Computer Science Journal of Moldova, vol.**9**, no.1(25), 2001

The system of molecular–genetic triggers as self–organizing computing system

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Abstract

In this paper is shown, that the system of molecular–genetic triggers can solve the SAT problem. The molecular–genetic trigger represents the self–organizing structure and has attractors. The signal from one attractor is transmitted to other attractor, from the first level to the second level of the system. Molecular–genetic triggers work separately. The system of molecular–genetic triggers represents an example of parallel computing system. Suppose, that the system can receive two types of signals. In the first case, the system switches with the help of signals of a molecular nature (concentration of activators x_1, x_2, x_3, x_4). In the second case, the signals of wave nature of a resonant frequency can be utilized. It is possible to show, that the molecular–genetic system, can recognize images encoded by 2–dimensional vectors. Thus, the cells can be considered as parallel self–organizing system producing, receiving and transmitting the information.

Introduction

Beginning with paper [1] the models of DNA–based molecular computing are intensively researched. New formal parallel computing models such as P Systems with Active Membranes [2] and others have been recently built.

The phenomena of self–organization are met everywhere: both in animate and inanimate nature. By processes of self–organization are called such phenomena under which in systems, owing to instability, the initial organization in space and time is lost, and instead of it, a new one is installed. Synergetics – science dealing with self–organization in

physical, chemical, biological and social systems – [3] and the processes of self– organization of structures in cooperative systems [4] are researched. Conditions, indispensable for arising processes of self–organization, are as follows [5]:

1. The system is thermodynamically opened, i.e. it can exchange matter and energy with environment.

2. The dynamic equations of the system are non–linear.

3. The deviations from equilibrium exceed the critical value.

4. The microscopical processes in the system are cooperative.

The biosystems completely satisfy the above listed conditions.

In biological systems, due to cooperative actions of objects (molecules of enzymes, proteins, mRNA etc.), constituting a system, spatial, time, time–spatial and functional structures appear. Different forms of self–organization are widely spread and play a major role in the processes of receiving, developing and transmitting the wave information in biosystems [5].

Thermodynamics as a whole, however, is not sufficient for phenomenological treatment of animate systems because the latter have dynamic, but not statistical features, and are far from equilibrium. In order to describe kinetic processes, it is necessary to define production of entropy in one unity time. Thermodynamics of biosystems (open systems) is, as a fact, kinetics.

The development of thermodynamics of irreversible processes has shown, that the processes of self–organization are only possible far from thermodynamic equilibrium. In this field nonlinear thermodynamics now is entirely based on the initial mathematical models that use, as a basis, a qualitative analysis of the system of kinetic nonlinear differential equations which take into account the character of concentration change of reagents in chemical processes. It refers to self–sustained oscillations, trigger switching of the system from one regime to another and to processes of self–organization in full measure.

Characterization of the biological system behaviour, which is essentially nonequilibrium and heterogeneous in the whole, with the help of concept of entropy is not justified. This concept can only be applied to concrete metabolic processes. In order to find a stationary state of the far from equilibrium system, by analogy with the principle of entropy increasing (Prigogin theorem) [4, 8], adequate in nearby of equilibrium, the potential function $D(x)$ which called *a kinetic potential* is investigated.

The important property of a stationary state is its *stability*: if at a deviation small enough from a stationary state, the system never moves far from it and comes back to it again, the state is steady. If, in the consequence of taking out from the stationary state, the system continues moving away from it, the state is unstable.

From the thermodynamic point of view, the potential function $D(x)$ has minimum value in steady states. In unstable states the potential $D(x)$ has maximal value. In Fig. 1 the potential profile of the system (one–dimensional mathematical model [13, 14]), having three stationary states (trigger) is shown. By modeling biological phenomena one comes to the equations, which coincide with the equations that describe the movement of an usual ball in one small cavity or its re – jumping through between several ones. It happens because the equation identical in form describes different processes in physics, chemistry and biology [9, 10]. The steady points of the system (a and c) are called *attractors*.

The stationary states a and c - are steady. The ball can be in any of cavities, but its location in the first one is more likely. A stationary state b is unstable.

On the basis of quantum mechanics the theoretical models of generation of wave information by enzymes (so–called *transmitters*) and their transmission to genes (*receivers*) are determined. In biophysics the mechanism of quantum processes of generation by enzymes of radiation (wave information) [10, 11], quantum mechanisms of a fotoregulatory processes of DNA and the electron – conformation transformations of the DNA under effect of photons are investigated. In paper [12], for example, the molecular–genetic trigger is controlled by means

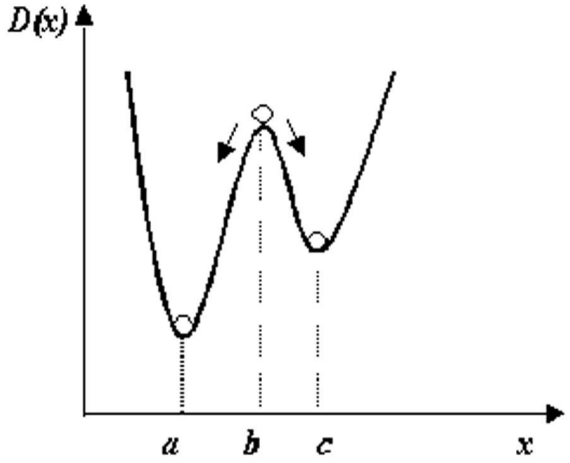

Fig. 1. The kinetic potential of the system having three stationary states.

of a molecular nature signal. In this paper we shall treat sites of a DNA (genes, genes – regulators, enhancer elements) as receivers, recognizing a signal of molecular and wave nature. The possibility of controlling the genetic structures by signals of wave nature (photons of a resonant frequency) is taken into account. Wave information encoded in the value of quantums of energy (photons), generated by enzymes, is received by genes. Time characteristic of wave processes is by a few orders higher than time describing interaction on a molecular level. For example, time of generation by an enzyme of photons is about 10–9 sec, time of electron conformational changes of DNA under the influence of 1–2 photons is approximatively 10^8 – 10^{11} sec [10, 11].

In this paper the problems related to different sciences such as synergetics, biophysics, molecular biology and computing theory are touched upon. Therefore, there is a necessity of using corresponding nomenclature in treating particular phenomena and processes. At the same time, for simplicity of presentation the mathematical calculations are not given. The mathematical models of MGT [12]–[15], self–sustained oscillations [16] and quantum mechanical models and calcu-

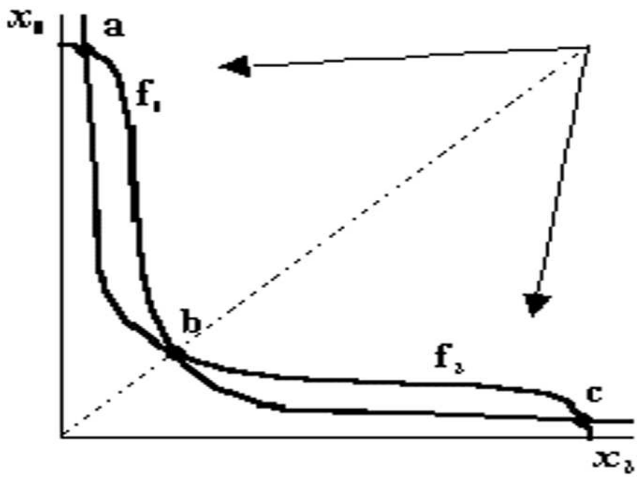

Fig. 2. A phase plane of the MGT_1. Intersection of the principal isoclines of the system of two kinetic equations [12].

lations of light generation by enzymes and interaction of a light with a DNA are explicitly surveyed in [10, 11].

1 The MGT as the self–organizing system

In molecular biology the bistable Turing structures, so-called molecular–genetic triggers, are researched [8]–[15]. Turing structures represent a system possessing two stable states (attractors) and capable of switching from one stable state to another.

Let us consider in more details what is the MGT and its mechanism. In trigger systems of steady–state the values of variables depend on the starting conditions. If the system operates in one of the stable conditions, it cannot be taken out from this regime by small deviations. However, in real biological systems there are ways of switching off the system from one state to another. It can be made in two ways: specific and parametric.

In a Fig. 2 the phase plane of the trigger system with two steady

singular points (attractors) is represented. x_1 and x_2 correspond to input signals (dimensionless concentrations of activators x_1 and x_2, accordingly). Intersection points a and c are "stable nodes", and point b is "saddle" one. The f_1-isocline of vertical tangents, f_2-isocline of horizontal ones. Arrows show the way of system relaxation (attraction of the system to one of the stable points a or c).

The amount of stationary states in the system is determined by a number of cross points of main isoclines of vertical and horizontal tangents (bold lines). The cross point of isoclines b represents a saddle (unstable point), and the cross points of main isoclines a and c, laying on both sides from a separatrix of a saddle (dotted line) – steady states. If the initial position of point, which corresponds to initial state of the system, is situated more to the left of a separatrix of a saddle, the system is placed in the field of influence of a singular point a and tends to this steady stationary state (area of attraction of an attractor is spread up to a separatrix). From the initial points laying more to the right of a separatrix (area of attraction of other attractor), the system moves to a steady singular point c. (Phase plane corresponds to two–dimensional mathematical model [12].)

More thin is the way of parametric nonspecific switching. Here, to direct expose effect, not variables are subjected, but parameters η of the system, for example, temperature, ph etc. In Fig. 3 the dependence of stationary states of the system on the controlling parameter is represented.

In areas $(0, \eta_1)$ and (η_3, ∞) the system has only one stationary state. In area (η_1, η_3) there are three stationary states, two from which (branch AB and CD) are steady, and one (branch BD) is unstable. The points B and D are bifurcation states of the system, in which the steady and unstable states merge.

The parameter value η_1 is critical and its name is a *bifurcation point.* The bifurcation point is a point of a stability limit of the system.

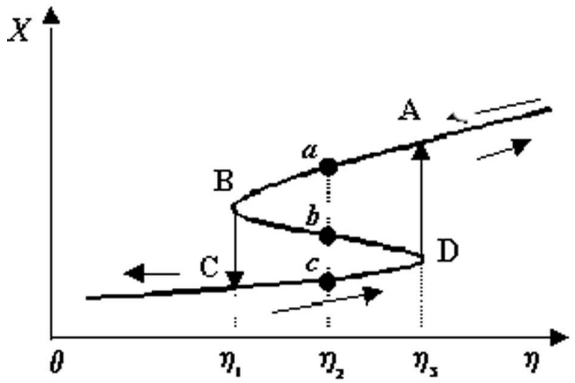

Fig. 3. Dependence of stationary states of the system on the controlling parameter η.

2 The self–organizing system can solve SAT problem

In paper [2] it was shown that the SAT (Satisfiability of propositional formula in the conjunctive normal form) problem can be solved by P system with active membranes in a time which is linear in the number of variables and the number of clauses. In the paper it is shown that the cooperative system of molecular–genetic triggers with given relationships can solve the concrete example of SAT problem and namely "a logical sentence" like this one:

$$\alpha = (x_1 or x_2) and (x_3 or x_4) \tag{1}$$

(Fig. 4). In this case we have 4 variables x_1, x_2, x_3, x_4 and two clauses. It is satisfiable, when any of the following truth–assignments makes the formula *true*

$$(x_1 = false, x_2 = true), (x_3 = true, x_4 = false), \tag{2}$$
$$(x_1 = true, x_2 = false), (x_3 = true, x_4 = false), \tag{3}$$

$$(x_1 = false, x_2 = true), (x_3 = false, x_4 = true), \quad (4)$$
$$(x_1 = true, x_2 = false), (x_3 = false, x_4 = true), \quad (5)$$
$$(x_1 = true, x_2 = true), (x_3 = true, x_4 = false), \quad (6)$$
$$(x_1 = false, x_2 = true), (x_3 = true, x_4 = true), \quad (7)$$
$$(x_1 = true, x_2 = false), \ (x_3 = true, x_4 = true), \quad (8)$$
$$(x_1 = true, x_2 = true), \ (x_3 = false, x_4 = true), \quad (9)$$
$$(x_1 = true, x_2 = true), \ (x_3 = true, x_4 = true). \quad (10)$$

(see Table 3). In this case variables x_1, x_2 and x_3, x_4 are independent. It use three connectives: or, and, not. The molecular–genetic triggers of the first (MGT_1 and MGT_2) and the second (MGT_3) levels work independently and the SAT problem (1) can be solved in linear (parallel) time [2].

MGT are genetical systems of trigger type reacting to external effects (signals). It is possible to present MGT as an automaton. In this case it is assumed that each automaton (MGT_1, MGT_2 and MGT_3) has two inputs and one output. Signals x_1, x_2 and x_3, x_4 in Fig. 1 correspond to variables in (2)–(10) and Boolean values *true* will be further designated as 1, and values *false* as 0 (see Tables 1–3).

For the MGT_1 the inputs are designated as x_1 and x_2 and the output is designated as y_1. If both input signals $x_1 = 1$, $x_2 = 1$, then output signal is also $y_1 = 1$ as the system relaxes and is attracted to one of the two attractors. When $x_1 = 0$, $x_2 = 0$ (i.e. absence of a signal on the input) there is no signal on an output(see Table 1).

Table 1 contains the values of the output signals y_1 for MGT_1 depending on values of the input signals x_1 and x_2.

Table 1. LOGICAL OR.

x_1	x_2	y_1
1	0	1 (true)
0	1	1 (true)
1	1	1 (true)
0	0	0 (false)

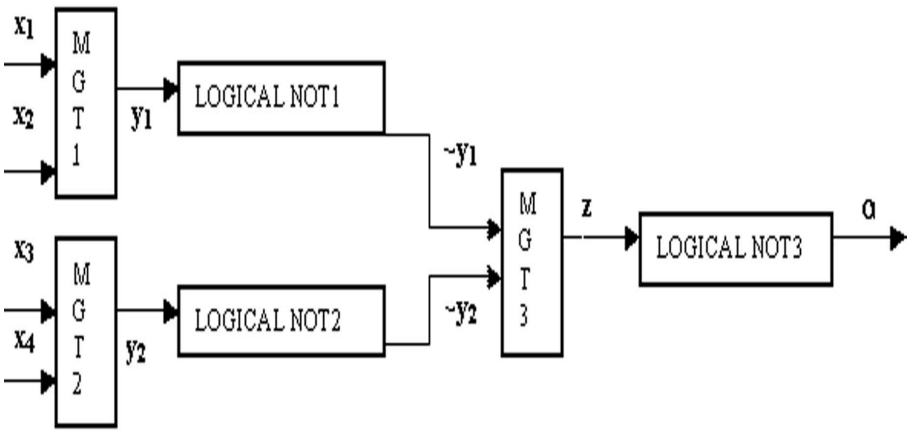

Fig. 4. The elementary scheme of two level system containing three molecular-genetic triggers (MGT) with set connections.

The genetic scheme is represented in Fig. 6. The logical element *not* represents a gene with a negative type of transcription control.

Table 2 represents the values of the output signals, for LOGICAL NOT, depending on values of the input signals z.

Table 2. LOGICAL NOT.

z	$\alpha(notz)$
1	0 (false)
0	1(true)

Table 3 includes the values of the output signals, for the system consisting of three molecular-genetic triggers, with set connections depending on values of the input signals x_1, x_2, and x_3, x_4. The output signal 1 corresponds to the value *true* and the output signal 0 – to the value *false*.

Table 3.

	x_1	x_2	x_3	x_4	y_1	y_2	$noty_1$	$noty_2$	z	$\alpha(notz)$
1	1	0	0	0	1	0	0	1	1	0
2	0	1	0	0	1	0	0	1	1	0
3	0	0	1	0	0	1	1	0	1	0
4	0	0	0	1	0	1	1	0	1	0
5	1	1	0	0	1	0	0	1	1	0
6	0	1	1	0	1	1	0	0	0	1
7	0	0	1	1	0	1	1	0	1	0
8	1	0	1	0	1	1	0	0	0	1
9	0	1	0	1	1	1	0	0	0	1
10	1	0	0	1	1	1	0	0	0	1
11	1	1	1	0	1	1	0	0	0	1
12	0	1	1	1	1	1	0	0	0	1
13	1	0	1	1	1	1	0	0	0	1
14	1	1	0	1	1	1	0	0	0	1
15	0	0	0	0	0	0	1	1	1	0
16	1	1	1	1	1	1	0	0	0	1

In Fig. 4 the phase plane of MGT_1 is represented [12]. For MGT_2 and MGT_3 the phase planes are similar. When both input signals are approximately equal to 1, the system is attracted to one of the two attractors (stable point a or c) and the output signal corresponds to the value *true*.

Thus, in the system there are attractors which correspond to stable points a, c. MGT represents a system working in two alternative regimes. The signal from one attractor is transmitted to another, from the first to the second level. Bistable Turing structures (MGT) with attractors occur in the biosystem due to cooperative actions of objects (molecules of proteins, mRNA, enzymes) constituting a system [8]–[15].

The problems of computational universality of the MGT system will be discussed in the paper that will follow.

3 The model of molecular–genetic trigger

It is known that there are two types of transcription regulation systems with positive and negative control. In case of *a negative control* regulatory locus (operator) admits free promotion of RNA–polymerase, but it is effectively locked at binding a repressor molecules. *The positive control* is stipulated by the operator, which impedes transcribing structural genes by the RNA–polymerase, but is capable of linking a specific activator which facilitates promotion of this enzyme. The trigger Jacob – Monod, for example, represents a system with negative control of structural genes [8]. Irrespective of control transcription type of the triggers, the scheme of MGT system, shown in Fig. 4, and in Tables 1–3, remains the same. Let us consider in more details the model MGT_1 with a positive transcription regulation [12]. In Fig. 5 the elements of the regulatory system of the genetic system of allelic pair of chromosomes with the system of transcription positive control are represented. Reg_1 and Reg_2 are the regulator genes, the result of action of which the molecules of activators x_1 and x_2 are synthesized. Molecules of activators reversibly interact with sites of structural gene – operators O_1 and O_2 (receptor sites), and activate transcription mPHK of structural genes G_1 and G_2, correspondingly. E_1, E_2 – enzymes, products of genes G_1 and G_2, have an activity (proteolytically) for instance related to the molecules of homologous chromosome activators (x_2, x_1). They destroy the molecules of activators x_2 and x_1, correspondingly. It is also assumed that the activator-controlled polycistronic sets also contain genes S_1, which synthesize proteins – repressors y_1 (for the LOGICAL NOT1) and y_2 (for the LOGICAL NOT2). The molecular–genetic schemes for MGT_2 and MGT_3 are similar to the scheme introduced in Fig. 5.

Suppose that genes – regulators Reg_1, Reg_2 (belonging to receiver MGT_1) and Reg_3, Reg_4 (belonging to receiver MGT_2) are closed and the initial concentrations x_1, x_2, x_3, x_4 are equal to zero. Let us consider two variants of input signals x_1, x_2, x_3, x_4:

1. Signals of molecular nature: high concentration of molecules activators x_1, x_2 and x_3, x_4 switches on the process of transcription of a

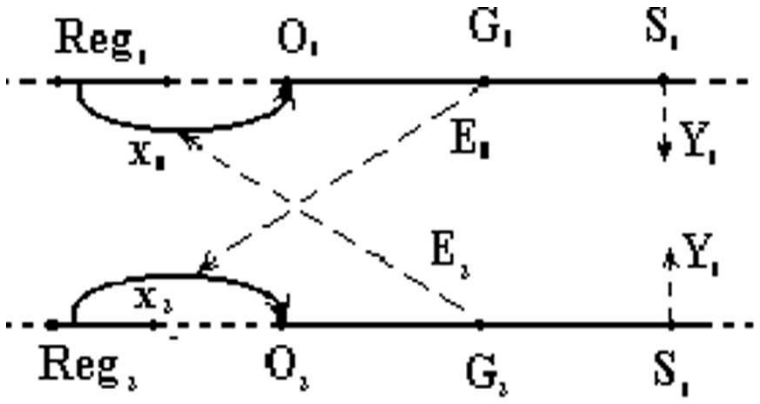

Fig. 5. The scheme of genetical regulation of homologous chromosomes with positive control of gene activation.

polycistron (i. e. genes G_1, G_2, S_1 etc. switch on) which is under control of operators O_1, O_2 and O_3, O_4. y_1 and y_2 are synthesized (product of genes S_1 and S_2). The molecules of repressors y_1 (output signal of MGT_1) and y_2 (output signal of MGT_2) are the signals recognized and received by the receiver at the second level – the LOGICAL NOT1 and the LOGICAL NOT2. The LOGICAL NOT1 and LOGICAL NOT2 is switched off by the molecules of repressors y_1 or y_2 (Fig. 7).

2. Signals of wave nature: let us take into account the possibility of controlling of gene activity by the signals of wave nature, i.e. the activation of DNA sites (genes, genes – regulators), so-called *receivers*, tuned in resonant frequencies, by tons of a resonant frequency ω_1,ω_2 and ω_3,ω_4 (Fig. 6). As a result gene – regulators Reg_1, Reg_2 and Reg_3, Reg_4 switch on. It has been proved, that gene activity can be controlled by signals of wave nature [10, 17].

In a living cell the role of the *transmitter* is played by enzymes, which generate the wave information as dipoles with the discrete frequency setting [10, 11, 17]. We shall treat sites of a DNA (genes, genes – regulators, enhanced elements) as *receivers* recognizing a signal of

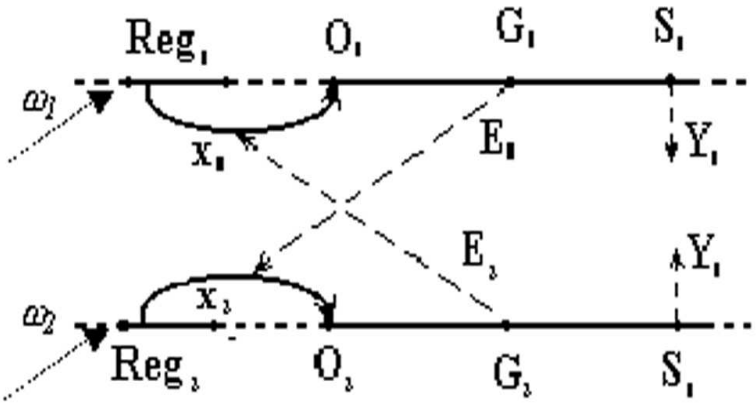

Fig. 6. Wave information, generated by enzymes (*transmitters*) , is received by genes (*receivers*).

wave nature. Thus, the information encoded in the value of quantum of energy (photons), generated by enzymes, is received at the level of DNA by genetic structures. The gene with concrete quantum characteristics should take reason and optical (wave) information for its activation [17]. The total sum of genes (thousand genes in a cell of higher eukaryotes [18]) react to changes of the quantum state of an energy field of the cell, receiving and transmitting the wave information.

Suppose that there come the following signals on an input: $x_1 = 1, x_2 = 0, x_3 = 1, x_4 = 0$. Proceeding from Table 1 $y_1 = 1$ (product of a gene S_1 of MGT_1), $y_2 = 1$ (product of gene S_2 of MGT_2). The signals y_1 and y_2 represent the input signals for LOGICAL NOT1 and LOGICAL NOT2. As y_1 and y_2 are repressors, which turn off genes S_3 and S_4, we shall obtain *not* $y_1 = 0$ and *not* $y_2 = 0$. The signals *not* y_1 and *not* y_2 are products of genes S_3 and S_4 and represent signals (activators) recognizing by MGT_3, under the effect of which the polycistron's transcription (under control of operators O_5 and O_6) is switched on. Since in this case *not* $y_1 = 0$ and *not* $y_2 = 0$ (absence of activators) the gene S_5 switches off and $z = 0$ (product of a gene S_5). The signal z is the repressor received by LOGICAL NOT3. In the absence of repressors z the gene S_6 is switched on and *not* $z = 1$

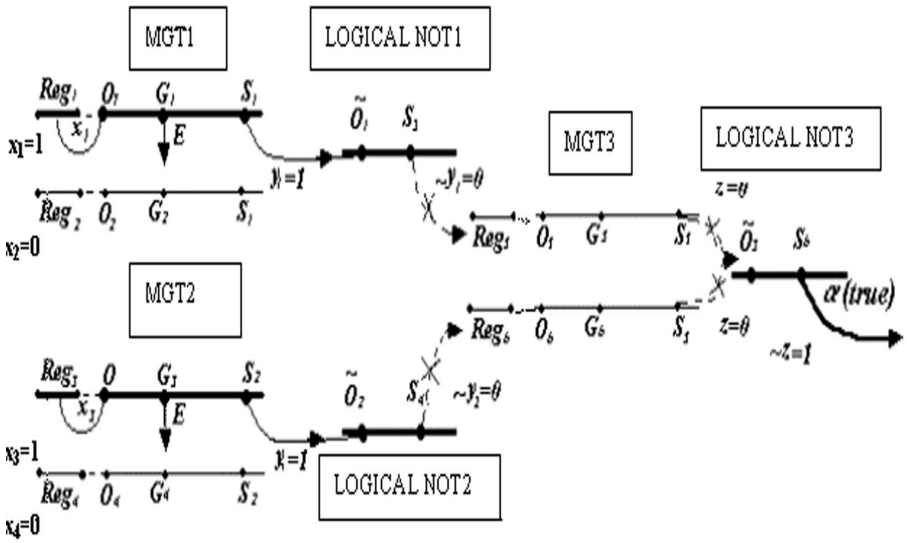

Fig. 7. The answer of the MGT system to input signals ($x1 = 1$, $x2 = 0$, $x3 = 1$, $x4 = 0$) is *true*.

(product of a gene S_6). When *not* $z = 1$, we consider the answer of MGT system to input signals to be *true*.

We notice, that in MGT the positive control of genes is carried out, i.e. the trigger switch on under effect of activators: signals x_1, x_2, x_3, x_4 for MGT_1, MGT_2 both $noty_1$ and $noty_2$ for MGT_3. In LOGICAL NOT1, LOGICAL NOT2 and LOGICAL NOT3 the negative transcription control of genes is realized. The signals y_1,y_2 and z are repressors. The presence of output signal α (product of a gene S_6) in the system is equivalent to an output true and specifies that on the input the combination of signals satisfying the equation (1) was received.

4 Living cell as parallel synergetic system and image recognition

By a simple example it is possible to show that the synergetic system, presented in Fig. 4, possesses several attractors and can recognize the images. To each image a vector or a point corresponds. Let us consider the simplest example, when the images in the sequence of string of two characters, is encoded by two–dimensional vectors. Instead of a vector we can consider its end – a point in a two–dimensional space. The components of this vector do not necessarily acquire numerical values 0 or 1, they can be continuous values. Each point j, for example, can be brought in correspondence with some intensity q_j.

Suppose that to characters q_1, q_2 and q_3 there correspond the combinations $(1,0),(0,1)$ and $(1,1)$. In such a case, we can say that the system shown in Fig. 4 is capable of recognizing a string of characters q_1 , q_2 and q_3. In other cases, when there are other combinations except $(1,0),(0,1)$ or $(1,1)$ on an input, the system will produce Boolean values *false* (see Table 3) on output.

q_2	q_1	*true*
q_1	q_1	*true*
q_2	q_2	*true*
q_1	q_2	*true*
q_3	q_1	*true*
q_2	q_3	*true*
q_1	q_3	*true*
q_3	q_2	*true*
q_3	q_3	*true*

In real conditions in a cell the set of external and internal signals of a different nature (the set of which represent great arrays of the information, i.e. images) is received and processed by corresponding receivers (sites of DNA). The images can be encoded by multidimensional vectors (more than two dimensions). The major role in recognizing, processing and information storage play MGT.

In a genome of higher plants and animals thousands of genes structures work simultaneously (parallel). It is known, that in a genome of higher eukaryotes, the genes are represented by single copies, clumps of identical genes or by sets of similar r genes. The number of copies in the set can vary from several up to several thousands [18]. In complex eukaryotes cells there are probably much more complex systems of MGT with set connection, rather than those represented in Fig. 4. At every stage of development the cells are able to recognize definite images.

5 Conclusion

The system of molecular–genetic triggers can solve the propositional formula in the conjunctive normal form: It has also been shown, that the cooperative (self–organizing) system of molecular–genetic triggers is able to recognize the elementary string of characters encoded by vectors $(1,0)$, $(0,1)$ and $(1,1)$. Since MGT of the first and the second levels of the cooperative system (corresponding to a gene structure of genome) work separately, it is possible to speak about parallel processes of recognitions, transmission and information processing. We also think that the living cell represents parallel synergetic computing system [5] and is capable of recognizing images.

Acknowledgments

The author thanks Iurii Rogozhin and Elena Boian for helpful discussions.

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Received 19 April, 2001