Reaction-Diffusion Risk: Chemical Signaling in a Conquest Game

Nathanaël Aubert-Kato[1] & Olaf Witkowski[2]

[1]Ochanomizu University, Tokyo
[2]The University of Tokyo, Tokyo
aubert.kato.nathanael@ocha.ac.jp, olaf@sacral.c.u-tokyo.ac.jp

Late-Breaking Abstract

The spontaneous generation of life has long been a central question investigated in the study of the origins of life [Szathmáry and Smith, 1995, Bedau et al., 2000]. The most common constructive approach to this problem might be artificial chemistry, the computer-inspired modeling of systems composed of chemical substances, either simulated with interaction rules and with more or less coarse-grained structures or implemented *in vitro*.

Reaction–diffusion (RD) systems, first introduced by Alan Turing [Turing, 1952], are models explaining how concentrations of spatially distributed chemical substances change locally with local reactions by which the chemicals are transformed into each other, and diffusion which causes the substances to spread out over a surface in space. One of the most famous artificial reaction diffusion system is the Belousov-Zhabotinsky chemical system, displaying complex temporal patterns [Zaikin and Zhabotinsky, 1970].

RD systems can be applied to molecular programming, involving the specification of structures, circuits and behaviors within living and non-living systems, in which decision-making will carried out by chemical processes themselves.

In the past, RD-based molecular programming has been showing impressive results, both from the experimental side [Chirieleison et al., 2013, Padirac et al., 2013] and the theoretical side [Scalise and Schulman, 2014].

In this paper, we use a molecular programming model (implementing a Risk-like game[1]-like simulation) to explore a minimalist type of signaling system, by which the state of an entity affects other entities. In particular, we explore the signaling between chemicals substances within the following set of reactions, with interactions based on an extension of the system presented by Padirac et al. [2012] (Figure 1):

$$A + land \rightarrow A + land + tA$$

$$A + tA \rightarrow 2A + tA$$

$$B + land \rightarrow B + land + tB$$

$$B + tB \rightarrow 2B + tB$$

The "land" are chemical species that template the production of other species, which in turn is used to catalyze the production of signal. "Land" species are considered to be tethered to the surface and thus do not diffuse. They are also protected against degradation. All other species are degraded over time.

To allow for competition, the reactions based on substance A (resp. B) are inhibited by substance B (resp. A). Substances tA and tB represent "agents", whereas A and B are "signals". Signals can propagate much further than the agents themselves, and are used to take over new areas on the board. Population can also be neutral when as roughly as much A and B are present (including when they are both 0).

In simulation, a transient fight was observed (see Figure 2) between the agents tA and tB, for the conquest of a central land area. Interestingly, even at equilibrium, areas of influence were observed to be maintained by the exchange of signals A and B. In certain runs, because of the signaling-induced areas of influence, both agents were kept from some land area, which remained "neutral".

To wrap up, our preliminary results showed, for a simple reaction-diffusion molecular programming model, new insights on the influence of proto-signaling, as an indirect and delayed behavior that impacts on

[1]Risk is a strategy game, played on a board depicting a political map of the Earth, divided into forty-two territories. Players control armies with which they attempt to capture territories, with results determined by dice rolls. To win the game, object of the game is to occupy every territory on the board and in doing so, eliminate the other players.

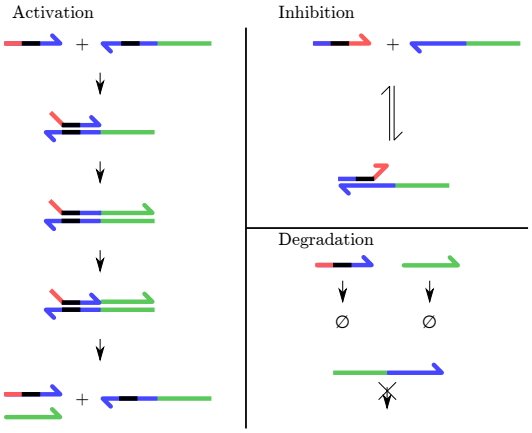

Figure 1: **Diagram of considered molecular programming reactions, displaying the three fundamental principles of the model: activation, inhibition and degradation.** Activation: a signal strand attaches to a template species, generating a new molecular species. Inhibition: A signal can inhibit templates based on its counterpart by partially attaching to it. No reaction ensues due to the mismatches. Black: part common to both signal species, used to ensure the basic stability of all complexes. Degradation: all generated species are degraded over time, except for "land" species, which are chemically protected.

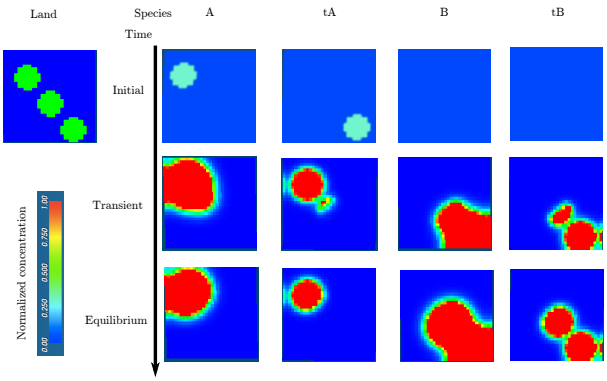

Figure 2: **Visualization of the different stages of a simulation.** Each square represents a local normalized heatmap of concentrations respectively in A, tA, B and tB, with values ranging from 0 (blue) to 1 (red). Simulated with Ready [Hutton et al.].

competition in multi-agent systems. In particular, it is interesting to notice the strong localization of "agents" in spite of the global catalysis from signal. While our approach relies on a DNA computing implementation for convenience, the principles of this study can be extended to various chemical systems. The next step will consist in developing the model further with variation, to study the coevolution between signaling and heredity. It would be also interesting to implement stochasticity to have non-deterministic behaviors.

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