Stochastic cellular automata modeling of excitable systems

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1 Introduction

Experimental and numerical study of excitable systems has a long tradition. The importance of these investigations lies in the general properties of the related models. Several phenomena of reaction kinetics like motion of reaction fronts, propagation of chemical waves can be put into the framework of the above models. In life sciences, spatiotemporal spread of epidemic diseases or migration of some species can also be successfully simulated by considering the population or the territory as an excitable system.

As for many other phenomena in the natural sciences a class of partial differential equations provides an accurate model for waves in an excitable system \cite{5}. At the same time, beyond the difficulties choosing (and programming) a proper numerical solver, the computational time (especially, in case of 3 dimensions) may be too long.

This practical problem called forth the cellular automata (CA) models, which have been substantially developed in the last decades. Besides the relatively low computational cost of these models, they became popular also due to their generality and simple setup. In this approach, usually a two dimensional lattice is associated to the excitable medium, consisting of individual cells and a well defined connection between them. Practically, for each cell we define its neighbors. We investigate discrete time models, considering the system in uniform
time steps. The cells are described in the way that we give their state in every time step. A given transition rule (function) provides the state of the cells after each time step depending on their present state and that of their neighbors.

The development of the CA models can be directed to the qualitative simulation of some important phenomena: diffusion [1], some kind of reactions [14] and pattern formation [1], [7], [8]. For a systematic overview and further references on these applications we refer to [1]. Moreover, many other real life processes like neural signal transport [14], highway traffic [10], propagation of forest fires or epidemics diseases [11] can be successfully simulated.

We follow another way: our objective here is to present an improved cellular automata model such that excitation waves and propagation of reaction fronts can be modelled in more details. In particular, shape of the reaction fronts, variation of propagation velocity, curvature effect and an interesting phenomenon: existence of target patterns in a Belousov-Zhabotinsky type reaction is explained and effectively simulated in the frame of our setting. For this we choose a probabilistic approach such that the propagation of waves is simulated using a Monte Carlo method.

Several types of stochastic CA models have been proposed in the literature [14] and successfully applied for modeling some phenomena in excitable systems. The transition rule in these models [2], [7] is substantially deterministic, only a careful post-processing is applied to ensure the conservation of mass (particle number) by the simulation of the reactions [13]. In other models [12] the transition probability was simply calculated in a heuristic way. However, the stochastic CA that we present can also conserve some quantities [6] and adaptive stochastic modeling has also been developed using CA [9]. Other authors suggested the addition of some stochastic term to take into account the noise in the system. In our approach the time step is fully probabilistic which results in a transparent structure of the model and the appropriate computer implementation. An early version present kind of CA has been initiated by Domany and Kinzel and many of its improved versions has been used in a number of simulations. The other starting point of our investigations is the systematic study in [7], [8] on excitable media using CA. We combine these two approaches: inserting a fully probabilistic approach into a detailed model of excitable systems results in a successful simulation of the above phenomena.

2 The model

In the presentation of CA we follow the lines in [1]. We also make use of the detailed study on 2D excitable systems in [2] by extending it with stochastic elements.

A cellular automaton consists of a set \( L \) of cells, which are usually represented with unit squares or even with their midpoints in a coordinate system. Each cell \( l \in L \) should have a fixed state at any given time; the set of the states will be denoted with \( Q \).

The cellular automaton (in our case, as a model of an excitable system) is described in the way that we give the state of each cells in discrete steps. The time evolution of the system is driven by the interchange of the cells. For this, we first define the neighbors of the cell \( l \) as a set \( \{l_1, l_2, \ldots, l_n\} \). Practically, in the classical cases the time step is characterized with a function \( f : Q \times Q^n \rightarrow Q \), which gives the state of a given cell in the subsequent time step depending on its present state (first component) and that of its neighbors (last \( n \) components).
Note that the number \( n \) is not necessarily the same for every cells, depending on the geometry of the investigated media: it can be reduced near to boundaries or walls.

Corresponding to the model in [2] we give then our model formally as follows.

\[
L \subset \{(c_1, c_2) : c_1 \text{ and } c_2 \text{ are positive integers}\}.
\]

The possible states are given as:

\[
Q = \{q_{-1} \text{ “refractory”}, q_0 \text{ “resting”}, q_1 \text{ “active”}\}.
\]

In the literature, instead of “active” one frequently uses the term “excited”, and accordingly, refractory cells are often called non-excitable ones. In this context, the boundary of the region formed by the active cell is often called “front”. For a cell \( l = (c_1, c_2) \) the neighbors are the following ones:

\[
\begin{align*}
l_1 &= (c_1 - 1, c_2 - 1), \quad l_2 = (c_1 - 1, c_2), \quad l_3 = (c_1 - 1, c_2 + 1), \\
l_4 &= (c_1, c_2 + 1), \quad l_5 = (c_1 + 1, c_2 + 1), \quad l_6 = (c_1 + 1, c_2), \\
l_7 &= (c_1 + 1, c_2 - 1), \quad l_8 = (c_1, c_2 - 1),
\end{align*}
\]

provided that they are in \( L \).

We modify, however, the classical definition of \( f \) in the way, that \( f : Q^d \times Q^n \rightarrow Q \) where the first \( d \) component gives the “past” of a given cell over \( d \) time steps. This modification is essential, since corresponding to the real life cases we prescribe in this way that any cell should be kept in the refractory state over \( d_1 \) time steps. Similarly, the number of the time steps while a cell resides in the active state is denoted by \( d_2 \) and with these, \( d := \max\{d_1, d_2\} \).

We give the time stepping function in the way that a cell \( l \) can turn into the active state (loosely say, it can be infected) by any of its neighbors \( l_1, l_2, \ldots l_8 \) with a certain probability:

- \( l \) can infect \( l_2, l_4, l_6 \text{ and } l_8 \) with probability \( p \),
- \( l \) can infect \( l_1, l_3, l_5 \text{ and } l_7 \) with probability \( \alpha p \),

where the parameter \( \alpha \) is determined such that we ensure the uniform propagation velocity of the active region in all directions. More precisely, the expected value of the propagation length within one time step should be the same in all directions. The details on the computation are given in the appendix. We point out that despite of the simplicity of this stochastic step function, the corresponding cellular automaton is capable to model a number of qualitative and quantitative properties of excitable systems.

While describing the step function \( f \) in details we distinguish three cases according to the state of the given cell after this time step. In the formal rules, \( a_i \) corresponds to the state of \( l \) (a given cell) \( i \) steps before \((i = 1, 2, \ldots, d)\) and \( b_j \) denotes the state of its neighbors \( l_j \) after the preceding time step \((j = 1, 2, \ldots, 8)\).

- A given cell will turn into resting state if either this was resting and none of its neighbors infected it or this was in refractory state over the preceding \( d_1 \) time steps. Formally:
  - If \( a_1 = q_0 \) then
    \[
    P[f(a_1, \ldots, a_d; b_1, b_2, \ldots, b_8) = q_0] = (1 - p)^{k_1}(1 - \alpha p)^{k_2},
    \]
where $k_1$ is the number of its active neighbors which has a common edge with $l$: $k_1 = \#\{ j \in \{2, 4, 6, 8\} : b_j = q_1 \}$ and $k_2$ is the number of its active neighbors which has a common vertex with $l$: $k_2 = \#\{ j \in \{1, 3, 5, 7\} : b_j = q_1 \}$.

If $a_1 = a_2 = \cdots = a_{d_1} = q_1$ then

$$f(a_1, \ldots, a_{d_1}; b_1, b_2, \ldots, b_8) = q_0.$$  

- A given cell will be in refractory state in a time step if either this cell was active during the preceding $d_2$ time steps or it was in the refractory state in the preceding steps over a period at most $d_1 - 1$. Formally:

  If $a_1 = a_2 = \cdots = a_{d_2} = q_1$ then

  $$f(a_1, \ldots, a_{d_2}; b_1, b_2, \ldots, b_8) = q_1.$$  

If $a_1 = a_2 = \cdots = a_{m-1} = q_1 \neq a_m, m \leq d_1$ then

$$f(a_1, \ldots, a_m; b_1, b_2, \ldots, b_8) = q_1.$$  

- A given cell will turn into active state in a time step if either it was resting and one of its neighbors infected it or this cell was in active state during the preceding steps over a period at most $d_2 - 1$. Formally:

  If $a_1 = q_0$ then

$$P[f(a_1, \ldots, a_{d_2}; b_1, b_2, \ldots, b_8) = q_1] = 1 - (1 - p)^{k_1}(1 - \alpha p)^{k_2},$$

with $k_1, k_2$ defined above. If $a_1 = a_2 = \cdots = a_{m-1} = q_1 \neq a_m, m \leq d_2$ then

$$f(a_1, \ldots, a_{d_2}; b_1, b_2, \ldots, b_8) = q_1.$$  

3 Simulation results, discussion

In the simulation, we executed the above time evolution using a C++ code. According to the formal transition rules we determined the states of the cells (in more precise terms, a realization of a discrete time stochastic process) stepwise using a Monte Carlo simulation. It is essential, that we should execute each time step simultaneously for all cells.

The propagation of a zone consisting of active cells are influenced only on the present position of this zone and that of the zones with refractory cells. Therefore, in all figures we depicted only these regions.

Test case 1.

In the first case we simulated an excitation wave generated by a point source using our stochastic model (Fig 1. (a),(b)).

The probabilities $p$ and $\alpha p$ in the transition rules were chosen to be $p = 0.35$ and $\alpha p = 0.06$, respectively with the identical length of the refractory and active period $d_1 = d_2 = 8$. We started the simulation from one single active cell and investigated the qualitative properties of the zone of the active cells which corresponds to an excitation wave.
Figure 1: Simulation of excitation waves originated from a point source. Black: active cells, grey: refractory cells.
Figures 1. (a),(b): simulation results using our probabilistic approach with the parameters $p = 0.35$ and $\alpha p = 0.06$ in 44 and 154 time steps, respectively.
Figures 1. (c),(d): simulation results using a deterministic approach after 24 and 80 time steps, respectively. The cells remain both in the active and the refractory state over 8 time steps.
Figure 2: Curvature effect in the simulations. The symbols ▲ and ■ show in each time step the average position of a planar and radially symmetric front of active cells, respectively. The slope of the dotted line corresponds to the constant propagation velocity of the planar front. In case of radially symmetric front, the lines (a), (b) and (c) have been fitted to the average positions of the front in the first 6, 12 and 24 time steps, respectively. The parameters in the simulation coincide with the ones in Fig. 1.

Using the stochastic approach the shape of the reaction front corresponds to the observations. This will be radially symmetric after a transient period, only some noise is present (arising from the Monte Carlo simulation) like in the real experiments.

For analyzing the propagation of a planar front we placed initially a vertical stage filled with active cells of horizontal position zero and considered the half plane with positive horizontal coordinates. The propagation is described with the average position of the front: in each time step we took the average of the horizontal position of those active cells, which have a resting right hand side neighbor. The average of the positions depending on the time step are depicted in Figure 2. The propagation velocity is constant, this corresponds to the slope of the dotted line which has been fitted to the observed data.

In a similar way, we analyzed the evolution of a radially symmetric front of active cells according to the test case 1. At the computation of the average distance from the midpoint we took into consideration those active cells which have at least two resting neighbors.
We track the curvature effect in the way that we fitted a linear curve to the first 6, 12 and 24 observations, respectively. The slope of these lines approximate that of the one corresponding to the planar front propagation. These results are shown in Figure 2.

Note that for these qualitative results it is essential that we used a stochastic model. Using a deterministic one the geometry of the cell network will highly influence the shape of the active zone and its propagation velocity does not properly change according to the shape of this zone. For a visible comparison we simulated the above excitation waves also using a deterministic approach, which can be interpreted as a special probabilistic approach with \( p = \alpha p = 1 \) (Fig. 1 (c),(d)). These results correspond to the ones in [2].

**Test case 2.**
In the second case we simulated the formation of a double spiral wave (Fig. 3 (a),(b),(c)). The probabilities \( p \) and \( \alpha p \) in the time stepping function were chosen to be 0.35 and 0.06, respectively. The length of the active and refractory period were equally \( d_1 = d_2 = 8 \), respectively. We started the simulation from a vertical stage consisting of active cells and after some steps the bottom half of the active and refractory region was removed and substituted with resting cells corresponding to the usual deterministic simulation technique [1].

Due to the extended period for being a cell in the refractory state also a resting region appears between the excitation waves. The shape of the active zone is again in a good accordance with the results of the real experiments [3].

**Test case 3.**
In the third simulation we modelled the propagation of the active zone around a circle shaped obstacle (Fig. 4 (a),(b),(c)). We have chosen again the probabilities \( p = 0.35 \) and \( \alpha p = 0.06 \) and the length of the active and refractory period were equally \( d_1 = d_2 = 20 \). Initially we took a single stage perpendicular to the obstacle with active cells and after 44 time steps we removed one half of the system as in the previous test case. The geometry of the active zone corresponds again to the experimental results [3] and also to some numerical simulations [5], [7]. In order to get a well visible picture with more thick region of active and refractory cells we applied longer period for these state of the cells: 20 time steps both for the active and the refractory state of the cells.

**Test case 4.**
In the frame of the above model we could reproduce a unique phenomenon which can hardly be simulated using any deterministic approach. In some real experiments “target patterns” can be detected, in more precise terms: the whole active region consists of concentric circles which propagate outward (i.e. their diameter is growing) according to the first test case. These are usually considered as degenerated double spirals. Under some circumstances such a pattern can form without any excitation in their center. [4].

In the deterministic simulations, in a rather unrealistic way, an artificial excitation is applied to simulate this phenomenon. In our approach, however, this can arise in a natural way: If the length of the refractory period is short compared to that of the active period, then the region of the active zone can infect also the resting cells accidentally which are normally separated by the zone of the refractory ones. This can happen, since the probabilistic transition rule makes possible that this separating region becomes thin or vanish occasionally. Through the appearing gaps the propagation of active cells can be directed backwards into the central region when the zone of the refractory cells is passed through. In the simulation
Figure 3: Simulation of double spiral formation using the parameters $p = 0.35$ and $\alpha p = 0.06$. Black: active cells, grey: refractory cells. At the beginning a single horizontal stage was filled with active cells. Figure 3. (a): after 18 time steps, the bottom half of the active and refractory cells was replaced by resting ones. Figure 3. (b) and (c): evolution of the system after 34 and 108 time steps, respectively. Length of active and refractory state were both 8 time steps.
Figure 4: Propagation of excitation waves around a circle shaped obstacle using the parameters $p = 0.35$ and $\alpha_p = 0.06$. Black: active cells, grey: refractory cells. Length of active state: 20 time steps, length of refractory state 20 time steps. Initially, the cells on a vertical stage (perpendicular to the obstacle) were active and after a few time steps, the left half of the active region was removed and replaced by resting cells. Evolution is shown after 44 (Figure 4. (a)), 164 (Figure 4. (b)) and 450 (Figure 4. (c)) time steps, respectively.
Figure 5: Self inducing concentric target pattern using the parameters $p = 0.35$ and $\alpha p = 0.06$, respectively. Initially, a couple of cells in the central region were in the active state. Evolution is shown after 23 (Figure 5. (a)) and 114 (Figure 5. (b)) time steps, respectively. Length of active state (black): 10 time steps, length of refractory state (grey) 3 time steps.

we used again $p = 0.35$ and $\alpha p = 0.06$, with the parameters $d_1 = 10, d_2 = 3$. The results are shown in Fig. 5 (a),(b).

Test case 5.

We have also simulated the spontaneous appearance of spirals and “target patterns” [] using the parameters $p = 0.35$ and $\alpha p = 0.06$, respectively. In each time step a randomly generated new excited cell was placed in the domain with uniform spatial distribution. In this way, after some time time, target patterns, spirals and double spirals can appear. A simulation result is shown in Fig. 6.

Pattern formation phenomena in a precipitation system may produce similar structures. Our new experimental investigations [15] have shown the coexistence of precipitation process and excitability without any external forcing. In such a way, spontaneous appearance of travelling waves and spiral formation inside of the precipitation front was described for the first time. The dynamics and spatial structure of the observed travelling waves suggest the similar origin of BZ waves and the phenomena in [15]. The result in a real experiment is depicted in Fig. 7.

Summarized, in this paper, while using the classical setup as sketched above we improved the existing models in some aspects

- In our model we can prescribe how long a cell can remains in active or resting state, which can be optionally given in the code.
- We can take into consideration stochastic effects like noise or material inhomogeneities without applying any perturbation.
- We can avoid the rather unrealistic property of many simulations that the shape of