5. Cellular Automata and Self-Organization

There are many examples in the animate and inanimate nature, where structure of various complexity evolves from simple beginnings, following very simple rules of regeneration which are embodied in the substance of interest itself. Each new generation evolves as determined by the local environment. This is how nanostructures assemble themselves, how possibly life has begun on Earth. Nanostructures are structured assemblies of 10^3 to 10^9 atoms or molecules. Examples are nanocrystals, supramolecular clusters, cellular organelles, or viruses. In certain environments, such self-assembly occurs and produces structure; in others it does not, leading to disordered media. We know, for example, that certain chemical reactions are made possible by the proximity of catalytic molecules close to the reagents.

Cellular automata, a concept discussed by von Neumann, illustrate a simple mechanism that is capable of showing a broad range of self-organizing behavior, producing anything from cooperative phenomena resulting, e.g., in global fractal structures, to complete disorder. The schematic concept considers the following properties of a system:

- The configuration (state) space is approximated by an n-dimensional lattice of equal cells.
- Each cell has a finite number of discrete properties.
- The automata develop in discrete time steps
- The automata develop according to deterministic rules.
- The rules only refer to the states of neighboring cells.

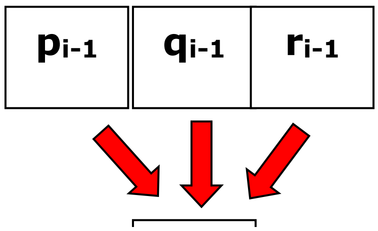


Figure 21

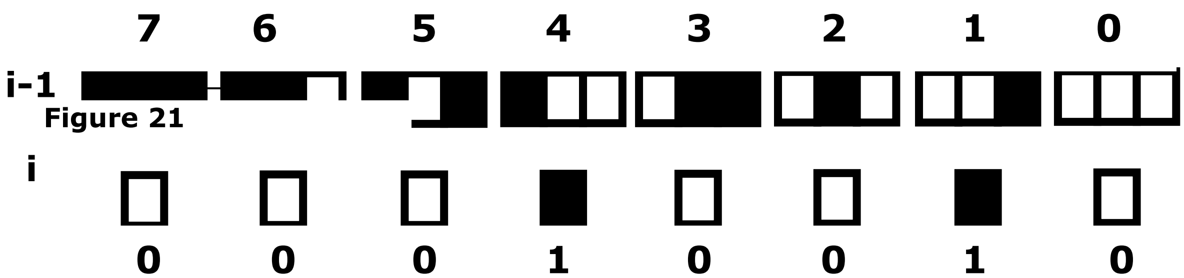


Figure 22

Consider a simple one-dimensional automaton with only two states, "occupied" (black) and "free" (white). Let the fate of a cell ***q*** at time step ***i*** be determined only by the state of its nearest neighbor cells, ***p*** and ***r*** at the previous time step ***i-1***. For example, there could be the rule that a cell could only be occupied if it had been free previously and if there was only one neighboring cell occupied. This rule can be graphically represented by showing for all combination of the states of cells p_{i-1}, q_{i-1}, r_{i-1}, the resulting q_i. The top row of 8 cell triplets shows all possible configurations, ordered and numbered according to their cumulative occupancy in p_{i-1}, q_{i-1}, r_{i-1}. The bottom row of cells depicts the corresponding states of cell q_i. There are obviously 256 (0-255) possible constructions of rules. They can be classified and numbered in the binary system just by quoting the bit sequence of results q_i for the sequence of initial conditions p_{i-1}, q_{i-1}, r_{i-1}, with Rule #0 leading to all white cells and Rule #255 to all black cells. The above sequence would hence be classified as Rule $\#10010_2 = \#(2^4+2) = \#18_{10}$. It can also be expressed in terms of Boolean Algebra as

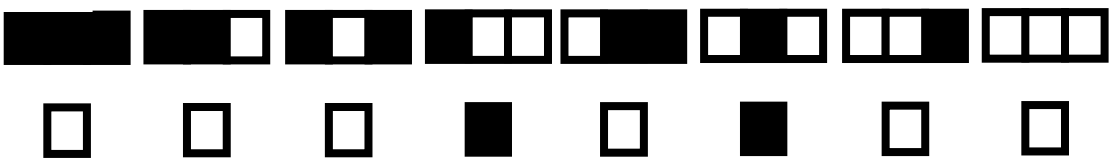
$$q_i = (p_{i-1} \oplus r_{i-1}) \wedge (\neg q_{i-1}) \tag{70}$$

where "true" implies "occupied" or "black" in the graphic representation. The operators in this equation are Exclusive OR, AND, and NOT. The formalism of cellular automata therefore avails itself to numerical exploration of patterns of self-organization using simple computer programs. A Mathcad program has been written for this purpose.

In the following, consider the 1D cellular automata for the rules #20, 90, 30, and 110. The corresponding pattern relations are shown in the figure below. It seems obvious to expect that Rule #20 would show a pattern with the largest white areas, since there are only 2 initial conditions leading to an occupied cell. On the other hand, Rule #110 should have the largest coverage of cells, since 5 of the possible 8 initial conditions lead to an occupied state. But how would Rules #30 and #90 compare, for which both 4 out of 8 possible initial configurations lead to occupancy? Furthermore, there is no simple way to predict a repetitive or random pattern of the sequence of automata. So, one simply has to construct and inspect the individual patterns (run the Mathcad program).

For the present illustrative purposes, a linear automaton with 200 cells is chosen, and 200 successive steps in its evolution are displayed in the graphs resulting from the calculations. In each case, the same simple initial condition was applied, where only the cell (0,100) was loaded and all other 99 initial cells were left blank.

20



90

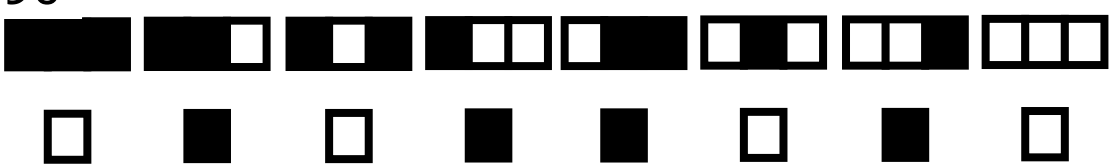
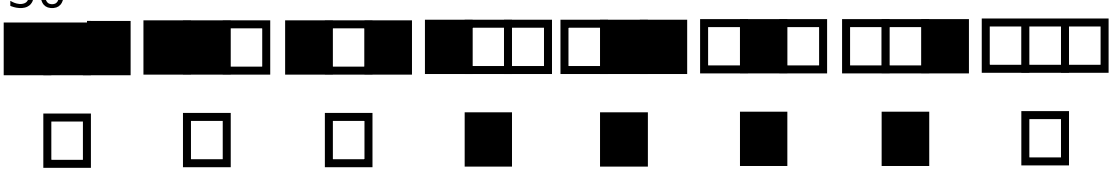
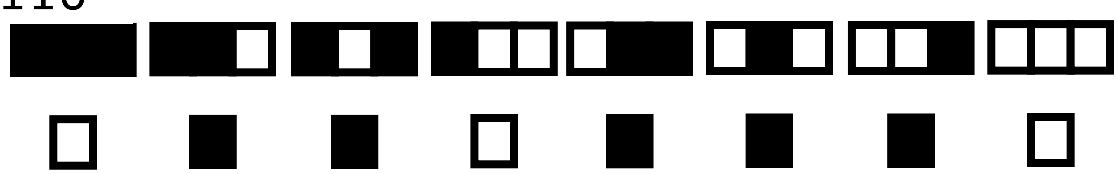


Figure 23

30



110



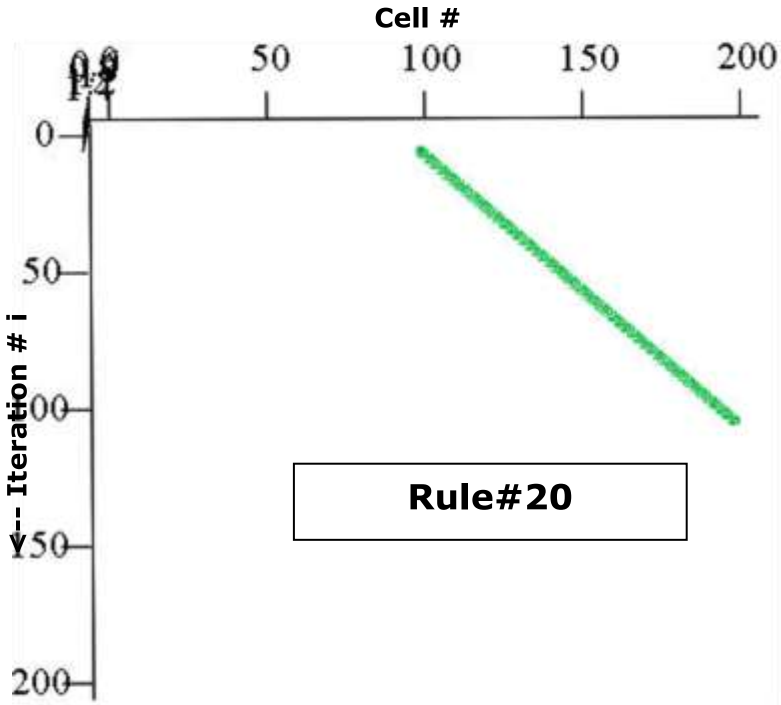


Figure 24

From the figure, it is clear that automaton #20 is indeed very simple. It is represented by a straight line to the right, starting from the initial point (100). The asymmetry is due to the rule, according to which a cell is occupied when it either was occupied before or its left neighbor was occupied, but not its right neighbor. Closer scrutiny reveals that the line is actually a succession of point triplets arranged in a diagonal fashion.

Automaton #30, with one more condition, is illustrated below. Its pattern is much more complex than that for Rule#20. Here, a region of repetitive structure is observed at the rim of the triangular figure. Overall, the pattern looks mostly filled, with white trian-

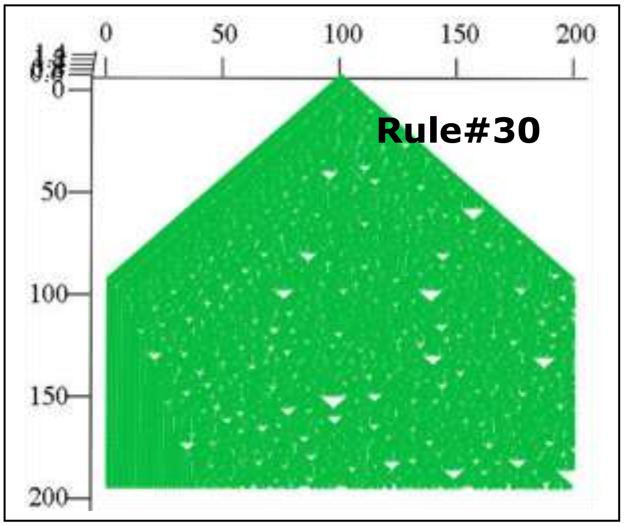
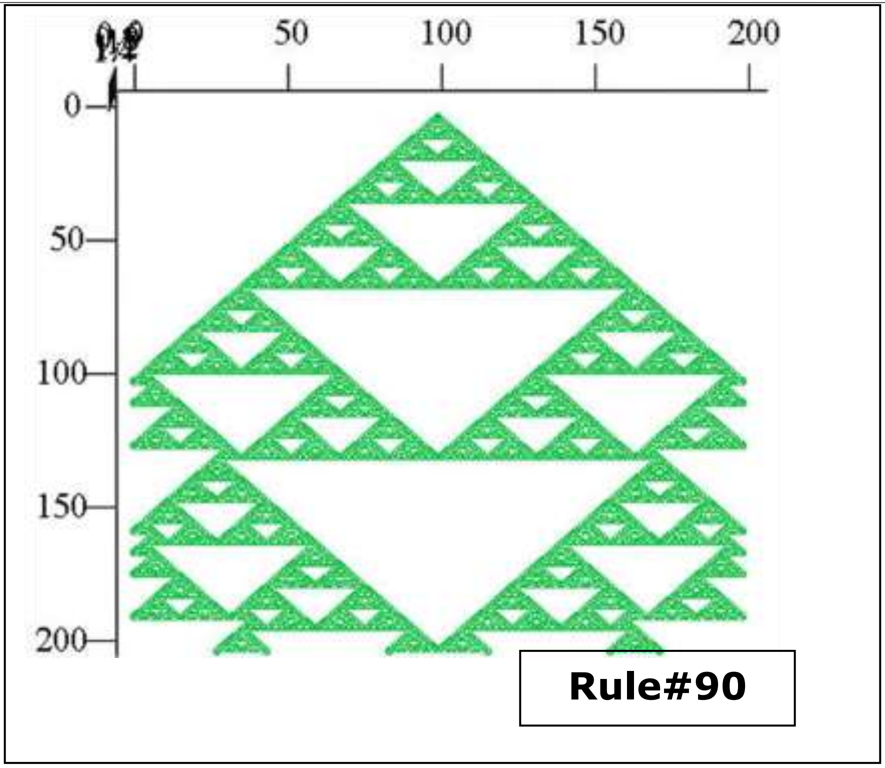


Figure 25

gles of different sizes cut out randomly.

Following is automaton #90, which might be expected to show similar randomness as automaton #30. This, however, is not the case. There is a highly repetitive pattern of nested triangles. Close inspection shows that this structure is fractal. It repeats itself on every length scale.



Finally, the automaton corresponding to Rule #110 is shown below with the expected random complexity. Its asymmetry comes again from the rule propagating cells which have occupied neighbors on the left, but not on the right.

Figure 26

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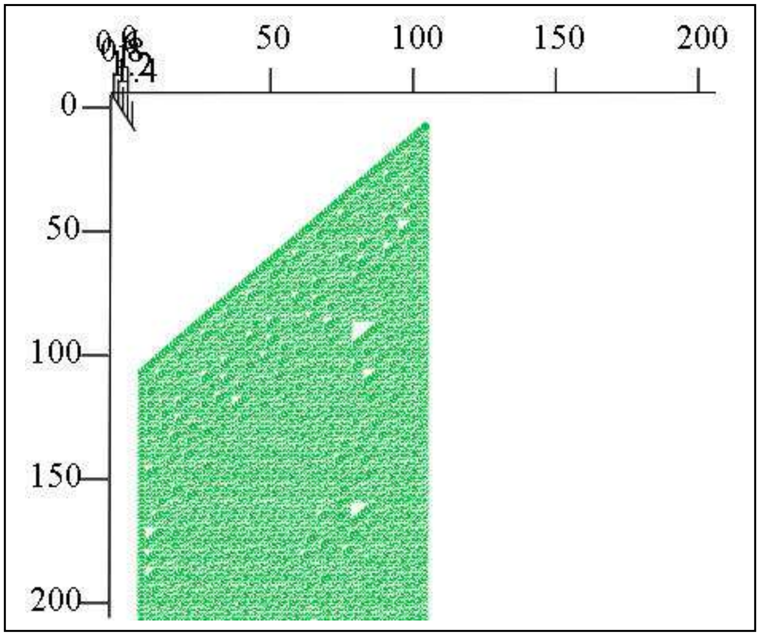

Figure 27

All these automata started from a single initial occupied cell #100. Some showed structure, others developed a random pattern even for the simplest of all initial conditions. One may wonder, if the structure survives random initial conditions, where several initial cells are randomly populated. The answer is that all considered automata show increased randomness. For the automata considered here, Rule#20 shows the most resilience, as might be expected from its simple pattern for each occupied cell. Automaton #90 retains some structure, if the random cells initially populated are not too dense.

A more detailed study of cellular automatons reveals that there are **4 classes of automata**:

- Class 1 reaches a homogeneous state (all cells free) after a few initial steps.
- Class 2 shows a periodic pattern after the first few steps, relatively independent of initial conditions.
- Class 3 develops into a chaotic pattern, independent of initial conditions.
- Class 4 produces a highly complex, nested fractal pattern.

In summary, we have seen that local microscopic interactions of coupled (non-linear) systems can lead to chaos or highly organized complex structure. Even though the underlying interactions are very simple, the outcome of multiple interactions cover the entire range from random independence to correlated self-organizing structures. The result for a given automaton does not dominantly depend on external influences but are due to peculiarities in the individual local interactions.