Journal of Statistical Physics, Vol. 55, Nos. 1/2, 1989

The Effect of Screening on Entropy Production in Pattern Formation

J. H. Kaufman,[1] O. R. Melroy,[1] and G. M. Dimino[1,2]

Received August 30, 1988; revision received November 29, 1988

Information theory is used to study the effects of screening on the rate of entropy production during pattern formation. Screening is an effect where the outermost parts of a growing fractal pattern influence the growth probability at interior sites. The results demonstrate that a state of maximum entropy production does exist for dynamical systems which generate patterns based on simple screening rules alone. This state corresponds to a critical point where the pattern exhibits self-similarity and fractal properties typical of random aggregates. Scaling occurs because the screening transmits information from the smallest to the largest scales of the system.

KEY WORDS: Pattern formation; fractals; information theory; entropy production; critical phenomena.

Recently, considerable effort has been directed toward the study of random fractals, whose static and dynamic properties scale with various exponents.[1,2] Experimental studies have demonstrated that real random fractals can be prepared in a variety of ways.[3-5] Many of these experiments (e.g., dielectric breakdown, diffusion-limited electrochemical deposition) suggest that the formation of fractals occurs when the dynamical system responsible for the pattern formation is at a critical point.[3-7]

In a recent letter, Bak *et al.*[8] demonstrated that many self-organized extended dynamical systems naturally evolve toward a critical state where the variables of the system begin to scale. Scaling represents a transmission of information from the smallest to the largest scale of the system. Furthermore, the rate of information produced by Bak's model system seems to

[1] BM Almaden Research Center, San Jose, California 95120-6099.

[2] Department of Physics, University of California at Santa Cruz, Santa Cruz, California 95064.

0022-4715/89/0400-0331$06.00/0

increase as the system approaches criticality. This contrasts with the suggestion of Prigogine that for self-organizing open systems in a steady state (e.g., of flow) one can apply a principle of minimum entropy production.[9] Important examples where Prigogine's principle may apply include living organisms which develop into highly ordered states that are stable for extended periods of time. The principle of minimum entropy production is valid for systems "not far from equilibrium,"[9] whereas Bak's sand dune constantly produces configurations on the brink of collapse. One might expect that Bak's system evolves to a state of *maximum* entropy production, since the growth is ruled by fluctuations (sand is added to the dune at random sites).

In an attempt to answer these questions for a simple dynamical system, we chose to study a primitive system which generates spatial patterns constrained only by connectivity and screening. Screening is an effect where the outermost parts of a growing fractal pattern influence the growth probability at interior sites. This property is common to many processes involving random aggregation. As the strength of the screening is varied, the rate of entropy production and the geometry of the spatial pattern will change. For each pattern, we use information theory to measure the rate of entropy production. The model is not intended to mimic any particular process; the intent is to determine if random fractals are produced at a critical point, to find the relative rate of entropy production, and to gain an intuitive understanding of the origin of scaling in such patterns.

To understand how loss of information (as particles are added) corresponds to entropy production in pattern formation, it is convenient to consider a process which adds points to a plane at random. This models, for example, a totally inept dart thrower. The information produced by the system is the final location of each dart thrown. If multiple darts can occupy the same site, the expectation of where the next dart will land is completely flat. This corresponds to a maximum production of entropy. If darts are constrained to one per site, then every dart which hits the plane also destroys information or possibilities for future darts to land. The maximum state of entropy production, given some set of constraints, is that process which destroys information at a minimum rate.[10,11]

A typical growing system adds new particles adjacent to existing parts of the pattern.[1,3–5] At any instant in time the possible locations for growth are limited to some subset of the surface area of the pattern. The pattern of maximum total surface area is not necessarily the maximum entropy producer. For example, on a square lattice, the maximum surface area is produced by growth in a straight line. For every site (possibility) destroyed by adding a point to the end of the line, the net surface area is increased by two. Any other operation produces new surface area at a slower rate. However, if one constrains growth to a straight line, never using vacancies on the sides, then the "active area" (the area where growth is permitted) is constant, as is the rate of information production and destruction. We expect the next point to be added at one of the two tips. Knowledge of both the "active area" and total surface area are necessary to determine the rate of entropy production of a growing pattern.

The relationship between the change in total and active area and the entropy follows from the information theory of a discrete noiseless system.[11] If P_{ji} is the probability that symbol r_j will be received, given that symbol(s) r_i have been received, then the unpredictability of a sequence of symbols is $-\sum_j P_{ji} \log P_{ji}$. The average information produced is this quantity weighted by the average probability P_i of the state i.[11,12] For pattern formation, the change in information on adding a particle to the system is the change in possible locations for future growth. For a particular labeled pattern (state i), let $P_{ji} = dA^{\text{act}}/dN$ denote the probability that site a_j will become active given the shape of the pattern (sites a_i are occupied). By analogy, the unpredictability is $-\sum_j P_{ji} \log P_{ji}$. Weighting the unpredictability by the average probability $P_i = dA^{\text{tot}}/dN$ of the particular pattern i, the change in entropy is $-\sum_{ij} P_i P_{ji} \log P_{ji}$ (where the sum is taken over every possible pattern at every stage in its growth). Obviously, it is not practical to take this sum even if the patterns are constrained to be finite subsystems of a finite medium. However, if the surface area and the active area both scale, then the corresponding probabilities for very large patterns (all of size N) will not vary much between patterns of the same fractal dimension. Such scaling also implies that the change in area $A = N^x$ per particle added tends to $dA/dN = A/N$ for large N. If there exist a value of the fractal dimension for which the number of distinct ways to grow is a maximum for every N, then the number of possible patterns will also be a maximum at that fractal dimension. Self-averaging of this kind would allow one to compare the number of choices open to particular patterns of different fractal dimension without summing over many configurations. The change in entropy δS per particle added is then given by the approximate relation

$$\delta S = -(A^{\text{tot}}/N)(A^{\text{act}}/N) \log(A^{\text{act}}/N) \tag{1}$$

where A^{act}, the number of active sites, and A^{tot}, the total surface area, both scale with N to some fractal dimension. N is the area occupied by the pattern.

It is not obvious from Eq. (1) that a unique solution exists which maximizes the entropy production. If, for example, the entropy scaled with the fractal dimension, then the pattern which maximizes δS would depend on the value of N. To see how the entropy production is influenced by the geometry of the pattern, it is useful to examine two limiting cases: the filled circle and the straight line. In the case of the circle, A^{act}/N and A^{tot}/N are identical. They both scale as $N^{-0.5}$. The rate of entropy production, from Eq. (1), is proportional to $(1/N) \log N$. For a straight line, A^{tot}/N is constant (two), while A^{act}/N scales as N^{-1}. The rate of entropy production is again proportional to $(1/N) \log N$. For all values of the fractal dimension d the total surface area per particle added scales as $N^{(1/d)}/N$. If A^{act}/N scales as $N^{(1-1/d)}/N$, the entropy production does not scale with d, and is proportional to $(1-1/d)(1/N) \log N$ for all values of N and d. The relative rate of entropy production then depends only on the fractal dimension and the appropriate prefactors of the area terms (which may themselves be functions of d) and is independent of the value of N. To test the validity of these relations, and to find the maximum state of entropy production (if it exists), it is necessary to produce patterns with various scaling properties.

Clearly, connectivity alone will only generate compact structures. The scaling properties can be varied by an additional constraint, namely screening. Screening is an important factor in the formation of random fractals.[1,6,7] In our model, a primitive definition of screening is used. The degree to which a point on a pattern is "unscreened" is determined by the solid angle in which that point "sees" the outside world. To investigate this phenomenon, a two-dimensional simulation is used where growth occurs at nearest neighbor sites on a square lattice. A particular surface area site is "active" if it is unscreened above some minimum solid angle threshold. While this screening constraint is simplistic, it elucidates the physics essential to answering the questions posed above. We will motivate the choice of a step function later. The simulation is performed for thresholds between 0 and 300 deg, for 50,000 points, or until the pattern reaches the border of a 1000×1000 grid. All active sites have equal probability, and the next growth site is chosen at random from a list of active locations. The initial condition was a cross of five particles centered on the grid. Each growth event can add new active area sites. After each growth event, every active site was checked to see if the addition of the new point reduced the unscreened angle below the threshold. If so, the screened site was removed from the active list.

Patterns obtained for various screening conditions are shown in Fig. 1. For small thresholds, the screening condition is weak and compact structures with small holes are formed. As the minimum unscreened angle is increased, the holes increase in size until holes as large as the pattern radius form. At this point the pattern is made up of numerous thick branches. Larger screening angles result in thinning of the branches. Eventually,

(a) (b) (c) (d)

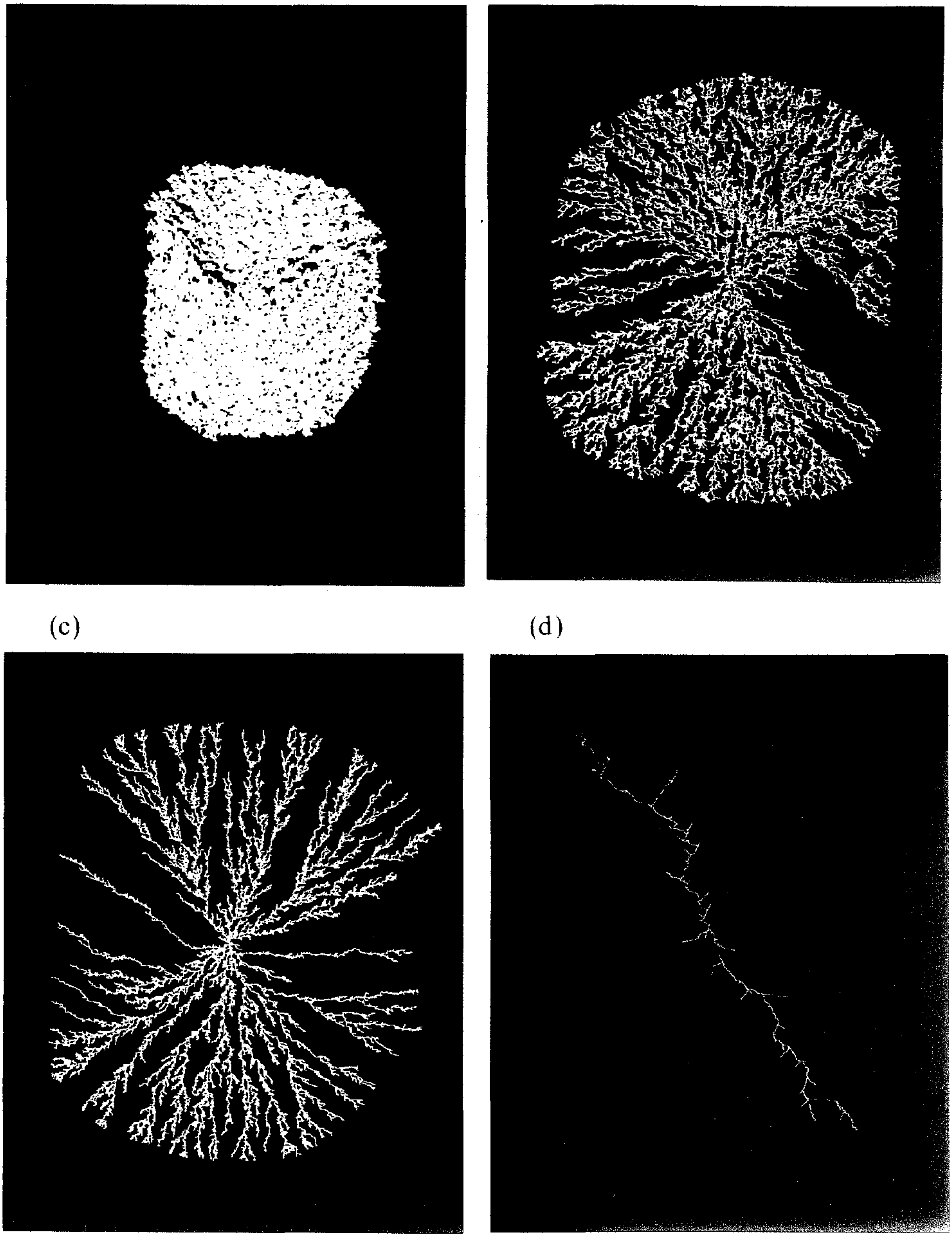

Fig. 1. The pattern formed at unscreened thresholds of (a) 60, (b) 125, (c) 140, and (d) 220 deg. Part (b) is near the threshold for the maximum rate of entropy production.

branches begin to screen themselves. Above 200 deg., patterns with fractal dimension near one are formed. Short branches form at the ends of these linear patterns, but as the tips advance the branches quickly become screened.

For each pattern, the active surface area and the total surface area were measured. The active area was indeed found to scale as $N^{(1-1/d)}$. The compact structures (small angles) had the lowest total surface area, but the highest active area, as expected. All of the surface sites on a filled circle are active. However, the final pattern is independent of the order in which the perimeter is filled in. Large screening angles result in the highest total surface area and smallest active area, as discussed above.

The minimum solid angle specified for each pattern corresponds only to the threshold above which surface area sites are active. There exists a distribution of unscreened angles (above the threshold) corresponding to the state of each active area site when it was chosen for growth. To determine the mean unscreened angle, this distribution was measured for each pattern and fit to a Gaussian. At low angles, the distributions were fairly broad. For example, at a threshold of 40 deg., the FWHM was 100 deg. This narrowed to a minimum of 32 deg. at a 160 deg. threshold.

It is possible to calculate the rate of entropy production of the various patterns from the measured active and total surface areas using Eq. (1). The results for $N = 50{,}000$ are shown in Fig. 2a. The data are plotted as a function of the mean unscreened angle $\langle \theta \rangle$ instead of the designated threshold, in order to compare consistently the current simulation to more realistic processes (see below). The maximum rate of entropy production occurs at a mean unscreened angle of about 160 deg. (Fig. 1b). The fractal dimension for each pattern was computed from the two-dimensional autocorrelation and is plotted in Fig. 2b. It is clear from the data in Fig. 2 that a peak in entropy production does occur. It corresponds to a critical point in the screening condition where the patterns become self-similar random fractals. It is evident from Fig. 2b that a phase transition between compact and one-dimensional structures occurs at this point.

To the extent that the growth of the compact and one-dimensional patterns is more stable with respect to variations in the screening constraint, one might consider the steady-state growth of compact or 1D patterns to be "closer to equilibrium" than the growth of a fractal pattern. That these patterns produce entropy more slowly than the fractals is consistent with Prigogine's minimum entropy principle. This observation does not prove that principle in a general sense. In fact, Landauer[13] proved that while many open systems (which satisfy the "not-far-form equilibrium" condition) evolve to ordered states, they are extremely sensitive to fluctuations. In particular, the lifetime of the ordered state can depend quite sensitively on the history of the system as it developed. It is interesting to consider the two "more stable" pattern geometries our system is capable of producing. Both the compact patterns and the one-dimensional patterns produce entropy more slowly than the fractals which form at the critical point. Of the two, the compact geometry produces slightly more entropy than the 1D case. This is evident in Fig. 1a, or if one simply considers the limits of filling in an area or growing in a straight line. Linear growth never produces more than two options. Is it meaningful to consider the stability of these two limits? Certainly one could conceive an automata to produce 1D and 2D patterns of arbitrarily large size. However, for all of our patterns, though self-consistent, the choice of the location for the next growth

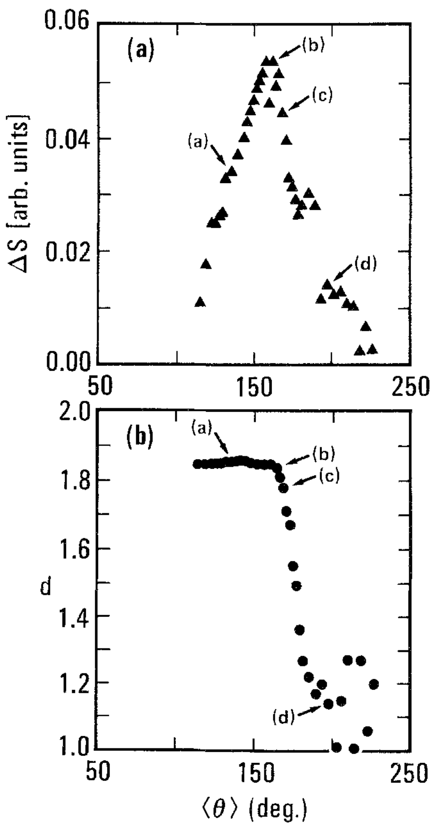

Fig. 2. (a) The rate of entropy production and (b) the fractal dimension, as a function of the mean unscreened angle. For every threshold angle there is a distribution of unscreened angles above threshold where the pattern grows (see text). The arrows indicate where the patterns in Fig. 1a–1d fit on these data.

event is determined by fluctuations (a random number generator). These fluctuations put no limit on the size of the compact (or the fractal) patterns, but they can limit the lifetime of the lower entropy 1D state. At very large values of the screening angle thresholds, there is a finite probability that a linear pattern will "die" (i.e., it can grow to a configuration with zero active area sites available for future growth, without violating its screening constraint). To study completely the kinetics of this process—what fraction of the patterns eventually die and on what time scale?—it is necessary to generate a large number of patterns at each screening threshold. This work is in progress and will be reported in a future publication. However, it is already evident that the only states of our system which die are the states of lowest entropy production. These states (the 1D patterns) are the most sensitive to the fluctuations which occur during growth.

An increase in the statistical error is evident above the 200 deg. screening threshold in Fig. 2. This occurs because there are fewer points in those patterns. For large screening thresholds, the pattern becomes essentially one dimensional and a pattern of 50,000 points will not fit on a 1000×1000 grid. For screening thresholds above 260 deg., the rate of destruction of active growth sites can exceed the rate of production of new ways to grow. As a result of this information loss, it is possible for such patterns to cease growing after only a few thousand points. For these patterns it was simple to extrapolate the active and total surface areas to 50,000 points, because the active area was constant and the total area was linear.

The patterns formed at the critical point in Fig. 1 are similar to the fractals observed in random aggregation experiments. In fact, the information theory applied to our patterns is meaningful for other processes. In a diffusion-limited aggregation (DLA) simulation, for example, one can measure the unscreened angles of (active) area sites when they are chosen for growth. The average of the resulting distribution for a DLA simulation of 10,000 points is 160 deg. with a FWHM of about 75 deg. This distribution, when integrated and normalized to the distribution for total area sites, yields the "activity" probability as a function of screening angle for DLA. The probability of being active rises smoothly from zero to one at about 160 deg. The transition is not a step function (used in our simulation). It has a width of ± 30 deg. The rate of entropy production of DLA at 10,000 points was 30% higher than the maximum entropy production in our simulation for patterns of the same size.

Several analogies can be drawn between the critical screening condition and other critical phenomena such as percolation. In particular, the distance to the farthest screening point diverges at the critical point, as does the range of the correlations in the case of percolation. It is evident from Fig. 1b that the separation of the most remote screening point from the site it screens is on the order of the largest hole in the pattern. When the holes grow to the pattern radius (Fig. 2b) this separation diverges with the radius of the pattern. While the influence of a remote screening point will decay with distance, the location of every point on the pattern stores information which determines the activity of every area site. As in the case of other critical phenomena, the exact screening angle where scaling occurs may depend on the size of the system. We intend to study finite-size effects in the future.

In conclusion, we have used information theory to study pattern formation governed only by connectivity and screening. As the screening constraint is made more severe, the pattern changes from compact to that of a random fractal and eventually to a one-dimensional structure. The rate of entropy production is found to reach a maximum at a screening angle near that observed in a true DLA simulation. At this point the pattern exhibits self-similarity and scaling. The only mechanism in our simulation which can transmit information from the smallest scales to the scales of the system is screening. While many critical phenomenon do not involve screening, it is characteristic of virtually all real dynamical systems which produce random fractal patterns. It is not unreasonable that in those systems the scaling is a consequence of the screening constraint on the pattern formation. Intuitively, the scaling occurs because the addition of a single particle (an operation on the smallest possible scale) can transmit information, screen, parts of the pattern as far away as the pattern radius. The formation of fractal patterns and maximization in the entropy production at the same structural phase transition reflect the fact that the dynamical system responsible for the pattern formation has reached a critical point. The changes in the pattern as the screening constraint is shifted away from criticality are analogous to those observed in other systems such as percolation.

ACKNOWLEDGMENTS

We thank Richard Voss and Per Bak for some very useful discussions.

REFERENCES

1. T. A. Witten, Jr. and L. M. Sander, *Phys. Rev. Lett.* **47**:1400 (1981).
2. B. B. Mandlebrot, *The Fractal Geometry of Nature* (Freeman, San Francisco, 1983).
3. J. H. Kaufman, A. I. Nazzal, O. R. Melroy, and A. Kapitulnik, *Phys. Rev. B.* **35**:1881 (1987).
4. J. H. Kaufman, O. R. Melroy, F. F. Abraham, and A. I. Nazzal, *Solid State Commun.* **60**:757 (1986).

5. L. Niemeyer, L. Pietronero, and H. J. Wiesmann, *Phys. Rev. Lett.* **52**:1033 (1984).
6. A. Coniglio and H. E. Stanley, *Phys. Rev. Lett.* **52**:1068 (1984).
7. P. Meakin, H. E. Stanley, A. Coniglio, and T. A. Witten, *Phys. Rev. A* **32**:2364 (1985).
8. P. Bak, C. Tang, and K. Wiesenfeld, *Phys. Rev. Lett.* **59**:381 (1987).
9. I. Prigogine, G. Nicolis, and A. Babloyantz, *Phys. Today* **25**(11):23 (1972); *Science* **201**:777 (1978).
10. S. Wolfram, in *Scaling Phenomena in Disordered Systems*, R. Pynn and A. Skjeltorp, eds. (Plenum Press, New York, 1985).
11. C. E. Shannon and W. Weaver, *The Mathematical Theory of Communication* (University of Illinois Press, 1962).
12. D. L. Goodstein, *States of Matter* (Prentice-Hall, Englewood Cliffs, N. J., 1975), pp. 43–46.
13. R. Landauer, *Phys. Today* (November 1987); *Phys. Rev. A* **12**:636 (1975).