Simple models for crystallisation processes

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ABSTRACT

Cellular Automaton (CA) modelling, the repeated application of simple rules can result in very complex behaviour and is being increasingly used to simulate physical processes. This paper outlines the technique with special emphasis on ordered states and order/disorder transitions.

keywords: Cellular Automata, Game of Life, Transmission Line Matrix (TLM), crystallisation, phase transitions

1. INTRODUCTION

At previous crystal conferences in Zakopane presentations have been made about the benefits of TLM, a numerical modelling technique which at one extreme can be interpreted in terms of electromagnetic theory[1,2,3]. At the other extreme it can be considered as the repeated application of a set of rules; an example of a cellular automaton (CA). This paper introduces some basic concepts of general CA modelling in one and two dimensions. Even a cursory inspection of the subje[4] reveals a bewildering expanse of interesting avenues. However, as will be demonstrated here, there has been much recent work on classification and this helps to reduce the apparent problems associated with disparity of formalism and dialect. In addition to introducing the subject, this paper presents details of work we have done in this area and discusses some of the wider work on crystallinity and phase transitions. We will start with a presentation of some interesting/amusing, but nevertheless useful two-dimensional CAs. We will then revert to one-dimension and demonstrate some of the CA aspects of one-dimensional TLM algorithms for diffusion. We follow this with a discussion on Wolfram's classification system and consider several specific cases. Finally, we will return to two-dimensional CAs and discuss recent developments in terms of the classification of CAs which distinguishes between those that lead to crystalline states, non-crystalline states and chaotic states.

2. SOME TWO-DIMENSIONAL CELLULAR AUTOMATA

2.1. *Game of Life*

'Life' was invented by J.H. Conway and was popularised by Martin Gardner in the Scientific American[5,6]. It involves a rectangular mesh where grid-points are either alive (state '1') or dead (state '0'). The population of any point at the next generation is determined only by the state of the 8 nearest neighbours at the present generation (see figure 1).

There are three possible transitions in *'Life'*:

Birth	If ${}_kP(x,y) = 0$ then ${}_{k+1}P(x,y) = 1$ if three of the neighbours are currently alive.
Survival	If ${}_kP(x,y) = 1$ then ${}_{k+1}P(x,y) = 1$ if two or three neighbours are currently alive.
Death (by crowding)	If ${}_kP(x,y) = 1$ then ${}_{k+1}P(x,y) = 0$ if four or more neighbours are alive .
Death (by isolation)	If ${}_kP(x,y) = 1$ then ${}_{k+1}P(x,y) = 0$ if one or no neighbours are alive.

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Intl. Conference on Solid State Crystals 2000: Growth, Characterization, and Applications of Single Crystals, Antoni Rogaski, Krzysztof Adamiec, Pawel Madejczyk, Editors, Proceedings of SPIE Vol. 4412 (2001) © 2001 SPIE · 0277-786X/01/$15.00

Life is totally deterministic but we generally have to run a simulation to see what any but the most trivial starting configurations will yield as the simulation progresses.

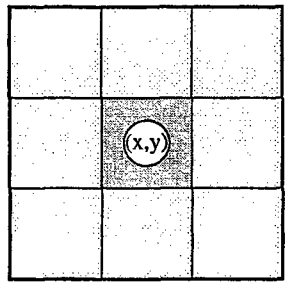

Figure 1. The eight nearest neighbours in Conway's *'Game of Life'*

2.2. *Forest fires*

The *'Forest Fire'* CA uses a square lattice but differs from the last case in that it has a stochastic element. Grid-points have three possible states: Red denotes a burning tree, White (blank) is either a dead tree or an empty site and Green is a living tree. The rules are as follows:

If ${}_kP(x,y)$ = Red then ${}_{k+1}P(x,y)$ = White (the tree has burnt).

If ${}_kP(x,y)$ = Green then ${}_{k+1}P(x,y)$ = Red, if one of the eight neighbours is currently Red

If ${}_kP(x,y)$ = White then ${}_{k+1}P(x,y) \rightarrow$ Green with probability p (growth)

If ${}_kP(x,y)$ = Green then ${}_{k+1}P(x,y) \rightarrow$ Red with probability f (fire initiated by lightning)

Values of $p = 0.3$ and $f = 6\times10^{-5}$ give very convincing results[4].

2.3. Others

Examples of CAs with different levels of random element that are discussed by Chopard and Droz[4] include *percolation*, *Ising spin* modelling and *road traffic* simulation.

3. TLM ALGORITHM FOR ONE-DIMENSIONAL DIFFUSION AS A CA PROCESS

The basics of Transmission Line Matrix (TLM) for diffusion can be found in a variety of references which are summarised by de Cogan[7]. It has two basic steps, *Scatter* and *Connect*. The *Scatter* process has two rules *Reflect* and *Transmit*. *Reflect* multiplies any data impulse which is incident on a spatial node by the reflection coefficient, ρ and reverses its direction of motion. *Transmit* multiplies any incoming pulse by the transmission coefficient $\tau = (1-\rho)$ and retains the direction of motion. These determine the magnitude and destination of the pulses for the *Connect* process which determines the total population distribution at the next generation. The resulting scatter algebra can be summarised for a unit pulse incident at position (x) from the left:

Reflect $\quad \hat{\rho}[(x)] \rightarrow \rho[(x-1)]$

Transmit $\quad \hat{\tau}[(x)] \rightarrow \tau[(x+1)]$

Thus, $\hat{\rho}\hat{\rho}[(x)] \rightarrow \rho^2[(x-1+1)]$, i.e. $\rho^2[(x)]$

The process is not commutative: $\hat{\rho}\hat{\tau}[(x)]$ (working outwards) $\rightarrow \rho\tau[(x+1-1)]$, i.e. $\rho\tau[(x)]$, while $\hat{\tau}\hat{\rho}[(x)] \rightarrow \rho\tau[(x-1-1)]$ or $\rho\tau[(x-2)]$. This is similar to the CA which can be used to model the behaviour of falling sand in an hour-glass. When $\rho = \tau$ this is identical to Galton's 'Quincunx' which was an early experimental method of demonstrating that such processes yield a Gaussian distribution[8].

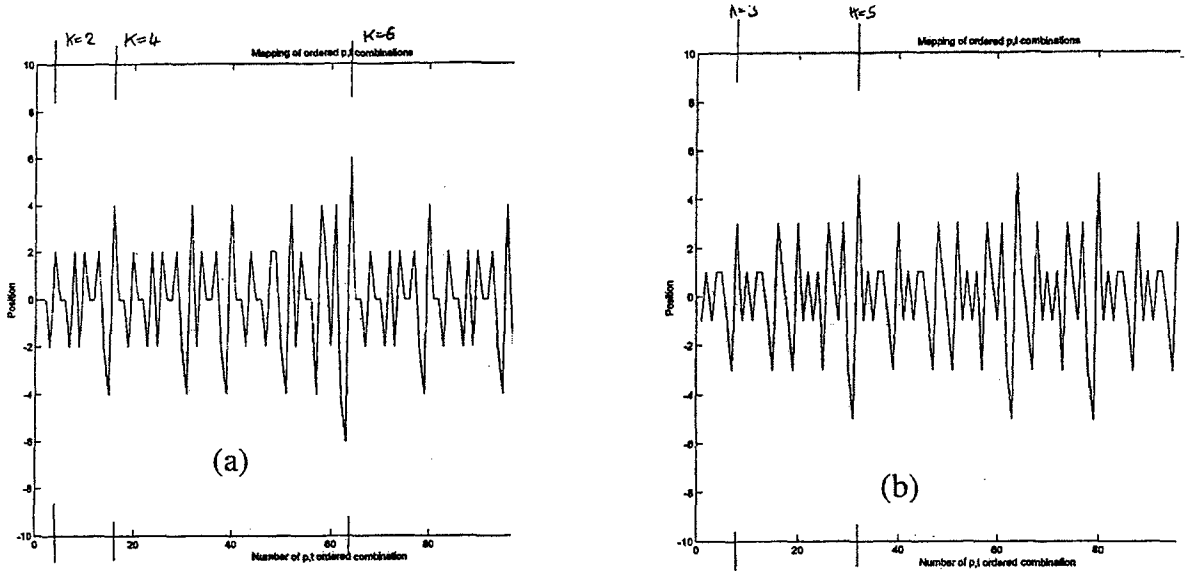

Figure 3 Displacement of successive elements in a ρ, τ binary sequence of length 2^k plotted against number in sequence (a) for (k =2, 4, 6),(b) for (k = 3, 5).

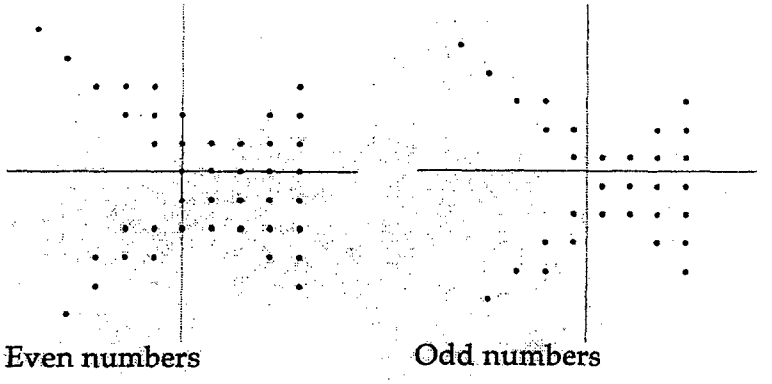

Figure 3 Displacement of successive elements in a ρ, τ binary sequence of length 2^k plotted as position of (s+1)th in sequence (vertical axis) versus position of (s)th (horizontal axis) for even and odd length sequences.

If we assume that the diffusion process described by TLM is an arrangement by which data-pulses, starting at the source take all possible paths then we can describe the situation three time-steps after the start of our simulation by means of a three-bit binary sequence of scattering operators $\hat{\rho}\hat{\rho}\hat{\rho}[(x)]$, $\hat{\rho}\hat{\rho}\hat{\tau}[(x)]$, $\hat{\rho}\hat{\tau}\hat{\rho}[(x)]$, $\hat{\rho}\hat{\tau}\hat{\tau}[(x)]$, $\hat{\tau}\hat{\rho}\hat{\rho}[(x)]$, $\hat{\tau}\hat{\rho}\hat{\tau}[(x)]$, $\hat{\tau}\hat{\tau}\hat{\rho}[(x)]$, and $\hat{\tau}\hat{\tau}\hat{\tau}[(x)]$. Similarly, the scattering algebra can be used to determine the final position due to the sixteen four-bit binary operations after the fourth time-step. If we can take a large binary sequence and estimate the final positions of successive components then it can be seen from figure 2 that there is a high degree of correlation. This can also be investigated using a technique borrowed from phase-space plots in chaos theory. A plot of P_{s+1}, the position of the (s+1)th component in the sequence vs P_s, the position of the (s)th component yields some very interesting, and as yet, unexplained results, which are shown for odd and even sequences in figure 3.

4. WOLFRAM'S CLASSIFICATION SYSTEM FOR ONE-DIMENSIONAL CAS

The few examples cited above give some indication of the complexity of the subject. Stephen Wolfram[9] made a systematic study of one-dimensional CAs and recognised that if there are k states involving r nearest neighbours then the total number of distinct rules is:

$$k^{k^{2r-1}}$$

Thus, if there are two states (1,0) and if the outcome at position (x) is determined by two nearest neighbours (x+1) and (x-1) then there are 2^8 rules. Wolfram used the same binary approach as we have used in the previous section and these are shown for some rules in the tables below. The top row represents the current states of (x-1), (x) and (x+1). The bottom row in each shows the state at (x) at the next time as a result of applying the particular rule.

k	(111)	(110)	(101)	(100)	(011)	(010)	(001)	(000)
k+1	0	0	1	1	0	0	1	0

If we take the sequence 00110010 as a binary number then it represents decimal 50. Wolfram termed this as *'Rule 50'*. The exclusive OR rule where the population at (x) is one at the next generation only if (x+1) or (x-1) is one is given in the table below and it can be seen why this is termed *'Rule 90'*. Chopard and Droz[4] discuss how rule 184 mimics a surface growth process.

k	(111)	(110)	(101)	(100)	(011)	(010)	(001)	(000)
k+1	0	1	0	1	1	0	1	0

Although there is the question of non-decidability (just as in nature) these rules can be divided into clearly empirical classes.

1. After a finite number of steps the system tends towards a unique homogeneous state (i.e. tends towards a limit point). *Rule 40* is an example of this.
2. The system develops periodic regions for almost all initial states (i.e. tends towards a limit cycle). *Rule 56* is an example of this.
3. Characterised by aperiodic or chaotic patterns, e.g. *Rule 18* (i.e. strange attractor).
4. Rules in this class yield persistent complex structures for a large class of initial states, the behaviour can only be determined by explicit simulation (e.g. *Rule 110*).

5. MORPHOLOGICAL STUDIES OF *RULE 90*

We were interested in *Rule 90* for two reasons. A single initial excitation in the middle of a string of zeros yields the beautiful Sierpinski gasket with its self-similar properties (figure 4).

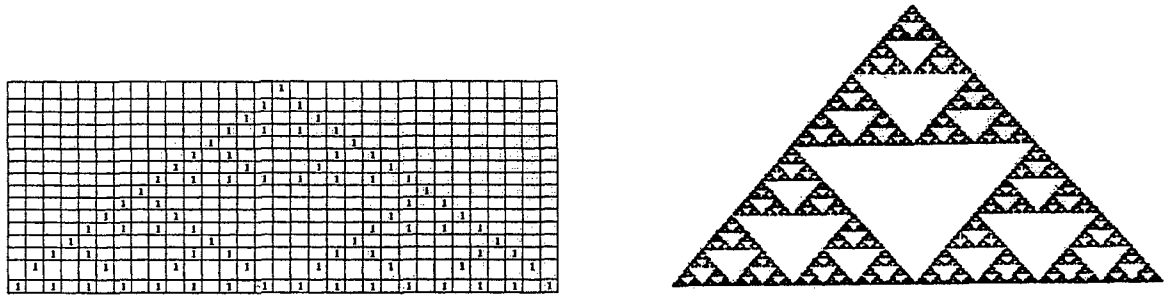

Figure 4 Wolfram's *Rule 90* for different numbers of iterations after a single initial excitation (Sierpinski Gasket)

The second reason for our interest was the fact that an excitation consisting of a random sequence of ones and zeros seems to 'develop' a level of order. We used techniques borrowed from image processing to identify the relative sizes of triangles. The situation is very simple in the Sierpinski gasket. The smallest triangles have 2 ones along each side. We call these class 2 triangles. The next smallest triangles are class 4 (they have 4 ones along each side), the next is class 8 and then class 16. There are no triangles with odd numbers of ones along each side. The total number of class 2 triangles at generation, k (where k>1) is 3^{k-2}. Class 4 triangles do not appear until k = 3. Thereafter they increase as 3^{k-3}. The analysis can be extended to higher classes. Any real simulation of a Sierpinski gasket is bounded by the size of the chosen array and the boundary conditions which are applied (zero boundary, unit boundary, mirror boundary, wrap-around boundary) will affect the population of triangles. The effect of bounding can be to have the concentration of triangles of a given class tend towards a steady state. Knowing the relationship between equilibria and entropy we investigated the time variation of different classes of triangles which evolve from random initial excitations. The model spaces were large and we examined only a central region so as to eliminate boundary effects within the number of iterations used. In no case were we able to identify a time-dependent change in the number of triangles of a given class. We are forced to assume that within the limits of our numerical experiments there was no persistent change in the state of order of the system.

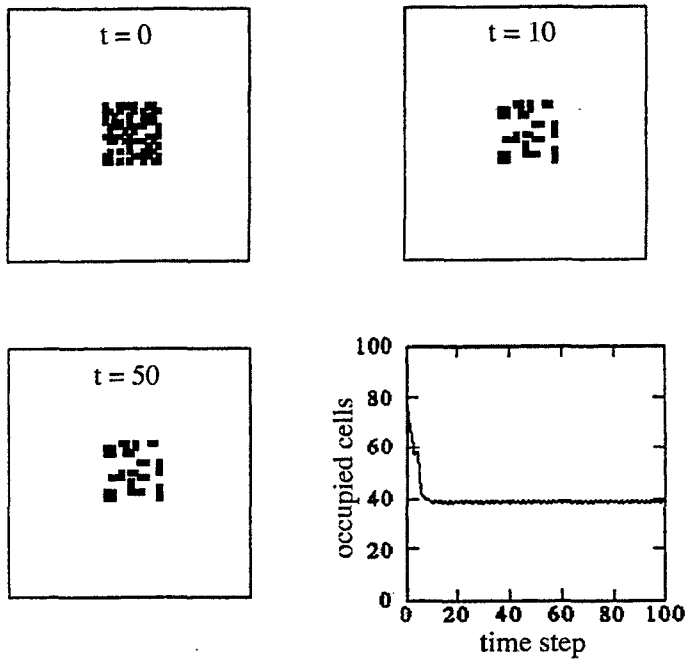

Figure 5 Population versus time for a rule which outputs zero except for $g(0,3)$, $g(1,1)$ and $g(1,2)$ which ouput 1.

6. CLASSIFICATIONS OF SIMPLE TWO-DIMENSIONAL CAS

Suzudo[10] has extended the classification techniques to two-dimensions but his analysis may difficult to assimilate on account of differences in formalism. He defines a generalised CA function, f which acts on the present population of states ${}_k a$ to generate ${}_{k+1}a(x,y)$, the value of a(x,y) at the (k+1)th generation.

$$ {}_{k+1}a(x,y) = f\left[{}_k a(x-1,y), {}_k a(x+1,y), {}_k a(x,y-1), {}_k a(x,y+1), {}_k a(x,y)\right] $$

He starts by insisting that $f(0,0,0,0,0) = 0$, ones are not generated from empty space. He then defines a function, g, where it is the sum of the neighbouring population that is important. (in the case of *Life* we are summing over the eight neighbours)

$$_{k+1}a(x,y) = g\left[{}_{k}a(x,y),\ {}_{k}a(x+1,y)+{}_{k}a(x-1,y)+{}_{k}a(x,y-1)+{}_{k}a(x,y+1)\right]$$

The condition $g(0,1)$ says that ${}_{k}a(x,y) = 0$ and at least one of its neighbours = 1.

$g(0,1) = 1$ is a 'Deposition' process and is the two-dimensional equivalent of Wolfram's *Rule 90*. This is an important rule, otherwise occupied cells may disappear or become locallised (see figure 5). However, there are other rules where we can get the opposite effect, namely locallised empty cells.

We can use the reverse of $g(0,1) = 1$, namely $g(1,3) = 0$ which causes empty states to advance into occupied territory. This is a 'Dissolution' or erosion process. A combination of $g(0,1)$ and $g(1,3)$ can be used to prevent localisation by occupied or empty cells. Figure 6 is an example of such a mixing process that can lead to 'crystallisation'.

Suzudo then introduces the concepts of spatial and temporal entropy, which we will designate as S_s and S_t which are arranged to be zero for ordered states and unity for disordered states. S_s can be plotted against S_t for all possible rules after a given evolution time and it is possible to distinguish those rules which lead to chaotic evolutions. They have large values of both entropies. Even after 2000 time-steps there is a significant clustering of rules with small S_t i.e. less than 0.1. This allows us to distinguish between rules that ultimately lead to a chaotic (liquid) state and those that will lead to a solid state. In order to distinguish between crystalline and amorphous states we need another parameter.

The Suzudo μ parameter is defined as $\mu = \dfrac{2^5 - m}{2^5}$ (m = number of rule entries which update the cell with no change)

This can be related to the λ parameter of Langton[11] which gives the percentage of non-zero transitions in the CA transition table and is closely related to the Wolfram classes rules. The process of crystallisation really only applies to class 3 rules. Accordingly, we can divide the λ, μ space into six classification areas as shown schematically in figure 7.

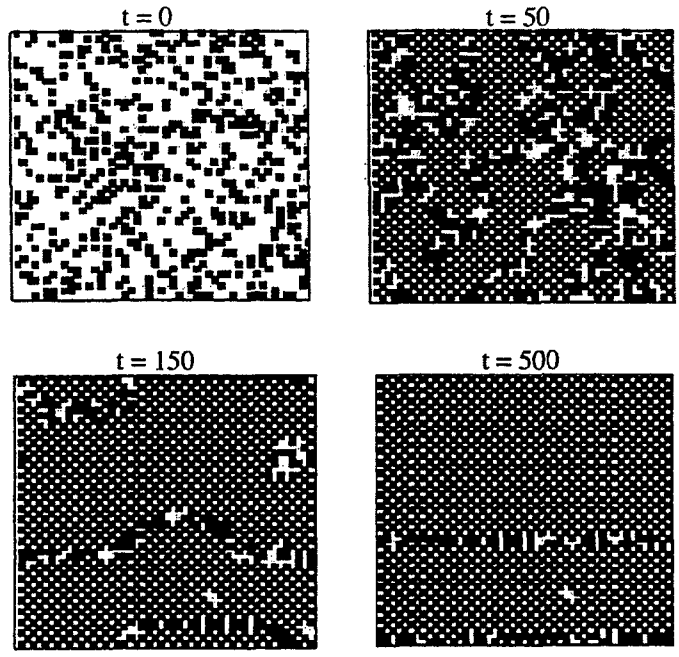

Figure 6 Evolution towards a crystalline state: $g(0,3) = 1$ and ($g(1,3) = 0$ or $g(1,4) = 0$).

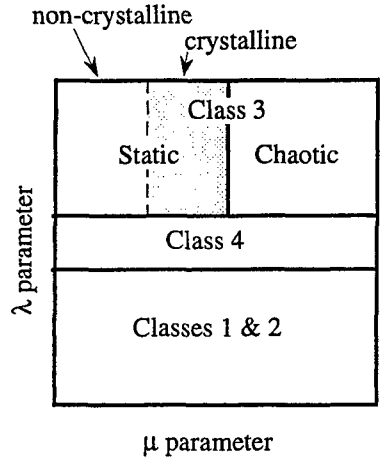

Figure 7 Crystalline/non-crystalline transitions in λμ space (μ can be considered as the CA equivalent of temperature).

7. CONCLUSIONS

This paper has given some indication of the complexity that can be achieved from the repeated application of simple rules. In spite of the fact that the number of rules is limited by the number of states and the number of neighbourhood sites it is possible to distinguish different behavioural classes, and states of order/disorder. Rules which lead to an ordered state have much in common with the normal processes of crystallisation, even the inclusion of persistent 'defects'. There has been relatively little work on three-dimensional CAs. It may be that in numerical terms the prospect appears to be daunting, but with only two states and six nearest neighbours, there are less rules than in *Life*. The challenge to create a CA which emulates real crystallisation processes remains.

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