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### End-Directed Evolution and the Emergence of Energy-Seeking Behavior in a Complex System

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Self-organization in a voltage driven non-equilibrium system, consisting of conducting beads immersed in a viscous medium, gives rise to a dynamic tree-structures which exhibits worm-like motion. The complex motion of the beads driven by the applied field, the dipole-dipole interaction between the beads and the hydrodynamic flow of the viscous medium results in a time-evolution of the tree-structure towards states of lower resistance or higher dissipation and thus higher rates of entropy production. Thus emerges a remarkably organism-like "energy seeking behavior". The dynamic tree-structure draws the energy needed to form and maintain its structure, moves to positions at which it receives more energy and avoids conditions which lower available energy. It also is able to restore its structure when damaged, i.e., it is "self-healing". The emergence of energy-seeking behavior in a non-living complex system that is extremely simple in its construct is unexpected. Along with the property of "self-healing", this system, in a rudimentary way, exhibits properties that are analogous to those we observe in living organisms. Thermodynamically, the observed diverse behavior can be characterized as end-directed evolution to states of higher rates of entropy production.

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Since its discovery in the 1960s, the study of self-organization in non-equilibrium systems [1-6] has given us insight into how several biological phenomena such as chemical oscillations, pattern formation, and chemotaxis may arise in physico-chemical systems [7-9]. More recently, synchronization in a large number of chemical oscillators akin to the behavior observed in cell populations was demonstrated by Taylor et al. [10]. These studies have revealed how self-organization arising from irreversible processes could explain the origin of phenomena we observe in biological organisms, a possibility noted decades ago [11-13]. Since these structures are generated and maintained by dissipative processes, they have been termed dissipative structures [2] with the rate of entropy production being a measure of dissipation.

While the insight we got through the study of chemical oscillations and pattern formation is certainly important, a fundamentally different aspect of organisms is their ability to seek energy and matter needed to maintain their structure. Broadly speaking, this may be viewed as "end-directed time-evolution" in which the system transforms to states of higher energy consumption. Thermodynamically, the evolution of closed systems to states that minimize Gibbs or Helmholtz energy may be viewed as "end-directed evolution" in which the final state is specified but not the path towards this state. The system may take any one of the many possible paths, but we can be sure that eventually it will find a way to the state of minimum free energy. The highly complex energy seeking behavior we have observed in our voltage-driven system can also be quantitatively characterized as evolution to states of higher rates of free energy dissipation or entropy production. While recognizing that other variables particular to this system, such as the total current, *I*, or the resistance *R*, could also be used, we note that the essential feature of our system is end-directed evolution, regardless of the particular variable used to characterize it. We choose entropy production because it is a more general measure that can be applied to all non-equilibrium systems.

The electrically driven self-organizing system, which is simple in its construct, is maintained by the flow of current and it physically moves to states in which the current flow is higher, or equivalently, evolves to configurations that lower the system's electrical resistance. Our study indicates that when a self-organizing system consists of a large number of interacting elements which are subject to a flow of energy and/or matter, new and unexpected behavior might arise as we have found and as was observed by Taylor et al. [10]. While a large number of individual self-organizing systems have been the subject to detailed study, the study of higher-level organization emerging from the interaction of a large number of such systems is relatively new field. Our work points to the promise of this area of research.

The remarkably simple system consists of *N* spherical chromium beads, of 4mm in diameter, immersed in 60 mL of viscous oil in a 15 cm petri dish. They are subjected to a high voltage in the 15-30 kV range. The applied voltage is across a source electrode, located about 4 cm above the surface of the oil, and a ring ground electrode in the oil (Fig.1). The current was found to be in the 25-100 micro-amp range causing very little heating and the oil temperature varied less then 0.1 K(see [20] for more details). The applied high voltage induces electric dipole moments in the beads and drives complex convection currents in the oil. The dipole moments in turn alter the local electric field resulting in a complex field-fluid-bead interaction. Above a threshold voltage, due to the strong gradient of the applied field and the dipole-dipole interaction between the beads, the beads begin to move in the viscous oil and alter the field in complex

ways, which in turn drives their motion. The total current of the system,  $I(X_i, v(r))$ , depends on the position of the beads  $X_i$ , and the fluid velocity field, v(r), and an analytical description of its time evolution is practically impossible.

The early studies of this system [14,15] focused on the static dendritic structures generated when 400-1200 small beads, 1.6mm in diameter, were used. For the evolution of the system to the final steady state, they proposed a qualitative theory that expressed equation of motion of the beads in terms of a potential, the steady state being the minimum of the potential. This was characterized as evolution to minimum dissipation, but the theory was too general and could not predict any aspects of the bead motion even qualitatively. These studies also noted that dependence of the resistance of the system R on the number of beads was approximately  $N^{-\alpha}$ but the value of the exponent  $\alpha$  was not consistent between the experiments (ref [14] reported  $\alpha = 0.73$  while ref [15] reported  $\alpha = 2.35$ ). In subsequent studies [16-18], analytical approaches to obtaining the time evolution of the total current  $I(X_i, v(r))$  was understandably abandoned in favor of a phenomenological approach which focused on the geometrical properties of the system and categorizing stages of evolution on the way to the final structure [18]. The statistics of the beads in the final dendritic structure were analyzed and it was shown that the number of beads at the branch tips and the number of beads from which side branches emerged both scaled linearly with N. To obtain good statistics, 400-1200 beads were used in these studies. The similarity between transportation networks in biological system and the dendritic structure was noted[18].

Our study, however, focuses on dynamical aspects of the system when the applied voltage is well above the threshold voltage needed to overcome the static friction of the beads. We use a relatively smaller number, in the range10-60, of 4mm beads. Since an analytical approach to the evolution of the total current through the system,  $I(X_b, v(r))$ , is practically impossible, we looked for a higher-level description in terms of an end-directed evolution that emerges out of the complexity. To this end we took a thermodynamic approach. Since the structure is created and maintained by entropy producing processes, we looked at the rate of entropy production. The end directedness is not towards a steady state minimizing a potential but towards dynamic states of higher rates entropy production. For the rates of entropy production, there is no associated potential[19].

The basic experimental set up is shown in Fig. 1A. When a high voltage is applied, the beads begin to move from their initial position in the center of the dish (Fig. 1B), aggregate into one or more strings toward the outer ring electrode(Fig.1, C and D); eventually one string of beads makes contact with the ring electrode and a dynamic tree with swaying branches forms (Fig. 1E). The process of tree formation is extremely variable and fascinating to watch. Supplementary Material [20] shows a video of the process of tree formation. At the applied voltage of about 26kV, repeated trials result in dynamic trees with very different structures.

The highly variable time-evolution of this system can be described by one general property: evolution towards states with higher energy dissipation or rate of entropy production, and in this sense it is "end-directed". With widely varying paths and tree-structures, the system reaches the same final rate of entropy production. Here the total rate of entropy production, expressed in terms of thermodynamic forces and flows is given by [19]:

$$\Sigma = d_i S/dt = V I(X_i, v(\mathbf{r})) / T$$
(1)

where V is the voltage,  $I(X_i, v(r))$  is the current that depends on the position of the beads  $X_i$  and the velocity field v(r) of the viscous fluid as noted above, and T is the temperature Since the structure is maintained by ohmic energy dissipation, we shall characterize the system using  $\Sigma$ . If the voltage is turned off, the tree will disintegrate. At this time there is no established general thermodynamic theory that explains what class of systems evolves to states of higher  $\Sigma$ . Indeed, when a constant voltage is applied to a simple resistor, the increase in temperature caused by ohmic heating increases the resistance and thus decreases  $\Sigma$ , contrary to what is observed in our system.

The system's energy-seeking behavior of increasing  $\Sigma$  appears both in the formation of the tree structure and in its subsequent dynamic behavior. Formation of tree structure by itself is an evolution to a state of higher  $\Sigma$ . When the structure forms, there is a sharp jump in  $\Sigma$  (Fig. 1F). The relationship between applied voltage and  $\Sigma$  is shown in Fig. 2A; the jump in  $\Sigma$  also depends on the number of beads N nearly linearly (Fig. 2B). While small variations in initial conditions across trials lead to considerable variation in the tree structure,  $\Sigma$  always reaches virtually the same value. Thus, it is rate of entropy production, not a particular tree structure, that defines the end-directedness.

The most dramatic energy-seeking evolution to states with higher  $\Sigma$  is in the dynamic behavior of the tree. The tree structure is topologically stable after its formation, but the tree exhibits complex motion: the branches and trunk sway from side to side, and the tree as a whole can move along the ring electrode, thus allowing it to move to different regions within the dish. In the tree's complex motion, there were indications that it might be directed towards increasing the current and thus higher  $\Sigma$ . This was indeed confirmed in the following experiment. Using a tree with no branches, first, two plastic gates are used to constrain the tree's point of contact, and thus the tree, to a region of lower  $\Sigma$  (see Fig. 3A). In the constrained region, the tree moves back and forth from one gate to the other. When a gate is opened allowing the tree to move freely, remarkably, with swaying organism-like motion, the tree moves to a location of higher  $\Sigma$ . (See [20] for a video of a tree moving to a location that draws more current.) Similarly, if the tree is allowed to move to its preferred location and then forced to a different location by briefly tilting the petri dish (by about 5 degrees for 5 sec), it will move back to the preferred region of higher  $\Sigma$ (Fig. 3B) when the dish is returned to its horizontal orientation.

The tree's dynamics also show that it avoids regions that decreased  $\Sigma$  When part of the ring electrode was coated with a material that considerably increased its electrical resistance, the tree does not move into the high resistance region. An unconstrained tree, initially formed and in contact with the ring electrode in the uncoated region, moved until it reached the boundary of the coated region in which  $\Sigma$  would be lower, but then backed away into the uncoated region where  $\Sigma$  is higher.

The higher-energy-drawing evolution of the system towards higher  $\Sigma$  can be seen in other aspects of the system in less obvious ways. Driven by the strong applied voltage, the beads can, in principle, all move independently from their starting point at the center of the dish to the ring electrode or form many small trees each with a distinct point of contact. However, this does not happen. The vast majority of beads invariably self-organize into a single tree with branches, never a multitude of small trees. This can also be seen in earlier work [18] when a large number of beads were initially at the center of the system: a single dendritic structure formed with one trunk making contact with the ring electrode. It is possible, however, to initially arrange a given number of beads into many small trees, each with a distinct point of contact with the ring electrode (e.g., 20 beads arranged as 4 trees with 5 beads in each), and measure  $\Sigma$ . As shown in Fig. 4A,  $\Sigma$ increases monotonically as the trees increase in length, thus showing that the system forms larger trees because  $\Sigma$ is higher.

Evolution to higher  $\Sigma$  is also revealed when systems are perturbed such that the tree structure temporarily breaks apart into several disconnected small bead strings. A fixed total number of beads (N=20) arranged into different number of trees (eg. 10 trees of 2 beads each), were repeatedly tilted by 5 degrees for 10 sec each time. After the perturbation, beads showed a strong tendency to form larger trees. Fig. 4B shows the average longest tree lengths before and after perturbation for 10 runs for each initial configuration. Two points are noteworthy: 1) longer trees are more likely to return to their original length and 2) the probability of transitioning to a longer tree, with greater  $\Sigma$  is quite high. Thus, given a path through a sufficiently large perturbation, the system will evolve to a structure with greater  $\Sigma$  which is more stable than a system with lower  $\Sigma$ 

Stable dissipative structures are endowed with the property of "self-healing" because the dissipative processes that create the structure also restore it when damaged. Self-healing in organisms may be attributed to such thermodynamic stability. The observed tree structure is stable or self-healing in the sense that if the tree is disrupted by breaking a branch, the branch is

restored; if a segment of a tree with several branches is severed, the severed beads reattach and restore the tree, sometimes with a different branch structure. However, the new tree restores  $\Sigma$  to its pre-perturbation value; in other words, the function of the tree that maintains  $\Sigma$  at a certain level is restored, not the exact tree structure. The process is not unlike healing in organisms in which exact structure may not be restored, but its function is.

#### **Concluding remarks**

Though the system is simple to set up, the underlying electro-hydrodynamics complexity makes an analytical explanation of the observed dynamic behavior essentially impossible. Interestingly, out of such complexity "energy-seeking" behavior emerges. Currently there is no theoretical explanation to the observed evolution of the total current  $I(X_i, v(r))$  to higher values thus increasing  $\Sigma$ . We note that, even for the well established Second Law, one can experimentally only show that all physical processes increase entropy, when and if the maximum possible value is reached is not crucial for its validity. Indeed, in the 20<sup>th</sup> century formulation of thermodynamic by Onsager and Prigogine, the statement of the Second Law is that physical processes increase entropy:  $d_iS = \Sigma dt \ge 0$ , in which  $\Sigma$  is expressed in terms of thermodynamic forces and thermodynamic flows [19]. Similarly, in our non-equilibrium system, the evolution is to states of higher  $\Sigma$ ; whether or not it reaches the maximum possible value is neither very important nor can it be established experimentally. We clearly see that our system has metastable states from which, given the necessary perturbation, it can evolve to a state of higher

Σ.

Our study suggests that systems that have a large number of components which generate internal thermodynamic forces and flows in response to an externally imposed thermodynamic force are good candidates for the emergence of organism-like behavior, such as the observed energy-seeking behavior. In the present case, the internal components are the beads and the fluid and the voltages gradients they generate locally are the internal thermodynamic forces. These internal forces give the system large number of degrees of freedom that drive local currents which add up to the total current  $I(X_b \ v(r))$ . These local currents seem to organize to increase the rate of entropy production. This process, in our case, manifests as "energy seeking behavior" of a self-organized tree, and there are several other features that are open for investigation. This line of thought provides us a way to design other systems in which other types of emergent behavior may be observed. The much more diverse end-directedness we see in organisms might have had its origins in complex systems with a large number of internal thermodynamic forces [21]. The observed energy seeking behavior is also in accord with the recent observation made by England on maximization of energy absorption [22].

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#### **References and Notes:**

- 1. A. N. Zaikin, A. M. Zhabotinsky, *Nature* **225**, 535 (1970).
- 2. G. Nicolis, I. Prigogine, *Self-organization in Non-equilibrium systems* (Wiley, 1977).
- 3. H. Haken, Springer series in Synergetics Vol. 1. (Springer ,1977).
- 4. V. Petrov, Q. Ouyang, H. L. Swinney, *Nature* **388**, 655 (1997).
- 5. V.K.Vanag,L.Yang,M.Dolnik,A.M.Zhabotinsky,I.R. Epstein, *Nature* **406**, 389 (2000).

- L. Rensing, N.J. Jaeger, (Eds) Temporal Order: Proceedings of a Symposium on Oscillations in Heterogeneous Chemical and Biological Systems (Springer-Verlag, 1985).
- 7. A. Goldbeter, *Biochemical Oscillations and Cellular Rhythms: The molecular bases of periodic and chaotic behaviour* (Cambridge University Press, 1996).
- 8. J. Horváth, I. Szalai, P. De Kepper, Science, **324**, 772-775, (2009)
- I. Lagzi, S. Soh, P. J. Wesson, K. P. Browne, B. A. Grzybows J. Am. Chem. Soc. 132, 1198 (2010).
- 10. A. F. Taylor, et al. *Science* **323**, 614 (2009)
- 11. M. Eigen, P. Schuster *The Hyper Cycle* (Springer-Verlag, 1979)
- 12. S. Kaufmann, Origins of Order (Oxford University Press, 1993)
- 13. R. Rosen, *Essays on life itself* (Columbia University Press, 2000).
- 14. B. Merté et al., Helv. Phys. Acta 61, 76 (1988).
- 15. G. Hadwich, B. Merté, A. Hübler, E. Lüscher, Helv. Phys. Acta 63, 487 (1990).
- 16. M. J. Dueweke, Ph. D thesis (Univ. of Illinois at Urbana Champagne. Urbana, IL)
- M. Marani, J. Banavar, G. Caldarelli, A. Maritan, A. Rinaldo. *J. Phys. A* 31, L337– L343 (1998).
- 18. J. Jun, A. Hübler. *PNAS* **102**, 536-540 (2005).
- 19. D. Kondepudi, I. Prigogine, *Modern Thermodynamics, From Heat Engine to Dissipative Structures* (Wiley, 1998).
- 20. See Supplementary Material at [URL to be inserted] for (A) Material and Methods, (B) A video of tree formation in real time (video #1) and (C) a video of energy seeking behavior in real time (video#2).
- 20. R. Swenson, M. Turvey. Eco. Psych. 3, 317-348 (1991).

21. J. L. England, J. Chem. Phys. **139**, 121923-1 -- 121923-8 (2013)

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#### **Figure Captions**

Fig. 1. (Color) Self-organization of a dynamic tree structure in a voltage-driven system. (A) Schematic of the basic set-up in which conducting beads, placed in 60 ml of oil, are subjected to voltage V = 26kV across the source and the ground ring-electrode. (B-E) Evolution of the tree structure at four time points. With swaying branches, the tree as a whole (E) can move while maintaining its contact with the ring. (F) The rate of entropy production,  $\Sigma$  (in mJ/Ks), during formation of the tree structure. When the tree makes contact with the ground electrode, there is a sharp increase in  $\Sigma$ .

Fig. 2. Entropy production  $\Sigma$  in the system. (A)  $\Sigma$  as a function of the voltage for  $N_{beads} = 20$ ; at a given voltage,  $\Sigma$  is on the lower curve (preformation) but jumps to the upper curve when the tree makes contact with the ground electrode (postformation). (B) for a fixed voltage of 26 kV the magnitude of the  $\Sigma$  jump depends on the number of beads. Error bars = ±1 SE.

Fig. 3. (Color) Energy seeking motion of the tree. (A) With off-center source electrode, the base of the tree is confined by two gates to a state of  $\Sigma$  (lower panel); when a gate is opened, the tree moves quickly to increase  $\Sigma$  (see Movies S2- Energy Seeking in the Supplementary Information) (B) When the tree is moved to a location with lower  $\Sigma$  by tilting the system (around 580 s) by 5 degrees for 5 sec (t=577-582), it moves back to the state with higher  $\Sigma$ .

**Fig. 4.**  $\Sigma$  as a function tree length. (**A**) With fixed total number of beads,  $N_{beads} = 20$ , trees of varying length were constructed (e.g., ten 2-bead trees, or five 4-bead trees).  $\Sigma$  increases when there are fewer but longer trees. A single 20-bead tree has the highest  $\Sigma$ . (**B**) The results of a perturbation of a set of trees of different length. When a system of smaller trees is perturbed, they reform into longer trees (e.g. 2-bead trees regroup to form 4-bead trees). Error bars =  $\pm 1$  SE.







