in:The Right Stuff: Appropriate Mathematics for Evolutionary and Developmenta Biology
Chrystopher L. Nehaniv and Guenter P. Wagner, Editors,
pp. 27-31, Technical Report, CS, Report No 315, Univ. of Hertfordshire, School of Information Science, 1998

Real Evolution in Artificial Chemistries

Peter Dittrich
University of Dortmund
Dept. of Computer Science, Systems Analysis
D-44221 Dortmund, Germany
dittrich@LS11.cs.uni-dortmund.de
http://ls11-www.cs.uni-dortmund.de

1 Overview

The intention of this contribution is to stimulate discussion concerning the following question: Are artificial chemistries a useful tool to study pre-biotic or chemical evolution ? Or more general: Are artificial chemistries a useful tool to study the evolution of organizations ? The latter question implies that the insights gained from the investigation of chemical-like systems can be transfered to other systems which are also forming organizations through local interactions of many components.

The first part gives an introduction to artificial chemistries. In the second part an example for "real evolution" in an artificial chemistry is shown. The term "real evolution" refers to the phenomena of self-evolution, where every variation and implicit selection is performed by the individuals (molecules) themselves and not by explicit external selection, mutation or recombination operators.

2 Introduction to Artificial Chemistries

An **artificial chemistry** is an artificial system, which is similar to a chemical system. Usually, an artificial chemistry consists of:

1. **a set of objects** S **:** These objects may be abstract symbols [16], character sequences [1, 12, 14], lambda-expressions [8], binary strings [3, 6, 15], numbers [4], or proofs [10].
2. **a set of rules** R**, describing the interaction among objects:** The rules can be defined explicitly [16, 7] or implicitly by using string matching/string concatenation [2, 13, 14], lambda-calculus [8, 9], Turing machines [15], finite state machines or machine code language [6], proof theory [9], matrix multiplication [3], or simple arithmetic operations [4].
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, 6, 8], an Euclidean discrete CA-like (fixed) topology [13, 16], a continuous 3-D space [17], or a self-organizing topology [5].

Both, the set of object and the interaction rules, can be defined explicitly or implicitly (e.g. by an algorithm or mathematical expression). An example for an implicit definition is the **number-devision chemistry** [4]: In the number-division chemistry the set of objects are natural numbers s $S = \{2, 3, 4, \ldots\}$. 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, $R = \{s_1 + s_2 \Longrightarrow s_3 | s_1 \bmod s_2 = 0 \wedge s_3 = s_1/s_2\}$.

A typical algorithm simulates a well-stirred tank reactor which contains a population P of molecules out of S. Here, the population is implemented as an array of fixed size M:

```
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
```

This simple 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 substrate X is kept constant. The population P can be initialized by randomly selecting elements out of S.

An important aspect of this framework is, that it allows to setup *constructive* dynamical systems. i.e., the collision of molecules can generate new molecules [8, 9]. A constructive dynamical system can be treated as a dynamical system where dimension and components are changing through interactions of the components [1].

A second important aspect is, that the dynamics is *not* abstracted from the structure, as it is the case for example in the works by Eigen and Schuster on hypercycles [7]. The definition of the reaction mechanism relies on the structure of the interacting substances. The mapping from structure to function plays a key role in the process of self-organization. It allows a structure (or an organization) to operate on itself.

Finally, the inherent parallelism should be noted which allows very efficient implementation on massively parallel hardware [14].

3 Example for Self-Evolution in an Artificial Chemistry

In Fig. 1 an example for evolution without any explicit mutation, recombination, or fitness operator is shown. Every variation and implicit selection are only performed by the interacting species.

In the example, molecules are represented by binary strings with constant length of 32 bits, $S = \{0,1\}^{32}$. An interaction among two strings $s_1, s_2 \in S$ is performed in two steps: (1) s_1 is mapped to a finite state automaton A_{s_1} by interpreting s_1 as 4-bit machine code [1]. (2) The automaton A_{s_1} is applied to s_2 to generate the output s_3. In addition elastic collisions are introduced by not allowing exact replications [8]. Thus, $R = \{s_1 + s_2 \Longrightarrow s_3 | s_3 = A_{s_1}(s_2) \wedge s_1 \neq s_3 \wedge s_2 \neq s_3\}$. The population is initialized with $M = 10^6$ strings out of S and the algorithm mentioned above applied.

During the run displayed in Fig. 1 a lot of completely new strings are produced. Some strings are generated with rapidly increasing concentrations. A few generations later they are replaced by "better" ones. It is also interesting to note that the structure of the strings is evolving (a string is similar to its "predecessor").

[1]The automaton is described in more detail in [6] and available as C++ source from ftp://lumpi.informatik.uni-dortmund.de/pub/biocomp/src/

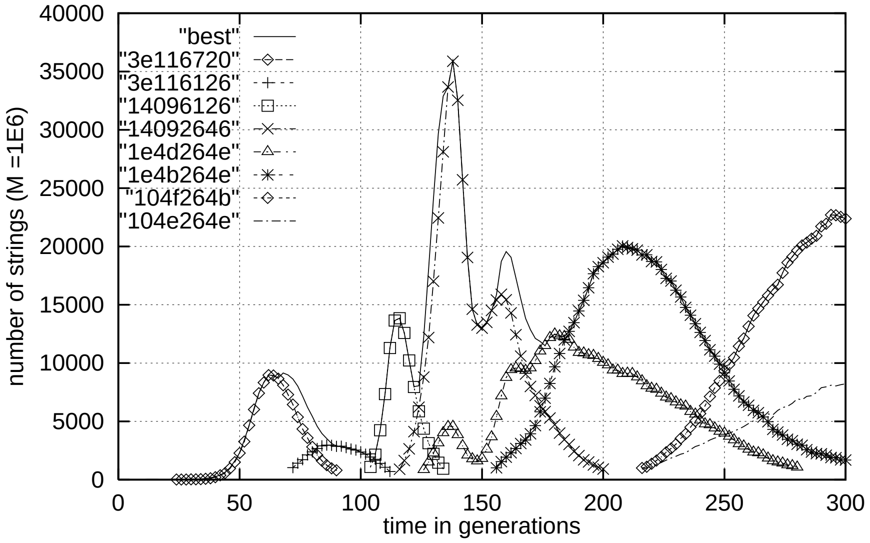

Figure 1: *Example for self-evolution in an artificial chemistry. Concentration of some representative strings are shown. Parameters: population size $M = 10^6$, automata reaction with table 2, no exact replication, population seeded with M random strings out of* $\{0,1\}^{32}$.

4 Questions for Discussion

(1) Is an artificial chemistry suitable to study molecular/prebiotic evolution ? (1a) What is missing ? (2) What level of abstraction is reasonable ? (2a) Do we have to incorporate detailed physical/chemical knowledge ? (3) How many meta-levels of evolution are there ? (4) How can "evolution" be measured ? (5) Does "information processing" emerges in the context of evolution ? And how ? (6) How can an artificial chemistry be investigated and analyzed ? (7) Is an artificial chemistry able to create information ?

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. [11]. 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 used as a social dynamics model, what can be kept and what should be added ?

Acknowledgments

The author is supported by the DFG (Deutsche Forschungsgemeinschaft), grant Ba 1042/2-1 and Ba 1042/2-2.

References

[1] R. J. Bagley and J. D. Farmer. Spontaneous emergence of a metabolism. In C. G. Langton et al. (editors), *Proceedings of the Workshop on Artificial Life (ALIFE '90)*, Redwood City, 1992, Addison-Wesley.

[2] R. J. Bagley and J. D. Farmer. Spontaneous emergence of a metabolism. In C. G. Langton et al. (editors), *Proceedings of the Workshop on Artificial Life (ALIFE '90)*, pages 93–140, Redwood City, 1992. Addison-Wesley.

[3] W. Banzhaf. Self-replicating sequences of binary numbers – foundations i and ii: General and strings of length n = 4. *Biological Cybernetics*, 69:269–281, 1993.

[4] W. Banzhaf, P. Dittrich, and H. Rauhe. Emergent computation by catalytic reactions. *Nanotechnology*, 7(1):307–314, 1996.

[5] P. Dittrich and W. Banzhaf. A topological structure based on hashing - emergence of a "spatial" oranization. *Fourth European Conference on Artificial Life (ECAL97), Brighton*, http://www.cogs.susx.ac.uk/ecal97/, 1997.

[6] P. Dittrich and W. Banzhaf. Self-evolution in a constructive binary string system. *submitted to Artificial Life, revision in preparation*, 1998.

[7] M. Eigen and P. Schuster. The hypercycle: a principle of natural self-organisation, part a. *Naturwissenschaften*, 64(11):541–565, November 1977.

[8] W. Fontana. Algorithmic chemistry. In C. G. Langton et al. (editors), *Proceedings of the Workshop on Artificial Life (ALIFE '90)*, pages 159–210, Redwood City, 1992. Addison-Wesley.

[9] W. Fontana and L. W. Buss. What would be conserved if 'the tape were played twice'? *Proc. Natl. Acad. Sci*, 91:757–761, 1994.

[10] W. Fontana and L. W. Buss. The barrier of objects: From dynamical systems to bounded organizations. In J. Casti and A. Karlqvist, editors, *Boundaries and Barriers*, pages 56–116. Addison-Wesley, 1996.

[11] J. Hofbauer and K. Sigmund. *Dynamical Systems and the Theory of Evolution.* University Press, Cambridge UK, 1988.

[12] S. A. Kauffman. *The Origins of Order.* Oxford University Press, 1993.

[13] M. W. Lugowski. Computational metabolism: Towards biological geometries for computing. In C. G. Langton, editor, *Artificial Life*, pages 341–368. Addison-Wesley, Redwood City, CA, 1989.

[14] J. McCaskill, H. Chorongiewski, D. Mekelburg, U. Tangen, and U. Gem. Configurable computer hardware to simulate long-time self-organization of biopolymers. *Ber. Bunsenges. Phys. Chem.*, pages 1114–1115, 1994.

[15] M. Thürk. *Ein Modell zur Selbstorganisation von Automatenalgorithmen zum Studium molekularer Evolution.* PhD thesis, Universit"at Jena, naturwissenschaftliche Fakult"at, 1993.

[16] F. J. Varela, H. R. Maturana, and R. Uribe. Autopoiesis: The organization of living systems. *BioSystems*, 5(4):187–196, 1974.
One of the first presentations of the concept of autopoiesis.

[17] K.-P. Zauner and M. Conrad. Simulating the interplay of structure, kinetics, and dynamics in complex biochemical networks. In R. Hofestädt et al. (editors), *Computer Science and Biology—Proceedings of the German Conference on Bioinformatics (GCB'96)*, IMISE Report, pages 336–338, Leipzig, 1996. Univ. Leipzig.