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Phase transition in cellular random Boolean nets

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Résumé. — Nous avons étudié par simulation sur ordinateur l'apparition de structures spatiales dans les cycles limites des réseaux aléatoires d'automates cellulaires Booléens. Ces mesures ont porté sur les périodes locales des automates comparées à la période globale du réseau et sur la percolation des structures oscillantes. Le seuil de percolation de ces structures est le même que celui observé par Derrida et Stauffer pour le comportement des distances entre configurations initialement différentes.

Abstract. — We have monitored by computer simulations quantities related to the spatial organization of random cellular Boolean nets during the limit cycles such as the local periods of automata, the global period of the whole net, and percolation of the oscillating structures, and shown that they obey a phase transition for the same value of the transition parameter as found by Derrida and Stauffer from overlaps between initially different configurations.

Random nets of Boolean automata have been proposed by Kauffman [1, 2] in 1969 as models for cell differentiation. Since then, their dynamical properties have been recognized as models for the properties of organization of complex biological [1-5] or physical [6] systems. They share some common features with spin glasses, but their structure is more general : interactions among units are non-symmetrical and more varied than in spin glasses. There exist no energy functions for Boolean automata, and their dynamics is thus more complex. From earlier studies two different regimes have been exhibited which depend upon the input connectivity K, i.e. the number of automata which directly influence the state of one automaton. For small connectivities (K=1 or 2) there exist a few limit cycles of short periods. For larger connectivities, very long periods (their size is exponential as compared to the number of automata) characterize a chaotic behaviour.

In addition to time organization during limit cycles, Boolean nets exhibit functional organization, best revealed by their cellular version. Cellular automata are arranged in a lattice (we shall deal here with square lattices) and connections are established among neighbours. Atlan *et al.* [3] worked with 2 input automata and reported the organization of independently oscillating clusters surrounded by fixed automata during the limit cycle. This functional organization, like time behaviour, has also two regimes which depend upon the selection of Boolean functions [3].

Instead of varying connectivity, Derrida and Stauffer [7] have proposed to study a square lattice of random Boolean automata, each automaton receiving inputs from its 4 nearest neighbours. The connectivity is thus constant and equal to 4. The transition between the two regimes is obtained by biasing the distribution of Boolean laws, by imposing a given internal homogeneity, a quantity first described by S. Kauffman [2]. The purpose of this paper is to study the spatial organization of the 4-inputs square lattice and to compare our results to those of reference [7] which concerns the evolution of overlaps. Definitions and properties of this model will be recalled in part 1 and local dynamics and its relation to the global dynamics of the net will be described in part 2. Part 3 is devoted to local properties averaged over several initial conditions and treats the problem of percolation [8] of oscillating clusters.

1. Definitions.

The system consists of a net of N spins σ_i which can take 2 possible values ($\sigma_i = 0$ or 1). Following common use in Computer Science they are from now on called automata. The time evolution of this system is given by

N Boolean functions of K variables each, randomly chosen among the $2^{(2^K)}$ inputs. K is called the input connectivity of the automaton.

$$\sigma_i^{(t+1)} = f_i\left(\sigma_{i_1}^{(t)}, \sigma_{i_2}^{(t)} \dots, \sigma_{i_K}^{(t)}\right) . \quad (1)$$

At each time step (from t to $t+1$), all the spins are simultaneously updated according to (1) (parallel iteration). In Kauffman's original model [1], for each automaton i the input automata $\sigma_{i_1}, \sigma_{i_2} \dots, \sigma_{i_K}$ are randomly chosen among the N automata. Cellular connectivity is a restriction of the randomness to the choice of the Boolean functions which allows a simpler interpretation of the dynamical interactions among spins. It has first been suggested in Atlan *et al.* [3] for $K = 2$. We use the square lattice with $K = 4$. Every automaton receives inputs from its 4 nearest neighbours (Derrida and Stauffer [7]). The edges of the lattice are connected to each other (periodic boundary conditions).

The system is defined once a function f_i and the input sites $i_1, i_2, \dots i_K$ have been chosen for each siste i of the net.

The dynamics of such a net is thus fully deterministic. Starting from any initial condition, since the system has only 2^N different configurations, after a time $t > 2^N$ the system must have been at least twice in the same configuration. It must then be periodic with a period T less or equal to 2^N. The set of configurations which occur between 2 consecutive occurrences of the same configuration (including this configuration) is a limit cycle. For different initial conditions, possibly different limit cycles are reached.

The dynamical properties of the model were studied by numerical simulations [1, 5]. Kauffman [1] reports that the period T of the limit cycles follows different regimes depending on K. For low K ($K = 1$ or 2), T increases as the square root of the number N of automata (to be called further frozen behaviour). For $K \geqslant 3$, T increases exponentially with N (chaotic behaviour).

In the 4 inputs square lattice model studied by Derrida and Stauffer [7], if all Boolean functions are sampled with a uniform probability, chaotic behaviour is observed as predicted by Kauffman for randomly connected nets. One can then bias the sampling of Boolean functions by deciding that the probability of function f_i to yield 1 for any input configuration is p, different from 0.5. Values of p close to 0 or 1 yield frozen behaviour. Because of the 0-1 symmetry, values of p symmetrical with respect to 0.5 give equivalent behaviours. For $p \simeq 0.26$ a phase transition between the two behaviours, frozen and chaotic, has been found by Derrida and Stauffer [7] for the square lattice. Their paper mainly concerns the convergence of initially different configurations. Two initial configurations are selected with a small given Hamming distance (the number of automata which are in a different state). For $p \leqslant 0.26$ after a large number of iteration steps, the Hamming distance remains small and proportional to the original distance. For $p \geqslant 0.26$ the Hamming distance evolves towards a non zero asymptotic value independent of the initial distance.

2. « Local and global » periods.

Local periods.

The first studies of cellular random nets have shown that not all automata of a network oscillate with the period of the limit cycle [3, 9]. Figure 1 shows that most of them oscillate with a smaller period, which is a divider of the period of the whole net, and that some are even stable during the limit cycle. The results are given for two 24*24 lattices differing only in the concentration p of the number of ones in the functions f_i. The numbers for each lattice site or automaton give the period observed for this site, with three stars *** indicating a period larger than the maximum observable in these runs (999). We see quite clearly that for $p = 0.2$ we have many finite clusters with finite periods, which we associate with the frozen regime, whereas for $p = 0.3$ one cluster of « stars » (chaotic sites) is percolating throughout the sample. Figure 2 indicates the fractal structure close to the phase transition.

In the frozen phase, the system splits into many dynamic clusters, as seen already in the above figure for $p = 0.2$. Each cluster is defined as a group of neighbouring sites with periods larger than unity. In general one cluster contains sites of different periods. The period of one cluster can be identified as the lowest common multiple of the periods of the single cluster sites ; usually it agrees with the largest period observed for any site in the cluster. The period T of the whole lattice then is the smallest common multiple of the cluster periods observed in this lattice. Figure 3 shows more quantitatively the distribution of limit cycle periods in the frozen phase, combined with the periods observed for the single sites. We see that only a rather limited number of times T in the observed interval are actually reached.

In the chaotic phase one has a large percolating cluster of sites with « infinite » period (for large lattices), surrounding islands of small periods.

Of course, one can also average the local finite periods on the whole lattice. These single-site periods scatter widely according to the site, to the net and to the initial configuration, and different moments of the period distribution thus may be described by different critical exponents. Figure 4 shows semiquantitative results for the average period and the rms average period ; both seem to have a divergence or cusp at about $p = 1/4$, consistent with our other critical concentrations.

Global periods.

We have investigated the variation of the global period with the size of the net for both regimes.

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 1  1  1  1 24 24 24 24  1  1  2  1  1  1  4  1  4  1  4  4  4  1  4  1
 1  1  1  1 24 24 24 24 24 24  2  1  1  1  1  1  1  1  1  1  1  1  1  1
 1  1  1  1  1 24 24  1  1  1  1  1  1  4  4  4  1  1  1  1  1  1  1  1
 1  1  3  1 24 24 24 24  1  1  1 36 36  4  1  1  1  1  1  1  1  1  1  4
 1  3  3  3  3  1 24  1  1  1  1  1 36  1  1  1  1  1  1  1  1  1  1  4
 1  1  3  3  3  3  1  1  1  1  1 36 36 36  1  1  1  1  1  1  1  1  1  8
 8  1  1  1  1  1  1  1  1  1  1 36 36 36 36  1  6  6  6  1  1  1  1  1
 4  1  1  1  4  1  4  4  1  1  1 36 36  1 36  1  1  6  6  1  1  1  1  4
 2  1  1  1  4  1  4  1  1  1  1 36 36 36 36  1  6  6  1  1  1  4  1  4
 1  1  1  1  1  1 12 12 12  6  1 36 36 36  1  1  1  1  1  1  1  4  1  4
 4  1  1  1  1  1 12  6  6  6  1  1  6 36  1  1  1  1  1  1  1  1  4  4
 1  1  1  1  1  1  1  1  1  1  6  6  6  6  1  1  1  1  1  1  1  1  4  1
 1  2  2  1  1  1  1 20  1  1  1  1  1  1  4  4  4  1  1  1  1  1  1  1
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 4  1  2  2  1  1 20 10 20 20  1  1  1  1  1  1  1  1  1  1  1  1  1  4
 1  2  2  1  1  1  1  1 20 10  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 1  1  1 12 12  1  4  1 10  2  2  1  1  1  1  1  1  1  1  1  1  1  1  1
 1  1  1  6  6 12  4  2  1  1  4  4  1  1  1  1  1  1  1  1  1  1  1  1
 1  1  1  1  1  1  1  2  1  1  1  4  1  1  1  1  1  4  1  1  1  1  1  1
 1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  4  4  1  4  1  1  1
 1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  4  1  1  1  4  4  1  1  1
 1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  2  4  4  1  1  4  1  1  1  4
 4  1  1  1  1  1  1  1  1  1  1  1  1  1  2  4  1  4  1  4  1  1  4  4
 1  1  1  1 24  1  1  1  1  1  1  1  1  1  4  4  4  4  4  2  1  1  4  1
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a)

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  1  1  4  2***************  1  1  1  4  4  1  8  1  1  1  1  1  1  1  1
  1 12 12  4  1  1  1  1  1  1  1  1  4  4  4  8  1  1  2  1  1  1  1  1
  3  3  1  4  4  1  1  1  1  1  1  1  4  4  4  1  1  1  2  1  1  1  1  1
***  3  1***  1*************  1  1  1  4  4  1***  1  1  1  1  1  1  1  1
***  3  1**********************  1  1  4  4  4*********  1  1  1  1  4***
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  1  1**********************************************************  1  1  1
  1  1************************************************************  1
  1  1  1***  1  1  1****************************************  1  1  1  4
  4  1  1  1  1  1  4****************************************  1  1  1  1
  4  1  1  1  2  2  4**********************************  1  1  1  1  1
  1  1  1  1  2  1  1************************  1  1  1  1  1  1  1  1  1
  1  1  1  1  1  1  1*********  1  1  1  1  1  1  1  1  1  1  1  1  1  1
  1  1  1  1  1  1  1*********  1  1  1  1  1  8  8  1  1  1  1  1  1  1
  1  1  1  1  1  1  1*********  1  1  1  1  4  8  8  1  1  1  1  1  1  1
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b)

Fig. 1. — Examples of local periods in 24*24 square lattices at $p = 0.2$ (top) and 0.3 (bottom). The numbers on each lattice site give the period of the site observed between 500 and 1 500 iterations with one initial configuration ; thus a 1 means that the automaton did not change at all during the limit cycle and three stars give a period larger than 999 (too large to be observed). (p is the probability that the output of function f_i is 1 for any input configuration.)

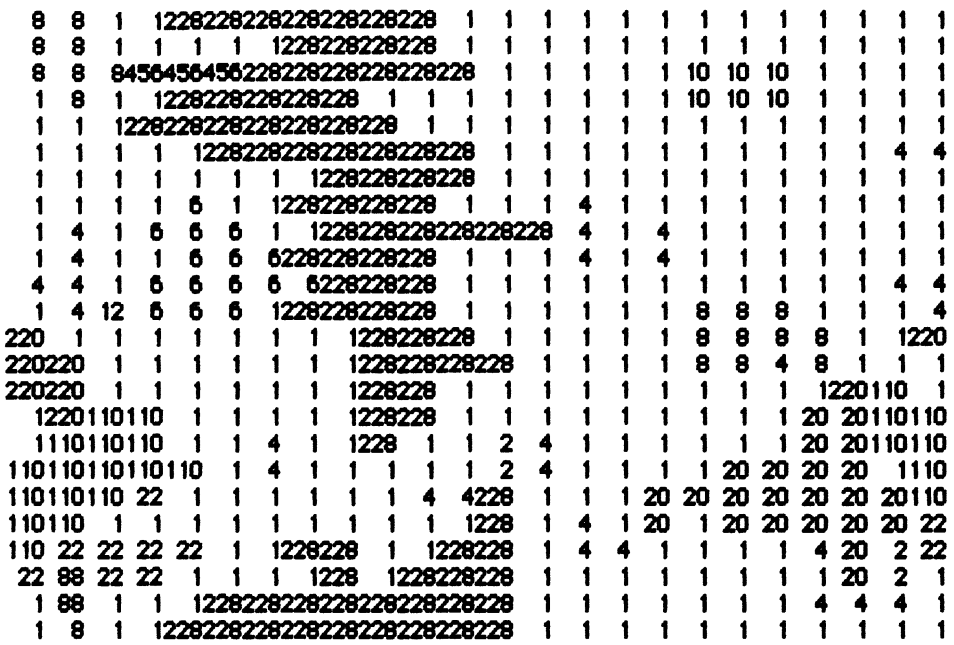


Fig. 2. — Local periods of a particularly complicated 24*24 sample net at $p = 0.23$, with two large clusters of period 456 and 440, and a lattice period $T = 25080$.

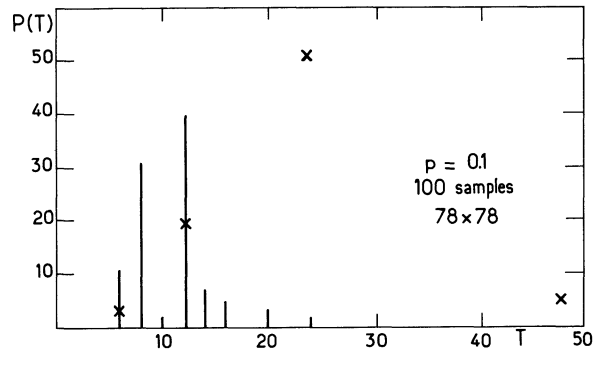


Fig. 3. — Histogram of the distribution of maximum periods for the single sites in the frozen phase. The four crosses denote the periods observed for the lattice as a whole.

For the chaotic phase, the periods of the limit cycles are very large, and thus one can investigate in this case only rather small lattices. For a finite lattice with $N = L*L$ sites, we have only 2^N possible configurations and thus after at most 2^N time steps we must have reached a limit cycle with a period not exceeding 2^N. Actually, the observed periods are much smaller, as shown in figure 5 : even for the strongest disorder, $p = 1/2$, we do not observe an increase as 2^N. In fact, Kauffman [2] predicted for randomly connected nets an increase as $2^{0.37\,N}/2$ for $K = 4$ and $p = 1/2$, which is compatible with our data. Closer to the phase transition the increase of the period T with system size N is weaker.

On the other side of the phase transition, in the frozen phase, the period is no longer exponential, as shown in figure 6. Because the periods are widely scattered, depending upon the net and the intial conditions, we usually plotted in figures 5 and 6 the « median » time t defined such that half of the observed times are larger, and half are smaller than this median value. (We produced usually 50 to 100 samples.) This

Table I. — *Summary of the differences between the frozen and the chaotic regime. The transition between the two regimes occurs for* $p = 0.26$. *The results concerning the convergence of configurations were obtained in reference* [7].

Behaviours	Frozen regime	Chaotic regime
Periods	Small	Large
Size dependence	Polynomial or logarithmic	Exponential
Oscillating clusters	Isolated	Percolating
Ratio of global over largest local period	Large (LCM)	Small, near 1
Convergence of different initial configurations	Small final distance close to initial distance	Finite final distance independent of initial distance

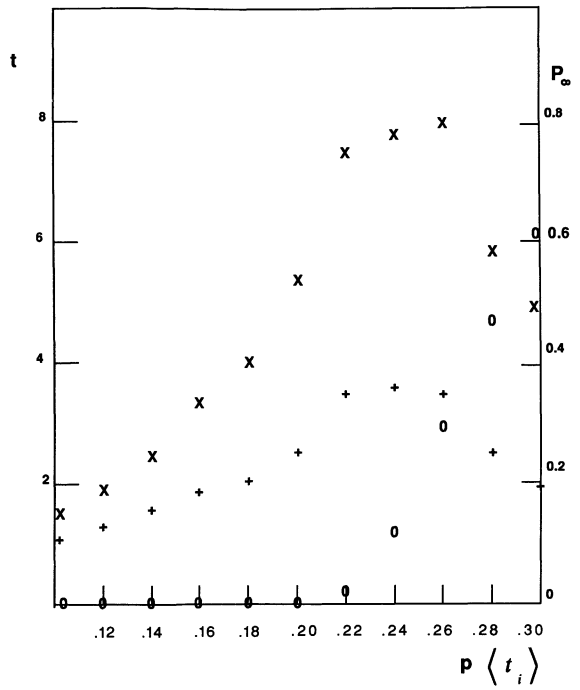


Fig. 4. — Variation of the average local period $\langle t_i \rangle$ (+), the r.m.s. period $\sqrt{\langle t_i^2 \rangle}$ (×) and the fraction P_∞ (0) of chaostic sites in a 60*60 lattice as function of p, observed over 400 time steps. (infinite periods are ignored in averaging).

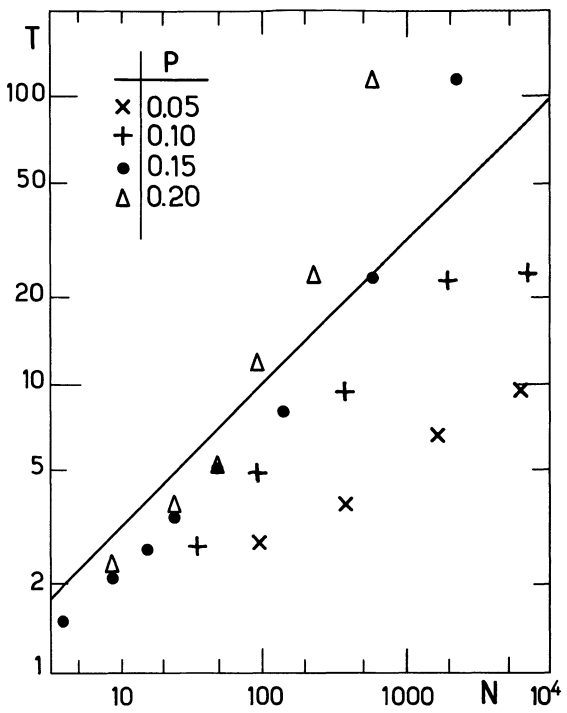


Fig. 6. — Median periods of lattice limit cycles in the frozen phase for much larger systems. In contrast to figure 5 this is a log-log plot. The straight line corresponds to $T = \sqrt{N}$, proposed by S. Kauffman [1] for $K = 2$ automata.

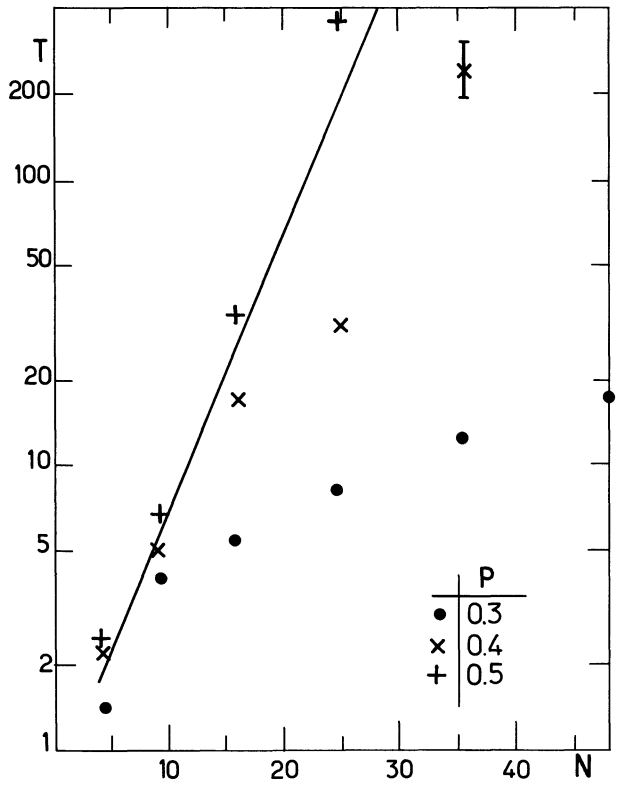


Fig. 5. — Median periods of lattice limit cycles in the chaotic phase, as function of the lattice size $N = L*L$, for different value of p. The straight line correspond to $T = 2^{0.37N}/2$, as predicted by Kauffman [2] for $p = 0.5$ for random nets.

definition is particularly useful for those cases, where for a small fraction of samples the period T was too long to be found within the finite observation time. However, while it works nicely in the chaotic phase where many different periods occur, its use for the frozen phase produces systematic errors when there are large gaps between the different observed values of the period (see again Fig. 3).

For p far below the percolation threshold we observed limit cycles even for rather large lattices. Most of seven 608*608 lattices had a period of 12 at $p = 0.05$. 14 samples of size 250*250 were found to give periods of 12 (once), 24 (7 times), 48 (once), and 120 (three times) for their limit cycles of the whole lattice at $p = 0.1$; the time to get into these limit cycles is of the same order of magnitude. For 250*250 lattices, even at $p = 0.15$ we could observe periods below 1 000.

(In percolation theory [8], the number of very large clusters for a fixed lattice size decreases exponentially with cluster size ; thus the size of the largest finite cluster increases logarithmically with lattice size. If this logarithmic law would be valid also for the Kauffman clusters, and if the typical cluster period increases exponentially (or with a power law) with cluster size, then the period of the largest cluster in the frozen phase would increase with a power law (or logarithmically) with the lattice size. We can also expect such a scaling law for the period of the whole lattice.)

One can also notice a difference in behaviour with

the ratio between the limit cycle period of the whole lattice and the largest period found for a single site. In the frozen phase the period of the whole lattice is appreciably larger than the largest period observed for a single site (see again Fig. 3), except for small lattices. This ratio becomes even larger when we get closer to the phase transition. In the chaotic regime one observes usually one large cluster, with most of its sites having the same period as tested on small nets ; this cluster is coexisting with a minority of sites of period usually one, i.e. of fixed sites. The ratio of lattice period to largest period of single sites is then nearly always unity, for not too large lattices and not too close to the phase transition.

Remarks about clusters.

The problems in evaluating the size dependence of T in the frozen phase might be circumvented by a detailed investigation of the average number of clusters with a given period, analogous to the average number of clusters with a given number of sites in percolation theory. However, even then there are problems, as shown by the 24*24 example ($p = 0.23$) of figure 2. Large clusters usually consist of sites having different periods. If two neighbouring sites have different periods, one of them usually is an integer multiple of the other. Therefore most clusters have a period equal to the maximum period of its sites. However, exceptions exist. Near the lower right corner of figure 2 we see a period 22 directly between a period 20, and the whole cluster (split by the helical boundary conditions into a left and a right part in the figure) has a period of 440, twice as large as the largest period of any of its sites. Apparently the functions f_i for these two sites are accidentally chosen such that they do not feel each other's influence. The other large cluster, mostly with site period 228, behaves more regular : three sites do indeed have the cluster period of 456. We have also observed other examples, where the cluster period was larger than the maximum period of its sites ; but those examples are rather rare.

It is also possible that geometrically one seems to have one connected cluster whereas dynamically it is split into several parts such that at all boundaries the sites of one part do not notice, *via* the function f_i, the status of the neighbouring sites of the other part. In this case the dynamic cluster structure could be investigated by randomly flipping a very small but finite fraction of the sites. The influence of this perturbation would be restricted to the dynamically connected parts of the cluster, which might be smaller than the geometrical cluster observed in our figures. The « susceptibility » investigated in reference [7] then might be related to the second moment of this dynamically corrected cluster size distribution. The fact that these authors observed about the same threshold concentration p_{over} suggests that the influence of these complication on p_{over} is much less drastic than the increase in computer time which their careful investigation would require.

3. Cores and clusters.

Instead of studying the behaviour of the net during one limit cycle, one can try to summarize information concerning different initial conditions. Figure 7 is such an example. It is an histogram which indicates for how many initial conditions (out of 9) each automaton of a square lattice has been oscillating at least once during a limit cycle. Blanks correspond to nodes which do not oscillate during any of these limit cycles (their set has been called the stable core by Fogelman-Soulié [9]). This set represents in fact the invariant part of the net under the different initial conditions. When the complement of the stable core is made of disconnected parts like in figure 7a, these clusters are functionally independent since no information is carried across the stable core. In this case we can expect :

— Short periods because the independent clusters are smaller than the complete net.

— A strong convergence of configurations. Large overlaps between configurations can be expected in the case of disconnected clusters since all the automata belonging to the stable core are already in the same state. The transition between the two behaviours occurs for a critical $p_{over} = 0.26 \pm 0.02$ as reported in reference [7].

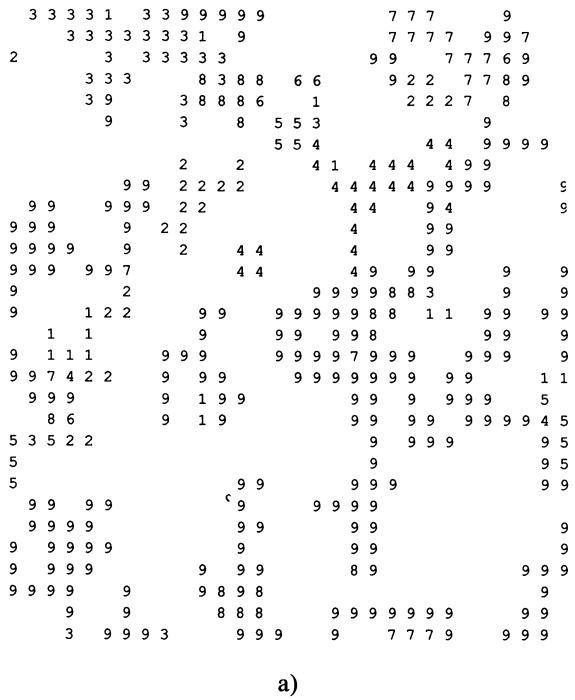
We have then investigated the probability that the complementary set of the stable core percolates through the lattice as a function of p and compared this percolation threshold p_{per} with p_{over}. We studied nets of size 10*10, 20*20, 30*30, 50*50, 70*70 and 100*100 by computer simulations. The histograms of oscillation were drawn for 10 initial conditions and the percolation of the oscillating set was tested. Figure 8 shows a typical plot of the probability of percolation as a function of p for 10*10 and 100*100 lattices (each dot corresponds to the simulation of 40 lattices). A threshold is reached when half the samples percolate. Figure 9 summarizes the results according to the size of the net. The size effects corresponding to the shift of the percolation threshold are small as compared to the error bars and we can conclude that the percolation threshold p_{per} is the same as p_{over} the threshold for the overlaps given in reference [7].

$$p_{per} = 0.26$$

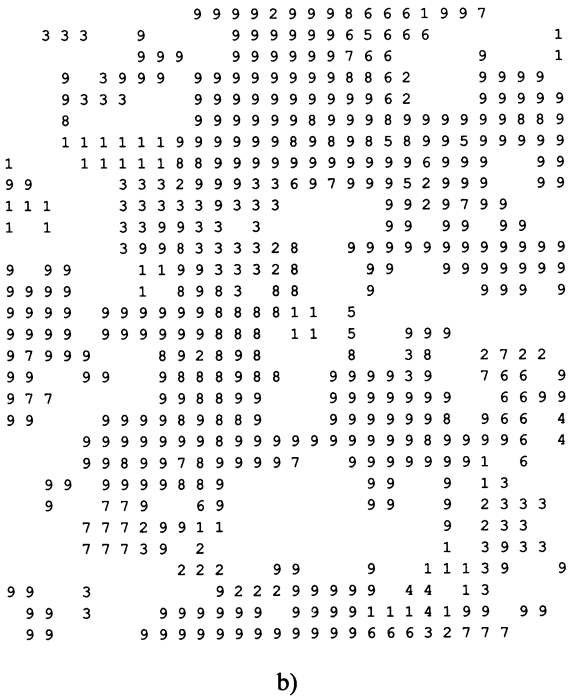
with a statistical error of about 0.01.

4. Conclusions.

The table summarizes the differences between the two regimes, frozen and chaotic. Further progress would involve considering three-dimensional nets, the measurements of the scaling laws governing the local and global periods, and the clusters' sizes in the vicinity of the phase transition. This would involve a lot of



a)



b)

Fig. 7. — Histograms of local oscillating behaviours for 9 different initial conditions for the same net. Each figure represent for how many initial conditions each site oscillates during the limit cycle. In order to facilitate the visualization of percolation of oscillating structures the zeroes have been replaced by blanks. The upper histogram corresponds to $p = 0.21$ and shows non percolating structures. The lower is for $p = 0.28$; the set of sometimes oscillating nodes percolates through the sample.

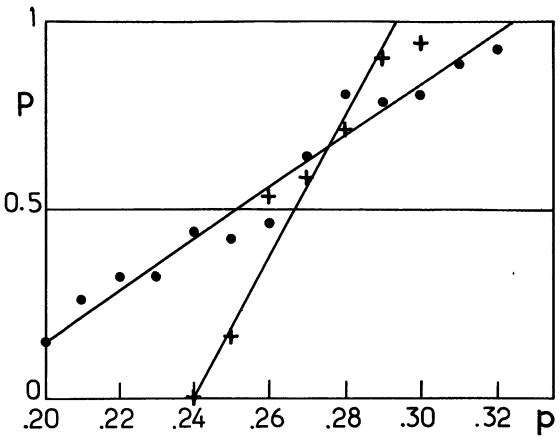


Fig. 8. — Probability of percolation of the set of oscillating nodes as a function of p, the probability of 1 as output of the f_i functions. Dots correspond to 10*10 nets and crosses to 100*100 nets.

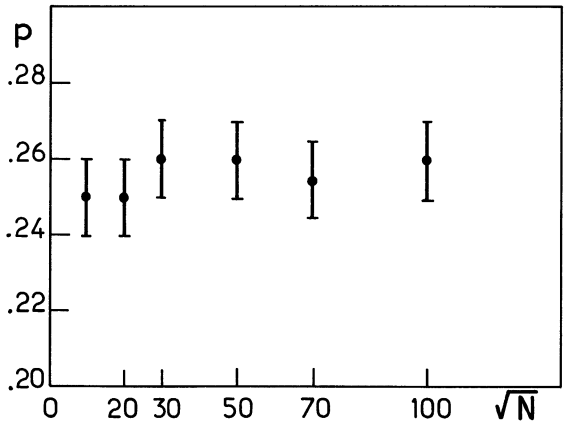


Fig. 9. — Size effects for the percolation threshold of the set of oscillating nodes. N is the number of automata of the net.

computer time. Other properties of interest include the possible existence of large attraction basins the size of which remains a finite fraction of the configuration space when N goes to infinity as in Derida and Flyvbjerg [6]. Finally a possible theoretical determination of p_{per} is to use the forcing structure approach of Fogelman-Soulié [9].

Acknowledgments.

We acknowledge discussions with S. Roux and H. J. Herrmann. Special thanks are due to B. Derrida for suggestions and interest in this work.

Appendix.

NUMERICAL TECHNIQUES. — In our Fortran program we tried to allow the simulation of relatively large systems with moderate computer memory, and to use algorithms which can be easily vectorized. The trivial method of storing each of the 16 possible functions f_i (depending on the configurations of the four neigh-

bours) for each site $i = 1, 2, ..., N$ in a separate computer word does not only require a large memory of $16*N$ words but also hinders vectorization since it now needs a « gather » operation. Instead, we stored these 16 function values for each site in one « integer » word 15, utilizing the 16 least significant bits only. The four neighbours $i + 1, i - 1, i + L$, and $i - L$ of site i in the $L*L$ square lattice give the position KA of the bit where the function value f_i for this particular neighbour configuration is stored. For parallel iteration the state of each automaton has to be kept in memory until all automata are updated to their new value and two state vectors, IS (i) the present state and ISN (i) the next one, are necessary. If LAW (i) stores the 16 bits of the function f_i, then the central loop with $i = 1, ..., N$ looks like

KA = IS ($i - 1$) + 2*IS ($i + 1$) + + 4*IS ($i + L$) + 8*IS ($i + L$)

ISN (i) = Shift (LAW (i), − KA) and 1

Here « Shift(IWORD, IBIT) » shifts the computer word IWORD by IBIT bits to the left (IBIT>0) or right (IBIT<0), and « and » is the Boolean bit-by-bit AND operation, which in the present application simply extracts the least significant bit. We used helical boundary conditions : the first L automata are connected to the last L automata.

For our largest systems (608*608) instead we worked with techniques very similar to multi-spin coding in Ising magnets : Each site occupied only one bit in the state arrays IS and ISN ; thus each array required only $N/32$ words of 32 bits each. The functions f_i were stored in LAW with two indices, the first going from 1 to $N/32$ to cover all sites, the second from 1 to 16 to denote the possible neighbor configurations. In this way every bit of memory is utilized but easy vectorization is lost.

Our computer simulations took 10^3 hours on several Macintosh microcomputers.

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