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The concept of invariants in reaction-diffusion cellular-automata

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Abstract. A concept of invariant in cellular automata (CA) models is introduced, being defined as a dimensionless value that characterizes the process simulated by a CA evolution irrespective of the form of its mathematical representation. The paper is concerned with asynchronous CA-models (ACA-models), simulating reaction-diffusion processes, although it may be expanded to synchronous case as well. Invariants associate the CA-model parameters with their physical counterparts, which is important in simulation of real life processes. Particularly, the invariants may be used for obtaining the scaling values for space and time. The invariants of some simple reaction-diffusion ACA-models are established and considered in detail.

1. Introduction

Modern computers are powerful enough to simulate complex physical and chemical phenomena imitating movements and transformation of real and abstract particles in discrete space and time. A broad class of such processes is represented by mathematical models, where particles displacement obey the diffusion law, and particles transformation are given by a nonlinear function or by simple substitution of the form "current state → next state "[1, 2, 3]. Nonlinearity and discontinuity of the process do not allow to use conventional models based on partial differential equations (PDE). Searching for alternative resulted in development of CA-simulation methods. It was found that cellular automata exhibit extremely useful properties being capable to represent complex phenomena by common functioning of many simple computing units [7].

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Moreover, the class of asynchronous CA (ACA) is adequate to describe reaction-diffusion processes which are stochastic by nature. Accordingly, nowadays, there is a wide class of ACA simulating reaction-diffusion processes on micro and nano levels, that are used in scientific investigation of heterogenous chemical reactions, phase transition phenomena, biological and ecological systems [4, 5, 6]. Nevertheless, there are problems of general type not yet solved. One of them concerns the relation between the ACA-model variables and the corresponding physical values in the system under simulation. In this paper such a relation is established using a concept of a *CA-model invariant*, which is a dimensionless characteristic of both: the model and the process under simulation. Since the most interest nowadays is in asynchronous reaction-diffusion CA, the paper is focused especially on asynchronous CA.

Apart from the introduction, the paper contains three sections. In second section the needed formalism is given. Third and fourth sections are devoted to invariants of diffusion and reaction asynchronous CA-models, respectively. In the fifth section invariants of reaction-diffusion ACA models are considered and the examples are given. The paper concludes by some considerations about the significance and benefit of the concept for ACA-simulation development.

2. Formal definition of reaction-diffusion asynchronous cellular automaton

ACA is defined by four notions: $\langle A, X, \Theta \rangle$, which represent a set of simple identical computing units, referred to as *cells*. A cell is given as a pair (u, x), where u is a cell state from a finite alphabet A, $x \in X$ - is a vector of coordinates in a m-dimensional space X. A set of cells $\Omega = \{(u_i, x_i) | i = 1 \ldots, |X|\}$ forms a *cellular array*. On the coordinate lattice X subsets

$$T_k(x) = \{x, x + a_1, \ldots, x + a_{k-1}\}, \quad T_k(x) \subset X, \tag{1}$$

called *templates*, are defined with $a_j \in \{(-c, \ldots, c)\}$, $|a_j| = m$, being a shift vector. The set of cells with coordinates from $T_k(x)$ form a *local configuration*

$$S_k(x) = \{(u_0, x), (u_1, x + a_1), \ldots, (u_k, x + a_{k-1})\}, \quad k = |T_k(x)|. \quad (2)$$

Functioning of the ACA is determined by the local operator $\Theta(x)$, which is a composition of a simpler local operators $\Theta_j(x)$ and elementary substitutions $\theta_i(x)$.

$$\Theta(x) = \Phi(\Theta(x)_1, \ldots, \Theta(x)_l, \theta_1(x), \ldots, \theta_n(x)), \quad (3)$$

where $\theta_i(x)$, $i = 1, \ldots, n$, is the following substitution of local configurations

$$\theta_i(x) : S_k(x) \to S'_{k'}(x), \quad (4)$$

the underlying templates of $S_k(x)$ and $S'_k(x)$ being related as follows: $|T_{k'}| \subseteq |T_k|$. The first k' cells of $S_k(x)$ comprise the *base* of $\theta_k(x)$ while the remaining ones play the role of a *context*. A substitution $\theta_i(x)$ is applicable to a cell $(u, x) \in \Omega$, if $S_k(x) \in \Omega$. Application of $\theta_i(x)$ consists of replacing the states of cells $(u_j, x + a_j) \in S'_{k'}(x)$ by the values of transition functions

$$f_j(u_1, \ldots, u_k) = u'_j, \quad j = 0, 1, \ldots, k'. \quad (5)$$

The following composition operations Φ in (3) are used in reaction-diffusion ACA.

- Sequential execution

$$\Phi_s(\theta_1(x), \ldots, \theta_n(x)) = \theta_1(x), \ldots, \theta_n(x). \quad (6)$$

- Random choice of one out of n substitutions:

$$\Phi_r(\theta_1(x), \ldots, \theta_n(x)) = \theta_j, \quad j > \text{rand} \times n \geq j - 1. \quad (7)$$

- Arithmetic operations on integers and reals

$$\Phi_{plus}(\theta_1(x) \ldots, \theta_n(x)) = \theta(x) \pm \ldots, \pm\theta_n(x). \quad (8)$$

- Arithmetic operations on Boolean values with their transformation into reals

$$\Phi_{plus-tr}(\theta_1(x),\ldots,\theta_n(x)) = Discr(Av(\theta_1(x)) \pm \ldots, \pm Av(\theta_n(x)), \tag{9}$$

where, according to [8],

$$Disc(\theta(x)) = \begin{cases} 1 & \text{if} \quad rand < v'(x), \\ 0 & \text{if} \quad rand > v'(x), \end{cases} \qquad Av(\theta(x)) = \frac{1}{|Av|}\sum_{Av} v'(x), \tag{10}$$

$Av(x)$ being an *averaging template*.

Application of $\Theta(x)$ to all $x \in X$ comprises an *iteration*, which transforms a global cellular array $\Omega(t)$ into a next global state $\Omega(t+1)$. *Asynchronous mode* suggests $\Theta(x)$ be applied sequentially to randomly chosen cells with immediate change of their states.

3. Invariants in CA-models simulating diffusion

Diffusion process is fully determined by the dimensionless value of a diffusion coefficient, referred to as *diffusion number*. When the process is represented in finite-difference form of a Laplace equation, the diffusion number

$$D = d \cdot \tau / h^2, \tag{11}$$

where d [$\mathrm{kg} \cdot \mathrm{m}^{-2} \cdot \mathrm{sec}^{-1}$], is a diffusion coefficient , τ [sec] is a time step, h [m] is a space.

A simple consideration based on the definition of a diffusion coefficient as a quantity of substance mass passing through a unit of space during a unit of time with a concentration gradient equal to one (the first Fick's law), makes possible to assess D for the ACA diffusion as follows. In a ACA with Boolean alphabet, the gradient between two adjacent cells, say $(1, x)$ and $(0, x-1)$, is 1, and so are space and time units. Hence, the probability of the states exchange between these cells equals D. Such a reasoning may not be taken as a proof and is further confirmed by computational experiments.

The *naive diffusion ACA* [9] mimics the movements of particles as follows: a cell, chosen randomly from X exchanges states with one of its adjacent cells randomly chosen as well. In two dimensional case, a

probabilistic substitution $\theta(i,j)$, based on local configurations $S_5(i,j))$ is used, the transition function (5) being as follows.

$$\begin{array}{rcl} v'_k & = & \left\{ \begin{array}{ll} v_0 & \text{if} \quad (k-1)/4 < rand < k/4; \\ v_k & \text{otherwise} \end{array} \right. \qquad k = 1,2,3,4. \\ v'_0 & = & v_k \quad \text{if} \quad (k-1)/4 < rand < k/4; \end{array} \tag{12}$$

Since in the course of an iteration particle exchange between a cell (i,j) and its neighbor $(i,j)' \in T_k$ is performed twice: when θ is applied to the cell (i,j), and when it is applied to $(i,j)'$, both times with $p = 1/4$, the invariant according to Fick's law should be $D = 0,5$.

In a one-dimensional case, $X = \{i : i = 0,1,\ldots,I\}$, the template $T_3(i)$ is used, $\theta(i)$ performs state exchange with one out of two neighbors with probability $p = 0.5$, the transition function differing from (12) only in the value of k, which is now $k = 2$.

In the course of an iteration each pair of adjacent cells makes the exchange twice, each time with $p = 0.5$, so, $D = 1$. Reasoning in the same way, the diffusion CA-model for a three-dimensional case $D = 1/3$, which is in agreement with [10] for nano particles moving in crystal lattice.

Asynchronous integer diffusion ACA-model [11] differs from its Boolean counterpart in two aspects: 1)alphabet is a finite set of integers, $A = \{0,1,2,\ldots,M\}$, and 2) only an n-th portion of state value is involved in the exchange of states. The transition function results in the following next states.

$$\begin{array}{rcl} v'_k & = & \left\{ \begin{array}{cl} (1-n)v_0 + nv_k & \text{if} \quad (k-1)/4 < rand < k/4; \\ v_k & \text{otherwise.} \end{array} \right. \quad k = 1,2,3,4. \\ v'_0 & = & (1-n)v_0 + nv_k \quad \text{if} \quad k-1)/4 < rand < k/4; \end{array} \tag{13}$$

One-dimensional case differs in in that the template used is T_3 and $k = 2$.

Relying on Fick's law the following diffusion numbers are suggested: $D = 0.5n$ for the two-dimensional diffusion and $D = n$ – for one-dimensional case.

Computational experiments for the above diffusion numbers confirmation consisted in comparing the values $\langle v(I/2,j)\rangle$, obtained by ACA simulation, with $u(I/2,j)$, obtained by numerical solution of the Laplace

Table 1. Invariants of diffusion ACA-models

Alphabet	Boolean		Integer	
	1-dimension	2-dimension	1-dimension	2-dimension
D_{ACA}	1	0.5	n	$0.5n$

equation with D_L as the diffusion number. The computations were performed for $t = 0, 1, \ldots, T$, where $T = 300$ is the number of iterations when the process practically terminates. If the values $\langle v(I/2, j)\rangle$ and $\langle v(I/2, j)\rangle$ coincide for all $j = 0, \ldots, J$, and for all $t = 0, 1, \ldots, T$, then $D_{ACA} = D_L$ and D_{ACA} is the ACA invariant. The obtained values of diffusion ACA invariants are given in Table 1.

The invariant helps to obtain the *scaling coefficients*, namely, the size of a cell h [m], and the time of an iteration τ. These two values correlate the model parameters with their physical counterparts. For example, the task is to construct an ACA-model simulating a diffusion process, the following being given:

- the size of the area S [m^2],

- the diffusion coefficient of the substance d [kg·m$^2 \cdot$ sec$^-$1], equal to d,

- the initial distribution of substance density $u_0(x)$ over the area under simulation.

According to the size of particles assumed as units of the substance, (atom, molecule, granule, etc.) and the required frequency of evolution observation, h and τ are obtained by (11). It gives the possibility to obtain the remaining data of the ACA: the size of the cellular array $|X| = S/h^2$, the probability of $\Theta(x)$ application $p = d \cdot \tau/(D_{ACA} \cdot h^2)$, and $\Omega(0)$ by calculating $v_0(x) = Discr(u_o(x))$ for all $x \in X$ [**?**].

4. Invariants in CA-models simulating chemical

The main characteristic of chemical reaction is its *reaction rate* , $r = \Delta C/\Delta t$ [kg$\cdot$ m$^{-2}\cdot$ sec^{-1}], which represents the relative increment of the substance per area (for surface reactions) and per second [12]. To associate the reaction rate with the ACA-model evolution it is reasonable

to use the dimensionless relative concentration change, which may be connected to the probability of the corresponding local operator. So, the value of the invariant is as follows.

$$\Upsilon_R = r \cdot h^2 \cdot \tau. \tag{14}$$

In the most known reactions on catalyzed surface, the reaction rate is proportional to the mole ratio of the gas from where the reactant is adsorbed, i.e. the invariant may is $\Upsilon = k_a \cdot Y(A)$, k_A being the reaction constant.

An example of such a reaction is *hydrogen dissociation* $H_2 = H^+ + H^+ + 2e$ on catalyzed surface, used in hydrogen energetics. The process consists of two reactions: adsorption of H_2 from the gas onto a catalyst with dissociation of the hydrogen molecule into two protons and two electrons, and desorption of the protons to the gas and the electron to the electric circuit.

ACA -model of the reaction has the alphabet $A = \{\emptyset, H, e, E\}$,where E is the amount of produced electrons, $X = C \cup \{x : x = (i, j), i, j = 0, \ldots, N\}$, C is a counter of electrons, and $\Theta = \Phi_r(\theta_{ads}, \theta_{dis}\}$, where

$$\begin{aligned} &\theta_{ads}: \quad \{(\emptyset, x), (\emptyset, (x + a_l))\} \xrightarrow{p_{ads}} \{(H, x)(H, (x + a_l))\} \\ &\theta_{dis}: \{(C, E), (H, (x))(H, (x + a_l))\} \xrightarrow{p_{des}} \{(C, E + 2)(\emptyset, (x))(\emptyset, (x + a_l))\} \end{aligned} \tag{15}$$

In (15) $(x + a_l) \in T_5(x)$, $l = 1, 2, 3, 4$, is chosen randomly. Since $r_{ads} \approx r_{des}$, the probabilities $p_{ads} = p_{des} = 0.5$.

Similar to the diffusion case, Υ_R helps to obtain the value of $h^2 \cdot \tau$, assuming that r_H and k_H are known. This allows to calculate all parameters of the ACA for simulating the reaction of hydrogen dissociation $S[\mathrm{m}^2]$ and Y_H being given.

5. Invariants of CA-models simulating reaction-diffusion processes

If an CA-model is represented as a composition of several diffusion and reaction ACA [8], then its invariant Υ_{RD} is defined as a specific characteristic of the whole process, which,usually, cannot be expressed as

a function of diffusion and reaction invariants. Hence, Υ_{RD} should be obtained by simulation for each type of ACA-models and treated as a physical constants.

Example 1. The *heterogenous reactions* on catalysed surface attract great attention. The most known is the so called ZGB-reaction [15], which initiated a wide application of ACA-simulation (kinetic Monte-Carlo method) [**?**, 16]. The reaction is given by the following system of chemical equations:

$$\begin{aligned} \emptyset &\xrightarrow{k_{CO}} CO_{ads} \\ 0_2 &\xrightarrow{k_O} 2O_{ads} \\ CO_{ads} + O_{ads} &\longrightarrow CO_2, \\ CO_{ads} + \emptyset &\xrightarrow{k_{Dif}} Z + CO. \end{aligned} \tag{16}$$

In (16) k_{CO} and k_O are adsorption rate constants, respectively. The fourth equation represents the diffusion of CO over the surface. The whole process proceeds as follows. On the catalyst surface ($\emptyset$) carbon monoxide (CO) and oxygen (O_2) are adsorbed from the gas, and when occurring in contact, they react producing carbon dioxide gas that leaves the surface. The adsorbed CO-particles tend to be distributed evenly. The probabilistic ACA of the reaction-diffusion process (16) has the alphabet $A = \{\emptyset, CO, O\}$, the naming set X, and a local operator

$$\Theta = \Phi_r(\theta_1, \theta_2, \theta_3, \theta_4)$$

where

$$\begin{aligned} \theta_1 :\ (\emptyset, x) &\xrightarrow{p_{CO}} (CO, x), \\ \theta_2 :\ \{(\emptyset, x), (\emptyset, x + a_l\} &\xrightarrow{p_O} \{(O, (i, j)), (O, (x + a_l)\}, \\ \theta_3 :\ \{(CO, x), (O, (x + a_l)\} &\longrightarrow \{(\emptyset, x), (\emptyset, (x + a_l)\}, \\ \theta_4 :\ \{(CO, x), (\emptyset, x + a_l) &\xrightarrow{p_{dif}} \{(\emptyset, (i, j)), (CO, (x + a_l)\}, \end{aligned} \tag{17}$$

In (17), $(x + a_l)$ is the k-th neighbor of x in $T_5(x)$, p_{CO},p_O and p_{Dif} are probabilities of θ_1, θ_2 and θ_4 application, depending on the reaction rates as follows

$$p_i = \frac{k_i}{k_1 + k_2 + k_4}, \quad i \in \{O, CO, Dif\},$$

The results of the CA simulation (Monte-Carlo method) of the above reaction are reported, for example, in [17, 18]. The investigation aimed at determining the influence of the diffusion number on the phase-transition critical values of the mole ratio $Y(CO)$. In these investigations $Y(CO)$ is treated as the invariant of the model. It is quite reasonable, since just this value determines the main features of the process, namely, the amount of each substance involved in the reactions at each iteration.

So, the ACA parameters may be obtained as follows. The invariant $Y(CO)$ and the adsorption rate r_{CO} be given, the value $h^2 \cdot \tau$ should be obtained from (14). Then, to allow for diffusion influence, τ is to be calculated by (11) with h chosen according to the nature of the process.

Example 2. A bright example of reaction-diffusion process is the *propagating front* process, studied in [13, 14] on the basis of the following partial differential equation:

$$u_t = Du_{xx} + F(u), \tag{18}$$

where D is a diffusion invariant and

$$F(u) = \alpha u(1-u), \quad \text{with} \quad F(0) = F(1) = 0, \quad 0 < \alpha \leq 1, \quad 0 \leq u \leq 1, \tag{19}$$

represents a reaction component. In [13] the asymptotic assessment of the dimensionless front propagation velocity value is obtained as a following function of the of the diffusion and the reaction invariants:

$$V_0 = 2\sqrt{D\alpha}, \tag{20}$$

being equal to a maximal front velocity with $t \to \infty$. Of course, the velocity is most important characteristic of the process and it should be taken as invariant.

An ACA analog $\aleph = \langle A, X, \Theta \rangle$ of equation (18), obtained by the composition method [8] has $A = \{0, 1\}$, $X = \{i : i = 0, \ldots, N\}$, and

$$\Theta(i) = \Phi_{plus-tr}(\theta_{diff}(i), \theta_{reac}(i)),$$

where $\theta_{diff}(i)$ is a local operator of a diffusion ACA, whose transition function (5) transfers $(u, i) \in \Omega(t)$ into $(v, i) \in \Omega_{diff}(t+1)$, and

$$\theta_{reac} : (v, i) \to Discr(\langle v \rangle + F(\langle v \rangle)$$

is a reaction contextless local operator.

Assuming the velocity be the invariant of the process, and to verify whether (20) is valid for the ACA-model the following computational experiment was performed.

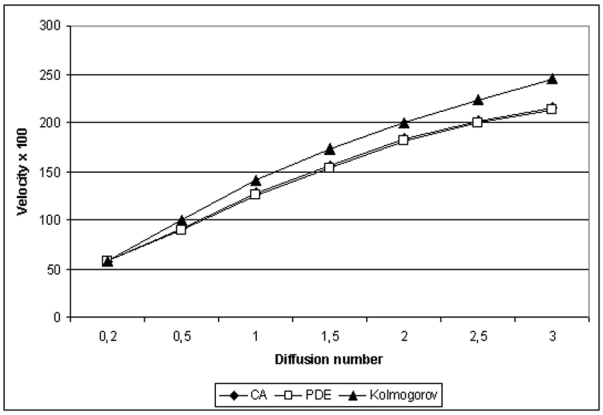

Figure 1. Dependence of front propagation velocity on α obtained by ACA simulation with D=0.5, by (20), and by (18)

Cellular array size was $I \times J = 200 \times 800$ with initial global state

$$v(i,j) = \begin{cases} 1 & \text{if} \quad 0 < i < 200,\ j \leq 40; \\ 0 & \text{if} \quad 0 < i < 200,\ j > 40 \end{cases}$$

For three above values of D and $\alpha = 0.1, 0.2, \ldots, 1.0$, the velocity V was computed as follows: $V = (j_2 - j_1)/(t_2 - t_1)$, t_2 and t_1 being such that $u(j_2, t_2) = u(j_1, t_1) = 0.5$ with $j_2 = 700, j_1 = 500$. The choice of j_1 and j_2 is approved by the experimental fact, that after t=300 the velocity becomes constant. The dependencies of front propagation velocity on α with $D = 0.2$, $D = 0.5$ and $D = 1$ were calculated by three methods: 1) by formula (20), 2) by PDE (18) solution, and 3) by ACA simulation. It is seen from Fig.1,that CA process coincide with that obtained by PDE solution, but is a little slower that the theoretical assessment.

The invariant is the normalized front velocity $\Upsilon = V$, which is related to the ACA scaling parameters as follows. In order to simulate front propagation with the maximum velocity v [m$\cdot$ sec^{-1}] in the medium with diffusion coefficient d [kg$\cdot$ m $\cdot$ sec^{-1}, the ratio of scaling parameters should be $\tau/h = V/v$, from what τ is obtained if h is chosen from physical conditions.

Example 3. Another example of a reaction-diffusion process is the so called *diffusion limited aggregation*, which represents the processes of crystallization, coral growth, snowflake formation etc.. In ACA-models of such processes the reaction intensity is given as probability of the reaction occurrence, known as a *sticking coefficient* which considered to be the invariant. A most simple ACA, simulating the diffusion limited aggregation has an alphabet $A = \{a, b.c\}$, discrete space $X = \{(i, j) : i, j = 0, 1, \ldots, M\}$,

$$\Theta = \Phi_r(\theta_{diff}, \theta_s ol),$$

where θ_{diff} is naive diffusion local operator (12) with $A = \{a, b\}$, and θ_{sol} is the local operator of solidification

$$\theta_{sol} : \{c, (i, j)), (a, (i + k, j + l))\} \xrightarrow{p_2} \{c, (i, j)), (c, (i + k, j + l))\}, \quad (21)$$

where $(k, l) \in \{(0, 1), (1, 0)), (-1, 0), (0, -1))\}$, p_2 is a sticking coefficient. The process suggests that initial cellular array has more than 90% of cells in the state b, less than 10% cells – in the state b, and some isolated cells in the state c (called *seeds*). In the course of the evolution a growing structure is formed around seeds (Fig.3), exhibiting fractal properties, and, hence, being characterized by the fractal dimension

$$\delta = log(N(R))/log(\pi R^2), \quad (22)$$

where R is a radius of a circle in the formed structure area with the center in the seed-cell, $N(R)$ is the a number of cells with c states in the circle area.

The dependence of fractal dimension on the invariant is investigated in [19] by simulation. So, given the invariant, it is possible to obtain the fractal dimension, i.e. to determine the velocity of the growth and the density of the structure. Then, comparing these model parameters with the natural process, find the needed scaling coefficients.

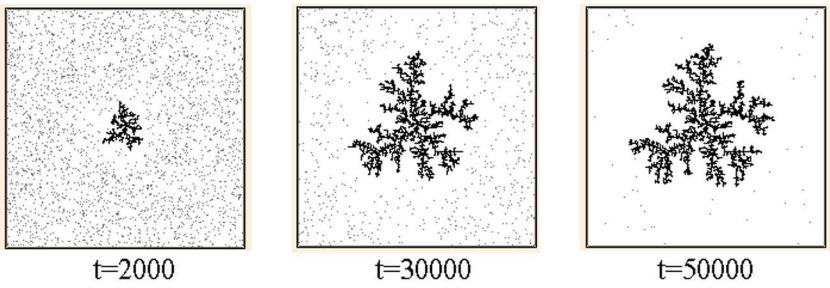

Figure 2. Three snapshots of diffusion limited aggregation ACA evolution

In Fig.2 three snapshots of the ACA evolution are shown obtained while simulating the process by an the ACA with the size of cellular array 200×200, initial density of cells $d(a,(i,j)) = 0.05$, $p_2 = 1$. Fractal dimension was calculated according to (22) as an averaged of values for $R = 40, 45, \ldots, 80$. The obtained value $\delta = 1.66$ is in accordance with those, given in [19].

6. Conclusion

For ACA-models of reaction-diffusion processes a concept of a invariant is introduced. It is a dimensional value which characterizes the process itself and is expressed in terms of ACA parameters. The concept is useful for constructing the ACA-model and calculating scaling ACA parameters: iteration time and size of the cell. The examples show, that for reaction-diffusion ACA invariants should be determined by computational experiments and stored in the same manner, that it is done for physical and chemical properties, obtained in-situ and stored in databooks. It is necessary for ACA-simulation working in practice.

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