Available online at www.sciencedirect.com

SciVerse ScienceDirect

Physics of Life Reviews 9 (2012) 219–263

PHYSICS of LIFE reviews

www.elsevier.com/locate/plrev

Review

Evolutionary dynamics of RNA-like replicator systems: A bioinformatic approach to the origin of life ☆

Nobuto Takeuchi [a,b,*], Paulien Hogeweg [b]

[a] *National Center for Biotechnology Information, National Library of Medicine, National Institutes of Health, 8600 Rockville Pike, Bethesda, MD 20894, USA*

[b] *Theoretical Biology and Bioinformatics Group, Utrecht University, Padualaan 8, 3584CH Utrecht, The Netherlands*

Received 26 February 2012; accepted 4 June 2012

Available online 13 June 2012

Communicated by J. Fontanari

Abstract

We review computational studies on prebiotic evolution, focusing on informatic processes in RNA-like replicator systems. In particular, we consider the following processes: the maintenance of information by replicators with and without interactions, the acquisition of information by replicators having a complex genotype–phenotype map, the generation of information by replicators having a complex genotype–phenotype–interaction map, and the storage of information by replicators serving as dedicated templates. Focusing on these informatic aspects, we review studies on quasi-species, error threshold, RNA-folding genotype–phenotype map, hypercycle, multilevel selection (including spatial self-organization, classical group selection, and compartmentalization), and the origin of DNA-like replicators. In conclusion, we pose a future question for theoretical studies on the origin of life.

Published by Elsevier B.V.

Keywords: RNA world; Early evolution; What is life?; Protocell; Mathematical modeling; Computational modeling

1. Introduction

This paper is centered on one question: How can a system of simple RNA-like replicators increase its complexity through evolution? Our motivation is two fold. The question is crucial to the RNA world hypothesis as explained in the next section. Moreover, the simplicity of RNA-like replicator systems makes it easier to investigate evolution as a process of pattern formation operating at multiple levels of organization such as genotypes, phenotypes, interactions, and spatiotemporal distributions of individuals. We approach the above question from the viewpoint of bioinformatics in a wide sense, namely, the study of informatic processes in living systems [1]. From this viewpoint, we will review

☆ This paper is based on the PhD thesis of the first author.

* Corresponding author at: National Center for Biotechnology Information, National Library of Medicine, National Institutes of Health, 8600 Rockville Pike, Bethesda, MD 20894, USA.

E-mail addresses: takeuchi@ncbi.nlm.nih.gov, takeuchi.nobuto@gmail.com (N. Takeuchi).

1571-0645/$ – see front matter Published by Elsevier B.V.
http://dx.doi.org/10.1016/j.plrev.2012.06.001

a variety of mathematical or computational models of RNA-like replicator systems. Emphasis will be placed on the use of models as a tool to discover the unforeseen rather than a tool to confirm the preconceptions.

1.1. Organization of this paper

In Section 2, we briefly review the RNA world hypothesis and motivate the central question of this paper.

In Section 3, we review the evolutionary dynamics of replicators that do not interact with each other. We first describe the quasi-species theory as an improvement on the "survival of the fittest" principle. We next show that there is a severe limit on the amount of information that can be maintained by evolution (the problem of information maintenance). In addition, we discuss error thresholds.

In Section 4, we review the evolutionary dynamics of replicators that have a complex genotype–phenotype map (no interactions assumed as in Section 3). We show that high redundancy in the genotype–phenotype map facilitates evolution toward a target phenotype. We also show that such high redundancy, however, does not solve the problem of information maintenance (phenotypic error threshold). In addition, we describe neutral evolution of mutational robustness.

In Section 5, we review the evolutionary dynamics of replicators that interact with each other. We first describe a replicator network known as a hypercycle and its limitation, namely, the problem of parasites. We then show how this problem can be solved by the consideration of spatial self-organization and discrete populations. We next introduce a simpler replicator network (one-replicase one-parasite system) and describe the phenomenon of multilevel evolution. In addition, we describe the effect of complex formation on the evolutionary dynamics of replicators.

In Section 6, we review the evolutionary dynamics of replicators that have a complex genotype–phenotype–interaction map. We show how complexity can evolve in an RNA-like replicator system through a positive feedback between the evolution of sequences and the evolution of ecosystems.

In Section 7, we review the evolutionary dynamics of compartmentalized replicators. We first describe the classical theory of group selection as applied to RNA-like replicator systems. We then describe a model of protocells and multilevel evolution that occurs in this model. We show that this multilevel evolution differs from that mentioned above and explain how this difference arises.

In Section 8, we review the evolutionary dynamics of DNA-like replicators (i.e., replicators that can serve as templates, but not as catalysts, of replication). We describe how the division of labor between templates and catalysts can emerge through the evolution of DNA-like replicators in RNA-like replicator systems.

In Section 9, after briefly summarizing the preceding sections, we suggest a possible direction for future research on the origin of life from the viewpoint of bioinformatics.

2. The RNA world hypothesis

Living systems are amusingly diverse at a glance, beautifully sophisticated on inspection, and staggeringly complex on reflection. Yet, in thinking about the origin of life, one can ask a question: What would be the simplest system conceivable if one simplified current living systems as much as possible? Then, the conjugate question is, How could this simplest system evolve into systems as complex as life as we know it?

A basic unit of biological systems is the cell (ignoring viruses for a moment). Very roughly speaking, half the dry mass of an *E. coli* cell is proteins, a quarter RNA, an eighth phospholipid, and a sixteenth DNA [2]. Proteins catalyze various chemical reactions essential to cells including the synthesis of lipids, DNA, and RNA. Proteins are synthesized by the translation of mRNAs, which are, in turn, synthesized by the transcription of DNA. DNA molecules are (nearly) always synthesized by the replication of already existing DNA molecules as templates (except, e.g., telomeres). In other words, information flows from DNA to proteins (or more precisely, from nucleic acids to proteins), but not vice versa—i.e., the central dogma of molecular biology [3,4]. It, therefore, appears that proteins and DNA are the essential components of living systems.

However, a great surprise came from studies on ribosomes. These studies revealed that rRNAs, rather than ribosomal proteins, catalyze the synthesis of proteins (i.e., the polymerization of amino acids), discriminate between correct and incorrect codon–anticodon pairs, and prevent the premature hydrolysis of peptidyl-tRNAs (see, e.g., Ref. [5], for review). Therefore, "the ribosome is a ribozyme" [6]. These findings have two implications. First, it is conceivable that proteins can also catalyze the synthesis of proteins; in fact, proteins *are* the common catalysts of various chemical