_{55}

Figure 1

of the state $s(w_{ij})$ shows which of two substances (let us call them "zero" and "one") is present in the cell w_{ij}. A set of the states $s(w_{ij})$ of all cells $w_{ij} \in W$ at the same instant t is called a global state $\sigma(t) = \{s(w_{ij}) : i \in [1, I], \ j \in [1, J]\}$ of the cellular automaton. In a cellular automaton with a synchronous operation, each iteration is a replacement of states $s(t)$ in all cells by states $s(t + 1)$. The cellular automaton thus changes its global state $\sigma(t)$ by a new global state $\sigma(t+1)$. An iteration of an asynchronous cellular automaton is a sequence of events. Each event is a replacement of a randomly chosen cell state $s(t)$ by the state $s(t + 1)$. The number of the events per iteration is equal to $|W|$.

A model concentration of each substance c_0 and c_1 in any cell $w_{ij} \in W$ is calculated by means of summing up over an averaging vicinity $\mathrm{Av}(w_{ij})$ with some radius r:

$$
\begin{aligned}
c_0(w_{ij}) &= \frac{1}{|\,\mathrm{Av}(w_{ij})|} \sum_{w \in \mathrm{Av}(w_{ij})} (1 - s(w_{ij})), \\
c_1(w_{ij}) &= \frac{1}{|\,\mathrm{Av}(w_{ij})|} \sum_{w \in \mathrm{Av}(w_{ij})} s(w_{ij}).
\end{aligned}
\tag{1}
$$

The vicinity $\mathrm{Av}(w_{ij})$ consists of the cells which are not further than r from w_{ij}.

2.2. Multi-particle models. The multi-particle cellular automaton differs from Boolean one in that it has integer-valued states $s(w_{ij})$ of cells $w_{ij} \in W$; $s(w_{ij})$ being in the interval $s(w_{ij}) \in [0, S]$, where S is the number of particles, corresponding to a maximum concentration of substance "one" in a cell. The value of $s(w_{ij})$ shows the number of the substance "one" particles in the cell w_{ij}. Concentrations of substances "zero" and "one" in the cell w_{ij} are equal to $S - s(w_{ij})$ and $s(w_{ij})$, respectively.

The model concentrations c_0 and c_1 of each substance, respectively, are calculated as follows:

$$c_0(w_{ij}) = \frac{1}{|\operatorname{Av}(w_{ij})| \cdot S} \sum_{w \in \operatorname{Av}(w_{ij})} (S - s(w_{ij})),$$

$$c_1(w_{ij}) = \frac{1}{|\operatorname{Av}(w_{ij})| \cdot S} \sum_{w \in \operatorname{Av}(w_{ij})} s(w_{ij}). \tag{2}$$

A radius r of the averaging vicinity Av can be diminished up to zero, and this will not excessively increase the automaton noise, like in the Boolean models. So, it is possible to use an automaton with a smaller in comparison with the Boolean model amount of cells.

3. Naive diffusion

3.1. Boolean model. The Boolean asynchronous cellular automaton simulates a diffusion process as follows. Each cell of the automaton $w_{ij} \in W$ is located at some point of a plane and has four neighbors. In Figure 2, a cross template with the cell w_{ij} and its neighboring cells a, b, c, and d is given. At each iteration, the following steps are done:

i \ j	1	2	3	4	5
1					
2			a		
3		d	w_{ij}	b	
4			c		
5					

Figure 2

1. A random cell $w_{ij} \in W$ is equiprobably selected.

2. One of four neighboring cells $w_k \in \{a, b, c, d\}$ is equiprobably selected.

3. Cells w_{ij} and the selected one w_k exchange their states $s(w_{ij})$ and $s(w_k)$.

The above iteration is repeated many times. After that, averaging (1) should be executed for obtaining the concentrations c_0 and c_1 for every cell of the array. The effect of operation of such an automaton is infiltration of substance "zero" into substance "one" and vise versa.

3.2. Multi-particle model. At each iteration, the following steps are done:

1. A random cell $w_{ij} \in W$ is equiprobably selected.

2. One of the four neighboring cells $w_k \in \{a, b, c, d\}$ is equiprobably selected.

3. The quantities of particles s representing the state value in each of the cells w_{ij} and w_k are divided into the two groups s_k and s_{1-k} as follows:

$$s_k(w_{ij}) = \lfloor k \cdot s(w_{ij}) \rfloor + s'(w_{ij}), \quad s_{1-k}(w_{ij}) = s(w_{ij}) - s_k(w_{ij}),$$
$$s_k(w_k) = \lfloor k \cdot s(w_k) \rfloor + s'(w_k), \quad s_{1-k}(w_k) = s(w_k) - s_k(w_k),$$

where $k \in (0, 1]$ is a certain parameter determining a model diffusion rate; $s'(w) = 1$ with the probability $k \cdot s(w) - \lfloor k \cdot s(w) \rfloor$ and $s'(w) = 0$ otherwise; $\lfloor x \rfloor$ denotes the floor x.

4. A group of particles $s_k(w_{ij})$ moves from the cell w_{ij} to the cell w_k, while a group of particles $s_k(w_k)$ moves in the contrary direction, where $w_k \in \{a, b, c, d\}$. Thus, their new states are

$$s(w_{ij}) = s_{1-k}(w_{ij}) + s_k(w_k), \quad s(w_k) = s_{1-k}(w_k) + s_k(w_{ij}).$$

After the assigned number of iterations, averaging (2) should be executed for obtaining the concentrations c_0 and c_1. An expected result is the same as in the Boolean model, differing only in that the amount of the automaton noise is less.

4. Margolus diffusion

4.1. Boolean model. In the Boolean cellular automaton of the Margolus diffusion, a template is a square of 2×2 cells. In this model, the even and the odd iterations are distinguished. They are executed in a different way. In Figure 3a, the even partitioning (for using at the even iterations) is given; both indices i and j of the upper left cell of the blocks of 2×2 cells are even. In Figure 3b, the odd partitioning (for using at the odd iterations) is given; i and j of the upper left cell are odd. Because of the synchronous mode of the Margolus diffusion, the transition rule in all the blocks is applied simultaneously. At each iteration in each block, the following steps are carried out:

i \ j	1	2	3	4	5
1	c	d	c	d	c
2	b	a	b	a	b
3	c	d	c	d	c
4	b	a	b	a	b
5	c	d	c	d	c

a) even partitioning

i \ j	1	2	3	4	5
1	a	b	a	b	a
2	d	c	d	c	d
3	a	b	a	b	a
4	d	c	d	c	d
5	a	b	a	b	a

b) odd partitioning

Figure 3. Cellular array partitioning for the Margolus diffusion

1. The direction of rotation is selected either clockwise or counterclockwise equiprobably, independent of other blocks.

2. The cells a, b, c, and d in each block exchange their values $s(a)$, $s(b)$, $s(c)$, $s(d)$ around a circle, according to a selected direction ($a \to b \to c \to d \to a$ or $a \to d \to c \to b \to a$).

The necessary number of iterations is to be repeated. After that, averaging (1) should be executed for calculating the concentrations c_0 and c_1 in every cell of the array. In [2], it is proved that the Boolean Margolus block-synchronous cellular automaton exactly simulates the diffusion process.

4.2. Multi-particle model. At each iteration in each block, the following steps are carried out:

1. The direction of rotation is selected either clockwise or counterclockwise equiprobably, independent of other blocks.

2. The number of particles $s(a)$, $s(b)$, $s(c)$, and $s(d)$ in each of the cells a, b, c, and d is divided into the two groups s_k and s_{1-k} as follows:

$$s_k(a) = \lfloor k \cdot s(a) \rfloor + s'(a), \quad s_{1-k}(a) = s(a) - s_k(a), \quad \text{etc.},$$

where $k \in (0, 1]$ is a parameter of a model diffusion rate; $s' = 1$ with the probability $k \cdot s - \lfloor k \cdot s \rfloor$, and $s' = 0$ otherwise; $\lfloor x \rfloor$ denotes the floor of x.

3. The cells a, b, c, and d in each block exchange their values $s_k(a)$, $s_k(b)$, $s_k(c)$, $s_k(d)$ around a circle, according to a selected direction. In the case of the clockwise exchange, their states thus will be equal to

$$s(a) = s_{1-k}(a) + s_k(d), \qquad s(b) = s_{1-k}(b) + s_k(a),$$
$$s(c) = s_{1-k}(c) + s_k(b), \qquad s(d) = s_{1-k}(d) + s_k(c).$$

In the case of the counterclockwise exchange, their states thus will be equal to

$$s(a) = s_{1-k}(a) + s_k(b), \qquad s(b) = s_{1-k}(b) + s_k(c),$$
$$s(c) = s_{1-k}(c) + s_k(d), \qquad s(d) = s_{1-k}(d) + s_k(a).$$

After finishing all the iterations, averaging (2) should be executed for obtaining the concentrations c_0 and c_1.

5. Computer simulation

For validation of the proposed models, their program realization has been constructed. This allows carrying out computing experiments with both models. The code has been written in C. The computing experiments, performed with the multi-particle Margolus diffusion model only, are described below. Results of the experiments with the naive diffusion model are identical to the Margolus one we will not dwell on them here.

5.1. Diffusion of a round spot. The first example simulated by the proposed model is rather simple. The size of a cellular automaton is $I = 500$ by $J = 500$ cells. The cells $\left\{ w_{ij} : \left(\frac{I}{2} - i \right)^2 + \left(\frac{J}{2} - j \right)^2 \leq \left(\frac{IJ}{100} \right)^2 \right\}$ are initialized by ones, $s(w_{ij}) = 1$. The rest of the cells are initialized by zeros, $s(w_{ij}) = 0$. So, the substance "one" looks like a round spot on the substance "zero" background. In Figure 4a, the array of the averaged concentration c_1 of the substance "one" in the initial global state is shown. Because of the averaging radius $r = 20$ being significant for the selected size of the cellular array, the boundary between the substances is blurred. After the simulation is completed, the spot of the substance "one" diffuses into the substance "zero" background. In Figure 4b, the result of Boolean model implementation is given; in Figure 4c, the result of multi-particle model implementation is given. The obtained results allow us to conclude the following:

- the models simulate diffusion process correctly;

- the multi-particle model provides a less diffusion rate than the Boolean one;

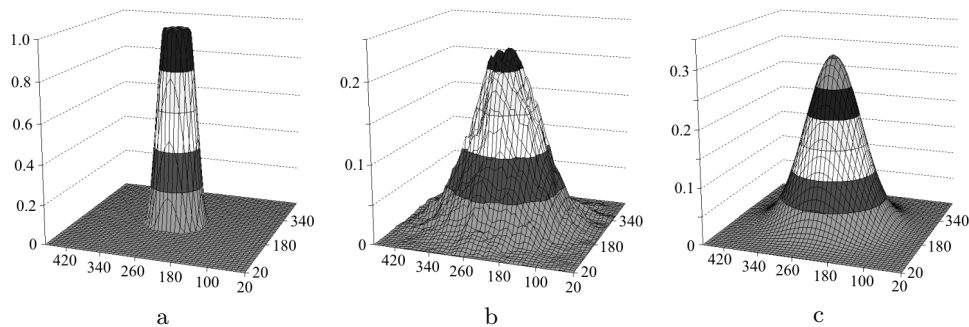- the multi-particle model gives much less noise than the Boolean one.

Figure 4. Diffusion of a round spot: a) the initial state for both models, b) the boolean model, 5,000 iterations, and c) the multi-particle model, 10,000 iterations

The following experiments deal with the automaton noise measurements, and making a comparison between the noise of the multi-particle model and that of the Boolean one.

5.2. Automaton noise measurements. The cellular array $W = \{w_{ij} : i \in [1, I], \; j \in [1, J]\}$ with the sizes $I = 1000$ and $J = 1000$ is homogeneously filled in with half-and-half substances "one" and "zero". The array borders are closed by a torus. The averaged concentration $c_1(w)$ is calculated in the cut, i.e., the set $W_{\mathrm{Av}} = \{w_{ij} : i \in [1, I], \; j = 500\}$. The number of iterations is 100. The quantitative representation of the automaton noise is dispersion $D(c_1)$, i.e., the mean square deviation of the concentration $c_1(w)$. It is calculated over W_{Av} as follows:

$$D(c_1) = \frac{1}{|W_{\mathrm{Av}}|} \sum_{w \in W_{\mathrm{Av}}} (c_1(w) - \bar{c}_1)^2, \quad \bar{c}_1 = \frac{1}{|W_{\mathrm{Av}}|} \sum_{w \in W_{\mathrm{Av}}} c_1(w),$$

where $\bar{c}_1$ is an average concentration.

Boolean model. The initial state $s(w_{ij})$ of each cell $w_{ij} \in W$ is chosen as $s(w_{ij}) = 0$ or $s(w_{ij}) = 1$, equiprobable.

In Figure 5, the dependence of dispersion $D(c_1)$ on the averaging radius r is shown. Experimental points for the Boolean model are approximated by the function

$$D(c_1) = \frac{k_{\mathrm{b}}}{r^2} \tag{3}$$
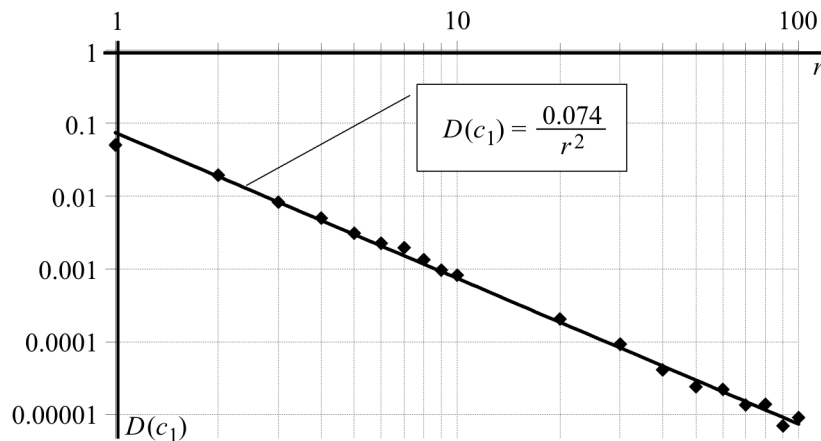
with $k_{\mathrm{b}} = 0.074$.

Figure 5. The dependence of dispersion $D(c_1)$ on the averaging radius r. Experimental points and approximating curve

Multi-particle model. The initial state $s(w)$ of each cell $w \in W$ takes the value that is equiprobable selected from the two ones: $\lfloor s_{\max}/2 \rfloor$ and $\lceil s_{\max}/2 \rceil$, where $s_{\max}$ is a maximum value of the number of particles in a cell, $\lfloor x \rfloor$ and $\lceil x \rceil$ denote the floor and ceiling of x, respectively. In the case $s_{\max}$ is odd, the rounding-off of $s(w)$ to an integer is performed up or down. If $s_{\max}$ is even, for preventing a degenerate case in which all the cells possess the same initial state, the Eldorado method is applied. It lies in using the decremented odd values $s_{\max} = 9, 99, 999$, etc. instead of the even ones $s_{\max} = 10, 100, 1000$, etc.

The averaging radius r was chosen as $r = 0$ for the greatest possible accuracy, i.e., the cardinal number of the averaging set $|W_{\mathrm{Av}}| = 1$.

In Figure 6, the dependence of dispersion $D(c_1)$ on a maximum value $s_{\max}$ with the model diffusion rate $k = 0.5$ is shown. Experimental points for the multi-particle model are approximated by the function

$$D(c_1) = \frac{k_{\mathrm{m}}(k)}{s_{\max}^2} \tag{4}$$

with $k_{\mathrm{m}}(0.5) = 0.48$.

Obviously, changing the model diffusion rate k implies changing the value of k_{m}. For each $k = 0.01, 0.02, \ldots, 0.99$, such an approximation curve was plotted and the coefficient k_{m} was obtained. In Figure 7, the experimental dependence $k_{\mathrm{m}}(k)$ is shown. The point $(0.5, 0.48)$ corresponds to the case given in Figure 6.
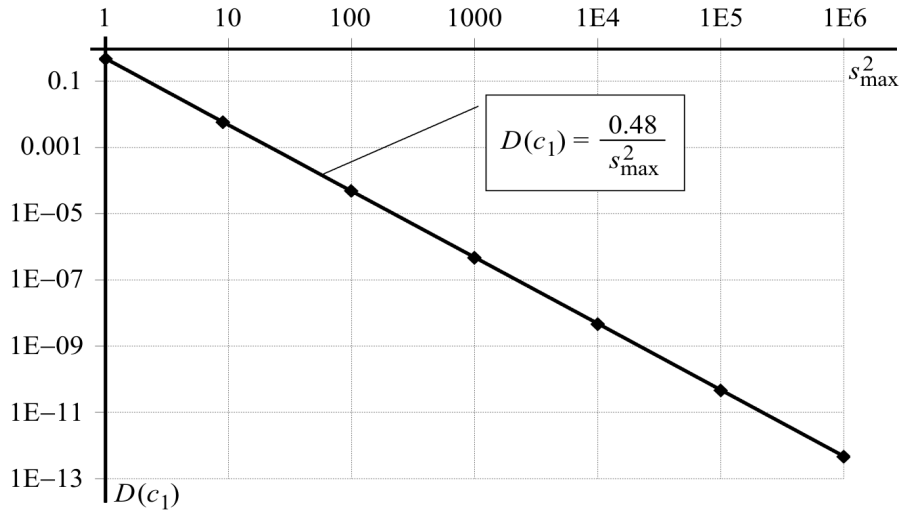

Figure 6. The dependence of dispersion $D(c_1)$ on $s_{\max}$. Experimental points and approximating curve
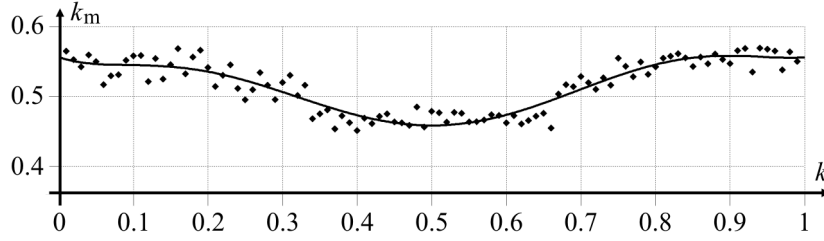
Figure 7. The dependence $k_{\mathrm{m}}(k)$

Comparison between the Boolean and the multi-particle models. The dependence of a maximum state value $s_{\max}$ of the multi-particle model on the averaging radius r of the Boolean model with equal dispersion $D(c_1)$ is obtained by equating the right-hand sides of (3) and (4):

$$s_{\max} = k_{\mathrm{bm}}(k) \cdot r, \tag{5}$$

where $k_{\mathrm{bm}}(k) = \sqrt{\dfrac{k_{\mathrm{m}}(k)}{k_{\mathrm{b}}}}$ is a coupling coefficient of the averaging radius r and a maximum value $s_{\max}$. All the possible values of the coefficient k_{bm} are given in Figure 8. Apparently, this coefficient possesses its value equal to $k_{\mathrm{bm}} = 2.6 \pm 0.2$. So, dependence (5) is linear. Now if in the Boolean model we know averaging radius r which leads to demanded automaton noise we can easily determine a maximum value $s_{\max}$ which is necessary for reaching of the same level of automaton noise in the multi-particle model.
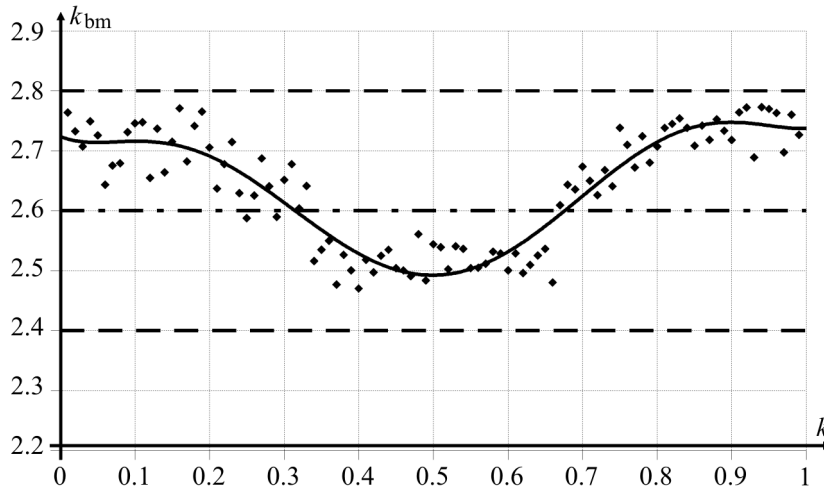

Figure 8. The dependence $k_{\mathrm{bm}}(k)$

6. Conclusion

The two new cellular-automata models of the diffusion process are proposed. The results of computer simulation allow us to conclude the following:

The models authentically feature the diffusion process because the results of simulation coincide with the results of the known models.

In the models proposed, the automaton noise with respect to the Boolean ones is extremely low that allows one to use a cellular array of a smaller size and to decrease the run time.

The dependence of a maximum state value of the multi-particle model on the averaging radius of the Boolean one with an equal automaton noise is obtained.

The parameter k in the proposed models affects the diffusion rate. Therefore, it is possible to simulate the diffusion process with various diffusivities.

In addition, the proposed models can be used in compositions with other multi-particle cellular-automata models [3].

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