Emergence of Adaptive behavior in simulations by using Abstract Rewriting System on Multisets

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Abstract

We have developed an Artificial Intelligence system by using a model of chemical reaction, Abstract Rewriting System on Multisets, ARMS, where "intelligence" means that the reaction system can "select" specific molecules to sustain their reactions. We have implemented the reaction system by using an ARMS sand have obtained several molecules modified mutated DNA sequences that can sustain the reactions. We confirmed that reaction behaviors in the time series of concentration of non-mutated input molecule and mutated input molecule show oscillations; it would show that the system selects higher concentration one in between non-mutated and mutated one according to its concentration. Since the system exhibits adaptive autonomous behaviors, this DNA reaction networks system realize ARMS.

Keywords: List four to six keywords which characterize the article.

1. Introduction

DNA molecular computing has recently advanced to the study of molecular robots. On the other hand, artificial intelligence is shifting from research to social implementation. Shortly, molecular robots and artificial intelligence will fuse. The purpose of this research is to realize artificial intelligence using the underlying technology of DNA molecular computation.

For this reason, we use the most commonly used DNA molecular reaction called molecular displacement called strand displacement reaction. As for intelligence, we aim to create a function that can autonomously adapt to environmental changes. ARMS is a theoretical computation model based on the Gillespie algorithm, which is a rigorous physicochemical algorithm. In this research, the design for artificial molecular intelligence performed using physicochemical simulation.

1.1. *Self-sustained Chemical Reaction Networks, CRN*

We utilize the results of artificial life research that can adapt to environmental changes. In artificial life, various adaptive self-sustained autonomous reaction systems have been proposed, such as Eigen and Schuster's Hypercycle[1], Kauffuman's NK network[1], Fontana's lambda chemistry[1] and so on. In this research, we take the simplest Self-sustaining Chemical Reaction Network, CRN;

$$A + B \rightarrow C + D, \quad (1)$$
$$C + E \rightarrow A + F. \quad (2)$$

Here, the concentration of A keeps on sustaining, we assumed that the concentrations of B and E are sufficient

and D and F flow out immediately and do not interfere with other reactions nor activities of other chemicals.

1.2. *Toehold mediated Strand Displacement Reaction, TMSD*

DNA strand displacement is a reaction between a double-strand DNA and single strand DNA, in which a strand in

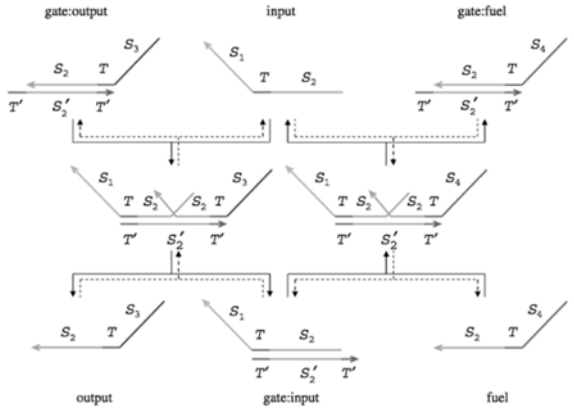

Fig. 1. Reprinted from the Journal of the Royal Society Interface, 2011 [4] (Open access)

a double-stranded DNA is replaced with the same or nearly identical single strand DNA. DNA strand displacement reaction is composed of the three single strands named the 'invader' 'incumbent' and the 'substrate'; this reaction is a swapping reaction between the invader and the incumbent strands on the substrate strand. The invader corresponds to an input signal, while the incumbent corresponds to an output signal. Toehold exchange reaction TER, which is Known as a class of strand displacements, since this reaction allows sequence- dependent control, it is peculiarly useful. In TMSD, the shorter incumbent forms a partial duplex with the longer, complementary substrate; then, the invader hybridizes with the toehold, which is the unbound region of the partially duplexed complement.

1.3. *Multiset Rewriting System on Multisets, ARMS*

We have been proposed a Chemical Reaction Networks, CRN, based on the Abstract Rewriting System, ARS; the ARS is a theoretical model of computation; we expand ARS on rewriting system on the multiset. A multiset is defined as a simple set and a map, which returns the duplication of element. We denote the duplication (multiplicity) of an element as M (a), for a $\in$ A and in case c /$\in$ A, M (c) = 0; for example M (a) and M (b) of {a, a, b, b} are 2, and M (c) = 0; in the mathematical description, a multiset is described as; < sup, M () >, in which sup is a simple set of elements, in this paper we describe a multiset by denoting the same alphabet in its number of multiplicity such as {a, a, b, b} or a vector w =(M (a1) M (a2) . . . M (an)).

The union of two multisets M1, M2 is the same as the union of simple set and in vector description, the union of multisets is addition of vectors w1 and w2. And inclusion of sets is also the same as the simple set, when M1(a) ≤ M2(a) for all a $\in$ A, the multiset M1 is included in M2 and we write M1 $\subseteq$ M2.

A reaction rule is a pair of multisets, we denote A# as a set of all combinations of multisets over A and in the combinations, an empty multiset is included. A reaction rule l → r, l, r $\in$ A# is described as a pair of multiset likewise chemical equations or a pair of its vector expression; and in some case, we can describe a reaction rule as a vector r, r = −l + r, it is simple and good for examining the dynamics of an ARMS, but this description cannot illustrate when there are the same species of element in the left-hand side and right-hand side such as a, b → a, c; in this case l = (1, 1, 0) and r = (1, 0, 1) and r = −(1, 1, 0) + (1, 0, 1) = (0, −1, 1).

A reaction is described as the rewriting of a multiset, if the left-hand side of a reaction rule is included in a multiset, these elements in the multiset are excluded and the right-hand side of the rule is merged to the multiset; the case when the multiset is a, a, b, b and the reaction rule is a, b → c, d, the left-hand side of the rule is included in the multiset, {a, b} $\subseteq$ {a, a, b, b} so the {a, b} is excluded from the multiset and it is transformed to {a, b} and the left-hand side of the rule {c, d} is merged to the set and we obtain {a, b, c, d} by this reaction.

Model

We model self-sustaining CRN with the seesaw gate reaction (Fig.1.) based on TMSD. In this reaction, first, TMSD occurs between the single strand DNA named' input 'and the double strand DNA named' gate:output

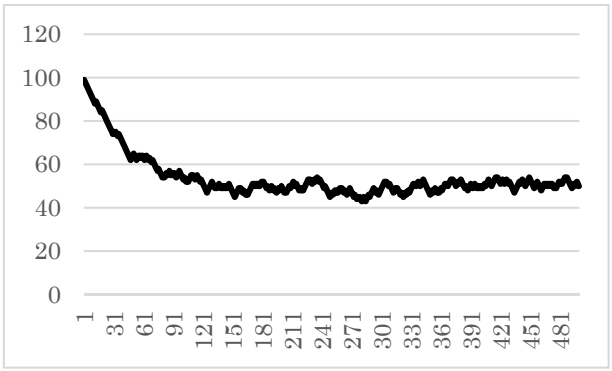

Fig. 2. Time change of the number of input molecules. The horizontal axis of the graph is the number of steps (one reaction is one step), and the vertical axis is the number of input molecules.

'and the single strand DNA named' output 'and the double strand DNA named " input:gate "are produced. Since the input:gate reveals a scaffold (T) for inter- action with the single stranded DNA named' fuel ', SDR occurs next on the fuel and input:gate, and the input and the gate:fuel are produced. Reactions of the first half and the second half occur like a seesaw, while the input consumed in the first half is supplemented in the second half; hence the reaction network sustains the input.

The self-sustaining CRN is implemented as;

$$\text{input} + \text{gate:output} \leftrightarrow \text{input:gate} + \text{output} \quad (1),$$
$$\text{input:gate} + \text{fuel} \leftrightarrow \text{input} + \text{gate:fuel} \quad (2).$$

In order to add perturbation to this reaction, an input 'molecule is introduced. input 'is an input molecule containing a miss-match pair. It is assumed that the binding force is weaker than the full match DNA strand as follows;

$$\text{input'} + \text{gate:output} \leftrightarrow \text{input':gate} + \text{output} \quad (3),$$
$$\text{input':gate} + \text{fuel} \leftrightarrow \text{input'} + \text{gate:fuel} \quad (4).$$

2. Method

We model and simulate the behavior of this reaction system using ARMS. This reaction system consists of eight reactions, including the reverse reaction. ARMS needs to determine the reaction rules to be applied, not random, but reasonably. Therefore, this model is regarded as a stochastic process model based on chemical kinetics (as for detail refer e.g. [3]).

We set the reaction rate constants as follows: the rate constants for the forward and reverse reactions are the same, the rate constant for the input' molecule is 100 times slower than the input molecule. This model assumes that the input' molecule has a mismatched pair. Therefore, we express this assumption by the difference in rate constants, which means that the affinity of strand matching will be lower, and the reaction will be slower.

3. Result

In the absence of perturbation, that is, without input', the reaction reaches an equilibrium state (Fig.2.). Add the input 'molecule and add perturbation. If the input molecule and the input' molecule are equivalent, the input' molecule hardly reacts. This simulation result is obvious because the reaction speed of the input' molecule is 100 times slower than the input molecule. If

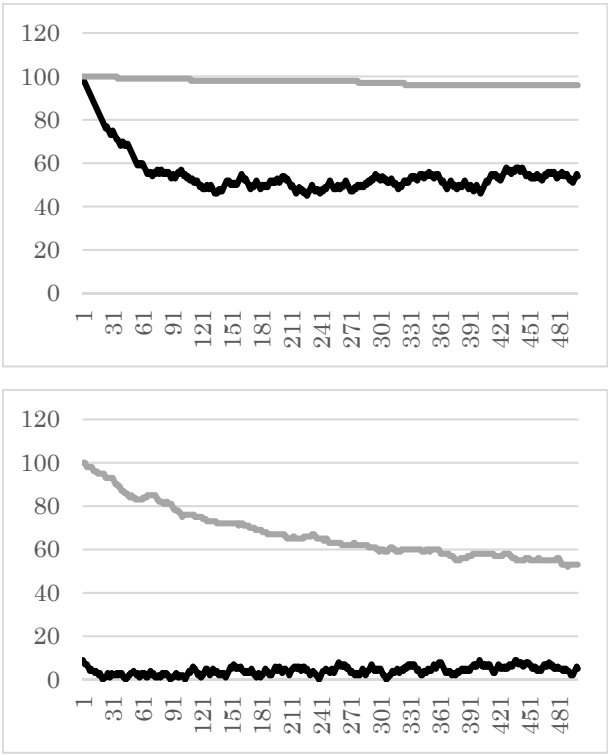

Fig.3. Time change of the number of input molecules and the number of input‘ molecules. When the same number of input and input’ molecule, input’ molecule does not react (top). (below) When the number of molecules containing mismatch is large, if the number of molecules of input' is 100 times that of input, the reaction system will use the molecules of input'. This result gives the DNA reaction system will be adaptive.

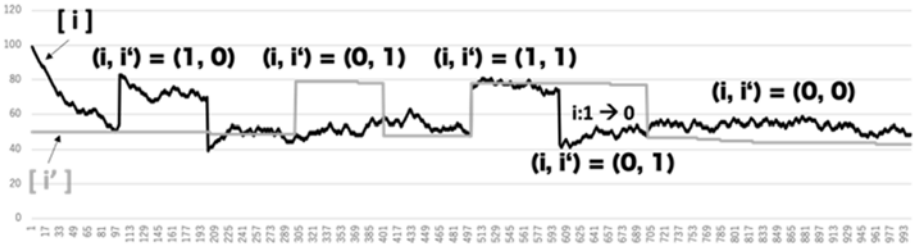

Fig. 4. 2-bit memory using DNA reaction. This memory realizes 2bit by on / off of input and input '. The equilibrium state of the input molecule and the input 'molecule is assumed to be (0, 0). And we regard the bit is set when the equilibrium state is changed by adding the input molecule or the input' molecule into reactions. In this simulation, at first i, which denotes the input molecules and i', input molecule, including mismatch, reached the equilibrium state. The equilibrium state is denoted as (0, 0) = (i, i'). Then 50 of input molecules added and (0, 0) transformed to (1, 0) and 50 of input molecules removed then (1, 0) back to (0, 0). Such adding and removing molecules realizes the states of bit change.

you set the number of input molecules to 100 times the amount of input molecules, the input molecules will be used. The simulation of this result predicts the environmental adaptation of a real DNA reaction system. If the input molecule containing the mismatch is high, the reaction system will use the molecule containing the mismatch (Fig.5.).

4. Discussion

The simulation results show that when the amount of input molecules is half the amount of input 'molecules, the concentrations of both become the same in the equilibrium state, and the equilibrium state shifts when the number of molecules is increased. Realize memory using this reaction system.

The case where the amount of the molecule is in the equilibrium state is 0, and the case where the equilibrium state is shifted by adding the molecule is 1. This method can realize n-bit, but for simplicity, this paper shows the example of 2-bit (Fig.4,5.). We confirmed through simulation that the DNA memory works. At first, when 30 molecules were added to the equilibrium state of the input and input 'molecules at the same amount, the shift of the equilibrium state was confirmed (Fig.5.). Then we confirm, do the bit on/off operations? Therefore, the input molecule and the input molecule were added and deleted. All states of input and input 'bit are (0,0), (0,1), (1,0), (1,1). It has confirmed that the transition between the four status bits can realize by adding and removing the numerator. We know that performing "removal" operations on real DNA reaction systems is not realistic.

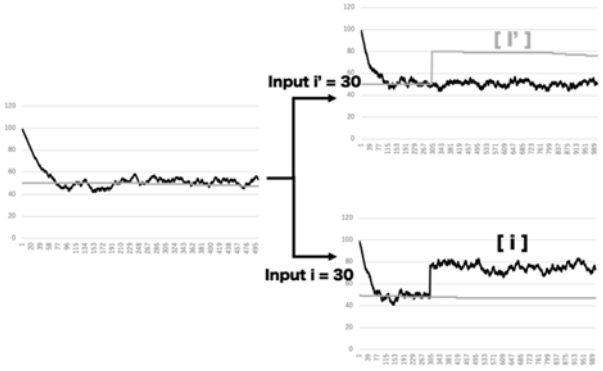

Fig. 5. This is the caption for the figure. If the caption is less than one line then it is centered. Long captions are justified manually.

However, it is more realistic to delete molecules as a result of using them instead of "deleting" them, for example, the DNA circuit by using this technique (Fig.4). In this paper, we show the realization of bit, but also show that this technology can realize "internal state" by input/output, which means that molecular artificial intelligence can be realized.

References

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