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Artificial Chemistries

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1 Aim

We are looking for the appropriate mathematical and computational tools for describing, studying and understanding complex chemical systems. Especially the phenomena of self-organization, structure formation, (pre-biotic) evolution and information processing in chemical or chemical-like systems need to be investigated.

A *constructive* artificial chemistry provides an abstract model for a complex chemical system which consists of a potentially infinite number of different substances. This becomes possible through the implicit definition of the reaction mechanism which relies on the structure of the interacting substances.

The aim of the working group *Artificial Chemistries* is to provide a forum for discussion and information exchange about artificial chemistries and related systems.

2 Introduction to Artificial Chemistries

An **artificial chemistry** is an artificial system, which is similar to a chemical system. Bagley and Farmer write in [1]: *An artificial chemistry is a set of rules stating which catalyzed reactions occur and with what strength.* Here, we describe an artificial chemistry as a system which consists of the following three parts:

1. **a set of objects** S **:** These objects may be abstract symbols [2], character sequences [1, 3, 4], lambda-expressions [5], binary strings [6, 7, 8], numbers [9], or proofs [10].

2. **a set of rules** R**, describing the interaction among objects:** The rules can be defined explicitly [2, 11] or implicitly by using string matching/string concatenation [1, 4, 12], lambda-calculus [5, 13], Turing machines [8], finite state machines or machine code language [7], proof theory [13], matrix multiplication [6], or simple arithmetic operations [9].

3. **an algorithm** A **driving the system:** The algorithm describes how the rules are applied to a collection of objects (soup/population). The algorithm may simulate a well-stirred reaction vessel with no topology [1, 5, 7], an Euclidean discrete CA-like (fixed) topology [2, 12], a continuous 3-D space, or a self-organizing topology [14].

Both, the set of objects and the interaction rules, can be defined explicitly or implicitly (e.g. by an algorithm or mathematical expression).

2.1 Example: Number-Division Chemistry

An example for an implicit definition is the **number-devision chemistry** [9]:

Set of objects. In the number-division chemistry the molecules are represented by natural numbers $S = \{2, 3, 4, \ldots\}$.

Interaction rule. Two objects can interact, if one object can be divided by the other. The result of the interaction is the divisor and the division of the two objects. Thus, $R = \{s_1 + s_2 \Longrightarrow s_3 | s_1 \bmod s_2 = 0 \wedge s_3 = s_1/s_2\}$.

Reactor algorithm. In addition to the set of molecules S and the set of collision rules R we need a description of how the rules should be applied to which objects and how the products should be handled. This is formalized by the following algorithm which instantiates a mass-action kinetics equivalent to second order dynamics of the form

$s_1+s_2 \longrightarrow s_1+s_3$. The following algorithms is applied to a population $P = (P[1], \ldots, P[M])$ which is an array of $s_i \in S$ of size M.

```
while not terminate() do
  s1 := P[randomInteger(1, M)]
  i2 := randomInteger(1, M)
  s2 := P[i2]
  if a rule (s1 + s2 => s3) exists in R
    P[i2] := s3
  fi
od
```

A slightly modified version of the preceeding algorithm instantiates a mass-action kinetics equivalent to second order catalytic reactions of the form $s_1 + s_2 + X \longrightarrow s_1 + s_2 + s_3$, where the concentration of the implicit substrate X is kept constant [5, 6, 7, 11]:

```
while not terminate() do
  s1 := P[randomInteger(1, M)]
  s2 := P[randomInteger(1, M)]
  if a rule (s1 + s2 => s3) exists in R
    P[randomInteger(1, M)] := s3
  fi
od
```

Note that this algorithm simulates a well-stirred reaction vessel with constant size. The production of new molecules s_3 creates an implicit competition for space which might lead to an evolutionary process [7, 15, 16].

It is also possible to rely the simulation of the dynamics on differential equations. This is much faster than an explicit simulation of every molecule if the number of molecules per species is high and the total number of different molecule types is low. The differential equation system may also change over time which is called **meta dynamics** [1, 15]. The meta dynamics aproach allows the investigation of constructive chemical systems by still using the differential equation framework.

2.2 Artificial Chemistry - A Formal Definition

The triple (S, R, A) is called an **artificial chemistry**, where S is a set of objects describing the molecules, R a set of collision rules describing the interaction among the objects, and A an algorithm describing how the rules are applied to a collection P of objects out of S.

Comments:

- By allowing A to be an algorithm the definition is universal in the computational sense and therefore might be too general.
- A rule in R may contain additional information such as rate constants, energy consumption etc.
- The algorithm A can be simple as in the examples above but also complex when e.g. a realistic spatially structured reaction vessel should be simulated.
- There are two other classes of systems which are also termed "Artificial Chemistry" : Cellular Automata and Corewars-like systems [17].

3 Related Work and Formal Frameworks

This section summarizes some related work and gives a brief overview about frameworks used to construct artificial chemistries.

3.1 Explicit Reaction Networks

Varela has defined an explicit spatial reaction system to explain his concept of autopoiesis [2, 18]. Eigen and Schuster used explicit reaction networks to demonstrate hypercyclic reaction dynamics [11]. Ziegler et al. applied in [19] an explicit artificial chemistry to control an autonomous mobile robot.

The common property of these explicit defined reaction networks is that the reaction rules are *not* based on the structure of the objects (molecules). In fact, the objects are only abstract symbols without a defined structure. These explicit approaches do not allow to study 1.) constructive dynamical processes and 2.) the structure-function relationship.

3.2 Typogenetics

The typogenics – introduced by Hofstadter – is an implicit defined, constructive artificial chemistry. It should illustrate the "logic of life", the DNA-RNA-Enzyme-DNA cycle [20]. The typogenetics has also been investigated by Morris [21].

3.3 Polymer Chemistry

In an artificial polymer chemistry the objects are symbol sequences and the reaction rules consist of concatenation and breaking (e.g. `AABBBA + BBB  <---> AABBBABBB`).

These systems have been intensively investigated by Kauffman, Farmer, Bagley, Packard, and others [1, 3, 15, 22]. They illustrate that a self-maintaining metabolism can emerge in a polymer chemistry without the need of template-based replication. The sorting chemistry in [9] can also be considered as a polymer chemistry.

3.4 Lambda-Calculus

Fontana applied the lambda-calculus to define an abstract constructive chemistry [5, 10, 13, 23, 24]. The lambda-calculus is an elegant framework which specifies how character sequences can be interpreted as operators acting on character sequences. Some advantages are the short and implicit definition of the interaction mechanism, the computational universality of the lambda-calculus, variable length objects (molecules), and different (in principal arbitrary) interaction schemes which can be formuleted as lambda-expressions. Disadvantages: Evaluation of lambda-expression may take a long time and have to be interrupted, and objects with variable length are harder to analyse.

Fontana indentfied several levels of organization. A **level 0 organization** consists of only a few molecules where self-replication is the dominant reaction. A **level 1 organization** maintains itself without self-replication. It consists of a potentially infinit number of different molecules where at a certain time only a finite subset is present. A **level 2 organization** consists of two or more coexisisting level 1 organizations. Level 2 organizations appear very seldom spontanously.

Fontana and Buss also demonstrate that molecules of a level 1 organization have syntactic simmilarities which allow a reduced description of the set of molecules of a level 1 organization by a grammar. In addition, the interaction can be described by an algebraic structure independently of the underlying lambda-calculus.

3.5 Simple Arithmetic Operators

Even simple arithmetic or logic operators can be used to construct artificial chemistries with interesting behavior, as shown in the number-division-chemistry example [9].

3.6 Matrix Multiplication

In [6], Banzhaf used matrix multiplication as a reaction mechanism in a binary string chemistry. In this case a binary string becomes an operator by "folding" it into a matrix. Self-replication and the emergence of nontrivial metabolic reaction networks have been observed even in simple 4-bit systems.

3.7 Binary String Automata

The idea of using a formal automata to define reaction mechanisms goes presumably back to John S. McCaskill. It has been implemented and investigated by Thürk [8], Ikegami and Hashimoto [25], and Dittrich [7, 16, 26]. Using mechanisms which are "compatible" to todays computer hardware allows very efficient implementations. The binary automata approach is especially usefull if huge spatially distributed systems should be simulated on reconfigurable computers [4].

4 Investigation

Designing a system that shows complex behavior is surprisingly easy. But to visualize and to explain in detail the behavior is much harder. The investigation of complex artificial chemical systems is still an unsolved problem.

The methods for investigation can be divided into macroscopic, mesoscopic and microscopic ones: A **macroscopic method** observes the whole system, by mapping its high-dimensional state into a low-dimensional space, where every component of the system should be considered. An example from thermodynamics is the temperature. A **mesoscopic method** considers only a small subset of the systems components. It still accumulates many microscopic events into low dimensional values (e.g. the concentration of specific substance in a region). **Microscopic methods** are visualizing elementary details of the system for instance the history of a specific object or memory cell.

Questions: How should the reaction network be visualized? How could the dynamics be visualized ? How can mesoscopic decomposition be achieved automatically?

5 Chemical-like Systems

It is interesting to note that the same models used to describe chemical systems can also be found in other domains, such as population dynamics, immune system, social dynamics, economy, memetics etc. [27]. Therefore we may suspect that artificial chemistries can also serve as a tool for understanding the formation and decay of organizations in other domains.

Here, a key question is: When an artificial chemistry should be applied to model e.g. social phenomena, what can be kept and what is missing?

6 Some Questions for Discussion

1. What level of abstraction is feasible ?
2. Does an artificial chemistry give insight into the process of prebiotic and/or biotic evolution ?
3. What is missing in current systems ?
4. What does evolution mean in the context of a chemical system ?
5. What does information processing mean in the context of a chemical system ?
6. How many levels of meta-evolution are present in a self-evolutionary chemistry ?
7. What are "natural laws" in the context of artificial chemistries ?
8. Is an artificial chemistry able to create information ?
9. How can an artificial chemistry be investigated and analyzed ?

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