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The Diversification of Proto-Cells Driven by Membrane Permselectivity

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Abstract

We consider how permselectivity as a function of the membrane is related to the cell evolution with an abstract proto-cell model. We construct an autopoietic proto-cell model having primitive auto-catalytic reaction cycle inside. In this model, several primitive membrane substances are assumed to be produced from the reaction cycle and the membrane is assumed to have a permeability to specific chemical species. We show that the permselectivity of the membrane induces the diversification of the cell volume. We discuss how the diversification of the cells is related to the Darwinian evolution.

1 Introduction

Recently there has been taken into account the prebiotic evolution based on membrane. In particular, Ségre proposed 'Lipid world hypothesis' in 2001[3]. In this hypothesis not one molecule but an aggregate of amphiphilic molecules can reproduce itself without a molecule which has genetic information and can evolve on the prebiotic earth. It should be, however, considered what will happen after the reaction which can produce membrane substances is separated from the environment. In particular, it is important to make sure whether the Darwinian evolution of the reaction cycle can occur or not and to elucidate the relation between the Darwinian evolution and the membrane functions.

The following three conditions is necessary for the Darwinian evolution[1].

1. Variation: There are differences among individuals.
2. Inheritance: The differences can be taken over to the descendant.
3. Selection: The differences influence the reproduction rate and the survival rate of the individuals.

The livings which fit an environment remain if these conditions above are met.

In the prebiotic condition, a proto-cell seems to be able to satify the conditions for inheritance and selecton. If a proto-cell is divided into two ones, the properties of the proto-cell can be inherited into the daughter proto-cells, and the proto-cells which have higher reproduction rate can be selected. It is, however, difficult to consider how the variation of proto-cells is generated and maintained without genetic molecules in the prebiotic condition.

We claim that the variation of proto-cells can be generated and maintained if a membrane function is taken into account. The membrane permselectivity which allows certain substances to permeate the proto-cell membrane can construct a specific internal condition and this effect may cause the variation of the reproduction and survival rate.

The purpose of this study is to answer the following question. How can the diversification of a proto-cell occur by membrane permselectivity?

2 Proto-Cell Model

We consider a simple proto-cell model which satisfies the following conditions.

1. It has an auto-catalytic reaction system inside.
2. Membrane substances are produced from the auto-catalytic reaction.
3. Membrane substances are self-assembled into a semipermeable membrane which separates the internal auto-catalytic reaction from the external environment.

The image of proto-cell model is shown in Figure 1. In the reaction k kinds of chemical species, $\mathrm{X}_1, \ldots, \mathrm{X}_k$, react auto-catalytically and some membrane substances, M_i, are produced from some of cheical species

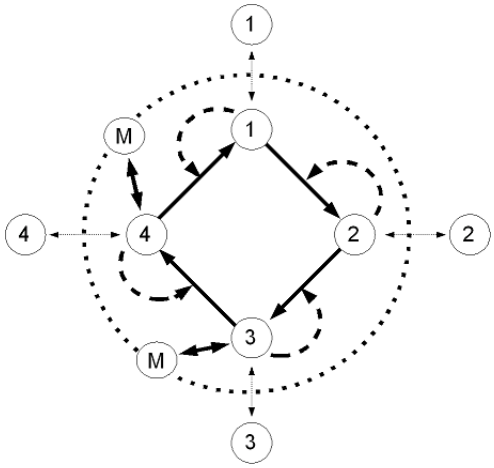


Figure 1: The image of proto-cell model. k kinds of chemical species react auto-catalytically and some membrane substances are produced from some of chemical species in the auto-catalytic reaction cycle. The numbers in the figure are the chemical species reacting auto-catalytically and 'M' means a membrane substance. The thick solid lines are the directions of reaction, the dashed lines indicate the catalyzed reactions, and the circular dotted line means the semipermeable membrane which separates internal and external condition. The thin solid lines across the circular dotted line indicate the permeation of the chemical species.

in the auto-catalytic reaction cycle as follows.

$$\mathrm{X}_i + \mathrm{X}_{i+1} \rightarrow 2\mathrm{X}_{i+1} \ (i = 1, \ldots, k; \mathrm{X}_{k+1} \equiv \mathrm{X}_1) \quad (1)$$

$$\mathrm{M}_j \leftrightarrow \mathrm{X}_j \quad (j \in \{1, \ldots, k\}) \quad (2)$$

In Figure 1, the number of reaction chemical species is $k = 4$ and memrane substances are produced from X_3 and X_4 $(j = 3, 4)$.

We assume the following conditions.

- Inside of the cell is well-mixed and the concentrations of all chemical species are even in the cell.
- The volume of the cell, V, is proportional to the amount of membrane substances.
- The molecules permeate and diffuse through the membrane with the diffusion coefficient D_i for the ith chemical species.

We use a stochastic method for calculating all the reaction processes and consider the number of molecules discretely. The effects of the discreteness of molecules and the smallness of the number of molecules should be considerd in the actual cell[4].

We use Gillespie's Direct Method[2]. The Probability of each reaction is calculated as the following equation,

$$P_{Ri} = r_i x_i x_{i+1} V = \frac{r_i N_i N_{i+1}}{V}, \quad (3)$$

where r_i is the reaction rate constant, V is the volume of the cell, and N_i is the number of chemical species. The probability of reaction of producing membrane substances is calculated from the Equation 4.

$$P_{C_i} = c_i x_i V = c_i N_i, \quad (4)$$

where c_i is the reaction rate constant of producing membrane substances. And the probability of reverse reaction is caclulated from Equation 5.

$$P_{B_i} = b_i m_i V = b_i Z_i, \quad (5)$$

where b_i is the rate constant of the reverse reaction, m_i and Z_i are the concentration and the number of membrane substances, M_i, respectively. The probability of efflux of chemical species from inside of the cell into the external envronment is calculated from Equation 6.

$$P_{Oi} = D_i x_i V = D_i N_i, \quad (6)$$

where D_i is the diffusion coefficient of efflux of chemical species, X_i. On the other hand, the probability of influx of chemical species is calculated from

$$P_{Ii} = D_i s_i V, \quad (7)$$

where s_i is the concentration of the ith chemical species in the external environment.

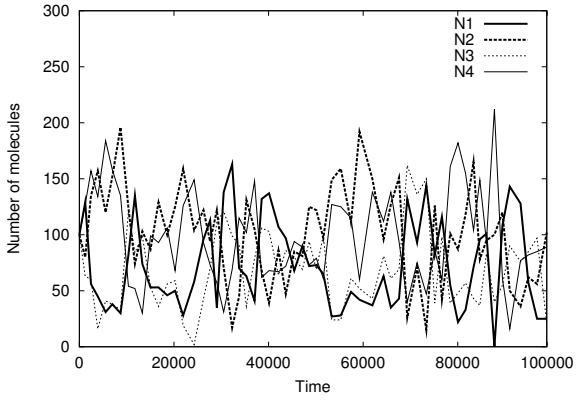
3 Results

The simulation parameters in all the simulations are set up as follows.

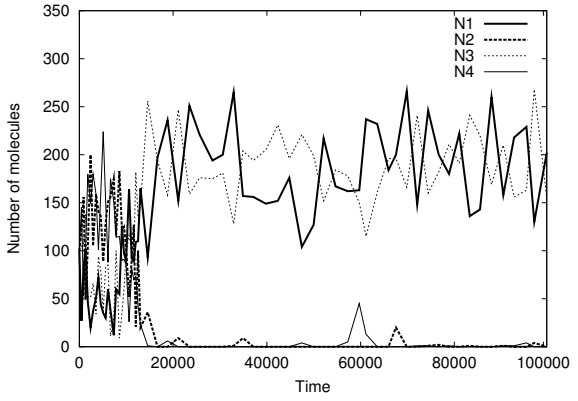
- The number of chemical species $k = 4$.
- All the reaction rate constants $r_i = 0.1 \quad (i = 1, \ldots, 4)$.
- Membrane substances are only produced from X_3 and X_4. Namely, there are two membrane substances, $\mathrm{M}_3, \mathrm{M}_4$.
- The reaction rate constants of membrane producing and reverse are $c_j = b_j = 0.01 \quad (j = 3, 4)$.
- Every initial number of molecules are $N_1 = N_2 = N_3 = N_4 = Z_3 = Z_4 = 100$.

3.1 Basic properties

Firgure 2(a)(b) show examples of the typical phenomena of each molecule without permselectivity in this model. Figure 2(a) shows the time-series of the number of chemical species when the diffusion coefficient $D_i = 0.001 \quad (i = 1, \ldots, 4)$ in each molecule, and Figure 2(b) when $D_i = 0.0001 \quad (i = 1, \ldots, 4)$. In the case of higher diffusion coefficient, the number of molecules oscillates. On the other hand, when the diffusion coefficient is lower, only X_1 and X_3 oscillate and X_2 and X_4 are mostly zero after $Time = 20000$. The opposite case, namely X_2 and X_4 oscillate and X_1 and X_3 are mostly zero, can occur with the same probability. The cell volume is almost constant all through the time without permselectivity irrespective of the diffusion coefficient.



(a)



(b)

Figure 2: The time-series behavior of the number of molecules in a cell without permselectivity. (a) Diffusion coefficient $D_i = 0.001$, (b) $D_i = 0.0001$ for all i.

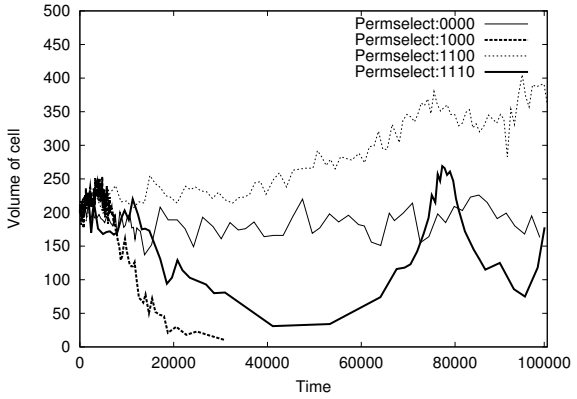


Figure 3: Examples of cell volume change as a function of time with permselectivity pattern.

3.2 Diversification driven by permselectivity

When each chemical species has a different permeability, the volume changes as a function of time. The time-series of cell volume are exemplified in Figure 3. In this figure 'Permselect:$p_1p_2p_3p_4$' designates the permselectivity pattern of membrane for each chemical species. $p_i = 1$ means high permeability $D_i = 0.001$, and $p_i = 0$ means low permeability $D_i = 0.0001$. For example, 'Permselect:1000' means $D_1 = 0.001, D_2 = D_3 = D_4 = 0.0001$. As shown in the previous subsection, in the case of no permselectivity, 'Permselect:0000', the cell volume is almost constant all through the time. This is shown by the thin solid line in Figure 3. The cell volume is increasing as shown by the thin dashed line in Figure 3 in the case that only D_1 and D_2 are high value. The cell volume changes with big fluctuation when D_1, D_2, and D_3 are high(thick solid line in Figure 3). The low value of only D_1 makes the cell volume tend to decay and terminate the reaction finally. This is shown by the thick solid line in Figure 3. Note that these results do not necessarily mean that the same trajectories are realized every time, because these simulations are calculated stochastically.

Figure 4 shows the standard deviation of cell volume as a function of time for some representative permselectivity patterns. Note that the value is the standard deviation of one hundred simulations with different random seeds in each permselectivity pattern. The patterns are classified into three groups. First, the value of standard deviation is under 100 at $Time = 100,000$. Second, the value of standard de-

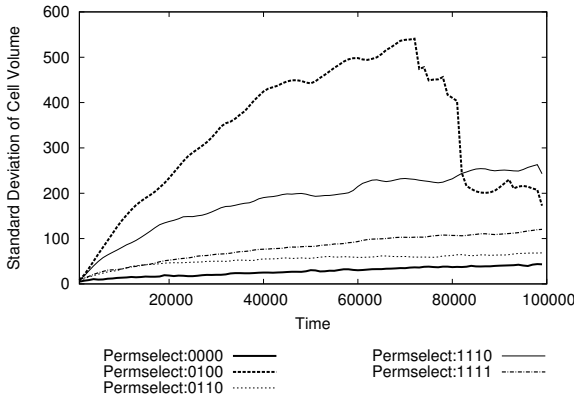


Figure 4: Standard deviation of cell volume as a function of time for each permselectivity pattern.

Table 1: Class of permselectivity

Class	Pattern
1	0000
2	1000, 0100, 0010, 0001
3	1010, 0101
4	1100, 0110, 0011, 1001
5	1110, 1101, 1011, 0111
6	1111

viation goes over 200 at $Time = 100,000$. Last, the value increases over 400 once but decreases drastically at $Time = 70,000$ around. The differences of cell volumes can occur despite that the reaction and the other conditions are totally the same.

We define the rate of standard deviation change of cell volume as the rate of diversification, because we can think that the reproduction rate and the survival rate depend on the cell volume. The rate of diversification in each permselectivity class are shown in Figure 5. The class of permselectivity is summerized in Table 1 from the view of symmetrical property of permselectivity. The way to indicate permselectivity in Table 1 is the same as 'Permselect:$p_1p_2p_3p_4$' in Figure 4. The class 1 and 6 show the rate of diversification without permselectivity. The class 2 and 3 show much higher value than the others, but the standard deviations of cell volume decay halfway through the time in these classes as shown in Figure 4('Permselect:0100'). The class 5 has the next higher value. Averagely the rates of diversification with permselectivity are higher than without permselectivity.

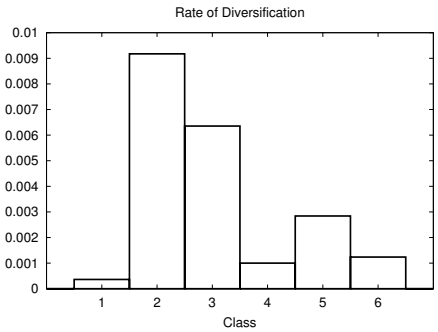


Figure 5: The rate of diversification in each class.The 'Pattern' in Table 1 means permselectivity pattern.

4 Conclusion

We construct a simple autopoietic proto-cell model in which auto-catalytic reactions produce membrane substances, and consider how the membrane permselectivity influences the proto-cell diversification. The simulation results of this model show that the permselectivity of membrane can induce the diversification of the proto-cell volume. This indicates that the reproduction and survival rate of proto-cells can also diversify by the membrane permselectivity if the reproduction and survival rate are assumed to depend on the cell volume even though the internal reaction system does not change. It is, however, not directly simulated how the diversification is related to the Darwinian evolution yet. We should do the numerical experiment to prove that the variation of proto-cells is generated and maintained by the membrane permselectivity and the proto-cells can evolve by the Darwinian evolution.

References

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