

## Is There an Optimal Level of Open-Endedness in Prebiotic Evolution?

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**Abstract** In this paper we explore the question of whether there is an optimal set up for a putative prebiotic system leading to open-ended evolution (OEE) of the events unfolding within this system. We do so by proposing two key innovations. First, we introduce a new index that measures OEE as a function of the likelihood of events unfolding within a universe given its initial conditions. Next, we apply this index to a variant of the graded autocatalysis replication domain (GARD) model, Segre et al. (*P Natl Acad Sci USA* 97 (8):4112–4117, 2000; Markovitch and Lancet *Artif Life* 18(3), 2012), and use it to study - under a unified and concise prebiotic evolutionary framework - both a variety of initial conditions of the universe and the OEE of species that evolve from them.

**Keywords** Complexity · Comptype · Compositional Information · Simulations · Replication

### Open-Ended Evolution

Open-ended evolution may be thought of as referring to a “system in which components continue to evolve new forms continuously, rather than grinding to a halt when some sort of ‘optimal’ or stable position is reached” (Taylor 1999). Notably, open-ended evolution does not necessarily imply evolutionary progress or complexification. Yet, a system in which complexity increases along the evolutionary time axis fulfills a sufficient (even if not necessary) condition for open-endedness.

Indeed, evolution of complexity and the related concept of open-ended evolution have been a topic of scientific enquiry since Darwin and Wallace introduced the Theory of Evolution by Natural Selection. There is no doubt that a complexification process took place over the extended evolutionary time frame, with some endosymbiotic events (Neef et al. 2011). With the advent of powerful computational tools in which one could seamlessly

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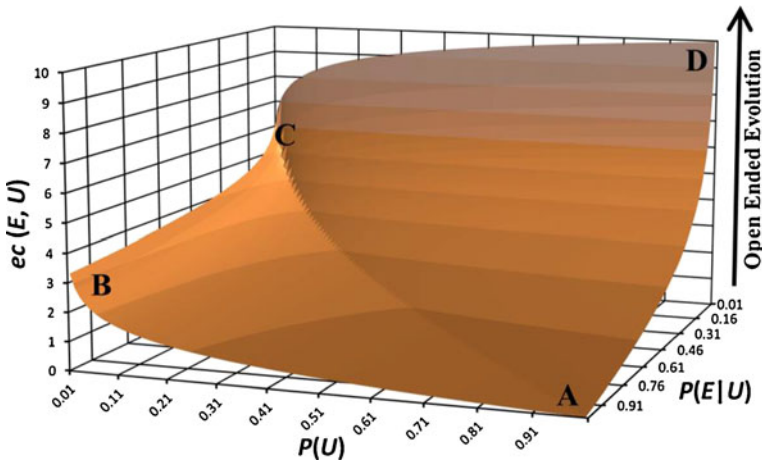
run “what-if” scenarios about the origins of life, the questions of how complexity emerges from evolution-like processes and how open-ended the emergent processes have gained renewed impetus (Bedau et al. 2000). Researchers have proposed multiple definitions of both open-ended evolution and (pre)biotic complexity and have applied these measures to several, more or less convoluted, “Artificial Life” and prebiotic systems. Common definitions of open-ended evolution consider an increase in the internal complexity of species (McMullin 2000; Ruiz-Mirazo et al. 2004) or species occupying ever more diverse niches of the natural design space (McShea 1994; Korb and Dorin 2011). A difference between the two approaches is apparent when considering the case of a few species in an ecosystem becoming more and more complex vs. the emergence of multiple species that might each be relatively simple but overall occupy a relatively large portion of the natural possible design space. The former definition can be viewed as “species-centric” whereas the latter as more “system-centric” (Korb and Dorin 2011).

Korb and Dorin discuss at length the various attempts made at measuring open-endedness and suggest a two-part measure based on message minimum length required for conveying (or encoding) information (*MML*). They propose that a measure that considers the complexity of events of species evolving (part 1) and of the related hypothesis (part 2) would be a better measure for evolutionary complexity as it is a relative measure that takes into account not only the end product but the context in which these are produced. Building on this concept, we address the question of whether there is an optimal set up for a putative prebiotic universe that leads to greater OEE of the species evolving within it. We define an index of the excess-complexity of species (event,  $E$ ) in relation to the universe in which they evolve ( $U$ ), as a proxy for OEE. This index is  $ec(P(E|U), P(U))$ , that relates the probability of observing events ( $P(E|U)$ ) to the probability of the initial conditions ( $P(U)$ ). Our index, like suggested by Korb and Dorin (2011), is a two part index but with the additional advantage of having the following properties:

1.  $P(E|U)$  and  $P(U)$  are normalized such that  $0 \leq P(E|U), P(U) \leq 1$ .
2.  $P(E|U) \rightarrow 0$  and  $\rightarrow 1$  respectively represents improbable and probable outcomes unraveling from the initial conditions  $U$ . Similarly,  $P(U) \rightarrow 0$  and  $\rightarrow 1$  represents improbable and probable initial universe conditions.
3.  $ec \geq 0$  and can grow arbitrarily large. The larger the value of  $ec$ , the more complex are the unfolding events in relation to a given universe.
4.  $\lim_{P(E|U) \rightarrow 1, P(U) \rightarrow 1} ec(P(E|U), P(U)) = 0$ , that is, probable initial conditions that lead to probable events receive the lowest rank (i.e. no surprises can be expected from this universe under the given initial conditions). This is marked as Scenario A in Fig. 1.
5.  $\lim_{P(E|U) \rightarrow 1, P(U) \rightarrow 0} ec(P(E|U), P(U)) = K; K > 0$ , that is, improbable initial conditions that lead to probable events are ranked slightly higher than 0 (Scenario B).
6.  $\lim_{P(E|U) \rightarrow 0, P(U) \rightarrow 0} ec(P(E|U), P(U)) = L; L > K > 0$ , that is, an improbable initial state that leads to improbable events ranks even higher as this clearly represents an unexpected observation emerging from an unexpected initial condition (“Garden of Eden”, scenario C).
7.  $\lim_{P(E|U) \rightarrow 0, P(U) \rightarrow 1} ec(P(E|U), P(U)) = M; M > L > K > 0$ , that is, a probable set of initial conditions throws out surprising outputs thus ranking at the top of the scale (“Elegant Garden of Eden”, scenario D).

We now define  $ec$  (Eq. 1) with exactly the above characteristics:

$$ec(E, U) = -\frac{1}{2} \log_2(P(E|U) \cdot P(U)) + \log_2 \frac{\text{Max}[P(E|U) \cdot P(U)]}{P(E|U)} \quad (1)$$



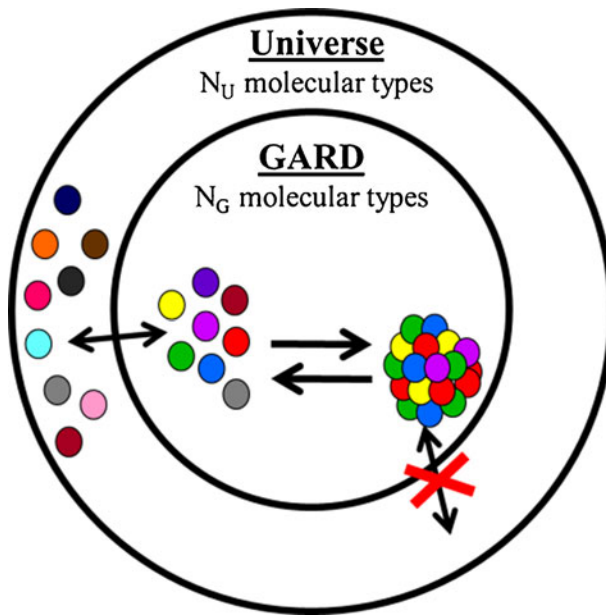
**Fig. 1**  $ec$  as a proxy for open-ended evolution (OEE). A, B, C and D mark different scenarios, as explained in the text

where the first part is an embodiment of MML and is scale invariant, and the second part is different from zero only when added value in the complexity of events has occurred (i.e.  $U$  is simpler than  $E$ ). An increase in  $ec$  during a simulation will serve as a proxy to identify OEE, as an increase in complexity is generally considered to be indicative of OEE. Moreover, following the previous discussion,  $ec(E, U)$  is a species-centric measure of OEE but can easily be “system-shifted” by encompassing all outcomes  $E$ .

In Fig. 1 we identify the four extreme  $ec$  values a simulated universe might receive. As one moves from A, to B, to C and finally to D the level of  $ec$  increases, thus OEE is observed. In fact, as the likelihood of the initial conditions increases ( $P(U) \rightarrow 1$ ) and the likelihood of the events decreases ( $P(E|U) \rightarrow 0$ ) the level grows, potentially without limit.

## Universe-GARD

In order to address the question of whether there is an optimal set up for a putative prebiotic “universe” with events unfolding inside such that OEE is observed, we extend the well-studied lipid-world framework, the GARD model (Segre et al. 2000). GARD simulates molecular assemblies formed by accretion from an immediate buffered environment containing a defined set of  $N_G$  amphiphilic compound types, where the rate of accretion is biased by a network of mutually catalytic interactions,  $\beta$ . The assembly is kept out of equilibrium by imposing a fission action when it reaches a predefined size, producing two progeny of the same size, one of which grows again generating a growth-fission cycle of consecutive generations. GARD dynamics portray composites, sets of faithfully replicating compositional states that may be regarded as analogous to species or quasispecies (Eigen and Schuster 1977; Shenhav et al. 2007; Markovitch and Lancet 2012). Typically up to eight different composites are being cycled, suggesting that GARD does not appear to display high levels of  $ec$  to begin with, which impends on its OEE. The new proposed model, to be termed universe-GARD (U-GARD), will allow us to systematically study the tradeoff between the initial conditions of the universe and the emerging composites (i.e. map the  $ec$  surface). In U-GARD, the immediate environment is embedded in a larger “universe” with  $N_U (\geq N_G)$  different compound types, instances of which are continually being exchanged with the immediate environment (Fig. 2). This is physicochemically feasible, as



**Fig. 2** Open-ended GARD (Universe-GARD, U-GARD). Assemblies undergo growth-fission cycles in the immediate environment, obeying the GARD dynamics. At any given time step exchange of compound types between the two environments occurs only for compounds not included in compotypes

exemplified by the immediate environment being absorbed to a mineral surface, contained in a mineral pore or constituting an ineffectively stirred sub-region of a larger prebiotic aquatic body. As a compotype constitutes a set of molecules that function better as a whole in their particular environment and thus faithfully replicate, the organization of a compotype is also assumed to protect its constituting molecular types from being “washed out” to the larger universe.

### ***ec* in U-GARD Simulations**

When a simulation starts, the universe is defined by the initial configuration of the  $N_U$  compounds.  $E$  and  $U$  respectively represent the compositions of compotypes encountered and the initial-environment.  $P(E|U)$  and  $P(U)$  will be measured as the probabilities of getting  $E$  and  $U$  by random picking. It is also possible to measure  $P(E|U)$  as the probability of finding new compotypes, never encountered before in that simulation, after a sufficiently long time course. OEE will be identified when a universe will exhibit an increase in  $ec$ . Different universes with different  $N_U$ ,  $N_G$  and  $\beta$  parameters can be compared by using the expected value of  $ec$ :

$$\langle ec\{N_U, N_G, \beta\} \rangle = \sum_U [ec(E, U) \cdot P(ec(E, U))] \quad (2)$$

in order to find the optimal set of parameters exhibiting the highest  $\langle ec \rangle$ .

### **Conclusions**

We have presented a new version of the GARD model that, through a simple extension, allows us to address the question of whether there is an optimal level of open-ended

evolution that can be expected from a prebiotic world. To quantify this we have proposed a new index that incorporates several intuitive expectations of what “open-endedness” should look like. Namely, predictable and simple universes producing predictable and simple outputs are at the bottom of the scale and unlikely universes producing simple output score only slightly higher. Next on the scale we find the unlikely universe producing unlikely and complex output (Garden of Eden scenario) and finally, at the pinnacle, close to where true-emergence lies, we find those probable prebiotic universes that throw out unlikely and complex events (Elegant Garden of Eden scenarios, a hallmark of emergence). In our future work we plan to systematically chart what kind of dynamics GARD and U-GARD provide and how they map into *ec*.

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## Comment on Is There an Optimal Level of Open-Endedness in Prebiotic Evolution?

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The lipid world framework and, specifically, the GARD model have been considered as a kind of alternative to the RNA world scenario (Segre et al. 2001). The talks, which we have heard during this meeting, suggest that these two approaches could complement each other.

Indeed, the current versions of the RNA world scenario imply that, starting from a certain level of complexity, the RNA replicators should have been encased by amphiphilic membranes to avoid collapsing by parasites (Takeuchi and Hogeweg 2012). It seems extremely unlikely that the very first replicators could possess systems of lipid biosynthesis. Hence, replicators should have recruited abiotically synthesized amphiphilic molecules to build their envelopes. It has been suggested that replication of ribozymes may have driven the fission of replicator-encasing vesicles (Schrum et al. 2010). Then, however, even a perfect, template-guided RNA replication event, followed by a division into two vesicles, would yield two different vesicles because their probability of inheriting identical sets of amphiphilic molecules should have been negligible. Hence, the survival of each membrane-encased replicator would depend on the quality of its abiotically synthesized and self-assembling membranes. In my opinion, the outlined scenario represents a merger of the RNA world model and the Lipid world framework. This kind of scenarios might be explored by the GARD model or its modification.

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