Emergent Rhythms in an Artificial Chemical World Using 'Genetic Switches'

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Abstract

This paper describes a model of the artificial chemical world and its computer simulation, in which rhythms emerge. The model specifies four items of the artificial chemical world: (1) components (five kinds of particles and DNA having Genetic Switches); (2) space (2-dimensional polar grids); (3) simple reaction rules (construction and destruction of molecules, etc.); (4) simple behavioral rules (stochastic movements and stochastic collisions, etc.); The simulation demonstrates the capability of the system to exhibit emergent behavior: that is, global order of the system (regular rhythms in this case) emerges out of randomness (thorough stochastic movements and collisions) of its components.

1 Introduction

We are now trying to build "celloids" [3] that 'grow' thorough cell divisions and differentiation. One of the problems to achieve this is the variation in amounts of gene products through time. Actually, 'the timings of gene expressions' seems very important in the process of development. Therefore, we focus on 'temporal processes of gene expressions' and selected the phenomenon of 'circadian rhythms' as a simple example related to 'temporal gene expressions'.

Many lifeforms on earth exhibit circadian rhythms, in which processes the amounts of some gene products oscillate regularly. Genes contributing to circadian rhythms are found [1][2] but details of circadian clocks are still unclear. Under these circumstances, we designed the model of an artificial world and made some computer simulations.

2 The Model

Four items of the model, i.e. (1) components, (2) space, (3) reaction rules, (4) behavioral rules; are designed as follows:

1 ⟨ the components ⟩ : The world consists of (1) five kinds of particles $\{g, e, f, d, b\}$ and (2) DNA containing two genes ('E' and 'F') and their Genetic Switches[4]. (See fig.1 (left))
Particles are assumed to make **hierarchical structure**: { particle (**P**), molecule (**M**), complex (**C**) }. For example, a particle exists either as a 'free' one or as a member of a 'molecule'. We assume three kinds of molecules $\{G, E, F\}$ and their component-parts to be g's, e's, f's, respectively. The particle 'd' (for "destroyer") catalyzes the dissociation of E's and F's, whereas the particle 'b' (for "builder") catalyzes the synthesis of E's and F's, as follows:

$$E \xrightarrow{d} \alpha e; \quad F \xrightarrow{d} \beta f; \qquad \alpha e \xrightarrow{b(e)} E; \quad \beta f \xrightarrow{b(f)} F; \quad (\ \alpha \text{ and } \beta \text{ are integer parameters})$$

Note(1): The particle 'b' takes one of the three states: $\{\ b(), b(e), b(f)\ \}$, and this state determins its catalytic capability.
Note(2): All particles are assumed to be **conserved**. Denotating $N(X)$ as the amount of the particle (or molecule) X, and $\dot{N}(X)$ as $(d/dt)N(X)$, $\dot{N}(g) = \dot{N}(e) = \dot{N}(f) = \dot{N}(d) = \dot{N}(b) = 0$. We also assume $\dot{N}(G) = 0$; but $\dot{N}(E) \neq 0$; $\dot{N}(F) \neq 0$;

2 ⟨ the (grid) space ⟩ : Each of P's or M's or C's exist in one of the grids. (The current version of the space is the 2-dimensional polar grids: see fig.1 (center)) The P's or M's or C's move around and/or collide one another (according to the behavioral rules) and react, if possible, when collide (according to the reaction rules).

3 ⟨ the reaction rules ⟩ : Dimer 'GE' is assumed to be more stable than dimers 'GG' or 'EE'. Only one dimer, either 'GG' or 'EE', is assumed to be bindable to DNA. (See fig.1 (left & right)) When a particle 'b' collides to DNA, the state of 'b' changes as follows:
(1) If a dimer 'GG' is binding to DNA, then $b(*) \rightarrow b(e)$; $(b(*) \in \{b(), b(e), b(f)\}$
(1) If a dimer 'EE' is binding to DNA, then $b(*) \rightarrow b(e)$; $(b(*) \in \{b(), b(e), b(f)\}$
Otherwise, the state of 'b' does not change. (See fig.1 (right))

4 ⟨ the simple behavioral rules ⟩ : See fig.2(left).

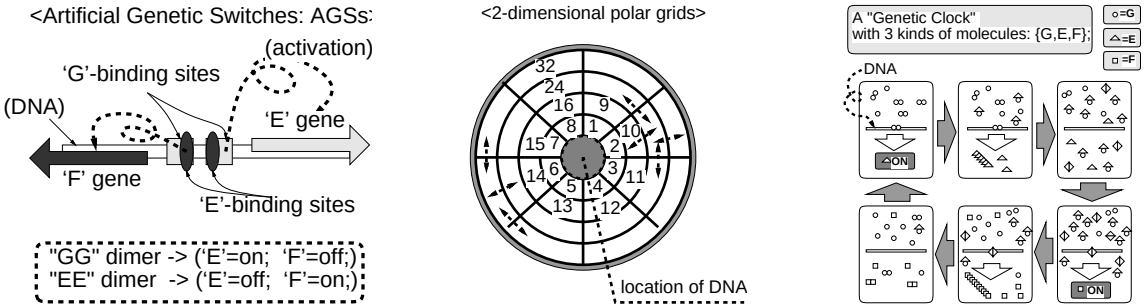

Figure 1: (L)= Artificial Genetic Switches; (C)= 2D polar grids; (R)= Clock cycle with {G,E,F}'s

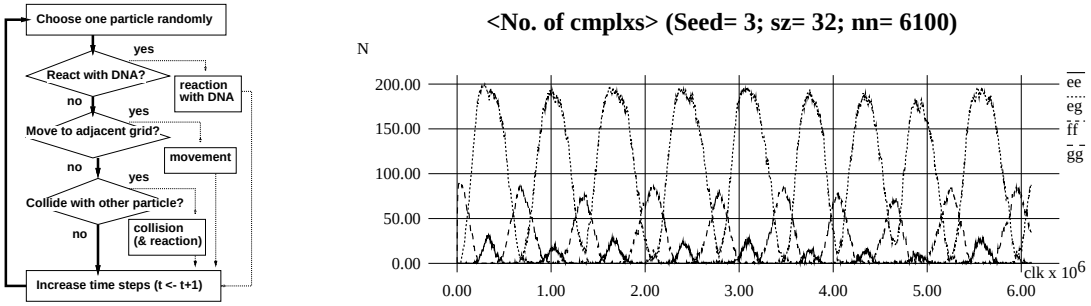

Figure 2: (L)= Behavioral flow chart; (R)= An example of the simulation;

3 Results

As is shown in fig.2 (right), almost regular rhythm in the amount of dimers 'GE's emerged.

Acknowledgement

This work was supported in part by a Grant-in-Aid (8293103) for Scientific Research on Priority Areas from The Ministry of Education, Science, Sports and Culture in Japan.

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