

# Artificial Chemistries – Towards constructive dynamical systems

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**Abstract.** *In this contribution we consider constructive dynamical systems, taking one particular Artificial Chemistry as an example. We argue that constructive dynamical systems are in fact widespread in combinatorial spaces of Artificial Chemistries.*

## 1. Introduction

The notions of self-assembly of structures, of self-formation and of self-organization are sometimes used interchangeably. Here we would like to offer a clear-cut discrimination between these terms, based on our understanding and what has been discussed in the literature [1-3].

We propose to consider self-assembly [1] as the most special term in this regard. It comprises the assembly of parts into a whole, directed by the assembling parts and their interactions. In exceptional cases, this might include changes in the interactions, depending on the growth of the self-assembling (partial) whole, but most of the time it is determined from the outset of the process by features of the parts. Notably, a self-assembling process is usually not recursive, i.e. it cannot move through successive stages of first assembling some elementary parts into more complex parts, which in turn self-assemble into the whole.

Self-formation [2], on the other hand, we propose to have a clear notion of sequence. Processes of self-formation can be used to generate more complicated wholes. This requires the developing system to change state repeatedly, with each state determining subsequent states and the sequence of events to follow. Much more complex wholes can be constructed by such a mechanism, and indeed it is possible to generate spatial patterns of enormous complexity. Self-formation finds its limits in the problem of repair and maintenance of the structures formed. Due to the very specific sequence of events that lead to the original result, these needs are virtually impossible to achieve with self-formation.

We propose self-organization [3,4] to be the most general term in this order, including both self-assembly and self-formation, but also self-maintenance, and probably development. Self-organization is much more dynamic in that it does not require a specific sequence to arrive at the end result. Rather, it has a multitude of paths toward the desired goal (usually a steady state). Self-organization allows phenomena on different time scales, and thus on a hierarchy of levels, which in turn allows for a recursive consideration of its mechanisms.

All three terms try to encircle the phenomenon of constructiveness of processes that we see so much at work in our surrounding environment. Obviously, a growth of complexity can be observed, if only qualitatively, not yet quantitatively. New wholes or new phenomena emerge through the constructive effects of various processes, with their effects not explainable by recurrence to the parts alone.

Artificial Chemistries [5] offer a useful tool to examine effects of constructiveness in a world completely defined by the researcher. An Artificial Chemistry allows the definition of arbitrary objects that interact according to arbitrary rules set by the programmer. They are then run in a dynamical system fashion and the results of myriads of interactions are observed and examined. If the underlying objects have a combinatorial structure, Artificial Chemistries allow to observe constructive systems dynamics. Such observations might teach us how to understand the effects and power of constructiveness in other systems as well.

A general phenomenon in this regard is that constructiveness is a way of emergence, in that the structure of a system changes over time. Many natural and also man-made systems exhibit a particular characteristic, that is related to stabilizing emergent phenomena once they have appeared: networks. Networks are a fundamental object of consideration, especially since they offer a smooth way to grow complexity. Sometimes this complexity growth of networks is unintended, as is the case, for example, in Law. This can be seen from the following two statements in recent discussions about the development of law:

*“Originally, the structure of the existing[1936] law was a logical arrangement of the sections. Adding so much law over the years has made it difficult for readers to find their way around the Act ... [which] no longer has a readily discernible structure” [7]*

*„The single largest threat to the modern administrative state is itself. The sociolegal system is an adaptive system, and as such is nonlinear, dynamical, and complex in its behavior and governed by complexity theory. Organized, hierarchical, centralized societies tend to increase their structural complexity to confront internal and external sources of stress. At some point, the complexity of law begins a feedback loop. Society's desire to create certain predictable outcomes causes it to rely increasingly on new and interrelated laws to "fine tune" the picture.” [8]*

This paper is organized as follows: Section 2 will review the general principles of Artificial Chemistries and give an example for an AC. Section 3 will discuss this particular artificial chemistry in more detail, that can be considered constructive if looked at from the proper perspective. Section 4 will summarize the results and try to give some future directions.

## **2. Artificial Chemistries - Principles and an Example**

Artificial Chemistries generally consist of a 3-tuple of (a) a set of objects or molecules with specific features, (b) a set of interaction rules between these objects, and (c) an algorithm driving the dynamics of a population of objects reacting according to the prescribed interaction rules.

More formally, an Artificial Chemistry AC can be written as a tuple  $AC = \{S, R, A\}$  with  $S$  a set of objects (molecules),  $R$  a set of reaction rules of arity  $n$ :  $R: S^n \rightarrow S \cup \emptyset$  to determine the interaction between  $n$  elements of  $S$  (with no reaction,  $\emptyset$ , a possibility), and  $A$  an algorithm driving the systems dynamics. Usually, the systems dynamics is based on the reaction kinetics of a continuously-stirred tank reactor, assuming full mixing of reactants. Alternatively, notions of topology can be introduced which change the kinetics substantially [6].

In recent years, Artificial Chemistry models have been used to model processes in Biology, Social Science and Computer Science, to name a few areas. Artificial Chemistries were also applied in information processing, notably optimization. For a more detailed review, readers are referred to [5].

An Artificial Chemistry with constructive potential is usually based on a combinatorial space. In the example discussed here we consider bit-strings of arbitrary length as the (macro-) molecules to be considered. There is a particular reaction rule between such bit-strings that is based on the formation of 2-dimensional operators from these strings, and the performing of matrix multiplication operations between matrices and bit strings. This system has been considered under various driving algorithms, see for example [9], including a notion of space [6] and complexity growth [10]. It has been confirmed that various equivalent ways exist to describe system behaviour, at least for small systems of this type. Notably, a rate equation approach, a reaction table based discrete dynamics and a single molecule simulation have all resulted in the same quantitative behaviour, at least in systems where the higher level descriptions could work.

In this section we want to restrict ourselves to the most simple non-trivial system of this kind, the 4-bit string matrix chemistry, which is based on a space of  $2^4 = 16$  species of strings. The rate equation model for this system reads like

$$\dot{x}_i(t) = A(t) + \left[ B_i x_i(t) + \sum_{k \neq i}^{n_S} C_{ik} x_k(t) - D \right] x(t)_i + \sum_{j, k \neq i}^{n_S} W_{ijk} x_j(t) x_k(t) - \frac{x_i(t)}{\sum_k y_k(t)} \Phi(t)$$

where  $B_i, C_{ik}, W_{ijk}$  are rate constants for self-replication, replication and other reactions, with  $n_S$  being the number of different string types. The rate constants can be read off from the reaction table of participating string types. Based on the interactions defined on the level of matrix-string multiplications, this reaction table is (see [9]):

Operator $s_1$	operand string $s_2$															
	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1	0	1	0	1	4	5	4	5	0	1	0	1	4	5	4	5
2	0	0	1	1	0	0	1	1	4	4	5	5	4	4	5	5
3	0	1	1	1	4	5	5	5	4	5	5	5	4	5	5	5
4	0	2	0	2	8	10	8	10	0	2	0	2	8	10	8	10
5	0	3	0	3	12	15	12	15	0	3	0	3	12	15	12	15
6	0	2	1	3	8	10	9	11	4	6	5	7	12	14	13	15
7	0	3	1	3	12	15	13	15	4	7	5	7	12	15	13	15
8	0	0	2	2	0	0	2	2	8	8	10	10	8	8	10	10
9	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
10	0	0	3	3	0	0	3	3	12	12	15	15	12	12	15	15
11	0	1	3	3	4	5	7	7	12	13	15	15	12	13	15	15
12	0	2	2	2	8	10	10	10	8	10	10	10	8	10	10	10
13	0	3	2	3	12	15	14	15	8	11	10	11	12	15	14	15
14	0	2	3	3	8	10	11	11	12	14	15	15	12	14	15	15
15	0	3	3	3	12	15	15	15	12	15	15	15	12	15	15	15

**Figure 1:** Reaction table of a 4-bit matrix-multiplication chemistry. A "0" indicates an elastic collision, i.e. there is no reaction product defined so that in case of a collision the molecules do not react.

If a population of strings is seeded with a particular initial condition, the dynamical system will approach an attractor state. That is, a number of string types will dominate the dynamics, with most others being suppressed by the nonlinear competitive dynamics of the system.

In a more recent paper we have pointed out that the Artificial Chemistry realized by the above reaction table erects a lattice of organizations. Organizations in this context can be defined in the following way (see [11-13]) using the properties of closure and self-maintenance which should be self-evident:

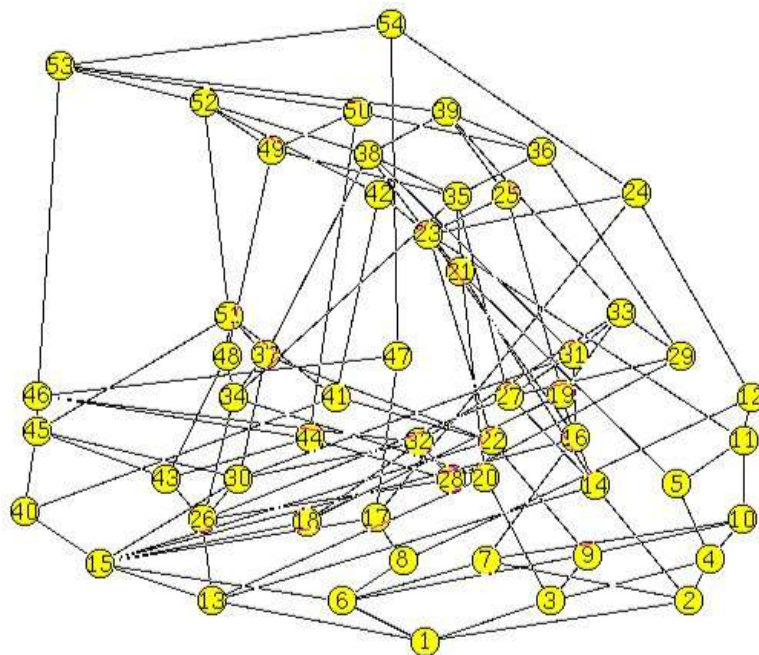
### Definition

Let  $O$  be a set of elements, subset of  $S$ , ( $O \subseteq S$ ). Then  $\mathbf{O} = \langle O, R \rangle$  is an **organization** iff  $\mathbf{O}$  is closed and self-maintaining. That is if  $\forall x_1, \dots, x_n \in O, R(x_1, \dots, x_n) = y, y \in O$  (property of **closure**) and  $\forall x \in O, \exists y_1, \dots, y_n \in O$  such that  $R(y_1, \dots, y_n) = x$  (property of **self-maintenance**).

This notion of an organization is algebraic, not referring to the dynamics of the state space. However, organizations correspond to order parameters of the system, i.e. quantities whose analysis allows us to understand the dynamics of the system to a fuller extent [3].

If one continues with the definition of unions and intersections of organizations (see [11]) one can produce a lattice of organizations which can be depicted as a graph with the nodes being different organizations and the edges being relations of indicating which organization is a sub-organization to which other.

The example above will therefore lead to a graph summarizing the lattice as in Figure 2.



**Figure 2:** Lattice of organizations of the 4-bit matrix-multiplication chemistry shown in Figure 1. Numbers indicate different organizations.

It is interesting to note that a small system of 4-bit strings and matrices has such a richness in behavior (at least statically). This reflects, of course, the fact that we are dealing with a combinatorial system.

### 3. Constructive Dynamical Systems

In what sense can we speak of a constructive dynamical system? We have to consider the development of a population of strings in such a lattice. As is clear from the dynamics of a population, starting, for instance, with two different string types that do not obey the feature of closure and self-maintenance, say,  $x_1 = x_5 = 0.5$ , the population of strings will begin to develop somewhere near to one of these organizations and wander around in the lattice, until it hits an organization which is stable.

$S_1$	$S_2$	
	1	5
1	1	5
5	3	15

$S_1$	$S_2$			
	1	3	5	15
1	1	1	5	5
3	1	1	5	5
5	3	3	15	15
15	3	3	15	15

**Figure 3:** The table on the left summarizes the interactions initially at work. New strings are produced by this interaction and the table has to be expanded to observe the fuller picture. The table, right, contains the full organization.

In the course of this wandering, new string types might appear and disappear. If they are bound to stay (because of the appropriate organization requiring them, see Figure 3) we can speak of the system being constructive. A more general definition can be given as follows:

### Definition

A dynamical system  $DS$  implemented by an artificial chemistry  $AC = \{S, R, A\}$  is said to be constructive if its complexity with respect to a complexity measure  $C$ , defined as the number of components present at a time and the cumulative interactions between components happening until that time  $C(DS(AC))$ , grows over time:  $C(t_2 > t_1) > C(t_1)$ .

Thus, as new elements from the set  $S$  are being generated, or new reactions happen,  $C$  starts to grow. This definition implies, however, that it is not merely innovation that is important for constructivity, but an expansion of activities, here in terms of number of participating species and interactions between them.

Why would any of the organizations ever be unstable, given its features of closure and self-maintenance? Admitted, if modeled at the level of rate equations with their idealizing assumption of infinitesimally small concentrations of strings to be able to participate in the dynamics this would never happen. This is, however, an idealizing model assumption that is not borne in reality of such systems. Rather, one would need to look at a simulation at the molecular level: A concentration below one molecule in the reactor vessel is simply not feasible. Even at concentrations of between 1-10 molecules, chances are that the randomly acting flow term flushes out an entire species, thus rendering a transition in the lattice.

Alternatively, one could use the trick of introducing a cut-off in the simulation of rate equations, a minimal threshold of concentration for string types, below which a string type is considered to be non-existent [14].

There is another source of constructiveness, apart from the internal effect of reaching an organization from anywhere in state space: Noise in terms of random injection of new types. An example of this would be, that one or more strings of type 4,  $x_4 > 0$ , would suddenly appear in the system. One could imagine that to happen either by manual injection, or by mutation of strings. In fact if there is an abundance of  $s_5$ ,  $s_4$  would be a single bit-flip away. This would result in the immediate growth of the reaction table from the example above. Then, the reaction table would look like this:

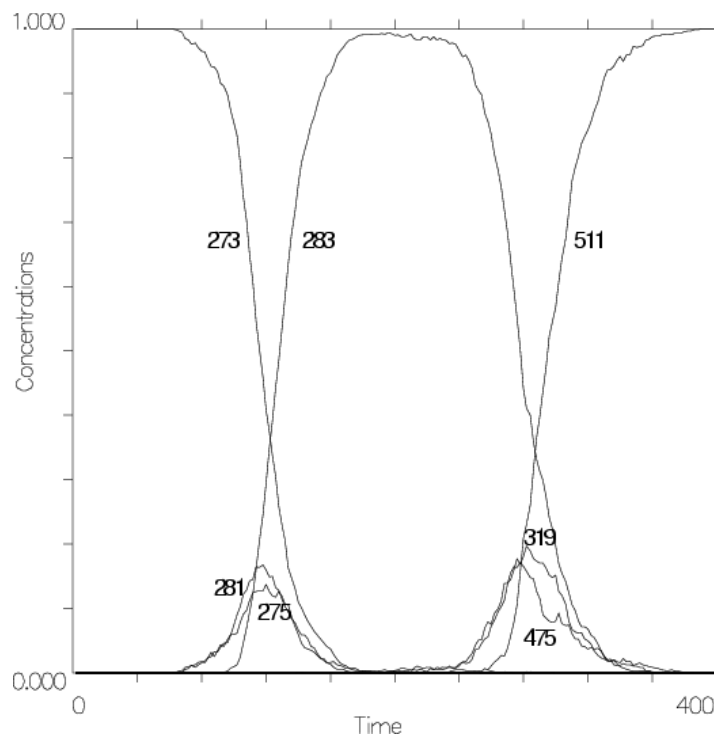
$S_1$	$S_2$				
	1	3	4	5	15
1	1	1	4	5	5
3	1	1	4	5	5
4	2	2	8	10	10

5	3	3	12	15	15
15	3	3	12	15	15

But given the products resulting from this interaction, the reaction table would then further expand:

$S_1$	$S_2$									
	1	2	3	4	5	8	10	12	15	
1	1	0	1	4	5	0	0	4	5	
2	0	1	1	0	0	4	5	4	5	
3	1	1	1	4	5	4	5	4	5	
4	2	0	2	8	10	0	0	8	10	
5	3	0	3	12	15	0	0	12	15	
8	0	2	2	0	0	8	10	8	10	
10	0	3	3	0	0	12	15	12	15	
12	2	2	2	8	10	8	10	8	10	
15	3	3	3	12	15	12	15	12	15	

At this point, a new organization (closed and self-maintaining) has been reached, and the system becomes stable again. Thus, as was indicated in [12], a certain degree of noise in a dynamical system of this type would help to perturb the systems dynamics' occasionally in such a way as to cause a new equilibrium state to occur. We might add here, that the noise, indeed, is a perfect vehicle to find more stable organizations in a lattice, as sooner or later different sorts of string types are introduced by random fluctuations. It would therefore cause the system to generate the most encompassing organization. It should be noted, however, that in order for the noise to be realistic, a notion of similarity between strings is helpful, if not necessary.



**Figure 4:** Development of a 9-bit string system. A total of 512 string types are possible. Initial condition is  $x_{273} = 1$  with a mutation that hits each bit string with a certain probability. We can see organizations coming and going destabilized by mutations.

In the example discussed next, a 9-bit string system has been simulated which has, due to combinatorics,  $2^9 = 512$  different string types. If we seed a population of strings with one self-replicating string type, and allow for single bit-flip mutations to occur in the population, we observe the occurrence of a succession of different organizations. The full reaction table of the system is too large to be reproduced here (512 x 512 entries), so we only reproduce some relevant parts.

The system dynamics starts out with  $x_{273} = 1$ . Two 1-bit-flip mutations generate strings  $s_{275}$  and  $s_{281}$ .

$S_1$	$S_2$			
	273	275	281	283
273	273	275	281	283
275	281	283	281	283
281	275	275	283	283
283	283	283	283	283

Because of further mutations after  $s_{283}$  dominates, namely to 1-bit variants  $s_{347}, s_{411}$ , a new organization occurs according to another part of the reaction table.

$S_1$	$S_2$					
	283	319	347	411	475	511
283	283	319	475	475	283	511
319	475	511	475	475	475	511
347	319	319	511	511	283	511
411	319	319	511	511	283	511
475	319	319	511	511	511	511
511	511	511	511	511	511	511

As a result,  $s_{511}$  dominates after a transitional period through  $s_{319}, s_{475}$ .

#### 4. Conclusion

Whereas this was just a discussion of one particular instance of the problems of constructive dynamical systems, the results generalize to many systems. In fact, as long as there is a certain degree of noise in the system, there is potential for the organization presently being dominant to become instable. We plan to further study this behavior in the context of a rigorous mathematical framework. One important ingredient will be the nature of the noise added to the system. We would like to argue that the most interesting type of noise is the one that is related to the species already present, because it shall provide us with a notion of neighborhood.

In a biological sense, the type of mutation considered here is analogous to radiation from outer space or spontaneous mutations, whereas the other mutation mentioned would be a production error in the reactions. Both of these are natural, and obviously very important to arrive at more stable organizations.

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