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Relationships between cellular automata model parameters and their physical counterparts*

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Abstract. When constructing a Cellular Automata (CA) model of a natural process one meets a problem of determining scaling relations, i.e. the quantitative relationships between the CA dimensionless parameters and corresponding values characterizing the prototype process given in terms of a physical system of units. The problem has no general solution. Moreover, till now there is no strict statement and detailed investigation of the problem despite the fact that for some classes of CA models certain approaches have been proposed. The most formalized and substantiated approach is based on the similitude theory, which studies dimensionless characteristics of natural processes that are equal both for a model and its prototype. Certain attempts have been made to use the approach when developing and investigating particular CA models of natural phenomena, but no systematic methods have been created. In this paper the problem is discussed, and basic principles of finding scaling relations are formulated and shown at work for two most advanced classes of CA models: Lattice–Gas CA simulating viscous flows and stochastic CA models of Reaction–Diffusion processes.

1. Introduction

The CA is a mathematical model, which maps a natural process onto a sequence of spatial configurations, each being a cellular array whose entries are states, given by a finite set of symbols that characterize a simulated phenomenon [1]. The array is given by a lattice of finite size with the distance between the adjacent cell centers $\Delta l = 1$. Each next configuration results from the current one by application of local transition rules to all cells of the array. The cell states adjustment happens at discrete time moments $t = 0, 1, \ldots, \hat{t}$, $\hat{t}$ being the final iteration number. Briefly speaking, a CA model is represented by a set of parameters $\Pi = \{\pi_1, \ldots, \pi_q\}$, denoting the subject and the medium of the process, and a set of transition rules $\Theta = \{\theta_1, \ldots, \theta_n\}$, denoting operations governing the process evolution. The CA models are highly abstract, parameters $\pi \in \Pi$ being discrete and dimensionless. In practice, it makes CA modeling valuable only when the relations $\mu(\pi) = \pi'/\pi$ between parameter values expressed in physical terms π' and their model dimensionless counterparts π are available. Hence, the

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problem of determining $\mu(\pi)$ also being referred as *scaling CA parameters* is an important part of the CA model synthesis.

The CA model parameters may be divided into the three groups:

- *Basic parameters* of the process domain: the space step Δl, and the time step Δt;
- *Cell states*, representing objects of simulation: density of a certain species (integer), averaged density of a certain species (a real number), dimensionless velocity (Boolean vector), averaged velocity (a real number), and pressure (integer).
- *Medium properties* expressed in terms of CA dimensionless characteristics: diffusion coefficient, heat and electric conductivity, viscosity, resistivity, reaction rate, etc.

The problem is also complicated by the diversity of the CA models properties related to the features of simulated phenomena which may have an unpredictable behavior, exhibiting all features of complexity [2].

Based on the current state of the CA simulation experience, the two classes of CA models are distinguished:

- *Lattice–Gas CA models* are the most known and well studied models of a viscous flow called FHP-models according to the names of the authors [3]. The models are synchronous CA with a hexagonal array of cells, where particles are moving and colliding governed by probabilistic transition rules. Although these models are not intensively used due to the Reinolds number limitation, they have served as prototypes for a series of more practical modifications [4–6]. Hence, the methods of the CA parameter scaling for FHP models is considered to be basic for the whole Lattice–Gas CA class.
- *Reaction–Diffusion CA models.* This class comprises CA models 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 [7–9]. The processes under simulation are represented by a set of interacting particles, which move, collide, and undergo transformations, all those events being represented by probabilistic transition rules.

The parameter scaling may be performed correctly when a simulated phenomenon is completely determined, i.e. properties of substances and a medium involved in the process are known. This problem is quite different from that of finding unknown values of constants, which should be implemented by solving the inverse problem. The latter is similarly stated as is done in the numerical analysis and hence not considered here.

In what follows, an approach to the CA models parameters scaling based on similitude theory [10] is proposed. The main idea is to determine a dimensionless characteristic for a simulated process, which is equal both for the model and the prototype called the process invariants, and use its value for finding the relation between all the other CA parameters and their physical counterparts. Further on, to be concrete in the state of the problem, $\mu(\pi)$ is expressed in MKS unit system (meters, kilograms, seconds).

2. Formal problem statement

The formalism that is further used for representing CA models is Parallel Substitution Algorithm [11], modified for the CA simulation objectives. According to this, a CA model $\aleph$ is represented by four notions $\aleph = \langle A, X, \Theta, \varrho \rangle$, where A is a set of symbols of any kind, called *state alphabet*, $X = \{x_1, x_2, \ldots, x_N\}$ is the finite set of *cell names*, $\Theta = \{\theta_1, \ldots, \theta_n\}$ is a set of *local operators*, and ϱ is the *mode of operation*, which determines the time-space distribution of operator application. The central concept in the CA model is a *cell*, which is the pair (a, x), where $a \in A$ is the cell state, and $x \in X$ is the cell name. The set of cells $\Omega = \{(a_i, x_i) : \ i = 1, \ldots, N\}$ containing no cells with identical names is called a *cellular array*.

On the set X, the *naming functions* $\varphi(m)$ are defined whose values indicate to the location of cells communicating with a cell named x. When the Cartesian coordinates $X = \{(i, j)\}$ are used for names, the naming functions are given in the form of shifts $\phi_k = (i+a, j+b)$, a, b being integers. A set of the naming functions

$$T(x) = \{x, \phi_1(x), \ldots, \phi_q(x)\}, \quad q \ll |X|, \tag{1}$$

is referred to as the *neighborhood* of x. A subset of the cells

$$S(x) = \{(u_0, x), (u_1, \phi_1(x)), \ldots, (u_q, \phi_q(x))\}, \tag{2}$$

having the names from $T(x)$, is called the *local configuration* with $T(x)$ as its *underlying neighborhood*. A local operator $\theta_i \in \Theta$ is expressed in the form of a *substitution* [11] as follows:

$$\theta(x) : S(x) \star S''(x) \to S'(x), \quad \forall x \in X, \tag{3}$$

the underlying neighborhoods of $S(x)$ and $S'(x)$ being identical, i.e. $T'(x) = T(x)$, and that of $S''(x)$, $T''(x)$ being allowed to be arbitrary.

An application of $\theta(x)$ to a certain cell $(u, x) \in \Omega$ consists in removing the cells of $S(x)$ from Ω and replacing them by the cells given in $S'(x)$. Such a concept of a local operator allows one to simulate living organisms which may grow and die. When simulating physical phenomena *stationary* local operators [11] are used which do not change the naming set, only replacing the states of cells from $S(x)$ in (2) by the states of cells from

$$S'(x) = \{(u'_0, x), (u'_1, \phi_1(x)), \ldots, (u'_h, \phi_h(x))\},$$

u' being obtained according to transition functions

$$u'_k = f_k(v_0, v_1, \ldots, v_q), \quad q = |S(x)|, \;\; h = |S'(x)|, \;\; h < q. \tag{4}$$

There are two basic modes $\rho = \{\sigma, \alpha\}$ of ordering a local operator application to $x \in X$ to perform the global transition $\Theta(X)$ from $\Omega(t)$ to $\Omega(t+1)$.

Synchronous mode σ of the operation provides for any substitution $\theta \in \Theta$ to be applied to all $(u, x) \in \Omega(t)$, the cell states being adjusted in any order or all at once in parallel.

Asynchronous mode α of the operation suggests the cells $x \in X$ to be chosen at random, the cell states in $S'(x)$ to be computed and adjusted immediately.

In both cases, the transition to the next global state is referred to as *iteration* occurs when all substitutions $\theta \in \Theta$ are applied to $\Omega(t)$.

The sequence

$$\Omega(0), \Omega(1), \ldots, \Omega(t), \ldots, \Omega(\hat{t})$$

is called *CA evolution*, $\hat{t}$ denotes a terminal iteration number.

Performing a CA simulation task comprises the three stages:

1. Constructing the CA model, i.e. determining $\aleph = \langle A, M, \Theta, \varrho \rangle$ and its initial global state $\Omega(0)$;
2. Obtaining the resulting data by running the CA program; and
3. Interpreting the results by transferring the model parameters to habitual physical values.

The first and the third stages require the scaling coefficients to be known. The problem is solved differently for different types of CA models, but the techniques rely on the same above-mentioned principles and the same formalism.

3. The scaling coefficients in Lattice–Gas models of viscous flows

The Lattice–Gas CA models comprise a special class of CA intended to simulate processes in gas and liquids. A medium is represented by abstract particles, moving and colliding in a discrete hexagonal space. The most known and well studied models comprise a series of probabilistic Lattice–Gas CA called FHP-models according to the names of the authors [3]. Formally, they are synchronous CA $\aleph = \langle A, X, \Theta, \sigma \rangle$, where $X = \{x_k : \; k = 1, 2, \ldots, N\}$ enumerates hexagons on a 2D plane. A cell neighborhood includes the cell

names of 6 adjacent cells. Accordingly, 6 moving and a number of the rest particles may be located in a cell. To represent the cell states with 6 moving and one particle at rest (FHP–1), the alphabet $A = \{s = (s_0, \ldots, s_6)\}$, $|A| = 2^7$ comprises Boolean vectors 7 bit long. A component of the state vector $s_i = 1$ indicates that the cell (s, x) has a particle moving towards the ith neighbor $(i = 1, \ldots, 6)$ with the velocity $v_i = 1$, or if the cell has a particle at rest, then $s_0 = 1$ having the velocity $v_0 = 0$. The particle mass is equal to 1.

Two local operators determine the functioning of a CA. The first θ_1 makes all particles in all cells simultaneously propagate: one cell towards the neighbor pointed by its velocity vector. It is convenient to represent θ_1 as a set of six substitutions $\theta_1^{(i)}, i = 1, \ldots, 6$, each being applied to the ith component s_i of the state vector

$$\theta_1^{(i)} : \{(s_i, x)\} \to \{(s_i, \phi_{(i+3) \bmod 6}(x)\}, \quad i = 1, 2 \ldots, 6. \tag{5}$$

The second contextless local operator simulates the collision of particles:

$$\theta_2(x) : \{(s, x)\} \to \{(s', x))\}. \tag{6}$$

The transition function $s' = f(s)$ is given in the form of a table, some arguments having two equiprobable outcomes. The collision rules principles are shown in Figure 1.

The mode of operation of Lattice–Gas CA is two-stage synchronous, i.e. each iteration consists of the two stages: at the first stage, six propagation

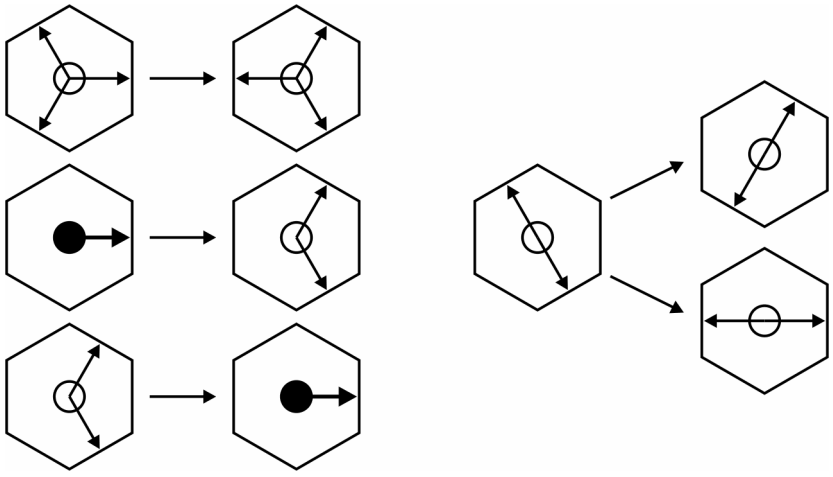

Figure 1. Graphical representation of collision operators in FHP-1 Lattice–Gas model. Deterministic rules are given on the left, the probabilistic ones — on the right

operators (5) act simultaneously, at the second stage the collision operator (6) completes the transition to the next global state.

In [3], FHP-model is proved to be identical to the Navier–Stokes equation in describing the viscous flow velocity. A 3D version of the FHP-model called RD-1 is also known [4]. Its naming set is a discrete space with cells having the form of rhombododecahedra. The neighborhood of RD-1 has 12 cells. The model allows the simulation of flows in a large enough space, as compared to the FCHC model proposed and investigated in [3]. Although the model approximately meets the isotropic conditions, its experimental tests have shown an acceptable plausibility to the phenomenon being simulated [4].

The Lattice–Gas CA models dimensionless parameters can be divided into three groups:

1. Basic parameters associated with all types of CA models: $\Delta l = 1$, i.e. the distance between the adjacent cells centers (spatial step), and $\Delta t = 1$, i.e. the duration of an iteration (temporal step).
2. Parameters inherent to a concrete Lattice–Gas model: the sound speed v_s, the mean particle density per cell at equilibrium ρ_0, the mean particle density per the velocity direction d, and the viscosity $\nu(d)$.[1] For the model FHP-1, that is further used in Example 1, the above parameters have the following values [3]:

$$v_s = \frac{1}{\sqrt{2}}, \quad \rho_0 \in [1,3], \quad d = \frac{\rho_0}{6}, \quad \nu(d) = \frac{1}{12d(1-d)^3} - \frac{1}{8}. \qquad (7)$$

3. Parameters, characterizing the process under simulation: the velocity field $V = \{(v_x, t) : \ x \in X, \ t = 0, 1, \ldots, \hat{t}\}$, the pressure field $P = \{(p_x, t) : \ x \in X, \ t = 0, 1, \ldots, \hat{t}\}$.

The task of simulation fluid flow through a reservoir is usually stated as follows.

Given are the following values in physical units:

- the size and geometry of the reservoir X' [m] including a subset of input cells X'_{in} and a subset of output cells X'_{out}.
- the fluid density ρ' [kg/m^3],
- the fluid viscosity ν' [m^2/s], and
- the pressure drop $\Delta p'$ [kg/(m $\cdot$ s^2)].

To be obtained are the following data also in physical units:

[1] As distinct from [3], we use the term *mean particle density per cell* for denoting mean value of $\sum_{i=1}^{6} s_i$, while in [3] this term is used for denoting d.

- the field of velocity vectors $V' = \{(u'_x, x) : \ \forall x \in X'\}$, u'_x [m/s];
- the field of pressure values $P' = \{(p'_x, x) : \forall x \in X\}$, p'_x [kg/(m $\cdot$ s^2)];
- any additional characteristic of the flow, (i.e. the flow output per second, the time of transferring a given volume of liquid) may be calculated provided the above two fields are obtained.

In-between the above parameter transformations, the simulation procedure is performed, that consists of constructing the CA, programming and running a CA program, and scaling the results obtained.

- *CA construction.* Since the alphabet, local operators and operation mode are defined by Lattice–Gas model, the construction of the CA consists of the two procedures:

  1) Transform the given X' [m] into the hexagonal naming set X, and provide cells of X with initial states to obtain $\Omega(0)$. This requires Δl to be known, which may be chosen according to required spatial precision of the simulation results. It is important to remark that only one basic parameter scale is allowed to be chosen, the other is related to it through a fluid viscosity value.

  2) Provide cells of X_{in} with initial states to obtain $\Omega(0)$. It is done by choosing the mean density per cell ρ_0 according to (7) and calculating the mean particle density $p = \rho_0 v_s^2$.

- *Running the program.* The CA model should be programmed and run until the stationary process is attained, resulting in the velocity and pressure fields:

$$V(X) = \{(\langle v_x \rangle, x) : \ \forall x \in X\}, \quad P(X) = \{(\langle p_x \rangle, x) : \ \forall x \in X\}, \quad (8)$$

  where $\langle v_x \rangle$ and $x\langle p_x \rangle$ are averaged over a given vicinity of the values x of v and p, respectively.

- *Scaling results.* Resulting values from (8) should be expressed in KMS physical units as

$$V'(X) = \{(v'_x, x) : \ \forall x \in X\}, \quad P'(X) = \{(p'_x, x) : \ \forall x \in X\},$$

  where $v'_x = \mu_v \cdot \langle v_x \rangle$, $p'_x = \mu_p \cdot \langle p_x \rangle$, the scaling coefficients being calculated according to the following scaling expressions:

$$\mu_\nu = \frac{\nu'}{g\nu} \ [\text{m}^2/\text{s}], \quad \mu_v = \frac{mu_\nu}{\Delta} \ [\text{m/s}], \quad \mu_\rho = \frac{\rho'}{\rho_0} \ [\text{kg/m}^3],$$
$$\mu_p = \frac{p'}{p} \ [\text{kg} \cdot \text{m/s}^2], \quad \Delta t = \frac{\mu_l}{\mu_v} \ [\text{s}]. \quad (9)$$

The simulation results together with the scaling coefficients comprise a complete set of data for determining any additional value about the simulated process, such as the fluid flow per second, the time required to transfer Q kg through the reservoir, the Reinolds number.

Example 1. The Lattice–Gas FHP-1 CA model is used for simulating the flow of heavy oil through a tube. The following data are given:

- A tube with diameter 0.7 m and length 7 m. On one end of the tube the pressure $p'_{\text{in}} = 3$ atm is imposed, the other end is opened to be left, i.e. $p'_{\text{out}} = 1$ atm. So, the pressure drop $\Delta p' = 20000$ kg/(m $\cdot$ s^2).
- Heavy oil properties: kinematic viscosity $\nu' = 1.4 \cdot 10^{-3}$ m^2/s and density $\rho' = 880$ kg/m^3.

Simulation aims to obtain velocity and pressure fields.

To construct the Lattice–Gas CA, the model constants $\rho_0 = 2.4$ and $d = 0.4$ are chosen, and the dimensionless viscosity and the correcting coefficient $\nu(d) = 0.839$, $g(d) = 0.166$ are computed.

The basic scaling coefficient $\Delta l = 0.01$ m is chosen. The cellular array size and the naming set is designed: $|X_i| = 700, |X_j| = 70$, $X_{\text{in}} = \{(0, j) : j = 0, \dots 69\}, X_{\text{out}} = \{(699, j) : j = 0, \dots 69\}$,

The initial state $\Omega(0) = \{(s_{\text{in}}, x) : x \in X_{\text{in}}, (0, x) : x \in X \setminus X_{\text{in}}\}$, where ($s_{\text{in}}$ are the state vectors with $|s_{\text{in}}| = \rho_0/v_s = 1.2$, chosen with equal probabilities to be the states of $x \in X_{\text{in}}$.

The model $\aleph$ is programmed and run until the global stable state is reached, and, hence, fields of averaged velocities $V(x, t)$ and the pressure values $P(x, t)$ are obtained.

The scaling coefficients are calculated according to (9):

$$\mu_\nu = \frac{1.4 \cdot 10^{-4}}{0.839} = 1.66 \cdot 10^{-4} \text{ m}^2/\text{s}, \quad \mu_\rho = \frac{880}{2.4} = 336.7 \text{ kg/m}^3,$$
$$\mu_v = \frac{\mu_\nu}{\Delta l} = 0.0167 \text{ m/s}, \quad \mu_p = \frac{20000}{1.2} = 16667 \text{ kg/(m} \cdot \text{s}^2).$$

The obtained values $\langle v_x \rangle$ and $\langle p_x \rangle$ are expressed in KMS units by multiplying them by the corresponding scaling coefficients. The resulting mean velocity vector length is 0.8, which yields $v'_m = 0.8 \cdot 0.0167 = 0.0133$ m/s.

The Reinold number of the process is as follows:

$$\text{Re}' = \frac{l'_0 v'_m}{\nu'} = \frac{0.7 \cdot 0.0133}{1.4 \cdot 10^{-4}} = 83.5, \quad \text{Re} = \frac{|X_i| \cdot v_m}{\nu} = \frac{70 \cdot 0.8}{0.839} = 83.5,$$

where Re$'$ is computed in physical terms, Re—in the Lattice–Gas CA terms.

4. The scaling coefficients in stochastic reaction-diffusion CA models

Mathematical modeling and computer-aided simulation are now primarily focused on nonlinear dissipative phenomena in chemistry and biology [1], rather than on conventional physics. Formally, RD CA model is characterized by Boolean, symbolic or integer alphabet, the Cartesian lattice-like cell naming set X, a set of substitutions $\Theta = \{\theta_1, \ldots, \theta_n\}$ corresponding to a set of elementary actions. In a simple case, Θ contains the two substitutions: θ_d is the modeling diffusion, and θ_r is the modeling reaction. In a general case, there may be any number of both. The mode of operation is asynchronous ($\rho = \alpha$).

The scaling problem solution for RD CA model may be correctly stated if all properties of the species, involved in the process under simulation, are known, and hence, for all components of scaling coefficients can be obtained.

There are a number of diffusion CA models, described in [12] in detail. All of them are characterized by a dimensionless parameter, called *diffusivity*. This parameter is obtained analytically or experimentally and may be tuned by a varying probability of the corresponding substitution. It is considered to be an invariant, like the Reinold number for fluid flows, being equal in physical terms to

$$D = \frac{c\Delta t}{(\Delta l)^2}, \tag{10}$$

where c [m^2/s] is the diffusion coefficient of the substance, Δl and Δt are the scaling coefficients for length and time.

Since in any certain simulation task c is known, it is sufficient to choose one of the basic parameter scales for finding the other. Usually, the CA size is determined based on the required resolution of a resulting spatial function and available computing resources. Herefrom (10), the time scaling coefficient is direct. The concept of reaction in RD phenomena is assumed to include in addition to chemical reactions all kinds of particle transformations, such as adsorption, desorption, phase transition, mostly inherent to micro and nano kinetic processes. The displacements of particles are represented as the diffusion or the convection steps, obeying conservation laws, while transformations simulate the phase transitions, or chemical reactions, or some biological transmutations, being dissipative by nature. All reactions are simulated by probabilistic substitutions $\theta_i \in \Theta$, probabilities being computed depending on the reaction rates.

Accordingly, the mode of the CA model operation is *stochastic* [13], which is an extension of the asynchronous mode, operating as follows:

- a cell $x \in X$ is chosen with probability $p_x = 1/|X|$;

- a substitution $\theta_i \in \Theta$, $i = 1, \ldots, n$, is chosen with probability p_i, and immediately applied to x;
- an iteration consists of repeating the two above-mentioned time steps $|X| \cdot |\Theta|$ times.

The stochastic CA model parameter set contains the three groups:

- the two basic parameters Δl and Δt,
- dimensionless properties of the species, involved in the process (e.g. density, viscosity, diffusivity), and
- substitution probabilities reflecting the rates of corresponding elementary actions involved in the process.

The above parameters are obtained when a CA model is constructed using the following given data:

- the size of an area under simulation in meters,
- properties of the species involved in the process, expressed in physical units,
- the rates of elementary actions, usually given as rate constants k [s^{-1}].

In the first group, Δl is chosen according to a required spatial resolution of simulation process, Δt is then calculated according to (10). The scaling coefficients of the second group is calculated as the ratio $\mu_w = w'/w$, where w and w' are characteristics of any property of a species involved in the process under simulation.

The computation of substitutions probabilities in the stochastic CA models is the most complicated part of the CA synthesis. There are the following three reasons for it.

1. The rates of many elementary actions are not known exactly, especially, the rates of complex chemical reactions, the rates of nano particles sticking or agglomeration.
2. The rate of diffusion is some orders lower than that of reactions. In order to simulate a process, where they act in common, the two time scales are used: the diffusion time scale Δt_d, and the reaction time scale Δt_r, such that $\Delta t_r = \kappa \Delta t_d$, where κ is an integer usually that is usually equal to some tens hundreds.
3. The reaction rate constants are usually given as real numbers k_1, ..., k_m [s^{-1}], m being the number of reactions. Probability values are computed according to the stochastic CA methodology [14] as follows:

$$p_i = \frac{k_i}{\sum_{j=1}^{m} k_j}, \quad \Delta t_r = k_{\min}^{-1}. \tag{11}$$

In order to pack both time scales into a common iterative process, the iteration should include κ applications of θ_d and an applications of $\theta_i \in \Theta$ with

$$\Delta t = \Delta t_r + \kappa \Delta t_d. \tag{12}$$

The substitution is determined as follows: a random number in the interval $[0, 1]$ is got, if its value is between p_{i-1} and p_i, then θ_i is applied.

The simulation procedure aimed at obtaining:

- the fields of averaged densities

$$R_i = \{(\langle \rho_i \rangle, x),\ \forall x \in X\}, \quad i = 1, \ldots, m, \quad \langle \rho_i \rangle\ [\mathrm{kg/m^3}],$$

- the time per iteration Δt [s].

This is done by executing the following computations:

1. Choose Δl according to the required resolution, which is associated with the smallest size of a particle and determine the size and geometry of X.
2. Define the state alphabet as a set of symbols corresponding to the set of species in the process, and calculate the scaling coefficients of their properties.
3. Compute probabilities p_i, $i = 1, \ldots, n$, according to (11), and write down the substitutions $\theta_i \in \Theta$.
4. Write the program and run the CA model until the required resulting fields $R_i(X)$ for all $i = 1 \ldots m$ are obtained.
5. Transform the obtained dimensionless values $\langle u_i(x) \rangle$ into the physical terms: $u' = u/\mu_u$, where u being any dimensionless parameter.

Example 2. *A simplified model of epitaxial growth of a silicon (Si) crystal.* The process [15] comprises the two following actions: 1) adsorption of Si-atoms from an external gas flow; 2) the diffusion of absorbed atoms (adatoms) over the crystal surface. Being deposited on the surface layer-by-layer adatoms form pillars and islands of different height and size. The top atom on a pillar may diffuse to the adjacent site allocated higher than its neighbor. The process is simulated by a stochastic CA$= \langle A, X, \Theta, \sigma \rangle$, where $A = \{0, 1, \ldots\}$, $X = \{(i, j) :\ i, j = 0, \ldots, N\}$, $N = 200 \times 200$. A cell $(u, (i, j))$ corresponds to a site on a Si crystal surface, the thickness of the adsorbed layer being equal to u atoms. The cell size is equal to $\Delta l \times \Delta l$, these values being equal to the size of a conditional atom, the set of substitutions $\Theta = \{\theta_{\text{ads}}, \theta_{\text{diff}}\}$, θ_{ads} being responsible for absorption and θ_{diff} — for diffusion:

$$\theta_{\text{ads}}: \{(v,(i,j))\} \xrightarrow{p_{\text{ads}}} \{(v+1,(i,j))\},$$
$$\theta^{(l)}_{\text{diff}}: \{(v,(i,j)),(v_l,\phi_l(i,j))\} \xrightarrow{p_{\text{diff}}} \{(v-1,(i,j)),(v_l+1,\phi_l(i,j)\},$$
$$l=1,2,3,4.$$

Here $\phi_l(i,j)$ is a lth neighbor of the cell (i,j) such that $v > v_l$.

The simulation process is performed as follows:

The adsorption rate constant k_{ads} is obtained according to the given partial pressure P_{ads} in the gas over the crystal surface and the sticking coefficients. The simulation is carried out for $k_{\text{ads}} = 0.4\ \text{s}^{-1}$.

The diffusion rate constant k_{diff} depends on the bond strength between the adjacent adatoms $B = 0.08$ in the following way. If a cell has n adjacent cells occupied by adatoms, then $k_{\text{diff}}(n) = 0.08^n\ \text{s}^{-1}$. According to (11) the probabilities

$$p_{\text{ads}} = \frac{k_{\text{ads}}}{k_{\text{ads}} + k_{\text{diff}}(n)}, \quad p_{\text{diff}} = \frac{k_{\text{diff}}}{k_{\text{ads}} + k_{\text{diff}}(n)}.$$

Since p_{diff} depends on n, its value varies from cell to cell, being equal to $8 \cdot 10^{-2}$, $64 \cdot 10^{-4}$, $512 \cdot 10^{-6}$, for $n = 1,2,3$, respectively. The ratio between the reaction and the diffusion time scales may be chosen as $\kappa = 10^2$. Hence, according to (12), each iteration includes an application of θ_i and 100 applications of θ_{diff}.

Program output contains the CA evolution $\Omega(t)$, the total islands perimeter $\text{Per}(t)$, the average expectancy $H_{\text{av}}(t)$, and the dispersion of island height $H_{\max}(t)$, $H_{\min}(t)$.

To express all the results obtained in the physical terms Δl should be chosen as a Si molecule size, let $\Delta l = 10$ Å, then $\text{Per}'(t) = \Delta l \cdot \text{Per}(t)$, $H'_{\text{av}}(t) = \Delta l \cdot H_{\text{av}}$ and the dispersion of H are computed in the same way.

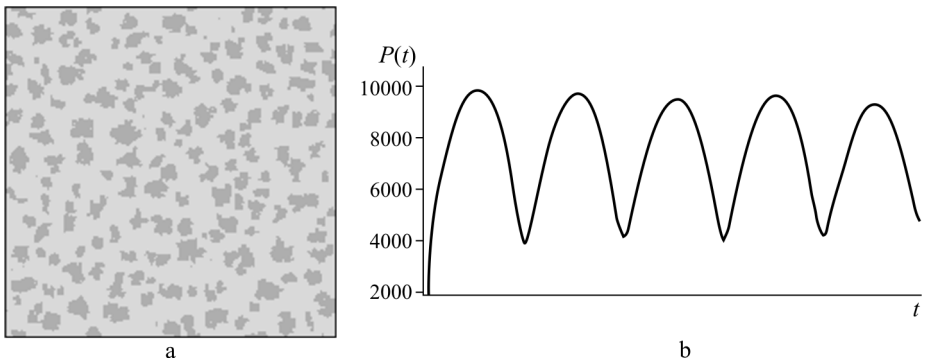

Figure 2. Simulation results of the epitaxial growth process: (a) cellular array after $t = 100{,}000$ iterations; intensity of the gray color corresponds to the height of the island; (b) dependence of total islands perimeter $P(t)$ during the process

A snapshot of the CA evolution is shown in Figure 2a, where the formed islands on the crystal surface are seen. In Figure 2b it is seen that $\mathrm{Per}(t)$ oscillates.

5. Conclusion

The problem of finding the adequate relations between a physical phenomenon and its CA model is discussed. Some general principles are formulated and, based on them, the scaling coefficients are derived apart for the two different types of CA models: lattice–gas CA for the simulation of a viscous flow, and the stochastic CA for the simulation of reaction–diffusion processes. It is clear from the presented examples that the construction of a CA model as well as transformation dimensionless values obtained by running the programmed CA model, are significant parts of the CA simulation procedure. A method proposed for finding the relations between the CA model parameters and their physical counterparts is based on the theory of similitude and requires a profound knowledge of physical fundamentals of a phenomenon under simulation.

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