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# Protocells under the Chemoton hypothesis do evolve: Emergence of species

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## 1. INTRODUCTION

Almost all life forms known today are composed by cells, fundamental constituting units which are able to self-replicate and evolve through changes in genetic information. These highly sophisticated devices are the product of about four billion-year evolution, and, in this respect, represents the relic of primordial life bricks, the *protocells*. The latter were most probably exhibiting only few simplified functionalities, that required a *primitive embodiment structure*, a *protometabolism* and a *rudimentary genetics*, so to guarantee that offsprings were “similar” to their parents [6, 8].

Artificial protocells have not yet been reproduced in laboratory and intense research programs <sup>1</sup> are being established aiming at developing reference models [5] that capture the essence of the first protocells appeared on earth and enable to monitor their eventual subsequent evolution. In 1971, Gánti [4] proposed a pioneering theory that provides a minimalist description of a protocell, termed *Chemoton*: roughly speaking a model to describe growing and multiplying microspheres controlled by a template duplication process. The Chemoton hypothesis includes a *membrane* which protects the inner bulk, while filtering the access of high energetic “food”, which is made available in the surrounding environment. The food is processed through chemical reactions and transformed into basic materials that are needed to stimulate both template duplication and membrane growth, hence a *metabolic process*. Finally, in the simplest scheme, the template-polymer is assembled from one specific type of monomer (homopolymer), which acts as an effective *carrier of information*: its length determines in fact the division time, a phenotype property of paramount importance. After such a time, the protocell attains a critical size, above which a division into two perfect halves occurs. Each daughter cell contains an identical portion of material, which is equally shared from the mother constituents. Thus according to the definitions given by [8, 1, 6, 7], the Chemoton hypothesis is an *uniti of life*, hence a natural question is [4]: is it also a *unit of evolution*?

Assume that the external food is periodically available, each cycle being for instance associated to tides in the pond were the protocells supposedly live, or the metabolic process to be driven by a periodic source of energy, e.g. the light from the sun. Then the *regular functioning* of the model, i.e. periodic growth and division in time of the protocell, relies on the *synchronization* of the three chemical networks.

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<sup>1</sup>For instance PACE – Programmable Artificial Cell Evolution – an European Integrated Project in the EU FP6-IST-FET Complex Systems Initiative.

With respect to the original Chemoton picture, we developed an improved formulation [2, 3]: chemical reactions occur in a varying volume, not known a priori, but intrinsically determined by the protocell membrane growth. This effect is explicitly accounted for. Moreover, the deterministic model is further modified to accommodate for a mutation mechanism: during the template duplication extra monomers are added (removed) according to a pre-assigned probability.

Within this novel scenario, the time evolution of a single protocell is monitored as functions of a number of selected variables of key relevance, e.g. the amount of food initially available and the template length at start. This knowledge translates into a State Function which unambiguously predicts the ultimate fate of the protocell, once the initial conditions are specified, e.g. the length of the polymer ( $N$ ) and its ability to self-replicate ( $V^*$ ).

Motivated by the synchronization hypothesis and due to the absence of intermittency in the protocell dynamics, it is assumed that only protocells with regular behavior give rise to next generation offsprings, while non-synchronized protocells will eventually die <sup>2</sup>

Using the State Function concept we are able to perform for the first time simulations on a large population of protocells, following their evolution for long intervals of time <sup>3</sup>. The protocells are subjected to the pressure of the environment, here exemplified through the amount of available food, which changes in time and depends self-consistently on the size of the population: the larger the number of protocells, the lower the amount of available food, and vice-versa. This open-ended mechanism mimics therefore an effective Darwinian evolution.

The main result of our analysis is that the *speciation* is an emergent property of the model: protocells with different templates can develop from a common ancestor. The occurrence of a speciation mechanism in a Chemoton-like population is here demonstrated for the first time and contributes to shed new light into the important issue of protocells evolution and dynamics: the Chemoton hypothesis defines not only a reliable unit of life, but also a unit of evolution.

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*keywords:* Protocell; Chemoton model; Evolution; Speciation; Chaos

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<sup>2</sup>Let us observe that our results will hold even if we remove this “conservative” assumption as we will show later.

<sup>3</sup>Each protocell behavior is described by more than one hundred of equations, computing the State Function once for all, enables to formally assimilate each protocell belonging to the population under scrutiny to a black box, which produces specific output, once selected input values are provided. This reduces considerably the computational costs and allows to significantly enhance the statistics over previous investigations.

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