

The Behavior-Based Hypercycle: From Parasitic Reaction to Symbiotic Behavior

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Abstract

Most researchers in the science of the origin of life assume that the process of living is nothing but computation in the chemical domain, i.e. information processing of a genetic code. This has had the effect of restricting research to the problem of stability, as epitomized by the concept of the hypercycle and its potential vulnerability against parasites. Stability is typically assumed to be ensured by a rigid compartment, but spatial self-structuring is a viable alternative. We further develop this alternative by proposing that some instability can actually be beneficial under certain conditions. We show that instability can lead to adaptive behavior even in the case of simple prebiotic reaction-diffusion systems. We demonstrate for the first time that a parasitic side-reaction on the metabolic level can lead to self-motility on the behavioral level of the chemical system as a whole. Moreover, self-motility entails advantages on an evolutionary level, thus constituting a symbiotic, behavior-based hypercycle. We relate this novel finding to several issues in the science of the origin of life, and conclude that more attention should be given to the possibility of a movement-first scenario.

Introduction

The scientific debate about the origin of life has traditionally been centered on the competing claims of the ‘replicator-first’ scenario and the ‘metabolism-first’ scenario (e.g. Anet, 2004; Pross, 2004). We have argued extensively that these scenarios are currently in the process of merging into two versions of an information-compartment-metabolism-first scenario (Froese et al., in press). The essential components of the consensus are not new; they are already familiar from Ganti’s (1975) idea of the ‘chemoton’, for example. To be sure, it is commendable that the replicator-first approach is beginning to recognize the value of metabolism, and that the metabolism-first approach is paying more attention to the historical-collective dimension of life. Nevertheless, we have criticized this consensus because it completely ignores the intermediate timescales of life where an individual’s behaviors unfold. Although biologists assume that behavior is a decisive factor for Darwinian fitness in the later stages of life, existing attempts to ground evolution in a prebiotic scenario have tended to focus on chemical factors:

Darwinian competitive exclusion is rooted in the chemical competitive exclusion of metabolism, whether through differential rates of growth or differential resource capture. (Morowitz and Smith, 2007, p. 58)

Indeed, even attempts to generate a more encompassing list of features that could be used to classify the transition from pre-life and life, such as the one compiled by Schuster (2009), fail to even mention the possibility of motility and behavioral interaction. We reproduce Schuster’s list in detail, because it serves as a useful summary of the ideal goalposts of current efforts in artificial life and synthetic biology.

- i. multiplication and inheritance,
 - ii. variation through imperfect reproduction and recombination,
 - iii. metabolism for the production of molecular building blocks,
 - iv. individualization through enclosure in compartments,
 - v. homeostasis and autopoiesis,
 - vi. organized cell division (bacterial cell division or mitosis),
 - vii. sexual reproduction and reductive division (meiosis), and
 - viii. cell differentiation in germ line and soma
- (Schuster, 2009, p. 7)

Schuster’s list is paradigmatic of what we called the new information-metabolism-compartment consensus. Again, it is not that we disagree with the importance of any specific items on this list. But the list as a whole presents an impoverished view of life that neglects the contribution of behavior. We can understand this omission from the standard perspective of the neo-Darwinian synthesis, which integrated biochemistry with population statistics at the expense of ethology. At the same time, however, it should be remembered that even the oldest forms of life, such as the *Archaea* whose lineage dates back to over 3.5 billion years ago, are capable of adaptive behavior including chemotaxis and phototaxis. Indeed, the whole world of single-celled organisms is full of behavior, which suggests that life involved self-motility from the beginning.

Fortunately, a serious appreciation of motility at the origin of life is starting to develop. Although it is widely assumed that intermediate timescales of behavior could not have played a role at the very beginning of life, it has been demonstrated that even simple dissipative structures can exhibit a variety of life-like behaviors (e.g. McGregor and Virgo, 2011; Froese et al., 2011; Virgo, 2011; Hanczyc and Ikegami, 2010; Suzuki and Ikegami, 2009). And there is a small but growing body of research supporting the idea that self-movement and adaptive behavior could have played a crucial role for the origin of life

and proto-cell evolution (e.g. Egbert et al., 2012; Hanczyc, 2011; Froese, et al., in press). In order to distinguish this work from the information-compartment-metabolism framework we refer to it as a ‘movement-first’ scenario.

In this paper we add support to the idea that a movement-first scenario is applicable even in the case of simple prebiotic systems. We address potential criticisms that using a minimal dissipative structure, as an example of a proto-living system, is implausible. For instance, it could be argued that a non-compartmentalized autocatalytic cycle is unsuitable for the origin of life and early evolution, because of (1) a lack of a clearly defined ‘individual’ that could serve as the target of natural selection (Maynard Smith, 1979), (2) a lack of internal functional differentiation for natural selection to choose from (Mossio et al., 2009), and (3) a lack of sufficient protection against the evolution of parasitic side-reactions (Bresch et al., 1980; Maynard Smith, 1979). We have provided an extended response to the first two concerns elsewhere (Froese, et al., in press). Here we focus on the problem of parasitic reactions, because this is one of the most widely discussed issues. The main worry is that prebiotic systems, lacking the selectivity of specialized enzymes, would quickly succumb to side-reactions that receive benefit from the system but do not provide any benefit in return. In the words of Orgel:

The most serious challenge to proponents of metabolic cycle theories—the problems presented by the lack of specificity of most nonenzymatic catalysts—has, in general, not been appreciated. If it has, it has been ignored. Theories of the origin of life based on metabolic cycles cannot be justified by the inadequacy of competing theories: they must stand on their own. (Orgel, 2008, p. 12)

However, this problem may be overstated. Following the pioneering research of Boerlijst and Hogeweg (1991) it has been recognized that spatial embedding and self-structuring of chemical systems plays an essential role in reducing the negative impact of parasites (May, 1991). This has given rise to a tradition of modeling research into what particular aspects of spatiality modify the evolutionary dynamics of populations (e.g. Cronhjort, 1994; Boerlijst and Hogeweg, 1995; Cronhjort and Blomberg, 1997). For example, it was found that spatial self-structuring can constitute a stable composite structure that can serve as a new individual unit of natural selection (e.g. Savill et al., 1997; Hogeweg and Takeuchi, 2003).

Here we push this approach in a novel direction by shifting the current focus from spatial self-structuring to self-generated movement. The upshot of our argument is that the threat of parasitic side-reactions for early proto-metabolic systems may in fact have been overestimated, because the possibility of an adaptive response at the behavioral level of the system has so far been ignored. In brief, *parasites are less of a problem as long as the reaction system tends to move away from them, such as when searching for a more metabolically desirable region of the environment.*

The idea of a chemical system capable of chemotaxis like a bacterium may appear to be implausible, but this behavior has now been demonstrated in different models (e.g. Froese, et al., 2011; Suzuki and Ikegami, 2009) and even in actual chemistry (e.g. Hanczyc and Ikegami, 2010). Thus, while most research is still focused on how spatiality can enhance stability, we are

interested in how instability can be harnessed as a means to do useful behavioral work in space. Using an illustrative example first introduced by Virgo (2011), we show that under some conditions a parasitic reaction on the metabolic level can constitute movement on the behavioral level of the system as a whole, which is adaptive on the evolutionary level.

In the next section we provide some general background to the proposal that current approaches to the origin of life need to be enriched with a movement-first scenario by appealing to a related development in the history of cognitive science. We then take a closer look at one famous proposal for the origin of life, namely the ‘hypercycle’ (Eigen, 1971). On this basis we discuss a simple reaction-diffusion model in order to show that taking the possibility of motility into account is a useful extension to the traditional hypercycle model, thereby leading to the generalized notion of a *behavior-based hypercycle*.

Historical background

Synthetic and molecular biology are largely defined by the assumption that the process of living is essentially nothing but information processing in the chemical domain. Half a century ago a similar idea, namely that the process of cognition is nothing but information processing in the brain, gave birth to cognitive science. What can we learn from its history?

We argue that progress in the science of the origin of life is hampered by a familiar set of misguided assumptions. Just as in the heyday of ‘Good Old-Fashioned Artificial Intelligence’ (GOFAI) and its idealized toy worlds, in today’s molecular biology there is no concern for the requirements and benefits of adaptive behavior in the real world. Indeed, in an implicit agreement with the computational theory of mind, the most widely accepted theories of life are centered on the notion of information processing of symbolic representations, in this case the genetic code. The metabolism-first scenario is only a sub-symbolic alternative to this view, just like sub-symbolic AI was a version of GOFAI that also continued to share the commitments of the computationalist framework.

And just like this computationalist AI had locked the mind inside of the head, synthetic biology (and much artificial life) has constrained life to reside inside a membrane boundary. In recent versions of the RNA-world scenario, for instance, all essential processes involved in the first instances of life are assumed to take place inside of an insulating compartment. This compartment ensures a fundamental division between an internal ‘system’ and an external ‘environment’, where the former is controlled by the genetic system. This insistence on the notion of internal control and on a dualistic distinction between controller and body, as well as between body and environment is, of course, familiar from traditional cognitive science. Even life’s requirement of continuous material and energetic exchange with the environment is conceived of as nothing but a contingent feature of the chemical domain. It is conceptually treated as no different than a robot’s ‘need’ for an external power supply. Accordingly, it is assumed that the process of living can be synthesized and studied in relative disregard of the metabolic body and the environment, which in any case is practically kept as pure and sterile as is possible.

However, as we know from the history of AI and cognitive science, the guiding principles of computationalist AI turned out to be inadequate for the construction of mobile robots that

behaved flexibly and robustly in the real world, especially in environments that were noisy, unpredictable, and fast-paced (Froese and Ziemke, 2009). Although there were examples of successful engineering applications, it became evident that the minds of living creatures must be operating according to other fundamental principles. Eventually the practical shortcomings of classical robotics resulted in a paradigm shift to behavior-based robotics (Brooks, 1991). The assumption that cognition is essentially information processing of abstract symbols was decisively rejected in favor of a treating cognition as primarily an embodied and situated engagement with the world. On this view, mind is a relational phenomenon that emerges out of the distributed dynamics of brain, body and environment (Beer, 1995). The processes of mind are no longer limited to the neural domain of the brain (Clark, 2008). Finally, embodied action became a core concept in the latest developments of an enactive cognitive science (Stewart et al., 2010).

We propose that the science of the origin of life is in need of a similar paradigm shift toward an enactive approach that treats life as a relational phenomenon (Di Paolo, 2009). Life emerges out of the distributed dynamics of a genetic system, metabolism, and the environment. It is primarily a form of goal-directed movement like embodied action.

Synthetic biology can play an essential role in this new endeavor. Previously, robotics made a significant contribution to progress in cognitive science by putting the computational theory of mind to a practical test that turned out to highlight its shortcomings. And given the recent advances in synthetic biology, it is likely that there will be increasing opportunities to practically test out different theories of life as well. In addition, given that synthetic biology still shares some of the core assumptions of the computational theory of mind, it is reasonable to expect that its computational theory of life will also face significant shortcomings as experimental situations become progressively more realistic. Fortunately, we have the benefit of hindsight. We are in a position to learn from the failure of computationalist AI and to draw inspiration from the subsequent development of an embodied and situated robotics and cognitive science. In particular, we emphasize one lesson that may help in understanding the origin of life, namely the role of active movement for embodied and situated agents.

Robots that have been designed according to the principles of GOFAI are easily recognizable by their carefully controlled environment, as well as by their unnatural movements. More importantly, their behavior is inflexible, brittle, and does not degrade gracefully. These undesirable characteristics largely result from an explicit attempt to prevent the messy details of the body and the environment from having any influence on the control system. In contrast, robots that have been designed in a relational manner, in order to properly take advantage of the passive dynamics and material properties of the body and the environment, spontaneously exhibit a surprising amount of robustness and versatility. Moreover, active movement of the sensing body facilitates the self-structuring of sensory flows into perceptual forms (Pfeifer and Scheier, 1999). Movement also increases the resolution of what is perceived, as when the sensation of an isolated tactile contact turns into the complex perception of texture through movement along a surface. Note that the particular structure of a sensorimotor loop is related to the agent's potential for embodied action in a given situation, which grounds its cognition. Accordingly, a mixture of messy

embodiment and situated movement can enhance an agent's behavioral performance, while at the same time significantly reducing the need for a specialized internal control system.

A behavior-based hypercycle model

We will now demonstrate the relevance of this 'movement-first' approach to a specific debate in the science of the origin of life. A fitting starting point are the extensive arguments surrounding the 'hypercycle' theory developed by Eigen and Schuster (e.g. Eigen and Schuster, 1977; Eigen, 1971; Eigen and Schuster, 1978a, 1978b). They identify three requirements for Darwinian evolution by natural selection to take place on the molecular level:

Metabolism. Following the pioneering work of Schrödinger (1944), Eigen and Schuster accept that living systems belong to the general class of far-from-equilibrium systems, and that they maintain that status by means of ongoing degradation and formation of molecular components, i.e. metabolism. It is on this basis that complexity can be generated, maintained, and eventually selected by natural selection.

Self-reproduction. The eligible molecular structures must have the inherent ability of instructing their own synthesis, e.g. they are autocatalytic. Autocatalysis serves to preserve the existing structure of the system, and hence the information it has accumulated. It is on this basis that complexity can be inherited by subsequent generations.

Mutability. Noise ensures that self-reproduction is not 100% reliable, and errors of copying provide the main source of new information in evolution. This ensures that new variants of the molecular structures are made available for selection.

Eigen and Schuster famously showed that the mechanisms of selective accumulation of information involve an upper limit for the number of elements that can be assembled into one genotype, a limit that is inversely proportional to the average copying error rate per element. If this threshold is exceeded there is an 'information crisis': the information that has been accumulated in the evolutionary process so far becomes lost over generations. Accordingly, an increase in the amount of inheritable complexity depends on an increase in the fidelity of genetic transmission.

Eigen and Schuster argue that at the molecular level this enhanced fidelity requires the mutually beneficial *functional linkage* among several autocatalytic or self-reproductive units into one hypercycle. The basic idea is that each autocatalytic component aids in the replication of the next component in a chemical regulatory cycle that is closing on itself. Later on we will modify this basic idea by following the notion of life as an extended process that can incorporate behaviors into its self-constitution (e.g. Di Paolo, 2009; Virgo et al., 2011). We show that a generalized concept of functional linkage enables us to conceive emergent adaptive behavior as another potential form of beneficial linkage, which we denote with the concept of a *behavior-based hypercycle*.

There have been many critiques and elaborations of Eigen and Schuster's original proposal. One important shortcoming was highlighted by Maynard Smith (1979). He pointed out that since each self-reproducing unit within a hypercycle is

assumed to be an independent target of natural selection, they couldn't evolve in such a way that would increase the overall fitness of the hypercycle as a whole on the basis of their mutual cooperation. It is worth quoting Maynard Smith at length, because similar reasoning is still guiding much research into the origin of life today.

How then can a hypercycle evolve characteristics which favour the growth of the cycle as a whole, rather than merely its constituent parts? So long as there is no compartmentalisation, it cannot. For natural selection to act, there must be individuals. (Maynard Smith, 1979, p. 446)

We can now better understand why many researchers insist on the necessity of compartments at the origin of life (e.g. Szathmáry and Demeter, 1987). But as we have argued at length elsewhere (Virgo, et al., 2011), to identify an individual by its external spatial boundaries alone is a misguided. This confuses the organizational limits of the living system as a network of processes with its physical interface. A physically distinct spatial boundary may appear to be important for the structure of an individual, at least from the perspective of the internalist framework of the computational theory of life and mind. On that view, individuation is identical with physical containment. But this is not the case for a relational theory of life and mind, which views individuation as a process and its physical boundary as an interface for exchange. For instance, as we will show in the next section, it is in fact possible for a system of autocatalytic processes to constitute an individuated dissipative structure even without a dedicated compartment, and this individual can be subject to natural selection. Similar results have also been found in related work (e.g. Savill, et al., 1997; Hogeweg and Takeuchi, 2003).

Another influential critique of the hypercycle theory was put forward by Bresch, Niesert and Harnasch (1980). Their model reiterated a worry raised by Maynard Smith. Mutations of self-replicating units that only benefit other self-replicating units in the hypercycle, although beneficial to the hypercycle as a whole, will not be favored by natural selection due to the independent fitness evaluation of the individual autocatalytic units. Instead it is likely that a hypercycle will succumb to so-called 'parasites', i.e. mutant reactions that receive benefit from the hypercycle without providing any benefit in return:

A hypercycle open to new members, i.e. to evolution, is equally open to its killers. How, then, could a hypercycle evolve? Protection could apparently be achieved by spatial separation – be it a wide geographic heterogeneity of RNA populations, a complex formation, or the encaging of entire hypercycles in compartments – a fate, which will sooner or later overtake a hypercycle anyhow. (Bresch, et al., 1980, p. 403)

Out of these three options of protecting a network of self-reproducing units against an invasion of parasites, Bresch, Niesert and Harnasch choose to follow the classical tradition in the study of the origin of life. They claim that a simplified version of a hypercycle must be enclosed as a 'package' in order to evolve in a stable manner. It has been widely debated whether the addition of a compartment can facilitate Eigen and Schuster's hypercycle scenario (Niesert et al., 1981), or if perhaps it can circumvent the need for a hypercycle entirely,

because selection at the level of the compartment is equivalent to group selection of the enclosed, competing self-reproducing units (Szathmáry and Demeter, 1987). In any case, there is a general agreement that a compartment reduces the detrimental impact of parasitic side-reactions (Eigen et al., 1980).

But what about the other two options indicated by Bresch, Niesert and Harnasch, namely a wide heterogeneous spatial distribution and complex formations? These alternatives may not have received sufficient attention, especially considering the difficulty of explaining how several self-reproducing units could fortuitously come to be enclosed inside a compartment so as to give rise to a functioning hypercycle (or some kind of alternative). We speculate that the probability of a successful enfolding would be helped considerably, if there were already a relatively stable network of reactions existing even before the enclosure takes place. In fact, other research has shown that as soon as we move away from models based on ordinary differential equations, and include at least a minimal form of spatial embodiment in an incompletely mixed medium, it is clear that the problem of parasites has been exaggerated in the literature (Boerlijst and Hogeweg, 1991). In some conditions a heterogeneous spatial distribution and/or a complex formation are sufficient conditions for the emergence of group selection and for protection against parasites. Following this tradition, the assumed necessity of pre-biotic compartments at the origin of life must therefore be reevaluated.

In addition, as we will demonstrate, a complex formation can give rise to adaptive behavior at the collective level, i.e. directed movement or 'chemotaxis', which ensures a suitable spatial distribution of the population and thereby reduces that species' vulnerability to local extinction events. In the same model we also demonstrate another possibility that has not yet received sufficient attention. In some cases what looks like parasitic behavior at the metabolic level of the individual self-reproducing units, may instead turn out to be a mechanism of symbiotic behavior when we consider its emergent effects at the level of the system as a whole. The idea that a hypercycle could be conceived of as symbiosis in the chemical domain is not new (Lee et al., 1997). But we extend this idea by showing that this symbiosis can take the form of behavioral interaction in addition to chemical interaction, and that this behavioral symbiosis can even be constituted by parasitic reactions.

The Gray-Scott model

We chose to study a certain kind of dissipative structure that can be found in the Gray-Scott reaction-diffusion system. We use reaction-diffusion patterns because they exhibit some of the essential features of living systems, yet they are easy to simulate and their dynamics can be understood. As with living cells, reaction-diffusion patterns persist by chemically altering their environment, using up available 'food' molecules and temporarily converting them into the substance that makes up their own structure. This process can be thought of as a highly simplified prebiotic metabolism. The 'spot' patterns that can emerge in the Gray-Scott system have the additional property of being composed of many distinct 'individuals', separated by regions in which little chemical activity takes place. We see this process of individuation as analogous to the division of living matter into populations of individual organisms (Virgo, 2011). These individuated spots can exhibit behavior

that depends on the chemical details of their metabolism, as will be shown below.

Although the Gray-Scott reaction-diffusion spots exhibit minimal analogues of metabolism, individuality and behavior, they lack some other properties often associated with living organisms. In particular, they lack specialized genetic material and they lack a physically distinct bounding membrane. This demonstrates that neither a bounding membrane nor the replication of genetic information is a necessary requirement for metabolism and behavior to occur. The existence of distinct individuals despite the lack of a strong separation between their interior and exterior should help to illustrate our point that it might not be necessary for membrane-bound compartmentalization to occur before the onset of evolution by natural selection, even in a metabolism-first scenario.

The Gray-Scott reaction-diffusion system was first studied in a 2D context by Pearson (1993). This is a minimal model of chemical reactions taking place on a flat surface. The reaction modeled is a simple autocatalytic one, $A + 2B \rightarrow 3B$, meaning that when two molecules of B collide with one of A , they react to produce a third molecule of B , while using up one A in the process. A second reaction, $B \rightarrow P$, represents the decay of the autocatalyst into an inert waste product, which is assumed to instantly leave the system. The molecules A and B have a separate concentration at each point on the surface, which are represented by a and b (note that the concentration of P is not modeled). In addition, the ‘food’ molecule A is fed into every point at a rate proportional to $1 - a$. This can be thought of as due to the entire surface being immersed in a solution of A at a constant concentration of 1. In addition to reacting and being added to the system, the chemical species can diffuse across the surface. Overall this gives rise to Equations 1 and 2

$$\frac{\partial a}{\partial t} = D_A \nabla^2 a - ab^2 + r(1 - a) \quad (1)$$

$$\frac{\partial b}{\partial t} = D_B \nabla^2 b + ab^2 - kb \quad (2)$$

where concentrations a and b are functions of space as well as time, r and k are parameters determined by the rates of the two reactions and the ‘feeding’ process (note that the rate of the autocatalytic reaction has been set to 1 without loss of generality). D_A and D_B are the rates at which the molecular species diffuse across the surface. These equations can be solved numerically using a method that is akin to a cellular automaton, except that each ‘cell’ point contains a continually variable amount of the two chemical species.

In this original Gray-Scott model we find different kinds of dissipative structures. Some of these are spatially individuated as self-maintaining spots of autocatalytic chemicals. The spots can divide and replicate. They are also sensitive to gradients of nutrient chemicals, and can react with chemotaxis, although they do not move spontaneously. The spots mutually exclude each other, and therefore during replication will be pushed away from each other. The spots serve as an abstract model of minimal pre-biotic life, but we found them to be limited because they do not have a capacity for open-ended behavior, development, and evolution (Froese, et al., 2011). In a follow-up study we argued that an important but neglected aspect of the pre-biotic scenario of the origin of life was the emergence of motility. We also showed how self-motility could arise in a modified Gray-Scott model (Froese, et al., in press). Here we

continue this research by focusing on what happens to the original Gray-Scott reaction-diffusion spots when they are threatened by the addition of parasitic side-reactions.

We modified the original Gray-Scott model by introducing a second autocatalyst to the system, which feeds not on the ‘food’ molecule but directly on the other autocatalyst (Virgo, 2011). That is, the reactions $B + 2C \rightarrow 3C$ and $C \rightarrow P$ are added to the system, so that Equations 1 and 2 are extended to Equations 3-5, where D_C is the rate of diffusion of C , and k_1 , k_2 and k_3 are the rate constants for the reactions $B \rightarrow P$, $B + 2C \rightarrow 3C$ and $C \rightarrow P$, respectively.

$$\frac{\partial a}{\partial t} = D_A \nabla^2 a - ab^2 + r(1 - a) \quad (3)$$

$$\frac{\partial b}{\partial t} = D_B \nabla^2 b + ab^2 - k_1 b - k_2 bc^2 \quad (4)$$

$$\frac{\partial c}{\partial t} = D_C \nabla^2 c + k_2 bc^2 - k_3 c \quad (5)$$

With an appropriate choice of parameters, the effect of this modification of the Gray-Scott system is to produce the usual spots of the primary autocatalyst, but this time accompanied by a small region of the secondary, parasitic autocatalyst. Since the secondary autocatalyst feeds on the primary one, the spot of primary autocatalyst tends to avoid it by moving away, while the secondary spot follows. This gives the secondary autocatalyst the appearance of being attached as a ‘tail’ behind the primary spot. Thus, the spot-tail system as a whole moves around spontaneously even in a homogeneous environment.

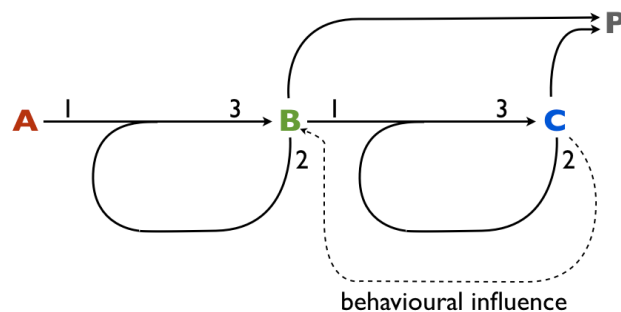


Figure 1. Diagram showing the interactions between chemical species in the reaction-diffusion model. Solid lines represent the chemical reactions $A + 2B \rightarrow 3B$, $B + 2C \rightarrow 3C$, $B \rightarrow P$ and $C \rightarrow P$. The autocatalyst C is parasitic on autocatalyst B . In our simulations, individuated regions of chemicals form, which are composed either out of B or of both B and C . The presence of C changes the behavior of such an individual; it starts to move around spontaneously. This is represented in the diagram by the dotted line marked ‘behavioral influence’.

The spot-tail system is not strictly speaking an autocatalytic hypercycle, because the direct chemical dependency between the two catalysts is not mutual. However, the relationship can still be considered to be an instance of a beneficial functional linkage under some conditions. This is because, although the tail is parasitic on the primary autocatalytic spot (since it does not directly contribute to it metabolically), their co-constituted movement within the environment is adaptive, at least under some conditions. When the chemical interaction (k_2) between the parasite and the spot is strong, a spot can move only in a straight manner and no reproduction occurs. When we weaken

the interaction, the self-moving spots can also reproduce. This transition is important; in the strong interaction regime, self-moving spots will eventually die out by being outcompeted by non-moving spots, but in the weaker regime, the population of self-moving droplets will be sustained by reproduction. With certain parameter settings of the simulation, the spot-tail systems can reproduce more frequently than the spots without tails. Interestingly, at the time of reproduction the self-moving spots can change direction so that they can occupy the whole space. That is, they are more adapted than spots without any ‘parasites’. This is unexpected from the traditional perspective on parasites. It seems that the tail-induced movement tends to split the primary autocatalyst into two distinct spots after some time. Both offspring frequently preserve a tail of their own as well, which means that the trait, once it has been acquired, is passed down the generations like a gene that is transferred from one generation to the next. The movement of the spot-tail systems also tends to make them colonize new areas of nutrients more rapidly. This ‘parasite’-enabled exploratory behavior additionally helps to prevent localized extinction events, in which random areas of the surface are periodically wiped clean of autocatalyst, from eventually killing the whole population (Froese, et al., in press). Here we demonstrated that the spot-tail systems can outcompete spots without ‘parasitic’ tails even in situations that do not include such extinction events (Figure 1).

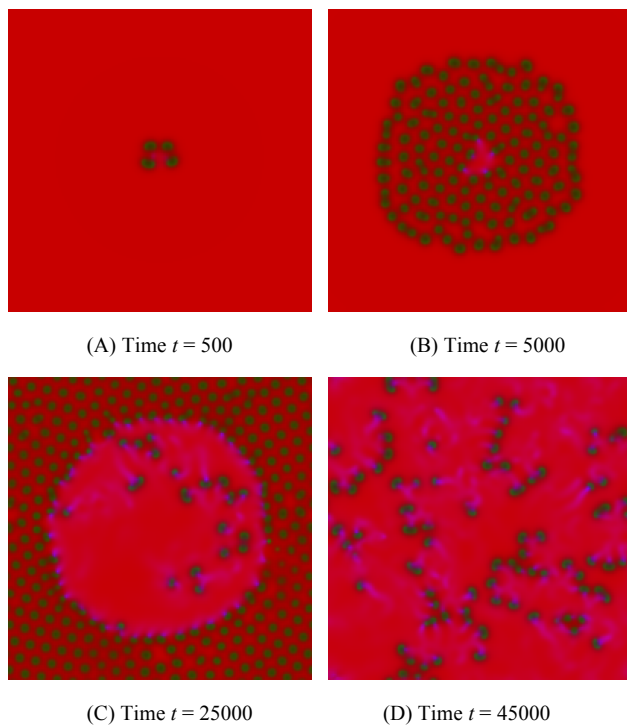


Figure 1. Screenshots of the modified Gray-Scott system with a parasitic side-reaction. At each point the concentrations of A , B , and C are visualized by scaling each of them by 200 and displaying the resulting Red, Green, and Blue (RGB) color value. The surface dimensions are 200 by 200 points. Constants r , k_1 , k_2 , and k_3 are set to 0.025, 0.085, 0.1, and 0.005, respectively. The diffusion rates of A , B , and C are set to 0.1, 0.05, and 0.0025, respectively. Initially, all points are

set to $a = 1$; only in a small 10 by 10 area in the center of the surface are b and c set to small random values drawn from the range $[0, 0.3]$ and $[0, 0.2]$, respectively. (A) At $t = 500$ we can see that the initial seeding of autocatalyst B and parasite C has already given rise to four individual spots that are just about to replicate again. (B) At $t = 5000$ almost the entire surface has been taken over by the spots. In the center we can see that a handful of spot-tail systems have emerged. (C) At $t = 25000$ the remaining outer surface has been occupied by spots. But in the middle there is a growing region in which only spot-tail systems survive. (D) At $t = 45000$ the spot-tail systems have managed to outcompete all of the spots without a parasite.

To be sure, the sequence of events that are shown in Figure 1 is not a necessary result of this modified Gray-Scott system; it is dependent on a certain range of parameters. We have not performed an exhaustive analysis of the parameter space, but we have some practical insights. For example, it is important that the diffusion rate of the parasitic autocatalyst C is significantly slower than the diffusion rate of the original autocatalyst B . Interestingly, in that case the rate of reaction of the parasite C can actually be slightly faster than that of the original autocatalyst B . It seems that the difference in the diffusion processes between B and C is responsible for the break of concentration symmetry, which eventually causes a spot-tail system to move forward. Note that this mechanism of motility is different from the symmetry breaking found in the case of an oil droplet, which is governed by an internal convection flow structure (Hanczyc, 2011). Future work could try to determine more precisely the range of conditions under which relatively stable spot-tail systems emerge.

Previous research about potential benefits of parasites had revealed that their introduction to a model can result in spatial self-structuring (Sardanyés and Solé, 2007). But true benefits have so far remained elusive; to demonstrate symbiosis some researchers relied on the inclusion of catalytic benefit from the parasite to the hypercycle, thereby turning it into a hypercycle by design (Kim and Jeong, 2005). Thus, to our knowledge this model is the first existence proof that a parasitic side-reaction of an autocatalytic system can actually be beneficial in some conditions. This benefit can only be observed when spatiality, self-individuation without containment, and the possibility of movement are taken into account. We can therefore extend the original idea of an autocatalytic hypercycle by including the emergence of system-level behavior as one possible beneficial functional linkage between the chemical components. In other words, the spot-tail system is a behavior-based hypercycle.

Note that this idea of integrating a parasite in order to take advantage of behavioral benefits is not as outlandish as it may appear. For example, the human body can also be seen as a behavior-based hypercycle in just the same way: the brain is metabolically parasitic on the rest of the body, since it uses up metabolites and does not contribute anything back directly on the chemical level. However, it enables us to breathe and find food (i.e. adaptive behavior), and so metabolism of the body is dependent upon the parasitic brain for its own continuation.

Discussion

In order to develop a better understanding of the origin of life we have to pay more attention to all of the various dimensions

and timescales in which this event unfolded. We have insisted on the importance of including more consideration of the role of spatial embodiment and intermediate timescales, because these space-time dimensions are necessary for the emergence of adaptive behavior. More specifically, we contributed to the development of a ‘movement-first’ approach to the origin of life by evaluating the possible role of movement and adaptive behavior in attenuating the problem of parasitic side-reactions.

A particular challenge for metabolism-first scenarios is the recognition that the first metabolic cycles presumably had to take place without the help of specialized enzymes, which could have significantly enhanced reaction efficiency. Also, it seems that only enzymes could have discriminated between very similar substrates and thus selectively avoided parasites. Accordingly, it appears that a simple dissipative structure, like the reaction-diffusion system in our model, must be especially vulnerable to parasitic side-reactions. It is for these kinds of reasons that Orgel (2008) has argued for the implausibility of metabolic cycles on the prebiotic earth.

It is clear that the existence of a sequence of catalyzed reactions that would constitute an autocatalytic cycle is a necessary condition for the cycle to function in a sustained way, but it is not a sufficient condition. It is also necessary that side reactions that would disrupt the cycle be avoided. [...] Lack of specificity rather than inadequate efficiency may be the predominant barrier to the existence of complex autocatalytic cycles of almost any kind. (Orgel, 2008, p. 8)

Specialized enzymes are clearly an important evolutionary milestone to ensure the increased efficiency and specificity of a metabolic system. However, they are a *necessary* solution only from an internalist perspective on life. On the other hand, if we adopt the relational perspective of the movement-first approach, then an unexplored alternative is made conceivable. We know that if the autocatalytic system is an individuated dissipative structure, such as the reaction-diffusion spots in our model, then the system spontaneously exhibits chemical gradient following, i.e. chemotaxis. The emergence of this self-motility and adaptive behavior is an alternative solution to Orgel’s challenge. Chemotaxis (1) enhances the *efficiency* of the chemical reaction by moving the autocatalytic system into regions with higher concentrations of nutrients, and (2) it also enhances the *specificity* of the reaction, because it moves the autocatalytic system away from the negative influence of parasitic side-reactions. In other words, *selective behavior in relation to the environment can partially substitute for the efficiency and selectivity of enzymes within the boundary of a protocell*. Finally, we note that this potential contribution of movement is not restricted to the metabolism-first scenario in as far as the replicator-first scenario is arguably also faced by the same problem of insufficient selectivity due to a lack of specialized enzymes (Shapiro, 2000).

Conclusions

The main points of this paper can be summarized as follows:

- The formation of a pre-biotic individual system does not necessarily require a special compartment; some dissipative

structures are able to self-organize their own spatiotemporal individuation, for instance in the form of chemical gradients.

- These kinds of individuals can exhibit adaptive behavior in an incompletely mixed spatial medium, especially selective self-movement in a chemical gradient (e.g. chemotaxis).
- Chemotaxis reduces the necessity for internal catalytic *efficiency*, such as provided by specialized enzymes, because the individual seeks out regions of its environment that tend to increase its chemical concentrations.
- Chemotaxis thereby enhances an individual’s chances of reproduction, because it increases its access to regions that are rich in nutrients.
- Chemotaxis reduces the necessity for internal molecular *selection*, such as provided by specialized enzymes, because the individual avoids regions of its environment that tend to decrease its chemical concentrations.
- Chemotaxis thereby reduces an individual’s vulnerability to parasitic side-reactions, because it moves away from any regions that reduce the concentration of its constituents.
- Interaction between an individual and a parasite can give rise to movement of the individual-parasite system as a whole, which in turn is an adaptive behavior in some environments.
- This kind of emergent symbiotic behavior can substitute for a lack of autocatalytic functional closure by constituting a novel behavior-based linking function in a hypercycle.
- A hypercycle that incorporates a behavior-based linking function confers advantages similar to a standard autocatalytic hypercycle; it enhances replicative success of both reactions together and enables group selection.

In sum, the model has demonstrated a novel possibility, i.e. that a parasitic interaction on the metabolic level can result in a symbiotic interaction on the behavioral level of the spatially embedded reaction-parasite system as a whole. It constitutes a new integrated individual that confers evolutionary advantage on the interaction processes of its components. It is easy to imagine that if the evolutionary advantage of such moving-information is strong enough, then the original autocatalytic reaction and the parasitic reaction may eventually evolve to form a proper autocatalytic hypercycle in order to reduce the chances of the parasite killing the host or the host losing its parasite. Chemical endosymbiosis may be an interesting target for future research in this direction.

To be clear, we are not trying to suggest that the Gray-Scott reaction-diffusion system is a realistic model of the origin of life. We have used that system as a proof of concept to show that already extremely simple pre-biotic chemical systems can exhibit individuality, movement, and adaptive behavior – even without a rigid compartment, digital genetic system, or any specialized sensory-motor interface. Arguably, such behavior could have made a significant contribution to resolving some of the problems faced by the earliest forms of life.

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