INFORMATION AND SYMMETRY IN THE CELLULAR SYSTEM

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1. INTRODUCTION

Very few approaches in theoretical biology have dealt with the cellular system in its entire functioning [1]. In this work we try to develop the concepts of Information and Symmetry within the framework of theoretical physics in order to be applied to the whole dynamics of the living cell. We make a closer examination of the selective action mechanisms of enzymes and enzyme networks ("the society of enzymes") and we study how the concept of symmetry for a stochastic dynamical system [2] can help us "to map" the information dynamics of the cell in relation to its environment. For this purpose, we work out a "symmetry transformation" and ponder the possibility of "conserved quantities" in the cellular system.

We also explore the interdisciplinary peculiarities this model-system shows within the framework of both Physics and Biology, and how the emergent "Information Science" can throw new light on the study of living beings (bioinformation).

2. THE CELL AS A "SOCIETY OF ENZYMES"

Certainly, the cellular system is one of the most complex entities --as we will discuss, it is a genuine "society". Not only because of the heterogeneity of its components, the complicated arrangements of interacting macromolecules in its subsystems, and the host of physico-chemical processes involved, but on other hand, because it is a system not quite amenable to experimental testing in its "in vivo" state [3]. Hence, simplified approaches seem necessary, in both methodological and formal aspects.

Biochemists and enzymologists have been taken as a matter of course that most metabolic activity of the cell results from the *superposition of action* of individual enzymes [4] dissolved in an aqueous phase, the dynamics being governed by simple mass-action laws and random thermal motion of metabolite molecules in weak-electrolyte solution. The cell (and each of the organelles therein) basically becomes a "bag" of enzymes and metabolites operating in homogeneous solution. The unitary space-time [4] events of the material transformations in such cell metabolism can be associated with localized enzyme-proteins.

In general, the action of enzymes entails two discrete stages: binding/recognition and chemical catalysis. The substrate molecules must diffuse to the enzyme "active center", where they bind selectively. The following step is the electronic transformation of the substrate, taking into account the impact of effectors (activators and inhibitors) at the binding sites and the influence of other thermodynamic variables (temperature, pH, etc.).

The above simplified approach allows us to see the cell as a "society of enzymes" [5] which exchange material and information among themselves and with the environment. It conduces us towards population-dynamics models not far away from the classical Lotka-Volterra approach. We can model the enzyme "population" as a stochastic dynamic system whose behaviour is described by trajectories within a state space.

The point of each trajectory at time t is determined by the n-dimensional vector $x(q,t)$. We assume that the process $y_t=x(q,t)$ obeys a stochastic differential equation of Stratonovich type.

$$dy_t = \mathbf{B}(y_t,t)dt + \sum_{r=1}^{m} \mathbf{A}_r(y_t,t).dw_t^r \qquad (1)$$

Each component of this vector stands for the value of a population (occupation) number, which has a certain measurable property q_t that can change in time. The state of this population is therefore an element of a certain vector space. In the course of the dynamics of the system, the state vector should not leave this space.

$\mathbf{B}(y_t,t)$ and $\mathbf{A}_r(y_t,t)$ are non-linear functions of y_t; dw_t^r is an m-dimensional stochastic Wiener process. In (1) $\mathbf{B}(y_t,t)$ corresponds to the deterministic part of the process and $\mathbf{A}_r(y_t,t)$ to fluctuating forces which depend themselves of the function y_t; the latter can be interpreted as a "community matrix" too, its anti symmetric part corresponding to the web of effectors (activators and inhibitors) and substrate-product transformation (e.g. the transfer of free energy through the "society") while its symmetric part reflects a collective dissipation.

Within this framework, the whole cellular dynamics can be understood as changing the occupation number, e.g. entering (or acting) new points of q-space and leaving old ones by means of the action of specific enzymes and network of enzymes.

3. SYMMETRY, INFORMATION AND COMPLEXITY

Let us now attempt an interpretation of the q properties of this enzyme population. The exchange of information between the different enzymatic functions occurs through the sharing and networking of substrates, products, activators, and inhibitors. This complicated network of exchanges allows the emergence of an overall functionality for the whole population of enzymes which can be extremely rich. (Here, we will not enter in the complementary dynamics of protein synthesis, converter enzymes of the signaling system, and the protein degradation phenomenon.)

We can now formally discuss how every individual enzyme receives and sends [6] a message. We can clearly distinguish between the reception of information through the effectors and substrate, and the carrier of information, the product. This kind of "gradient field" inside the cell can be "measured" by the individuals of the enzyme population. Then, we take the q-space of the properties of enzymes, as the pattern recognition capacity of this population which has its dynamics described by the equation (1). Therefore, we can set the q's as a state vector,

$$q(t) = [q_1(t), q_2(t),...,q_n(t)] \quad (2),$$

as for the stochastic differential equations, we can write them in the form

$$dy_t(\mathbf{q},t) = [\,\partial_t + Q_0\,]y_t(\mathbf{q},t) + \sum_{r=1}^{m} Q_r y_t(\mathbf{q},t).dw_t^r \quad (3),$$

where: $\partial_t = \dfrac{\partial}{\partial t}$, $Q_0 = \sum_{i=1}^{n} B^i \dfrac{\partial}{\partial t}$, $Q_r = \sum_{i=1}^{n} A_r^i \dfrac{\partial}{\partial q_i}$ (4)

are differential operators defined by (4).

We can see the equation (3) as a *symmetry transformation* for the process defined by the temporal change of a point in the q-space, consequently the dynamics of $q(t)$ must obey,

$$d\mathbf{q}(t) = \mathbf{B}(\mathbf{q}(t),t)dt + \sum_{r=1}^{m} \mathbf{A}_r(\mathbf{q}(t),t).dw_t^r \quad (5),$$

with; $q(t_0)=c(\alpha)$, $t \in [t_0]$, where α is a order parameter.

It can be demonstrated [2] that the condition for (3) being a symmetry transformation of (5) is that the function satisfies

$$\mathbf{B}(y_t(\mathbf{q},t),t) = [\,\partial_t + Q_0\,]y_t(\mathbf{q},t) \quad \text{and}$$
$$\mathbf{A}_r(y_t(\mathbf{q},t),t) = Q_r y_t(\mathbf{q},t) \qquad (6)$$

In this context we can consider the y_t as a "conserved quantities" for any system having its dynamics described by (5). In a similar fashion, this means (in our interpretation) that if the receiver properties of the enzyme can be described as a stochastic dynamical system (5) we can make a transformation to a population space the "form" of which (5) is invariant (under this transformation).

4. CONCLUDING REMARKS

The above mathematical description just maps an abstracted aspect of the "territory" of biomolecular information processing and control [7]. By following this approach, we can further formulate the notion of symmetry operator [2] which yields a more general

conserved quantity for the system, which in its turn can help us to find other possible conserved quantities. The explicit form of the process $y_t=x(q,t)$, as well as its component functions $\mathbf{B}(y_t,t)$ and $\mathbf{A}_r(y_t,t)$, will be the subject of future enquires.

The use of theories based on the intrinsic *symmetries* in the space-time structure of the natural world has been a fruitful strategy of physics in its attempt to unify its various levels of complexity. Among the symmetry principles of physics, the most abstract one is the set of "gauge symmetries". In this respect we can speculate how "form" (structure) and function are invariants under a gauge transformation (e.g., specific recognition).

It is a reasonable approximation to consider the populational species as being in quasi-stable equilibrium of growth with respect to its environment. The "chemical fields" (effector and substrate web), which are invariant to the gauge transformation, compensate for any local change of any "enzymatic field" within the populational number, and preserve (save) the global invariance. A local input in this system is a factor for a change in "local condensation" - nucleation. Through this nucleation process, the symmetry of the system suddenly and spontaneously lowers, and it does so in a non-predicable, random event. The symmetry of the system is "broken". In this context the enzyme populational action emerges as a "thermodynamic coordinate"--because of a fundamental symmetry principle grounded in the concept of broken symmetry.

5. REFERENCES

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