UIUC Physics 563: Term Paper. Self-Organization

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1. :
   This essay addresses the question of self-organization in open systems, i.e. a process in which the internal organization of a system, increases in complexity without being guided or managed by an outside source. First some general issues about possibility of self-organization are discussed, then two examples are considered. The first example, reaction-diffusion model, is related to bio-chemistry, and the second one - to population dynamics.

2. **General Remarks** :

   The first question that arises thereupon is how the processes of self-organization are consistent with the second low of thermodynamics, which states that entropy or chaos can only increase with time, while the order, or information should decrease? The answer is that such processes are only possible in thermodynamically open systems, i.e. systems that exchange energy and matter with the environment. The 2-nd law of thermodynamics is only valid for closed systems. If one includes environment into consideration, the total entropy will still increase with time, as it should. It is obvious, that nothing interesting can happen in an open system that is in equilibrium with environment (since then the environment can be removed from consideration without disturbing the system).

   Thus, in a search for self-organization, open systems out of equilibrium should be considered. Since we are looking for organization or ordering without any external reasons for this order, it is reasonable to consider steady states, i.e. states that can be maintained for a long time under the condition that external parameters are not changing. The environment then comes into the game as a boundary conditions imposed on the system. The typical problem of this type would be to consider some spatial region, where different chemical reactions can occur and concentrations of certain products are kept constant at the boundaries. The steady state where all concentrations are constant in time can be reached, but it should not be confused with the equilibrium. Detailed balance is lost in this state.

   But how close to the equilibrium can we expect to find self-organization? It can be shown that within the applicability of linear non-equilibrium thermodynamics, the state corresponding to minimum entropy production allowed by boundary conditions is stable. Which means that started close enough to the equilibrium (so that linear non-equilibrium thermodynamics is valid) the system will tend to stay as close to equilibrium as possible and no self-organization can occur. This result is not surprising - it is somehow intuitively clear that for order to arise from nowhere we need non-linearity.

   For systems far from equilibrium (linear non-equilibrium thermodynamics is not valid), the state of minimum possible entropy production (which is closest state to equilibrium which corresponds to zero entropy production) is not necessarily stable [1].
   So, one should look for self-organization in open systems far from equilibrium, which are sometimes called dissipative system.

H. Haken proposed the adiabatic technique to deal with complex systems, which suggests to divide modes of the system into 2 types: slaving modes and order parameters [2]. Slaving modes are those which damp very fast with comparison to others, which becomes order parameters. If such division is possible, slaving modes follow the order parameters almost immediately, and self-consistency condition then can be applied to find the values of order parameters. To clarify this, consider the simplest example of non-linear system of equations:

$$\frac{dq_1}{dt} = -\gamma_1 q_1 - a q_1 q_2$$
$$\frac{dq_2}{dt} = -\gamma_2 q_2 + b q_1^2$$

With $\gamma_2 >> \gamma_1$.

In this case q_2 is a slaving mode. Assuming that it fallows the order parameter q_1 immediately, we may solve the system approximately by putting $\frac{dq_2}{dt} = 0$, which leads

$$q_2(t) = \gamma_2^{-1} b q_1^2(t)$$

and

$$\frac{dq_1}{dt} = -\gamma_1 q_1 - \frac{ab}{\gamma_2} q_1^3$$

which have zero steady state solution for $\gamma_1 > 0$ and non-zero for $\gamma_1 < 0$.
q_1 can now be seen as a "force" but which obeys equation of motion itself.
The same idea can be repeated for more complex systems. One should separate stable modes with finite positive damping and assume that they are slaved by remaining order parameters, for which damping can become very small or even negative when external parameters of the problem change.

This approach obviously has it's limitations, but gives some kind of intuitive picture.

We now consider some examples of self-organization.

3. **Reaction-Diffusion Model** :

Probably, the most famous early examples of self-organization phenomena are reaction-diffusion equations describing autocatalytic chemical reactions. To clarify the mechanism of the appearance of temporal and spatial order, consider first the simplified case without diffusion. Assume that we are interested in chemical reaction

$$A \to X$$
$$2X + Y \to 3X$$
$$B + X \to Y + D$$
$$X \to E$$

Where concentration of initial and final products A, B, D and E are maintained constant (open system) whereas two intermediate components X and Y may have concentrations that change in time. To investigate temporal behavior of these concentrations assume that the production rate of the reaction is proportional to the product of the concentrations of reactants and a reaction rate that is taken to be

1 for simplicity. Inverse reactions can be ignored since far from equilibrium state is considered. The kinetic equations then read:

$$\frac{dX}{dt} = A + X^2Y - BX - X$$
$$\frac{dY}{dt} = BX - X^2Y$$

Which admits the steady state

$$X_0 = A$$
$$Y_0 = \frac{B}{A}$$

Linearizing this system around this point and applying the normal mode analysis, it is easy to see that for

$$B > 1 + A^2$$

the steady state solution becomes unstable. More detailed investigations show that the system has a limit cycle, i.e. for any initial concentrations X and Y the system approaches the same periodic trajectory. The oscillation frequency depends only on A and B, but not on the staring point in XY space, thus one can say that temporal self-organization has occurred (in contrary with Lotka-Volterra equation where frequency of oscillation depends on initial displacement from steady state solution, see below).

Even more interesting event happen when diffusion is included into consideration. It is done by considering X and Y as functions of both time and coordinates and including the terms describing change of concentration at a given point due to diffusion. equations then read:

$$\frac{dX}{dt} = A + X^2Y - BX - X + D_X\frac{\partial^2 X}{\partial r^2}$$
$$\frac{dY}{dt} = BX - X^2Y + D_Y\frac{\partial^2 Y}{\partial r^2}$$

This system is called "Brusselator". It was proposed by Ilya Prigogine and his collaborators at the Free University of Brussels. Another famous example of reaction-diffusion model is called "Oregonator".

It terns out that these models exhibit quite complicated spatially and temporally self-organized structures when sufficiently far from equilibrium.

The time evolution of spatial structure obtained by numerical computations as well as in real experiment is shown in Fig.4

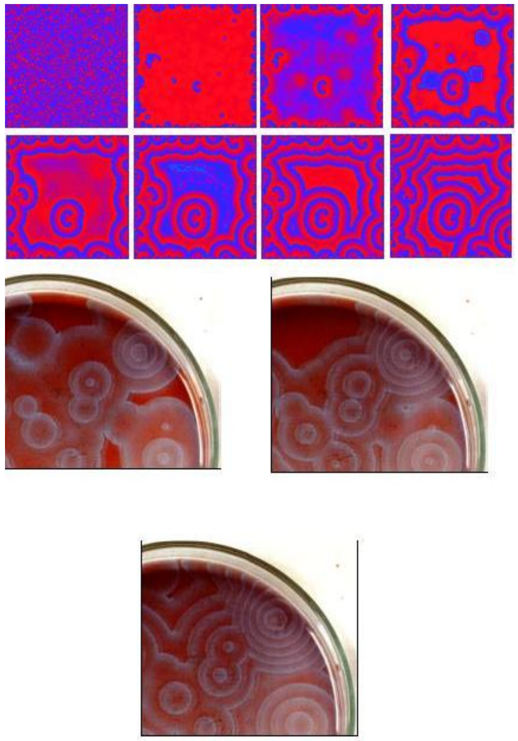

Fig.4 (from [3])

It should be mentioned that the above approach to reaction-diffusion equations, namely rate equations approach, is in some sense a mean field theory. One can also introduce probability distributions $P_X(N,t)$ of finding N molecules of type X at time t and establish the master equation for the temporal change of $P_X(N,t)$. One can then write an equation for temporal change of average number of molecules $\langle N_x \rangle$. The resulting equation is in complete agreement with "mean field theory" discussed above only if P is a Poisson distribution, which is generally not true far from equilibrium.

4. **Ecology, Population-Dynamics.** :

Non-equilibrium phenomena and self-organization play a central role in population biology. Attempts to understand distribution and abundance of species by modeling the ecological system as a dissipative system, started with Lotka-Volterra equations. This is a system of first order non-linear equations modeling the dynamics of biological system consisting of one predator and one prey species. The equations read:

$$\frac{dx}{dt} = x(\alpha - \beta y)$$
$$\frac{dy}{dt} = -y(\gamma - \delta x)$$

Where x is a number of prey and y - number of predator.

Non-zero fixed point of this system has a marginal stability. This means that being disturbed from steady state by fluctuations, the system performs cycles around this steady state, number of predators and prey oscillate around their steady state values. Frequency of the oscillations, however, depends on the initial deviation from these values, which doesn't allow us to call this periodicity temporal self-organization.

I now want to focus on recent research done by Szabo and Czaran who studied more sophisticated ecological model with predator-prey relations and observed the self-organizing pattern [4].

The authors of the paper consider a system of 9 species of bacteria each of them being "eaten" by another 3 species, being able to "eat" 3 species and being competitively neutral with remaining 2 (and itself).
The authors start by writing the system of equations for the time evolution of the population

$$\frac{d\rho_i}{dt} = \rho_i \sum_j A_{ij}\rho_j$$

Where A_{ij} is an adjacency matrix of the competition network. $A_{ij} = 1$ if i is superior to j, $A_{ij} = -1$ if i is inferior to j and zero otherwise.
These equations represent a kind of mean field theory for a given problem, which doesn't include any spatial characteristics of the system. Basically, it is the same approach as Lotka-Volterra model with birth and death rates being equal for each of the species ($\alpha = \gamma = 0$).
Because of the symmetry of matrix A (which is a fact specific to the model) one can find few conserved quantities, for example the product of three densities within each cyclic defensive alliance (the group of three species with competitive relations $1 \to 2 \to 3 \to 1$) remains constant. This fact somehow singles out these groups of three species which will act as alliance even after including spatial distribution into consideration.
The spatial model is realized on the square lattice with periodic boundary conditions and solved by Monte Carlo method. Each site is occupied by a single bacteria. The dynamics of the population is driven by interactions between neighboring sites - competitive replacements and diffusion events. The diffusion is realized as non-zero probability X for the two mutually neutral but different bacteria to switch places if they happened to be at neighboring sites.
It terns out the final state of such system depends drastically on the diffusion probability X. For $X < X_{c1}$ the system started from uncorrelated distribution evolves into domains of the three cyclic defensive alliances. (See Fig.1) Each alliance consists of tree types of bacteria coexisting in the same spatial region. These groups of three correspond to those found in the mean field theory approximation. Note that ignoring all other species (they are spatially separated) the mean field equations for the members of alliance are satisfied if densities of all members are equal. The domains grow with time and, since the lattice is finite, of them (with equal chances) will take over eventually.

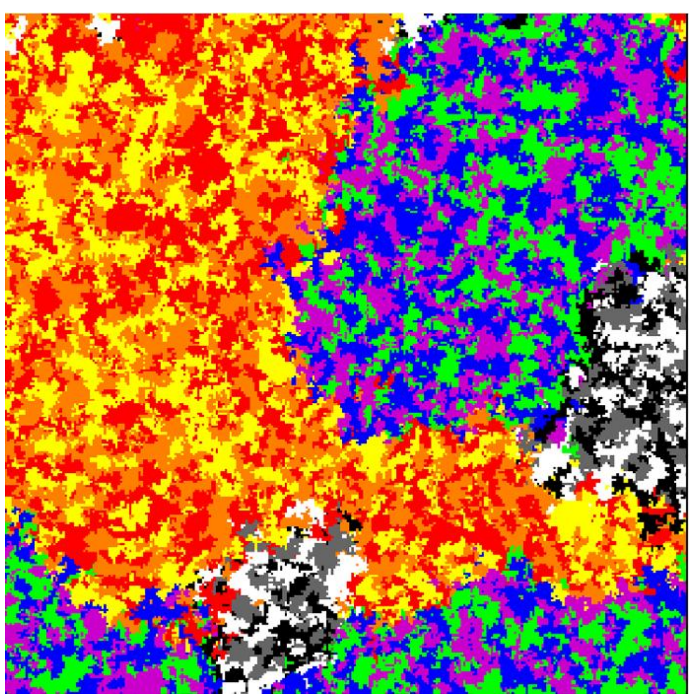
Fig.1 (from [4])

When diffusion probability is increased, two subsequent phase transitions occurs. Let me describe the third phase (large values of X). For the large diffusion probability the system forms again three domains but this domains consist of mutually neutral species (see Fig.2). It is interesting that these domains themselves form a cyclic dominant structure. The alliance 1 (for example) dominates alliance 2, alliance 2 dominates the 3-d one, and alliance 3 dominates alliance 1. So we have the same steady state situation as in the first phase, but now for the alliances of mutually neutral species. The domain walls will now move in a cyclic manner, leaving the average domain sizes (dependent on X) constant. One can say that self-organization pattern controlled by diffusion probability X appeared.

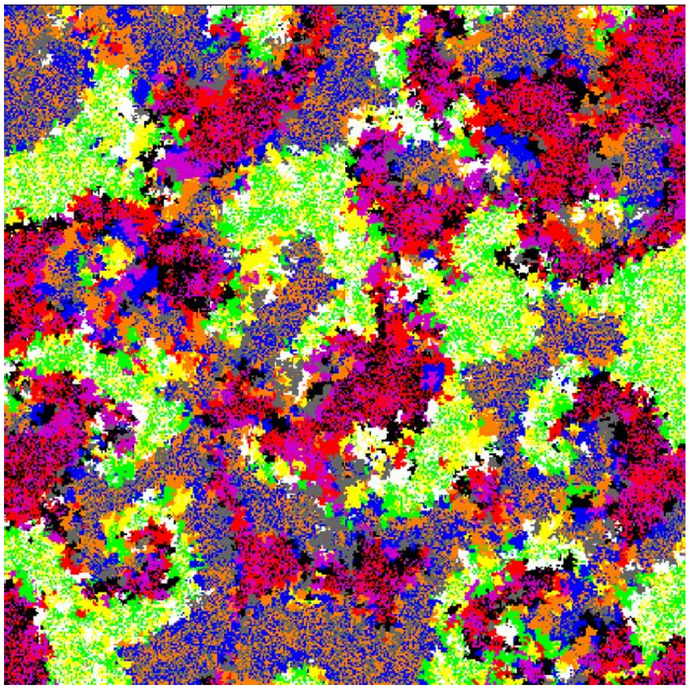

Fig.2 (from [4])

The second phase (intermediate values of X) resembles both the first and the third phase (See Fig.3). The evidence of the two phase transitions though is the discontinuity in the behavior of quantity p_n which is the probability of finding two neutral pairs on two neighboring sites. As pointed out by authors, quantitative analysis of fluctuations also indicate striking differences between these phases.

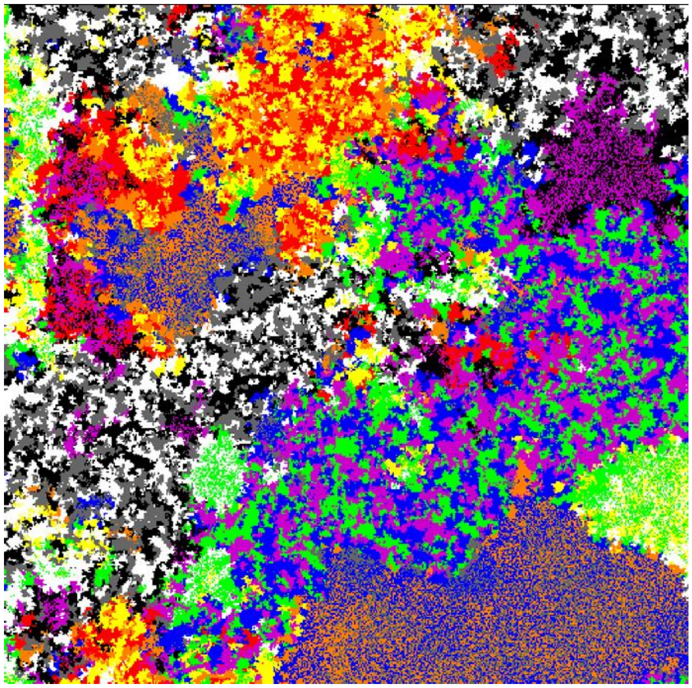
Fig.3 (from [4])

It should be pointed out, that essential role in deriving the results above played the symmetry of the problem - all invasion rates were considered to be equal, which is definitely a reduction of possibilities. Further development of the same idea but in a less symmetric problem is given in [5], where six-species predator-prey model with two different invasion rates is studied. Self-organizing spatio-temporal pattern in which the three alliances of neutral pairs dominate cyclically each other is observed in this model. In addition, the new phase is found where both the domains of cyclic three-species alliances and the neutral two-species alliances can coexist.

5. **References**:

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[5]Gyorgy Szabo, Attila Szolnoki, and Istvan Borsos, Self-organizing patterns maintained by competing associations in a six-species predator-prey model, (February 2008)