A Model of Reaction-diffusion phenomena with Multiset Processing

Yasuhiro Suzuki
Nagoya University, Furocho, Chikusa-ku, Nagoya, 464-8601, Japan

Abstract

We propose a model of reaction-diffusion phenomena using Abstract Rewriting System on Multisets ARMS, which is a model of Multiset Processing. Although proposed model is simple, computer simulations confirm that the Turing pattern is generated.

Keywords: Reaction-Diffusion, Activator-Inhibitor, Multiset Processing , Abstract Rewriting System on Multisets, ARMS

1. Introduction

A reaction-diffusion system is a mathematical model of how the concentration of one or more substances distributed in space changes under the influence of two processes: local chemical reactions, in which substances change each other, and diffusion, in which substances spread in space. One of the most famous reaction-diffusion systems is that proposed by Alan Turing. Turing showed a system that is locally stable but destabilized by diffusion. The spatio-temporal pattern that occurs in this system is called the Turing pattern [1].

The reaction diffusion model, which Alan Turing proposed is one in which two oscillators are coupled by diffusion (Eq. 1), where the two oscillators mutually activate and inhibit each other.

$$\frac{\partial u}{\partial t} = f(u,v) + D_u \nabla^2 u, \qquad (1)$$
$$\frac{\partial v}{\partial t} = g(u,v) + D_v \nabla^2 v,$$

In the equation (1), $u \equiv u(\boldsymbol{r},t), v \equiv v(\boldsymbol{r},t)$, f, g are reaction terms, D is a diffusion coefficient and ∇^2 is Laplacian.

2. Methodology

We model a system that performs activation and inhibition by diffusion coupling with two oscillators by a multiset rewriting system, Abstract Rewriting System on Multisets, ARMS.

2.1. Abstract Rewriting System on Multisets, ARMS

Abstract Rewriting System on Multisets, ARMS is a multiset rewriting system [2]. 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 ∈ A and in case c /∈ 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 ∈ A, the multiset M1 is included in M2 and we write M1 ⊆ M2.

A reaction rule is a pair of multiset, 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 ∈ 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 can not 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} ⊆ {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. By using vector ex- pression, a reaction is the addition of vectors as w − l + r,

in which l and r are vector expression of a reaction rule; the case when M = {a, a, b, b}, w = (2, 2, 0, 0) and the reaction rule is a, b → c, d, ({1, 1, 0, 0}, {0, 0, 1, 1}); and the reaction is denoted as {2, 2, 0, 0} − {1, 1, 0, 0} ={1, 1, 0, 0} and {1, 1, 0, 0} + {0, 0, 1, 1} = {1, 1, 1, 1}.

2.2. Activator-Inhibitor model

In the activator-inhibitor model, activator X increases themselves by autocatalytic reaction (Eq. 2); X → X, X. The reaction of activator X produces inhibitor Y is, X -> Y, X. X is put in both reaction equations because X does not increase by this reaction, while only Y increases. X, Y -> Y describes the inhibition of increasing X by Y, where X decreases while Y does not change. Y → ∅ denotes the decreases of Y, ∅ illustrates an empty set. We give reaction coefficients for each rule. We give reaction coefficients for each rule as k_1, k_2, k_3, k4. Each coefficient gives the probability of firing of the rule.

$$\begin{aligned} &X \underset{k_1}{\rightarrow} X, X\text{: r\_1,}\\ &X \underset{k_2}{\rightarrow} Y, X\text{: r\_2,}\\ &X, Y \underset{k_3}{\rightarrow} Y\text{: r\_3,}\\ &Y \underset{k_1}{\rightarrow} \emptyset\text{: r\_4.} \end{aligned} \tag{2}$$

Modelling diffusion：

The Eq. 2 above does not include diffusion. So, we need to consider diffusion separately. Why does diffusion occur? If we put a drop of ink on clean water and watch it for a long time, the ink spreading on the water's surface will eventually dissolve into the water. No matter how long we keep looking at the surface of the water where the ink has dissolved, there is no return of the drop of ink when the dissolved ink is dropped on the surface of the water again. In other words, diffusion is the process of homogenizing things.

If the state quantities of cells i and j are x_i and x_j, and diffusion occurs between these cells, the amount of diffusion from cell j to cell i can be expressed as d=(x_j - x_i)×D. D is called the diffusion coefficient. For example, let us consider a sequence of cells [2,3,1,2]. (The sequence of cells is indicated by enclosing the amount of state in each cell). For the cell with state 1, the state to the left of this cell is 3, and the state to the right is 2. The state of this cell is less voluminous than the left and right states. Therefore, an inflow occurs from the left and right cells to this cell, changing its state. The degree of inflow is determined by d=(x_j - x_i)×D. If the diffusion coefficient D is 0.1, the inflow from the left neighbour d_left=(3-1)×0.1=0.2 and the inflow from the right neighbour d_right=(2-1)×0.1=0.1. Thus, the sequence of cells [2,3,1,2] becomes [2,2.8,1.3,1.9] due to this diffusion. (Here, only the cell with state one is shown, but in reality, other cells change in parallel as well.) In this way, the state of each cell is averaged by diffusion.

2.3 Diffusion in a two-variable system

The active/inhibited system of Eq (2) consists of two variables, X and Y. Therefore, we will use a one-dimensional sequence of X-only cells and a one-dimensional sequence of Y-only cells. For example, if the sequence of cells representing the state of X is [2,3,1,2] and the sequence of cells representing the state of Y is [0,0,1,0], the states of X and Y in the cell located second from the leftmost are (1,1). When the diffusion coefficient of X is 0.1, and that of Y is 0.3, if diffusion occurs in cell (1,1), the state of the cell changes (Again, only cell (1,1) change is shown).

3. Results and Discussion

We assume that the rightmost cell is connected to the leftmost cell; the ten cells are considered to be connected in a ring. We show the result of simulation whose initial states are;

X=[0,10,0,10,0,10,0,10,0,10,0,10],

Y=[0,10,0,10,0,10,0,10,0,10,0,10].

We set the reaction coefficients are $k_1=k_2=k_3=k_4=0.01$. The state quantity is first updated by diffusion, as described in the previous section. Next, reaction rules are applied in parallel to update the state quantities. The update by diffusion and the update by reaction rules are repeated, and this process is repeated.

When the diffusion coefficients of X and Y are $D_X=D_y=0.0$, when there is no diffusion, there is no change from the initial state. Such a state is called an equilibrium state (equilibrium means "balanced"). As will be explained in detail in the next section, if X=Y (the amount of state of X is equal to the amount of state of Y), neither the amount of state of X nor the amount of state of Y will change in this reaction system. Therefore, since X=Y holds in the corresponding cell in the initial state, the system would remain in the initial state if there were no diffusion.

What would happen if diffusion were to occur in a state where the reaction is in equilibrium (X=Y)? First, assuming that X and Y diffusion coefficients are the same with $D_X=D_y=0.1$, X and Y change but always remain X=Y. In other words, the reaction is always in equilibrium. Eventually, X and Y are homogenized by diffusion, and the entire reaction reaches equilibrium. This is true even if the diffusion coefficient is changed as $D_X=D_y=0.2,0.3\cdots$.

Next, when X's diffusion coefficient is more significant than Y's with $D_x=0.3$ and $D_y=0.1$, X and Y become homogenized and almost X=Y, and the reaction approaches equilibrium. On the other hand, when the diffusion coefficient of Y is more significant than X's with $D_x=0.01$ and $D_y=0.3$, Y becomes homogenized. However, a larger or smaller pattern appears in X (Fig. 1) shows an example of the results). In this case, X does not equal Y, and X and Y continue to change (increase).

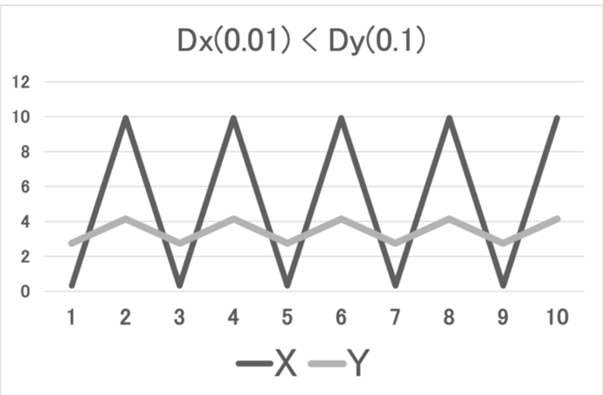

Fig.1 Turing Pattern like behavior, where the diffusion coefficient of X is 0.01, while Y, 0.1.

4. Conclusion

The reaction-diffusion phenomenon has been modelled and investigated as a partial differential equation by modelling the activator-inhibitor system. We used ARMS by modelling the activator-inhibitor system and confirmed that the ARMS model shows Turing pattern-like behavior.

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Authors Introduction

Dr. Yasuhiro Suzuki

He received his Doctor degree in Informatics in 2001 from Graduate School of Informatics, Kyoto University, JAPAN. He is currently an associate professor of Graduate School of Informatics, Nagoya University, JAPAN