Physics AUC, vol. 24, 130-151 (2014) **PHYSICS AUC**

Elimination of less-fit information variants during competition between low complexity dynamic systems

Vily Marius CIMPOIAŞU[1] and Radu POPA[2*]
[1] *Frontier Biology and Astrobiology Research Center, University of Craiova, 13 A.I. Cuza Str., 200585 Craiova, Romania*
[2] *University of Southern California, Los Angeles, CA, USA*

Abstract

Evolution of dynamic systems requires balance between information variance and the rate of eliminating less-fit system variants. When competing systems are simple and advantages of novel phenotypes are petite or implement slowly, networks of systems become cluttered with information variants. This chokes evolution and adaptation analogous in consequence with Manfred Eigen's "error catastrophe". Using the simulation platform BiADA (i.e. Biotic Abstract Dual Automata), we have studied extinction controllers and rates when primitive energy dissipative networks with similar cyclomatic complexity compete. Potential controllers included the stability of individual system parts, the abundance of free energy, variation in free energy availability, catalysis of uptake/dissipation of free energy and autocatalysis. Results indicate that: (a) Elimination of the less-fit is more efficient in energy limitative environments and difficult in energy copious environments; (b) Evolving prebiotic networks may have required environments progressively richer in free energy (albeit limitative); (c) The rate of increase in energy availability has to be low relative to the rate of information evolution; (d) In energy-rich environments, synergism between energy availability and autocatalysis amplifies minute differences in performance and facilitates extinction events; and (e) Autocatalysis is a major controller of prebiotic selection by increasing the stringency of selection and correlating it with energy availability, thus allows extinction of the less-fit to keep pace with information innovation. We hypothesize that the evolution of prebiotic automata required an environment progressively rich in free energy, and that the rate of this change must have been slow enough relative to the rate of adaptation. Excess free energy in a primeval environment or speedy increase in energy availability repressed the evolution of prebiotic chemical networks toward life.

1 Introduction

Modern life forms use a translation machinery to decipher encrypted information, which classifies them as informata. Systems that use solely analogical mechanisms for functioning and inheritance are classified as automata [1]-[2]. During prebiotic evolution, automata most likely preceded informata, which means that understanding evolution of simple dynamic systems toward life requires explaining competition between automata.

*e-mail address: rpopa@usc.edu

The evolution of modern biological informata occurs by Darwinian selection, but the principles controlling the evolution of automata (which are much simpler) are different. Informata keep records of historical changes in organization successful in the past (within information storage limits), and thus store either as individuals or collective, a cache of "virtual states". These backup system states represent potential responses to variations in the environment (based on past experiences). In contrast, automata have no specialized means of remembering the past, and as such, have poor, if any, "recollection" of former states. This makes automata less efficient with regard to response strategies in variable environments. Henceforth, informata are better adapted to withstand variable environments, while the robustness of automata increases in homogeneous environments. Automata contain little if any hidden information. The number of virtual states in automata is very low relative to informata, and therefore, the only automata that survive environmental challenges (such as limitation in resources and stress from complex and variable environments), are those open to innovation. Because they never learn from the past, automata have less competitive potential of automata; this explains why once informata have emerged in evolution they easily took over the world making all present living systems informata. During this transition, control has also shifted from being thermodynamics-based to being information-assisted as well. Last but not least, most informata have sufficient information content to evolve the capacity to reproduce; henceforth, they are better at filling the habitable space with copies of themselves. During competition, informata multiply fast, because in their case information too (apart from thermodynamics) controls the final equilibrium between system variants. In doing this, informata can eliminate competitors even when differences in performance between phenotypes are petite. Automata too, can evolve toward many information variants, but because they do not have an efficient strategy for selection-to-elimination of the less fit they end up in thermodynamic equilibrium among competitors.

A continuing problem of the origin of life is explaining the evolution of automata (or very simple systems) toward increased complexity and elimination of less-fit competitors prior to the advent of replication of information and informata systems. In homogeneous environments, rather than competitive elimination information variants evolve toward thermodynamic equilibrium and endless diversity (an indirect agreement with the 2^{nd} law of thermodynamics). Such clusters of systems will accumulate large collections of information variants, analogous in consequence with Manfred Eigen "quasi-species" and "error catastrophe" [3], instead of eliminating the less fit. During this crisis the pace of corralling diversity is lower than the pace of creating diversity. The habitat populations of automata occupy fills with random diversity, mediocre information, low order and poor networking, low complexity and thermodynamic equilibrium; these trends are opposite to the origin of life. Solutions to these problems are key to any origin of life theory. In theory, evolution via competition-to-elimination of the less fit automata could not have occurred if the environment was poor in free energy; i.e. insufficient for supporting the maintenance and the buildup of information. At the other end of the spectrum, in energy copious environment energy starvation cannot occur. This demonstration has not been made and implications have not been studied. Informata show extensive self-controlling capabilities. On the opposite, automata are to a large extent controlled by their environment and the stability of their parts. The questions we tackle in this study are:

- What properties should a primitive environment have, to drive the elimination of less competitive systems when differences in performance between competing systems are petite?

- In what circumstances do catalysis (and autocatalysis) help this elimination process?

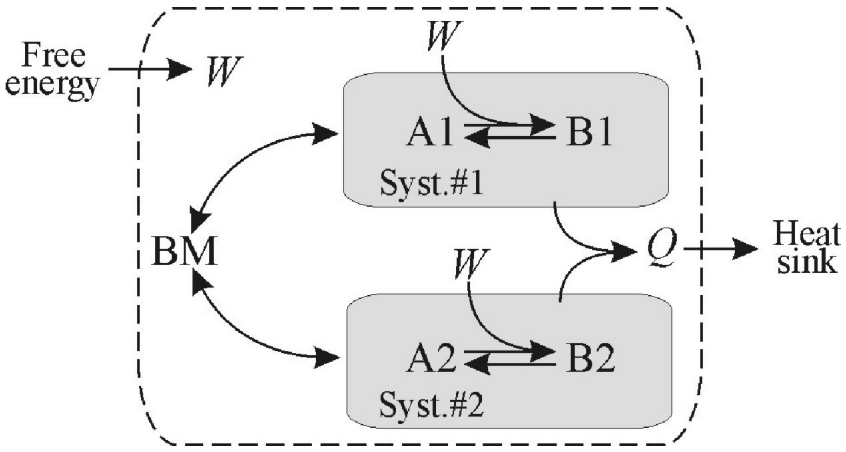

Figure 1: Diagram of the model used in this study for analyzing competition between two types of low complexity automata with similar cyclomatic complexity (Syst.1 and Syst.2). The two systems compete for building materials (BM) and free energy (W) in a closed environment (i.e. with energy exchanges, but no exchanges of materials with the exterior). Q = heat energy released from activity. Albeit changes in proportion between internal components occur within each system during simulation, no inheritable variation exists (typical for automata). Details of the structure and function of these systems are given in the Appendix section.

- From an information and energy point of view, catalysis (and autocatalysis) are not free. How are their costs and benefits balanced? And how are they used in prebiotic competition simulations?

2 Materials and Methods

Basic structure and functioning of systems analyzed

The model created for this study is that of competition for building materials and energy between low complexity automata (Figure 1). In this study we analyze how competition is influenced by three factors: energy availability (in an energy homogeneous environment with bottomless heat sink); thermodynamic stability of system parts and catalysis/autocatalysis. We also discuss advantages and pitfalls of increase in order (an expected outcome of prebiotic evolution). A Stella8 implementation of this model is available at: http://www.ksg.ro/Buildingmodel71vmc.STM . The model is explicit, so that readers can re-construct it in another dynamic simulation program.

Principles for model construction

Explaining the origin of life requires knowledge of disequilibrium thermodynamics [4]-[6], theory of information and statistical mechanics [7]-[9], as well as drivers of transformation and basic trends of prebiotic evolution [10]-[18]. Because the essence of life is composition independent, but also because "not everything that is measurable is worth measuring", many prebiotic simulations have been created that sacrifice mimicking minute details of the real world, for the sake of explaining the origin of life broadly by means such as meta-chemistry, non-earth centric, non-chemical centric and using abstract modeling principles [13], [19]-[27].

The modeling avenue chosen for this study is BiADA (acronym for Biotic Abstract Dual Automata), [28]-[29]. BiADA models use the following set of rules:

1) Modelled systems are abstract. Units of measure common in chemical system analyses, such as the Avogadro number (N_A), molar concentration (M), Boltzmann's constant (kB) and a universal energy content per unit of information (Landauer bound, see below), are optional and not absolutely needed to explain prebiotic evolution.

2) Each system or form of organizing building blocks has two energy features: free energy content (eg); disorder (or entropy)-related energy content (es) (equivalent to heat content from chemistry),

3) Each system or form of organizing building blocks has two information features: residual information (I_{Rs}) and remnant information (I_{Rm}).

4) For computational simplicity, E_G, E_S, I_{Rs} and I_{Rm} only take absolute (zero or positive) values.

5) All transformations are discrete increments or decrements of building blocks, energy and information, and transformations are expressed in integers of both units of transformation and units of organization.

6) Forward and reverse transformations are analyzed separately (i.e. as uni-flows). Flows too only have absolute values and a model measures both the brut and net changes and exchanges.

7) The direction and equilibrium of a process is not derived from changes in entropy and standard free energy values, but rather from net rates of forward and reverse transformations. Albeit not using conventional equilibrium calculations the meaning of free energy, entropy and equilibrium remain the same as in conventional thermodynamics.

8) During transformations, the efficiency of exchanging free energy between two forms of organization (i.e. source and target) depends, among others, on similarity/differences between information content (i.e. meaningful information). Because the exchange of meaningful information between source and target is seldom 100% efficient, most transformations require import of free energy even in exergonic directions.

Energy and information in BiADA models

Features of BiADA models explained in earlier publications explain: basic model layout; justifications for various formulas; software-specific commands for Stella software implementation and sequence of actions for introducing data in a model [28], [2], [29]. Here, we only summarize parameters important for this study. E_S is the disorder-related (i.e. entropy-; heat-, or I_{Rs}-related) energy content of a system or form of organization. For homology, in thermodynamic systems $E_S = T \cdot S^*$ (where: T = temperature; and S^* (or absolute entropy) = $k_L \cdot I_{Rs}$). The k_L parameter is explained below. E_G is the order-related (i.e. free energy- or I_{Rm}-related) energy content of a system or form of organization. Homologous to thermodynamic systems, E_G = -G^* (where: G^* = the sum of all standard bond energies or bond dissociation enthalpies) [32]. I_{Rs} or residual information (i.e. unused information or information capacity), is the information capacity of the disordered part of a system or form of organization. For homology to statistical mechanics and theory of information, $I_{Rs} = D = \log_2\Omega$ (where: D = information capacity or Shannon entropy measured in bits [7]; and Ω = the total number of potential microstates of a given system state). I_{Rm} is the removed (or remnant) information of a system or form of organization and represents information capacity lost to order (dI_{Rs} = -dI_{Rm}). I_{Vt} (= I_{Rs} + I_{Rm}) is the virtual information, or maximum information capacity of a system in fully disordered state. Relative to the theory of information, I_{Vt} is equivalent with Shannon's channel capacity [7]. A system is assumed to be fully disordered when $I_{Rm} = 0$ and $I_{Vt} = I_{Rs}$, while order is present in a system when $I_{Rm} > 0$ and $I_{Rs} < I_{Vt}$. Because in most cases the energy amount per bit varies between the disordered part and the ordered part of a system (i.e. $E_S/I_{Rs} \neq E_G/I_{Rm}$), changes in the E_S/E_G of a system are not quantitatively

correlated with changes in I_{Rs}/I_{Rm}. Meaningful information (I_{Mn}) is a difficult concept if analyzed for a single system [38]. In BiADA, I_{Mn} is a measure relating two or more systems or forms of organization. E.g., I_{Mn} is the amount of the I_{Rm} describing the organization of a source system (say: A) that is meaningful to the I_{Rm} of a receiver system (say: B): $I_{Mn}(AB) = I_{Rm}(A) \cap I_{Rm}(B)$. In BiADA models, one hundred percent efficient information transfer means that: when $I_{Rm}(A) > I_{Rm}(B)$ all information content needed by B is available in A (i.e. $I_{Mn}(AB) = I_{Rm}(B)$); and also that when $I_{Rm}(A) < I_{Rm}(B)$ all information content of A is shared unaltered towards B.

Relationship between energy and information in BiADA models

The parameter k_L ($= S^* / I_{Rs}$) is the energy equivalent of a unit of information capacity [28], [2], [29] homologous in meaning to the Landauer bound (or Landauer limit) from statistical mechanics [31], [36]. It is assumed that k_L is constant for a whole class of systems made of similar building blocks, yet may vary between systems of dissimilar type [30], [33], [34], [35], [37] or systems at various scales. One should reasonably expect for k_L to vary between dissimilar systems such as chemical systems vs. cybernetic systems and vs. socio-economical systems. This issue becomes important when analyzing non-conventional life analogues, systems at various levels of hierarchical organization and in chemistry-independent artificial life models. Although k_L may vary, the basic principles of organization and evolution of such systems remains the same. For example, at standard temperature, k_L (k_L^o) $= E_S \cdot T^o / (I_{Rs} \cdot T)$. For models of chemical systems we assume that k_L (or E_{bit}) $= kB \cdot T \cdot \ln 2 = 2.8 \cdot 10^{-21}$ J bit^{-1} at 20^oC [28], [2], [29]. Similar to absolute entropy (S^*), the E_S and I_{Rs} of a system are difficult to determine in the real world. Yet, this does not make these parameters less real. From a thought experiment point of view, E_S is the integrated heat capacity at constant pressure (C_P), or heat absorbed by the degrees of freedom of a system, between 0 K and the temperature of observation [28]. In practice, such measurement would only be straightforward if no changes in order (i.e. phase transitions) occur, as a system is cooled to zero K. In reality, various bonds and novel forms of organization emerge and are destroyed at various temperatures, due to ordering effects of fundamental forces, altering the I_{Rs} and C_P of a system. Yet, in abstract system modeling (BiADA included), S^*, E_S and I_{Rs} take absolute and quantifiable values. This helps explain in an empirical way why transformations occur in a system and the effect of internal heat and temperature on the stability of a system or form of organization. The parameter $k_G = E_G / I_{Rm}$ from BiADA models, called "Gibbs bound" is the free energy associated with adding or removing order (or I_{Rm}) in a system. Unlike k_L, the k_G parameter may vary with each type of organization and organization upgrade (e.g. analogous to various types of bonds from chemistry). One form of organization often consists of many types and layers of order. Thus, in models, specific k_G values are introduced (or deduced) for each system, form of organization or order upgrade. In a thought experiment E_G and I_{Rs} may be measured by combining results of calorimetry with prior knowledge of E_S, as temperature increases until all bonds are broken, all order is disintegrated, I_{Rm} becomes zero and $I_{Vt} = I_{Rs}$. Yet, because E_S and I_{Rs} cannot be measured with precision and will vary with temperature, the E_G and I_{Rm} of real world systems are difficult to determine precisely. An E_G approximation for chemical systems can be obtained by adding all bond energies, albeit evaluating I_{Rm} (and thus k_G) is still difficult. Yet again, this does not mean that E_G, I_{Rs} and k_G are unreal physical realities; such parameters are meaningful and very useful in abstract models.

Controllers of order in a prebiotic system

Presence of order (Ord) in a system depends on balance between ordering and disordering factors. In simple models, it can be assumed that $I_{Rm} > 0$ requires that $E_G \geq$

E_S. Yet, overall $E_G < E_S$ does not exclude the existence of order. The Ord $\because$ E_G-$E_S \geq 0$ constraint works at local scale, or when the distribution of E_G and E_S is homogeneous throughout space, or when interaction is possible between I_{Rs} and I_{Rm}. Yet, if the distribution of building blocks (or of E_G vs. E_S) is heterogeneous, (such as when areas of order are separated from areas of disorder with little interaction between them) order may yet exist locally even if the overall $E_G < E_S$. As temperature increases heat is absorbed in the E_S reservoir proportional to I_{Rs} until $E_S = E_G$. When this threshold is reached (and contingent upon I_{Rs} and I_{Rm} partition) order is degraded (beginning with the weakest bonds first) and part of I_{Rm} is lost to I_{Rs}. This change enhances the capacity of the system to absorb heat (because $E_S = T \cdot k_L \cdot I_{Rs}$), and more order destruction occurs. The process continues until only the strongest bonds and structures remain, where at least locally and for the given temperature $E_G > E_S$. This is the empirical explanation why phase transitions are fast during heating and cooling. Abstract models of prebiotic networks should include this effect as well, because they can produce systems where minute changes in phenotype have major consequences on competition success.

In real world systems, order is mixed with disorder and E_G and E_S are not fully separated. Their separate accounting in abstract models is yet useful because it allows discussing their individual contribution to the behavior of a system. For example, one can deduce from such analysis that pure order has no temperature, because only degrees of freedom (i.e. I_{Rs}) have the capacity of absorbing heat. It follows that a fictional system with one hundred percent order (i.e. $I_{Rs} = 0$; and $E_S = 0$) and no material exchanges with the exterior, will have zero heat content and heat conductivity and (at least in theory) should be indestructible by heat alone. In the real world however, I_{Rs} is never zero, and S^o all systems and forms of order are heat sensitive. This avenue of reasoning also explains why systems with larger E_G values tend to be more heat resistant and generally have lower heat capacity (C_P) than systems with lower E_G values (at comparable composition and k_G). No universal relationship exists between E_G and (C_P), because k_G varies among various levels and forms of organization.

Absolute and relative values for free energy and entropy

Equilibrium thermodynamics calculations circumvent the need for absolute entropy (S*) and absolute free energy (G*) by using relative parameters such as standard entropy (S^o) and standard free energy (G^o). With regard to the energy exchanged, the S^o-based and G^o-based calculations do not analyze uni-sense transformations, but only net differences between forward and reverse transformations. This approach works well in simple reaction models, but underestimates the energy dissipative potential and energy flow of systems in state of dynamic kinetic stability, (which is common in energy dissipative systems and biochemical networks). The BiADA approach to modeling aims addressing this limitation [28]-[29]. In chemical systems another solution exists: a reference form of organization has been selected (i.e. H^+(aq)), and given by default a $S^o = 0$ and $G^o = 0$. The reason H^+(aq) is used as zero reference is because it is the smallest and simplest chemical nucleus analyzed, and because it is analyzed in a aqueous environment under standard conditions of temperature and pressure (i.e. common for the natural chemistry). Extraterrestrial chemists however, living on a planet where another fluid and another temperature regime may be more common may choose another set of standard conditions for equilibrium thermodynamic calculations.

The S^o value of all chemicals and ions is measured relative to the zero reference (i.e. chemicals in the simplest, stable elemental form). S^o and S* are linearly correlated and measured in similar units. They can be placed on the same scale, yet shifted with the zero point in different position, analogous to ^{o}K and ^{o}C on the temperature scale; consequently

albeit $S^o \neq S^*$, $dS^o = dS^*$. Unlike entropy, G^o and G* have dissimilar meaning and, on a graph, they will appear independent of each other; consequently, $dG^o \neq dG^*$. dGo values measure differences in stability in standard conditions relative to the standard state, and thus measure changes in free energy during net transformations. dG^o measures changes in free energy content (the energy content of bonds) during uni-sense transformations. dG* alone cannot be used to predict whether a transformation was exergonic or endergonic. To obtain such information, models have to include parameters such as K, Q, G^o and T or have to monitor forward and reverse transformations. In BiADA, E_G = -G* because order (and bonds) are assumed to only contain positive energy.

3 Results and Discussions

Series 1 of simulations

In this series, two systems (network types or forms of organization) called Syst.1 and Syst.2 compete, no free energy is available from the exterior, and the A and B units of organization (i.e. components from the systems) form only due to software rules external to the systems (analogous to fundamental forces). The structures A and B only contain building materials (BM), free energy and heat and the information used in their construction is not resident in the systems or controlled by the systems. The model has the architecture shown in Fig.1 and the initial conditions from Table 1. Table 1 also gives the meaning for the various parameters used in the model. We have analyzed how changes in the degradation rate of A2 and B2 influence competition between the two types of systems (Syst.1 and Syst.2). The competitive success of Syst.2 was examined based on two factors: (1) changes in the rate of reduction of Syst.1; and (2) the ability to totally eliminate Syst.1.

Table 1. Input variable used in the series 1 of simulation.		
Init. no. of units of transformations	Forward transf. rates	Reverse transf. rates
Units BM init=1e10	Ro BM to A1=1e-3	Ro A1 to BM=1e-3
Units A1 init=2e8	Ro A1 to B1=1e-6	Ro B1 to A1=1e-5
Units B1 init=1e3	Ro BM to A2=1e-3	Ro A2 to BM=1e-3
Units A2 init=2e8	Ro A2 to B2=1e-6	Ro B2 to A2=1e-5
Units B2 init=1e3		
Run conditions: DT=1; N0. of steps: 32500 or DT=10;		
No. of steps:325000 or DT=20; No. of steps: 650000		
E input and Euptake effieciency	Catalysis and Energy availability	
free E input =0	Cat natrl A1 to B1 =1	
F Euptake A1 to B1 =1	Cat natrl A2 to B2 =1	
F Euptake A2 to B2 =1	Autocat B1=0	
Eff Etransfer A1 to B1=1	Autocat B2=0	
Eff Etransfer A2 to B2=1		

As expected from basic reasoning, results show that if no Ro differences exist between Syst.1 and Syst.2, no successful competition occurs and the two systems of organization end up with similar ratios at the end of simulations (Fig.2, Panel A, Plot 1). Next, we have analyzed changes in competitive success due to two parameters: lower degradation rate of A2 than A1 (i.e. "Ro of A2 to BM" < "Ro of A1 to BM") and lower degradation rate of B2 than B1 (i.e. "Ro of B2 to A2" < "Ro of B1 to A2"). These changes are expected

to favor the B2 form or organization and Syst.2. Lower "Ro of B2 to A2" should also increase the relative abundance of B2 vs. B1, while lower "Ro of A2 to BM" should increase the capacity of Syst.2 to over-compete Syst.1. Simulation results confirmed these expectations (Fig.2). When the value of "Ro A2 to BM" was 1e-7, total elimination of B1 has occurred within 560,000 steps (for a D.T. Stella parameter of 100). We have also verified the effect of lowering the "Ro B2 to A2" in the 1e-10 to 1e-5 range. At "Ro B2 to A2" of 1e-10 (and D.T. = 500), B1 has decreased to 1,561,500 units after 1.5e7 steps (results not shown). For the initial conditions used in this simulation the maximum duration allowed by the program did not result in B1 = 0. Yet, the asymptotic trend suggests that elimination of B1 may occur after approximately 1e+10 steps. Naturally, the information regarding the construction of B1 and A1 cannot be lost when A1 and B1 are eliminated because this information is resident in the rules of assembly (which are external to the competing systems). This is unlike complex networks where blueprint information is also stored in the systems themselves.

Without free energy from the exterior, we started from A and B having similar degradation rates between Syst.1 and Syst.2 (i.e. "Ro of A1 to BM" = 1e-6; "Ro of A2 to BM" = 1e-6; "Ro of B1 to A1" = 1e-6 and "Ro of B2 to A2 = 1e-6"), and compared effects on competition between the two types of systems. Fig.2 illustrates the effect of: (1a) Decrease in the degradation rate of A2 vs. A1; (Fig.2, Panel A); and (Fig.2, Panel B, Plots 1 vs. 2); (1b) Decrease in the degradation rate of B2 vs. B1; (Fig.2, Panel B, Plots 1 vs. 3); and (1c) Combined lower changes in the rate of A2 and B2 vs. A1 and B1 respectively, and relative to the above simulations from (1a), (Fig.2, Panel B, Plot 4).

Table 2	Ro A1 to BM	Ro A2 to BM	Ro B1 to A1	Ro B2 to A2
Plot (1)	1e-6	1e-6	1e-6	1e-6
Plot (2)	1e-6	1e-8	1e-6	1e-6
Plot (3)	1e-6	1e-6	1e-6	1e-8
Plot (4)	1e-6	1e-7	1e-6	1e-7

Results show that lowering the degradation rate of A2 has more beneficial effects on the competitive edge of Syst.2 than lowering the degradation rate of B2. Also, decrease in the degradation rate of both A2 and B2 is a very efficient strategy to increase the competitiveness of Syst.2 (i.e. synergism). From prebiotic perspective, it is more likely for an automaton to succeed in eliminating other automata through smaller (i.e. less costly) changes in the rates of transformation of many of its internal components, than by a very large change in the degradation rate of one or only a few of its internal components. It indicates that at this stage of system organization, similarity in the effect of change of various components from a system was an important selective factor.

Series 2 of simulations

In this series free energy was available from the exterior in uniform rate of supply. We have used the conditions shown in Table 1, except that the rate of degradation of A2 was lower (i.e. 1e-4 rather than 1e-3; similar to differences in competition between Syst.2 and Syst.1 in Fig.2 Panel A Plot 1 vs. Fig.2, Panel A, Plot 3. In Series 1 of simulations this difference in thermodynamic stability favors Syst.2. In Series 2 we have analyzed how the availability of external free energy influences competition between the two types of systems. This competition was studied from four perspectives (explained below in the sections 2a, 2b, 2c and 2d).

(2a) Changes in the rate of Syst.1 removal; and

(2b) Changes in the final equilibrium between Syst.1 and Syst.2

A first tier series of simulations has indicated that when free energy becomes avail-

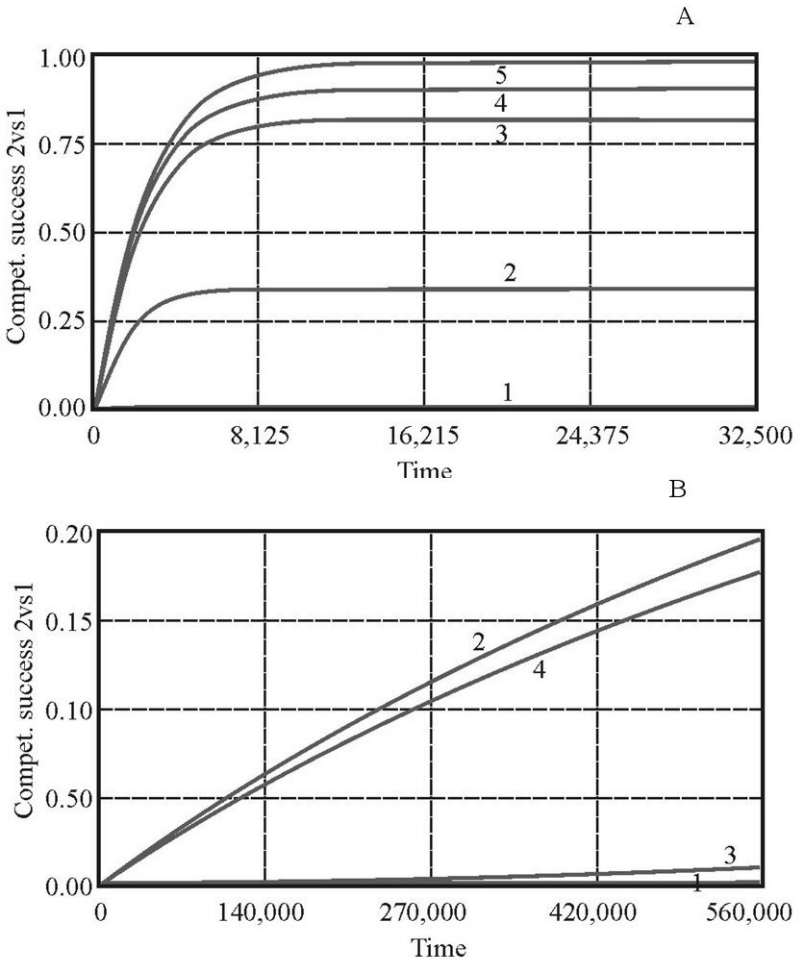

Figure 2: Graphs summarizing the results of Series 1 of simulations. Evolution of the competitive success of Syst.2 relative to Syst.1 in response to changes in "Ro A2 to BM". In the model, "Compet success 2 vs 1" is measured as ((A2+B2) - (A1+B1)) / (A1+B1+A2+B2). Panel A shows that lower values for "Ro A2 to BM" (i.e. decrease in the rate of degradation of A2 relative to Table 1 favor Syst.2. "Ro A2 to BM" = 1e-3 in Plot (1); 5e-4 in Plot (2); 1e-4 in Plot (3); 5e-5 in Plot (4) and 1e-5 in Plot (5). Panel B shows results of lowering the degradation rate of A2. Plot (1) is a control with similar values for the degradation rates of A1 and A2 and for the degradation rates of B1 and B2. Plot (2) shows that lowering the degradation rate of A2 relative to A1 increases the competitive success of Syst. 2. Plot (3) shows that lower rate of B2 degradation favors Syst.2, and that lowering the degradation rate of A2 is more important to the competitive success of Syst.2 than lowering the degradation rate of B2. Plot (4) shows that lowering the degradation rate for both A2 and B2 relative to A1 and B1 respectively favors Syst.2 almost as much as very low degradation rate of A1 (Plot 2); a typical example of synergism. This is important because in this material we seek to study circumstances leading to large competitive success when differences in parameters between systems are petite.

able Syst.2 becomes less competitive, and also that the competitive edge of Syst.2 was lost when the free energy level reached 1e-10 (Fig.3, Panel A). At first glance, this may indicate that differences in transformation rates (expected to drive competition success) may be cancelled by an excess of free energy in the environment. However, upon careful examination, not all levels of free energy lower the competitive advantage of Syst.2. For 0 < free energy < 3e-13, Syst.2 is actually favored (Fig.3, Panel B). An optimal free energy value exists for this particular set of conditions (approximately 1.5e-13; relatively similar to the Fig.3, Panel B, Plot 4) where Syst.2 has the advantage above the competitive level that is expected based on differences in degradation rates alone.

Results of the *2a* and *2b* series of simulations show that free energy helps those system containing components with largest stability (decay rate or survival rate), but only within a specific free energy range. In fact, excess free energy cancels the competitive benefit of a larger survival rate. The exact values are model dependent. In our model, this effect was produced by the fact that free energy unused by Syst.2 (the system with components having lower decay rate), became available to Syst.1; consequently, no energy limitation has occurred and free energy stopped being a controller of information selection. An optimal level of free energy was also found where energy availability and lower rate(s) of degradation had synergic effects on competition-to-elimination. This is important with regard to the origin of prebiotic networks, because it shows that the efficiency of catalysis and energy dissipative potential must have evolved "in tune" with the availability of free energy in the environment. It may also indicate that one purpose of the catalytic energy dissipation is deliberate creation of energy limitation and thus starvation of competitors. Because BiADA models are abstract, this observation is also meaningful for analyzing competition between other types of systems. It includes for example optimization strategies in socio-economical systems. For example when socio-economical systems compete, the choice for using cheap and disposable system components (commonly linked with short half-life, high turnover of materials and energy, which also make systems more tolerant to variability and change), as opposed to more costly and long lasting components (linked with curbing waste, traditionalism in organization and lesser tolerance for variability and quick-fixes) should be a strategy dependent upon predicted availability of resources. Albeit not analyzed in prebiotic networks, this observation is common in socio-economics where excess free energy is linked with consumerist and poor recycling strategy, and vice versa, resource limitation is linked with traditionalism and more efficient recycling. The most interesting part here is the connection between energy availability and the pace of adaptive evolution.

The effect of E availability on:

(2c) The competitive success of the fittest system; and on

(2d) The time threshold to eliminate the less-fit.

Fig.4 Panel A shows the final equilibrium between Syst.2 and Syst.1 after 325,000 steps using the conditions from Fig.2, Panel A, Plot 3, and various levels of free energy. In this series of simulations we have used free energy levels between 1e-15 and 1e-4. For Fig.4, Panel B we have selected a set of degradation rates where Syst.1 was totally eliminated, even when the available free energy was zero (Table 1 input conditions, Fig.4, Panel B), and analyzed the effect of energy availability on the time needed to eliminate Syst.1. Competition-to-elimination is a means to "sanitize" the environment of useless information variants and to corral diversity in the future. Anything less than total elimination of competitors is unacceptable because it increases the diversity of information variants when free energy becomes copious. We found that if the A2 and B2 components were more stable than A1 and B1 respectively, the addition of free energy helps Syst.2

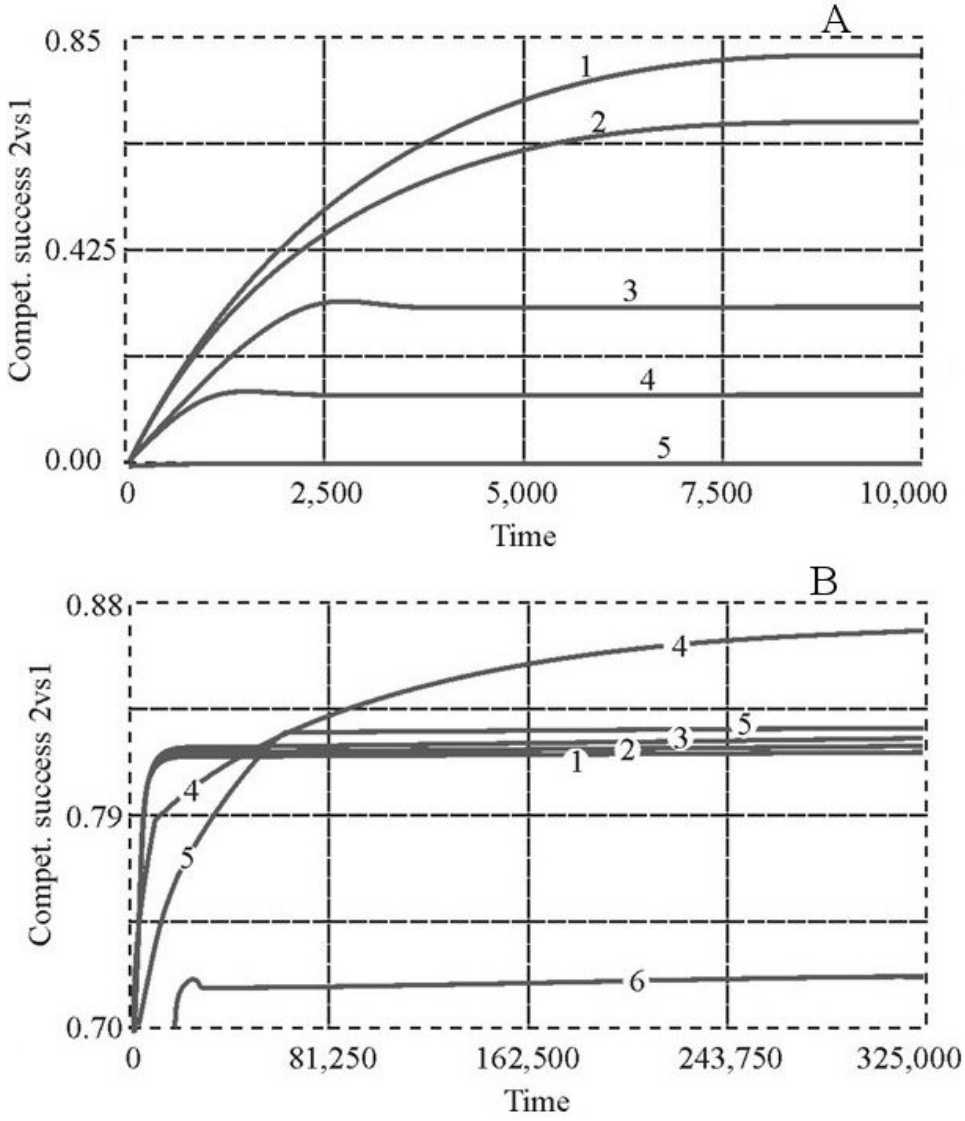

Figure 3: Graphs summarizing results of Series 2 of simulations (2a and 2b). Panel A shows the effect of energy availability on the competition between two systems: Syst.1 and Syst.2 (measured with regard to the rate of change) in the early part of the simulation (up to 10,000 steps). The proxy for the competitive success of Syst.2 is a parameter called "Compet success 2 vs 1" (see: the caption of Fig.2). "A2 to BM" = 1e-4. The "free E input" is: 0 in Plot 1; 2e-12 in Plot 2; 5e-12 in Plot 3; 9e-12 in Plot 4 and 1e-10 in Plot 5. Panel B shows results of simulations for analyzing the effect of the availability of free energy from an external homogeneous source on the competition between Syst.1 and Syst.2. When no external free energy exists, i.e. "free E input" = 0 (Graph A, Plot 1) the B2 type of information is favored (homologous to thermodynamic advantage) because "Ro A2 to BM" < "Ro A1 to BM" and "Ro B2 to A2" < "Ro B1 to A1". The addition of free energy in the range 0 < "free energy input" < 1e-13 results in increasing the abundance of Syst.2. Above 1e-13, but when "free E input" < 3e-13 (Graph A Plot 5) free energy still benefits Syst.2, relative to "free E input" = 0, albeit less than when "free E input" = 1e-13. "Ro A2 to BM" = 1e-4. The "free E input" is: 0 in Plot 1; 1e-15 in Plot 2; 1e-14 in Plot 3; 1e-13 in Plot 4; 3e-13 in Plot 5 and 6e-13 in Plot 6.

eliminate its competitor (Syst.1) more efficiently. In order for the external energy to increase the stringency of this competition, the external energy has to be within a specific range. Either too little or too much energy is unfavorable for competition-to-elimination. In most cases the energy level alone was insufficient to produce total elimination of the lesser efficient Syst.1, and free energy hastened the elimination of an information package (in this case Syst.1), that was going to be eliminated anyway. Albeit not impossible, it is more difficult however, to find a level of free energy that could lead to elimination of a system if the potential for elimination (based on differences in transformation rates) do not exist already. This effect caused by free energy did not occur when only one form of organization (either A2 or B2) was more stable than its homologous competitor (i.e. A1 or B1 respectively), (results not shown). Both A2 and B2 had to be more stable than A1 and B2 (respectively) in order for this effect (i.e. enhancement of competition-to-elimination with the help of external free energy) to be produced. In the future, it would be very interesting to study this effect in complex networks (i.e. automata with more types of internal components), in order to analyze the correlation between the pervasiveness of stability among the components of a network and its competitiveness.

We found that the free energy level available in the environment is very important for accelerating the elimination of over-competed information. With regard to the origin of life, a narrow relationship had to exist between differences in degradation rates between competing systems and the free energy available in the environment. Because free energy is in this case the independent variable, the stability of prebiotic information must have followed changes in the availability of free energy, or in the efficiency of up-taking free energy (see: Appendix, Fig. 6).

Series 3 of simulations

In this series we have analyzed the effect of B2 autocatalysis (parameter "Autocat B2" in the model) on competition between Syst.2 and Syst.1, and on the response of this competition to the availability of free energy in the environment. We still assume that free energy was homogeneously available. Except for "Autocat B2" and varying levels of free energy, input conditions were similar to those from Simulation *2d* (Fig.4, Panel B). When the free energy level was very low (e.g. 1e-13) autocatalysis did not help Syst.2 over-compete Syst.1. When the free energy level was 5e-12, and autocatalysis was little, Syst.2 was less competitive relative to the Control conditions, and Syst.1 was not eliminated. Increasing the efficiency of "Autocat B2" also increased the competitiveness of Syst.2. When the free energy was abundant (e.g. 1e-10) and "Autocat B2" was zero, no elimination of Syst.1 has occurred. Yet, under the same conditions, increasing "Autocat B2" to 0.6 level helped Syst.2 eliminate Syst.1.

Next we have asked whether a specific relationship exists between the free energy level and the autocatalysis of B2 that can help Syst.2 eliminate Syst.1 more efficiently. Fig.5, Panel B analyzes this relationship. Another question is: are some levels of free energy so extreme that changes in Autocat B2 cannot help this competition? We found this to be true for very low free energy levels and low Autocat B2 values. When the free energy level was little, small changes in "Autocat B2" had sizable effects on competition-to-elimination. When the free energy level was very large (e.g. 1e-4) Syst.1 was eliminated at "Autocat B2" > 1.25, but not at "Autocat B2" < 1. In this program any Autocat values larger than zero represent catalysis and negative value represent inhibition.

We found that relationship exists between energy availability, autocatalysis and the stringency of competition between low complexity automata. The optimum autocatalysis value for fast elimination of competition depends on the free energy level. In environments with low levels of homogeneous free energy, and where competition-to-elimination already

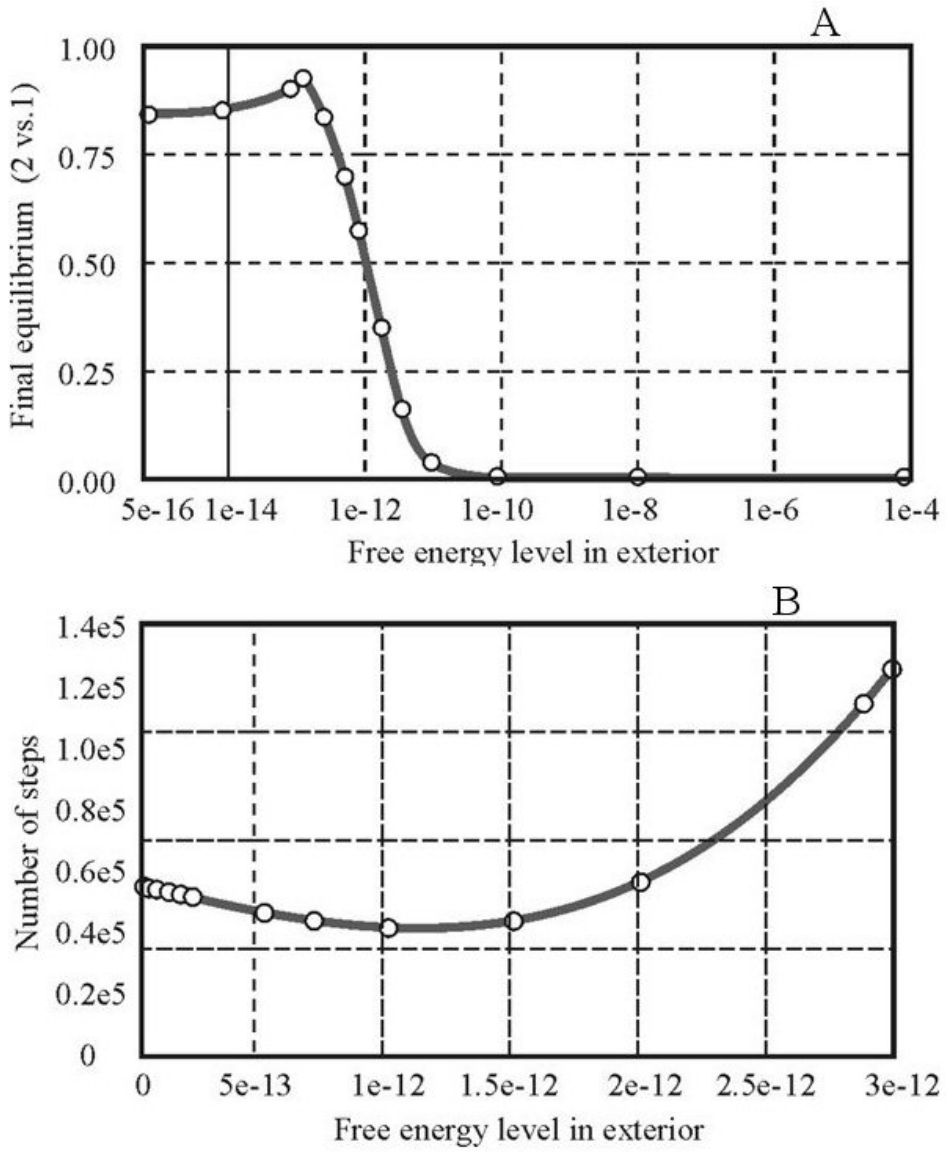

Figure 4: Graphs summarizing the results of Series 2 of simulations (2c and 2d). Panel A shows the effect of energy availability on the final equilibrium between Syst.2 and Syst.1 using the input conditions from Fig.2, Panel A, Plot 3. Panel B. Graph based on input conditions selected so that Syst.1 was totally eliminated(see Table), showing how fast Syst.1 is eliminated, as a function of the available free energy. If "free E input" = 3e-12, total elimination of Syst.1 occurs after 127,730 cycles. If "free E input" = 4e-12 Syst.1 is not eliminated. The fastest elimination of Syst.1 (i.e. 41,240 steps), occurred when the"free E input" was 1e-12 (i.e. the point of optimum free energy availability for helping Syst.2 over-compete Syst.1).

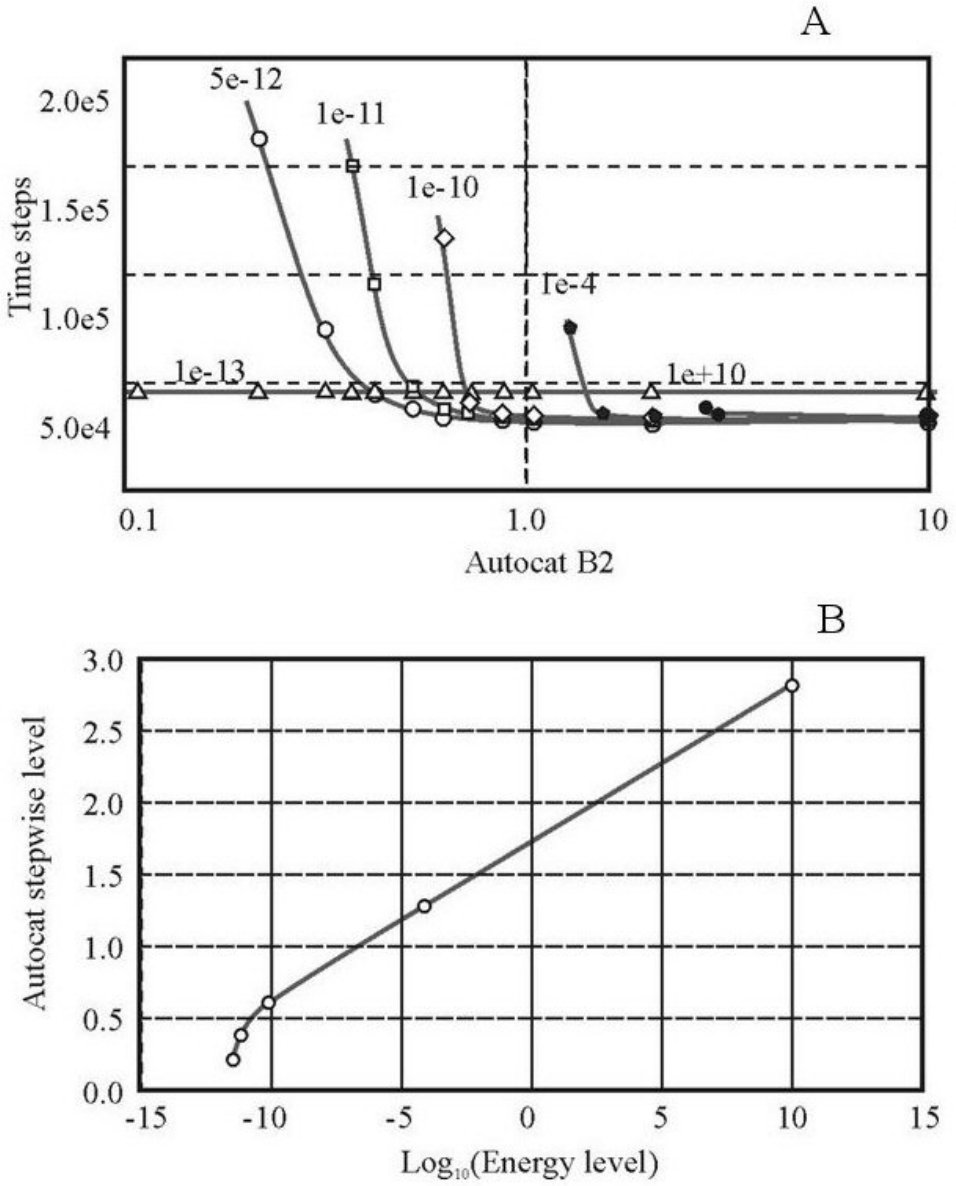

Figure 5: Graphs summarizing the results of Series 3 of simulations. Panel A. The effect of changes in autocatalysis at different levels of free energy on the competition between two systems of organization. The plots represent various energy levels and the OY axis represent the time of death (in simulation steps) of Syst.1. Panel B. Graph showing the "Autocat B2" level for various free energy levels where Syst.2 begins eliminating Syst.1. Prior to this level Syst.1 is not eliminated.

existed, autocatalysis did not help. Autocatalysis became more useful for selection-to-elimination at higher levels of free energy. When the level of free energy has increased, differences between unsuccessful and successful competition have narrowed, and small changes in autocatalysis sharpened the selective effects. We reason that after competitivity has peaked there is no advantage in further increasing the efficiency of autocatalysts, and therefore selection toward more efficient autocatalysis will lose momentum. Without autocatalysis however, competition between simple automata is highly sensitive to variation in free energy availability. Our interpretation is that free energy only helps systems compete within a narrow range of free energy availability, and that autocatalysis helps systems by making competition-to-elimination more efficient over a broader range of free energy availability. We have also found that linear correlation exists between the autocatalysis of a form of organization (i.e. B2 components in this model) and the log of the free energy level where Syst.2 could no longer eliminate its competitor. Henceforth, we propose that for a given competition situation it is possible to predict an energy level were elimination of less efficient competitors is not possible. Vice versa, the level of autocatalysis that may help a type of information (system of organization) eliminate its competitors should also be predictable. These results support that during prebiotic evolution one potential solution pushing systems toward "error catastrophe" (analogous to [3]) is synergism between energy availability and autocatalysis.

The effect of internal order on prebiotic competition of simple automata

Earlier simulations have shown that the relationship between energy availability and the efficiency of autocatalysis is an important controller of the time needed for eliminating the less efficient competitors (Fig.5, Panel A). When free energy becomes more abundant more efficient catalysts are needed to starve the competitors. This in turn, also increases the risk of an "error catastrophe". In this section we discuss how changes in internal order may influence competition-to-elimination. This subject is extensive and its full analysis will require a separate study. Here we only discuss the guiding principles of such analysis.

This problem can be simplified to the following: Increase in the level of order in a system (i.e. increase in I_{Rm}/I_{Rs} ratio) is expected to influence fitness. Increase in the specificity (and efficiency) of catalysts, improves competitiveness, but requires information. Very often, albeit not always, increase in order has the added benefit of also increasing the half-life of a form of organization (or system). On the flip side however, remnant information (i.e. the basis of order) comes with higher free energy costs, which may lower competitiveness. In systems with high compositional diversity, the number of possible forms of order increases exponentially with the number of types of components. Hence, albeit increase in catalytic specificity requires more order, increase in order does not guarantees that an increase in catalytic efficiency will also occur. In order to move toward this next step in evolution systems need sufficient time to explore numerous system stats and select the most appropriate form of order. Finding the environmental conditions that will give competing systems incentive to change, yet also give them the time they need to "experiment with", and to screen among f, numerous information variants is one of the most important subjects in the study of the origin of autocatalysis. This is important because once this step is taken (i.e. fast screening of variance and autocatalysis) the evolution of information toward life gains both momentum and direction. Albeit the model we have constructed here allows it, this subject is too extensive to be explored in this manuscript. Readers can yet use the model to study the effect of the following variables on the competitivity of Syst.2:

−Decrease the I_{Rs} of B2. This will increase the I_{Rm}, increase the Order level of Syst.2, increase the E_G of B2, and make the construction of each Syst.2 more expensive. In this

situation one can study the cost of added order on the competitiveness of a system.

−Changes in the availability of free energy. Too little free energy is expected to handicap Syst.2, which is more expensive to make, while too much energy will make some unused free energy available to Syst.1, thus diminishing the stringency of elimination of Syst.1 by Syst.2.

−The effect of changes in order on changes in stability; i.e. larger "I_{Rm} R2" values can be mathematically linked with the degradation rate of B2 ("Ro B2 to A2"). Lower degradation rate of B2 helps by making Syst.2 more stable than Syst.1. The faster turnover of Syst.1 will make this system "leak" building materials in the environment and help Syst.2 expand its habitable space.

−The effect of changes in the order of Syst.2 on changes in the autocatalytic efficiency of B2. Increase in "Autocat B2" is expected to increase the competitiveness of Syst.2, but only if sufficient building materials and free energy are available.

We posit here that the properties of the environment, in particular the availability of free energy, were a key regulator of the prebiotic evolution of self-controlled order. Interestingly, this autocatalysis conjecture links free energy with selfish information, i.e. creates a causal relationship between energy availability and prebiotic evolution toward self-rewarding order.

4 Conclusions

In this study we have analyzed the effect of energy availability, differences in thermodynamic stability and autocatalysis on competition between low complexity automata. We found that energy limitation and differences in thermodynamic stability can produce competition-to-elimination even in the absence of autocatalysis. Yet, the margin of error for this selection is narrow and different competing systems and levels of organization require different energy availability levels. When differences in competitiveness exist between systems, low energy availability speeds up the selection-to-extinction process. With regard to the origin of life, this means that selection of low complexity automata could not have occurred in energy copious environments, but have required environments that were either poor in energy (in general) or energy-limitative (relative to a specific system's needs).

Subsequently, selective evolution became more complicated due to the fact that as prebiotic networks have evolved and became more ordered and more complex their energy needs have also increased. In the absence of adaptive innovations (such as increase in the efficiency of free energy uptake), biogenic environments must have also become progressively richer in free energy in order to support competition between more complex networks. During the origin of life, the pace of evolution in complexity and the energy cost of order must have been tightly correlated with the evolution of energy availability, because insufficient free energy prohibits order and complexity and excess free energy negatively influences the odds for competition-to-elimination between automata. Without the addition of more innovative mechanisms, the pace of this increase in energy availability could not have been faster than the time needed for information variation and selection to occur. Therefore, it is assumed that the pace of increase in energy availability in the biogenic environment must have been slow, and prebiotic evolution, albeit it could have been faster, lagged behind the evolution of energy availability.

An important adaptation to increased energy availability to a system was autocatalysis, which allows automata to express competition-to-elimination at larger free energy lev-

els and over broader range of free energy availability. Selection-to-extinction is E$_S$sential for prebiotic evolution. Without it, information variants accumulate and choke the habitable space with excessively diverse information. Our results indicate that prebiotic systems are likely to have originated in an energy-limiting environment that had progressively (albeit slowly), changed toward a state of higher energy availability (albeit never copious in free energy relative to the needs of resident systems). In such environments, autocatalysis helped selection-to-extinction during episodes when energy availability has steadily increased.

We hypothesize that the most deeply rooted biogenic event, which led to the creation of the first prebiotic network, was symbiosis between an automaton capable of harvesting free energy from the environment and a selfish gene (i.e. an autocatalytic replicator preserving the specificity of the internal information). During competition between low complexity networks, selection was controlled mainly by differences in the stability of internal components, availability of free energy and autocatalysis. We speculate that the next major innovation in prebiotic evolution was the origin of dynamic systems capable of adjusting their energy dissipative potential to the availability of free energy. This adaptation produced systems capable of energy-starving their competitors, yet capable of withstanding wide range of energy availability. This also shifted evolution toward a novel paradigm where selection-to-elimination and equilibrium between competing systems (i.e. information variants) changed from being predominantly controlled by thermodynamics and kinetics to being controlled by internal information as well.

5 Appendix

The automatons used in this study have the structure and free energy exchanges shown in Fig. 6.

Principal external controllers of low complexity automata (such as those from Fig. 1 and Fig. 6) are proposed to include: energy availability, free energy homogeneity, temperature and the magnitude of the terminal heat sink. Low energy availability means that free energy from the environment is insufficient to maintain a given system state. Environments where free energy is the first resource to be exhausted are defined as "energy-limiting". In such environments dynamic systems are streamlined. Either the internal order decreases, or systems assume states of lower free energy per unit mass or require less free energy to maintain. The time averaged energy density in an environment may appear to be sufficient for maintaining a system's state, but the availability of energy may vary considerably with time, reaching sub-liminal or harmfully large levels for periods of time that are too long for the system state to survive. Systems not making sufficient reserves of energy during periods of bounty may change irreversibly during extensive periods of energy paucity. In such environments, successful survival strategy for automata includes making reserves of free energy, or rebuilding the system by using structures (forms of organization) with increased stability. Last but not least, environments with unlimited capacity to absorb heat influence the selection of dynamic systems based on their energy dissipative potential. Systems that cannot dissipate heat energy efficiently will overheat and become unstable. A cold, infinitely large and ever-expanding universe may explain ordering and stability of natural energy dissipative systems such as energy dissipative storms, the great ocean belt, convection cells, stars and many others. It is believe that this driver may have also played a role in the organization needed for the origin of life [16].

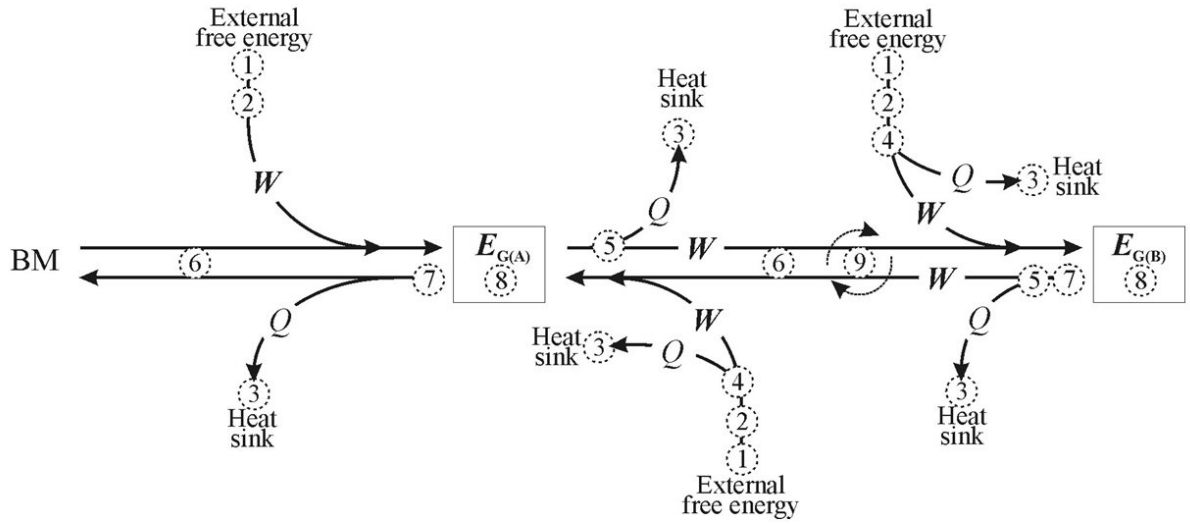

Figure 6: Energy-related controllers of the evolution of an automaton (low complexity system) containing two forms of organization (A and B). "A" is produced *de novo* from disordered building materials (BM). $E_{G(A)} < E_{G(B)}$ (where: $E_{G(A)}$ and $E_{G(B)}$ are the free energy content of A and B respectively). The energy content and energy exchanges associated with the entropy of the system (E_S) can also be included in a model, but are not shown in this figure. W = free energy exchanged with the environment and between A and B. Q = heat released during the exchange of free energy. The potential energy-related controllers of the system's evolution are marked with circles: (1) Available free energy; (2) Unevenness in free energy availability; (3) Heat sink magnitude; (4) The efficiency of up-taking free energy from the exterior; (5) The efficiency of exchanging free energy between A and B; (6) Thermodynamic equilibrium transformations; (7) The stability of order; (8) The free energy content of order; and (9) The rate of A⇔B transformations.

With regard to internal controllers of automata, the uptake of free energy from external sources into internal forms of organization (i.e. Fig. 6(4)) is in most situations less than 100% efficient. During this uptake, energy is released in a degraded form such as heat or thermal radiation. Energy uptake efficiency may vary considerably between various systems and influence competition between systems. Differences in information content also exist between forms of organization involved in various transformations within a system. These differences lead to free energy being exchanged also with less than 100% efficiency (e.g. "5" in Fig. 6). This topic is seldom analyzed in thermodynamic models of chemical transformations, because in most chemical analyses the free energy exchanged when one form of organization becomes another is either assumed to be 100% efficient, or the missing order comes from a combination of encounter probabilities, kinetic energy and the intrinsic order of fundamental forces. Should no order come from such sources, a transformation involving two forms of organization (A$\Leftrightarrow$B where $E_{G(A)} < E_{G(B)}$) that is 100 % efficient with regard to free energy exchanges means that:

- During A$\Rightarrow$B transformations, all free energy released from $E_{G(A)}$ is used into $E_{G(B)}$; and

- During B$\Rightarrow$A transformations, all free energy needed by $E_{G(A)}$ comes from $E_{G(B)}$.

Other internal controllers of prebiotic evolution of automata are the thermodynamic equilibrium of various transformations, the stability of order and the energy cost of order. Competition between dissimilar systems is influenced by changes in transformation rates (i.e. in Fig. 6(6)), which is a combination of factors such as thermodynamic stability, catalysis and inhibition.

This model is organized in sectors.

Sector: *Initial conditions*, contains user imputed values for: universal constants; temperature; the system's volume; the initial amount of various units (i.e. forms of organization); the stoichiometry between BM, A and B; the mass per unit of organization; the standard rates for the various transformations; the effect of temperature on these rates; the number of degrees of freedom for various forms of organization (Ω); the Landauer bound (k_L) chosen by the user for the specific for the type of system analyzed (i.e. in chemical systems $k_L \simeq 9.572{\cdot}10\text{-}24$ J bit^{-1} K^{-1}); the E_G per unit of organization; an energy availability factor describing how much free energy can enter from the environment; the efficiency of up-taking free energy into E_G; the auto-catalytic and self-inhibitory potential of various forms of organization (Ref); the energy dissipative potential associated with various forms of transformation; and the heat conductivity of the environment (a proxy for the magnitude of the terminal heat sink).

Sector: *Theoretical Transformation Rates*, gives forward and reverse rates for all unisense transformations from the model, in energy unlimited conditions.

Sector: *Energy Hunger Level and Energy Inputs*, calculates a parameter called "Hung" (abbreviation for hunger), which establishes the partition of input energy between competing systems.

Sector: *Main Model Evolution of Units of Transformation*, describes the evolution of units of transformation and flow of materials based on the input conditions and calculations from other sectors.

Sector: *Free Energy Flow Model*, is optional for this study, but useful in addressing other prebiotic evolution questions; it describes the flow of energy through the various E_G reservoirs.

Sector: *Model Variables and Monitored Parameters*, describes the main variables manipulated in this study and the model parameters indicative of changes in order, competition, growth and fitness.

In the model constructed for this study, the space that can be occupied by ordered structures has a finite number of building materials BM with $E_G = 0$. Only four types of structures (forms of organization) exist in the system (A1, A2, B1 and B2). The composition, the E_G value and the E_S value are similar between A1 and A2 and between B1 and B2. The only types of transformations allowed, and the stoichiometry of transformations chosen for this study, are the following: 2BM⇔2A1⇔ 1B1 and 2BM⇔2A2⇔1B2. E_G increases, while E_S decreases, in the BM⇒A⇒B direction. The outcome of competition between the two systems of organization (Syst. 1 = A1B1 and Syst.2 = A2B2) is measured through changes in their abundance relative to the total amount of construction materials (BM + A1 + 2B1 + A2 + 2B2). The order level depends on the abundance of B relative to A.

The competition success of the two systems of organization is measured as:

Competition success of Syst.1 vs. Syst.2 = ((A1+B1)-(A2+B2))/((A1+B1)+(A2+B2))

Competition success of Syst.2 vs. Syst.1 = ((A2+B2)-(A1+B1))/((A1+B1)+(A2+B2))

where: A1+B1 = Syst.1 and A2+B2 = Syst.2 are systems of organization; and A1, A2, B1 and B2 are units of organization.

The Order level is defined as:

Ord = (B-A)/(B_{eq}-A_{eq}) where: A and B represent the number of units of transformation; and A_{eq} and B_{eq} represent the number of units of transformation at equilibrium.

The following notations for model' variables have been used:

· energy availability ("E factor");

· variation in energy availability ("Period");

· heat sink magnitude ("Heat conductiv");

· the efficiency of up-taking free energy from the exterior ("Effc free E uptake");

· the efficiency of free energy exchange between forms of organization ("Effc free E uptake"); and

· the effect of catalysts and inhibitors on the kinetics of transformation between the forms of organization ("Cat").

Acknowledgements

We acknowledge support from University of southern California, Dr. Kenneth Nealson, Razvan Balasa and Mihai Moldovan.

References

[1] Popa R (2004), Between Necessity and Probability: Searching for the Definition and Origin of Life, Springer-Verlag Heidelberg, Germany

[2] Popa R, Cimpoiasu VM (2012), Energy-driven evolution of prebiotic chiral order (Lessons from dynamic systems modeling), In: J. Seckbach J (ed) Genesis "In the Beginning, Precursors of life, Chemical models and Early biological evolution", Springer, Heidelberg, Germany, pp 525-545

[3] Eigen M, Gardiner W, Shuster P, Winkler-Oswatisch R, (1981), Sci Am 244:88-118

[4] Prigogine I (1967) Introduction to Thermodynamics of Irreversible Processes, Interscience Publishers, New York

[5] Prigogine I, Stengers I. (1984) Order out of chaos : Man's New Dialogue with Nature. Heinemann, London

[6] Branscomb E, Russell MJ (2012), Biochim Biophys Acta 1827(2):62-78

[7] Shannon CE (1948), Bell Syst Tech J 27:379-424; 623-659

[8] Kerson H (1990) Statistical Mechanics, Wiley, John Sons, New York

[9] Arieh BN (2008) Statistical Thermodynamics Based on Information A Farewell to Entropy. World Scientific Publishing Co., Singapore

[10] Ken D, Sarina B (2002) Molecular Driving Forces : Statistical Thermodynamics in Chemistry Biology, Garland Science, New York

[11] Ganti T (1997), J Theor Biol 187:583-593

[12] Kauffman SA (1993) The origins of order. Oxford University Press, New York

[13] Bro P (1997), Complexity 2(3)38-44

[14] Deamer DW (1997), Microbiol Molec Biol Rev, 61:239-261

[15] Hazen RM (2001) Emergence and the origin of life, In: PÃ¡lyi G (ed) Fundamentals of life, Elsevier, New York, pp 41-50

[16] Chaisson E (2003), Intern J Astrobiol 2(2):91-101

[17] Pulselli RM, Simoncini E, Tiezzi E (2009), Biosystems 96(3):237-241

[18] Bywater RP (2012), Naturwissenschaften 99:167-176

[19] Rosen R (1973), Bull Math Biophys 35:1-9

[20] Ray TS (1991) Evolution and optimization of digital organisms, In: Billingsley KR, Derohanes E, Brown H Scientific Excellence in Supercomputing: The IBM 1990 Contest Prize Papers, 30602, The Baldwin Press, The University of Georgia, pp 489-531

[21] Fontana W, Buss LW (1994), Proc Natl Acad Sci USA 91:757-761

[22] Pargellis AN (1996), Physica D 98(1):111-127

[23] McMullin B (1997) SCL: an artificial chemistry in swarm, Working Paper 97-01-002, Santa Fe Institute, Santa Fe, NM 87501, http://www.santafe.edu/sfi/publications/Working-Papers/97-01-002

[24] Adami C (1998) Introduction to artificial life. Springer- Verlag, New York

[25] Moran F, Moreno A, Minch E, Montero F (1999) Further steps toward a realistic description of the E$_S$sence of life, In: Langton CG, Shimonara K (eds) Artificial Life, V. MIT Press, London, pp 255-263

[26] Bedau MA, McCaskill JS, Packard N, Rasmussen S, Adami C, Green DG, Ikegami T, Kaneko K, Ray TS (2000), Artificial Life 6(4):363-376

[27] Wilensky U, Rand W (2006) NetLogo 3.1: Low threshold, no ceiling, South Bend, IN

[28] Cimpoiasu VM, Popa R (2012), Astrobiology 12(12):1123-1134

[29] Popa R, Cimpoiasu VM (2013), Astrobiology 13(5):454-64. doi: 10.1089/ast.2012.0933

[30] Bennett CH (1982), International Journal of Theoretical Physics 21:905-940

[31] Bennett CH (2003), Studies in History and Philosophy of Modern Physics 34:501-510.

[32] Bndenrgy, 2013, http://www.cem.msu.edu/ reusch/OrgPage/bndenrgy.htm Accessed 28 April 2013

[33] Jarzynski C (1997a),Phys Rev E 56:5018-5035

[34] Jarzynski C (1997b), Phys Rev E 56:2254-2256

[35] Jarzynski C (1997c), Phys Rev Lett 78:2690-2693

[36] Landauer R (1961), IBM Journal of Research and Development 5:183-191

[37] Norton JD (2005), Stud Hist Phil Sci B 36:375-411. doi: 10.1016/j.shpsb.2004.12.002

[38] Yockey HP (2002) Information theory, evolution and the origin of life, In: PÃ¡lyi G, Zucchi C, Caglioti L (eds.) Fundamentals of life, Elsevier, New York, pp335-348