On the Evolution of Chemical Organizations

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Abstract

Chemical evolution describes the first step in the development of life, such as the formation of complex organic molecules from simpler (in-)organic compounds. A deeper understanding of this period requires not only a refinement of our chemical knowledge but also improved theoretical concepts that help to explain how complex chemical systems evolve in principle. Here we investigate how chemical evolution appears in the light of chemical organization theory. We identify two main dimensions of chemical evolution: the "actual evolution" of the reaction vessel and the "organizational evolution" of the set of molecular species reachable from the actual set of chemical species present in the vessel. The organizational evolution can be described precisely as a movement through the set of chemical organizations. We describe three types of such movements: upwards, downwards, and sidewards. The concepts are illustrated by simulation studies on a constructive artificial chemistry.

1 Introduction

Chemical evolution (*i.e.*, prebiotic evolution) is concerned with the period of life's history that precedes the arrival of the first living organism [17]. Since Miller's pioneering work [19, 20], prebiotic chemistry has been studied in various laboratory experiments [16]. On the other hand, there are theoretical attempts to study chemical evolution. These theoretical approaches can be classified roughly into replicator centered and network centered approaches. The first approach assumes replicating molecules as the central unit of chemical evolution. Models like the Quasispecies [7] or *in-silico* RNA evolution [10] have characterized the capacity of chemical systems to store, transmit, and gain information.

The other line of research investigates how autocatalytic networks [7, 14, 21] emerge and evolve. An autocatalytic set can be defined as a set of molecules where each molecule is catalytically produced by at least one molecule from that set [12]. Therefore replication¹ like in the Hypercycle model [8] are not required for an autocatalytic set to maintain itself. It has been shown in silico that autocatalytic networks emerge under various conditions [9] and can possess complex dynamical properties [13].

¹For example, a reaction $A + B + S \rightarrow 2A + B$ where A is replicated under the catalytic activity of B and by using up a substrate S.



Figure 1: Schematic description of the static and dynamics analysis of a reaction system using chemical organization theory. Left: Based on the static network structure, the reaction network is decomposed into overlapping sub-networks called organizations. The hierarchical organizational structure of the network is visualized by a Hasse diagram. Middle: To analyze the system's dynamics, a movement from state \mathbf{x}_g to a state \mathbf{x}_{g+1} in state space is mapped to a movement from organization O_g to organization O_{g+1} . The actual evolution of the state \mathbf{x} from g to g + 1 does not necessarily lead to a change of the organizations, that is why we distinguish the actual evolution of the set of molecules actually present in the reactor from the organizational evolution of the organizations reachable from that molecules. **Right:** The organizational evolution is categorized into three movements: upward, downward, and sideward. See text for detail.

In order to study such complex dynamics new methods are required that can deal with constructive systems [11], *i.e.* systems where new components (molecular species) appear, which may change the present network topology. In this paper we study how chemical organization theory [22, 4] can help to explain the dynamics of constructive evolving chemical systems.

2 Chemical Organization Theory

The central concept of the theory is the definition of a chemical organization as a set of molecular species that is closed and self-maintaining [4, 11, 22]. In order to find the organizations of a reaction systems, the theory requires only the reaction network, which can be represented as an algebraic chemistry [5] without any dynamics. An algebraic chemistry is a 2-tuple $\langle \mathcal{M}, \mathcal{R} \rangle$ where \mathcal{M} is a set of molecular species and \mathcal{R} is a set of reaction rules among the species. A reaction rule describes a transformation of molecular species and can be represented as a pair of multisets of molecules, the left hand side and right hand side, respectively. Requiring only the algebraic structure, the reaction network is searched for the organizations. The first property closure — ensures that there exists no reaction that produces new species not yet present in the organization using only species of that organization. The second property — self-maintenance — is a theoretical capability of an organization to maintain all of its members, (possibly) involving complex reaction pathways. Since the maintenance (possibly) involves complex reaction pathways, the stoichiometry of the whole reaction network must be considered, in general. Here, however, we investigate a specific class of reaction systems where all molecules are catalysts and where there is a general dilution flow. In this specific case, a set of molecules is self-maintaining if and only if every molecule within the set is produced by at least one reaction among molecules of that set.

By locating the organizations from all combinations of molecular species, the given reaction network is decomposed into overlapping sub-networks of organizations. As shown in Figure 1 (leftmost), we visualize the set of all organizations by a Hasse diagram, in which organizations are arranged vertically according to their size in terms of the number of their members. Two organizations are connected by a line if the upper organization contains all species of the lower organization and there is no other organization between them. The Hasse diagram represents the hierarchical organizational structure of the reaction network under study.

2.1 Dynamical Analysis

Chemical organizations are proposed to be an appropriate abstraction level to describe complex dynamical behaviors of reaction systems [22]. Central to this dynamical analysis is a function that maps a state $\mathbf{x} \in X$ of the reaction vessel to an organization generated by that state. Since the state space X is usually much larger than the set of all possible organizations (a subset of the power set of \mathcal{M}), this mapping provides a significant reduction of dimensionality. Given a state \mathbf{x} (e.g., a concentration vector) we generate the organization in three steps:

First, the quantitative state \mathbf{x} is mapped to a qualitative state $S = \phi(\mathbf{x})$, namely the set $S \subseteq \mathcal{M}$ of species present in \mathbf{x} . The function $\phi: X \mapsto \mathcal{P}(\mathcal{M})$ is called *abstraction*. Second, given the set of molecular species $S \subseteq \mathcal{M}$, we generate its closure $C = G_{CL}(S)$ by the algorithm shown in Tab. 1 (left). The closure of S is the smallest closed set containing S. Third, we generate the organization $O = G_{SM}(C)$ by finding the biggest self-maintaining set² ($O = G_{SM}(C)$) contained in the closure C (Tab. 1 (right)). All together the organization generated by a state \mathbf{x} is defined as:

$$O = G_{SM}(G_{CL}(\phi(\mathbf{x}))) = G_{Org}(\phi(\mathbf{x})).$$
(1)

Given an algebraic chemistry $\langle \mathcal{M}, \mathcal{R} \rangle$ and dynamics of the reaction system as a movement in the state space X, the dynamical movement can be followed in the set of organizations L using Eq. (1) [4]. We call this movement organizational evolution in order to distinguish from the actual evolution of the state **x** of the reaction vessel (Figure 1). The dynamical movement on the organizational level can be categorized into three directions: upwards, downwards, and sidewards. Regarding two states $\mathbf{x}_{t_1}, \mathbf{x}_{t_2} \in X$ at time points t_1 and t_2 , the organizations $O_{t_1}, O_{t_2} \in L$ can be generated: $O_{t_1} = G_{Org}(\phi(\mathbf{x}_{t_1})), O_{t_2} = G_{Org}(\phi(\mathbf{x}_{t_2}))$. In case $O_{t_1} \supset O_{t_2}$, the movement in the state space is classified as a downward movement. The other way of inclusion, namely $O_{t_1} \subset O_{t_2}$, is an upward movement. The dynamical change $(O_{t_1} \neq O_{t_2})$ that is neither downwards nor upwards is called a sideward movement. We exclude the equality $O_{t_1} = O_{t_2}$, since no movement is detected on the level of organizations.

3 Organizations and Evolution

When we investigate the dynamical behavior of the reaction system on the level of the chemical organization, the dynamical behavior is categorized into there directional movements. Downward movement is ascribed mostly by the disappearance of a molecular species from the reaction vessel, consumed by internal reactions or decay. Upward movement, on the other hand, is brought by external perturbation such as mutation or insertion of new molecules. New molecular species are necessary to be produced for the system to move upwards. Furthermore, the new species must be impossible to be produced by chemical reactions among the species present in the reaction vessel because the closure generation function G_{CL} includes those species in the original organization.

Upward and downward movements are generally sufficient to describe the dynamical behavior. The other movement, sideward movement, occurs usually in a combination of the two movements. The system is excited by some external perturbation and triggers an upward movement. Then some species would disappear and cause a downward movement. If the series of movements results in an organization in which some of the original species are missing and some of the members are new, the movement is categorized as sidewards.

 $^{^{2}}$ The generated self-maintaining set is not always unique for a set of molecular species in arbitrary reaction systems, but is determined uniquely in the autocatalytic reaction system considered in this paper.

| Table 1: Listing of functions to generate closed (left) or self-maintaining | (right) se | set |
|-----------------------------------------------------------------------------|------------|-----|
|-----------------------------------------------------------------------------|------------|-----|

Function: Generate closure G_{CL} **Function:** Generate self-maintaining set G_{SM} **Input**: Set of species (S)**Input**: Set of species (S)**Output**: Closed set of species (CL)**Output**: Self-maintaining set of species (SM) $CL \leftarrow S$ $SM \leftarrow S$ $A \leftarrow \emptyset$ $B \leftarrow SM$ while $SM \neq B$ do while $A \neq \emptyset$ do $A \leftarrow \emptyset$ $B \leftarrow \emptyset$ foreach $(s_i, s_j) : s_i, s_j \in CL$ do foreach $(s_i, s_j) : s_i, s_j \in SM$ do $p \leftarrow s_i + s_j$ $p \leftarrow s_i + \check{s_j}$ if $p \notin CL$ then $A \leftarrow A \cup \{p\}$ $B \leftarrow B \cup \{p\}$ end end $CL \leftarrow CL \cup A$ $SM \leftarrow SM \cap B$ end end

The upward and sideward movement are particularly significant in the field of evolution. When considering all sub-organizations in the reaction network, upward movement and sideward movement effect the new sub-organizations in the reaction network. Each (sub-)organization can be interpreted as a dynamical function of the reaction network [3], so the new sub-organization could be a new niche of the reaction system. By seeing the evolution of reaction network as the movement in the space of organizations, it could be practicable to analyze the functional evolution of the reaction system. The sideward movement is especially noteworthy since it captures the evolution without increasing the network size.

4 Experimental Setup

In this section, we demonstrate how the chemical organization theory gives an insight to chemical evolution. An artificial chemistry system called automata chemistry [6] is used to generate chemical evolution. Molecular species are binary strings $s \in \{0,1\}^{32}$ with a constant length of 32 bit. Two strings can catalyze the production of a third string: $s_1 + s_2 \Rightarrow s_3$. One of the strings s_1 is mapped to an automaton A_{s_1} according to a well defined instruction table (we used code table II in [6] allowing self-replication). The other s_2 serves as input to A_{s_1} . The result of the program execution on the input string is the product $s_3 = A_{s_1}(s_2)$. Preparing a reactor (or reaction vessel) containing N string objects, multiple copies of the species are placed in the reactor to simulate the dynamical behavior of the reaction system. In each time step, two string objects are randomly chosen to react, and the reactants are inserted back into the reactor without deleting the two reactands. One randomly chosen molecule in the reactor is replaced by the product in order to keep the total number of the objects in the reactor constant. In short, the system is a catalytic flow system in a well stirred reactor. In one generation, N steps are executed.

4.1 Analysis Method

Theoretically speaking, the automata chemistry consists of $2^{32} = |\mathcal{M}|$ binary strings as molecular species and reactions among them, forming the algebraic chemistry $\langle \mathcal{M}, \mathcal{R} \rangle$. Since it is impractical to consider the entire network, however, only the small part related to the reactor state $\mathbf{x}_g \in X$ at generation time g is considered as $\langle \mathcal{M}_g, \mathcal{R}_g \rangle$ where $\mathcal{M}_g = G_{CL}(\phi(\mathbf{x}_g))$ is the set of molecules that can be generated from \mathbf{x}_q .

Representing the reactor state as a multiset: $\mathbf{x}_g = \{m_1, m_2, \dots, m_N\}$ where N is the size of

the reactor, the abstraction of the reactor state is the set S_g of molecular species present in the reactor and calculated by ignoring the multiplicity: $S_g = \phi(\mathbf{x}_g) = \{s \in \mathbf{x}_g | \#(s \in \mathbf{x}_g) > 0\}$ where $\#(s \in \mathbf{x}_g)$ denotes the number of occurrences of element s in multiset \mathbf{x}_g . Taking the closure of the set of species: $C_g = G_{CL}(S_g)$ [23] listed as the pseudo code in Table 1 (left), the algebraic chemistry is constructed by setting $\mathcal{M}_g = C_g$. The set of reaction rules $\mathcal{R}_g = (\mathcal{C}_g \cup \mathcal{D}_g)$ is composed of two kinds of reactions: catalytic reactions \mathcal{C}_g and decay reactions \mathcal{D}_g . Decay reactions $\mathcal{D}_g = \{(m \to \emptyset) | m \in \mathcal{M}_g\}$ are included since every object is subject to be replaced by a reaction product. In passing we note that it is not possible in the dynamical simulation of the reaction vessel to be empty even though every object species is defined to decay in the algebraic chemistry. Since two objects initiating a reaction are not altered by the reaction, the process is defined as a catalytic reaction $\mathcal{C}_g = \{(m_i + m_j \to m_i + m_j + m_k) | m_i, m_j \in \mathcal{M}_g, m_i + m_j \Rightarrow m_k$ according to the automata chemistry $\}$. Note that $m_k \in \mathcal{M}_g$ because of the closure property of the algebraic chemistry. As a result, there are $|\mathcal{R}_g| = |\mathcal{C}_g| + |\mathcal{D}_g| = |\mathcal{M}_g|^2 + |\mathcal{M}_g|$ reaction rules in the algebraic chemistry because the automata chemistry is designed to halt always by excluding the control statements.

Considering the characteristics of the reaction network, the function G_{SM} to generate the selfmaintaining set can be defined as listed in Table 1 (right). The reaction network is designed so that every molecule decays but the reactants of all catalytic reactions are conserved. Therefore, the set is self-maintaining if all of the elements are produced by the catalytic reactions. In order to generate the biggest self-maintaining set contained in the original, species not produced by the reactions are excluded from the set until every molecule is produced.

Given the algebraic chemistry $\langle \mathcal{M}_g, \mathcal{R}_g \rangle$, we compute all organizations to extract the hierarchical organizational structure in the reaction network. The set of all organizations is denoted as L_g . It forms together with the union \sqcup and intersection \sqcap of organizations an algebraic structure $\langle L_g, \sqcup, \sqcap \rangle$ called a lattice³. The biggest organization $O_g \in L_g$ is generated from the whole set of the species present in the reaction vessel: $O_g = G_{Org}(S_g)$. The other sub-organizations are generated from any subset of the set: $O'_q = G_{Org}(S'_q \subset S_g)$

5 Results

In order to study down movements, we simulate our artificial chemistry without any external perturbations like mutation (Sec. 5.1). Then, in Sec. 5.2, we will demonstrate upward and side movements by introducing moderate mutations, which cause constructive perturbations.

5.1 Dynamical behavior as downward movement

The reactor of size N = 1000 is heterogeneously initialized with N random objects. Figure 2 shows the typical dynamical behavior of the simulated chemical evolution in three forms. The concentration change of some species (with relatively high quantity) is plotted to view the dynamical change of the reactor state. As in the middle graph, the number of molecular species present in the reactor is plotted as diversity. A tendency to decrease diversity may describe this evolutionary behavior. This dynamical behavior is analyzed with the theory of chemical organization, and the results are given as a series of Hasse diagrams, visualizing the lattice of organizations L_{200} , L_{400} , L_{500} , and L_{700} (Figure 2, bottom). The labels in the box indicate species that are new in the corresponding organization and are not contained in any of the organizations below it. Since the organizational structure depends on the qualitative state of the reaction vessel the result is not affected as long as the diversity stays the same.

³Since the algebraic chemistry is designed as a reactive flow system, the set of all organizations in such a system is proved [4] to form a lattice.



Figure 2: Dynamical behavior of automata chemistry showing several downward movements. The reactor of size N = 1000 is filled initially with one copy each of N species of random binary string with fixed length 32 bits. Top: concentration profile of the reactor with respect to some prominent species. Middle: diversity as the number of different species present in the reactor. Bottom: lattice of organizations at generation 200, 400, 500, and 700. Dotted boxes and lines are the organizations and links missing compared with the previous lattice structure.

At g = 200, there are eight species in the reactor, and those species form the biggest organizations: $O_{200} = G_{Org}(S_{200}) = S_{200}$. Forty-six organizations are found as shown in the leftmost Hasse diagram. In the next 200 generations, four species are drained so that the diversity value of the reactor becomes four. The lattice of organizations L_{400} consists of ten organizations including the biggest organizations formed by the remaining four species. Comparing two sets of the organizations L_{200} and L_{400} , we found that $L_{200} \subset L_{400}$ so that it is possible to impose the lattice L_{400} on L_{200} as shown in the figure. The solid lines represent the lattice at g = 400, and the organizations vanished during the 200 generations are drawn by the dotted lines

This dynamical change of the reactor state can be explained as a downward movement. The sets of species present in the reactor at generation g = 200 and 400 are the organizations: $O_{200} = G_{Org}(S_{200}) = S_{200}$ and $O_{400} = G_{Org}(S_{400}) = S_{400}$. The inclusion $O_{400} \subset O_{200}$ is true since species present in the reactor only disappear and no new species appears within that 200 generations. Similarly, this argument is applicable between S_{400} and S_{500} and between S_{500} and S_{700} . In this simulation settings, only the reactions can produce possibly new species, but applying the chemical reactions to the set of existing species cannot disrupt the closure property of the organization. Only the downward movement is thus feasible.

5.2 Upward and sideward movement

To demonstrate upward and sideward movement, a mutation process is introduced. Every 100 generation, ten objects are chosen randomly, and each binary string object is mutated by inverting one randomly chosen bit. The reactor is initialized homogeneously with N = 1000 copies of a certain species, so the diversity value is 1 in the beginning. Figure 3 (top) shows the



Figure 3: Dynamical behavior of automata chemistry exhibiting upward and sideward movement. The reactor of size N = 1000 is initialized heterogeneously. Every 100 generations, 10 string objects are chosen to be mutated by an one-bit negation. Top: dynamical change of concentration profile of the reactor with respect to prominent species. Second top: the number of unique species in the reactor as diversity and the size of the biggest organization generated, calculated every 10 generations. Third top: the number of the organizations in the reaction network. Bottom: Hasse diagrams depicting organizational structure in the reaction network. Starting from g = 360, two upward movements are achieved until g = 610 although the lattice immediately shrinks (downward movement). From 800 to 900, a sideward movement is observed.

dynamical behavior of the concentration profile with respect to the prominent species, and the number of the species existing in the reactor is plotted as diversity. The rapid increase of the diversity every 100 generation is caused by the ten new mutants. The organizational structure in the reaction network is computed every 10 generation. At the moment of the mutation event, the network is analyzed just before the mutation, and the effect of the mutation is observed only after ten generations. At the bottom, the dynamical change of the lattice structure from g = 360 is depicted. The organizations and links are drawn by bold lines if inherited from the previous structure, and the dotted lines are used if vanished.

Starting with two organizations (empty set and set of two species), the mutation at g = 400 introduces new species to the reaction system and the reaction network is expanded. After ten generations, the reaction system settles to the state with four species. The reaction network with the four species is composed of six organizations, and the biggest organization is the set of those four species. This lattice structure is sustained in the next 200 generations including one mutation at g = 500. Temporarily, the next mutation at g = 600 brings up the system to the organization of ten species and thirty-four organizations in the reaction network as observed at g = 610. After 20 generations, all of the new organizations are vanished, and the lattice structure comes back to that prior to the mutation at g = 600.

These are typical upward and downward movements. The mutation process produces new species outside of the closure and causes upward movement. The dilution flow removes species from the reaction vessel randomly, and the system goes to the organization below. Since the concentration of the new species is very low, the new organizations brought about by the upward movement has a disadvantage statistically. Thus, the upward movement is canceled mostly.

The sideward movement is observed between O_{800} and O_{900} . The mutation process at g = 800 introduces new species to the reactor system and pushes the system into the bigger organization consisting of sixteen species. Ninety-eight organizations are found in the reaction network. Each of the sixteen species is maintained for a relatively long period (90 generations), but four of the species are eventually depleted. In consequence, lattice structure L_{900} has 32 organizations. As illustrated in Figure 3 bottom, four organizations associated with species e and f are missing in L_{900} in comparison with L_{800} .

5.3 Diversity and Organization

In the previous examples, the generated organization from the reactor state is mostly the same as the abstraction (i.e., $G_{Org}(\phi(\mathbf{x})) = \phi(\mathbf{x})$). In other words, the set of species present in the reactor is an organization. In that case the diversity (number of different species present) seems an adequate representation of the evolutionary behavior. However, the benefit to apply the generate function becomes evident in Figure 4, where we can see that a decrease in diversity does not necessarily imply a decrease of the generated organization.

For this simulation the reactor of size N = 1000 is initialized with sixteen species, which form a reaction network holding 146 organizations as shown in Figure 5 (left). Mutation is disabled so that the only downward movement can occur. The reactor is in the biggest organization at the top of the lattice structure, and there are four organizations directly below as shown in Figure 5 (right). The organizational structure is sustained for a long time ≈ 800 generations until a series of species destruction causes the reaction system to move downwards. Around generation 200, the diversity is reduced due to the disappearance of the species from the reactor, and the reduction is dynamically compensated by regenerating the disappeared species. When the set of species present in the reactor is not the organization anymore, violating the closure property in this case, the dynamical reaction system tends to move the state so as to satisfy the two



Figure 4: Dynamical behavior of automata chemistry exhibiting long-term preservation of an organization and then downward movement. The reactor of size N = 1000 is initialized with sixteen species, and the organizational structure in the reaction network among those species consists of 146 organizations as shown in Figure 5 (left). Top: concentration profile of the reactor with respect to the prominent species and diversity as the number of unique species present in the reactor. Bottom left: zoomed into [150:250] to show in detail the dynamical behavior compensating qualitative disturbance. Bottom right: zoomed into [780:850] where stochastic effects eventually caused downward movement.

properties of the organization since the organization is a candidate of the steady state and the other species combinations are not stable [4].

The organization generated from the reduced set of species is, however, unchanged during that period. Applying the generate function takes the structure of the reaction network into consideration. By representing the dynamical behavior on the level of the organization, the dynamical change of the underlying reaction network is focused. Furthermore, temporal stochastic effects can be separated from the permanent effects, causing downward movements.

6 Discussion and Conclusion

In this paper, we have demonstrated that chemical organization theory can provide another level of explanation to understand chemical evolution. With the help of the theory, we can consider two levels of chemical evolution: (1) the actual evolution of the reaction vessel, that is, the arrival and disappearance of chemical species; and (2) the "organizational evolution", that is, the change of the organization generated by the current set of molecules present in the vessel (Figure 1, middle). Our results suggest that actual evolution of the reaction vessel does not trivially imply its organizational evolution and vice versa.



Figure 5: Organizational structure in the reaction network of the sixteen species with which the reactor for Figure 4 is initialized. Left: the whole lattice structure containing 146 organizations. **Right:** four organizations directly below the biggest organization (labeled as 145). For each link to below, the missing species are listed. Since twelve species constitute the organization labeled as 144, for instance, the link to that organization is associated with four species. The downward movement demonstrated in Figure 4 is from organization 145 to 140.

We have characterized, as usual in evolution theory, the actual evolution of the reactor by the change of its diversity, which reflects the arrival and disappearance of chemical species. The evolution on the organizational level was characterized as downward, upward, or sideward movement in the organization space. As suggested by our experimental results (Figures 2-4), downward movement correlates with decreasing diversity whereas an upward movement correlates with increasing diversity. However, in general, the relation between the actual level (actual state of the system) and the organizational level (organization the system is in) is not that simple. In fact, we have shown that there can be a decrease or increase in diversity without any change on the organizational level (*i.e.*, the organization generated does not change). Even a process that appears like a creative evolutionary process on the actual level can in fact be just a downward movement on the organizational level (see e.g. Figures 6 and 7 in Ref. [6]). In other words, an increase in diversity or the appearance of new molecular species (on the actual level) does not necessarily imply an upward or sideward movement but can go hand-in-hand with a downward movement (on the organizational level). Finally, it is even possible that an upward movement is accompanied by a decrease of diversity, e.g., in case some new molecular species take a large portion of the reaction vessel, although we have not experimentally demonstrated this case, yet.

An important aspect left for future research is to characterize the intrinsic stability of organizations. As we observed, not all organizations show the same level of stability: some organizations are sustained over very long periods while others are inherently unstable, or unstable under the smallest external noise. What exactly makes an organization stable or unstable is at the moment only a speculation, yet the topology of the reaction network [24, 15] and the existence of an attractor inside the organization could be important aspects to take into account.

When investigating evolutionary processes, the issue of complexity is inevitable and controversial. Previous studies suggest that evolution shows unlimited growth of complexity [1]. According to a recent analysis [18], the research about machines that grow in complexity can be traced back to works by John von Neumann or even further to western philosophical and theological thinking. Fontana and Buss [11] presented an artificial chemistry in which systems' complexity would increase by combining multiple non-complex systems. Another example, a natural one, are biochemical signaling pathways which are coupled and display emergent behaviors, such as bistability [2]. We speculate that the organizational structure of the reaction network (the lattice structure of organizations) has a close relation to the complexity of the dynamical reaction system. Where the number of organizations in the network is a facet of the system complexity, because of the association between sub-organizations and dynamical functions. However the structural features of the lattice, not only the size of the organizational structure, must also be taken into consideration. Do the sub-organizations contain each other like a chain, or do they form a hypercube or even more complex patterns. All these aspects are obviously relevant to the evolution of the system, yet the exact way in which they would affect it are still to be investigated and evaluated.

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