Thermodynamics of Fractal Networks

Andrea Rinaldo,[1,2] Amos Maritan,[3] Francesca Colaiori,[3] Alessandro Flammini,[3] Riccardo Rigon,[2] Ignacio Rodriguez-Iturbe,[2] and Jayanth R. Banavar[4]

[1]*Istituto di Idraulica "G. Poleni," Università di Padova, I-35131 Padova, Italy*

[2]*Department of Civil Engineering, Texas A & M University, College Station, Texas 77843*

[3]*International School for Advanced Studies, Istituto Nazionale di Fisica della Materia and Sezione INFN di Trieste, I-34014 Grignano di Trieste, Italy*

[4]*Department of Physics and Center for Materials Physics, The Pennsylvania State University, 104 Davey Laboratory, University Park, Pennsylvania 16802*

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Optimal channel networks are fractal structures that bear a striking resemblance to real rivers. They are obtained by minimizing an energy functional associated with spanning trees. We show that large network development effectively occurs at zero temperature since the entropy scales subdominantly with system size compared to the energy. Thus these networks develop under generic conditions and freeze into a static scale-free structure. We suggest a link of optimal channel networks with self-organized critical systems and critical phenomena which exhibit spatial and temporal fractality, the former under generic conditions and the latter on fine tuning. [S0031-9007(96)00007-5]

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The existence of fractals, i.e., the ubiquity of scale-free structures that look "alike" on many scales of observation [1], and the origin of the widespread phenomenon called $1/f$ noise (the property of a time signal having components of all durations) have recently found a powerful linkage through the idea of self-organized criticality developed by Bak and co-workers [2]. In this Letter we attempt to link different aspects of the spatial and temporal properties of fractal structures on thermodynamic grounds.

Observational evidence suggests that the characteristics of real river networks are extremely well reproduced by optimal channel networks (OCNs) [3] (Fig. 1) obtained by selecting the spanning tree, characterized by a variable s, that minimizes the Hamiltonian of the system defined as

$$H_\gamma(s) = \sum_{i=1}^{L^2} A_i^\gamma , \qquad (1)$$

where i spans the L^2 sites occupied by, say, a $L \times L$ square lattice, $\gamma \sim 0.5$ is an exponent capturing the physics of the erosional process [4], and A_i is a measure of the number of upstream sites to i connected by the network, defined by $A_i = \sum_{j \in \mathrm{nn}(i)} A_j + 1$ [where nn(i) are the neighbors of i in the lattice draining into i]. Thus a network configuration can be represented by a rooted spanning tree, with a set of oriented links between connected nearest neighbor sites. The orientations correspond to the drainage directions, and the root of the tree, i.e., the outlet, is taken in one of the corners of the $L \times L$ lattice for convenience at no cost of generality (Fig. 1).

The structure of the configuration minimizing the functional H_γ strongly depends on the parameter γ. We can distinguish different behaviors: For $\gamma < 0$, OCNs are attained by the so-called "Hamiltonian paths" [5] in which only one stream drains all the basin area; for $\gamma > 1$, the patterns minimizing Eq. (1) are such that the average length of the path from each site to the outlet is the shortest ("explosion paths"), and there is as little aggregation as possible [6]. The range $0 \leq \gamma \leq 1$ is more interesting, and in this region the system

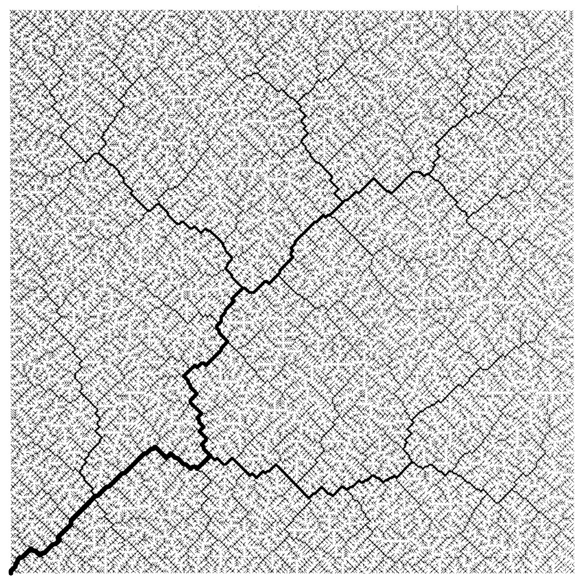

FIG. 1. An example of an OCN with $\gamma = 1/2$ ($L = 128$). The network is computed selecting the optimal configuration through a traveling-salesman-like algorithm starting from random initial conditions. The algorithm proceeds selecting a site i at random and perturbing the configuration ($s \rightarrow s'$) by locally assigning a change in the matrix of connections. This leads to a rearrangement of A_i's (all areas formerly and currently linked to i are modified). The change is accepted if $H_{0.5}(s') < H_{0.5}(s)$. The procedure stops after a prefixed number of attempts are rejected. For a brief discussion of related algorithms see [3] and references therein. Note also that the width of the channels in the plot is proportional to $\sqrt{A}$.

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exhibits rich structures and aggregation patterns. OCNs, which were originally obtained [3] by minimizing the functional in Eq. (1) with $\gamma = 0.5$, are fractals leading to power laws for the statistical distributions of suitable geometrical parameters [notably, using the definition of total contributing area A, the area distribution is $P(A) \propto A^{-(1+\beta)} f(A/L^{\phi})$ with $\beta = 0.43 \pm 0.02$ [3], $\phi \sim 1.8$, and $f(\cdot)$ is a suitable function that takes into account finite size effects [7]]. These attributes prove indistinguishable from those observed in nature [8].

For a given drainage basin B overlaid with a lattice of L^2 sites, let S be the set of spanning loopless trees rooted in a given point, say, 0. For any configuration $s \in S$ we define a Boltzmann-like probability of the tree s as

$$P(s) \propto e^{-H_{\gamma}(s)/T}, \tag{2}$$

where T^{-1} is the Gibbs' parameter mimicking the inverse of temperature of classic thermodynamic systems [9,10]. For a fixed γ, let $H_{\gamma}(S)$ denote the finite set of all possible values that may be taken on by $H_{\gamma}(s)$ for trees $s \in S$. Given an energy level, say, $E \in H_{\gamma}(S)$, let $N(E)$ be the degeneracy, i.e., the number of different spanning trees s for which $H_{\gamma}(s) = E$. One therefore obtains $P\big(H_{\gamma}(s) = E\big) = \sum_{s:H_{\gamma}(s)=E} P(s) \propto N(E)\exp(-E/T)$. Defining the thermodynamic entropy as $\sigma(E) = \ln N(E)$, one obtains

$$P\big(H_{\gamma}(s) = E\big) \propto e^{-F(E)/T}, \tag{3}$$

where a formal free energy $F(E) = E - T\sigma(E)$ has been introduced. Indeed, the most probable states correspond to an energy E that minimizes $F(E)$.

Our central result is that the entropy scales subdominantly with system size compared to the energy so that even for a nonzero value of the Gibbs' parameter the most probable spanning tree configurations determined by minimizing the free energy can be equally well obtained by minimizing the energy, provided that L is large enough. As a result, in the thermodynamic limit the system described by the probability in Eq. (3) always tends to operate at zero temperature, i.e., the total energy in Eq. (1) is minimized.

Our exact result is that, for the set s of OCNs, one has

$$E = \mathrm{Min} H_{\gamma}(s) \propto L^{2+\delta}, \tag{4}$$

with $\delta > 0$ for $\gamma > 1/2$. This result is obtained by dividing the sum in (1) into the sum over rows of sites in the direction transverse to the flow and the sum over sites within the rows, and using the inequality $\sum_i (X_i^{\gamma}) > (\sum_i X_i)^{\gamma}$ for $X_i \geq 0$. Physically, δ turns out to be greater than zero because of the aggregating properties of the river network. The result $\gamma = 1/2$ has $\delta = 0$, but with a logarithmic correction leading to an effective δ of 0.1–0.2 as shown by detailed examination of data in computer studies of accessible local minima. This result can also be derived through a renormalization group argument employing a coarse graining which preserves the mean elevation of OCN topographies [11] and, independently, by scaling arguments [7].

For spanning loopless trees the number $N(E)$ of configurations s with given energy E scales, at most, as $N(E) \propto \mu^{L^2}$, so that $S(E)$ scales, at most, as L^2, where μ is a real number depending on lattice properties and the energy. This follows from noting that the total number N of spanning trees is less then the number of possible ways of choosing $L^2 - 1$ links (number of link s in a spanning tree) among all the $2L(L + 1)$ possible links. Thus

$$N < \binom{2L(L+1)}{L^2 - 1} \sim 2^{2L^2}.$$

Since the number of configurations with a given energy is less than or equal to N, $N(E) \leq 2^{2L^2}$ and the above scaling of entropy is satisfied.

We conclude that for spanning trees (with $\gamma \geq 1/2$) the entropy scales subdominantly to the energy with system size and, in the thermodynamic limit $L \to \infty$, $\min F(E) \propto L^{2+\delta}$ because $\delta > 0$. Hence the configuration s that minimizes H_{γ} also minimizes $F(E)$, whatever the Gibbs' parameter T^{-1}, provided the system is large enough. Hence OCNs, which correspond to the zero-temperature assumption [i.e., the configuration yielding $\min F(E)$ is that with $\min E$ only for $T \to 0$], reproduce natural conditions at any temperature for large L. Since fluvial networks usually develop migration of divides and competition for drainage in the absence of geologic controls over domains large with respect to the lower cutoff scale (the scale of channel initiation [8]), it is likely that natural networks operate most in conditions that well approximate the thermodynamic limit. We suggest that this is the reason for the outstanding ability [3] of OCNs to reproduce observational evidence regardless of diversities in surface lithology, geology, vegetation, or climate. This also strongly suggests that size effects of samples of real networks may lead to spurious results for small sizes [10].

Conventional OCNs have a constrained structure (loopless and spanning) and entail the minimization of the total energy dissipation. Thus they do not exhibit a set of dynamically recursive states but have a frozen structure and behave as a $T = 0$ cold system. This follows from the subdominant scaling of the entropy with system size compared to the energy while the spatial critical behavior of OCNs originates from the correlated nature of their constrained structure. Hints that other fractal structures arise in the context of minimum energy dissipation for open systems come from experimental evidence on the development of stationary dendritic structures in injected electric fields [12].

We have run an example of entropy-dominated OCN with $\gamma = 1/2$ using the Metropolis algorithm [13] at a nonzero (and fixed) value of T. The example is meant to show the implications of entropy maximization, i.e., if $T > \text{const} \times L^{\delta}$, entropy dominates over the energy. We started with any initial condition and accepted configuration changes ($s \to s'$) when they (i) lowered the energy

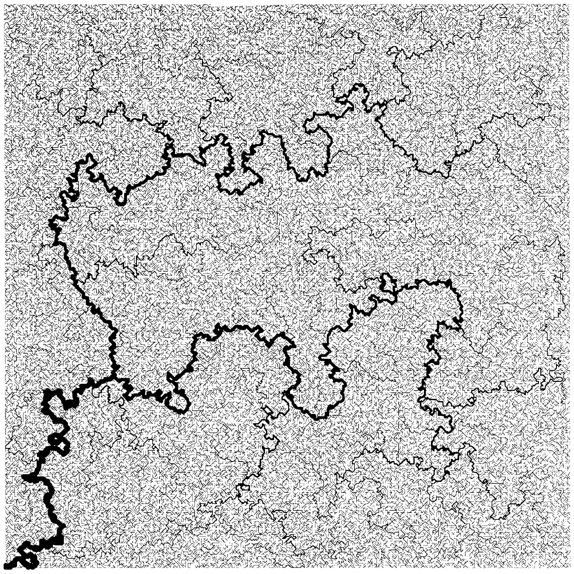

FIG. 2. One of the configurations of a "hot" OCN with $\gamma = 1/2$, obtained at $T = 100$ after 10^7 iterations. A perceptible difference with the structure in Fig. 1 is the less directed character of the network.

[i.e., $H_\gamma(s') < H_\gamma(s)$] or (ii) with probability $P(s') \propto \exp\{-[H_\gamma(s') - H_\gamma(s)]/T\}$ otherwise. Figure 2 shows one of the configurations of a $T = 100$ OCN which, for the system size $L = 128$, is large enough to ensure the dominance of entropy. The resulting networks are clearly fractal with properties none of which match those found in nature [8]. Nevertheless, it is striking that *hot* OCNs yield stable statistics of spatially scale-free structures and are characterized by a preponderance of time scales once the system reaches the set of recursive states, in a process reminiscent of ordinary self-organized critical (SOC) phenomena [2,14]. Hot OCNs and SOC have several common attributes and a key difference. They both lead to fractals, in space and time. They both have a set of recursive states. Nevertheless, hot OCNs are obtained by minimizing a free energy, whereas SOC is obtained by dynamical rules. It is thus tempting to speculate that classic self-organized critical systems [2], for which the concept of recursive states is meaningful [15], are *hot* and may maximize the entropy (with appropriate constraints) in the thermodynamic limit. In fact, in classic SOC systems like Abelian sandpiles, the number of possible configurations in two dimensions (i.e., recursive states) scales as μ^{L^2} [15]. Therefore $\sigma(E) \propto L^2$. Since energy dissipation is measured by the number of active sites [16] and occurs through the boundaries, its scaling is likely to be subdominant to the entropy in the thermodynamic limit. Entropy-controlled critical structures have been found [17] in neural networks of mobile elements with random activation—reminiscent of self-organized ant societies. Such networks operate at the edge of chaos with critical fluctuations that indeed maximize the entropy. In this case entropy maximization and the critical behavior are obtained by tuning a density parameter which quite accurately corresponds [17] to the self-organized value observed in nature.

Finally, conventional critical phenomena obtained by fine-tuning a parameter (e.g., temperature) might be the outcome in which the scaling properties of the energy and entropy are similar.

It is indeed possible that OCNs and SOC systems are distinct because the latter are not obtainable through any free energy minimization principle. However, an intriguing alternative is that natural evolution of fractal structures in open, dissipative systems with many degrees of freedom is generally the by-product of chance and necessity, the latter being embedded in the strive for optimality that we see everywhere [18] in natural forms.

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