A Conductivity-Dependent Phase Transition from Closed-Loop to Open-Loop Dendritic Networks

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Abstract

Motivated by a principle of minimum dissipation per channel length, we introduce a model for branching, hierarchical networks in an open, dissipative system. Global properties of the resulting structures are observed to scale with the ratio of conductivity in the dendrite material to conductivity in the lattice material. Beyond a critical conductivity ratio, the resulting structures are naturally self-avoiding and possess scale-independent branching ratios. Our findings suggest that the conductivity ratio determines the geometric properties of naturally-arising dendritic structures. We discuss empirical verification in the context of a system of self-organizing agglomerates of metal particles in castor oil.

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Open dissipative systems giving rise to self-similar, branching networks are ubiquitous in nature. Examples include naturally forming river basins [1–4], biological networks [5–7], and agglomerates of metal particles in castor oil [8–10]. Additionally, many nonequilibrium processes such as nucleation, gelation, polymerization, and tumor growth can be modelled as dendritic aggregates in the context of open dissipative systems [11–15]. Several computational models for dendritic network formation have recently been studied, particularly within the context of river networks. This work has followed three main approaches.

(i) Simple statistical and random walk models have been used to simulate the evolution of branching networks [11, 12, 16–18]. While such models have been very successful in explaining colloidal aggregation and other primarily statistical phenomena, their import into the domain of open, dissipative systems has been less empirically successful [19]. Consider, for example, the absence of closed loops in river networks, metal agglomerates, and other open, dissipative systems. All variants of these random walk models either obtain closed loops or enforce a condition of no closed loops *a priori*. That this condition is not obtained as the result of some local, physical principle suggests that such models do not accurately describe the evolution of these systems.

(ii) Open, dissipative systems have been modelled within the framework of self-organized criticality by assuming that global energy dissipation is minimized in their stationary states, and using computational methods, such as simulated annealing, to search for structures of minimum dissipation [1, 10, 20–22]. This procedure has reproduced the critical scaling exponents of river networks with reasonable accuracy suggesting a tenable physical principle. Unfortunately, such models do not give insight into the local physical processes responsible for the distinctive global geometries that minimize dissipation. In particular, the absence of closed loops is, again, enforced *a priori* rather than recovering this as a local manifestation of the hypothesis of minimum energy dissipation.

(iii) River networks have been modelled by postulating a dynamical equation for the evolution of eroding surfaces, and seeking self-consistent solutions to the proposed equation [23–26]. Again, however, a condition of no closed loops is generally enforced in the initial landscape condition or in the application of the landform evolution rules. This approach has been fruitful for studying river network formation, but its reliance on the specific physics of surface erosion indicates that it cannot yield a general theory for the common structural characteristics of dendritic networks in diverse physical systems.

Whereas most previous models for dendrite growth have enforced a condition of no closed loops *a priori*, we relax this assumption in the model presented below and study the formation of closed loops systematically. While the guiding objective of previous research has been to reproduce the topological and geometric scaling exponents that have been empirically measured in river-networks and other dendritic systems, our goal is to analyze the assumption of self-avoidant growth that underlies these previous models. Many of the scaling statistics recovered in these models rely implicitly upon the assumption of no closed loops, and in this paper, we will argue that this assumption can be replaced by a physical assumption on the conductivities of the dendrite material and the ambient material.

In this paper, we present a deterministic discrete dynamic for the evolution of physical networks in an open, dissipative system. While our model is primarily motivated by a system of self-organizing, conducting agglomerates in castor oil [8, 9], it is applicable to large class of open, dissipative systems. Two global properties of the resulting structures, namely self-avoidance and branching frequency, are defined and studied as a function of the ratio of conductivity in the network material, σ_1, to conductivity in the ambient lattice material, σ_2. Throughout this paper, we set $\delta = \sigma_1/\sigma_2$. We evaluate the model in a high δ limit and recover known properties of a system of conducting agglomerates in castor oil, most notably the absence of closed loops. Whereas most previous models for dendrite growth have enforced a condition of no closed loops *a priori*, we observe that the frequency of closed loops depends upon δ, suggesting that the parameter δ may be used to distinguish universality classes of dendritic structures.

Consider an NxN square grid with each node (i, j) assigned a potential ϕ_{ij}. Each adjacent pair of nodes (i, j) and (i', j') is assigned a conductivity $\sigma_{iji'j'}$, where (i, j) adjacent to $(i'j')$ means $(i', j') \in \{(i+1, j), (i-1, j), (i, j-1), (i, j-1)\}$. Current, $J_{iji'j'}$, across the (i, j) to (i', j') link is given by Ohm's Law.

$$J_{iji'j'} = \sigma_{iji'j'}(\phi_{ij} - \phi_{i'j'}) \tag{1}$$

Define s_{ij} to be an imposed current source at (i, j). Then conservation of charge at (i, j) is expressed:

$$\sum_{i'j'} J_{iji'j'} - s_{ij} = 0 \tag{2}$$

Where we adopt the convention that a sum over $i'j'$ runs only over those pairs of indices adjacent to (i, j). With specified boundary conditions, equations (1) and (2) uniquely determine

ϕ_{ij}. Let $\phi_{ij} = s_{ij} = 0$ on boundary nodes of the lattice, and $s_{ij} = s$ be identically constant for interior nodes. Then the dynamics for $\sigma_{iji'j'}$ determine ϕ_{ij}. As shown below, these dynamics consist of high-conductivity channels (dendrites) forming in a low-conductivity lattice.

$\sigma_{iji'j'}$ takes on only two values. It is initialized by $\sigma^0_{iji'j'} = \sigma_2$. In each subsequent timestep, one link attains a higher conductivity $\sigma_1 >> 1$. A node (i,j) is considered connected if it is on the boundary of the lattice or if its connection to some neighboring node has conductivity σ_1. Connections are grown via the discrete dynamic for $\sigma_{iji'j'}$ given below.

$$\sigma^{t+1}_{iji'j'} = \begin{cases} \sigma_1 & \text{if } P_{iji'j'} = P^{max}_{iji'j'} \\ \sigma^t_{iji'j'} & \text{else} \end{cases} \tag{3}$$

Where $t = 0, 1, 2, \ldots (N-2)^2 - 1$, and $P_{iji'j'} = \sigma_{iji'j'} J^2_{iji'j'}$ is the energy dissipated in the (i,j) to (i',j') link. We define $P^{max}_{iji'j'}$ as the maximum value of $P_{iji'j'}$, where (i,j) is a connected node, and (i',j') is a node adjacent to (i,j). Thus, each new high-conductivity link originates at an unconnected node, and attaches to an adjacent node (which may be either unconnected or previously connected via one of its three alternate neighbors). We grow $(N-2)^2$ links because this completely fills the lattice when no closed loops form. Whether there are closed loops or not, we consider a lattice with $(N-2)^2$ high-conductivity links to be fully grown.

We assume a separation of mechanical and electrical timescales and update ϕ_{ij} according to the Laplacian relaxation algorithm between each mechanical timestep in (3). The relaxation iteration, obtained from (1) and (2), is given by

$$\phi^{m+1}_{ij} = \sum_{i'j'} \phi^m_{i'j'} \sigma_{iji'j'} / \sum_{i'j'} \sigma_{iji'j'}. \tag{4}$$

A single iteration of the relaxation algorithm consists of N^2 applications of equation (4), one for each pair (i,j), where $0 \geq i \leq N-1$ and $0 \geq j \leq N-1$. After each timestep t in equation (3), we iterate the relaxation algorithm for $m = 0, 1, 2, \ldots K$, where K is chosen sufficiently large so that ϕ^m_{ij} has converged to a constant in eight significant digits for each pair (i,j). For a 50x50 lattice, we observe that ϕ_{ij} converges to eight significant digits in about 2000 iterations.

When the relaxation algorithm is applied with sufficiently many iterations as discussed above, we observe that the dynamic in equation (3) has a unique fully-grown state for given boundary conditions on ϕ_{ij} and given parameters N and δ (recall that δ is defined as

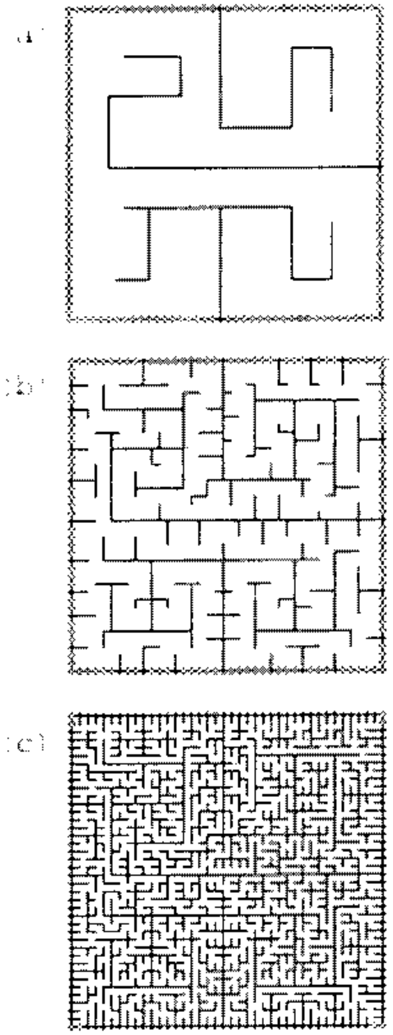

FIG. 1: Network evolution for a 40x40 lattice at (a) t=180 (b) t=500 (c) t=1444. Here $\delta = 10^9$, greater than the necessary threshold for no closed loops.

σ_1/σ_2). If the initial boundary conditions for ϕ_{ij} are asymmetric, the simulation produces asymmetric growths, whose shoots tend in the direction of the potential gradient. Since this is a less natural physical scenario, we set our boundary conditions as $\phi_{ij} = s_{ij} = 0$ throughout this study, and vary N and δ only. A sample evolution with $N = 40$ and $\delta = 10^9$ is displayed in fig. 1. For all sets of physical parameters observed thus far, global energy dissipation is a decreasing function of t under this dynamic.

We wish to characterize the self-avoidance of the proposed growth dynamic. We define $C(N, \delta)$ to be the number of closed loops in a fully-grown dendritic structure with linear dimension N and conductivity ratio δ, and study this measure of self-avoidance as a function of δ. We observe that when our growth algorithm is implemented with noise [1] , $C(N,\delta)$ is a robust parameter and the scaling behavior reported in this paper remains intact. Thus, we systematically study the phenomenon of self-avoidance through a robust, global parameter, rather than enforcing a local assumption of self-avoidance. Numerical simulations indicate that there exists a critical conductivity ratio $\delta_c(N)$, such that $\delta > \delta_c(N)$ implies $C(N,\delta) = 0$. Thus, $\delta_c(N)$ defines the location of the phase transition from closed-loop to open-loop structures. This threshold value scales with the linear dimension of the grid as:

$$\delta_c(N) = AN^{\alpha} \tag{5}$$

Where A and α are scale-independent constants. By the least-squares fit shown in fig. 2, their values are determined to be $A = .022 \pm .008$ and $\alpha = 4.03 \pm .21$ [2]. Hence, $\delta_c(N)$ scales approximately as the square of lattice area.

For $\delta < \delta_c(N)$, $C(N,\delta)$ displays power-law scaling as:

$$C(N,\delta) = B_N \delta^{\beta} \tag{6}$$

Where B_N is a constant dependent on N and β is a scale-independent constant. Fig. 3 shows $C(N,\delta)$ plotted against N, and $\beta = -.77 \pm .05$ from the displayed least-squares fit line. Furthermore, we have $B_{50} = 6.3e3 \pm 1.1e3$, $B_{40} = 2.4e3 \pm .6e3$, $B_{30} = 7.0e2 \pm .8e2$.

We have seen that δ determines the self-avoidance of dendritic growth. Next, we investigate the branching of fully-grown dendritic structures as a function of δ. Branching is quantified as follows: for $k = 1,2,3,4$, define a k-node to be an interior lattice node which has k neighboring connections of conductivity σ_1. Let $f_k(N,\delta)$ be the number of k-nodes in

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[1] Noise is implemented in the growth algorithm by modifying eq. 3 as follows: Rather than setting $\sigma^{t+1}_{iji'j'} = sigma_1$ for the $iji'j'$ link in which $P_{iji'j'} = P^{max}_{iji'j'}$, we randomly select an $iji'j'$ link among the set of links for which $P_{iji'j'} > cP^{max}_{iji'j'}$ where $0.82 < c < 1$ and for this link we set $sigma_{iji'j'} = sigma_1$. In other words, rather than choosing the link of maximum power dissipation to grow a dendritic connection, we randomly select a link among those with high power dissipation. This modification destroys the determinism of the growth dynamic, but we observe that for for $.82 < c < 1$, the global features of the resulting dendritic growths are not greatly affected. In particular, $C(N,\delta)$ for these non-deterministic implementation varies little from the value obtained in deterministic simulation.

[2] The standard error for each parameter estimate in this paper was computed using Origin's curve fitting tool, and is equal to $\sqrt{(C_{ii}\chi^2)}$ where C_{ii} is the diagonal entry of the variance-covariance matrix corresponding to the relevant parameter and χ^2 is the reduced chi squared value of the fitting curve (see [27] for details).

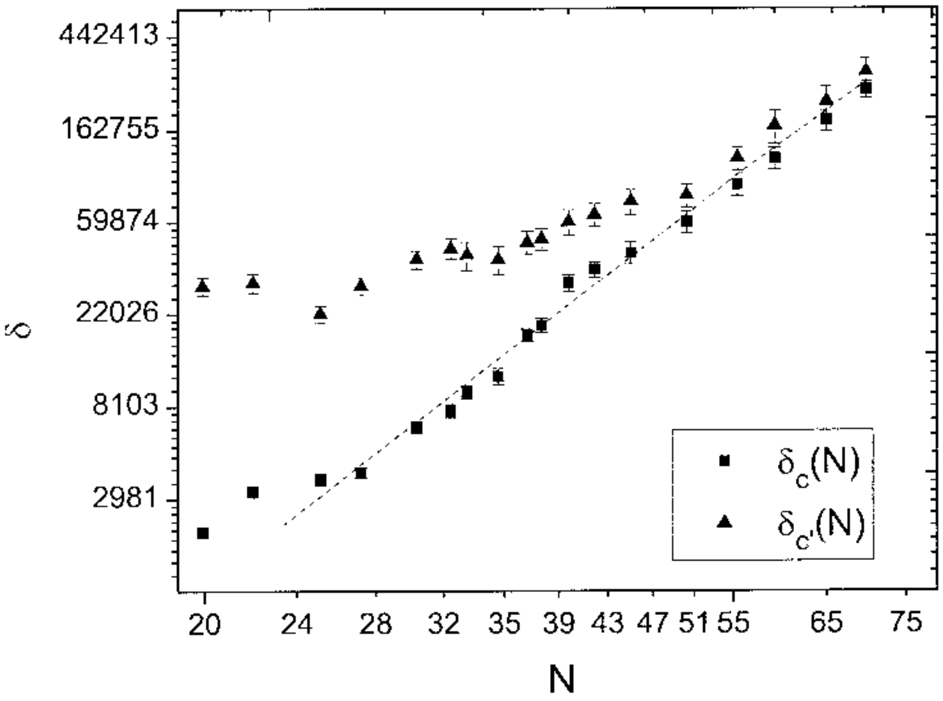

FIG. 2: Ln-ln plot of critical conductivity ratios $\delta_c(N)$ and $\delta_{c'}(N)$ against linear dimension of the lattice. Here, $\delta_c(N)$ defines the location of the phase transition from closed-loop to open-loop structures and $\delta_{c'}(N)$ defines a conductivity cutoff, beyond which the structures possess scale-independent branching ratios. The error bars indicate that $\delta_c(N)$ and $\delta_{c'}(N)$ have only been determined to within the specified range; an exact determination of these values is infeasible since it would require full simulations with the parameter δ set to every value contained in the indicated range. The least-squares best-fit line has slope 4.03 ± .21. The quantities in this plot and in each subsequent plot are dimensionless.

a fully-grown dendritic structure with linear dimension N and conductivity ratio δ (boundary nodes are excluded from this count). Numerical simulations indicate that there exists a critical conductivity ratio $\delta_{c'}(N)$ such that $\delta > \delta_{c'}(N)$ implies $f_k(N, \delta)$ is independent of δ. Both $\delta_{c'}(N)$ and $\delta_c(N)$ are plotted against N in fig. 2. Although, $\delta_{c'}(N)$ does not scale for small N, this appears to be a finite size effect. At the upper limit of numerical simulations, $\delta_c(N)$ and $\delta_{c'}(N)$ are seen to coincide.

If we let $f_k(N)$ denote $f_k(N, \delta)$ for $\delta > \delta_{c'}(N)$, then we have the further result that $f_k(N)$

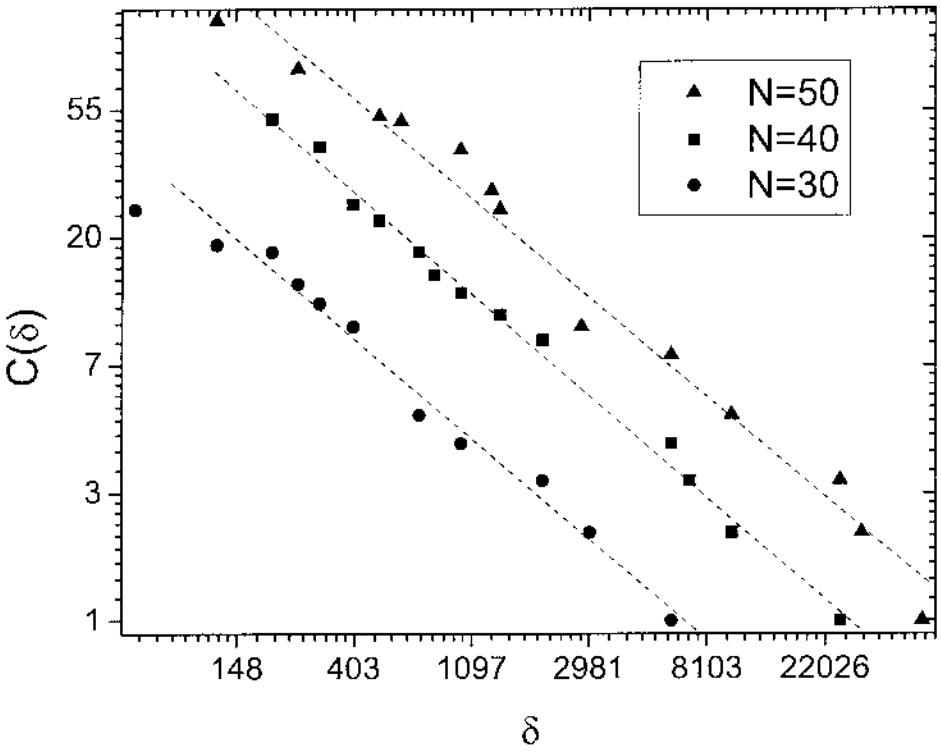

FIG. 3: Ln-ln plot of closed loops against δ for $\delta < \delta_c(N)$. The best-fit lines for lattices with linear dimensions $N = 50$, $N = 40$, and $N = 30$ have slopes $-.76 \pm .04$, $-.78 \pm .03$, and $-.77 \pm .03$ respectively.

scales approximately as the square of N as seen in fig. 4. Thus, we may define universal constants H_k (for $k = 1, 2, 3, 4$) as $f_k(N)/(N-2)^2$, the ratio of k-nodes to the total number of interior nodes in the lattice. Numerical simulations indicate that $H_1 = .423 \pm .008$, $H_2 = .311 \pm .015$, $H_3 = .210 \pm .012$, and $H_4 = .062 \pm .005$.

The existence of universal constants H_k and the absence of closed loops for high δ is in good correspondence with empirically-observed properties of a system of self-organizing agglomerates of metal particles [8–10]. The dimensionless H_1 corresponds to the number of tips of the conducting agglomerate and is observed to be a good order parameter for the stationary states of this system [8]. The total absence of closed loops is also an observed property of the stationary states of this system [8, 9]. The local dynamic proposed herein has recovered these properties in the high δ limit, in good correspondence with the large

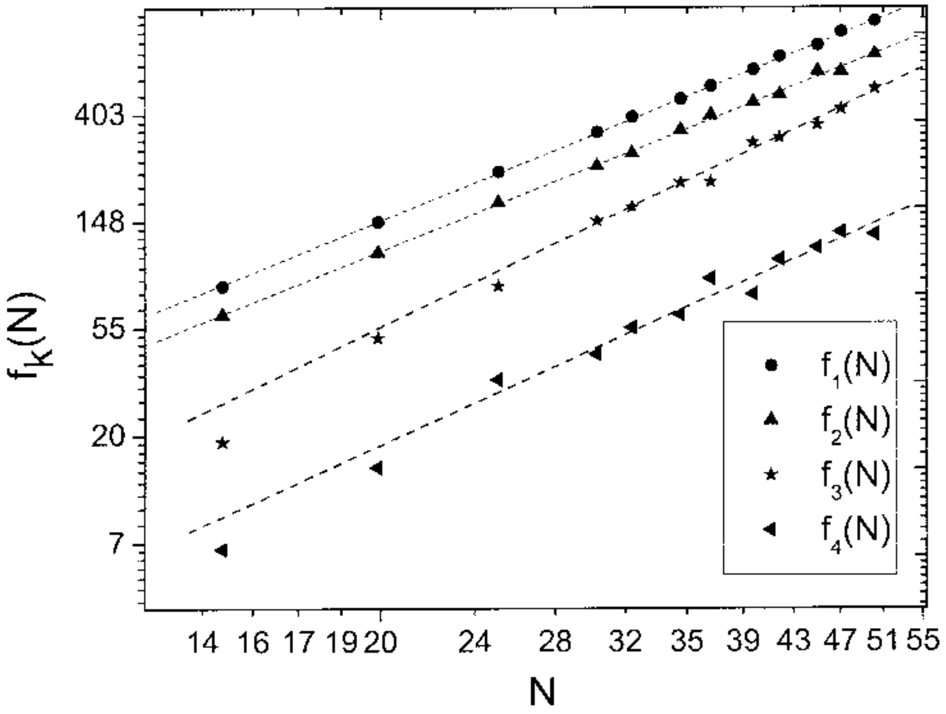

FIG. 4: Ln-ln plot of frequency of k-nodes against linear dimension of the lattice for $\delta > \delta_c(N)$. The least squares best-fit lines have slopes $2.04 \pm .01, 2.01 \pm .02, 2.4 \pm .11, 2.23 \pm .21$ for $k = 1, 2, 3, 4$ respectively.

conductivity ratio of conducting particles to low-conductivity castor oil.

Furthermore, several aspects of this dynamical model are applicable to the modelling of other open, dissipative systems, such as naturally-forming river basins and biological networks. In fact, our model provides a framework for separating basic universality classes of dendritic growth via the fundamental parameter delta, and for doing a comparative study of the varied geometries of dendritic systems. In this paper, we have restricted our focus to empirical verification in the high-delta limit, but our preliminary investigation into the model's statistics at medium and low-delta values suggests that the basic scaling of river basins is recovered at these subcritical delta values. Qualitatively, the high-delta universality class is characterized by two or three large dendrites covering the majority of the lattice (as in fig. 1), but the distribution of dendrite sizes becomes more regular as delta is lowered from the threshold $\delta_c(N)$. At these lower delta values, the size distribution of dendrite growths appears to obey power-law scaling, as has been empirically observed in river basins [2].

In conclusion, we have introduced a dynamic for the evolution of high conductivity dendrites in a low-conductivity medium, which is applicable in the context of many open, dissipative systems. We have found that for $\delta > \delta_c(N)$, closed loops are absent and branching frequencies stabilize to a set of universal constants, H_k. We have also observed scaling in the parameters $\delta_c(N)$ and $C(N, \delta)$, and have discussed empirical verification within the context of an experimental system of conducting agglomerates in castor oil. Preliminary investigation suggests that for $\delta < \delta_c(N)$, the properties of the resultant structures correspond to alternate universality classes of open, dissipative systems. Therefore, further investigation of the model in these contexts is a promising avenue for further inquiry into the phenomenon of self-avoidant growth.

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