

# CRYSTALLISATION OF TWO-DIMENSIONAL CELLULAR AUTOMATA

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October 15, 1998

The cellular automata (CAs) which asymptotically lead to uniform regular patterns, namely crystalline CAs are discussed. The two-dimensional and two-states-per-cell CAs with five neighbour structure are particularly focused. First, various CA evolution patterns are analysed by the entropy function, and it is suggested that there are two types of CAs with static or chaotic evolution. Analyses using a newly-introduced rule parameter, called  $\mu$  parameter, ensure that the crystalline CAs appear at the phase transition point between static and chaotic CAs. The observed phenomena are probably considered as a generalised model of liquid/solid phase transition.

## 1 Introduction

Many systems composed of countless elements in nature have their own temporal and/or spatial patterns, e.g. galaxies, the weather, biological and ecological systems and societies. These patterns appear without explicit pressure or constraint from outside the systems, and such phenomena are called self-organisation. The objective of studies of self-organisation is to understand the underlying properties of such phenomena in general, and has been explored by many scientists, e.g. [1, 2, 3, 4].

Crystallisation from a liquid state, which is a common example of self-organisation, governs physical characteristics of solid-state materials and is of great importance in science and engineering. The traditional explanation of this phenomenon starts from the microscopic laws applicable to their components, the quantum mechanics in this case. However, as seen in **Figure 1**, it is possible to embody similar dynamics by exploiting dynamical systems artificially defined in the discrete space with a simple rule of evolution. This fact indicates that the essence of crystallisation in general is not quantum force but something else: This paper attempts to describe what this is.

Cellular Automaton (CA) is a common tool for studying such self-organising phenomena, e.g. [5, 6, 7, 8, 9], and was adopted also in this paper. Due to the simplicity of method, CA is expected to yield the results which could be applicable to crystallisation in general. Another advantage of using CAs is easy implementation of the computer algorithm.

This paper discusses two-dimensional CAs causing crystalline patterns from theoretical and empirical perspectives, and focuses on their statistical features to extract some general properties of such phenomena.

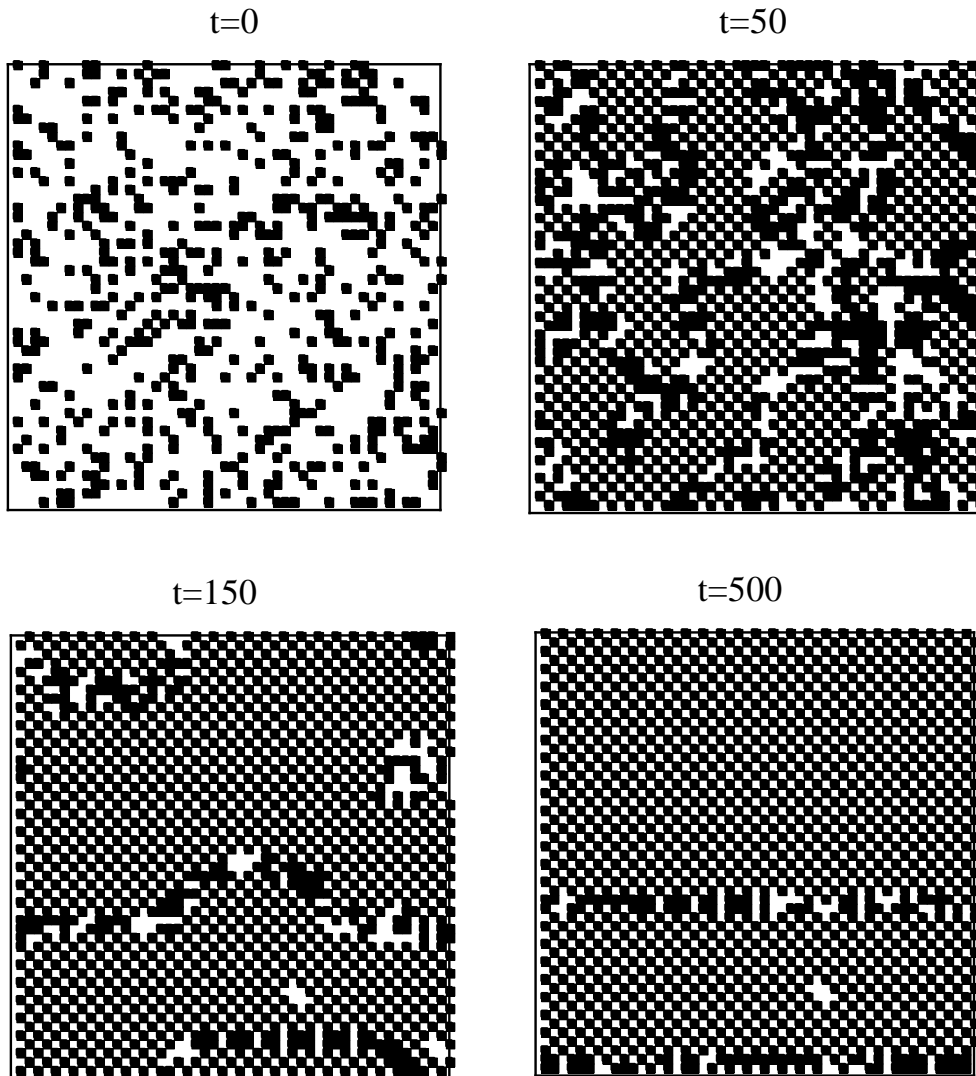


Fig. 1. Crystalline structure created from a random configuration by a particular CA rule.

## 2 Notation and the scope of analysis

Consider an integer value  $a_{i,j}(t) \in \{0, 1\}$  assigned at a two-dimensional discrete site  $(i, j)$ ,  $i \in \{0, 1, \dots, N\}$  and  $j \in \{0, 1, \dots, N\}$ , where  $t \in \{0, 1, 2, \dots\}$  is a time step. The site value  $a_{i,j}$  at the next time step is deterministically given by the mapping

$$a_{i,j}(t) = f[a_{i-1,j}(t-1), a_{i+1,j}(t-1), a_{i,j-1}(t-1), a_{i,j+1}(t-1), a_{i,j}(t-1)], \quad (1)$$

where  $f$  is an arbitrary function which specifies the CA rule, hence the value of a given site depends on the last values of five “neighbour” sites. This neighbourhood pattern is called five neighbour structure, and is sometimes referred to as the von Neumann neighbourhood. The total number of neighbour state patterns is  $2^5 = 32$ , therefore a CA rule is composed of 32 mapping functions. In other words, there are 32 rule “entries” per rule. In this paper the value-0 state (or the “empty” state) is considered as a quiescent state, which means

$$f(0, 0, 0, 0, 0) = 0, \quad (2)$$

is satisfied, i.e. the value-1 state (or “occupied” state) is never generated only by “empty” neighbours. This requirement is useful when the CA is used to model interacting particle systems. In addition, the CA space is assumed to be isotropic, i.e. the rule is always

rotationally and reflectionally symmetric. If a CA rule is defined such that each site value at the next time step is calculated by the “home” site value and the sum of the last value of the other neighbour sites such as

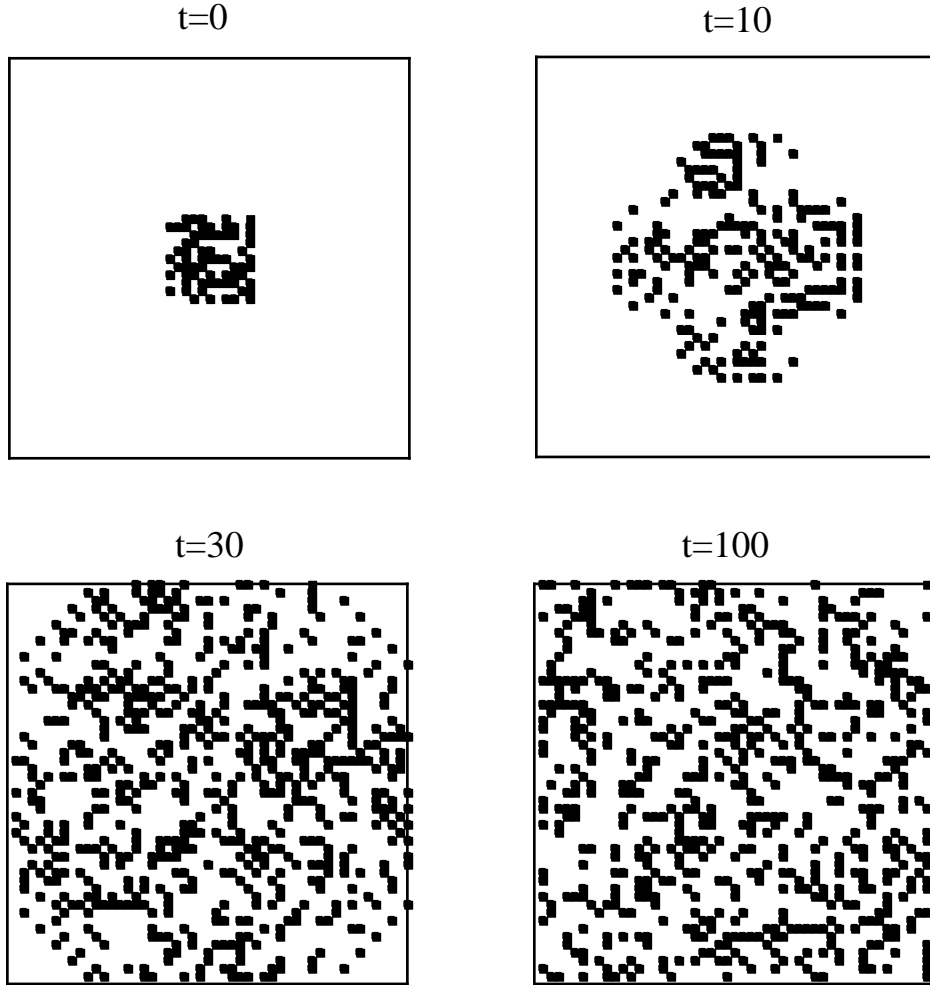
$$a_{i,j} = g[a_{i,j}(t-1), a_{i-1,j}(t-1) + a_{i+1,j}(t-1) + a_{i,j-1}(t-1) + a_{i,j+1}(t-1)], \quad (3)$$

the rule is called an *outer-totalistic rule*, and provides a subset of symmetric CA rules. The Game of Life [10, 11] is an example of the outer-totalistic rule with the nine neighbour structure.

It is surmised that the occupied cells in the background of empty cells always multiply toward the four directions when

$$g(0, 1) = 1 \quad (4)$$

is satisfied, as in **Fig. 2** for example (see **Appendix A** for the reason). The analyses in this paper focus on CAs satisfying eq. (4), otherwise the occupied cells may disappear, or may become localised, as in **Fig. 3**. Such CAs must be eliminated from our scope in advance.



**Fig. 2.** An example of expanding CAs given by the rule outputting 0 except for  $g(0, 1) = 1$ .

Let us tentatively swap the empty and occupied states in **Fig. 2**, and consider empty cells expanding into an occupied-state background. The expandable condition for an empty state can be derived by reversing all the input and the output states of eq. (4) such as

$$g(1, 3) = 0. \quad (5)$$

By taking account of this condition it is possible to remove the CAs whose evolution leads to localized empty cells such as in **Fig. 4**. Together with eq. (4), the condition of eq. (5) ensures that both occupied and empty cells do not become localised. In this way, the two types of cells are mixed with each other so that the CA pattern may become crystal-like, as in **Fig. 1**.

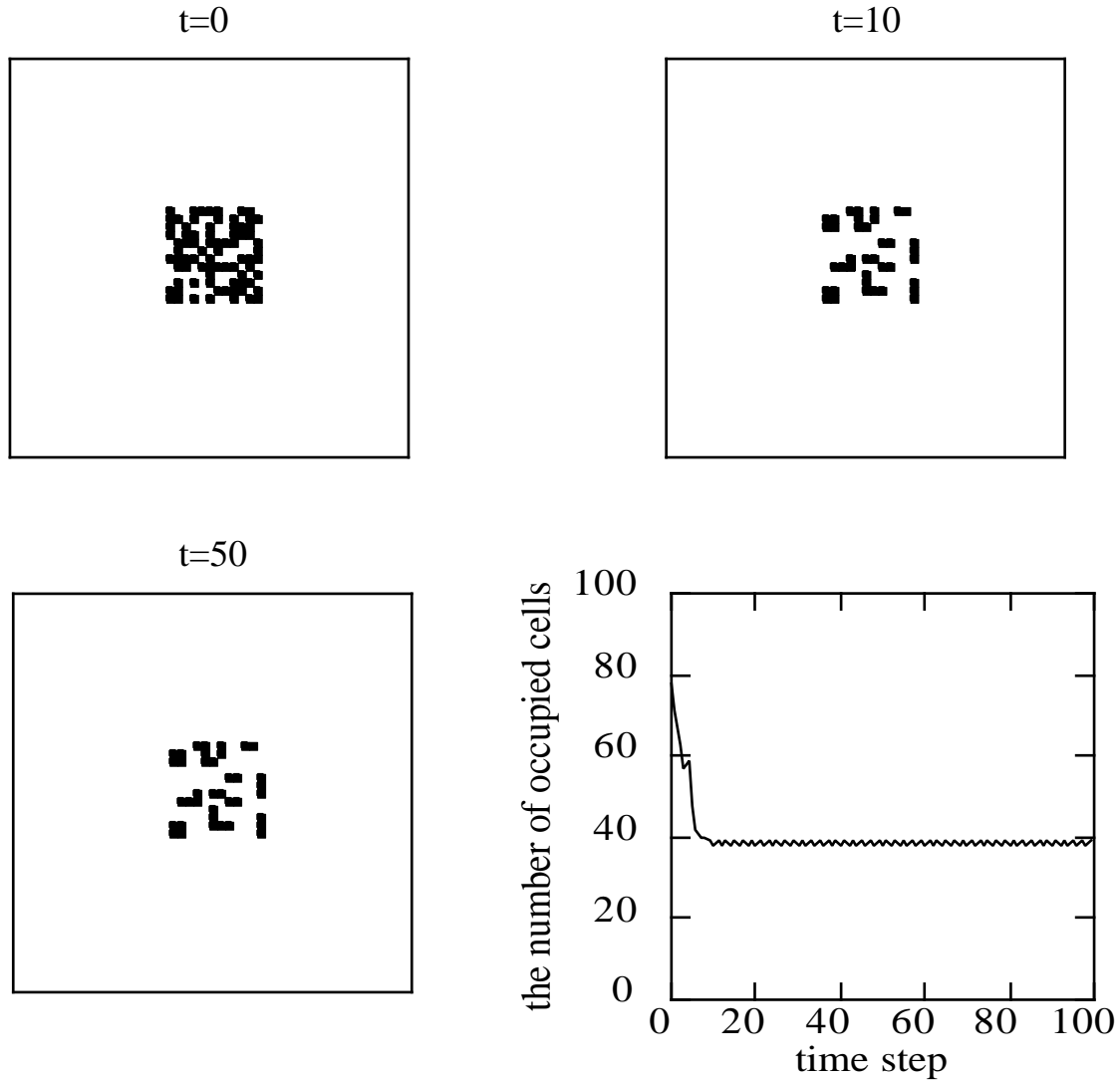
If eq. (2) is not satisfied, i.e. if

$$g(0, 0) = 1 \quad (6)$$

is satisfied, then the “empty” background as seen in **Fig. 2** will change to an occupied-state background one time-step later. As mentioned above, rules that include such a mapping are not considered in this paper, but the reverse of eq. (6)

$$g(1, 4) = 1 \quad (7)$$

does not violate the quiescent condition, and prohibits a large space filled with occupied sites such as in **Fig. 4**. Therefore, as with eq. (5), eq. (7) can also avoid the localisation of empty cells in the background of occupied cells.

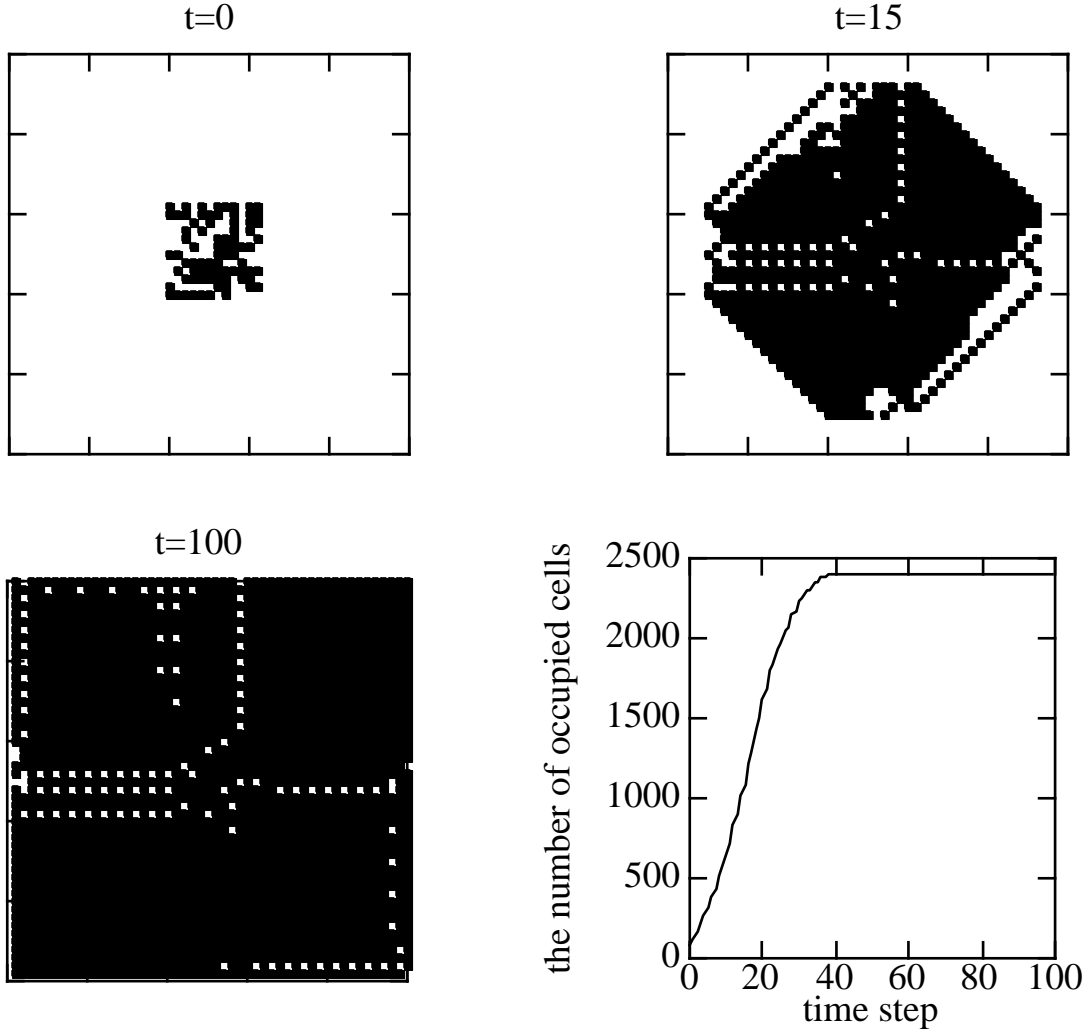


**Fig. 3.** The evolution leads to localized occupied cells: The rule outputs 0 except for  $g(0, 3) = g(1, 1) = g(1, 2) = 1$ .

From the discussion above, CA rules satisfying

$$g(0, 1) = 1 \text{ and } \{g(1, 3) = 0 \text{ or } g(1, 4) = 0\} \quad (8)$$

are expected to lead random configurations to become neither homogeneous nor localised patterns of both empty and occupied cells, which was confirmed by empirical studies. Consequently the CAs in this condition are those which can potentially cause a crystalline structure, and are examined in the next section.



**Fig. 4.** The evolution leads to localized empty cells: The rule outputs 0 except for  $g(0, 1) = g(0, 2) = g(1, 2) = g(1, 3) = g(1, 4) = 1$ .

### 3 Analyses

#### 3.1 Statistical measures of the CA

To understand the crystalline structure of CAs, it is useful to look at the entropy associated with their spatial pattern. The information entropy  $H$  is defined as

$$H \equiv - \sum_k P^k \log(P^k), \quad (9)$$

where  $P^k$  is a probability of the event  $k$  [12], and this can be used to evaluate the randomness (or regularity) of statistical variables. Consider four adjacent sites such as  $(i, j)$ ,  $(i + 1, j)$ ,  $(i, j + 1)$  and  $(i + 1, j + 1)$ ; there are  $2^4 = 16$  possible patterns for this local patch. The

entropy of the spatial pattern of CA configuration  $H_s$  at an arbitrary time step  $\tau$  can be defined by

$$H_s(\tau) \equiv - \sum_k P_s^k(\tau) \log_{16}(P_s^k(\tau)), \quad (10)$$

where  $P_s^k(\tau)$  is the probability for a particular pattern of the local patch at the time step  $\tau$ . Note that a base of 16 is used for the logarithmic function as the entropy assumes a position between nil and unity. Typical CA configurations varying with  $H_s$  are shown in **Fig. 5**. CAs with high  $H_s$  have random spatial patterns, whereas those with low  $H_s$  have regular patterns, i.e. crystalline structure. **Figure 6** shows the distribution  $H_s$  for all 768 cases satisfying eq. (8). The figure indicates that low- $H_s$  (i.e. crystalline) CAs are in the minority and most CAs have random spatial patterns.

Similarly to  $H_s$ , it is possible to define the entropy associated with the temporal pattern. Consider an arbitrary site  $(i, j)$ . There are four mapping patterns to the next time step per site, i.e.  $0 \rightarrow 0$ ,  $0 \rightarrow 1$ ,  $1 \rightarrow 0$  and  $1 \rightarrow 1$ , and assume we sample the mapping pattern of the site during a certain period. From the probability of each mapping pattern, the entropy of the temporal CA development at the site can be defined by

$$H_t^{(i,j)} \equiv - \sum_k P_t^{k,(i,j)}(\tau_0, \tau_1) \log_4(P_t^{k,(i,j)}(\tau_0, \tau_1)), \quad (11)$$

where  $\tau_0$  and  $\tau_1$  are the respective initial and final time steps of the data collection. The base of 4 is used for the logarithmic function as the entropy assumes a position between nil and unity. By collecting the entropy of all sites the average entropy of the temporal CA development ( $H_t(\tau_0, \tau_1)$ ) can be given. **Figure 7** shows the distribution of the CAs on the  $H_s - H_t$  space, where the data  $H_s$  are collected at the time step 2000 and those for  $H_t$  are collected during 1900 – 2000 time steps. The  $H_t$  clearly classifies the CAs into two groups, random and regular time-developing groups. Some points with moderate  $H_t$  correspond to CAs which are still transient even after 2000 time steps, and are expected to drop to the low- $H_t$  region soon or later according to their past tracks. The high- $H_t$  CAs always have a high- $H_s$  value, and these are generally recognized as *chaotic*. The  $H_s$  of *static* (low- $H_t$ ) CAs, on the other hand, have various values and it is difficult to clearly separate crystalline CAs from non-crystalline ones. The graph also indicates that the crystalline structures are stable once they are produced, because all the crystalline (low- $H_s$ ) CAs have regular time-development (low- $H_t$ ) after the transient period.

### 3.2 The $\mu$ parameter

If a rule is configured such that all cell states never change whatever state the neighbour sites have, that is,

$$g(0, i) = 0 \text{ and } g(1, i) = 1 (i = 0, \dots, 4), \quad (12)$$

then it is expected that the evolution leads to a constant development. On the other hand, if a rule is configured such that all cell states perpetually change whatever state the neighbour sites have, that is,

$$g(0, i) = 1 \text{ and } g(1, i) = 0 (i = 0, \dots, 4), \quad (13)$$

then the CA evolution becomes periodic with the period two. These are the two extreme cases, and in the case of general rules, the mapping may or may not change cell states depending on the neighbour state. As a descriptor of how the cell state is changeable, we consider a parameter uniquely determined for each rule

$$\mu = \frac{2^5 - m}{2^5}, \quad (14)$$

where  $m$  is a total number of the rule entries which update the cell state unchanged. The value of eq. (14) is hereafter called the  $\mu$  parameter. For instance, the  $\mu$  parameters for

the rules of eqs. (12) and (13) are nil and unity respectively. Note that the  $\mu$  parameters is different from the  $\lambda$  parameter [13].

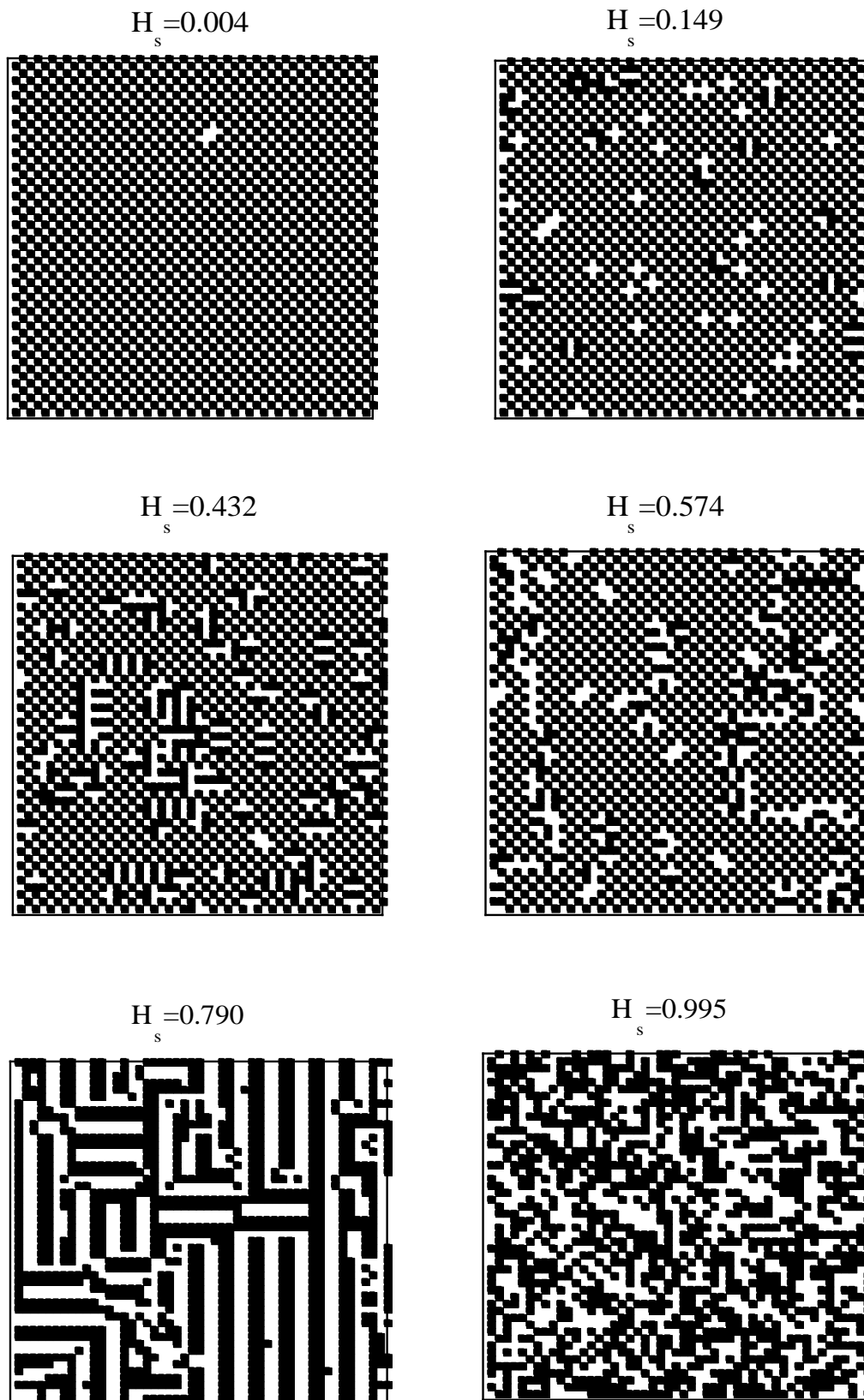


Fig. 5. Typical CA patterns with various  $H_s$ .

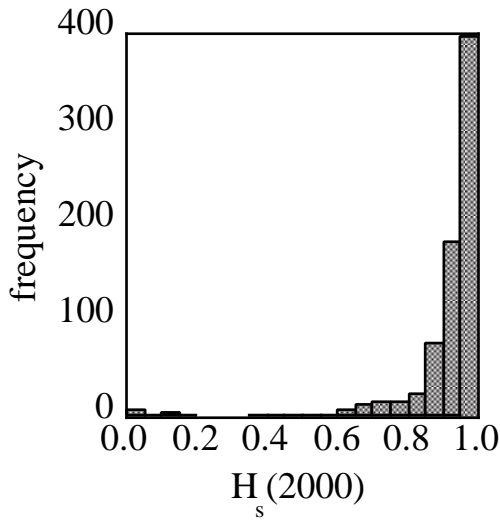


Fig. 6. Distribution of the entropy of spatial pattern of CAs after the long term evolution.

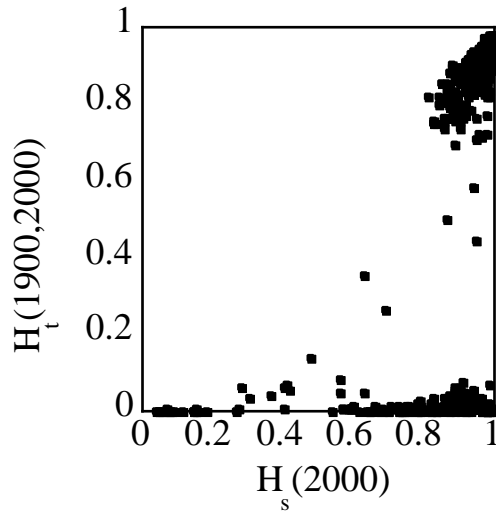
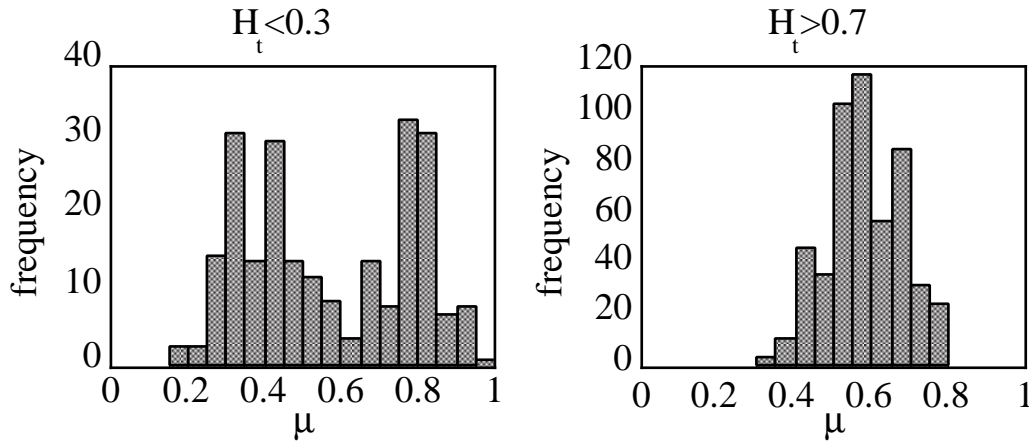


Fig. 7. Distribution of the CAs on the  $H_s$ - $H_t$  space

**Figure 8** shows the frequency distribution of the  $\mu$  parameter for static and chaotic CAs. CAs in the static group have a  $\mu$ -value near the extrema, and the value for those in the chaotic group is in the central range of  $\mu$ . Thus the graphs imply that the transition from static to chaotic takes place as the  $\mu$  parameter changes from  $\mu_0$  (or  $\mu_1$ ) to the moderate value, where  $\mu_0$  and  $\mu_1$  are the smallest and largest values of  $\mu$  parameter satisfying eq. (8) ( $\mu_0 \approx 0.156$ ,  $\mu_1 \approx 0.968$ ).



**Fig. 8.** The  $\mu$  parameters of static ( $H_t < 0.3$ ) and chaotic ( $H_t > 0.7$ ) CAs.

Consider CAs with  $\mu_0 \leq \mu \leq 0.5$ . If a rule has  $\mu$  close to  $\mu_0$ , we can presume that from the definition of  $\mu$  that there are many kinds of local patterns which remain unchanged through the updating by the rule. Therefore, CA evolutions starting from a random configuration remain random, although these time-developments are regular; these CAs are thought to be located at the high- $H_s$  and low- $H_t$  range in **Fig. 7**. As the  $\mu$  parameter increases the number of such constant local patterns decreases, and accordingly the CA's spatial pattern after the transient period becomes less random. At the same time, the position of the CA on the  $H_s - H_t$  space (**Fig. 7**) shifts gradually to the low- $H_s$  and low- $H_t$  range. If  $\mu$  becomes so large that only a few kinds of local patterns can remain unchanged, these particular patterns must be spread all over the CA space through the continuation of this process, because each local pattern keeps changing unless it fits one of the particular patterns: This is considered



to be the mechanism of crystallisation. For this reason, relatively longer transient times can be observed for the crystalline CAs compared to the others. There is a certain point in the  $\mu$  parameter, say  $\mu_c$ , at which all constant local patterns disappear. The rules with  $\mu \geq \mu_c$  therefore lead to random time development and random spatial configuration, and correspond to the high- $H_s$  and high- $H_t$  group (namely the chaotic group) in **Fig. 7**. The value of  $\mu_c$  is, however, not uniquely determined, because the largest  $\mu$  which leads to the crystalline structure is dependent on the type of patterns.

A similar discussion is possible for the CA rules with  $0.5 \leq \mu \leq \mu_1$ . The crystalline structure in this case is determined not by the constant local pattern but by the period-2 local pattern.

**Figure 9** shows the  $\mu - H_s$  distribution of CAs with  $H_t < 0.1$ , namely static CAs. Crystalline CAs have moderate values of  $\mu$ , while the non-crystalline ones have values near the extrema. These results also support the above scenario.

To sum up, the  $\mu$  parameter statistically parameterises the CA rules, and is a key value of the crystallisation and the phase transition between static and chaotic performances. As mentioned in [13], the  $\lambda$  parameter is related to the four Wolfram Classes [6]:

- 1) Evolution leads to a homogeneous configuration.
- 2) Evolution leads to a set of separated simple stable or periodic structures.
- 3) Evolution leads to a chaotic or aperiodic pattern.
- 4) Evolution leads to a complex localized structure, sometimes long-lived.

Because the two parameters are independent, these combinations can give more detailed classifications. As already mentioned in section 2, the classes 1,2 and 4 are eliminated from the scope of this study, and the above analysis suggests that the remaining CAs are classified into three groups: Two more classes (crystalline and noncrystalline-and-static classes) can be added. These six classes are roughly located in the landscape of the rule space drawn on the  $\lambda - \mu$  plane as seen in **Fig. 10**.

It is worthwhile to compare such CA dynamics to crystallisation in nature. The static and chaotic classes correspond to solid and liquid phases, respectively; the  $\mu$  parameter corresponds to temperature. The initial condition is “liquid” as shown in **Fig. 1**. The “liquid” is cooled rapidly when  $\mu$  is low, and a non-crystalline structure (or amorphas) is produced. If the “liquid” is slowly cooled at around melting point, i.e. at  $\mu_c$ , crystal is produced. The initial “liquid” continues to be liquid if  $\mu$  is high. The major difference is only that the  $\mu_c$  is not uniquely determined like the melting point. Consequently, the macroscopic properties of the crystallisation in CAs is fairly similar to those in nature. The microscopic mechanism of crystallisation is commonly understood to be that existing crystalline structures allow a local pattern (a molecular) join if it is matching in structure, whereas those unsuitable (impurities) are likely to remain in solution. This is clearly similar to the mechanism of CA crystallisation as explained above.

## 4 Concluding remarks

Two-dimensional CAs causing the crystalline structure were studied. The spatial and temporal pattern entropy functions successfully characterise them, and classified them into two groups, static and chaotic. The background for this classification was investigated using the  $\mu$  parameter, the probability for a cell-state to remain unchanged at the next time step; the  $\mu$  parameter is uniquely determined by the rule definition. Theoretical and experimental studies confirmed that the  $\mu$  parameter statistically parameterises the CA rules, and that it is a key value to the phase transition between static and chaotic performances. In addition, it was surmised that crystallisation appears when the rule has a  $\mu$  parameter near the critical point between static and chaotic CA evolutions. The observed phenomena are probably considered as a generalised form of crystallisation, including ones in nature and computers.

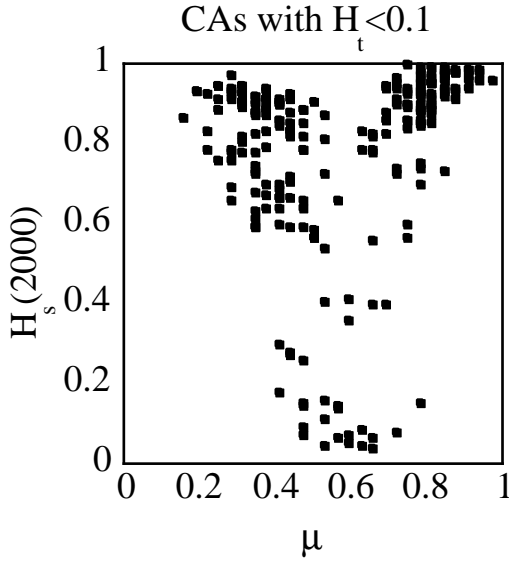


Fig. 9  $H_s$  of static CAs varying with the  $\mu$  parameter

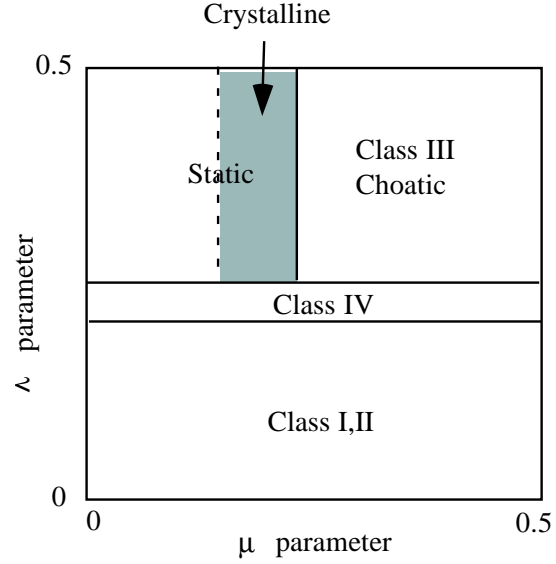


Fig. 10. The landscape of the rule space characterized by the  $\mu$  and  $\lambda$  parameters: The graph in the range of  $0.5 < \mu < 1$  ( $0.5 < \lambda < 1$ ) is produced by the symmetric transformation of that for  $0 < \mu < 0.5$  ( $0 < \lambda < 0.5$ ) at  $\mu=0.5$  ( $\lambda=0.5$ ).

## A The expandability of CAs

One-dimensional CAs with 3-neighbour structure are defined by

$$a_i(t) = f_1[(a_{i-1}(t-1), a_i(t-1), a_{i+1}(t-1))], (a_i \in \{0, 1\}, i \in Z) \quad (15)$$

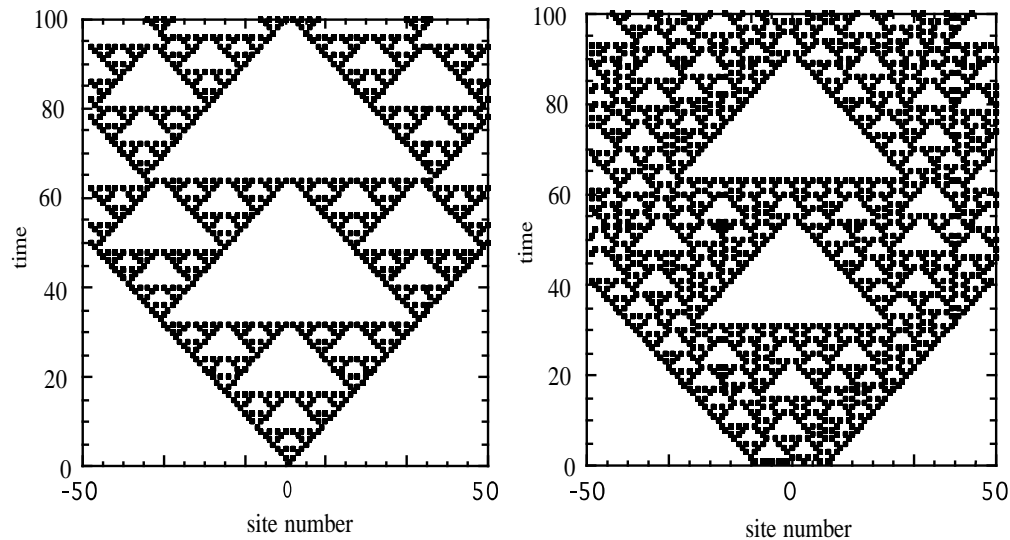
and rules satisfying the quiescent condition considered as

$$f_1(0, 0, 0) = 0, \quad (16)$$

and

$$f_1(1, 0, 0) = f_1(0, 0, 1) = 1. \quad (17)$$

Let us assume an initial condition of a single occupied site at the position of  $i = 0$  with the background of empty sites. When  $t = 1$ , two cells at the position of  $i = 1$  and  $-1$  are occupied. Similarly, two cells at  $i = 2$  and  $-2$  become occupied when  $t = 2$ . Generally, when  $t = \tau$ , the sites at  $i = \tau$  and  $-\tau$  have an occupied state, and a "triangle" is formed in the spatio-tempo CA space, as seen in **Fig. A1**. The sites inside the triangle have either an occupied or an empty state, but it is never totally empty because an isolated occupied cell at  $i = \tau$  again becomes another "seed" of the triangle. In this way, occupied cells spread all over the CA space, and this property is not influenced by the other entries such as  $f_1(1, 1, 0)$ . The evolution from the random configuration also leads to expansive dynamics as seen in **Fig. 11a**. Therefore the condition of eq. (17) ensures the expandability of the 1-dimensional CA. Equation (4) is the extension of this condition to two dimensions and ensures the expanding dynamics of 2-dimensional CAs.



**Fig. 11.** One-dimensional expandable CAs given by the rule outputting 0 except for  $f_1(1, 0, 0) = f_1(0, 0, 1) = 1$ .

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