

The Problems of Replication in the Early Stages of Evolution: Enumeration of Variants and Spatial Configurations of Replicators

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Abstract Two main problems of replication in the early stages of evolution are discussed: the problem of exponentially large number of conformational degrees of freedom and the problem of enumeration of variants.

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The conditions under which replication is possible remain unknown. There are two problems with the replication of molecules having many conformational degrees of freedom: different spatial configurations of the same molecule, represent, in fact, different molecules (they are no longer copies); and for a relatively small genome of size 10^2 - 10^3 , the evolution through undirected mutations is realistic, but with a further increase in genome size, the rate of non-directional evolution of the genome is too small and should include other mechanisms (see, for details, Melkikh 2014a).

As it was shown previously (Melkikh 2014b) potentials between molecules, which could provide the rapid folding of biologically important molecules (proteins, RNA, DNA), are not known. All currently known potentials do not allow for the organization of a funnel-like landscape, which is a condition of such a folding. Replicators that existed on Earth in the early stages of evolution had another problem - the number of possible reactions of such macromolecules (taking into account all possible conformations) is exponentially large. All this means that the replicators could not stably exist and reproduce.

Solving the problem of the rate of evolution of replicators presupposes the existence of a priori information, such that the evolution becomes partially directed. Any acceleration mechanisms of evolution compared to enumeration of all variants presuppose the existence of such information, but their storage mechanisms remain unclear.

An analysis of the task of gene control (directed mutations) and process of control of RNA (DNA, proteins) folding shows a significant similarity between these problems. In both cases,

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the problem is to make the choice of an exponentially large number of possible states of the system. It can be assumed that the same mechanism that is responsible for the accurate folding of replicators could also be responsible for their directed evolution.

In the paper (Melkikh 2014a) a model of partially-directed evolution on the base of the theory of learning automata was constructed. Let's transform the equations of partially-directed evolution from the most general form into a form that would allow clarify the physical meaning of the individual terms.

First, let's select in these equations *truly random processes*. In terms of partially-directed evolution this refers to those processes which are not directed a priori to any particular area in the phase space. We emphasize that this does not mean that these truly random processes will be expressed in the independent and equally point mutations. It is known that random processes are very diverse.

Secondly, we consider a sufficiently large population; therefore, we assume that, for the population as a whole, the change in the genome per generation of replicator is small. Effects associated with genetic drift in small populations are known, but do not contribute anything new to the mechanism of evolution. Therefore we can write the equation of balance of the number of replicators in the population as a differential equation. We will use the well-known equations for the evolution of replicators:

$$\frac{dx_k}{dt} = W_k x_k + \sum_l \chi_{kl} x_l - E x_k, \quad (1)$$

where x_k – number of replicators (information sequences) of the k -th species; W_k – reproductive fitness of individuals of the k -th species; χ_{kl} – the parameters characterizing the mutational fluxes; and E – is the parameter characterizing the overall dilution of the population. Equation (1) can also be written in discrete time.

In the case of partially-directed evolution, the overall structure of the evolution Eq. (1) remains the same, but the structure of the variable χ_{kl} will be different. Let's write χ_{kl} as follows:

$$\chi_{kl} = \chi^*_{kl} + \chi^D_{kl},$$

where χ^D_{kl} – are mutational fluxes not directed a priori to achieve any goal in the phase space, which corresponds to Darwinian evolution, χ^*_{kl} – mutation fluxes, directed a priori to achieve any «goal» in the phase space. In this case, the “goal” is a region in the phase space in which the system tends, in accordance with the equation of motion.

Then the basic equation of evolutions of replicators will be:

$$\frac{dp_k}{dt} = W_k p_k + \sum_l \chi^D_{kl} p_l + \sum_l \chi^*_{kl} p_l - E p_k,$$

where p_k – are probabilities of existing of certain species of replicators in population.

In the paper (Melkikh 2014b) it was shown that quantum effects are fundamental for solving combinatorial problems (storage of priori information), as well as for the effective transfer of information within the cell. Consequently, we can assume that the solution of proposed problems of replication in the early stages of evolution must also include quantum effects.

Experiments to test the hypothesis may be associated with a more detailed study of the replication process (see, e.g., Matsuno 2012) and a study of interaction with biologically important molecules in real time. The process of cell division is relatively slow compared to,

for example, a process of protein folding. This makes it possible on the basis of X-ray diffraction (neutron diffraction) to try to find the actual interaction potentials between nucleotides, as well as between other important molecules. In particular, it will be possible to answer the question whether such potential is many-particle or not.

Thus, we can give the following answer to the question 01 (How can we make ordered sequences of amino acids, or mononucleotides by prebiotic means?): we can make ordered sequences (replicators), only taking into account quantum effects and collective interactions between atoms.

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