Artif Life Robotics (2004) 7:210–213
DOI 10.1007/s10015-003-0278-0

ORIGINAL ARTICLE

Yasuhiro Suzuki · Peter Davis · Hiroshi Tanaka

Emergence of auto-catalytic structure in stochastic self-reinforcing reaction networks

Received and accepted: November 26, 2003

Abstract We consider a chemical reaction network model in which some of the reactions are stochastic and depend on past history. In this chemical reaction network, we found the emergence of autocatalytic sets (ACS) and complex dynamics in which ACS are repeatedly created and destroyed.

Key words Self-organizing systems · Self-repairing systems · Self-replicating systems

1 Introduction

A living system of any scale has many states so that it can reform itself in order to fit its environment. If a system has only a few states, it would have only a limited number of choices. Such a system would not be able to keep up with dynamic changes in the environment, and would not have a great potential to develop or evolve. Having many states and the potential to form a variety of dynamic structures is essential for living systems. We can see this at any scale of living systems, e.g., immune systems, the genetic code, and species in ecological systems. In this paper we present a model system which exhibits the ability to form and reform a variety of dynamic structures, with a complex dependence on the accumulated effects of past dynamics, and the memory or history of the system. The system is an abstract model of a chemical reaction network. We describe the model and the typical dynamic behavior of the system, in particular the spontaneous creation and destruction of self-reinforcing reaction structures. Finally, we briefly discuss similarities and differences with other model systems, and the significance for modeling biochemical and living systems.

Y. Suzuki (✉) · H. Tanaka
Bioinformatics Medical Research Institute, Tokyo Medical and Dental University, 1-5-45 Yushima, Bunkyo-ku, Tokyo 113-8510, Japan
Tel. +81-3-5803-5840; Fax +81-3-3818-0247
e-mail: suzuki@gentzen.mri.tmd.ac.jp

Y. Suzuki
ATR Human Information Science Research Laboratories, Kyoto, Japan

P. Davis
ATR Adaptive Communications Research Laboratories, Kyoto, Japan

This work was presented in part at the 7th International Symposium on Artificial Life and Robotics, Oita, Japan, January 16–18, 2002

2 Model

We consider an abstract model of chemical reactions, a type of "abstract chemistry." The model assumes that substances can interact with each other according to reaction rules which change the amounts of the substance, and that reaction tendencies change depending on the reaction history. Reaction rules are assumed to be of the form $x \rightarrow y$, which means that the amount of substance x decreases and the amount of substance y increases. Reactions occur at rates which depend on the amount of the first substance x and the strength of the reaction $x \rightarrow y$. The strength of each reaction is increased in proportion to how often the reaction has occurred recently.

Specifically, we considered a form of this model which is implemented according to the following procedure. The state of the system is represented by the amounts $[x]$ of the chemical substances, and the strengths $w_{y:x}$ of the reaction rules. (For generality, we use "amount" rather than "concentration" or "number of molecules.") Reactions are executed one at a time. The first substance and the reaction rule are each selected stochastically. The probability of selecting substance x is proportional to the relative amount of the substance $[x]$, and the probability of selecting the reaction $x \rightarrow y$ is proportional to the relative strength $w_{y:x}$ of the reaction. When the reaction $x \rightarrow y$ occurs, the amount of substance x changes from $[x]$ to $[x] - 1$ and the amount of substance y increases from $[y]$ to $[y] + 1$. The strength of the reaction $x \rightarrow y$ is $w = (q^*R + 1)$, where q is the number of times the reaction has occurred in the last M reactions of

x, and R is the strength of the reinforcement. If reactions have not been selected recently, or there is no reinforcement, then reactions have a minimal strength of $w = 1$.

In order to implement the reaction dynamics, we used abstract rewriting system on multisets (ARMS).[1] A multiset is a type of set which allows duplication of the same element. A reaction $x \rightarrow y$ rewrites the multiset $\{x,x,x\}$ to $\{x,x,y\}$.

The stochastic model we use is based on a well-known model in probabilistic theory, Polya's urn.[2] Selecting a node is equivalent to picking a ball out of an urn, where a node name is painted on each ball. In the urn, there are $N - 1$ types of ball, excepting itself. Before picking a ball out of the urn, R balls are added to the urn for each of the M most recently selected nodes, in addition to one extra ("permanent memory") ball for each node in the network. Initially, the urn will contain just one ball for each node, and the probability of choosing any node will be the same. The model reaction system can be thought of as a network. Each substance corresponds to a node of the network, and each directed connection between one node and another corresponds to a catalyzed reaction rule. However, since each connection has a probability which depends on recent activity, it is different from other models such as models based on a random graph.[3] We can think that each node has a "memory store" where it memorizes the names of the M most recent outgoing links, and then uses this memory to determine the probability of selecting an outgoing link. Another description is as follows. There are two types of link. Each node has $(N - 1) + M$ outgoing links, $(N - 1)$ permanent links, and M dynamic links. There is one permanent link to every one of the other $(N - 1)$ nodes. Other dynamic links are created and destroyed dynamically. Once a link is activiated to a node, then an additional replica link is added, and the oldest dynamic links are destroyed. One of the $(N - 1) + M$ links is chosen randomly with a bias weight of R for dynamic links compared with permanent links.

3 Dynamic behavior: emergence of structures

This model exhibits an interplay between population dynamics and a reaction rule dynamics. This interplay results in a variety of complex behaviors. A unique feature of the model is the mechanism for reinforcement of the reaction strengths. If this reinforcement is strong enough, it creates a tendency for the accumulation of substances in closed reaction paths, resulting in the emergence of structures. Here, we present some examples to describe typical behavior.

Figure 1 illustrates a sample run for a particular set of parameters. In this example, there are 15 types of substance of the same amount in the initial state: reinforcement parameter $R = 10$. (Other parameter values are described in the figure caption.) The dynamic behavior is complex, with the amounts of substances varying dramatically.

Figure 2 shows an example of typical behavior when the value of the reinforcement is increased. Even though the amounts of substances and the strengths of the reaction rules were all equal initially, after some time the reactions are dominated by just a few substances, and the set of reactions among this limited number of substances is strongly self-reinforcing. This is an example of the spontaneous formation of dynamic structures. Eventually, the structures collapse, and are later replaced by other structures.

The reinforcement parameter R is an important parameter governing the tendency for the emergence of self-reinforcing structures. The memory storage capacity M also plays a key role: when the capacity is small, structures do not emerge, and when it is very large, structures are more stable.

As explained above, the reinforcement of reaction strengths creates a tendency for an increase in the amounts of substances in closed reaction paths and the decrease of amounts elsewhere. The amount of a substance will tend to go to zero unless there is a feedback reaction path. For

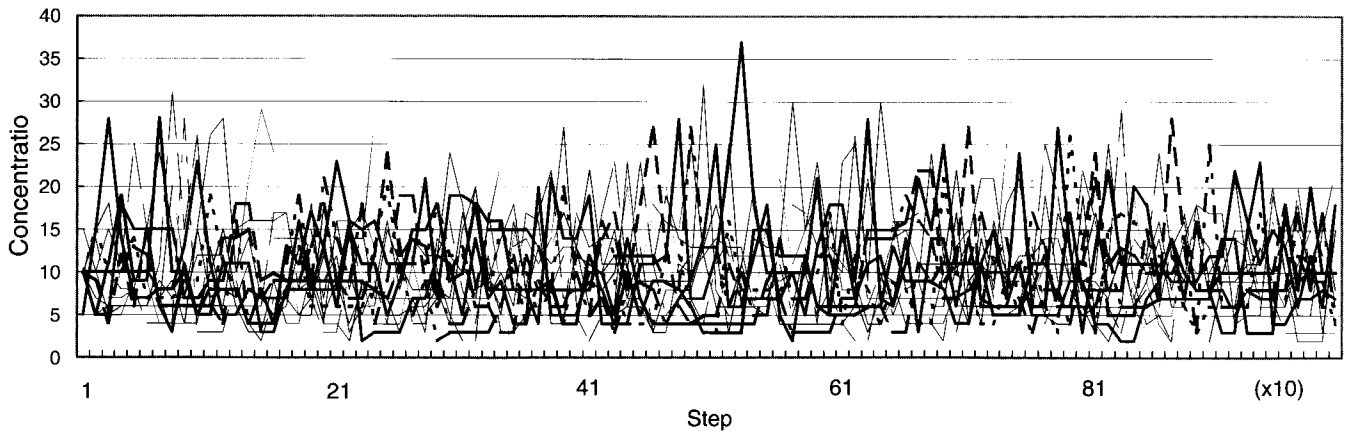

Fig. 1. Changing amounts of substances with time (1–1000 steps). This is a typical run for 15 substances with a reinforcement parameter $R = 10$ and a memory parameter $M = 400$. The amounts of each substance are equal in the initial state (amount = 10). Different line patterns correspond to different substances

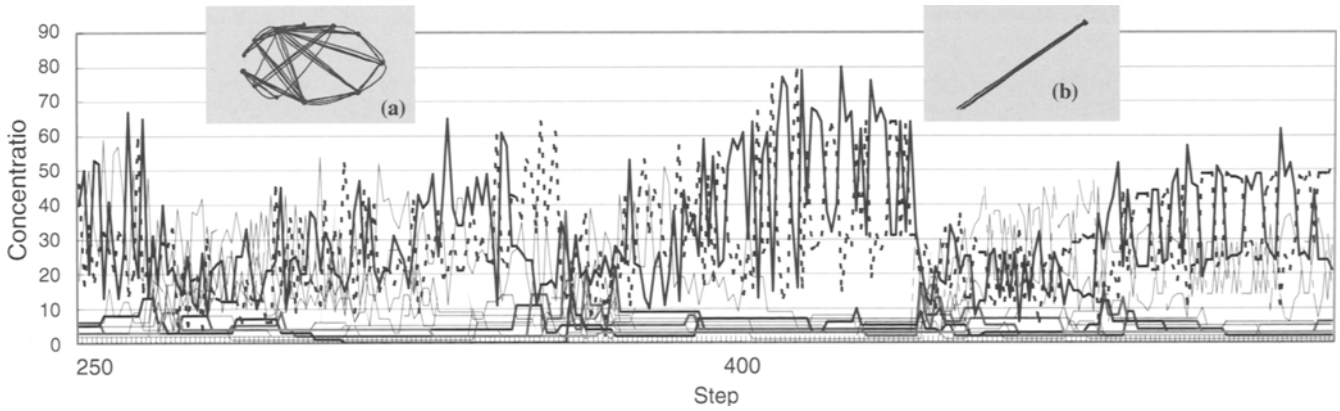

Fig. 2. Changing amounts of substances with time, showing the spontaneous emergence and collapse of an autocatalytic structure. This is a typical run with a reinforcement parameter $R = 300$. Other parameters and conditions are the same as in Fig. 1. **Inset a** Topology of the network after 300 time-steps, where each vertex stands for a type of substance, and each edge stands for a reaction. Only strong reactions with a strength greater than 10 are shown. The reaction direction is not shown. **Inset b** The topology of the network after 400 steps

example, consider a linear chain of reactions $a \rightarrow b \rightarrow c \rightarrow \ldots$. If there is no reaction creating substance a, the amount of a will decline to zero, and eventually b and c will also decline to zero. If the population of the start substance of the reaction goes to zero, the rule can never be selected and in a sense becomes dormant until the action of other rules creates some of the start substance. However, in our model, since we assume that permanent links remain between all substances, there is always a finite possibility of a reaction creating any substance. This provides a persistent mechanism for the decay of structures, and seeding the growth of new structures.

4 Discussion

We have shown that our abstract reaction model exhibits the spontaneous creation and destruction of self-reinforcing structures. Catastrophic events and recoveries have been found in various dynamic network models.[4,5] The structures in our model can be described as autocatalytic structures, or autocatalytic sets (ACSs).[6] An ACS in a reaction network is defined as a set of nodes (substances) which have at least one incoming link from other nodes in the set. Thus, an ACS has the property of catalytic closure, i.e., it contains a catalyst for each of its substances. A model which is similar in some respects is the model of Jain and Krishna,[6] which incorporates interplay between the network, population dynamics, and the environment. The Jain–Krishna model corresponds to a directed weight graph, where positive and negative edges represent "catalytic" and "inhibitory" interactions, respectively. The network evolves as the least populated species, or "less fit" species, are replaced by new ones. A small autocatalytic set, appearing by chance, provides the seed for the spontaneous growth of connectivity and cooperation in the graph, which corresponds to highly structured chemical organizations. Our model differs from the Jain–Krishna model in key aspects, including the facts that the nodes are not explicitly eliminated or replaced by new ones, the evolution proceeds by a stochastic selection of reactions, and the probability of reaction is affected by edge weights which are changed dynamically by self-reinforcement. We emphasize, that the self-reinforcing reaction mechanism results in the emergence of autocataytic sets even without the explicit removal of "unfit" species. In the Jain–Krishna model, the least-fit substances could sometimes be "keystone" substances,[4,5] which play important organizational roles in the network despite their low populations. When such a node is eliminated, many other nodes can become disconnected from the ACS, causing the catastrophic collapse of the ACS. On the other hand, in our model there are no explicit external operations of removing least-fit substances or adding new types of substance into the reaction network. A recognition and understanding of this intrinsic mechanism to generate a variety of reaction structures, to create and recreate spontaneously, and to self-organize and reorganize without the influence of external interactions could be important for understanding the developmental and evolutionary processes of complex biochemical and living systems.

5 Conclusion

We have presented an abstract model of a chemical reaction system that incorporates the interplay between population dynamics and a reaction network structure. We have shown that a reaction reinforcement mechanism based on a recent memory of reactions can result in the spontaneous creation and destruction of complicated reaction structures without needing external operations. This type of mechanism could potentially be useful in modeling the dynamic evolutionary processes of various complex biochemical and living systems.

Acknowledgments This research was supported by Grants-in-Aid for Scientific Research No. 14085205 and RCAST (at Doshisha University) from the Ministry of Education, Culture, Sports, Science and Technology of Japan, and the Telecommunications Advancement Organization of Japan.

References

1. Suzuki Y, Tanaka H (1997) Symbolic chemical system based on an abstract rewriting system and its behavior pattern. J Artif Life Robotics 1:211–219
2. Feller W (1957) An introduction to probability theory and its applications. Wiley, New York
3. Erdos P, Reny A (1960) On the evolution of random graphs. Publ Math Inst Hung Acad Sci 5:17–61
4. Ikegami T (2002) An origin of combinatorial complexity in replicator networks. Proceedings of the 7th International Symposium on Artificial Life and Robotics, vol 1, p. 300–301
5. Dittrich P, Kron T, Banzhaf W (2003) On the scalability of social order: modeling the problem of double and multi-contingency following Luhmann. J Artif Soc Soc Simulation 6. http://jasss.soc.surrey.ac.uk/JASSS.html
6. Jain S, Krishna S (2001) A model for the emergence of cooperation, interdependence and structure in evolving networks. Proc Natl Acad Sci 98:543–547