

Artificial Chemistry's Global Dynamic. Movements in the Lattice of Organisation

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Abstract

As *artificial life* is the study of life as it could be, *artificial chemistry* can be seen as the study of chemistry as it could be. In such systems molecules interact to generate new molecules, possibly different from the original ones. Here, we will focus on a general theoretical approach to study artificial chemistries. In this approach we consider the set of all possible organisations (closed and self-maintaining sets) in an artificial chemistry. As was shown in [2, 3] this set generates a lattice. We consider the dynamical movement of a system in this lattice, under the influence of its inner dynamic and random noise. We notice that some organisations, while being algebraically closed, are not stable under the influence of random external noise. While others, while being algebraically self-maintaining, do not dynamically self-maintain all their elements. This leads to a definition of attractive organisations.

1 Introduction

Artificial chemistries (AC) are a way to model natural systems. They have been used to model chemical systems, biochemical, ecological, sociological, and linguistic systems (refs. in [1]).

With the term artificial chemistry we refer to a system that can be described by three parts: the molecules \mathcal{M} , the operation \oplus , and the dynamic. The molecules are a set of elements¹. Depending

on the modelling aim, those elements can represent atoms, real molecules, animals, communication symbols, etc. Common in all those systems is that from the interaction of those elements new elements are generated. From this follows that in artificial chemistries the operation (the exact law that describes, given a set of interacting elements what comes out) is also important. In mathematical terms, if \mathcal{M} is the set of all possible molecules, the operation is a reaction that (usually) goes from $\oplus : \mathcal{M} \times \mathcal{M} \longrightarrow \mathcal{M} \cup \{\emptyset\}$. In other words the operation does not need to return a molecule for all possible couples. Some couples do not react, thus are called elastic. Some artificial chemistries use a more general product, where the product takes more than two elements, or returns more than one element. The last important element in an AC is the dynamic. The dynamic is an algorithm or formal system that specifies how the molecules are to be handled. In general the molecules are considered to live in a reaction vessel (e.g., a multiset, which is a set where the same element can appear multiple times). This reaction vessel is often called the soup or population, but the exact procedure that governs how the soup should be handled may vary from interaction to interaction. For example the soup could be a well stirred reactor, or from another medium. The dynamic also describes how the new molecule should enter the soup. Should they substitute the interacting ones, should they just be added to the set of existing molecules, or should they substitute another molecule randomly taken from the soup. In this paper we will not focus on a particular system, but we will investigate some characteristics common to many artifi-

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¹Not to be confused with chemical elements.

cial chemistries. A similar work was presented in the German Workshop on Artificial Life 2000 [3]. This work is set as a short general presentation of the field of artificial chemistries, as well as a deepening of that work.

2 Static Theory

If we consider only the set of molecules, along with the operation we can define two basic algebraic structures: closed and self-maintaining sets.

A **closed set** C is a set of molecules such that $\forall a, b \in C, a \oplus b \in C$. A **self-maintaining set** is a set of molecules such that $\forall a \in C, \exists b, c \in C$ such that $b \oplus c = a$. Closed sets are sets of molecules that cannot generate anything outside themselves. Self-maintaining sets are sets of molecules where each molecule can be generated by at least one interaction between the elements of the set. The concept of closure and self-maintenance are not mutually exclusive, in fact: let O be a closed and self-maintained set, we define O as an **organisation**.

Given a set $S, S \subset \mathcal{M}$, it is always possible to generate its **closure** $G_c(S)$ [3]. $G_c(S)$ will be the smallest closed set containing S . To generate the closure of a set we expand it by interacting the molecules of the set and adding to the set any newly generated molecule. When no new molecule is generated the set is closed.

Given a set $S, S \subset \mathcal{M}$, it is always possible to define its biggest self-maintaining subset [3]. We define this as the self maintaining set $G_{sm}(S)$ generated by S . To generate $G_{sm}(S)$ we contract S by eliminating one by one each molecule that cannot be generated from any possible reaction in S . When no element can be eliminated the set is self-maintaining. Note: if S is closed, then $G_{sm}(S)$ is closed too.

From the last property follows that given any set $S, S \subset \mathcal{M}$, it is always possible to define the organisation it generates [3]: $G_o(S) \equiv G_{sm}(G_c(S))$. Of course if O is an organisation $G_o(O) = O$. The organisations are the fixed points of the “generate organisation operator” G_o .

Given two organisations U and V , the organisation generated by their union ($U \sqcup V$) and intersection ($U \sqcap V$) is uniquely defined:

$$U \sqcup V \equiv G_o(U \cup V), \quad U \sqcap V \equiv G_o(U \cap V).$$

Let us now consider the set of all organisations

\mathcal{O} in an artificial chemistry, along with the operations organisation-union (\sqcup) and organisation-intersection (\sqcap). $\langle \mathcal{O}, \sqcup, \sqcap \rangle$ form a common algebraic structure called, a **lattice**.

Example. Let us consider an artificial chemistry composed of 10 molecules $\mathcal{M} = \{0, 1, \dots, 9\}$. The reaction network can be written as a table, where an entry $r_{i,j}$ denotes the interaction result of $i \oplus j$. A “-” denotes an elastic collision (an interaction that does not produce any molecule):

| | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|---|---|---|---|---|---|---|---|---|---|---|
| 0 | - | 0 | - | - | - | - | - | 6 | - | - |
| 1 | 2 | - | - | 5 | - | - | - | - | - | - |
| 2 | - | - | - | 1 | - | - | - | - | - | 0 |
| 3 | 5 | - | - | 0 | - | - | - | - | - | 1 |
| 4 | 8 | - | 6 | 6 | 4 | - | 8 | 4 | 8 | 5 |
| 5 | - | - | - | 1 | - | 9 | - | - | - | 8 |
| 6 | - | 8 | 0 | - | - | - | - | 7 | 2 | - |
| 7 | - | 5 | - | - | - | 5 | - | 9 | - | - |
| 8 | 1 | 2 | 9 | 1 | - | 6 | 3 | - | - | 2 |
| 9 | 0 | 8 | - | 0 | 3 | - | 6 | - | 0 | 0 |

This AC holds exactly 9 organisations: $\emptyset, \{4\}, \{4, 8\}, \{0, 6, 7, 9\}, \{0, 1, 2, 8, 9\}, \{0, 1, 2, 3, 5, 6, 8, 9\}, \{0, 1, 2, 3, 5, 6, 7, 8, 9\}, \{0, 1, 2, 3, 4, 5, 6, 8, 9\}, \{0, 1, 2, 3, 4, 5, 6, 7, 8, 9\}$. Its lattice of organization is shown in Fig. 1, left.

3 Dynamics

The static theory deals with molecules \mathcal{M} and reaction rules \oplus , but not with time. Now we add dynamics, which describes how the AC evolves over time. In general, the dynamics is given by a **state space** X and a formal definition (mathematical or algorithmical) that describes all possible movements in X . Given an initial state $\vec{x}_0 \in X$, the formal system (or algorithm) describes how the state changes over time. A state $\vec{x} \in X$ represents the state of a reaction vessel (or reaction space), that contains molecules from \mathcal{M} .

Example: $X = \mathcal{R}^{10}, \vec{x} = (x_0, x_1, \dots, x_9)$, x_i denotes the concentration of molecular type i in the reaction vessel presented before.

Dynamics can be introduced in different ways, for example, by an ordinary differential equation (ODE) or by a stochastic simulation where every single molecular collision is simulated explicitly.

Example: We use an ODE to describe how the state \vec{x} evolves over time. The dynamics is given as $dx_k/dt = \sum_{i,j \in \mathcal{M}} \alpha_{i,j}^k x_i x_j - x_k \Phi(\vec{x})$, with the dilution flow $\Phi(\vec{x}) = \sum_{i,j,k \in \mathcal{M}} \alpha_{i,j}^k x_i x_j$ and rate constant $\alpha_{i,j}^k = 1$ if $i \oplus j = k$, otherwise $\alpha_{i,j}^k = 0$.

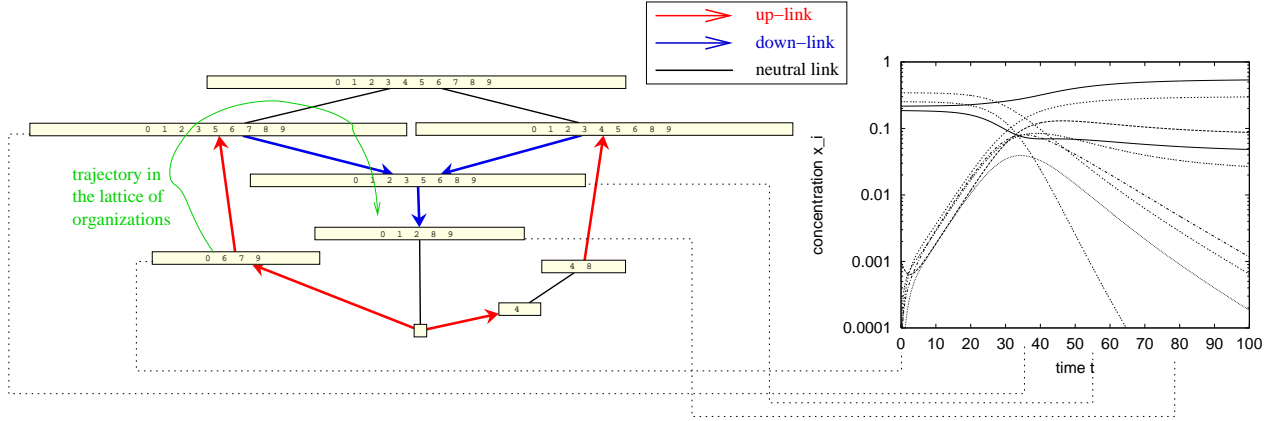


Figure 1: Left: Example of a lattice of organisations with up and down-links. Right: Simulation starting in organisation $\{0, 6, 7, 9\}$ with molecule 1 added in small quantity.

In order to connect the dynamics to the static theory we have to map a state, in the dynamical system, to a set of molecules, used to derive the algebraic organisation we are in. To do this we apply a threshold θ and consider present only the molecules above θ . We can define this as an operator $f_{Mol} : X \rightarrow 2^{\mathcal{M}}$ that defines the set of molecules that are present in the state x . Once defined f_{Mol} , we apply the generate organisation operator G_O to derive the present organisation $G_O(f_{Mol}(\vec{x})) = O \in \mathcal{O}$. Note that at each time the system is exactly in one organisation. We can also define the set of all states of an organisation $O \in \mathcal{O}$: $X_O = \{\vec{x} | \vec{x} \in O\}$.

3.1 Stability and Movement in the Space of Organisations

There are different ways how a system can move from one organisation to another. Basically there are two fundamental types of movements: (1) a movement caused by the internal dynamics, e.g., given by the ODE, and (2) a movement caused by a “constructive” disturbance (perturbation). Accordingly, we can also distinguish two types of stability: (1) stability within an organisation, and (2) stability against new molecules which are not coming from the organisation.

From an algebraic point of view we say that an organisation is stable, because it is closed and every molecule of the organisation is produced by at least one reaction among molecules inside the organisation. This does not necessarily mean that it is stable from a dynamic point of view.

In order to display a movement in the lattice of organisations, we consider three types of links between organisations: down-link, up-link, and a neutral link. A down-link is related to movement and stability type (1). An up-link is related to movement and stability type (2). A neutral-link is a link between organisations that is neither an up-link nor a down-link. We say that there exists a **down-link** from organisation O_1 to O_2 , $O_2 \subset O_1$, if there exists a trajectory starting in O_1 that would lead to a state in O_2 . We say that there exists an **up-link** from organisation O_1 to O_2 , $O_1 \subset O_2$, if there exists a trajectory starting from a perturbed state \vec{x} of the original organisation ($\vec{x} = \vec{x}_O + \vec{x}_\epsilon$, $\vec{x}_O \in O_1$) that would lead to a state in O_2 for $t \gg 0$. The perturbation is caused by new molecular types from $\mathcal{M} \setminus O_1$.

The dynamic stability of an organisation depends on whether a trajectory that is starting within the organisation remains there, or whether it “drops” to an organisation below, or it leaves the organisation by a “constructive” perturbation, such as mentioned above. We call an organisation **attractive**, if there exists a constructive neighbourhood such that all trajectories starting in that neighbourhood tend to the organisation for $t \rightarrow \infty$. We call an organisation **stable**, if for all neighbourhoods U^* containing O , there exists a constructive neighbourhood U , such that all trajectories starting in U are contained in U^* .

Example: In the example above, we consider those “constructive” perturbations where only one new molecular type appears:

$\vec{x}_\epsilon = (0, \dots, 0, \delta, 0, \dots, 0), \delta > 0.$

In Fig. 1 we can see 3 down-links, 4 up-links, and 4 neutral links. The organisation $\{0, 1, 2, 8, 9\}$ is clearly attractive and its basin of attraction touches every other organisation.

4 Conclusion

Artificial chemistry research has mainly concentrated in producing particular systems, to recreate and study particular natural systems or to study the behavioural spectrum of abstract reaction systems [1]. An exception on this was the work of Fontana and Buss [2], where a more general position was taken, and the general problem of study systems whose reaction can generate new component was faced. This led to the definition of organisation, and its use to face large ODE. Normally only few ordinary differential equations are solvable. This number decreases rapidly as the size of the system grows. If we are interested in studying an artificial chemistry we might not be able to solve its general ODE system. In this context the concept of organisation becomes important. An organisation is an independent subsystem and in absence of an external input, the system will remain bounded in the organisation. As such can be studied more easily than in the general case. This was part of the results of the Fontana/Buss work. The work was expanded in [3], where the concept of union, intersection and lattice of organisations were introduced. This permitted to address, from an algebraic point of view, the concept of what happens when two organisations interact.

Here we deepened the study by adding the dynamic. In our study we observed that often organisations are not stable, and the system *slides* (move) to a simpler one. This knowledge can, again, be used to focus the study only to the simpler system, ignoring the complex, unstable ones.

Of course to gather the data for a particular AC we need to confront ourselves with the system of equations in their more general form. But, interestingly, we do not need to completely solve them. We can in fact study the down-links from the more complex organisations through a statistically meaningful set of starting points. This would lead us to the really stable sub-systems, to solve which we can finally apply all our resources and

creativity.

Often AC include an external input of random noise. This noise can represent mutations; slow, non catalytic, spontaneous chemical reactions; a physical external input; etc. In all those cases the system, which has reached a simpler organisation through the previously explained down-links, has to interact with a new impulse, often being in this way sent to a different basin of attraction, and through other down-links to a different organisation. This type of dynamic is quite common in evolution, where a random impulse acts upon a stable situation, causing a global change and the movement to a different attractor.

We observed this behaviour, again from a disembodied prospective, looking at all the possible simple (1 molecule) disturbance. We discovered that the system were often attracted to very few, stable states, and to fewer organisations (*one in the example presented*). This led us to suggest that the evolutionary stochastic approach, where periods of natural evolution are alternated with random external influences, is a good way to find the attractors in an artificial chemistry too complex to be analytically solved.

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References

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