Mapping Physical Phenomena onto CA-models *

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Abstract. Simulation of natural phenomena using CA-models attracts more and more attention of researchers and enters into practical use. However, the methodology of constructing CA-models for simulating certain natural process as well as analyzing simulation results, are not yet completely developed. The reason lays in a high level of CA-models abstraction which causes difficulties in establishing correspondence between CA parameters and physical values characterizing the process under simulation. In the paper an attempt is made to formulate general principles of constructing CA simulation models, and to show in detail their application to three types of CAs: diffusion CAs, Lattice-Gas CAs, and asynchronous probabilistic CAs. In all cases algorithms for scaling coefficients are developed and illustrated by Examples.

1 Introduction

Cellular Automata (CA) is nowadays an object of growing interest as a mathematical model for spatial dynamics simulation. Due to its capability to simulate nonlinear and discontinuous processes, CAs are expected [1, 2] to become a complement to partial differential equations (PDE), especially in case when there is no other mathematical model of a phenomenon which is to be investigated. By now, a great variety of CAs are known whose evolution simulates certain kinds of spatial dynamics in physics, chemistry, biology, as well as a behavior of colonies of animals or crowds of peoples.

The most known and advanced CA-models may be divided into three classes: 1) CA-models of processes containing diffusion in explicit form, simulating diffusion-reaction processes, [3–6], 2) Lattice-Gas CAs simulating waves and fluids [7–9], and 3) asynchronous probabilistic CA-models simulating molecular kinetics [10–15]. Although the above CA-models are well studied, there is no systematic approach to establish relations between real values characterizing the process to be simulated and the parameters of its CA-model. Meanwhile, the abstract nature of CA-models causes sometimes significant difficulties in constructing an appropriate CA, i.e. in determining the size of the CA, expressing initial and border conditions in CA terms, defining transition rules, probabilities of

* Supported by Russian Academy of Sciences, Basic Research Program of N 14-16(2007)

their application and so on. The inverse problem arises when transforming the obtained CA simulation results into the real physical values.

To make the situation a bit more clear, a general approach to put into correspondence a real process and its CA-model is proposed. Based on it the techniques for determining scaling coefficients for three above classes of CA-models are presented.

Apart from Introduction and Conclusion the paper contains four sections. In Section 2 some formal definitions are given and general principles for CA-models construction are formulated. The next three sections are devoted to detailed considerations of obtaining scaling coefficients relating physical phenomena and its CA-model for the three classes of CAs.

2 General Principles of CA-models Construction

A CA simulation problem is usually stated by defining the following data.

- Size and form of the domain under simulation.
- Properties of the medium where the simulated process is going on.
- Initial and border conditions.

The results to be obtained are scalar $u(\mathbf{x}, t)$ or vector $\mathbf{u}(\mathbf{x}, t)$ functions, which may represent spatial dynamics of certain physical phenomenon. To achieve simulation goal a CA-model should be properly constructed, which may be done according to the following principles.

- The CA should be valid for the whole domain of values of the phenomenon to be simulated. For example, when simulating the fluid flow using Lattice-Gas model it is necessary to be sure that the Reynold's number does not exceed the Lattice-Gas CA limits.
- Implementation of CA simulation should be feasible on available computer systems during the acceptable time.
- It is important to chose the set of basic parameters of a CA-model, whose scales are straightforward. Usually, they are invariant of the phenomenon to be simulated. Such invariants are Reynold's number in fluid dynamics, dimensionless diffusion coefficient, reaction rates. Based on them all other scales may be derived.

It is worth to notice, that the choice of scaling parameters in CA-simulation is similar to that in PDE solution in mathematical physics. The main difference is in the fact that in numerical methods only two scaling values are needed: time step h and space step τ. All other computed values need not to be transformed, except in the special methods.

As for CA-modeling, the choice of CA parameters is more complicated, which is caused by the following factors.

1) The scales should be chosen for all the values involved in the simulation process, including the medium properties such that density, viscosity, pressure, sound velocity, etc.

2) CA-simulation application experience is not rich enough for obtaining quantitative values of above properties in CA-model terms. So, sometimes, they should be obtained by experiments on typical, a priory studied, processes, which is both time consuming and not very accurate.

3) CA-models are very diversified, most of them are essentially nonlinear with nonpredictable behavior, exhibiting all features of complexity [16], and, hence, all problems associated with it.

In what follows the measure system MKS (meter, kg (mass), sec) is used for physical values. As for CA-model, their parameters are mostly dimensionless, expressed in numbers of cells, whose side length $l_{CA} = 1$, number of particles Np_{CA} with mass $m = 1$, sum of velocity vectors with $|\mathbf{v}_{CA}| = 1$ and so on. Scaling coefficients (*scales* for short) are defined as relations of the physical value to its CA counterpart and denoted by $\mu_z = z/z_{CA}$, z being any value involved in the model.

Scales are divided into three groups.

The first group includes two *fundamental scales* which are defined in all types of numerical models, they are time step $\mu_l = h$ and space step $\mu_t = \tau$. In CA-models they represent the linear size of a cell and the time elapsing between two sequent global states, respectively.

The second group comprises *medium properties scales*, such as viscosity, sound speed, substance density, which characterize the medium where the process proceeds, but are not the simulated values. The CA properties of this group are the characteristics of the model derived from CA transition rules or, if it is not possible, they are obtained by simulation experiments.

The third group comprises the *scales of simulated values,* i.e. the values of functions $u(t, \mathbf{x})$, which are the objectives of the simulation, such as the velocity of a fluid flow or an acoustic wave, the rate of a crystal growth or of quantity of a substance obtained by a chemical reaction, etc.

Scales from the second and the third groups are strongly dependent of the nature of the phenomenon under simulation. Hence special methods for any process are further needed considered each in its own section.

A formalism further used for representing CA-models is Parallel Substitution Algorithm [17]. According to it a CA-model $\aleph$ is represented by four notions $\aleph = \langle A, M, \Theta, \varrho \rangle$, where A is a set of symbols of any kind, $M = \{m_1, m_2, ...\}$ is an enumerable set, Θ is a set of local operators, and ϱ is a mode of operation, which determines the time-space distribution of operator application. The central concept in the CA-model is a *cell*, which is a pair (a, m), where $a \in A$ is a cell state, and $m \in M$. The set of cells $\Omega = \{(a_i, m_i) : i = 1, ...\}$, containing no cells with identical names is called a *cellular array.*

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

set of naming functions

$$T(m) = \{m, \phi_1(m), \ldots, \phi_n(m)\}, \quad n \ll |M|, \tag{1}$$

is referred to as a *template*, m being called as *active cell* of a template.

A subset of cells

$$S(m) = \{(u_0, m), (u_1, \phi_1(m)), \ldots, (u_n, \phi_n(m))\}, \tag{2}$$

having the names from $T(m)$, is called a *local configuration* with $T(m)$ as its *underlying template*.

A local operator $\Theta_i \in \Theta$ is expressed in the form of a *substitution* [17] of local configurations as follows

$$\Theta(m) : S(m) \star S''(m) \to S'(m), \quad \forall m \in M, \tag{3}$$

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

An application of $\Theta(m)$ to a certain cell $(u, m) \in \Omega$ (a single-shot application) consists in removing the cells of $S(m)$ from Ω and replacing them by the cells given in $S'(m)$. Such a concept of a local operator allows to simulate living organisms which may grow and die. When simulating physical phenomena *stationary* local operators [17] are used which do not change the naming set, only replacing the states of cells from $S(m)$ in (2) by the states of cells from

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

u' being obtained according to transition functions

$$u'_k = f_k(v_0, v_1, \ldots, v_n, v_{n+1}, \ldots v_{n+h}), \tag{4}$$

where the last h variables are the states of cells from $S''(m)$. The latter in not changed by application of Θ to the cell named m, but provides f_k with additional variables, playing a role of a context [17].

There are different modes of local operator application ordering to perform a global transition $\Omega(t) \to \Omega(t+1)$. *Synchronous mode* provides for transition functions (4) to be computed using the current cell-states, i.e. $S(m) \subset \Omega(t)$. It may be performed at once (in parallel) or in any order. *Asynchronous mode* of operation suggests the substitution of cell states in $S(m)$ being done immediately after $\Theta(m)$ is applied. So, $S(m) \subset \Omega(t) \cup \Omega(t+1)$. In both case the transition to the next global state is referred to as an *iteration* occurring when all cells have completed their computations. The sequence

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

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

Performing a CA simulation task comprises three stages:

1) constructing the model, i.e. determining the CA $\aleph = \langle A, M, \Theta, \varrho \rangle$ and and its initial global state $\Omega(0)$,

2) obtaining resulting data by running the CA program , and

3) interpreting the results by transferring the model parameters into habitual physical values.

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

3 CA-models of Phenomena which Include Diffusion

Diffusion components are present in the majority of natural spatially distributed processes, in PDEs being represented by a Laplacian

$$d(u_{xx} + u_{yy}) \tag{5}$$

where d - is a diffusion coefficient in $\mathtt{m}^2\mathtt{s}^{-1}$. Being discretized by means of the "cross template" (5) takes the form

$$C(u_{i-1,j} + u_{i,j+1} + u_{i+1,j} + u_{i,j-1} - 4u_{i,j}), \quad i = x/h,\ j = y/h, \tag{6}$$

with

$$C = \frac{d\tau}{h^2}, \tag{7}$$

where h and τ are length and time steps, respectively. In other words, they are length and time scales, denoted further as μ_l and μ_t. In computational mathematics they are chosen according to performance constraints, convergence and stability conditions, and, perhaps some special requirements.

As for CA diffusion, determination of scales is more complicated and less studied. The reason is in the fact that each CA-model is characterized by its own CA-diffusion coefficient C_{CA}, which may be obtained analytically, as it is done in [4], or experimentally [3]. The coefficient is dimensionless and plays the same role that C in (6), being an invariant of a diffusion model. So, when a CA-model is chosen C_{CA} is easily obtained.

Taking into consideration (7) the derivation of a diffusion CA-model scaling coefficients is based on the following relation.

$$C_{CA} = d\frac{\mu_t}{\mu_l^2}, \tag{8}$$

Since in any certain simulation task d is a known characterizing property of the medium and the size of the area under simulation $L_x \times L_y \times L_z$ is given, it is sufficient to chose the CA dimensions $N_i \times N_j \times N_k$ for obtaining all scales. Usually CA size is determined based on the required resolution of resulting spatial function and the available computing resources. Herefrom all scaling coefficients are straightforward.

$$\mu_l = \frac{L}{N}\ \mathtt{m}, \quad \mu_d = \frac{d}{C_{CA}}\ \mathtt{m}^2\mathtt{s}^{-1}, \quad \mu_t = \frac{\mu_l^2}{\mu_d}\ \mathtt{s}. \tag{9}$$

There are several CA diffusion models. Two of them are the most popular. The first is a *two-stage synchronous* probabilistic model (CA-synch), proposed in [1] and studied and founded in [4]. The second, called in [1] a *naive diffusion* (CA-naive), is an asynchronous probabilistic CA . For all models C_{CA} is a function of the probability used in the local operators, the maximal values $\hat{C}_{CA}$ being fixed for each diffusion CA.

In Table 1 $\hat{C}_{CA}$ for the above two CA-diffusion models are given for 1D, 2D, and 3D cases. For $C_{CA-synch}$ they are proved in [4], for $C_{CA-naive}$ they are obtained by comparing simulation results with analytically known values.

Table 1. Maximum values of diffusion coefficients of synchronous and asynchronous CA-models

n	$\hat{C}_{CA-synch}$	$\hat{C}_{CA-naive}$
1D	1.0	1.0
2D	3/2	1/2
3D	23/18	1/3

By varying probabilities of local operators application it is possible to simulate processes with diffusion coefficient changing in space or in time, for example, depending on temperature.

Example 1. *Application a diffusion-convection CA-model to simulate vapor propagation through a porous membrane.* The objective of simulation is to investigate the impact of pore walls properties on the percolation velocity. A fragment of the membrane in a 2D approximation is considered, the pore diameter being equal to its width. The fragment has three vertically located pores with equal diameters: a hydrophilous, a hydrophobic and a neutral one (Fig.1). The process is represented as a stream of abstract particles, moving under convective and diffusive forces. The source of particles is on the fragment top area where the pressure of the vapor is imposed having equal effect to the three pores. The convective force makes the vapor particles move downwards. The diffusion component accounts for anisotropic properties of the medium by varying probability values of particles displacements along the pore diameter, depending on pore wall properties. The mode of percolation is characterized by the relation of the impact of convective component to that of the diffusion one, defined as $Pe = 0.5$ [18]. The porous sample to be investigated has the size $L_i = L_j = L = 0.03\ \mathtt{m}$, pore diameter being $Dp = 8 \cdot 10^{-3}\ \mathtt{m}$. Diffusion coefficient of vapor is $d = 10^{-4}\ \mathtt{m}^2\mathtt{s}^{-1}$, the density is $\rho = 0.5 \cdot 10^3\ \mathtt{kg} \cdot \mathtt{m}^{-3}$.

The model to be used is an asynchronous naive CA-diffusion with $A = \{0, 1\}$ and the naming set $M = \{(i, j) : i, j = 0, \ldots, N - 1\}$. The local operator is the superposition of two substitutions: $\Theta = \{\Theta_{conv}, \Theta_{diff}\}$, both being probabilistic. The probabilities p_{conv} and p_{diff} are determined according to the given coefficient $Pe = p_{conv}/p_{diff} = 0.5$ [18],

$$\Theta_{conv}(i,j) = \{(1,(i,j))(0,(i+1,j))\} \xrightarrow{p_{conv}} \{(0,(i,j))(1,(i+1,j))\}, \qquad (10)$$

advances a particle along the pore with a probability equal to p_{conv}.

$$\Theta_{diff}(i,j) = \{(1,(i,j))(0,(i+a,j+b))\} \xrightarrow{p'_{diff}} \{(0,(i,j))(1,(i+a,j+b))\}, \quad (11)$$

exchanges the cell-state $u = 1$ with one of its neighbor according to the pair $(a, b) : a, b \in \{-1, 1\}$, which is chosen with the probability $p = 1/q$, q being the number of empty neighbors. So, $p'_{diff} = p_{diff} \cdot p_w$, with p_w accounting for pore type and depending of the distance g_w between the cell (i, j) and the wall. When a pore is neutral or if $g_w > \beta$, then $p_w = 1$, β being the distance where wall influence may be neglected. If $g_w \leq \beta$, then for hydrophilous and hydrophphobic pores

$$p_w(\texttt{phil}) = 1 - \exp(-g_w/n_1\beta_1), \quad p_w(\texttt{phob}) = \exp(-g_w/n_2\beta),$$

respectively, n_1, n_2 depending of the wall properties.

The above data are sufficient for obtaining physical scales of CA-model parameters.

1) *Length scale.* According to porous medium simulation practice [18] minimal diameter of the pore should be several times larger than 10. Taking $h = \mu_l = 10^{-4}$ the CA-diameter yields $Dp_{CA} = 80$, and the linear size of the whole CA $L_{CA} = 300$.

2) *Diffusion scale.* Since the 2D naive asynchronous CA diffusion is used, $C_{CA} = 0.5$, and $\mu_C = d/C_{CA} = 2 \cdot 10^{-4}$ $\texttt{m}^2\texttt{s}^{-1}$.

3) *Time scale* $\mu_t = \mu_l^2/\mu_C = 0.5 \cdot 10^{-4}$ s.

4) *Density scale* (mass of an abstract particle) $\mu_\rho = \rho/(\rho_0/h^3) = 1.25 \cdot 10^{-9}$ kg.

5) *Flow scale* (mass of vapor propagating through the cross-section of a pore per second, relative to the number of particles passing through the pore per iteration). Accounting for a pore square $Sp = 5024$ cells, $\mu_Q = \mu_\rho/\mu_t = 2 \cdot 10^{-5}$ kgs^{-1}.

CA-simulation results in the following flows, obtained in particles numbers passing through a pore per iteration

$$Q_{CA}(\texttt{phob}) = 3939, \quad Q_{CA}(\texttt{phil}) = 1975, \quad Q_{CA}(\texttt{neutr}) = 2812,$$

which are recalculated into physical values by multiplying the obtained Q_{CA} by μ_Q resulting in the following flows.

$$Q(\texttt{phob}) = 0.079\ \texttt{kgs}^{-1}, \quad Q(\texttt{phil}) = 0.039\ \texttt{kgs}^{-1}, \quad Q(\texttt{neutr}) = 0.058\ \texttt{kgs}^{-1}.$$

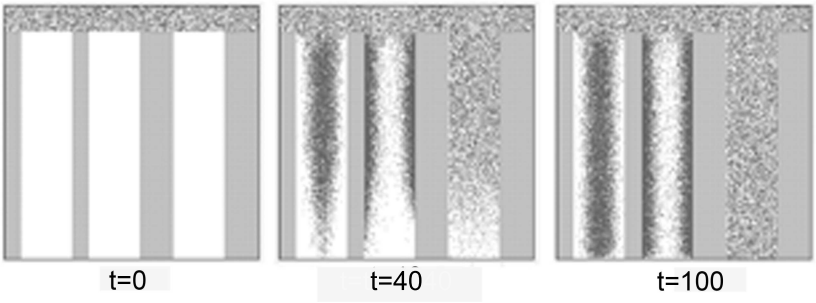

Fig. 1. Three snapshots of CA simulation of vapor propagation through porous membrane

4 Lattice-Gas Models of Viscous Flows

Gas-Lattice CA-models comprise a special class of CA intended to simulate processes in gas and liquids. The medium is represented by abstract particles, moving in a discrete space and colliding. The most known and well studied model is a series of stochastic Lattice-Gas CAs called FHP-models according to the names if the authors [9]. Formally, they are synchronous CA, characterized by the following parameters. The naming set $M = \{m_k : k = 1, 2, \ldots, |M|\}$ enumerates hexagones on a 2D plane. A cell neighborhood includes the cell names of 6 adjacent cells. Accordingly, 6 moving and some rest particle may be located in a cell. To represent the cell states with 6 moving and one rest particle the alphabet $A = \{s = (s_0, \ldots, s_6)$, $|A| = 2^7$ comprises Boolean vectors 7 bit long. A component of a state vector $s_i = 1$ indicates that the cell (s, m) has a particle moving towards the ith neighbor $(i = 1, \ldots, 6)$ with a velocity $c_i = 1$, or if the cell has a rest particle, then $s_0 = 1$ having the velocity $c_0 = 0$. 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 it as a set of 6 substitutions each being applied to ith component of state vector.

$$\Theta_1(m, i) = \{(s_i, m)\} \star \{(s'_i, \varphi_i(m))\} \rightarrow \{(s'_i, m))\}, \quad i = 1, 2 \ldots, 6. \tag{12}$$

The second contextless local operator simulates the collision of particles.

$$\Theta_2(m) = \{(s, m)\} \rightarrow \{(s\prime, m))\}. \tag{13}$$

The transition function $s\prime = f(s)$ is given in the form of a table, some arguments having two equiprobable outcomes. The principles of collision rules functioning is shown in Fig. 2.

The mode of operation of Lattice-Gas CA is two-stage synchronous, i.e. each iteration consists of two stages: on the first stage the six6 propagation operators (12) act simultaneously, on the second stage the collision operator completes

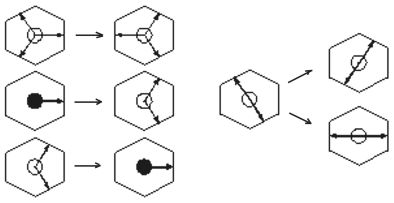

Fig. 2. Graphical representation of collision operators in FHP-I Lattice-Gas model. Deterministic rules are given on the left, the probabilistic ones – on the right

the transition to the next global state. In [9] FHP-model is proved to be identical to Navier-Stokes equation in describing the velocity of viscous flow and to be identical to the wave propagation when being regarded relative to particles density.

The 3D-version of the FHP-model called RD-1 is also known. It is based on the discrete space with cells having the form of rhombododecahedra. The template of RD-1 has 12 neighbors. It allows to simulate flows in large enough space, as compared with the FCHC model proposed and investigated in [9]. Although the model meets the isotropic conditions approximately, its experimental testing showed acceptable plausibility to the phenomenon [19].

Each Lattice-Gas CA-model is characterized by by the following parameters: equilibrium density $\tilde{\rho}_{CA}$, sound velocity Cs_{CA} and and viscosity $\nu_{CA}(\rho_{CA})$, the latter being a functions of particle density. In (Table 2) these parameters are given according to [9, 19].

Table 2. Main parameters of Lattice-Gas CA $\tilde{\rho}_{CA}$

CA-model	Cs_{CA}	$\tilde{\rho}_{CA}$	$\nu_{CA}(\tilde{\rho}_{CA})$ [1]
FHP	$1/\sqrt{2}$	1.2	0.85
RD-1	$\sqrt{7/13}$	3.9	0.325

In its turn a simulation task statement includes the following data in physical terms.

1) Size of the reservoir where the simulated process proceeds, l $\mathtt{m}$ being its characteristic length.

2) Location of source and of the outlets of the fluid.

3) The fluid properties: density ρ $\mathtt{kgm}^{-3}$, kinematic viscosity ν $\mathtt{m}^2\mathtt{s}^{-1}$.

3) External and initial conditions: working pressure P or pressure drop ΔP $\mathtt{kgm}^2$.

[1] CA-viscosity values are given already corrected with regard to the isotropy coefficient $g(\rho)$ [9, 19]

4) The wanted velocity value u or the Reynolds number

$$Re = \frac{u \cdot l}{\nu}. \tag{14}$$

The above CA parameters and given physical values allow to obtain all scaling coefficients. Namely, the viscosity and the density scales are straightforward.

$$\mu_\nu = \frac{\nu}{\nu_{CA}}\ \mathtt{m}^2\mathtt{s}^{-1}, \quad \mu_\rho = \frac{\rho}{\tilde{\rho}_{CA}}\ \mathtt{kgm}^3. \tag{15}$$

Moreover, from the limiting CA Reynold's number [9]

$$Re = Re_{CA} = Cs_{CA}\frac{l_{CA}}{\nu_{CA}}$$

it is possible to find the characteristic CA-values of length l_{CA} or velocity u_{CA}, depending on the simulation task objective, and then calculate the following scales.

$$\mu_l = \frac{l}{L_{CA}}\ \mathtt{m}, \quad \mu_u = \frac{\mu_\nu}{\mu_l}\ \mathtt{ms}^{-1}, \quad \mu_t = \frac{\mu_l}{\mu_u}\ \mathtt{s}. \tag{16}$$

The pressure scale may be obtained in two ways:

$$\mu_P = \frac{\mu_u^2}{\mu_\rho}\ \mathtt{kgm}^{-2}, \quad \text{or} \quad \mu_P = \frac{P}{\rho_{CA}}\ \mathtt{kgm}^{-2}. \tag{17}$$

Since the alphabet, local operators and operation mode are defined by the Lattice-Gas model, only the linear dimensions and external pressure are to be determined in order to construct a Lattice-Gas CA-model.

1) The linear dimensions l_{CA} along the three directions l_i, l_j, l_k are computed by dividing the given real dimensions of the reservoir l_x, l_y, l_z by μ_l.

2) The external pressure is represented by the value of ρ_{CA} at the source location $\rho_{CA} = \frac{P}{\mu_P}$.

Example 2. *The Lattice-Gas 3D model RD-1 is used for simulating the flow of motor oil through a tube partly barred up by a choker.* The follwing data are given.

1) Tube diameter $Dt = 0.7$ m, the length l= 7 m, on one end of the tube the pressure $P = 1.07$ atm is imposed, the other end is left opened. So, pressure drop $\Delta P = 7000\ \mathtt{kgm}^{-1}$. The choker is placed at the distance 3.5 m from the source and barres up a half of the tube cross section.

2) Motor oil viscosity $\nu = 4.5 \cdot 10^{-3}\ \mathtt{m}^2\mathtt{s}^{-1}$.

3) Motor oil density $\rho = 880\ \mathtt{kgm}^{-3}$.

Simulation aims to obtain the velocity field behind the choker-bar.

Properties of the fluid being known the scales of density and viscosity are straightforward.

$$\mu_\nu = \frac{\nu}{\nu_{CA}} = 13.8 \cdot 10^{-3}\ \mathtt{m}^2\mathtt{s}^{-1}, \quad \mu_\rho = \frac{\rho}{\tilde{\rho}_{CA}} = 225\ \mathtt{kgm}^{-3}. \tag{18}$$

Taking the averaged CA-density $\rho_{CA}(0) = 8$ in source cells twice as large as the $\tilde{\rho}_{CA}$, the pressure scale is obtained according to (17). Then, accounting for (18) it is possible to calculate all others scales as follows.

$$\mu_P = \frac{\Delta P}{\rho_{CA}(0)} = 875\ \mathtt{kgm}^{-2}, \quad \mu_u = \sqrt{\frac{\mu_P}{\mu_\rho}} = 1.97\ \mathtt{ms}^{-1},$$

$$\mu_l = \frac{\mu_\nu}{\mu_u} = 7 \cdot 10^{-3}\ \mathtt{m}, \quad \mu_t = \frac{\mu_l}{\mu_u} = 3.55 \cdot 10^{-3}\ \mathtt{s}. \tag{19}$$

Having the scales in hands CA length values are computed as follows.

$$Dt_{CA} = \frac{Dt}{\mu_l} = 100, \qquad l_{CA} = \frac{l}{\mu_l} = 1000,$$

l_{CA} being the CA length of the tube (along the j-axis).

Simulation results are obtained as an 3D array of vectors $\langle \mathbf{u}_{CA} \rangle (i, j, k)$, each being equal to the averaged value of CA-velocity in a cell. The corresponding physical values

$$\mathbf{u}(x, y, z) = \mu_l \cdot \langle \mathbf{u}_{CA} \rangle (i, j, k), \quad x = i\mu_l, y = j\mu_l, z = \mu_l.$$

A fragment of the velocity field behind the choker is shown in Fig.3.

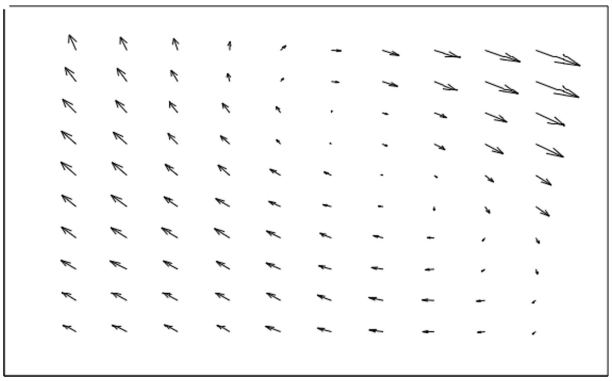

Fig. 3. A fragment of a lengthwise projection of of the velocity field behind the choker obtained by applying MathCad tools to RD-1 simulation results of the fluid flow through a tube

Maximum averaged value of the velocity over the choker is $\langle \mathbf{u}_{CA-max} \rangle = 0.9$ which yields $u_{max} 1.77\ \mathtt{ms}^{-1}$. The mean velocity through the tube is computed as the average lengthwise velocity component at distance $l_{CA} = 700$ from the source, which occurred to be $\langle u_{CA} \rangle = 0.67$, which after scaling yield $\langle u \rangle = 1.3 \mathtt{ms}^{-1}$.

5 Asynchronous CAs Modeling Nano-Kinetic Processes

Kinetic asynchronous CA (ACA) simulate phenomena consisting of sets of elementary actions, directly mimicking physical movements and interactions of molecules or atoms, in CA-models being referred to as called*particles*. Nowadays a number of surface nano-kinetic processes simulation by ACA are known, being, sometimes, referred to as Monte-Carlo methods [10, 11, 14, 20]. In brief, the methods are as follows. The domain where the process should proceed is divided into sites. A site (a cell in the CA) may be occupied by a particle representing a species from a given set of species involved in the process. The particles move and interact according to the laws prescribed by the phenomenon under simulation. The symbols, denoting different particles of the set comprise the ACA alphabet. The following alphabets are mostly used.

- Boolean alphabet $A = \{0, 1\}$, when it suffices to indicate presence or absence of a particle in the cell.
- A set of characters or symbols representing the notations of particles ($\emptyset$, Al, CO, H_2, etc.), a symbol $\emptyset$ denoting the state of unoccupied site.
- A set of integers, when several particles are allowed to be allocated in a single site.

The set of cell coordinates $M = \{(i, j) : i, j = 0, \ldots, N\}$ is frequently appended by a contextual domain consisting of a single generalized cell, say Gas, which represents the external space, where nothing happens, but wherefrom particles emanate and whereto the desorbed ones are gone. There is no restriction on the naming set structure, the most popular are arrays based on crystalline lattices, as well as those providing structural anisotropy.

Local operators which simulate the most used elementary actions in kinetic ACA are as follows. *Adsorption*. A particle $a \in A$ is adsorbed from the gas onto an empty site on a solid surface with the probability p_a.

$$\Theta_a : \{(\emptyset, m)\} \star \{(a, Gas)\} \stackrel{p_a}{\rightarrow} \{(a, m)\}. \tag{20}$$

Desorption. A particle b is desorbed from a surface site with the probability p_b.

$$\Theta_a : \{(a, m)\} \stackrel{p_b}{\rightarrow} \{(\emptyset, m)\}. \tag{21}$$

Reaction. If the particles a and b occur in the adjacent sites on the surface, they react forming a molecule ab, which outgoes to the gas with probability p_{ab}.

$$\Theta_{ab} : \{(a, m)(b, \varphi(m)) \stackrel{p_{ab}}{\rightarrow} \{(\emptyset, m)(\emptyset, \varphi(m))\}. \tag{22}$$

Diffusion. If a particle occur in the neighborhood of an empty site, it moves there with the probability p_d

$$\Theta_d : \{(a, m)(\emptyset, \varphi(m))\} \stackrel{p_d}{\rightarrow} \{(\emptyset, m)(a, \varphi(m))\}. \tag{23}$$

Of course, the above local operators do not exhaust all possible actions in surface kinetic processes, but they are typical and the most commonly encountered.

Nano-kinetic ACA-model simulation aims to investigate the behavior of the process both qualitatively (finding out whether it tends to a steady state, or to oscillation, or exhibits instability, etc.) and quantitatively (calculating amounts of obtained reactants, real rates of the reactions). The given data comprise a set of species, involved in the process, prerequisites to be accounted for, initial conditions. As for the size of the sample where the process should proceed, it is mostly constrained by the available computational resources rather than by researcher's request, the latter being usually "the larger the better".

From the above it is clear that local operators of a kinetic ACA model are very simple being easily derived from the chemical representation of the reaction mechanism. The problem is to determine the time scale and to find correct probabilities for reaction operators. The latter ones are computed according to chemical and physical properties of the process under simulation, usually calculated on the basis of molecular dynamics laws [21]. So, there are no general method to obtain their values. But, based on available experience, some following considerations may be made.

For a chemical reaction $R_i \in R$, $i = 1, \ldots, n$, R being a set of reactions in the process, the probability in Θ_i is equal to

$$p_i = \frac{k_i}{\sum_{j=1}^{n} k_j},$$

where $k_i, k_j(\ \mathtt{s}^{-1})$, $j = 1, \ldots, n$, are known rate coefficients.

Adsorption probability p_a is obtained apart for each type of particles according to given partial pressure of the corresponding species in the Gas and sticking coefficients. If any deposited atom is assumed to be adsorbed, then $p_a = 1$.

Diffusion probability p_d strongly depends on bond strength between particles and is computed based on bond energy values [21].

Time scale is calculated basing on the assumption that all time intervals Δt between a certain sequential event are identical, and, hence, may be put into correspondence with CA iterations Δt_{CA}, depending of what value is given. In [20] two methods of establishing a relation between Δt and Δt_{CA} are given: 1) when the real flow of atoms $F\ \mathtt{m}^{-2}\mathtt{s}^{-1}$ to be involved in the process per second is known, and 2) when the deposition rate (numbers of monolayers deposited onto the surface per second) $ML\ \mathtt{s}^{-1}$ is measured. Accordingly,

$$\mu_t = \frac{N_d \cdot t_{CA}}{\mu_l^2 \cdot F \cdot |M|}\ \mathtt{s}, \quad \text{or} \quad \mu_t = \frac{1}{ML \cdot |M|}\ \mathtt{s}. \tag{24}$$

where N_d is the total number of particles involved into the process during the whole simulation, t_{CA} is the number of iterations per second measured during the simulation, $|M|$ is the cardinality of cellular array in the ACA. In [11] the physical time interval between two deposition acts t_{eff} is taken to correspond to the averaged time taken by adatoms to jump to the adjacent site.

$$\Delta t_{eff}^{-1} = \frac{k_B T}{2\pi\hbar} \exp(-\frac{E_c}{k_B T}).$$

The following scaling coefficients establish the correspondence between the ACA parameters and their physical counterparts.

1) *Length scale* $\mu_l = l$ m, l being the real linear size of the largest atom.

2) *Mass scale* $\mu_m^{(i)} = m_i$ kg, m_i being the real mass of an atom of ith species.

3) *Time scale* $\mu_t = \Delta t/\Delta t_{CA}$, Δt_{CA} being the computing time of an iteration measured during the simulation.

Moreover, CA-evolution being visualized allows the process to be observed in detail.

Example 3. *The simplified model of epitaxial growth of a silicon (Si) crystal*. The process [20] comprises two following actions: 1) adsorption of Si-atoms from an external flow; 2) diffusion of the absorbed atoms (adatoms) over the surface. If any atom deposited on the surface is adsorbed, then the rate coefficient $k_a = 1$. 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 an adjacent site $(i + a, j + b)$, $a, b \in \{-1, 0, 1\}$, if $u(i + a, j + b) \leq u(i, j)$. Probability of such an action depends on bond strength between the adjacent adatoms, characterized by a constant $B = 0.05$ in the following way. If a site has n adjacent adatoms, then the probability of the diffusion is $p'_d = (4 - n) \cdot 0,05^n$. The choice among the sites whereto the adatom is allowed to move is equiprobable, which yields $p_d(k) = p'_d/(4 - n)$.

The process is simulated by an ACA= $\langle A, M, \Theta \rangle$ where $A = \{0, 1, \ldots\}$, $M = \{(i, j) : i, j = 0, \ldots, N\}$. A cell $(v, (i, j))$ corresponds to a site on a Si crystal surface, the thickness of the adsorbed layer being equal to v atoms. The transition rule $\Theta(i, j)$ is a superposition of Θ_{ads} responsible for absorbtion, and $\Theta_{diff}(i, j)))$ responsible for diffusion.

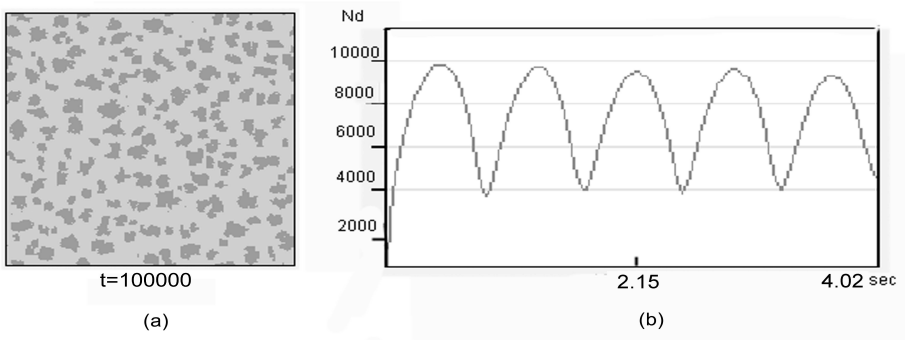

Fig. 4. Simulation results of epitaxial growth process. (a) Cellular array after t=100000 iterations (b), the dependence of islands perimeter $P(t)$ on real time. $|M| = 200 \times 200$. Intensity of gray color corresponds to the height of the island

$$\begin{aligned} \Theta_{ads} &= \{(v_0,(i,j))\} \star \{(1,Gas)\} \stackrel{p_a}{\rightarrow} \{(v_0+1,(i,j))\}, \\ \Theta^{(k)}_{diff} &= \{(v_0,(i,j)),(v_k,\varphi_k(i,j))\} \stackrel{p_{d(k)}}{\rightarrow} \{(v_0-1,(i,j)),(v_k+1,\varphi_k(i,j)\}, \\ & \quad k=1,2,3,4. \end{aligned} \tag{25}$$

where $\varphi_k(i,j)$ is a kth neighbor of the cell (i,j).

A snapshot of the ACA evolution is shown in Fig.4 (a), where the formed islands on the crystal surface are seen. One of the important characteristic of the process is the dependence of total island perimeter $P(t)$ on time. The perimeter P is computed at each iteration as a number of pairs of adjacent cells having different states. During the process this parameter exhibits oscillations shown in Fig.4 (b), which are of interest for the researcher. The time scale is computed according to (24) based on the given rate of the deposition $ML = 1.4\ \mathtt{sec}^{-1}$ (monolayers per second $\mu_t = (ML \cdot |M|)^{-1} = 0.178 \cdot 10^{-4}\ \mathtt{s}$.

6 Conclusion

The problem of finding out the adequate correspondence between physical phenomenon and its CA-model is approached form the position of researcher who exploits CA simulation in studying certain natural phenomenon. Some general principles are formulated and, based on them, scaling coefficients are derived apart for three different types of CA-models. It is clear from the presented examples, that construction of a CA-model as well as finding out the correct interpretation of the simulation results, require a profound knowledge of physical fundamentals of the phenomenon under simulation. It affirms the fact that users of CA-simulations tools should be the physicists or engineers not experienced in CA theory. It makes the methodology of CA simulation yet more important and requested, thus implanting aspirations that the development of CA-models should include procedures of computing scaling coefficients.

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