AUTOCATALYSIS AS THE NATURAL PHILOSOPHY UNDERLYING COMPLEXITY AND BIOLOGICAL EVOLUTION

Güngör Gündüz*

Department of Chemical Engineering, Middle East Technical University Ankara, Turkey

Regular article

Received: 28. March 2011. Accepted: 27. June 2011.

ABSTRACT

The importance and different aspects of autocatalysis in evolution was analyzed. The behaviour of autocatalytic reactions mainly the Lotka-Volterra and the Schlögl equations were discussed in terms of phase change, entropy, and their oscillation frequency. The increase of complexity as the general direction of evolution was examined on some patterns in terms of both their entropy and information content. In addition, the relation between stability and functionality, stability and cohesion were discussed. It was concluded that evolution drifts in the direction of increasing complexity as a kind of natural philosophy to counteract the increase of entropy in the universe.

KEY WORDS

autocatalysis, entropy, evolution, complexity, information, oscillation frequency, cohesion

CLASSIFICATION

JEL: C02, Z19 PACS: 01.70.+w, 89.75.-k

INTRODUCTION

The theory of biological evolution did not only have a spectacular impact on human knowledge of biological systems, but also founded a close relationship between many disciplines of science such as, chemistry, physics, geology, and philosophy; yet sociology, psychology, economy, and similar other fields use evolutionary concepts to evaluate long term changes. In early 19th century physical and chemical principles had not yet been strongly introduced into biology, and Darwin could make his reasoning on some philosophical and observational facts. He used the 'causality principle' of ancient natural philosophy and Newtonian mechanics to establish a physical ground for the evolution of living organisms. He considered the Malthus principle of 'limited food supplies but geometric multiplication of populations' as the driving force in Newtonian sense for the fight for survival. And then Adam Smith's principle of economic progress 'speciation brings in gain for competition' helped Darwin to come up with the idea of 'competition for food is the driving force, and speciation may bring in advantage for survival'. The molecular basis of 'speciation' could be understood decades later with mutations on DNA through different mechanisms which could be described by statistical mechanics, chemical kinetics, and biochemical interactions. The intricate relations of parameters in evolution are too complicated [1].

The apparent paradox between the entropy principle and the evolution has been the concern of physicists, because the former drifts everything in the universe into disorder while evolution drifts into order and complexity. Schrödinger's suggestion 'living things feed on negative entropy' somehow surmounts the problem, but stays as a natural fact rather than a proof. The problem has been much better tackled by the concepts of nonequilibrium thermodynamics, nonlinear phenomena, chaos, and complexity. In the last few decades the nonlinear theory revolutionized our understanding of natural phenomena, because, most natural phenomena come out through a process, and in the words of Prigogine anything which comes out through a process is 'happening', not an 'event'. Time appears in almost all physical equations as second order derivative, and the physical equations cannot differentiate between the past and future; that is, $t \rightarrow -t$ substitution leaves the physical equation invariant, therefore most of the equations of physics describe 'event' not 'happening'. However, Boltzmann's H-theorem is first order in time, and entropy has a time direction. In nonlinear theory the evolution of any process is described by multiple equations which provide correlation of some of the parameters, and the irreversibility is naturally embedded within the process. It is now generally accepted that irreversibility is not identical to entropy but more than that. Irreversibility can increase both entropy and information, and the increase of information content of a system runs parallel with the increase of its complexity. Complexity is not sufficient for survival but it is necessary [2].

'Competition for survival' can well explain the mechanism of natural selection but lacks to explain the 'molecular evolution' in nonliving world. Darwin's second important contribution to the 'selection' mechanism of evolution is 'sexual selection' which does not also a have direct correspondence in nonliving world, but 'chemical affinity' may somehow explain the preference of occurrence of certain products in the soup of many reactant chemicals. The 'adaptability' of living organisms can be explained in terms of 'thermodynamic stability'. In Ancient times the philosopher Thales claimed that magnet has the properties of animate because it moves. Hippias and later Aristotle objected to this idea and they said magnets do not have the fundamental attributes of animates such as, autonomous locomotion, perception, primitive desires, judgment, and act of will. In biological world discussion goes on viruses whether they are living species or not. The fundamental property of all living organisms is that they self-multiply, and viruses cannot do it by themselves but must use host cells. The

theories proposed to explain evolution must in fact come out from very general natural principles, and physical laws. Evolution is one of the most general natural phenomenon, therefore, evolution theories must also base on very general universal facts. The first biological evolution theory in the history was proposed by the great philosopher Anaximander (~610-550 BC), and irreversibility of forms once generated plays a predominant role in his explanation of the existence of different species in nature. He was the first person before Darwin claiming that all living beings sprang out of sea long ago.

All living organisms desire to multiply, and so do viruses. In nonliving world the increase of entropy also fragments the objects and increases the number of pieces, but this is not self-multiplication. There are different examples on similarity growth in nonliving world such as crystal growth, or chain growth of a polymer where monomers combine to make bigger and complex structure. The question is then, does entropy decrease in crystal growth or polymer chain growth as in the case of living organisms? In fact they are both ordered structures. Whether it is biological world or nonliving world self-multiplication stands as the most general phenomenon to understand evolution in the most general sense. It is better to use the term 'autocatalysis' instead of self-multiplication, because it involves the concept of converting others into itself usually in an irreversible manner.

AUTOCATALISYS

An autocatalytic reaction is simply given by $A+B \xrightarrow{k} A+A$, where the reactant A converts B into A, and the product is all A. The chemical reaction rate constant 'k' denotes the probability of reactions taking place. Fisher proposed in early 1920s that prey-predator interactions are random phenomena like the collisions of atoms. Around the same time Lotka proposed a chemical kinetic basis of prey-predator interactions, and the model was improved by Volterra in 1930s. Considering only three species grass (G), rabbit (R), and fox (F) we can write their interactions in the form of the following chemical reactions.

$$G + R \xrightarrow{k_l} R + R$$
(1)

$$R + F \xrightarrow{k_2} F + F$$
(2)

$$F \xrightarrow{k_3} E$$
 (3)

The differential equations governing the rate of growth of rabbit and fox can be given by,

$$\frac{dR}{dt} = k_1' GR - k_2 RF = k_1 R - k_2 \beta_R^{-1} RF$$
(4)

$$\frac{dF}{dt} = k_2 \beta_F^{-l} RF - k_3 F \tag{5}$$

where the rates are based on the number of species on the right side of equations since each rate is irreversible, and *R* and *F* denote the number of rabbits and foxes, respectively. Volterra called the constant β^1 equivalence number. Specifically, β_R^{-1} denotes the ratio of number of rabbits lost per unit time to the number of foxes gained. The solution of these equations yield sinusoidal change for both species and one can simply show this by Fig. 1.

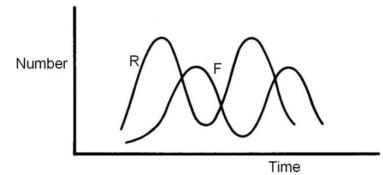


Figure 1. Change of rabbit-fox populations in Lotka-Volterra problem.

The increase of rabbit population makes increased amount of food available for fox, which, in turn increases in number in time. Then rabbit population decreases, and after a while some of foxes die due to starvation and fox population also starts to decrease with a time lag. Then rabbit population starts to increase, and so on. The kinetics of reactions entirely depend on the chemical reaction constant 'k' in (4) and (5). We can interpret 'k' in terms of characteristic properties of prey and predator. The meaning of 'k' is very clear for two interacting gas molecules 'A' and 'B'. For A and B to react the sum of their kinetic energies must be above a threshold energy so-called activation energy.

In Lotka-Volterra problem 'k' is a resulting constant of all properties and characteristics of animals. For instance in (4) and (5) ' k_2 ' denotes the ability of foxes to catch rabbits. For simplicity we may not mind about most of the biological characteristics such as vision, hearing, being at alert, brain functions, etc. of the both animals but consider only their ability to run. So we can show their speed distribution by the first distribution in Fig. 2.

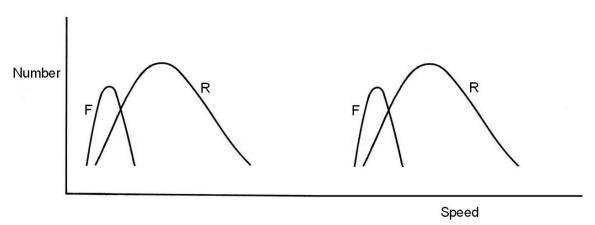


Figure 2. Speed distribution of prey (R) and predator (F).

It is clear that only fast running preys can survive as they can easily run away from the predators, and also only fast running predators can survive as they have advantage over low speed predators for catching low speed preys. In this respect the mechanism of survival has resemblance to the dynamics of chemical interaction, i.e. equations (1)-(5) are based on this principle. Evolution tells us that in the long run the characteristics of species change; and in our simple case both prey and predator evolve to become fast runners as in the second distribution of Fig. 2. The distribution of F&R at higher speeds (e.g. the second case) is an oversimplification, and it can occur only if the proportions among k_1 , k_2 , and k_3 do not change. However k_1 , k_2 , and k_3 at higher speeds are naturally different than the ones at lower speeds. This is, because, even for simple gas molecules chemical reactivity expressed in terms of rate constant 'k' depends on energy (i.e. on temperature) through Arrhenius or

similar relations. The change of 'k' with temperature is actually due to increase of kinetic energies of molecules, which, changes the impact parameter between colliding molecules. In turn, the number of electronic excitations increase and more number of molecules get involved in reaction. The occurrence of any chemical reaction changes either thermal or configurational entropy, or both; otherwise, the product molecule wouldn't be stable. A change of entropy does not warrant the persistence of the new state occurred; it is likely that the process may reverse. However, evolution is an irreversible process in the long run.

ENTROPY OF OSCILLATING SYSTEMS

The entropy of prey-predator can be determined by following the usual procedure. The change of chemical potential ' μ ' due to change in number from a steady ' n_s ' by a fluctuating number of 'n'' can be given by the following equation where R_G is gas constant.

$$\mu - \mu_s = R_G T \log \frac{n}{n_s} = R_G T \ln \left(\frac{n_s + n'}{n_s}\right) = R_G T \log \left(1 + \frac{n'}{n_s}\right) \approx R_G T \left(\frac{n'}{n_s}\right)$$
(6)

The entropy production rate ' σ ' due to fluctuations in populations can be expressed by,

$$\sigma = \frac{dS}{dt} = \sum_{j} X_{j} J_{j} = \frac{1}{T} \sum_{l}^{k} \left[-\mu_{l} \frac{dn_{l}'}{dt} \right] = \frac{1}{T} \left[-\mu_{R} \frac{dn_{R}'}{dt} - \mu_{F} \frac{dn_{F}'}{dt} \right]$$
(7)

where J is reaction rate (i.e. flux), and X is the gradient of the driving force. The substitution of (6) into (7), along with replacing $n_R = R$, and $n_F = F$ gives,

$$\sigma \approx R_{\rm G} \left[-\frac{R'}{R_s} \frac{dR'}{dt} - \frac{F'}{F_s} \frac{dF'}{dt} \right]$$
(8)

One can also show after some algebra that,

$$\frac{dR'}{dt} = -k_2 \beta_R^{-l} R_s F'$$

$$\frac{dF'}{dt} = k_2 \beta_F^{-l} F_s R'$$
(9)

Now these two equations can be substituted in (8) to find entropy. However, (8) does not include equivalence numbers which need to be introduced. Then one gets,

$$\sigma \approx R_G k_2 \left(R'F' - F'R' \right) = 0 \tag{11}$$

This shows that the system is stable against small fluctuations around the steady state values. The system rotates around the steady state without getting into it. The point corresponding to the steady state is a center. In other words the oscillating populations as shown in Fig. 1 do not produce any entropy. So we can say that autocatalytic processes do not produce entropy but provide oscillations in the system. Zero entropy change means the system resists to persistent changes, and the system accomplishes this by moving from a thermodynamic equilibrium point to a limit cycle, because, the plot of the change of populations of prey and predator with respect to each other gives a limit cycle. So the Lotka-Volterra model or other kinetic models cannot explain the irreversible and persistent changes in the course of evolution.

The persistent changes in evolution yield new changes in the shapes of living organisms, and these structural changes can be discussed in terms of 'configurational entropy'. The structural changes come out from the accumulation of mutations on DNA, and therefore configurational entropy has one-to-one correspondence with the change of mutations and thus the information content of DNA, as if the change of the meaning of a word by changing the order of characters. The mutations thus change the constants ' k_i ' for all types of interactions of

species, their physical abilities to sense preys or predators around, their communications with the things in their environments, and thus their abilities for their fitness or adaptability, their sexual attraction, etc. Therefore the shape of the second distribution in Fig. 2 depends on how k_1' , k_2' and k_3' change in time with respect to each other. Actually, the constants are time dependent for an evolutionary process, and the differential equations like (4) and (5) must involve time dependent rate constants; but there is no way to express the exact timely changes of k' values as nobody knows the future pathways of evolution; nevertheless, short term predictions can be done for the evolutionary dynamics of interaction rates between species since k' does not change fast in time. All dynamical equations of physics like classical mechanics, electromagnetism, relativity, and quantum are insensitive (i.e. exhibit symmetry) to the change of sign of time; one cannot go to past or future, and they tell exactly what happens at present. The only equation which has a time direction is Boltzmann's H-theorem as mentioned earlier, though Lorentz and coriolis forces have some kind of time symmetry problems. Therefore evolution has a very close relation to entropy, because both have time direction.

DIRECTION OF EVOLUTION

Evolution has two fundamental characteristics, (i) time asymmetric, and (ii) drifts to higher complexity. The former is like entropy, while the second is exactly opposite to entropy. In the philosophical sense evolution stands as the dialectic counter part of entropy, they share a common root (i.e. time asymmetry or irreversibility), and they also contradict each other; entropy drifts the system towards fragmentation in time while evolution pushes the existing system towards complexity. Irreversibility is not identical to entropy and disorder, it can also generate order.

In the earlier discussions it was shown that the creation of order in the form of periodic oscillations in time domain from disorder (e.g. from Maxwellian like distributions) is possible through autocatalytic reactions (e.g. Lotka-Volterra problem). It was also shown that such systems do not exhibit irreversibility as they have zero entropy for overall change. The irreversibility in autocatalytic reactions comes out through nonlinear or chaotic growth.

The simplest autocatalytic reaction is the growth of microorganisms on an agar plate, and first studied and modeled by Verhulst in 1870s. The rate of growth of population 'x' on agar obeys the following equation,

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \mu x (1 - x). \tag{12}$$

where the constant ' μ ' denotes the growth rate constant. Then on, there have been several models for population growth but logistic equation popularized by May has drawn much attention used for discrete time demographic model [3]. It is nonlinear difference equation, and given by

$$x_{n+1} = \mu x_n (1 - x_n). \tag{13}$$

The population x_n becomes x_{n+1} after a discrete time interval. There are two parameters here; x_n corresponds to the growth parameter whereas $(1 - x_n)$ corresponds to the controlling parameter. The large magnitudes of μ can push the system into chaotic growth. In fact the growth described by the Verhulst and the Lotka-Volterra equations can be chaotic depending on the magnitude of μ [4, 5].

Whether the change of population is oscillatory or chaotic does not help to understand the persistent change due to evolution. However nonlinear dynamics and chaos has a number of interesting properties exhibited exactly by evolution, and they can be summarized as:

• it is irreversible; you cannot revert the anatomy of man to its homo erectus or earlier shape,

- irreversibility introduces pattern formation; the anatomy of organisms change in a persistent way,
- entropy increases with irreversibility; the higher the extent of irreversibility the higher the entropy produced. The larger the extent the species changed in evolution, the less they are alike to their ancestors,
- pattern formation occurs through the change of parameters (or dimensions) at certain proportions. The scaling of dimensions gives 'fractal dimension'. The course of evolution results in dimensional changes and the proportions in anatomic changes may follow scaling relations that can be traced from the measurements on fossils. These changes can even turn into geometric proportions as first noted by D'Arcy Thomson [6],
- system has memory; all organisms carry the memory of their parents, the closer the chronological parent the more it is memorized. Darwin noticed that the toe of human fetus separates out from forefinger as in monkeys, but then comes back near forefinger before birth. Human coccyx is a remnant of tail,
- the thermodynamics of chaos is non-equilibrium thermodynamics, and resonance interactions may dominate over random interactions. A chaotic system has many periodicities and thus frequencies, so resonance interactions play an important role. Organisms exhibit cyclic or periodic behaviors. Seasonal migration of birds, butterflies, etc., hatching or menstruation in some animals in integer multiples of seven days in accordance with periods of tides, and insect clocks all imply the periodicities involved in the lives of organisms [7],
- the complexity increases as the system grows; the complexity of evolved organisms increased in the course of evolution from prokaryotes to humans.

All these similarities between chaos and evolution introduced a new aspect to understand the dynamics of evolution [8-12]. What is naturally selected, sexually selected, adapted to environment, or has better fitness, etc., can be all expressed in terms of interaction rate constant k in mathematical modeling. It is the collection of k's of all kinds, and the coordination of the appropriate biochemical reactions that provide survival. At the molecular level it is the information content of DNA that determines the values of different k's of an organism. The change of k is possible only if mutations occur on DNA by changing the order of existing bases. In other words information originates from the sequence of several bases; that is, a segment of polymeric chain generates information. Naturally, some mutations are passive, and the information content is not actively changed.

ENTROPY, INFORMATION, AND COMPLEXITY

According to Ancient philosopher Anaxagoras 'there is everything in anything, and everything in nature is *sperma* (i.e. seed)', and some sperma multiplies itself and becomes dominant. Finally the attributes of objects result in from the dominant spermas. According to this way of thinking atoms are sperma of molecules, molecules are of higher order structures, unit cells are of crystals, monomers are of polymers, nucleotides are of DNA, words are of sentences, musical notes are of melodies, and individuals are of society. Whether it is biological, or social, cultural, molecular, cosmological, etc. evolution, it is the information (which is the sperma) that evolves. It is the information of 'gene' (selfish or not) that tries to multiply itself. Since evolution drifts towards complexity the information content in an evolving system should increase in a firm manner to hold up the uniformity of the system. In other words there must be a kind of synchronized correlation between components of the system. However, it is known that the entropy increases also as the complexity increases. So for an evolving system towards higher complexity the increase of information should exceed the increase of entropy. As an example consider Fig. 3.

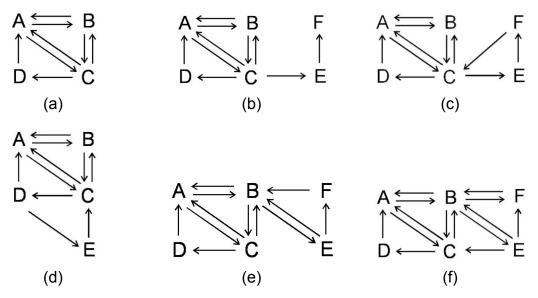


Figure 3. Evolving complexity.

Figure 3a represents a configuration made from two subsystems ACD and ABC, the former is a directed cycle, whereas the latter is reversible either direction. ACD can well represent prey-predator system of three species, as well as three subsequent information obtained from the transcription of DNA such that information A induces C which induces D, and it induces back A. The ABC cycle is an extreme case, it may not be realistic but it is mathematically important as the limiting case of extreme complexity. The entropy and information of each pattern seen in Fig. 3 can be found from the following equations utilising logarithm function with base 2:

$$S = \sum_{i} p_i \log_2 p_i \tag{14}$$

$$I = S_{\max} - S. \tag{15}$$

The probability is based on the controlling parameter, for instance D controls only A in Fig. 3a. Values calculated are tabulated in Table 1.

Figure	S	Ι
3a	1,05	1,95
3b	1,26	2,06
3c	1,52	1,94
3d	1,20	2,12
3e	1,16	2,65
3f	1,19	2,62

Table 1. Entropy and information of patterns depicted in Fig. 3.

In Fig. 3b branching occurs at C, and compared to Fig. 3a entropy increases from 1,05 to 1,26, and information from 1,95 to 2,06. The increase in entropy is more than the increase in information, that is, $\Delta S_{ba} = S_b - S_a = 0,21 > \Delta I_{ba} = I_b - I_a = 0,11$, therefore the system is not going in the direction of complexity as we go from Fig. 3a to Fig. 3b. In Fig. 3c the new triangle FCE is the mirror image of ACD. Although entropy keeps increasing ($\Delta S_{ca} = 0,47$)

information keeps almost constant ($\Delta I_{ca} = -0.01$), and therefore FCE is not recognized as something similar to ACD by the system.

However, if a new triangle is generated on the already existing ACD as DEC as seen from Fig. 3d, then entropy decreases but information increases when compared to Fig. 3c, such that $\Delta S_{dc} = -0.32$ and $\Delta I_{dc} = 0.18$. So the order in Fig. 3d is higher than the order in Fig. 3c; thus, the pattern of Fig. 3d is much more favored than the pattern of Fig. 3c. The system recognizes DEC something similar to ACD in Fig. 3d. In other words, ACD behaves as a template creating its own copy DEC, that is, ACD autocatalyzes itself, and it also acts as a kind of nucleation site. A well known and well studied example of the geometry repeating itself is Benard convection, where repetition of hexagonal pattern takes place. Here autocatalysis decreased entropy and increased order and information. If we consider Fig. 3a and 3d we see that both entropy and information increases as we go from Fig. 3a to 3d, but the increase of information is slightly more than the increase of entropy, that is, $\Delta S_{da} = 0.15 < \Delta I_{da} = 0.17$. Therefore the system is ready to go into further complexity on the repetition of the same procedure. Thus it can be said that ACD has been the generator of DEC in the mathematical sense, i.e. ACD reproduced itself in the form of DEC. In autocatalytic reactions the increase in information can come out to be more than the increase in entropy. In Fig. 3e ABC reproduced itself as BFE. Compared to Fig. 3a entropy increased little bit ($\Delta S_{ea} = 0,11$), but the increase in information is quite large ($\Delta I_{ea} = 0,70$). Fig. 3a is duplicated in Fig. 3f, that is, ABCD repeats itself as BFEC. Although Fig. 3f seems to be more symmetric than Fig. 3e the entropy slightly increases ($\Delta S_{\text{fe}} = 0.03$) but information decreases ($\Delta I_{\text{fe}} = -0.03$). It seems that there is a kind of two competing structures (or configurations) in Fig. 3f; one is ABC and BFE and the other is ACD and BEC. However in Fig. 3e E is not connected to C, and the contribution of ACD is somehow depressed by ABC and BFE. The generation of BEC in Fig. 3f enhances the contribution of the similar structure ACD, and thus each of the competitive structures make significant contributions to entropy, which, in turn, decrease information. This situation is similar to the case of entropy of mixing, where, maximum entropy is achieved when two species were mixed at equal molar concentration. The repetition of ABCD on two-dimensional surface results in tessellation, which has two different structures: one is ABC with reversible (i.e. two-way) paths and the other ACD with irreversible (i.e. one way) path. If ACD also had two-way pattern then the tessellation would be perfectly symmetrical with minimum entropy. Such structures naturally cannot easily branch and cannot easily evolve to other structures. Therefore, similarity which is provided by autocatalysis acts like the controlling parameter in evolution. In other words branching pushes the system to gain new entropies while autocatalysis counteracts and tries to decrease entropy. In wild life the increase of the population of one type of species at the expense of others naturally decreases the overall entropy of that territory. If one species overdominates through overmultiplication all others may go extinct drifting the system towards minimum entropy. Co-evolution sustains entropy at a fluctuating but certain level.

The increase of complexity of pathways for metabolic reactions or to synthesize proteins for structural materials is in accordance with the increase of the complexity of the whole organism; naturally reptiles and birds have more complexity than bugs, and mammalians than all others. The increase of complexity more or less correlates with the size of DNA; larger size implies larger information content. However this is not always true, lungfishes have much more DNA than other fishes, and amphibians than reptiles and birds. This is called 'C-paradox' and solved by the discovery of noncoding DNA.

COMPLEXITY AND PHASE CHANGE

There must be some explanation for the extraordinary increase of DNA in some species. While mammals have a mean C-value of 3,5 pg and most species less than 3,3 pg, there are some striking jumps in a some groups of organisms. For instance cartilaginous fishes have a mean C-value of 5,7 pg, amphibians 16,2 pg and lungfishes 90,4 pg [13]. These species are transient species; bone has evolved after cartilaginous fishes, atmospheric oxygen could have been utilized by lungfishes, and animal life on earth (e.g. land) has become possible with amphibians. These major changes resemble to phase changes in materials, and the group dynamics of molecules in each phase displays entirely different collective behavior; for instance molecular dynamics of carbon black is much different than that of graphite, and of liquid water than that of vapor. Mutations occurring on a certain portion of DNA are naturally expected to yield new informations, perhaps at the expense of loss of some part of previous information. Evolutionary diversification depends on gains and loss, and one can trace the diversification by studying the changes in metabolic pathways [14, 15]. Small changes if they are critical can yield sharp morphological changes [16].

For the type of information needed for major changes mutations should accumulate not on the existing part but preferably in some other parts of DNA. So the increase in the size (e.g. length) of DNA provides new regions for the accumulation of new mutations and thus new information, which, in time overwhelms the former information in an effective way, and a new group of species evolve in time. So whenever major changes are needed such as change from cartilage to bone, from fin to lung, or from sea life to land life, long DNA is needed. The network of all information resulting from the transcription of DNA, the network of protein synthesis, the network of metabolic reactions, or reactions to synthesize structural materials wouldn't depict major change in the long run if mutations took place on the already existing units of DNA. Such mutations could probably introduce smooth changes from one type of form to another such as the change of eye or skin color, or the change of length of tail, ear etc. The information needed for the major change from fin to lung should not occur on the same portion of DNA; it will cause nothing but confusion, because an organ will otherwise be two-functional, and a conflict occurs between them. However, this is not what happens in living species. For instance each enzyme has only one function and catalyzes only one reaction. Only in very primitive cases confusions are allowed, for instance overlapping transcription is allowed in viruses but not in bacteria. The absorption of dissolved oxygen in water by fins and the respiration of atmospheric oxygen by lung can be both achieved simultaneously during evolutionary period only if they are separated from each other and controlled by different network of reactions.

In evolutionary period fins and lung have the same functionality except that the mechanisms of oxygen intake are different, and the mechanism of oxygen absorption from water is substituted by the mechanism of oxygen absorption from atmosphere. This substitution reaction can be simply evaluated by autocatalytic reactions. In market economy the substitution of one commercial product in the market by a new product in time can be well evaluated by (12) or (13), i.e. by Fisher-Pryer type of equations [17, 18]. Two competing mechanisms one overwhelming the other in evolution can also be studied by the same logic. Fins and lung are two different systems though they serve the same purpose. The change from one system to another can be viewed as a change from one state to another, or from one phase to another. The question then is, 'can we understand phase change by autocatalytic reaction systems?' The answer of this question was given several decades ago by Schlögl [19]. In fact pattern formation was first studied by Turing in a seminal paper to investigate chemical morphogenesis [20]. Different autocatalytic reactions are presented in Table 2.

As mentioned earlier the Lotka-Volterra type of autocatalytic reactions yields oscillations. The intermediate agents *B* and *C* seen in the first column of Table 2 disappear in the final step, and the overall reaction is simply, $A \rightarrow E$. In the Brusselarator the overall reaction is $A + B \rightarrow D + E$, and it also gives oscillations [21]. The Schlögl equations are in between and two initial reactants transform to a single product, as $A + B \rightarrow C$.

Lotka-Volterra	Brusselator	Schlögl-1	Schlögl-2
$A + B \rightarrow B + B$	$A \rightarrow X$	<i>A+2X</i> ≥ <i>3X</i>	$A + X \gtrless 2X$
$B+C \rightarrow C+C$	$2X + Y \rightarrow 3X$	$B + X \gtrsim C$	$B + X \gtrless C$
$C \rightarrow E$	$B + X \rightarrow D + Y$		
	$X \rightarrow E$		
Overall:			

 Table 2. Autocatalytic reactions.

$A \to E \qquad A + B \to D + E \qquad A + B \gtrless C$	<i>A+B</i> ≥ <i>C</i>

The solution of Schlögl-1 gives [19],

$$k_{\rm c}C = X^3 - 3X^2 + fX \tag{16}$$

where the rate constant k_C is for the reverse direction from *C* to *B* and *X*, and $f=k_BB$ where k_B is the rate constant for the reaction of *B* and *X* to yield *C*. For f < 3 equation (16) has three possible roots. Then (16) has the same mathematical form for the first order phase transition equation, that is the Van der Waals equation or the virial equation of state given by,

$$p = \frac{RT}{V} - \frac{a_1}{V^2} + \frac{a_2}{V^3}.$$
 (17)

Actually the potential leading to this equation is fourth order in X, and it, in turn, gives a double-well solution each representing a different phase [19].

Schlögl also showed that there exists a relation between g and f as follows,

$$g = f - 2. \tag{18}$$

where $g = k_c C$. This equation is of the same form with Gibbs phase rule with zero variance, with *f* corresponding to the number of phases and *g* to the number of components. If we have a many component system (i.e. many predators besides *B*) the number of phases will change accordingly. Every persistent change is irreversible and g = 0, because $k_c \rightarrow 0$ for irreversibility, so f = 2. That is, *C* is one of the phases, and the other is A + B.

The solution of Schlögl-2 gives [19],

$$c = X^2 - (1 - b)X,$$
 (19)

where $c = k_C C$, and $b = k_B B$. Note that *c* was used instead of *g* in (19). First order transitions are reversible such as liquid-vapor transitions. However, second order transitions such as demagnetization are irreversible. The irreversibility can be imparted in the final step in Schlögl-2 by setting $k_C = 0$, which in turn yields c = 0. Then (19) gives,

$$X = \begin{cases} 1 - b, & b \le 1, \\ 0, & b > 1. \end{cases}$$
(20)

This is the condition of second order phase transition. If X, b, and c stand for the magnetization M, temperature T, and magnetic field H, respectively, then b = 1 corresponds to the critical temperature (*Curie temperature*) above which magnetization disappears.

There is in fact a close resemblance between magnetization and autocatalytic change [22]. A magnet magnetizes iron particles and converts them into new magnets, and in an autocatalytic

reaction like $A + B \rightarrow A + A$ the molecular configuration of B is converted into the molecular configuration of A. So an existing magnetic field (i.e. the predator) induces a change in the randomly configured spins and re-orientates and align them (i.e. predator uses the proteins of the prey for its own growing structure or to sustain its own molecular configuration), and as temperature increases the order is lost (i.e. if preys gain new properties beyond a threshold value, then, predators may not catch them and they die of starvation and go extinct). The same logic can be applied also to the change in DNA. If a mutation or set of mutations improve the adaptability of a species then they multiply more in number, and if mutations exceed a certain threshold the configuration on DNA so changes that the species gains a relatively strong new property or functionality not owned or weakly owned by its predecessors.

IRREVERSIBILITY AND FUNCTIONALIT

The Schlögl-1 and the Schlögl-2 equations are essentially similar, and 2X is needed in Schlögl-1 whereas only X is needed in Schlögl-2 for autocatalysis. So Schlögl-1 is more difficult to achieve than Schlögl-2, as also the case in first and second order phase transitions; the former needs large energy at the transition temperature. To have permanent change we need to have irreversibility that can be achieved when $k_{\rm C} = 0$ as mentioned above. So whether it is small changes due to mutations or sharp changes in the long run can be explained in terms of second and first order phase transitions, and the kinetics of these transitions can be explained in terms of Schlögl autocatalytic reactions. Prigogine and his colleagues studied the irreversibility by so-called Λ -transformation and the complex spectral theories. These two approaches are not equivalent [23]. However, it is very easy and somehow trivial to understand the irreversibility in chemical world in terms of chemical reactions; because, chemical reactions are noncommutative and thus persistent irreversibility is apt to survive. The irreversibility is related to the gradient of driving force, and the higher the gradient the higher the irreversibility. In nonequilibrium thermodynamics a current associated with a flow such as heat, mass, electric, or chemical change can be put into a general form of

$$J_{\rm i} = \sum_{\rm j} L_{\rm ij} X_{\rm j} \tag{21}$$

where *L* is known as phenomenological coefficient, and *X* is the gradient of the driving force. The dissipation function σ which is the rate change of entropy *S* per unit time is given by,

$$\sigma = \frac{\mathrm{d}s}{\mathrm{d}t} = \sum_{j} X_{j} J_{j} = \sum_{i} \sum_{j} L_{ij} X_{j} J_{j}. \tag{22}$$

Thus the increase of the magnitude of driving force increases the entropy production rate and thus the extent of irreversibility. River running slowly in a valley may have eddy currents pushing the flow backward whereas water flow through steep landscape is irreversible. In chemical systems the gradient disappears at equilibrium conversion, and if the chemical potential between the reactant and product is too high the equilibrium is achieved at complete conversion, which is named as irreversible reaction. Since the chemical potential of any chemical substance is never zero, there is no absolute irreversibility in the chemical sense. As a consequence, Aristotle's philosophical view of continuous 'combination-dissociation' forms the foreground of evolution. This view needs to be coupled with entropy to provide stability of the new forms, patterns or structures formed. Usually a functionality is associated with the change occurred. Otherwise too many mutations helping nothing may devastate the working system of organism, and its fight for survival may become inefficient and difficult.

Autocatalysis is a kind of intermediate step to convert A into C through employing X, which disappears in the final state, otherwise there would be no change of A into C. Although it is possible also to convert A into C by means of ordinary catalysis, this process is usually an entropy increasing process. It is very difficult to evolve complexity without autocatalysis,

which essentially minimizes entropy production and induces order which is needed for the increase of complexity. According to the Curie principal 'the symmetry of an effect is no higher than a cause'. In chemical transformations the configurations change from one form to another. The change like $A + X \rightarrow X + X$ is a symmetry increasing (i.e. entropy decreasing) process. The overall entropy increases if we consider not only the configurational but also thermal component. In fact the motions will be reversible if the driving forces depend only on geometric configurations; the irreversibility sets in when the forces or velocities of interacting components vary in time if the dependence is asymmetric [24]. The reversibility occurs if the reversibility of momentum is not different than the reversibility of time [25].

It is known from the analysis done on spin glass systems that in the low-temperature limit the ground state entropy is negative. The proof is given in literature [26] and utilizes an equation having the same mathematical form as (20). So it can be said that at ground state where fluctuations are minimized autocatalytic reactions of type Schlögl-2 also has negative entropy. It is logical to extend it to other autocatalytic reactions also.

Autocatalysis naturally inherits nonlinearity and distorts the symmetry of the Onsager's phenomenological coefficients. Consider the chemical system given in Fig. 4, where cross-effects occur.

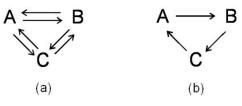


Figure 4. Reversible and irreversible cyclic reactions.

The one-way cyclic balancing seen in Fig. 4b is prohibited by the principle of detailed balancing. It says when equilibrium is established between reactants in a reaction system, any branch of reaction and its reverse must take place at the same rate or equal frequency. This is called the principle of microscopic reversibility [27]. In fact one-way cyclic reactions especially seen in ecology like 'fox feeds on bird which feeds on frog which feeds on flies, which feed on dead fox' never reach true equilibrium although asymptotically stable equilibrium is achieved; that means the change in the number of any of the species with time has oscillations. The equilibrium for the reaction seen in Fig. 4a can be achieved only when the Onsager phenomenological coefficients defined by 'L' in (23) have symmetric properties,

$$L_{11} = \frac{(k_{\rm AB} + k_{\rm AC})n_{\rm Ae}}{R}, L_{12} = -\frac{k_{\rm BA}n_{\rm Be}}{R}, L_{13} = -\frac{k_{\rm CA}n_{\rm Be}}{R}$$
(23)

where n_e refers to equilibrium numbers. The symmetry properties imparts $L_{12} = L_{21}$, $L_{23} = L_{32}$, and $L_{31} = L_{13}$. Under these conditions the irreversibility cannot be achieved and no change occurs since entropy change is zero. However the nonlinearity inherited in autocatalytic reactions as seen from (4), (5), (12), (16) and (19) distorts the equilibrium conditions and favors the temporary rise of one species against others. It naturally invalidates the Onsager principle which is good only at small driving forces which can be Taylor expanded.

According to (11) autocatalytic reactions yield zero entropy at small fluctuations. This result was achieved as the chemical potential was approximately taken to be equal to $R_{\rm G}T n'/n_{\rm S}$ which was obtained after linearization of (6). The nonlinearity can be taken into account by taking the chemical potential to be equal to $R_{\rm G}T\log(1+n'/n_{\rm S})$ from (6). Its substitution in (7) yields, for $\sigma > 0$,

$$-(k_2\beta_{\rm R}^{-1}R_{\rm S}F')\log\left(1+\frac{R'}{R_{\rm S}}\right)(-k_2\beta_{\rm F}^{-1}F_{\rm S}R')\log\left(1+\frac{F'}{F_{\rm S}}\right) > 0.$$
(24)

It can be put into the form,

where

$$\left(1 + \frac{R'}{R_{\rm S}}\right) < \left(1 + \frac{F'}{F_{\rm S}}\right)^{\alpha} \tag{25}$$

$$\alpha = \frac{R'}{F'} \frac{F_{\rm S}}{R_{\rm S}} \frac{\beta_{\rm F}'}{\beta_{\rm R}'}.$$
(26)

The fox population is always smaller than rabbit population, so it is logical to assume that $F_S \ll R_s$. So it is logical to assume $R'/R_S \ll F'/F_S$. By using the series expansion,

$$(1+x)\alpha = 1 + \alpha x + \dots$$
 (27)

we can write (25) in the form,

$$1 + \frac{R'}{R_{\rm S}} < 1 + \alpha \frac{F'}{F_{\rm S}}.$$
 (28)

Its simplification gives,

$$\frac{\beta_{\rm F}}{\beta_{\rm R}} > 1. \tag{29}$$

This condition seems trivial but it is essential to get irreversibility (e.g. $\sigma > 0$) in evolution. The number of predators lost must be sufficiently high to satisfy (29) in a three-body system. However, it does not have to be so in a many-species system of wild life, because, different possibilities may result in different varying ratios for (29) in the network formed from many feeding pathways. However, (29) essentially points out that the Malthus principle of 'limited food supplies but geometric multiplication of populations' can constitute the very basic irreversibility principle in evolution. In fact, Boltzmann believed that nonlinearity in the universe may underlie the origin of irreversibility.

Autocatalytic reactions tend to lower entropy as they push the system towards the domination of one type of species, but they also introduce irreversibility if the dominance of one species is controlled by rate of birth of preys and hunting capabilities of predators. In other words the coexistence and coevolution of many species provides sustainability and persistence of prevailing situation; the more the number of species the less the dominance of one species, and the more the irreversibility.

Another important implication of (29) is that the number of preys must be more than the number of predators, because, not all molecules of preys hunted by predators are transformed into molecules of new borne predators. So (29) is a kind of efficiency relation in terms of material content of species. In fact, in classical thermodynamics there is a very close relation between entropy and efficiency; the high entropy production leads to lower efficiency. Efficiency is inherent to all real processes taking place in a finite time interval in nature, and thus entropy production or irreversibility is inherent to all processes. Autocatalysis tries to minimize entropy production, but its inherent nonlinearity leads to entropy production, and thus provides irreversibility.

As a summary we can notice that autocatalysis introduces several fundamental issues; (i) it provides oscillatory changes between species as in Schlögl-1 and Schlögl-2 given in Table 2, (ii) lowers entropy due to speciation, (iii) leads to complexity, and (iv) provides nonlinearity and the reversibility of momentum becomes different than the reversibility of time; in other words, the reaction like Schlögl-2 prevails in evolutionary systems with $k_c = 0$. In fact this last property is the most important property of autocatalysis. It lowers configurational entropy but its nonlinear dynamics imparts irreversibility. The oscillations of autocatalytic reactions damp in time due to decrease of one of the components, and finally terminate with a pattern formation which is an irreversible end. A good example to this is Belousov-Zhabotinsky reactions [28, 29]. In biological evolution the rate constants *k*'s change in time as mentioned earlier, which in turn change the oscillatory dynamic balance (or quasi-equilibrium) between species. As a result new equilibria are established even though some of the species may go extinct or new species come into occurrence in the long run.

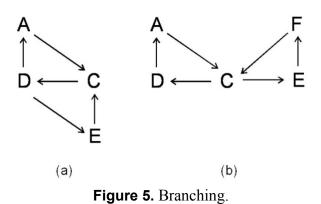
Let us assume certain functionality was achieved after a series of phenomenon as a useful property for the organism. If another one achieves slightly different mutations but gains the same property in a less cumbersome series of steps of reactions, then the second organism spends less energy in the overall and may utilize its remaining energy in somewhere else to achieve additional property. So the second organism gains higher chance for its survival. In other words the configurations of networks of biochemical reactions form the basis of the efficiency of the system. It, in turn, affects both the present adaptability of the species to their environment, and also the potentiality of their offsprings to the conditions in future. In fact the final system evolves from the contribution of many interactions. It is not only the network of reactions but also the chemical rate constants affect the efficiency of reactions. Two systems with same set of chemical reactions having different rate constants yield different entropies, because, entropy generated in the steps of reactions will be different. So in the overall the Kolmogorov-Sinai entropy will be different, and in the final step different configurations or patterns either in the form of network of reaction pathways or in the form of anatomical structure will come out. So reaction rate constant has decisive effect both on the form of final state, and also on the extent of irreversibility.

In nonlinear or chaotic growth entropy and complexity both tend to increase together. The pattern formation in chaotic growth or any change of form is mainly determined by the existence of singular or fixed points. In chemical reaction network systems the number densities, the reaction rate constants, and the equilibrium constants of reversible reactions all play important roles for the value of fixed points besides the way the pathways of the network are connected to each other. These parameters, therefore, also determine the way functionality evolves and also the memory developed since memory is related to fixed points [30].

The gain of information through mutations may not always be useful for a single species, but it is good for the entire herd; the more the mutations in the herd the more the chance to achieve future equilibrium for some of them. Mutations leading to functionality are the useful ones for success in survival. There, autocatalysis plays an important role; the set of reactions leading to functionality should be amplified. That is, a pattern representing certain functionality should form with high efficiency. In the chaotic behavior of logistic curve entropy keeps constant between two bifurcation points, but it increases right after the bifurcation [31]. Autocatalysis can reduce the increase of entropy while information content or complexity keeps increasing at larger extents, meanwhile the number of functionality. It is the complex property or quality not quantitative measures that evolve. Entropy increases fragmentation and quantity, evolution counteracts against fragmentation and enhances the complexity of properties.

The functionality must be unique and must not be interfered by other interactions. If we eliminate the B-pathways and the reversing paths in Fig. 3d and Fig. 3c we get Fig. 5a and Fig. 5b, respectively.

Figure 5a is a four component system, and Fig. 5b is a five component system. It is clear that Fig. 5a has lower entropy than Fig. 5b. This is, because, CD is common for both ACD and CDE in Fig. 5a, and ACD truly autocatalyzes itself in the form of CDE. In Fig. 5a C controls only D, and D controls both A and E, whereas in Fig. 5b C controls both D and E. The asymmetry in Fig. 5b leads to an increase in entropy, and thus Fig. 5b has relatively higher irreversibility



than Fig. 5a. In Fig. 5a the new patterns can be achieved through the growth on DE and CE. However, in Fig. 5b the new patterns can be achieved through the growth on CE, EF, and CF. In other words, CEF in Fig. 5b has three degrees of freedom while CDE in Fig. 5a has two degrees of freedom. Therefore Fig. 5b is more likely to result in more new patterns and thus associated functionalities. The increase of entropy naturally leads to new possibilities and thus branching in network configurations. In chaotic dynamics the changes are so sensitive to initial conditions that a tiny change can lead to an abrupt great change since differentiability is lost in chaos. Actually in chaos the frequent bifurcation points represent branching, and so the higher the chaos the more the chance for new patterns or new functionalities. Chaos brings in higher chance for differentiation.

The increase of the number of functionalities in a system is usually achieved through the increase of complexity. However, a specific functionality has its own set of operations and interactions not much interfered by others. Otherwise specific jobs couldn't be achieved. For instance, each enzyme does have and actually should have only one job. In this respect its functionality is unique and persistent. To achieve the stability the molecular size of enzymes are usually huge, and thus the configuration of the active site is not disturbed. So the evolution of a specific functionality takes place at the expense of the decrease of interfering reactions. For instance if we write down the entire chemical rate equations and put the rate expressions into a matrix form, then the matrix belonging to Fig. 3c will have less number of matrix elements than that of Fig. 3f; the former has 20 zeros while the latter has 15 zeros in the matrix. If we let F to denote certain functionality then it is controlled only by E in Fig. 3c, but by both E and B in Fig. 3f. The interference by B decreases the persistence of F and its due function in Fig. 3f. The symmetry breaking is necessary for the generation of new functionalities. There are more reversible reactions and thus more number of interfering elements in Fig. 3f than in Fig. 3c. So Fig. 3c is more likely to generate new functionalities. A similar situation also occurs in the transcription of DNA. The segment transcripted serves only one job, and some part of the same segment is never transcripted for another job, that is no overlapping occurs. However, overlapping transcription is allowed in viruses as mentioned earlier, which are the most primitive and the least complex organisms.

OSCILLATION FREQUENCY

As mentioned before a simple Lotka-Volterra system is an oscillatory system with zero entropy production. These oscillations originate from stochastic behavior, and are not limit cycle found in rate equations [32, 33]. The frequency of oscillations can be evaluated by linearizing the set of equations given by (4) and (5). That is, we look for the solution in the form,

$$R = R_{\rm s} + R' e^{\omega t} \text{ and } F = F_{\rm s} + F' e^{\omega t}, \tag{30}$$

where R_s and F_s are steady state values of R and F, respectively; and they can be found in terms of rate constants by setting the rate equations (i.e. eq.4 and 5) to zero. R' and F' are the fluctuations around their steady state values. Equation (30) can be substituted in (4) and (5) and the solution for ω can be obtained after linearization. One then gets,

$$\omega = \pm i \sqrt{k_1 k_3} \tag{31}$$

It is seen that ω is pure imaginary quantity and periodic fluctuations are undamped, that is, the oscillatory behavior seen in Fig. 1 lasts forever. The oscillation frequency is given as

$$v = \frac{\omega}{2\pi} = \frac{\sqrt{k_1 k_3}}{2\pi}.$$
(32)

The Lotka-Volterra problem can be expanded to include more species as seen from the first column of Table 3.

Expanded Lotka-Volterra	Branched Lotka-Volterra
$A+B \xrightarrow{k'_1} B+B$	$A + B \xrightarrow{k'_1} B + B$
$B+C \xrightarrow{k_2} C+C$	$B+C \xrightarrow{k_2} C+C$
$C+D \xrightarrow{k_3} D+D$	$C+D \xrightarrow{k_3} D+D$
$D+E \xrightarrow{k_4} E+E$	$C+F \xrightarrow{k_6} F+F$
$E \xrightarrow{k_5} extinct$	$D+E \xrightarrow{k_4} E+E$
Overall:	$F+G \xrightarrow{k_7} G+G$
$A \rightarrow extinct$	Overall :
	$E \rightarrow extinct$
Pathway :	$G \xrightarrow{k_s} extinct$
$A \rightarrow B \rightarrow C \rightarrow D \rightarrow E \rightarrow extinct$	
	Pathway :
	$D \rightarrow E \rightarrow extinct$
	$A \to B \to C$
	$F \to G \to extinct$

 Table 3. Other Lotka-Volterra problems.

As before, the solution can be found by substituting $k_1 = k_1'A$ since A does not essentially change. The β values also can also be dropped off or absorbed in the rate constants. One gets

$$\omega^{4} + \left(\frac{k_{1}k_{2}k_{5}}{k_{3}} + \frac{k_{1}k_{3}k_{5}}{k_{4}} + k_{3}^{2}\frac{k_{1}k_{3}}{k_{2}k_{4}}\right)\omega^{2} + \frac{k_{1}^{2}k_{2}k_{5}^{2}}{k_{4}} = 0.$$
(33)

For mathematical simplicity we set $k_1 = k_2 = k_3 = k_4 = k_5 = 1$. Equation (33) then becomes $\omega^4 + 3\omega^2 + 1 = 0.$ (34)

Its roots are

$$\omega_{1,2} = \pm 1,618i \text{ and } \omega_{1,2} = \pm 0,618i.$$
 (35)

The roots are pure imaginary as in the case of three-species Lotka-Volterra problem and the oscillations are not damped.

Now we can introduce branching to the Lotka-Volterra equation as seen from the second column of Table 3. The solution for this branched case yielded six roots, and they were all pure imaginary. Every new step introduced in prey-predator models introduces a new frequency. From oscillations point of view the system is a collection of different oscillations

in a way that they are somehow synchronized; the change in one frequency influences the overall behavior. The change in one of the frequency in the long run period can be due to mutations occurring. The other frequencies must cope up with the change; in other words the entire system must coevolve. Prey-predator interactions and competition with similar kinds both affect coevolution [34].

The Lotka-Volterra type interactions no matter how many species are involved or how they are branched always have purely imaginary ω values. In other words, in wild life the populations are oscillatory, and the entire system is somehow at steady state. So what pushes evolution is the change of rate constants 'k's in time, and it is due to mutations occurring at the genes of species.

When Schlögl-1 was examined with the same procedure it yielded two roots for ω . One is real positive and the other is real negative with no imaginary component. These roots denote that we have a saddle point. So it can go either direction towards stability or to instability. This is expected, because, Schlögl-1 represents a state with first order phase transition. The change from one phase to another phase can be well understood as a change from unstable to stable state, or vice versa.

The ω values for Schlögl-2 were also similar to those of Schögl-1 with one positive and one negative value. However if we set, $k_C = 0$, that is if $C \rightarrow B + X$ is prohibited in the last column of Table 2, then the roots come out to be,

$$\omega_1 = 0, \ \omega_2 = -(k_{AB} + k_{BC}), \tag{36}$$

where k_{AB} involves also 'A' in molar quantities. Therefore we get a straight line instead of a singular point or saddle point. Since the sign of ω_2 is negative it represents stability, i.e. the fluctuations die out in time. So the system is stabilized through irreversibility. This is an important conclusion, because, natural phenomena reach equilibrium by producing entropy in open systems. The condition $k_C = 0$ stabilizes the system, and the final stability is achieved through the accumulating formation of C.

COHESION OF INTERACTIONS

A network entropy is generally defined in terms of the number of vertices 'V', such that [35, 36],

$$\Delta S \sim \log V. \tag{37}$$

In prey-predator systems a predator feeds on many different preys, so this equation can be written in the form,

$$\Delta S \sim \sum_{i=1}^{V} p_i \log p_i \tag{38}$$

where V denotes the number of predators, and p_i denotes the probability (or the fraction) of preys that the predator feeds on. The number of prey-predator interactions can be visualized as a network, and the higher the number of edges emanating from a vertex the higher the cohesion of interactions. In other words the edges emanating from the vertex denotes the variety of preys that the predator feeds on. As V increases the entropy change also increases. A crowded wild life with increased number of predator species (i.e. high entropy state) makes evolution difficult, because, there will always be a predator around to hunt a mutated prey. The probability of survival of preys increases if predators diminish for some reason (i.e. if entropy decreases). In fact geological disasters accelerate the evolution of new species at the expense of disappearance of others. Mammals of mouse size first appeared by the end of third geological period, and they dominated the world by the mass extinction of about 90-95 % of species including dinosaurs about seventy five millions years ago. Mammalians would probably never so much evolved into their present forms if there had happened no geological disaster due to fall of giant meteorite on Yucatan region. The sexual preferences of males or females can also be represented by a network. The strong preferences decrease the number of edges emanating from a vertex which represents a male or female, and the cohesion naturally gets weaker. It, in turn, facilitates the occurrence of new species.

In a network, entropy increases as the number of vertices increases, but cohesion increases if the number of edges connecting different vertices increases, that is, cohesion depends on the density of connections of vertices. Complexity depends on both; the increase of the number of vertices and the increase in the number of edges connecting vertices contribute to the increase of complexity.

The decrease of the number of interactions or the decrease of cohesion in any network system leads to (i) increased chance of functionalization, (ii) increased rate of evolution by allowing species with different mutations to survive, and (iii) increased rate of speciation due to strong sexual selection.

COHESION AND OSCILLATION FREQUENCIES

The number of frequencies generated depends on the number of species in the system, and the reversing paths of interactions do not contribute to the number of frequency. The number of oscillation frequencies gives an idea about the complexity of a system, the higher the number of frequencies (i.e. the higher the number of vertices in a network) the higher the complexity. However, this is not sufficient, because Fig. 3b and Fig. 3d have equal number of steps, yet Fig. 3d has lower entropy and higher information than Fig. 3b as seen from Table 2. The interaction between the components of Fig. 3d is tighter than that of Fig. 3b; in other words, Fig. 3d has higher cohesion than Fig. 3b yielding higher complexity. As mentioned above complexity depends on both the number of vertices (i.e. species) and the interactions between them. It was also mentioned above that autocatalytic effect in Fig. 3d is stronger than that in Fig. 3b. In other words the structures which have higher uniformity or symmetry is naturally expected to depict higher cohesion as crystals have higher cohesion than amorphous materials of same atomic/molecular structure. By the same token the similarity of oscillation frequencies to each other in a complex system represents the level of cohesion in that system. Such systems are relatively more stable, and subject to a low profile evolution. In these systems the similarity of frequencies represents a state where resonant coupling is more likely, and coherence prevails. Systems with low level cohesion or with dissimilar oscillation frequencies involve higher asymmetries, and are apt to subject to higher level of branching and thus to evolution.

A system always reacts in a way to stabilize itself in a coherent form. Mutations destabilize it, and evolution forces it to stabilize at future conditions. Since the overall entropy in the universe always increases the matter falls apart from each other. In other words cohesion decreases in cosmological time in accord with the increase of entropy. The decrease of cohesion naturally decreases the interactions within the system, and it becomes more susceptible to interact with other objects outside the system. The decrease of cohesion and thus the decrease of mutual interactions in the system can be recovered by introducing new controlling parameters. It can be provided only by the addition of new components to the system. The new components naturally add new oscillation frequencies, and thus new behavioral modes, and increased complexity. So evolution drifts in the direction of stabilizing a loosened system by increasing its complexity. In other words, it is a reaction to the increase of entropy in the universe. Since the least action or minimum energy principle is a fundamental law of nature evolutionary processes obey it by frequently employing autocatalytic dynamics.

CONCLUSIONS

Autocatalysis forms the foreground of evolution, and natural selection as a mechanism of evolution takes place among different species which try to autocatalyze themselves either through competition for food or for sexual partner. Autocatalysis is an entropy reducing process since it attempts to decrease the number of other competitors. The mutations change the chemical reaction rate constants of interactions between species; therefore, the irreversibility in evolution is associated with the irreversible change in rate constants. Autocatalysis can also explain sharp changes like first order phase change, and irreversible changes like second order phase change. The increase of entropy due to irreversibility is counteracted by the increase of information which could be achieved through the increase of complexity, which depends both on the number of components and the number of interactions in a network system. Evolution is slow if the interactions between the components of the entire system are intense, or if cohesion in the system is high; otherwise, evolution is accelerated. Evolution propagates in the direction of increase of complexity. The number of oscillations associated with autocatalysis increases with the number of components in a system. The similarity of oscillation frequencies gives an idea about the cohesion strength in a system.

In this manuscript autocatalysis as the underlying principle of evolution and complexity was discussed from different aspects. Computer simulations need to be done to carry out specific case studies and to have better understanding of the evolving specific systems.

ACKNOWLEDGEMENT

The author is grateful to his wife Ufuk Gündüz, professor of Molecular Biology, Orta Doğu Teknik Üniversitesi, Ankara, for her invaluable help.

REFERENCES

- [1] Weber, M.: *Determinism, Realism, and Probability in Evolutionary Theory*. Philosophy of Science, Supplement **68**(3), S213-S214, 2001,
- [2] Elaydi, S.: *Is the world evolving discretely*? Advances in Applied Mathematics **31**(1), 1-9, 2003
- [3] May, R.M.: *Simple mathematical models with very complicated dynamics*. Nature **261**, 459-467, 1976,
- [4] Arneodo, A.; Coullet, P. and Tresser, C.: Occurence of strange attractors in threedimensional Volterra equations. Physics Letters A 79(4), 259-263, 1980,
- [5] Peitgen, H.O. and Richter, P.H.: *The Beauty of Fractals*. Springer-Verlag, p.24, 1986,
- [6] Thomson, D.W.: *On Growth and Form*. Vol. II. Cambridge University Press, Ch.17, 1968,
- [7] Saunders, D.S.: *Insect Clocks*. Elsevier, 2002,
- [8] Liebovitch, L.S.: *Fractals and Chaos Simplified for the Life Sciences*. Oxford University Press, 1998,
- [9] Kumar, S.: On Growth, Form, and Computers. Elsevier, 2003,
- [10] Collier, J.D.: *Entropy in Evolution*. Biology and Philosophy 1(1), 5-24, 1986,
- [11] Collier, J.D.: *Two Faces of Maxwell's Demon Reveal the Nature of Irreversibility*. Studies in History and Philosophy of Science A **21**(2), 257-268, 1990,

- [12] Collier, J.D.: Information Increase in Biological Systems: How does Adaptation Fit? In van der Vijver, G.; Salthe, S.N. and Delpos, M., eds.: Evolutionary Systems. Kluwer, Dordrecht, pp.129-140, 1998,
- [13] Gregory, T.R.: *The Evolution of the Genome*. Elsevier Academic, 2005,
- [14] Tanaka, T.; Ikeo, K. and Gojobori, T.: Evolution of metabolic networks by gain and loss of enzymatic reaction in eukaryotes. Gene 365, 88-94, 2005/2006,
- [15] Testa, B. and Kier, L.B.: Emergence and Dissolvence in the Self-organisation of Complex Systems. Entropy 2(1), 1-25, 2000, <u>http://www.mdpi.com/1099-4300/2/1/1/pdf</u>,
- [16] Honeycutt, R.L.: Small changes, big results: evolution of morphological discontinuity in mammals. Journal of Biology 7(3), No. 9, 2008,

http://jbiol.com/content/pdf/jbiol71.pdf,

- [17] Bergman, J.P.: Wireless e-business application methods for forecasting the demand of wireless services and technologies. M.Sc. Thesis.
 Lappeenranta University of Technology, Lappeenranta, 2002, http://www.doria.fi/bitstream/handle/10024/34548/nbnfi-fe20021156.pdf,
- [18] Marchetti, C.: Productivity versus Age. Co. No. 00-155, International Institute for Applied Systems Analysis, 2002, <u>http://www.cesaremarchetti.org/archive/electronic/prodage.pdf</u>,
- [19] Schlögl, F.: *Chemical reaction models for non-equilibrium phase transitions*. Zeitschrift für Physik A **253**(2), 147-161, 1972,
- [20] Turing, A.M.: *The chemical basis of morphogenesis*. Philosophical Transactions of the Royal Society B **237**, 37-72, 1952,
- [21] Glansdorff P. and Prigogine, I. *Thermodynamic Theory of Structure, Stability, and Fluctuations.*

Wiley-Interscience, 1971,

- [22] Saakian, D.B.; Hu, C.-K. and Khachatryan, H.: Solvable biological evolution models with general fitness functions and multiple mutations in parallel mutation-selection scheme. Physical Review E, **70**(4), No. 041908, 2004,
- [23] Tasaki, S.: On Prigogine's approaches to irreversibility: a case study by the baker map. Discrete Dynamics in Nature and Society 2004(1), 251-272, 2004, <u>http://downloads.hindawi.com/journals/ddns/2004/529759.pdf</u>,
- [24] Hutchison, K.: *Is Classical Mechanics Really Time-reversible and Deterministic?* British Journal for the Philosophy of Science **44**(2), 307-323, 1993,
- [25] Hong, F.T.: Towards physical dynamic tolerance: an approach to resolve the conflict between free will and physical determinism. Biosystems 68(2-3), 85-105, 2003.
- [26] Nishimori, H.: *Statistical Physics of Spin Glasses and Information Processing, An Introduction.* Oxford University Press, 2001,
- [27] Tolman, R.C.: *Principles of Statistical Mechanics*. The Clarendon Press, Oxford, p.163, 1938,
- [28] Markus, M.; Müller, S.C.; Plesser, T. and Hess, B. Characterization of Order and Disorder in Spatial Patterns.
 In Degn, H.; Holden, A.V. and Olsen, L.F., eds.: Chaos in Biological Systems, NATO ASI Series, Plenum Press, pp.295-303, 1987,
- [29] Zhabotinsky, A.M. and Rovinsky, A.B.: Mechanism and nonlinear dynamics of an oscillating chemical reaction. Journal of Statistical Physics 48(5-6), 959-975, 1987,

- [30] Pomeau, Y. and Manneville, P.: Intermittent transition to turbulence in dissipative dynamical systems.
 - Communications in Mathematical Physics 74(2), 189-197, 1980,
- [31] Baker, G.L. and Gollub, J.P.: *Chaotic Dynamics, An Introduction*. Cambridge University Press, 1990,
- [32] Dauxois, T.; Di Patti, F.; Fanelli, D. and McKane, A.J.: Enhanced stochastic oscillations in autocatalytic reactions. Physical Review E 79(3), No. 036112, 2009.
- [33] McKane, A.J. and Newman, T.J.: Predator-Prey Cycles from Resonant Amplification of Demographic Stochasticity.
 - Physical Review Letters **94**(21), No. 218102, 2005,
- [34] Lässig, M.; Bastolla, U.; Manrubia, S.C. and Valleriani, A.: *Shape of Ecological Networks*. Physical Review Letters **86**, 4418-4421, 2001,
- [35] Scarabotti, F.: *On a lemma of Gromov and the entropy of a graph*. European Journal of Combinatorics **23**(5), 631-633, 2002,
- [36] Dehmer, M.: Information Processing in Complex Networks: Graph Entropy and Information Functionals.

Applied Mathematic and Computation 201(1-2), 82-94, 2008.

AUTOKATALIZA KAO FILOZOFIJA PRIRODE KOJA JE PODLOGA KOMPLEKSNOSTI I BIOLOŠKE EVOLUCIJE

G. Gündüz

Odsjek kemijskog inženjerstva, Bliskoistočno tehničko sveučilište Ankara, Turska

SAŽETAK

Analiziran je značaj različitih vidova autokatalize u evoluciji. Ponašanje autokatalitičkih reakcija, prvenstveno opisanih jednadžbama Lotke-Volterre i Schlögla, razmatrano je u okviru promjene faze, entropije i pripadnih frekvencija osciliranja. Porast kompleksnosti kao opći smjer evolucije analiziran je jednim djelom pomoću njihove entropije i informacijskog sadržaja. Zaključeno je kako su evolucijski pomaci u smjeru porasta kompleksnosti jedna vrsta filozofije prirode koja se suprotstavlja porastu entropije svemira.

KLJUČNE RIJEČI

autokataliza, entropija, evolucija, kompleksnost, informacija, frekvencija osciliranja, kohezija