



Niche emergence as an autocatalytic process in the evolution of ecosystems

Roberto Cazzolla Gatti^{a,b,*}, Brian Fath^{c,d}, Wim Hordijk^e, Stuart Kauffman^f, Robert Ulanowicz^{g,h}

^a Biological Institute, Tomsk State University, Russian Federation

^b FACAI Lab (GFBI Hub), Department of Forestry and Natural Resources, Purdue University, USA

^c Department of Biological Sciences, Towson University, Towson, MD, USA

^d Advanced Systems Analysis Program, International Institute for Applied Systems Analysis, Laxenburg, Austria

^e Institute for Advanced Study, University of Amsterdam, The Netherlands

^f Institute for Systems Biology, Seattle, WA, USA

^g Department of Biology, University of Florida, USA

^h Chesapeake Biological Laboratory, University of Maryland, USA



ARTICLE INFO

Article history:

Received 21 July 2017

Revised 23 May 2018

Accepted 30 May 2018

Available online 1 June 2018

Keywords:

Autocatalysis

Symbiosis

Niche emergence

Diversity

Autocatalytic set

Biodiversity

Ecosystem evolution

ABSTRACT

The utilisation of the ecospace and the change in diversity through time has been suggested to be due to the effect of niche partitioning, as a global long-term pattern in the fossil record. However, niche partitioning, as a way to coexist, could be a limited means to share the environmental resources and condition during evolutionary time. In fact, a physical limit impedes a high partitioning without a high restriction of the niche's variables. Here, we propose that niche emergence, rather than niche partitioning, is what mostly drives ecological diversity. In particular, we view ecosystems in terms of autocatalytic sets: catalytically closed and self-sustaining reaction (or interaction) networks. We provide some examples of such ecological autocatalytic networks, how this can give rise to an expanding process of niche emergence (both in time and space), and how these networks have evolved over time (so-called evoRAFs). Furthermore, we use the autocatalytic set formalism to show that it can be expected to observe a power-law in the size distribution of extinction events in ecosystems. In short, we elaborate on our earlier argument that new species create new niches, and that biodiversity is therefore an autocatalytic process.

© 2018 Elsevier Ltd. All rights reserved.

1. Introduction

It is now well-accepted that all objects in ecological networks interact with and influence the others in the web and that there are no null community-level relations (Fath, 2007; Cazzolla Gatti 2016a). Moreover, the idea that species diversity can drive speciation was proposed (Emerson and Kolm, 2005) and tested (Gruner et al., 2008; Bailey et al., 2013). With the “Biodiversity-related Niches Differentiation Theory” (BNDT; Cazzolla Gatti, 2011), it was suggested that mutualistic networks of the ecosystem allow, through circular and feedback mechanisms, the enhancement of the number of species, generating a non-linear self-sustaining (or autopoietic) system. The BNDD stressed that species tend—directly, through interactions, or even indirectly, thanks to their simple presence and life roles—to increase the number of potentially available niches for the colonization of other species, enhancing the

limit imposed by the basal hyper-volume, until they reach the carrying capacity of the ecosystem. In this manner, the presence of the species expands the environmental openings for other species: i.e., diversity begets diversity.

Ulanowicz et al. (2014), analysing the behaviour of self-sustaining systems, considered three actors interacting in an autocatalytic cycle, each receiving benefit from its upstream partner and providing benefit to its downstream counterpart. Implicit in this configuration resides a positive form of selection. The end result is the phenomenon called centripetality, whereby internal selection pulls progressively more resources into the orbit of the autocatalytic cycle (usually at the expense of non-participating elements). The *Utricularia* communities, which dominated the oligotrophic interior of the Florida Everglades, but which disappeared when new resources (mostly phosphorus) became available, provide a good example. The *Utricularia* reappeared, however, in the eutrophic canals where the species could grow fast enough to stay ahead of the choke-off (Ulanowicz, 1995). It was proposed (Levin, 1998) that aggregation and hierarchical assembly are not imposed

* Corresponding author.

E-mail address: robertcazzolla@gmail.com (R. Cazzolla Gatti).

on complex adaptive systems (CAS), but emerge from local interactions through endogenous pattern formation. These patterns of aggregation constrain interactions between individuals and thereby profoundly influence the system's further development.

More generally, the existence of so-called ecological autocatalytic sets (EcoRAFs: species, or “guilds” of species that exploit the same set of resources in similar but slightly different ways), producing intermediate and final products/conditions that enable the appearance and existence of other EcoRAFs, was recently advanced (Cazzolla Gatti et al., 2017a). The simple conclusion coming from combining the BNDT and the EcoRAF hypothesis was that “new species create new niches”. Thus, biodiversity is autocatalytic, and increasingly diverse ecosystems are its emergent properties (Cazzolla Gatti et al., 2017a).

Here we explore the long-term effects of the idea that “biodiversity is autocatalytic”: at evolutionary time scales new species, simply by coming into existence, create ever new niches into which further new species can emerge, creating yet more new niches, and so on (Cazzolla Gatti, 2011; Kauffman, 2016).

2. Ecosystems and autocatalytic sets

Previously, we argued that an ecosystem can be viewed as a collection of autocatalytic sets representing species, or species guilds (Cazzolla Gatti et al., 2017a). An *autocatalytic set* is a (chemical) reaction network where each reaction is catalysed by at least one molecule from the set, and each molecule can be built up from a basic food set by a sequence of reactions from the set itself. The food set consists of those elements that are assumed to be available from the environment (although not necessarily in an unlimited supply). In other words, elements from the food set do not need to be produced by any of the reactions from the autocatalytic set itself (although they could be by-products of other autocatalytic sets). Thus, an autocatalytic set forms a catalytically (or *functionally*) closed and self-sustaining reaction network. The concept of autocatalytic sets was formalized mathematically as RAF sets: reflexively autocatalytic and food-generated sets (Hordijk and Steel, 2014, 2017).

Autocatalytic sets are assumed to be an essential underlying property of living systems, and to have played an important role in the origin of life. They have been shown to exist in computational models of chemical reaction networks, as well as in real chemical and biological reaction networks (Hordijk and Steel, 2017). For example, Sousa et al. (2015) showed that the metabolic network of *E. coli* forms a large autocatalytic (RAF) set, containing 98% of the reactions in that metabolic network. Assuming the same holds for most, if not all species, it seems a valid alternative to represent species by the RAF sets formed by their respective metabolic networks, as opposed to representing them by their genomes. This gives an outward framing of the species in its interactive environment, similar to the “envirogram” approach proposed by Andrewarthe and Birch (1984) and Fath (2014).

Cazzolla Gatti et al. (2017a) then argued that existing species (represented by their respective RAF sets) in an ecosystem create additional niches for new species to evolve or immigrate and occupy these new niches, in turn creating yet more additional niches, and so on. This process of niche creation happens due to each species (or rather their metabolic networks, or RAF sets) producing additional “food” elements and catalysts for other RAF sets (species) to come into existence (Cazzolla Gatti et al., 2017a). Occurrence of niche creation has been well studied and documented in ecological systems (Odling-Smee et al., 2013; Mathews et al., 2014). This is an important and related concept for the EvoRAF hypothesis, which has added focus on the process that generates the new niches. This process thus gives rise to an ever (and potentially exponentially) expanding niche space (Figs. 1 and 2), and

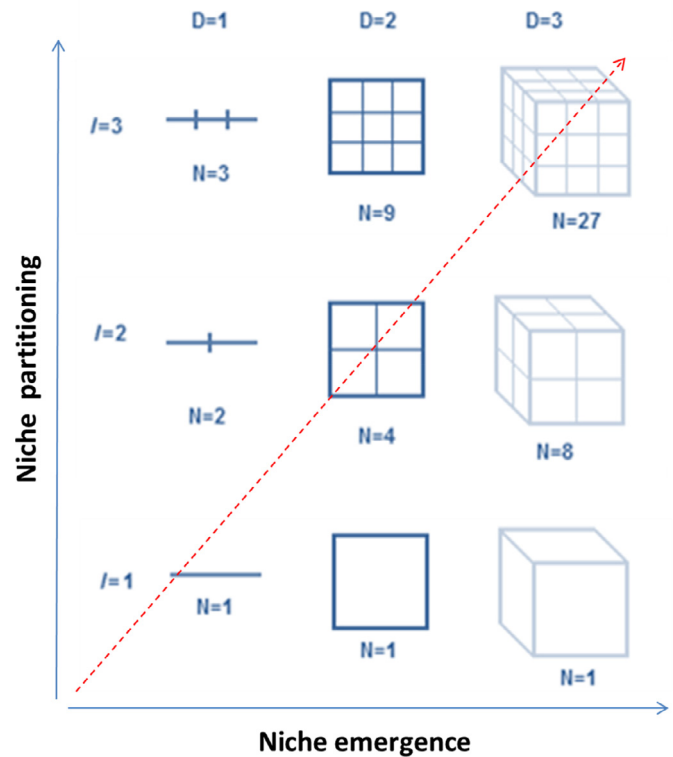


Fig. 1. Trade-off between niche partitioning and emergence. Only by niche emergence (horizontal development; increase of D = the fractal dimension from 1 to 3) it is possible to increase the number of niches of an ecosystem and, therefore, the number of coexistent species. In fact, if the niche partitioning (vertical development; I = the iteration of partitioning) were the only process, in the absence of niche emergence, the number of available niches (N) would be limited. The red-dotted arrow represents the species' trade-off between niche partitioning (iterativity) and emergence (fractality).

provides a realistic (metabolic) mechanism for how this can happen. A RAF set is based on “facilitation” processes (Bruno et al., 2003; Kikvidze and Callaway, 2009; Cazzolla Gatti, 2011; Calcagno et al., 2017), where the catalyst species is a “facilitator” in niche emergence (Cazzolla Gatti et al., 2017a).

Here we extend this line of reasoning to argue that an ecosystem itself can also be represented as an autocatalytic set. In this case, the nodes in the network are not molecules, but species. The equivalent of a chemical reaction is the transfer of biomass and energy from one or more species to another (i.e., individuals from one or more species being eaten by individuals from another species). So, the underlying “reaction network” consists of the usual food web representing a given ecosystem. However, the notion of catalysis can be added in the form of processes such as:

- one species providing safe nesting space for another species (such as trees and coral reefs do for birds and fish);
- one species helping to spread seeds or pollen for another species (such as birds and bees do for plants and trees);
- one species helping to digest food or produce essential vitamins for another species (such as gut bacteria do for humans and other animals);
- any kind of symbiosis, which would constitute “reciprocal catalysis” (such as with ants and aphids, or legumes and nitrogen fixing bacteria).

Note that in all of these examples the “catalyst” species allows or causes the other species to increase its fitness (i.e., reproduce at a higher rate than it would otherwise), without being “used up” (eaten, not in a predation process) in that process. This is simply

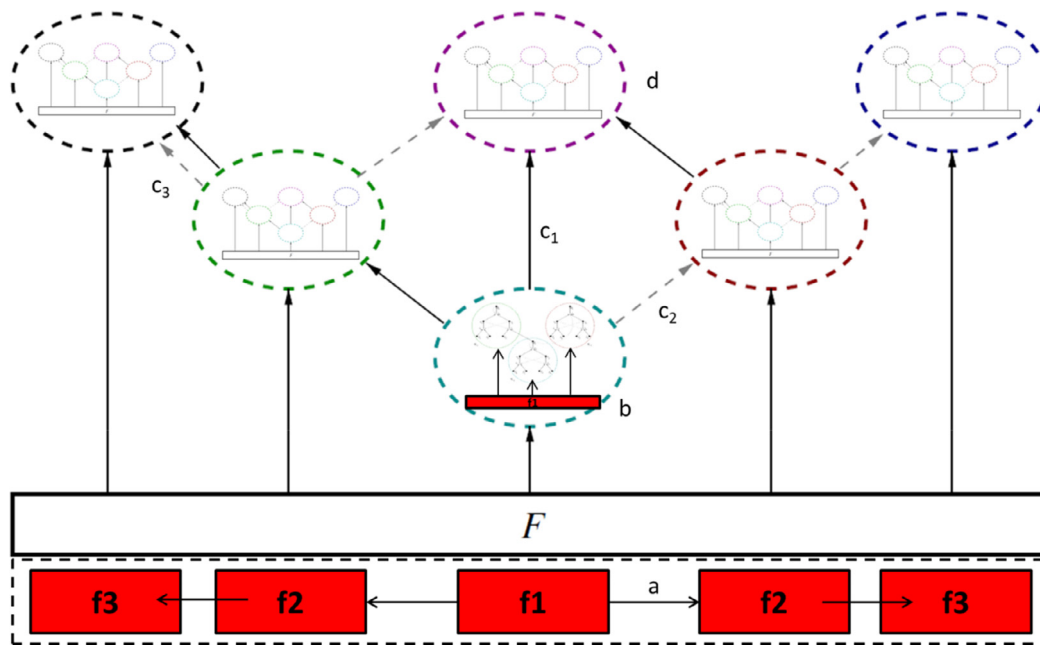


Fig. 2. Niche emergence through autocatalysis. The expansion (a) of food sets (F) created by each set (b) of interacting species guilds (Eco-RAFTs) allows guilds in each next level to use the extended resource sets ($f1$ to $f2$ to $f3...$). This creates the possibility to expand the original resource set ($F=f1+f2+f3...$) and, during time, to structure the ecosystem by evolutionary autocatalysis (Evo-RAFTs). The autocatalytic interactions between species guilds (Eco-RAFTs) can be either direct (solid arrows, c_1) or indirect (dashed arrows, c_2) or both (c_3). Some Evo-RAFTs and the related niches could emerge from the interactions among higher-order (>2) Eco-RAFTs (d). An example is given by the 3-species *Utricularia* system (Ulanowicz, 1995) and the 5-species Ladybug system (see Fig. 3). Within each set a self-similar set is represented to show the fractal nature of iterative autocatalytic sets (see Eq. (1) in the text).

a generalization of the chemical notion of catalysis (Hordijk and Steel, 2015; Montévil and Mossio, 2015).

Such a “food web + catalysis” representation, we argue, would most likely form an autocatalytic (RAF) set, where each “reaction” (trophic transformation) is “catalysed” by at least one species from the set, and each species can be maintained from a basic food source (the lowest trophic level) by a sequence of “reactions” from the set itself. In other words, a (complete) ecosystem itself most likely forms a catalytically closed and self-sustaining set. Note that this is then an “autocatalytic set of autocatalytic sets”: the ecosystem itself is an autocatalytic set in which the basic elements (species) themselves are represented as autocatalytic sets (metabolic networks).

Moreover, other hypotheses on the evolution of species diversity, such as cooperation-competition trade-offs (Calcagno et al., 2017), are also compatible with our hypothesis that “biodiversity is autocatalytic”.

3. The evolution of EcoRAF sets

Here we consider what happens to the evolution of EcoRAF sets (i.e., hereafter, “EvoRAF sets”) at an evolutionary time scale. Earlier it was already pointed out that there are two different time scales involved in this view of ecosystems as a network of mutually dependent RAF sets (Cazzolla Gatti et al., 2017a). First there is the (faster) time scale within one EcoRAF (species or guild of species). At this time scale, the stability and rate of reproduction of components of one particular EcoRAF is determined, phenomena such as centripetality play a role, and autocatalysis induces competition that drains resources from members not participating in autocatalytic cycles (Ulanowicz et al., 2014). Next, there is the (slower) time scale at which new EcoRAFTs come into existence, depending on which others are already present in the ecosystem. This is the time scale at which mutual “enablement” of RAF sets relates directly to the BNDT, and provides a mechanistic explanation for how biodiversity can increase proportionately. Calcagno et

al. (2017) proposed that the same ecological theory that predicts a negative diversity-diversification relationship due to saturation can also predict, in the very first stages of adaptive radiations, a positive, expansionary diversity-diversification relationship.

We explore the (slower) evolutionary time scale at which new EcoRAFTs (sustained by the biodiversity-related niche’s differentiation; Cazzolla Gatti, 2011, 2016b) came into existence since the beginning of life and its expansion into the current level of biodiversity. The actions at the different time scales appear to be antagonistic (one simplifies, the other complicates), but such complementary phenomena are common in nature (Brenner, 2008; Lupasco, 1947). This time scale separation should be considered as relative, because at the time scale of the life span of some individuals (K-selected species), other species have enough time to evolve (r-selected species).

In an evolutionary framework of the EcoRAF sets, we consider Fath (2007) and Ulanowicz et al. (2014)’s ideas that a species must not only preserve itself, but also engage in autocatalytic feedback cycles that contribute to the overall function of the local environment. This evidence relates to the changing nature of the autocatalytic biodiversity set over an evolutionary time scale. The phenomenon of autocatalysis can be considered a process of internal and external selection because natural selection “filters”, by the common evolutionary processes (e.g., avoidance of competition, cooperation, etc.), for the fittest EcoRAF sets which generates, as by-products, new emerging conditions available for the diversification of new life forms (i.e., biological diversity): this follows from the exaptation of unknown “preceding niches”, which represent the boundary conditions of selection. From recent hypotheses (Cazzolla Gatti et al., 2017a; Calcagno et al., 2017) and our current results, we are now able to better define how natural selection can act on whole EcoRAF sets, rather than only on single species (even better, on individual genotypes) and we have a strong support of the evolvability of autocatalytic sets from new emergent and unprestatable conditions.

This work builds on and extends the ideas of ecosystems as complex adaptive systems (CAS), which highlights how patterns of organization emerge across hierarchies (Levin, 1998). The functional role of that organization is central here, in how positive feedbacks become entrained and codified into autocatalytic structures that themselves operate across scales leading to evolutionary outcomes with greater biodiversity. However, CAS tends to emphasize the response of a system to external perturbations or drivers: it is somewhat a passive action to exogenous conditions. Autocatalysis, by contrast, originates within the system and serves to both order the system as well as affect its environment: it plays a more active dynamical role. CAS is more about phenomenology, those properties that we observe certain systems to have, whereas autocatalysis describes the process that achieves (some of) those properties. Nonetheless, Levin (1998) says that CAS exhibit three essential elements, such as: i) sustained diversity and individuality of components; ii) localized interactions among those components; iii) an autonomous process that selects from among those components, based on the results of local interactions, a subset for replication or enhancement. This last element is in line with our idea of EcoRAF sets, although with our theory of the Evolutionary RAF sets and niche emergence (see the next paragraph) we dig deeper into understanding some of the mechanisms suggested with CAS using the autocatalytic approach.

In order to discuss the notion of ecosystemic functions, philosophers have also pointed out the analogy between the organization of cells and organisms, and ecosystems (Nunes-Neto et al., 2014).

4. Niche's emergence as a property of EvoRAF sets

From the considerations above, it follows that the utilization of the ecospace (Cazzolla Gatti et al., 2017b) and the change in diversity through time could not only be because of the effect of niche partitioning, as a global long-term pattern in the fossil record was suggested by many authors (Finke and Snyder, 2008; Brokaw and Busing, 2000; Albrecht and Gotelli, 2001; Silvertown, 2004; Di Bitetti et al., 2010; Cardinale, 2011). Niche partitioning as a way to coexist could be a limited means to share the environmental resources and conditions during evolutionary time. In fact, a physical limit impedes a high partitioning without a high restriction of the niche's variables (Fig. 1). Moreover, only the extant niche with its related resources and conditions might be partitioned, but no new resources or conditions can be added. Instead, by the process of the emergence of new niches by means of diversity itself (Fig. 1), we propose that, because new resources and conditions are, at least, partly unprestatable, only niche emergence can push the ecosystem evolution ahead. Niche partitioning allows species coexistence, not speciation (i.e. creation of new niches). New niches can emerge as a result of species occupation following a fractal hypervolume expansion (Fig. 1). Consider the "capacity dimension" or "box-counting dimension" applied to fractal objects (Schroeder, 1991) of $N \propto \phi^{-D}$, where N is the number of available niches into the ecosystem, ϕ is the scaling factor and D the fractal dimension, then we can calculate the number of new emerging niches as

$$\log \phi N = -D = \frac{\log N}{\log \phi} \quad (1)$$

In other words, because the number of available niches is proportional to a scaling factor ϕ (which we will later call as "coefficient of niche's emergence biodiversity-related") and a fractal dimension, only by the emergence of new niches is it possible to enhance species coexistence, thus avoiding to partition the extant niches too much.

In nature, there should be a trade-off between niche partitioning and emergence, which moves towards the second process when the limitation of the first one is too high to sustain too many

coexistent species. This implies there is an emergence pressure but it also could occur through random, non-pressurized processes.

In space, this creates autocatalytic ecological sets (EcoRAF sets); in time, this creates autocatalytic evolutionary sets (EvoRAF sets). Thus, we defined species (or guilds of them) as an EcoRAF set and now we suggest that ecosystems (or, at least, food webs), which are an integration of emergent EcoRAF sets from autocatalytic processes, must be considered EvoRAF sets. Looking backward, we could find a selection line, but looking forward, the conditions are, at least, partly unprestatable. Rather (after Longo et al., 2012), there are "no entailing laws, but enablement in the evolution of the biosphere".

An ecosystem could then be seen as an autocatalytic set itself (a hierarchical system consisting of smaller autocatalytic sets). The description at this higher level (Fig. 2) envisions that species are the nodes in the network and they evolve (as for chemical reactions) into others. The catalysts are the species (or ecosystems) themselves and any one may facilitate other species (or ecosystems) in space, resources, and energy "usage". In this manner, these catalysts are not simply partitioning, but creating (expanding in adjacent possible space phase) new genetic, behavioural, and environmental niches (niche emergence). This can be well represented by the 5-species Ladybug system (Fig. 3).

In this system, aphids suck the sap from the plant who can suffer if the population of this insect increases too much, transforming their interaction from commensalism (+,0) to parasitism (+,-). Since aphids are one of the favourite ladybug's prey, their population size is top-down controlled (-,+) by predation. However, during their evolution, some aphid species established a mutualistic (+,+) relationship with ants. Aphids produce a honeydew that ants milk by stroking them with their antennae. This mutualism takes place because the aphids, by attracting ants, use them as a defence against the ladybugs. In fact, ants attack and, sometimes, kill ladybugs, directly reducing their populations by predation (+,-) and, at the same time, indirectly rising aphids' survival chances (+,+). The mutualism between aphids and ants is countered by plants which can produce attractive volatile substances that attract ladybugs when they feel heavily damaged by aphids (bottom-up control). This indirectly increases the number of ladybugs and, thus, decreases aphid populations. Similarly, the production of allelochemical substances by plants which attract more ladybugs, can reduce ant populations (bottom-up control) and, indirectly, reduce aphids because they start to be predated by an higher number of ladybugs, with a limited a top-down controller. This EvoRAF set 2 (Fig. 3) can take place only because of the endosymbiotic relationship established between aphids and the bacteria *Buchnera aphidicola* (EcoRAF set 1, Fig. 3). This endosymbiotic relationship occurred in a common ancestor 280–160 million years ago (Banerjee et al., 2004) and enabled aphids to exploit a new ecological niche that emerged autocatalytically. In fact, the possibility of phloem-sap feeding on vascular plants emerged because *B. aphidicola* provided its host with essential amino acids, which are present in low concentrations in plant sap, rich only of sugar and minerals.

The 5-species Ladybug system highlights the fact that during time, species autocatalyse their own and other species evolution increasing the rate at which the evolution happens (like jumps in the evolution: i.e., the punctuated equilibrium invoked by Gould and Eldredge, 1977), but without being used up in that process (in direct analogy with chemical catalysts). To better explain this point, in Cazzolla Gatti et al. (2017a) we suggested the example of a tree being a catalysts for birds, as it provides safe nesting space so that birds can reproduce at a higher rate than they otherwise would, but the tree is not "used up" in that process. Many other examples of such "ecological catalysis" can be found in nature, such as enteric fermentation, nitrogen fixation, etc.

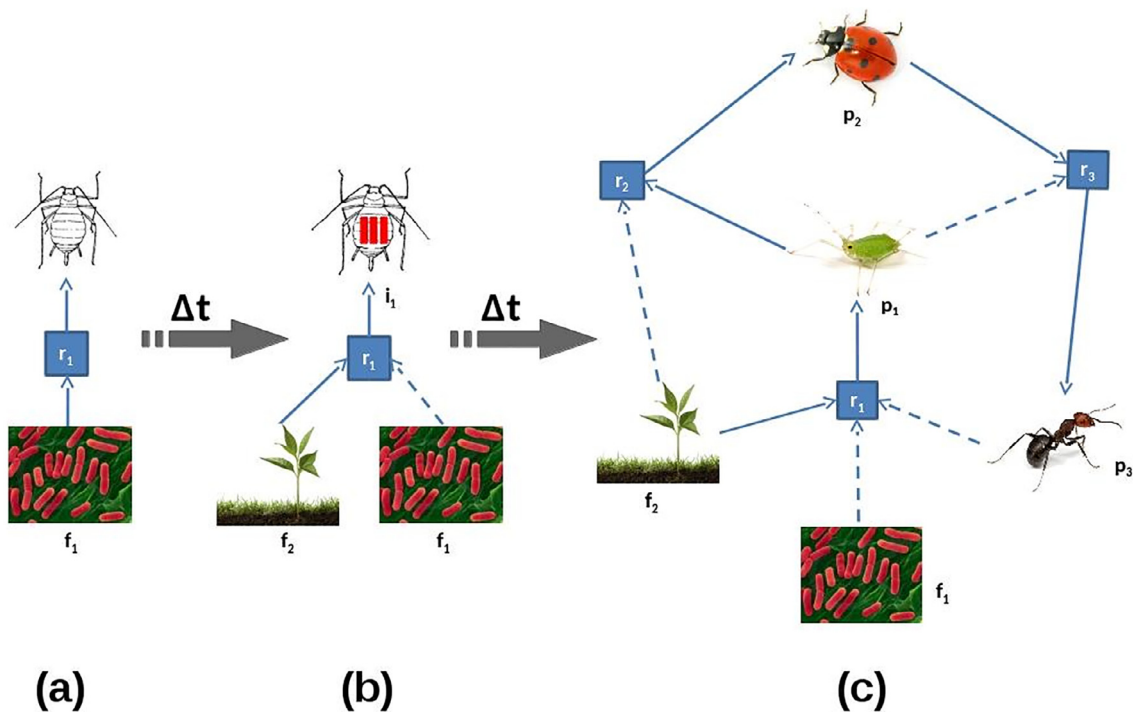


Fig. 3. A 5-species EvoRAF set. (a) Aphids depend on bacteria (f_1). This is not a RAF set in itself, but the bacteria (ecoRAF 1) allow aphids (ecoRAF 2) to come into existence (reaction 1, r_1), since now the aphids have something to live on, which they otherwise would not have had. (b) Over evolutionary time, this system changes to one where the bacteria (f_1) live inside the gut of the aphids (without being digested), which allows the aphids (i_1) to live on plant sap (f_2), since the bacteria produce additional nutrients (as by-products) not available in the plant sap. This is still only one reaction, but it is a proper RAF set (i.e., an EvoRAF), as the reaction is now "catalyzed" by the bacteria. (c) Over even longer evolutionary time this system grows into an even larger EvoRAF set consisting of five species. This network also forms a proper RAF set, where "reaction" 1 now has an additional catalyst. The emergence of a new ecological niche autocatalysed by the bacteria-aphids-plants EvoRAF set created the conditions for the existence of a 5-species EvoRAF set. In the 5-species EvoRAFs, p_1 and f_2 (which is a food source and, after some time Δt , a catalyser) react (r_2) to "produce" (i.e. "become the food source of", in ecological words) ladybugs (p_2). p_2 (ladybugs), by reacting (r_3) with p_1 (aphids), which during some time (Δt) evolved as a catalyser of r_3 by producing honeydew, became the food source of ants (p_3). Ants (p_3), in a certain evolutionary time, establish a symbiosis with aphids (p_1) by eating their honeydew in exchange for protection, that catalyses the reaction 1 (r_3). Solid arrows ("reaction arrows") indicate conservative substances (food, energy, etc.), while the dashed arrows ("catalysis arrows") indicate qualitative influences (protection from predation, attraction to food resources, etc.). Note that each "reaction" (transformation) in the set is catalysed by at least one species, and each species can be formed from the food set (bacteria + plants) through a series of reactions from the set.

Recent theoretical developments have shown that even simple models of intra and inter-specific ecological interactions can predict a positive effect of diversity on diversification (Calcagno et al., 2017), based on classical mechanisms such as competition and adaptive trait variation. Especially, interspecific interactions are found to promote diversification in initially diverse systems (i.e. more than one species), since individuals are selected to avoid engaging in competition with other species. However, the scale of interaction relevant for EcoRAF is at the species scale not the individual scale. Individuals obviously get consumed, i.e., used up, during predation, but the overall species remains as a pool of resources for the receiving node in the autocatalytic loop (assuming, of course, that the species is not driven to extinction, but that result would hurt the entire set of interactions). Indeed, it seems that all evolution is made by autocatalytic ecological systems. So, in this view, an ecosystem as a whole is a self-sustaining autocatalytic set (EvoRAF). This provides a formal view at an evolutionary time scale. So we have different levels of aggregation (hierarchical autocatalytic sets), which correspond to different time scales. Each set enables the (partly) unprestatable emergence of a new one. Each species by realizing its ecological niche, during the evolutionary time, facilitates the emergence (or the expansion) of new niches. As Jacobs (2001) observed, "the ensemble itself made the environment rich by expanding" (p. 45) as a first stage of emergence, followed by specialization and partitioning during which, "an ensemble grows rich on an environment that the ensemble itself made rich" (p. 60).

5. Power-laws of speciation and extinction

What does this view mean for biodiversity and its evolution? We asked if, in an hypothetical situation without mass extinction events during evolution, we would have either an unstoppable (exponential) increase of species richness, or whether there is a global carrying capacity for speciation, as was suggested in Cazzolla Gatti et al. (2017a).

It was proposed (Cazzolla Gatti, 2011) that over evolutionary time, the biosphere is subject to an increase in the number of niches proportional to the number of niches already present in the environment at time t , with available niches increasing in an exponential way until reaching an ecosystem carrying capacity (sigmoid growth).

Even without mass extinction events, it was suggested that there is a global carrying capacity, which represents a plateau (e.g., a successional climax) for speciation through autocatalysis (a sigmoid curve, as in every chemical autocatalytic growth), but that this is a dynamic, not fixed, threshold depending on the state and the energy of the planetary system (highest autocatalytic set) and the emergence of new technological-biological processes.

This means that, in our extended time frame of evolution, the deletion of a single element, i.e., a node in the autocatalytic set (a molecule type in a chemical reaction network, or a species in an ecosystem), leads to an extinction cascade of the other elements (i.e., other molecules or species). This pattern follows a power law (Taylor, 1961) distribution ($\sigma^2 = \alpha \mu^\beta$), which applies to both niche

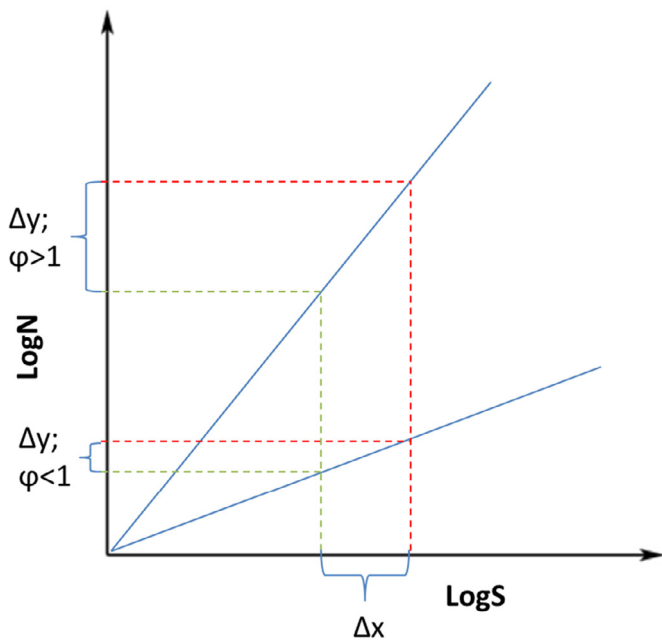


Fig. 4. The power law in niche emergence. With an increase of species Δx , the number of emerging niches Δy is higher for slope $\phi > 1$ (i.e. $\frac{i_{\Delta t}}{e_{\Delta t}} > 1$) than for slope $0 < \phi < 1$ (i.e. $0 < \frac{i_{\Delta t}}{e_{\Delta t}} < 1$). At the same time a reduction of species Δx has a bigger impact on the number of available niches Δy when the slope $\phi > 1$ (speciation rate > extinction rate) than when $0 < \phi < 1$ (speciation rate < extinction rate). This could be the reason why in high diverse ecosystems where the speciation rate is higher than the extinction one, such as tropical forests or reef barrier, the removal even of a limited amount of species can cause a stronger cascade effect on the available niches (i.e. on other species not directly interested by the removal). Similarly, the autocatalytic evolution of the ecosystems (EvoRAF sets) foresees that if the speciation rate is higher than the extinction one, at a certain increase of species richness, an emergence of new niches following a power law will correspond.

emergence and extinction:

$$\text{var}(N) = tS^\varphi \quad (2)$$

where $\text{var}(N)$ is the variance of the number of niches, S is the mean number of species in the ecosystem, t is the evolutionary time and φ is the coefficient of niche's emergence biodiversity-related (see Eq. (1)), derived from the BNDT (with $\varphi = i_{\Delta t}/e_{\Delta t}$, with $i_{\Delta t} > 0$; $e_{\Delta t} > 0$, where i is the rate of immigration/speciation and e the rate of emigration/extinction).

Thus, $N \propto S = S \propto \frac{i_{\Delta t}}{e_{\Delta t}}$, (i.e., species richness is proportional to niche's emergence biodiversity-related).

The emergence of the power-law distribution is a consequence of the assumption that the number of new niches (which must involve a minimum of 2 interacting species, otherwise we would have only an arithmetical progressions) is proportional to the quotient of $\log(N)/\log(S)$, because the quotient of two ordinary distributions is always Cauchy, or power-law distributed (Ulanowicz and Wolff, 1991).

In the log-log linear transformation, Eq. (2) becomes: $\log(\text{var}[N]) = \log(t) - \varphi \log(S)$. Deviation for the mathematical expectation of a power-law slope = 2 suggest that, when the extinction rate is higher than the speciation rate, then $\varphi < 1$ and the slope of a log-log plot is lower than when the speciation rate overtakes the extinction one (Fig. 4). The power law phenomenon is common in natural systems (Mellin et al., 2010). One should recall that power-law distributions were once called “joint distributions”, indicating that the behaviour is related to the structure of the underlying network of interactions and dependencies. For instance, the power law definitely shows up in the autocatalytic sets that exists within the *Escherichia coli* metabolic network (Sousa et al.,

2015) and in the binary polymer model (regardless of the catalysis assignment method, see below). In ecology, the distribution of magnitudes of trophic transfers follows the power-law (Ulanowicz and Wolff, 1991). It is interesting, however, that binary networks of trophic interactions are not distributed according to a power-law, a result that demonstrates how one can miss significant features of ecosystems by relying solely on unweighted networks (Ulanowicz et al., 2014).

Non-experimental approaches have emphasized the existence of statistical patterns in the structure of communities that seemingly reflect the operation of general principles or natural laws and emerge as scaling relationships with similar or related exponents (West et al., 1997). But what does this mean for true ecosystems such as a tropical forest or the Great Reef Barrier? We have now a useful theoretical mean to test, empirically, the hypothesised cascade effect of niche emergence and extinction).

6. An empirical test for the EvoRAF sets

One question we can now ask is how the removal of one or more species from such an “ecosystem autocatalytic set” affects the size of the original set. In other words, when one species (or, alternatively, the trophic transformation (“reaction”) that produces that species) is removed from the network, how many other species (or reactions) will also disappear because they depended on the removed species?

In the autocatalytic sets that were observed and studied in the past, such a removal of (random) reactions generates a power law in the frequency distribution of the sizes of the resulting “extinction events”. More specifically, given an autocatalytic set and the removal of one (random) reaction, one can measure by how many reactions the autocatalytic set is reduced (i.e., the number of reactions that depended fully on the product of the removed reaction, and which thus cannot be part of the autocatalytic set anymore). If this measurement is made for each reaction in the original autocatalytic set, and the frequency distribution of the sizes of the resulting “extinction events” is plotted, then a power law results.

Fig. 5 shows two examples. The left plot shows the frequency distribution of extinction sizes in an autocatalytic set that occurred in one particular instance of a simple polymer model where molecules are represented by bit strings that can be either “glued” together into longer bit strings (a ligation reaction) or “cut” into shorter bit strings (a cleavage reaction). In this model, bit strings are assigned as catalysts to reactions in a probabilistic way (although the power law in extinction sizes does not seem to depend on how exactly this is done). Note that the plot is on a log-log scale, with the straight line representing a power law fit to the data, which in this case results in a slope of -1.35 . The right plot shows similar results for the autocatalytic set that exists in the metabolic network of *E. coli*, resulting in a slope of -1.19 .

In short, autocatalytic sets (whether they exist in a simple computational model or in real biological networks) seem to generate a power law in the frequency distribution of extinction event sizes. If, as we argued above, ecosystems can be represented as autocatalytic sets too, we would also expect to observe a power law in extinction events in real ecosystems. Indeed, the power law was observed on the distribution of the magnitudes of the flows (Ulanowicz and Wolff, 1991).

Note that power laws appear in many different systems and can be generated by many different mechanisms. But the autocatalytic sets representation provides a very specific (and testable) mechanism for why and how power laws can be expected, and are indeed observed, in extinction events in ecosystems.

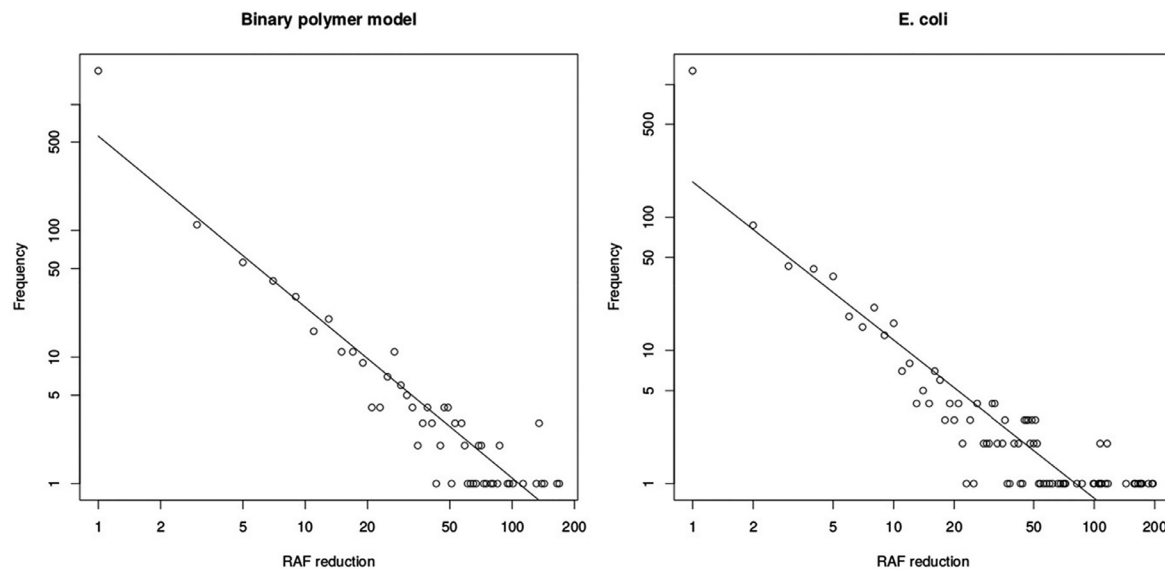


Fig. 5. Frequency distribution of extinction sizes in RAFs. The frequency distribution of extinction sizes in an autocatalytic set that occurred in one particular instance of a simple polymer model (left) and similar results (right) for the autocatalytic set that exists in the metabolic network of *E. coli*, resulting in a slope of -1.19 .

7. Conclusion

In the ecological theory "niche emergence" is a neglected process, while "niche partitioning" has been widely used as a hypothesis to explain species coexistence and evolution. The emphasis put on niche (resources and conditions) partitioning for new niche evolution has hidden the reality: there is a limited possibility to prestate niches in the ecosystems, because niches emerge when new species colonize the space or evolve in time.

In a previous paper (Cazzolla Gatti et al., 2017a), niche emergence in space was explored, but a discussion of its relevance over time and on the evolution of biodiversity was only outlined.

Here we demonstrated that an ecosystem as a whole (consisting of autocatalytic sets) can be described as an autocatalytic set itself. Ours is a hierarchical (top-down/bottom-up) RAF set description in space and time.

We are aware that it is quite impossible to mathematize the evolution of the biosphere, since we cannot fully prestate the forever new "adjacent possible" of that evolution, but – at least – we provided a formal description of the evolutionary patterns of the emergence of new adjacent possible. We can, in general, not fully identify or prestate which specific new adjacent possible (which new niche's resources and conditions) there will be, but we have formalised how an expanding phase space emerges during the evolution and identified it as a general common pattern in the biosphere's evolution.

In this regard autocatalytic centripetality plays an important role because, since "the trajectory of a system through time conceivably could be used in lieu of a set of its existing properties" (Ulanowicz, 2009), the evolution of ecosystems (as autocatalytic sets consisting of autocatalytic sets made by species) "becomes the centre of a centripetal vortex, pulling as many resources as possible into its domain" (Ulanowicz, 2009). This increases the positive feedback and energy flow for its own set (ecosystems become more resilient and self-sustaining) but, also, creates the new possibility for other adjacent niches (in these cases ecosystem's, and not species', niches) to emerge. The new species could not be an obligatory autocatalytic set themselves, but evolving by the "emergence" of new niches based on lower hierarchical autocatalytic set they could interact with other species creating a new EcoRAF set. The adjacent possible of an ecosystem (made up of EcoRAFTs) can

emerge and evolve (as an EvoRAF set) without species autocatalytic set but compulsory within another hierarchical level of autocatalysis. In other words, the adjacent possible niche space is the result of an autocatalytic reaction, even if the facilitating and resulting species are not autocatalytic if taken alone. It would not be a squirrel without an oak, both squirrel and oak are not autocatalytic if taken alone, but both are part of a larger autocatalytic set (in which they are some of the catalysts) that allow the emergence of their own consequent niches. The squirrel's niche emerges because of the presence of the oak (which produces resources as acorns and conditions as lairs) as foreseen by the BNDT, but both the oak and the squirrel are not isolated in the ecosystem since they react with other biotic and abiotic elements in autocatalytic ways.

The ecological perspective agrees with the statements so far that the species are nodes, doing their thing (transforming energy and nutrients), while in the context of the ecosystem. Building the hierarchy adds another level of complexity but still everything fits together in an evolutionary context. It would be interesting, in future, to develop a more formalised mathematical framework in order to include niche emergence in existing evolutionary models, and test our hypothesis against empirical data and other theories on the evolution of biodiversity.

Finally, the EvoRAF set (ecosystem) evolves over time through the evolution and interactions of the individual species, extinction-emigration/speciation-immigration events, as suggested by the BNDT. We stressed that niche emergence is more important than niche partitioning. A simple spatial model (Fig. 1) showed that, for instance, in a two dimensional land surface, any species (such as trees) that projects into the third dimension is multiplying the space for new niches. We cannot fully prestate which new species emerge, but can show the increased dimensionality of the niche. This also fits in with the ideas of Alexander (2012) and Fath (2014) that "interactions must be not only structure preserving, but also wholeness extending". That's where the new novelty arises.

References

- Albrecht, M., Gotelli, N.J., 2001. Spatial and temporal niche partitioning in grassland ants. *Oecologia* 126 (1), 134–141.
- Alexander, C., 2012. *The Battle for the Life and Beauty of the Earth: A Struggle Between Two World-Systems*. Oxford University Press, New York, NY.

- Andrewartha, H.G., Birch, L.C., 1984. *The Ecological Web: More on the Distribution and Abundance of Animals*. University of Chicago Press, Chicago, IL, p. 506.
- Bailey, S.F., Dettman, J.R., Rainey, P.B., Kassen, R., 2013. Competition both drives and impedes diversification in a model adaptive radiation. *Proc. R. Soc. Lond. B* 280, 20131253.
- Banerjee, S., Hess, D., Majumder, P., Roy, D., Das, S., 2004. The interactions of *Allium sativum* leaf agglutinin with a chaperonin group of unique receptor protein isolated from a bacterial endosymbiont of the mustard aphid. *J. Biol. Chem.* 279 (22), 23782–23789.
- Brenner, J., 2008. *Logic in Reality*. Springer Science & Business Media.
- Brokaw, N., Busing, R.T., 2000. Niche versus chance and tree diversity in forest gaps. *Trends Ecol. Evol.* 15 (5), 183–188.
- Bruno, J.F., Stachowicz, J.J., Bertness, M.D., 2003. Inclusion of facilitation into ecological theory. *Trends Ecol. Evol.* 18 (3), 119–125.
- Calcagno, V., Jarne, P., Loreau, M., Mouquet, N., David, P., 2017. Diversity spurs diversification in ecological communities. *Nat. Com.* 8, 15810.
- Cardinale, B.J., 2011. Biodiversity improves water quality through niche partitioning. *Nature* 472 (7341), 86–89.
- Cazzolla Gatti, R., 2011. Evolution is a cooperative process: the biodiversity-related niches differentiation theory (BNDT) can explain why. *Theor. Biol. Forum* 104 (1), 35–43.
- Cazzolla Gatti, R., 2016a. The fractal nature of the latitudinal biodiversity gradient. *Biologia (Bratisl)* 71 (6), 669–672.
- Cazzolla Gatti, R., 2016b. A conceptual model of new hypothesis on the evolution of biodiversity. *Biologia (Bratisl)* 71 (3), 343–351.
- Cazzolla Gatti, R., Hordijk, W., Kauffman, S., 2017a. Biodiversity is autocatalytic. *Ecol. Modell.* 346, 70–76.
- Cazzolla Gatti, R., Di Paola, A., Bombelli, A., Noce, S., Valentini, R., 2017b. Exploring the relationship between canopy height and terrestrial plant diversity. *Plant Ecol.* 218 (7), 899–908.
- Di Bitetti, M.S., De Angelo, C.D., Di Blanco, Y.E., Paviolo, A., 2010. Niche partitioning and species coexistence in a Neotropical felid assemblage. *Acta Oecologica* 36 (4), 403–412.
- Emerson, B.C., Kolm, N., 2005. Species diversity can drive speciation. *Nature* 434, 1015–1017.
- Fath, B.D., 2007. Network mutualism: positive community-level relations in ecosystems. *Ecol. Modell.* 208 (1), 56–67.
- Fath, B.D., 2014. Sustainable systems promote wholeness-extending transformations: the contributions of systems thinking. *Ecol. Modell.* 293, 42–48.
- Finke, D.L., Snyder, W.E., 2008. Niche partitioning increases resource exploitation by diverse communities. *Science* 321 (5895), 1488–1490.
- Gould, S.J., Eldredge, N., 1977. Punctuated equilibria: the tempo and mode of evolution reconsidered. *Paleobiology* 3 (2), 115–151.
- Gruner, D.S., Gotelli, N.J., Price, J.P., Cowie, R.H., 2008. Does species richness drive speciation? A reassessment with the Hawaiian biota. *Ecography* 31, 279–285.
- Hordijk, W., Steel, M., 2014. Conditions for evolvability of autocatalytic sets: a formal example and analysis. *Origins Life Evol. Biospheres* 44 (2), 111–124.
- Hordijk, W., Steel, M., 2015. Autocatalytic sets and boundaries. *J. Syst. Chem.* 6, 1.
- Hordijk, W., Steel, M., 2017. Chasing the tail: the emergence of autocatalytic networks. *Biosystems* 152, 1–10.
- Jacobs, J., 2001. *The Nature of Economies*. Vintage Books, p. 208.
- Kauffman, S.A., 2016. *Humanity in a Creative Universe*. Oxford University Press.
- Kikvidze, Z., Callaway, R.M., 2009. Ecological facilitation may drive major evolutionary transitions. *Bioscience* 59 (5), 399–404.
- Levin, S.A., 1998. Ecosystems and the biosphere as complex adaptive systems. *Ecosystems* 1 (5), 431–436.
- Longo, G., Montévil, M., Kauffman, S., 2012, July. No entailing laws, but enablement in the evolution of the biosphere. In: *Proceedings of the 14th Annual Conference Companion on Genetic and Evolutionary Computation*. ACM, pp. 1379–1392.
- Lupasco, S., 1947. *Logique et Contradiction*.
- Matthews, et al., 2014. Under niche construction: an operational bridge between ecology, evolution and ecosystem science. *Ecol. Monographs* 84, 245–263.
- Mellin, C., Bradshaw, C.J.A., Meekan, M.G., Caley, M.J., 2010. Environmental and spatial predictors of species richness and abundance in coral reef fishes. *Global Ecol. Biogeogr.* 19 (2), 212–222.
- Montévil, M., Mossio, M., 2015. Biological organisation as closure of constraints. *J. Theor. Biol.* 372, 179–191.
- Odling-Smee, et al., 2013. *Niche construction theory: a practical guide for ecologists*. Q. Rev. Biol. 88, 3–28.
- Silvertown, J., 2004. Plant coexistence and the niche. *Trends Ecol. Evol.* 19 (11), 605–611.
- Nunes-Neto, N., Moreno, A., El-Hani, C.N., 2014. Function in ecology: an organizational approach. *Biol. Philos.* 29, 123.
- Schroeder, M., 1991. *Fractals, Chaos, Power Laws*. Freeman, New York.
- Sousa, F.L., Hordijk, W., Steel, M., Martin, W.F., 2015. Autocatalytic sets in *E. coli* metabolism. *J. Syst. Chem.* 6 (1), 4.
- Taylor, L.R., 1961. Aggregation, variance and the mean. *Nature* 189 (4766), 732–735.
- Ulanowicz, R.E., 1995. Utricularia's secret: the advantage of positive feedback in oligotrophic environments. *Ecol. Modell.* 79 (1–3), 49–57.
- Ulanowicz, R.E., 2009. The dual nature of ecosystem dynamics. *Ecol. Modell.* 220 (16), 1886–1892.
- Ulanowicz, R.E., Holt, R.D., Barfield, M., 2014. Limits on ecosystem trophic complexity: insights from ecological network analysis. *Ecol. Lett.* 17, 127–136.
- Ulanowicz, R.E., Wolff, W.F., 1991. Ecosystem flow networks: loaded dice? *Math. Biosci.* 103 (1), 45–68.
- West, G.B., Brown, J.H., Enquist, B.J., 1997. A general model for the origin of allometric scaling laws in biology. *Science* 276 (5309), 122–126.