The Ideal Storage Cellular Automaton Model

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Abstract

We have implemented and investigated a spatial extension of the original ideal storage model by embedding it in a 2D cellular automaton with a diffusion-like coupling between neighboring cells. The resulting ideal storage cellular automaton model (ISCAM) generates many interesting spatio-temporal patterns, in particular spiral waves that grow and "compete" with each other. We study this dynamical behavior both mathematically and computationally, and compare it with similar patterns observed in actual chemical processes.

1 Introduction

In recent years, some of us began re-investigating pattern formation processes in oscillating systems [3], based on the *Ideal Storage Model* introduced in 1982 [2]. Our analyses show that, from a dynamical systems point of view, these models provide an amazingly rich class of toy examples for studying the onset of oscillating and chaotic behavior. As was observed already in the 1980s, this becomes even more apparent when the dynamical behavior of a coupled rectangular array of many such systems is studied, e.g. when they are placed on the lattice sites of a cellular automaton and coupled by spatial diffusion of one of its two parameters (see e.g. [5, 13, 6]). A little later, similar patterns were actually observed experimentally by Ronald Imbihl (then working at Gerhard Ertl's lab in Berlin who received the Nobel prize in 2007 for his work on chemical processes on solid surfaces) [11, 10, 8, 12, 7]. Furthermore, it turned out in subsequent studies that one can use such CA for modeling all sorts of complex processes, from phase transition in binary mixtures [14] to using them as a metaphor for cancer onset caused by only one short pulse of 'tissue dis-organzation' (changing e.g. for only one single time step the diffusion coefficient) as hypothesized in recent papers questioning the current gene/genome centric view on cancer onset [AO Ping references].

Here, we continue our own investigations, in particular by studying a spatial 2D cellular automaton version of the original ideal storage model, with a diffusion-like coupling between neighboring cells. We perform some mathematical analyses, investigate the dynamical behavior and pattern formation (in

particular the formation and stability of spiral waves) generated by an implementation of the spatial model, and compare these patterns with those observed experimentally in actual (catalytic) chemical processes.

2 The Ideal Storage Model

Consider the product space $X = \mathbb{R}^+ \times [0, 1]$ and the discrete time dynamics $D : X \to X = (S, R) \to (S' = S - RS + C_s, R' = f(RS))$, where C_s is a non-negative constant and $f(x)$ denotes a monotonously increasing map from $\mathbb{R}^+$ into $[0, 1]$, for example $f(x) = \frac{1}{1+e^{-5x+C_r}}$ with C_r a non-negative constant. The constants C_s and C_r are the control parameters of the model.

This model, known as the *ideal storage model* (ISM), is considered to describe the dynamic behavior of a system in which some substance (or resource) (S) is stored and, at each time step, part of the substance is released (or "used up") at a rate R while, simultaneously, it is replenished by an amount C_s. Moreover, the rate R itself is dynamic, depending directly (and in a monotonously increasing way) on how much of the substance is currently released. Thus, the system can be considered as describing some kind of exothermic process in which the released substance produces heat which, in turn, determines the value of the reaction rate at the next time step (going up if temperature goes up, and down if temperature goes down). A large amount of stored substance S as well as a high reaction rate R will lead to an even higher reaction rate R. This, however, will eventually lead to a decrease in S and, consequently, also in R, thus allowing S to build up again. So, we can expect the system to exhibit, for appropriate choices of C_s and C_r, some kind of periodic behavior.

The ISM was used to describe hetero-catalytic processes at metal surfaces in earlier work [2], in which it was discovered that such processes could potentially form interesting spatio-temporal patterns. This was later confirmed in a number of exciting and innovative experimental studies [11, 10, 8, 12, 7].

3 The Ideal Storage Cellular Automaton Model

The ISM is analyzed mathematically in more detail in [3] where fixed points and their stability are derived, and the existence of a Neimark-Sacker bifurcation is shown. However, as already suggested in [3], the model becomes even more interesting (but also much more difficult to analyze mathematically) when a spatial dimension is introduced with local interactions between neighboring elements. Here, we investigate such a spatial extension of the original model. In particular, we have embedded the ISM in a cellular automaton: the *ideal storage cellular automaton model* (ISCAM).

Cellular automata (CA) were introduced by John von Neumann already in the 1940s [15, 1], but only became more popular in the 1970s after the "invention" of what is probably the most well-known CA, the Game of Life [4]. A CA consists of a regular D-dimensional grid of "cells" (D is usually just one or

two), where each cell is in one of a finite number of discrete states. At discrete time steps, all cells simultaneously update their state according to a fixed deterministic update rule. This rule determines the new state of a cell depending on its current state and those of other cells in its local neighborhood. This local neighborhood is usually simply the adjacent cells (e.g., left and right for $D = 1$, or left, right, up, and down, or alternatively all eight surrounding cells for $D = 2$), or some extension of that. A variation on this basic scheme is to allow real values – or even n-tuples of real values – as state parameters (i.e., to work with continuous instead of discrete values), where the update "rule" is now a real-valued function – or an n-tuple of real-valued functions – with several arguments, giving the new state (value) of a cell as a function of its own current value(s) and those of its neighboring cells.

Using a $D = 2$ regular grid, each cell in our ideal storage cellular automaton actually contains two real-valued variables, S and R, the individual dynamics of which are governed by the ISM as explained in the previous section. However, before calculating the new R values, using the given function $f(x)$, first a "diffusion" step is included based on a cellular automaton (real-valued) update function. Instead of calculating $R' = f(RS)$ for a given cell, we calculate $R' = f(\overline{R}S)$, where $\overline{R}$ is a (weighted) average of the cell's own current R value and the (unweighted) average of its eight surrounding cells' R values. So, for cell i:

$$\overline{R_i} = (1 - p)R_i + \frac{p}{8} \sum_{j \in \mathcal{N}_i} R_j$$

where R_i is the current R value of cell i, $\mathcal{N}_i$ is the eight-cell (Moore) neighborhood of cell i, and $p \in [0, 1]$ is a parameter that determines the amount of diffusion. This "diffused" rate $\overline{R_i}$ is then used to calculate the new rate R'_i of cell i according to the ISM.

4 Mathematical Analysis of the ISCAM

— Lin Wei —

5 Experimental Results

We have implemented the ISCAM in a Java program, which allows us to empirically study the spatio-temporal behavior (pattern formation) for different values of the control parameters C_s, C_r, and p.

Figure 1 shows a typical sequence of patterns observed over time with parameter values $C_s = 0.5$, $C_r = 2.5$, and $p = 0.2$, on a CA grid of size 100×100 cells with periodic boundary conditions (i.e., the cells on the left and right boundaries are each others neighbors, and similarly for the top and bottom boundaries). Starting from a random initial configuration ($t = 0$), several independent spiral wave nucleation sites start forming, after a few hundred iterations, in an otherwise fairly homogeneous (but oscillating) background ($t = 300$). The indepen-

dent spiral waves then start growing and interacting with each other ($t = 1000$), and a few dominant spirals will start "competing" for space ($t = 2000$). Sometimes these competing spirals remain stable and several of them can coexist for a long time, or sometimes they become unstable again, disintegrate, and new spirals arise at the interfaces of the older ones. However, occasionally one spiral will destabilize the others ($t = 3500$), and eventually take over the entire grid ($t = 6000$). The exact behavior, of course, depends on the value of the control parameters, but is independent of the grid size (i.e., it can be observed for any large enough system size).

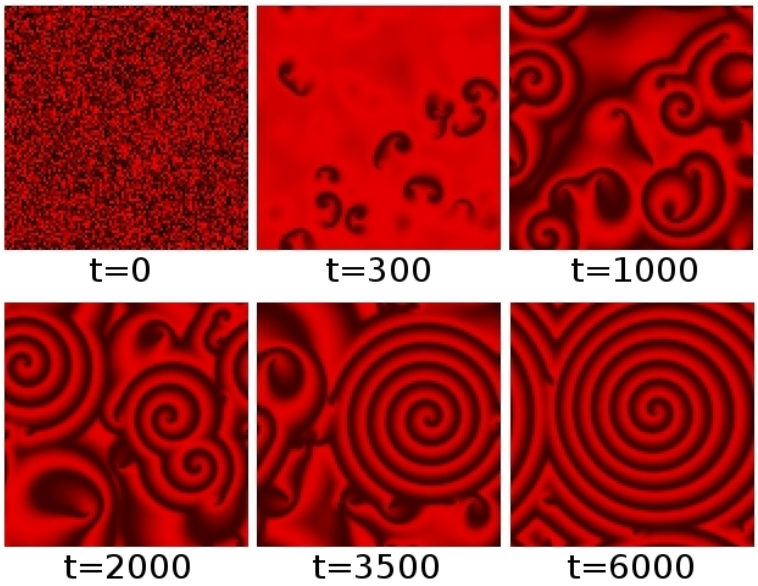

Figure 1: A typical sequence of patterns, with spiral waves forming, growing, and competing. In this example one dominant spiral eventually takes over the entire grid. The parameter values used are $C_s = 0.5$, $C_r = 2.5$, and $p = 0.2$, on a CA grid of 100×100 cells with periodic boundary conditions and a randomly generated initial configuration.

Alternatively, we can look at the behavior of the system as a collection of points moving through state-space. Figure 2 shows two examples. On the horizontal axis are the S values (in [0,2]) and on the vertical axis are the R values (in [0,1]). The blue dot (in the center) indicates the (unstable) fixed point of the ISM (for $C_s = 0.5$ and $C_r = 2.5$). Each black dot represents one cell in the CA grid (so in total there are $100 \times 100 = 10,000$ dots in each figure), plotted with the corresponding cell's current S and R values as coordinates. Both figures show one particular time step during the CA iteration. When viewing this state-space plot over time, one can observe the entire collection of dots moving around the fixed point in a counter-clockwise direction.

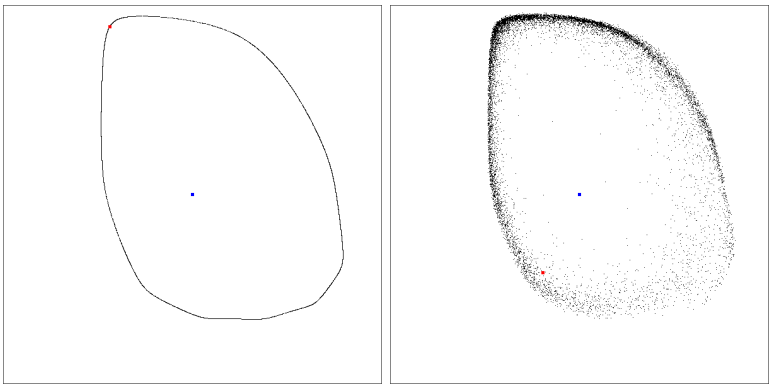

Figure 2: State-space view of the dynamic behavior. Left: No diffusion. All cells end up in the same limit cycle. Right: With diffusion, $p = 0.2$. The cell-states now occupy a cloud around the limit cycle.

Figure 2 (left) shows the state-space configuration when there is no diffusion ($p = 0$). Each cell updates its state independently, and very quickly all cells move onto the same limit cycle as shown in this plot (the exact position along this orbit depends on each cell's (random) initial value). Tracking the top-left cell in the CA grid over time (indicated by the red dot in the upper-left part of the limit cycle), it moves around the orbit in a counter-clockwise direction, but never seems to return to the exact same position. In other words, this limit cycle appears to be a chaotic attractor. In this situation, no spiral waves form in the CA grid (as there is no interaction between cells).

Figure 2 (right) shows the state-space for the same system, but with a diffusion value of $p = 0.2$. Now, the cells occupy a "cloud" around the original limit cycle. Tracking again the top-left cell (the red dot in the lower-left part of the cloud), it also moves around in a counter-clockwise direction and in a quasi-periodic way, as before. However, in this situation, the local interactions (diffusion) between neighboring cells cause them to be constantly perturbed from their independent limit cycles, eventually giving rise to spiral waves in their spatio-temporal behavior, as shown in Figure 1.

The actual long-term behavior depends on the exact control parameter values and the initial configuration, but the overall dynamics of spiral waves forming, growing, and competing seems to be a general phenomenon that occurs for a wide range of parameter values. Moreover, these spiral waves seem to be very robust. When a perturbation is introduced in the system, the spiral waves quickly "clean" up the perturbed area. An example is shown in Figure 3. The left-most diagram shows a spiral wave that has taken over the entire space at some time step t (on a 50×50 grid, with $C_s = 0.5$, $C_r = 2.5$, and $p = 0.4$). In the next picture, we have introduced a perturbation (noise) by resetting the values in a 3×3 block of cells to $S = 0$ and $R = 0$ (the black square near the center). The third diagram shows the configuration nine time steps later ($t+9$),

when the spiral has made exactly one full rotation. As the picture clearly shows, the perturbed area is already reduced to a vague smudge. After 10 rotations of the spiral ($t + 90$), the perturbation has disappeared altogether, and the spiral continues as before, seemingly undisturbed.

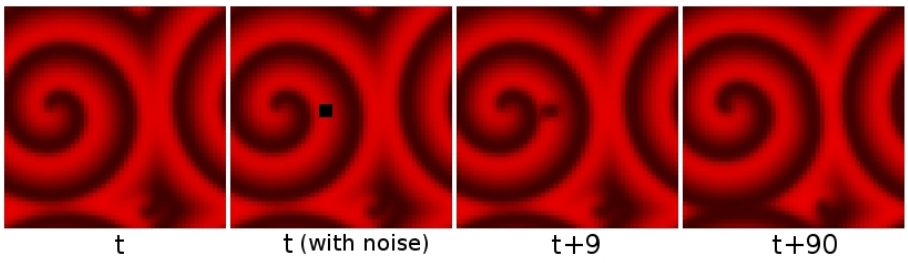

Figure 3: Stability of a spiral wave. At time t, a perturbation is introduced (second diagram). At $t+9$ (after one full rotation of the spiral), the perturbation is already reduced significantly, and has disappeared completely at $t + 90$.

As mentioned above, the ISM was originally used to describe hetero-catalytic processes at metal surfaces [2]. Comparing our spatial ISCAM model with experimental observations of such systems, we can indeed find striking similarities between the patterns generated by both systems (the chemical one and the model). Figure 4 shows an example. The image on the left is taken from [12] which describes the chemical system Rh(100)/NO+H_2. The image on the right was generated by the ISCAM program, using parameter values $C_s = 0.45$, $C_r = 2.5$, and $p = 0.2$. Note the resemblence between the patterns in the two images: a central spiral wave curving back onto itself, surrounding circular wave fronts, and wave fronts traveling in opposite directions canceling out each other when they collide.

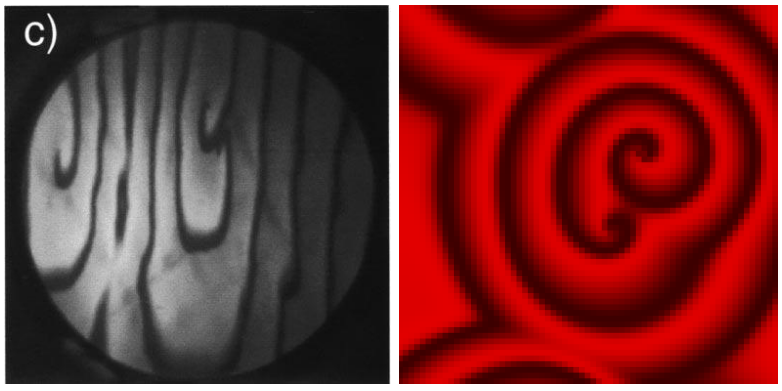

Figure 4: A comparison of an experimentally observed pattern (left, taken from [12]), and a pattern generated by the ISCAM program (right).

6 Conclusions and Discussion

We introduced, implemented, and studied a cellular automaton-based spatial extension of the ideal storage model: the ISCAM. The spatio-temporal patterns generated by this model closely match the patterns observed in hetero-catalytic processes on metal surfaces by which the ideal storage model was originally motivated. The ISCAM can be studied both mathematically and computationally to better understand this pattern forming behavior. For example, parameter values can be identified for which particular kinds of spatio-temporal behaviors occur, and it was shown that the spiral waves generated by the model are robust against perturbations.

Of course there are many other chemical and also biological processes that generate similar patterns, in particular interacting spiral waves [9]. The most familiar of these "excitable systems" are probably the Belousov-Shabotinsky (BZ) reaction and cAMP signaling in Dyctiostelium. As a consequence, our ISCAM provides a useful modeling tool and possible explanation for the observed pattern formation in such systems in general.

The ISCAM Java program is available for download from the following web page: `http://www.picb.ac.cn/ISCAM`. However, the program is still under development, and is not guaranteed to be bug-free, and there is only minimal help available (although most of the functionality is fairly self-explanatory). The program may be used and distributed freely as long as the original copyright notice is not removed.

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