Quantum Genetics, Quantum Automata and Computation

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ABSTRACT

The concepts of quantum automata and quantum computation are studied in the context of quantum genetics and genetic networks with nonlinear dynamics. In a previous publication (Baianu,1971a) the formal concept of quantum automaton was introduced and its possible implications for genetic and metabolic activities in living cells and organisms were considered. This was followed by a report on quantum and abstract, symbolic computation based on the theory of categories, functors and natural transformations (Baianu,1971b). The notions of topological semigroup, quantum automaton,or quantum computer, were then suggested with a view to their potential applications to the analogous simulation of biological systems, and especially genetic activities and nonlinear dynamics in genetic networks. Further, detailed studies of nonlinear dynamics in genetic networks were carried out in categories of n-valued, Łukasiewicz Logic Algebras that showed significant dissimilarities (Baianu, 1977) from Boolean models of human neural networks (McCullough and Pitts,1945). Molecular models in terms of categories, functors and natural transformations were then formulated for unimolecular chemical transformations, multi-molecular chemical and biochemical transformations (Baianu, 1983,2004a). Previous applications of computer modeling, classical automata theory, and relational biology to molecular biology, oncogenesis and medicine were extensively reviewed and several important conclusions were reached regarding both the potential and limitations of the computation-assisted modeling of biological systems, and especially complex organisms such as ***Homo sapiens sapiens*** (Baianu,1987). Novel approaches to solving the realization problems of Relational Biology models in Complex System Biology are introduced in terms of natural transformations between functors of such molecular categories. Several applications of such natural transformations of functors were then presented to protein biosynthesis, embryogenesis and nuclear transplant experiments. Other possible realizations in Molecular Biology and Relational Biology of Organisms are here suggested in terms of quantum automata models of Quantum Genetics and Interactomics. Future developments of this novel approach are likely to also include: Fuzzy Relations in Biology and Epigenomics, Relational Biology modeling of Complex Immunological and Hormonal regulatory

systems, n-categories and Topoi of Lukasiewicz Logic Algebras and Intuitionistic Logic (Heyting) Algebras for modeling nonlinear dynamics and cognitive processes in complex neural networks that are present in the human brain, as well as stochastic modeling of genetic networks in Lukasiewicz Logic Algebras.

Introduction

The Concepts of Quantum Automata and Quantum Dynamics in terms of the Theory of Categories, Functors and Natural Transformations

Molecular models in terms of categories, functors and natural transformations were formulated for unimolecular chemical transformations, multi-molecular chemical and biochemical transformations (Baianu, 1983, 2004a). Previous applications of computer modeling, classical automata theory, and relational biology to molecular biology, neural networks, oncogenesis and medicine were extensively reviewed and several important conclusions were reached regarding both the potential and limitations of the computation-assisted modeling of biological systems, and especially complex organisms such as ***Homo sapiens sapiens*** (Baianu,1987).

1. MOLECULAR MODELS IN CATEGORIES

A simple introduction of such a synthesis is based on set-theoretical models of chemical transformations (14).
Consider the simple case of unimolecular chemical transformations (14):

$$\mathbf{T : A \times I \rightarrow B \times I} \qquad (1)$$

where A is the original sample set of molecules, I = [0, t] is a finite segment of the real time axis and A x I denotes the indexing of each A-type molecule by the instant of time at which each molecule $a \in A$ is actually transforming into a B-type molecule (see also eq.3 in ref.14). B x I denotes the set of the newly formed B-type molecules which are indexed by their corresponding instants of birth.

MOLECULAR SET -**A**, with f: A →A are ENDOMORPHISMS that belong to H(A,A)

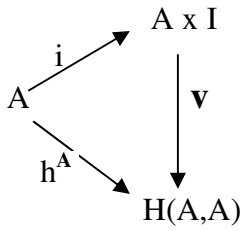
THE CATEGORY OF MOLECULAR SETS AND THEIR TRANSFORMATIONS is : **M** .

THE h^X FUNCTOR: h^A: ***M*** → ***Set*** is defined as:

$h^A(X\} = H(A,X)$ for any X in ***M***
$h^A(t) = m: H(A,A) \rightarrow H(A,B)$ for any t: A→B, where:

A = MOLECULAR SET
B= MOLECULAR SET OF REACTION PRODUCTS OF TYPE "B", RESULTING FROM a DEFINITION OF the MOLECULAR SET VARIABLE (m.s. v.), defined as follows.

The flexible notion of molecular set variable (m.s.v) is precisely represented by the morphisms **v** in the following diagram:



where morphisms **v** are induced by the inclusion mappings ***i***: A→A x I and the commutativity conditions $h^A = v \circ i$. The naturality of this diagram simply means that such conditions hold for any functor h^A defined as above.

THE REPRESENTATION OF UNIMOLECULAR CHEMICAL REACTIONS AS **NATURAL TRANSFORMATIONS**:

The unimolecular chemical reaction can be thus represented by the natural transformations

$h^A \xrightarrow{\eta} h^B$, as one can readily check in the commutative diagram :

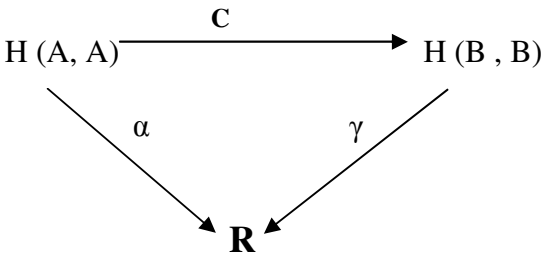
$$\begin{array}{ccc} h^A(A) = H(A,A) & \xrightarrow{\eta_A} & h^B(A) = H(B,A) \\ \downarrow h^A(t) & & \downarrow h^B(t) \\ h^A(B) = H(A,B) & \xrightarrow{\eta_B} & h^B(B) = H(B,B) \end{array}$$

if the states of the molecular sets $A_u = a_1, \ldots, a_n$ and $B_u = b_1, \ldots b_n$ are represented by certain endomorphisms in H(A,A) and H(B,B), respectively.

THE OBSERVABLE OF AN m.s.v, B, CHARACTERIZING THE CHEMICAL PRODUCTS "B" OF A CHEMICAL REACTION IS A MORPHISM:

γ : H (B , B) ------> R where R is **the set of real numbers** .

THIS OBSERVABLE IS SUBJECT TO THE FOLLOWING COMMUTATIVITY or NATURALITY CONDITION:



(5)

with c : $A_u^* \longrightarrow B_u^*$, and A*, B* being specially prepared **fields of states**, within a measurement uncertainty range, δ.

DEFINITION OF A ***MULTI-MOLECULAR REACTION*** :

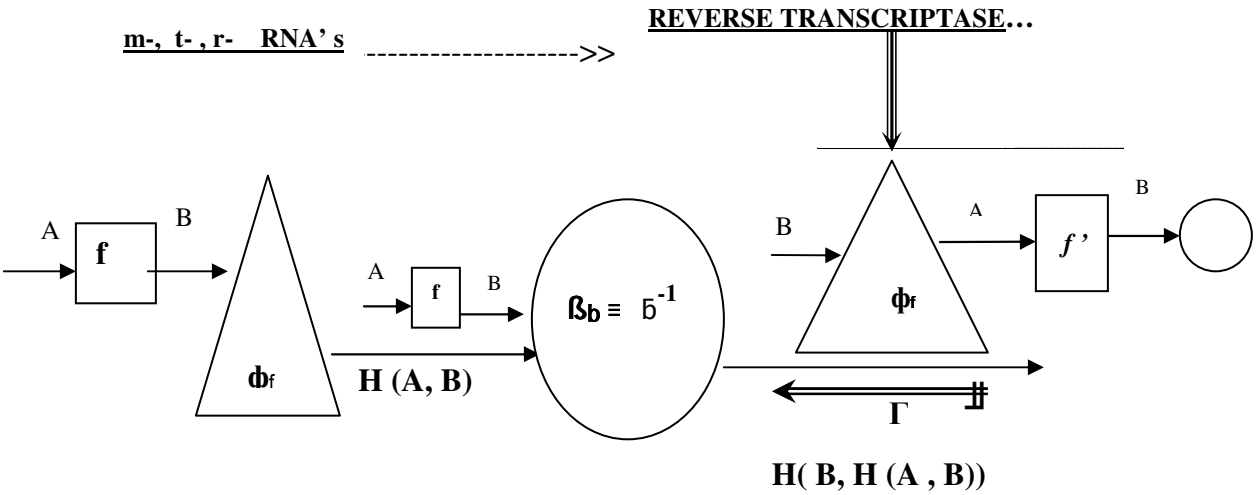
In the case of ***multi-molecular reactions***, the canonical functor of category theory:

$h : \underline{M} \dashrightarrow [M, Set]$ (4)

assigns to each molecular set A the functor $h^{A,}$ and to each chemical transformation **t**: : A $\longrightarrow$ B, the natural transformation $h^A \xrightarrow{\eta} h^B$.

The simplest METABOLIC-REPAIR (M, R)-System with REVERSE TRANSCRIPTION.

ENZYMES ----------->> ***DNA / GENOME***



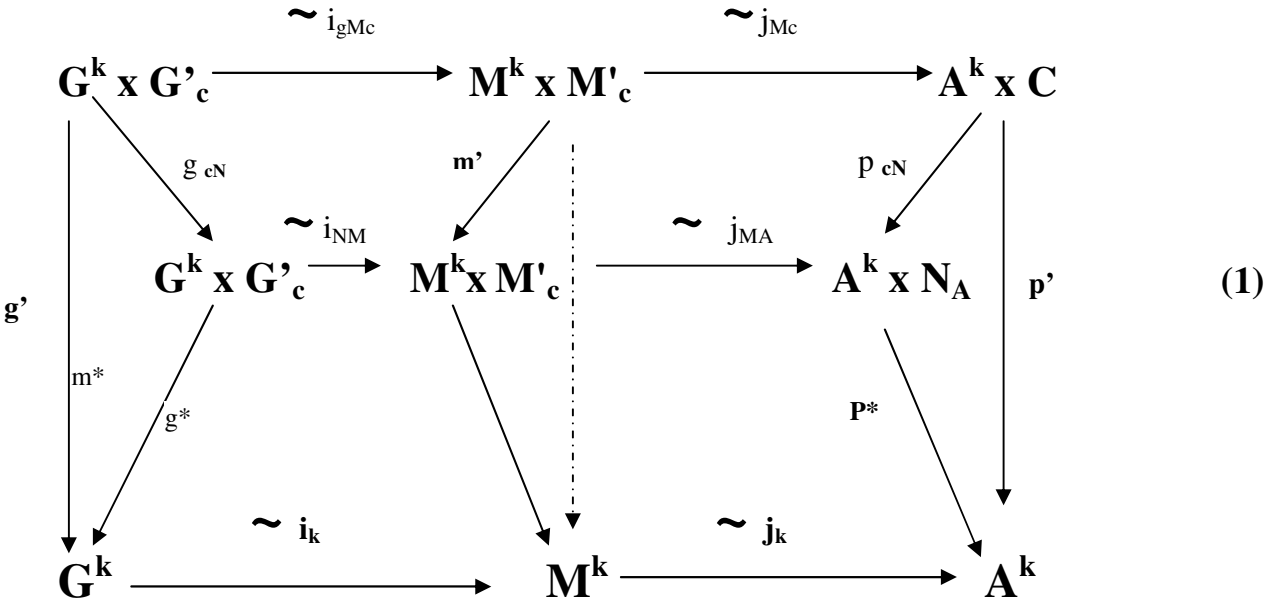
DNA DUPLICATION and CELL DIVISION
follows next in this series-type, or **linear** categorical diagram.

FIGURE 1. The simplest (M, R)-System model of a Primordial Organism..

Possible molecular candidates are indicated at the top of the diagram in Figure 1, above the corresponding METABOLIC (f) or REPAIR/ TRANSCRIPTION (ϕ_f) components. Surviving organisms have **non-linear** diagrams *with* **feedback** and **feedforward**. note in this case, the **'closure', functional mapping, r,** that physically regenerates the telomere and closes the dna-loop at the end of the chromosome. (note also that the above diagram in fig.1 was updated in 2004; the original diagram in 1983 was **completely linear**, and did not have the **closure map r,** the telomere, the **reverse transcriptase… and the dna duplication** ***that are now all represented in the updated diagram. Adding to this diagram an*** **hTERT** ***suppressor gene would provide a FEEDBACK mechanism for simulating the control of cell division and the possibility of cell cycle arrest that is present in somatic cells. the other alternative—which is preferred—is the addition of an*** **hTERT** ***promoter gene*** **that may need to be activated in order to begin 'perpetual' cell cycling, as in 'immortal' cell lines.** ***It would also allow us to introduce simple models of carcinogenesis or cancer cells.***

STRUCTURAL 'HOMOLOGY' OF C- and Nu3-PROTEINS is caused by THE OVERLAP OF THE GENE C WITH THE GENE Nu3 IN THE BACTERIOPHAGE

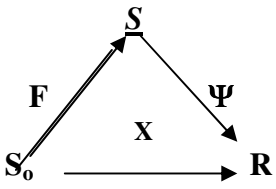
The mathematical representation of this HOMOLOGY-like sequence is given in diagraM (1):



(1)

The "homology" is mathematically represented by the isomorphisms i_{gMc}, i_{NM}, i_k, j_{Mc}, j_{MA}, j_k Regardless of the algebraic structure with which A^n , A^m, M'_c , M^k, M'_N, G^k, G'_c and G_N are endowed, the projections, p', p*, m', m*, g' and g* will always be defined. It is apparent from diagram (1) that transcription of the overlapping genes and the biosynthesis of the proteins for which they code will involve certain multi-molecular reactions. As shown in diagram (4) of ref. (l) these processes will lead to certain natural transformations, η, as specified in diagram (4) .

PHYSICOCHEMICAL MEASUREMENTS ON ORGANISMIC STRUCTURES, $\mathbf{S_o}$, YIELD CERTAIN ***OBSERVABLES*** **F**: S_o ----> ***S*** ; these are defined NATURALLY, such that the DIAGRAM OF CATEGORIES AND ALGEBRAIC THEORIES :



(2)

is commutative .

Such observables of $\underline{\mathbf{S}}_o$ associate to each of its elements, e_j, at each moment, the biological activities of $\underline{\mathbf{S}}_o$ and the products made as a result of such activities. ***S*** was shown to be an **algebraic theory** and is built from *cartesian products* of the sets describing the biological activities and biochemical products of such activities. Physicochemical measurements on $\mathbf{S_o}$ produce real numbers so that certain general observables X: $\underline{\mathbf{S}}_o \rightarrow \underline{R}$ are defined naturally.

NATURAL TRANSFORMATIONS IN PROTEIN BIOSYNTHESIS AND EMBRYOGENESIS.

THE SET OF r-PROTEINS is denoted as H (A,B)

THE SET OF r-PROTEIN mRNA's is denoted as H(B, H(A,B))

THE GENOME TRANSCRIBED INTO r-PROTEIN mRNA is then represented as:

H(H(A,B), H(B,H(A,B))

(see also FIGURE 1 for further details)

Let us consider:

- TWO SETS X and Y in THE METABOLIC CATEGORY, **M**
- and the MAPPING t: X → Y of **M** .

DEFINITION OF THE SPECIAL FUNCTOR $\mathbf{h^X : M \rightarrow Set}$

- $h^X(Y) = H(X,Y)$ for any set Y in M;
- $h^X(t) = m : H(X,X) \rightarrow H(X,Y)$ for any t: X → Y;
- $h^X(g)(t) = g \circ t : H(X,X) \rightarrow H(X,Y')$ for any g: Y → Y' in M ,

where X is a certain fixed object in M. The functor h^X carries Y into H(X,Y)

CONSTRUCTION OF THE SET H (B, H (A, B) of r-PROTEIN mRNAs USING THE CANONICAL FUNCTQR

h : M → [M, Set] is defined as

$$S \sim\sim\rightarrow h^X \text{ and } t\sim\sim\rightarrow h^X \xrightarrow{\eta_t} h^Y,$$

Where t: X→ Y and [M, Set] is a category of functors from M to Set.

An embedding I: M →Set

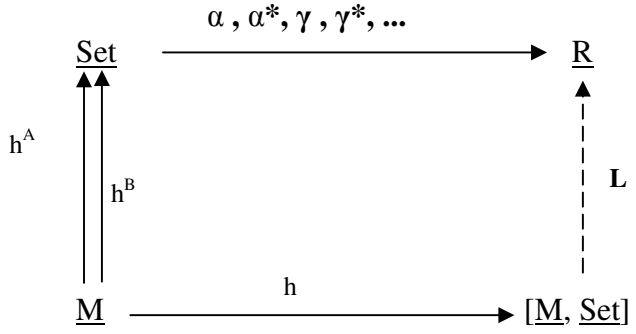
h^X are NATURAL TRANSFORMATIONS

and define r-PROTEIN mRNA's [represented by morphisms in H (X, H (X, Y))].

PROTEIN BIOSYNTHESIS DEFINED AS A MULTI-MOLECULAR REACTION VIA NATURAL TRANSFORMATIONS

Such multi-molecular reactions lead to GENERALIZED OBSERVABLES as defined next.

Such processes induce certain natural transformations $\upsilon : \alpha \dashrightarrow \alpha^*$, and $\omega : \gamma \dashrightarrow \gamma^*$, with α , α^*: Set →R and γ , γ^*: Set→ R being certain special functors. From the definitions of natural transformations and multi-molecular reactions (see formulae (2)-(4) in Section 1) one obtains the following commutative diagram:



with ***L*** playing the role of a ***generalized observable***. In this diagram, the *canonical* functor h assigns to each *molecular set A* the functor h^A and to each *chemical transformation* t: A→B, the natural transformation $\eta : h^A \rightarrow h^B$.

DISCUSSION

It is often assumed incorrectly that Quantum Computation was introduced in 1982. There are also numerous citations of Quantum Automata papers printed in the late 90's and recent quantum computation textbooks that also fail to report the first introduction of the concept of 'quantum automaton'in 1971. Quantum Automata were introduced in a paper published in the Bulletin of Mathematical Biophysics, 33:339-354 (Baianu, 1971a). Categorical computations, both algebraic and topological, were also introduced the same year based on adjoint functor pairs in the theory of categories, functors and natural transformations (Baianu, 1971b). The notions of topological semigroup, quantum automaton,or computer, were then suggested with a view to their potential applications to the analogous simulation of biological systems, and especially genetic activities and nonlinear dynamics in genetic networks. Further, detailed studies of nonlinear dynamics in genetic networks were carried out in categories of n-valued, Łukasiewicz Logic Algebras that showed significant dissimilarities (Baianu, 1977) from Boolean models of human neural networks (McCullough and Pitts, 1943).

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Applications of the Theory of Categories, Functors and Natural Transformations, N-categories, (Abelian or NonAbelian) to:

Automata Theory/ Sequential Machines, Bioinformatics, Complex Biological Systems /Complex Systems Biology, Computer Simulations and Modeling, Dynamical Systems , Quantum Dynamics, Quantum Field Theory, Quantum Groups, Topological Quantum Field Theory (TQFT), Quantum Automata, Cognitive Systems, Graph Transformations, Logic, Mathematical Modeling, etc.

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Note:

This is an effort to integrate Applications of the Theory of Categories, Functors and Natural Transformations (next... pushouts, pullbacks, presheaves, sheaves, Categories of sheaves, Topos.., n-valued Logic, N-categories/ higher dimensional algebra, Homotopy theory, etc.) to an entire range of: physical, engineering, informatics, Bioinformatics, Mathematical Biology , Computer simulations in Neurosciences and Cognitive Sciences – or other areas that are either utilizing or developing categorical formalisms for studying complex problems and phenomena appearing in various types of Dynamical Systems, engineering, Computing, Neurosciences, Bioinformatics, biological and/or social networks.