

Cellular Automata Simulation of a Bistable Reaction-Diffusion System: Microscopic and Macroscopic Approaches

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ABSTRACT: *The Cellular Automata method has been used to simulate the pattern formation of the Schlögl model as a bistable Reaction-Diffusion System. Both microscopic and macroscopic Cellular Automata approaches have been considered and two different methods for obtaining the probabilities in the microscopic approach have been mentioned. The results show the tendency of the system towards the more stable phase in both microscopic and macroscopic cases. It is shown that the fluctuation effect plays an important rule in the microscopic approach while it is negligible in the macroscopic case.*

KEY WORDS: *Reaction-diffusion systems, Bistable system, Schlögl model, Pattern formation, Cellular Automata.*

INTRODUCTION

Reaction-Diffusion Systems (RDS) are mathematical models that describe how the concentration of one or more substances which distributed in space changes under the influence of two processes: local chemical reactions in which the substances are converted into each other, and diffusion which causes the substances to spread out in space. As this description implies, RDS are naturally applied in chemistry. However, the equation can also describe

dynamical processes of non-chemical nature. Examples are found in biology, geology, physics, and ecology. Mathematically, RDS take the form of semi-linear parabolic partial differential equations. The most simple reaction-diffusion equation concerning the concentration u of a single substance in one spatial dimension is [1],

$$\partial_t u = D \partial_x^2 u + R(u) \quad (1)$$

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where D is a diagonal matrix of diffusion coefficients and R accounts for all local reactions. If the reaction term vanishes, then the equation represents a pure diffusion process. The solutions of reaction-diffusion equations display a wide range of behaviors, including the formation of travelling waves and wave-like phenomena as well as other self-organized patterns like stripes, hexagons or more intricate structures [2]. In recent times, RDS have attracted much interest as a prototype model for pattern formation. It has also been argued that reaction-diffusion processes are an essential basis for processes connected to morphogenesis in biology and may even be related to animal coats and skin pigmentation [3-7]. Another reason for the interest in reaction-diffusion systems is that although they represent nonlinear partial differential equation, there are often possibilities for an analytical treatment [8-12]. In some cases, RDS include sophisticated differential equations, and analytical methods could not lead to results. So, numerical and simulation methods may be used [8,11]. Cellular Automata (CA) is one of the simulation methods that seems to be a good candidate for description of RDS. The CA are discrete dynamical system, i.e. space, time, and the states of the system are discrete. Each point in a regular spatial lattice, called a cell, can have any one of a finite number of states. The states of the cells in the lattice are updated according to a local rule. That is, the state of a cell at a given time depends only on its own state and the states of its nearby neighbors at the previous time step. All cells on the lattice are updated synchronously. Thus the state of the entire lattice advances in discrete time steps. The theory of cellular automata is immensely rich, with simple rules and structures being capable of producing a great variety of unexpected behaviors. *Von-Neumann* was one of the first people to consider such a model, and incorporated a cellular model into his "universal constructor" [13]. Comprehensive studies of the cellular automata have been performed by *S. Wolfram* starting in the 1980s [14,15].

In this paper, both microscopic and macroscopic CA approaches are used to simulate the Schlögl model as a bistable reaction-diffusion system. In the next section, the *Schlögl* model is introduced and after that, the CA methods for simulation of the *Schlögl* model are described. Finally, the results of the microscopic and macroscopic approaches are shown and compared with each others.

The Schlögl Model

In physics, for an ensemble of particles, the bistability comes from the fact that its free energy has three critical points. Two of them are minima and the last is a maximum. By mathematical arguments, the maximum must lie between the two minima. By default, the system state will be in either of the minima states, because that corresponds to the state of lowest energy. The maximum can be visualized as a barrier. The *Schlögl* model is an example of a bistable system first introduced by Schlögl [16]. In a series of papers, *Schlögl* introduced two models for a chemical bistable system [16-18]. One of the models is described by



where A , B , and C are chemical species that are assumed to be in abundance and kept constant by appropriate feeding. Only X is allowed to vary. Note that this assumption about the species A , B , and C is only admissible in a mesoscopic setting, where the mean field equations are valid. These simplifications are not valid in low dimensional simulations of hard-spheres on a lattice [19]. Denoting the concentration of X by x , one could obtain the mean field rate law

$$f(x) = k_{-2}[C] - k_2[B]x + k_1[A]x^2 - k_{-1}x^3 \quad (3)$$

For appropriate values of the parameters, this third order polynomial has three real roots $x_1 \leq x_2 \leq x_3$ and can be written as

$$f(x) = -\tilde{k}(x - x_1)(x - x_2)(x - x_3) \quad (4)$$

It follows that the states x_1 and x_3 are stable steady states, and x_2 is an unstable steady state.

Cellular Automata Model

A CA model for simulation of RDS consists of a combination of two different parts, a diffusion step and a reaction step [20]. To clarify the separation into two steps, the reaction-diffusion equation could be discretized as follow (for one-variable system),

$$\frac{\partial x(r,t)}{\partial t} = D\nabla^2 x(r,t) + f(x(r,t)) \quad (5)$$

$$x(r, t + \Delta t) = x(r, t) + \Delta t D \nabla^2 x(r, t) + \Delta t f(x(r, t)) + O(\Delta t^2) \quad (6)$$

On the other hand, to be able to call the simulation method a cellular automaton, and to use a lookup table instead of calculating a nonlinear reaction term, the variables could be discretized. There are two different CA approaches for simulation of a reaction-diffusion system. The microscopic approach is used when microscopic fluctuations play an important rule in the system. In contrast, a macroscopic approach is used when fluctuations are not important. In this section, each method is shortly described.

Microscopic approach:

Molecules are considered as point particles. Particles move on the lattice with discrete velocities, that is, they move at discrete time steps from a cell to one of the neighboring cells as dictated by particle velocities. Each cell of the lattice possesses five channels where particles can reside, and an exclusion principle forbids more than one particle to reside in any channel. It also forbids more than one particle with the same velocity in each cell. Fig. 1 shows one cell with all possible particles in different velocities. The time evolution of particles occurs at discrete time steps based on the rule of the automata (operator ε) which can be separated into three basic operations: Propagation P, Redistribution R, and Chemical Transformation C.

$$\varepsilon = C \cdot R \cdot P \quad (7)$$

During the propagation, each particle moves from its channel to the corresponding channel of a neighbor cell as dictated by the particle velocity. In this step, the number of particles and their momentum are conserved. In the redistribution step, the velocity configuration is randomly shuffled in each cell. This operation conserves the number of particles in each cell but the momentum is not conserved. The momentum changes can be viewed as elastic collisions between particles. These two operations are considered as the Diffusion part. During the chemical transformation (or the Reaction part), particles are created or annihilated at each cell based on probabilities which are derived from reaction equations. There are two different approaches for obtaining the probabilities:

First approach is used when the detailed mechanism of a system is known. In this case, one could obtain

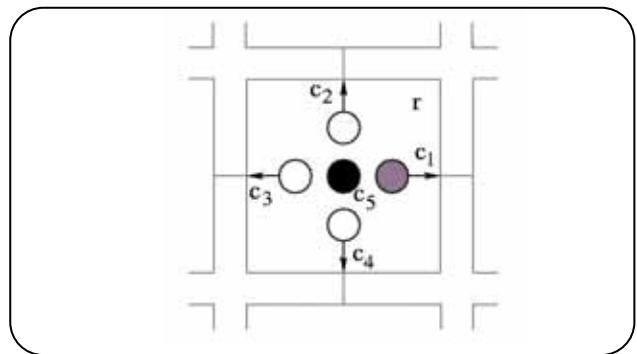


Fig. 1: A given cell with all possible particles with different velocities (c_5 is the halt state or zero velocity).

probabilities according to these equations (obtaining these equations are shown in details in [21]),

$$g_i(\alpha) = h \sum_{j=1}^r (v_i^j - v_i^{-j}) \left\{ -k_j \prod_{k=1}^n m^{v_i^k} \binom{m - v_i^j}{\alpha_k - v_i^j} \binom{m}{\alpha_k}^{-1} + k_j \prod_{k=1}^n m^{v_i^{-j}} \binom{m - v_i^{-j}}{\alpha_k - v_i^{-j}} \binom{m}{\alpha_k}^{-1} \right\} \quad (8)$$

and,

$$g_i(\alpha) = \sum_{\beta} (\beta_i - \alpha_i) p(\alpha, \beta) \quad (9)$$

$$p(\alpha, \alpha) = 1 - \sum_{\beta \neq \alpha} p(\alpha, \beta) \quad (10)$$

where α and β are particle numbers in a cell before and after a reaction, respectively, $g_i(\alpha)$ is the average value of particles transformation in α configuration, $p(\alpha, \beta)$ is the probability of the transformation of α particles to β particles, m is the number of channels (here 5), v and k are the reaction stoichiometry and reaction rate coefficients, respectively, r is the number of the reactions, and h is a normalization coefficient.

The second approach is used when the mechanism of a reaction is not fully understood. In this case, one could use these equations [21],

$$p_{\{x\}}(\alpha_i) = \prod_{i=1}^n \binom{m}{\alpha_i} x_i^{\alpha_i} (1 - x_i)^{m - \alpha_i} \quad (11)$$

$$f_i(x) = \sum_{\alpha} g_i(\alpha) p_{\{x\}}(\alpha) \quad (12)$$

Where $f(x)$ is the macroscopic reaction rate. By calculation of $g_i(\alpha)$ from Eq. 12, one could obtain the probabilities based on Eqs. 9,10.

Macroscopic approach

In this approach, for the diffusion step (Φ_D), each variable $x(r,t)$ is an integer number in the range $[0, M]$ whereas M is called the canal number. In each time step, the value of a given cell is added to those of its neighbors. After that, the result is distributed equally within the cell and its neighbors. So, the lattice will possess a uniform distribution of particles. There are also other approaches which use different algorithms for the diffusion step (see for example [20, 22, 23]).

The second step of the cellular automaton simulates the reaction part. The operator for the reactive part is defined as [20],

$$\Phi_R(c_0x(r,t)) = x(r,t) + \Delta t f(x(r,t)) \quad (13)$$

It is important to verify that the CA steps respect the discretization, i.e., the outcome of an operation on the integer variables is also an integer. As it was mentioned, the diffusion operator Φ_D acts on a field of integers in the range $[0, M]$ to give a field of integers in the range $[0, c_0M]$, where c_0 is the number of neighbors and the cell itself. The non-normalized result is also an integer, now in the range $[0, c_0M]$. The normalization, i.e., the multiplication by $1/c_0$ necessary to bring the range back to $[0, M]$, does not preserve the cell values as integers. So, some mechanism has to be introduced to ensure that the result of the reaction step is an integer in the permitted range. Therefore, it is needed to use another operator Φ_T for truncation. This operator takes the real numbers which result from operator Φ_R and produces an integer. The Probabilistic Minimal Noise Rule (PMNR) is used for rounding off numbers [20],

$$\Phi_T(x) = \begin{cases} [x] & \text{with probability}(1-p) \\ [x]+1 & \text{with probability}(p) \end{cases} \quad (14)$$

$$(p = x - [x])$$

where $[x]$ denotes a floor function. Therefore, a complete dynamics of a system in a macroscopic CA approach will be given by $\Phi_T\Phi_R\Phi_D$.

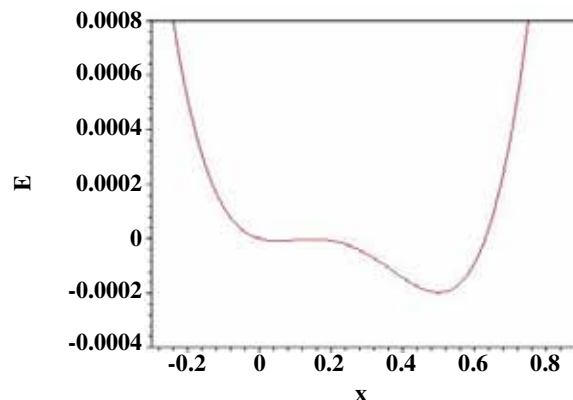
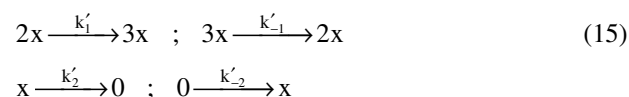


Fig. 2: The graph of energy versus a variable (here x in eq. 16) based on Eq. 16.

RESULTS AND DISCUSSION

The Schlögl model (Eq. (2)) could be separated in four pre-reaction terms (here means four elementary reactions),



where $k'_1 = k_1[A]$, $k'_{-1} = k_{-1}$, $k'_2 = k_{-2}[B]$, and $k'_{-2} = k_{-2}[C]$. A special case is considered where $k'_1 = 0.07$, $k'_{-1} = 0.1$, $k'_2 = 0.01075$, and $k'_{-2} = 0.000375$. Using these values, Eq. 3 could be written as,

$$f(x) = -k(x-0.5)(x-0.15)(x-0.05) \quad (16)$$

For determining stable and unstable concentrations, one could use the graph of energy versus concentrations

$$E = -\int f(x) dx \quad (17)$$

As it is shown in the Fig. 2, the system consists of one more stable (minimum energy with greater negative value, $x=0.5$), a less stable (minimum energy with smaller negative value $x=0.05$), and an unstable phase (maximum of the graph $x=0.15$). So, a system in an unstable phase tends toward a more stable phase.

First, the microscopic approach for the Schlögl model was considered. A two-dimensional square lattice with periodic boundary condition was used. Each cell was contained five channels for particles with different velocities and the Von-Neumann neighbors were considered. The diffusion part (Propagation and Redistribution steps) were done as it was described in the

Table 1: The probabilities for the microscopic CA approach based on the first method.

$\alpha \backslash \beta$	0	1	2	3	4	5
0	0.998125	0.001875	0	0	0	0
1	0.01075	0.987375	0.001875	0	0	0
2	0	0.0215	0.941625	0.036875	0	0
3	0	0	0.08225	0.810875	0.106875	0
4	0	0	0	0.243	0.545125	0.211875
5	0	0	0	0	0.201875	0.798125

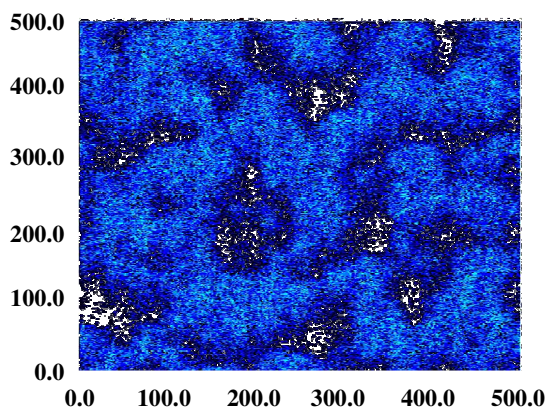


Fig. 3: The microscopic CA simulation of the Schlögl model based on the first probability calculation method (a 500x500 two-dimensional square lattice, initial state: $x=0.15$, $k=0.1$, after 1000 time steps).

previous section. For the reaction part, the first method was considered. According to pre-reactions, more or less than one unit particle transformation is forbidden (i.e. $\beta_i - \alpha_i = \nu_i^{-j} - \nu_i^j = \pm 1$). So, a general equation could be obtained for the probabilities based on Eqs. (8), (9) as follow,

$$p(\alpha, \beta) = \left((r_1^+(\alpha) + r_2^-(\alpha)) \delta_{\alpha+1, \beta} + (r_1^-(\alpha) + r_2^+(\alpha)) \delta_{\alpha-1, \beta} \right) (1 - \delta_{\alpha, m}) + (-r_1^+(\alpha) + r_1^-(\alpha) + r_2^+(\alpha) - r_2^-(\alpha)) \delta_{\alpha, m} \quad (18)$$

where

$$\begin{aligned} r_1^+(\alpha) &= hk'_1 \frac{m\alpha(\alpha-1)}{m-1} \\ r_1^-(\alpha) &= hk'_{-1} \frac{m^2\alpha(\alpha-1)(\alpha-2)}{(m-1)(m-2)} \\ r_2^+(\alpha) &= hk'_2\alpha \quad , \quad r_2^-(\alpha) = hk'_{-2} \end{aligned} \quad (19)$$

$h = m^{1-\nu}$, and $\delta_{i,j}$ is the kronecker's delta function.

The given probabilities based on Eqs. 18, 10 for this case are shown in Table 1.

For the Schlögl model, if a system starts from an unstable concentration ($x=0.15$), it tends toward more stable phases ($x=0.05$ and $x=0.5$), as it was mentioned before. This case was simulated using the microscopic CA and the result is shown in Fig. 3. The bright and dark regions show $x=0.5$ and $x=0.05$ concentrations, respectively. The detailed algorithm of the microscopic CA method for the simulation of the Schlögl model is given in the Appendix A.

In the next step, a simulation was done to show which concentration is more stable. So, for the initial state, half of the lattice was covered with $x=0.5$ while the rest of the lattice was included with $x=0.05$. The results are shown in Fig. 4 which show $x=0.5$ has more stability.

As it was mentioned, there are two different methods for obtaining probabilities. In the next simulation, the second method for the reaction part was considered. So, for the Schlögl model, a new probability table was used based on Eqs. 9-12. The results are given in Table 2. The CA simulation process is the same as the first method (the detailed algorithm is given in the Appendix A). A simulation was done to show the difference between these two methods. As it is obvious in Fig. 5, the difference is negligible, even though it is more considerable in the regions between two phases ($x=0.05$ and $x=0.5$) where the velocity of the movement phases plays an important rule.

For the macroscopic simulation of the Schlögl model, a two-dimensional square lattice with periodic boundary condition was considered. The Moore neighbors were used for each cell and the canal number was 55. The initial state was consisted of a lattice with unstable phase (dark color, $x=0.15$). The diffusion part was done based

Table 2: The probabilities for the microscopic CA approach based on the second method.

$\alpha \backslash \beta$	0	1	2	3	4	5
0	0.998125	0.001875	0	0	0	0
1	0.008875	0.991125	0	0	0	0
2	0	0	0.984625	0.015375	0	0
3	0	0	0	0.975375	0.024625	0
4	0	0	0	0.031125	0.968875	0
5	0	0	0	0	0.201875	0.798125

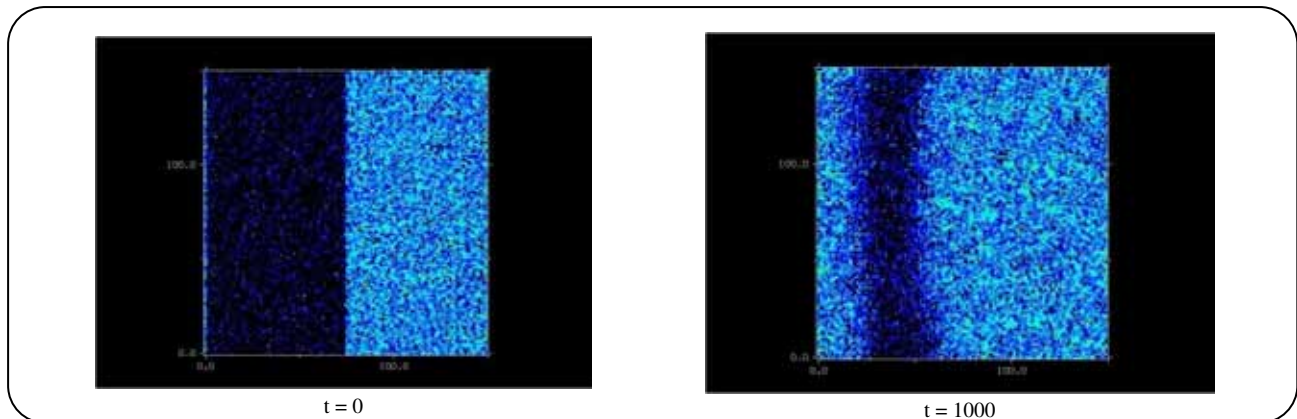


Fig. 4: The microscopic CA simulation of the Schlögl model based on the first probability calculation method (a 150×150 two-dimensional square lattice, $k=0.1$, initial state: half of the lattice=0.5, the rest of the lattice=0.05).

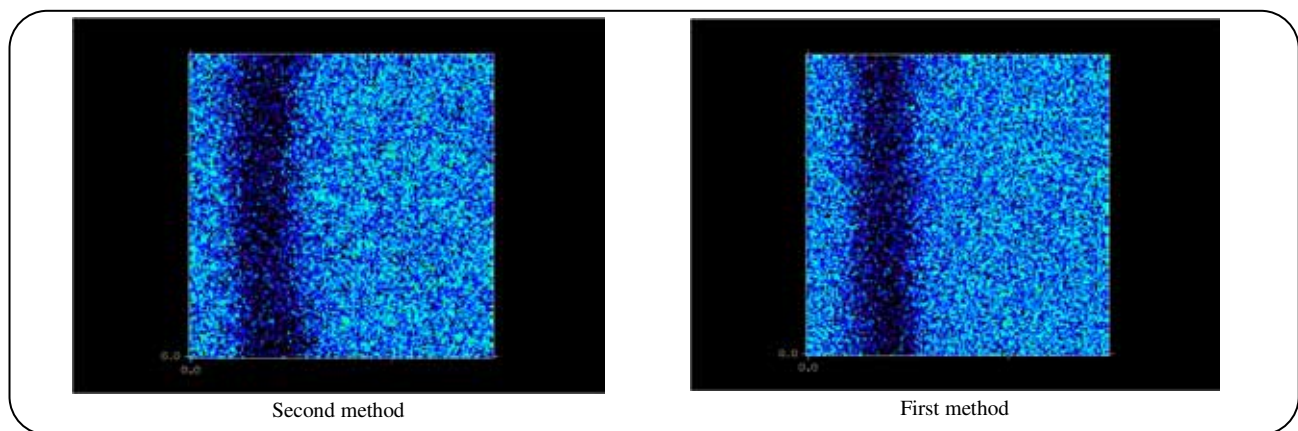


Fig. 5: The difference between two methods of obtaining the probabilities for the microscopic CA of the Schlögl model (a 150×150 two-dimensional square lattice, $k=0.1$, initial state: half of the lattice=0.5, the rest of the lattice=0.05, after 1000 time steps)

on the value of a given cell and those of its neighbors. After that, the reaction part was done according to Eq. (13), while the results were rounded off based on Eq. (14). The detailed algorithm of the macroscopic CA method is given in the Appendix B. The results are shown in Fig. 6 in which one could see the formation and growth of the more stable concentration (bright color, $x=0.5$) during the automat.

To show the competition of two stable phases, a symmetric case of the Schlögl model was considered where $x_2 - x_1 = x_3 - x_2$ in Eq. (4). So, the parameters $x_1=0.1$, $x_2=0.5$, and $x_3=0.9$ were chosen. The stability graph for this case is shown in Fig. 7 which shows one unstable phase ($x=0.5$) and the same stability for two phases ($x=0.1$, $x=0.9$). For the macroscopic simulation

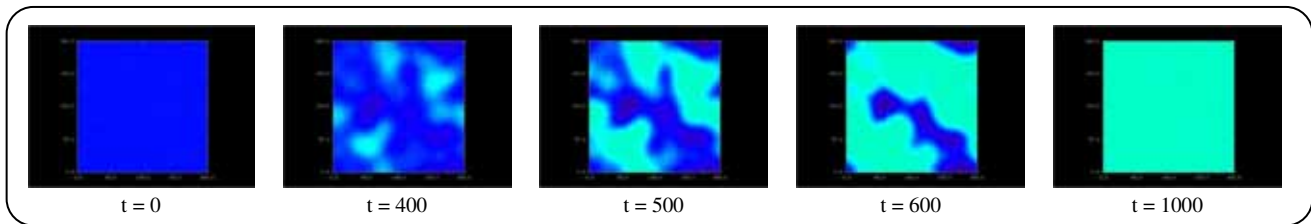


Fig. 6: The macroscopic simulation of the Schlögl model (a 200×200 two-dimensional square lattice, $k=0.8$, initial state: $x=0.15$, $\Delta t=0.4$, canal number=55).

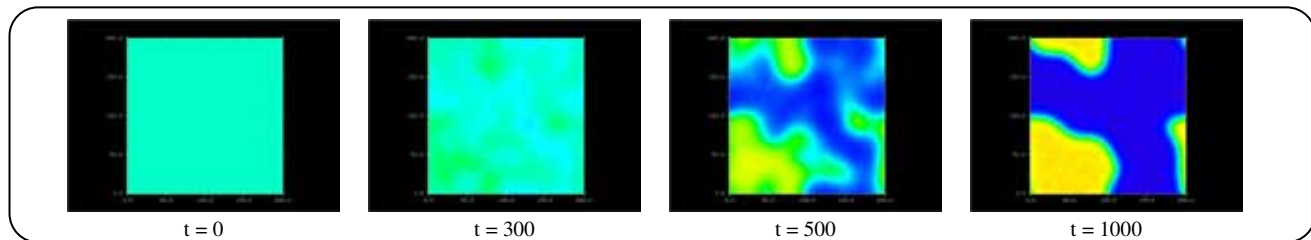


Fig. 8: The macroscopic simulation of the Schlögl model for the symmetric case (a 200×200 two-dimensional square lattice, $k=0.4$, initial state: $x=0.5$, $\Delta t=0.2$, canal number=55).

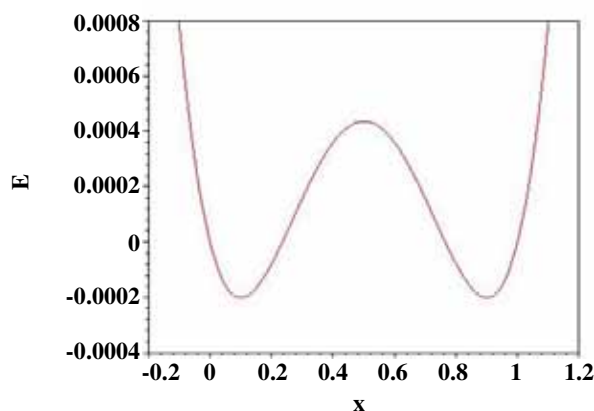


Fig. 7: The graph of energy versus x for Eq. (4) in a symmetric case.

of this case, a lattice was covered with the unstable phase ($x=0.5$) as the initial state. Other simulation parameters were the same as before. The results are shown in Fig. 8 in which one could see the formation and growth of two stable concentrations ($x=0.1$, $x=0.9$) during the automata.

Figs. 6 and 8 imply the macroscopic simulation does not include the fluctuations of the system, as it was mentioned in the previous section.

CONCLUSIONS

The pattern formation of the Schlögl model based on microscopic and macroscopic CA approaches has been

considered. Two different methods for obtaining the probabilities of a microscopic approach were mentioned. It was shown that the results are very similar to each other while there is a little difference in the regions between two stable phases, as the velocity of the movement phases plays an important rule. It was also shown the tendency of the system towards the more stable phase. For the macroscopic simulation, two different models have been considered. The same results of the tendency towards the stability were given. Moreover, the results imply the fluctuations effect in the microscopic approach, even though it is negligible in the macroscopic case. There are many cases which could be considered for the simulation of the Schlögl model such as movement of one phase among another phase, calculation of the velocity of the movable phase, etc. Some of these cases are of our interest and will be presented in near future.

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Appendix A

The microscopic CA algorithm for the *Schlögl* model;
Definition of the lattice
Definition of the initial state and boundary condition
Definition of the functions for the Propagation (P) and
Redistribution (R) steps
Beginning of the Automata

- Doing of the Propagation step based on its function
- Doing of the Redistribution step based on its function
- Doing of the Reaction part based on the probabilities (Tables 1 or 2)

(The automata will be done till the end of the time steps)
End of the Automata
Drawing the concentrations graphs of the system

Appendix B

The macroscopic CA algorithm for the *Schlögl* model;
Definition of the lattice
Definition of the initial state and boundary condition
Beginning of the Automata

- Choose all cells one by one
- The diffusion step will be done by knowing the state of a given cell and those of the neighbors
- The reaction will be done based on Eq. 13 and the results will be rounded off according to Eq. 14

(The automata will be done till the end of the time steps)
End of the Automata
Drawing the concentrations graphs of the system

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