Challenging the Robustness of Simulated Protocells

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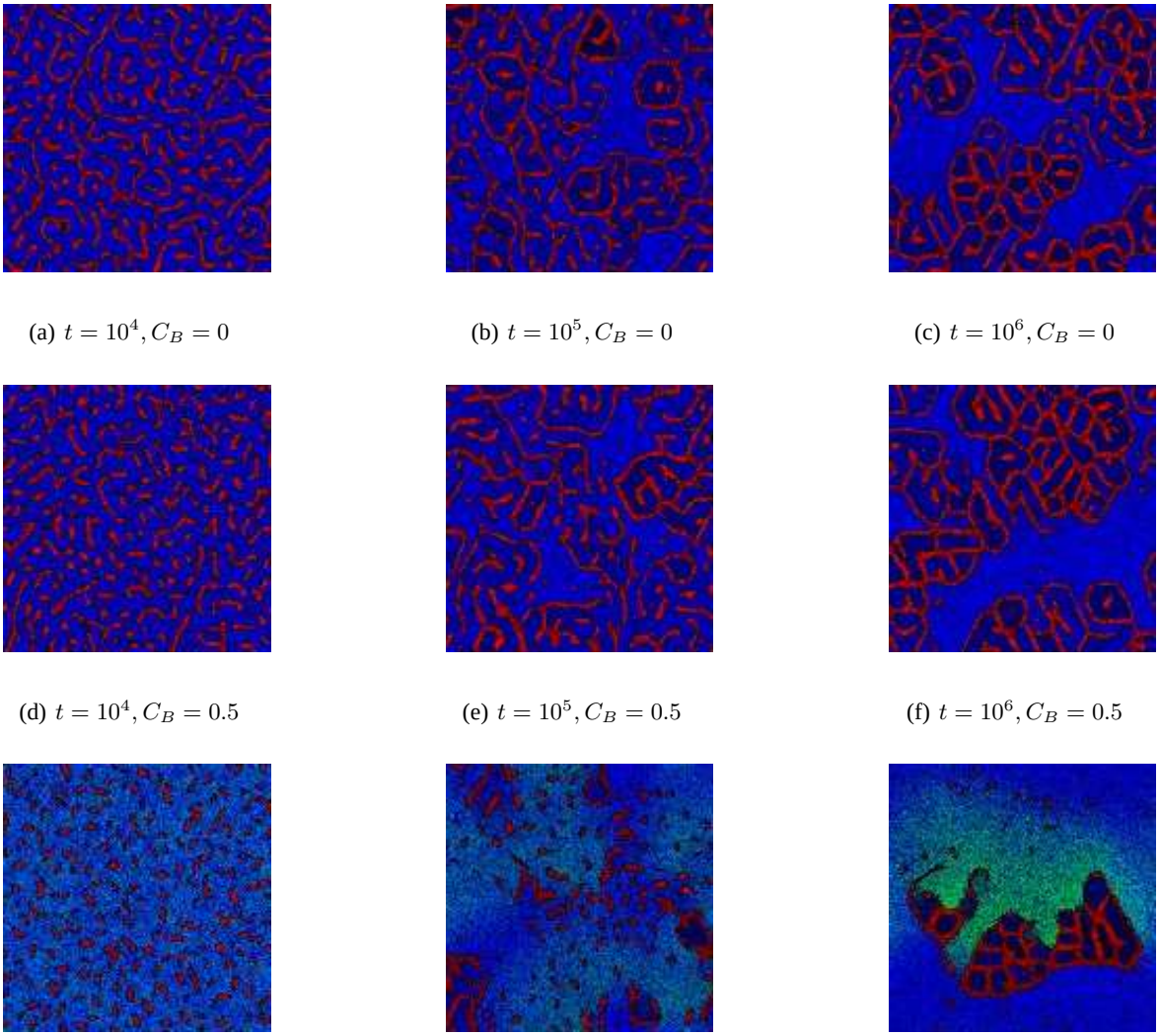
Extended Abstract

We have re-implemented and extended the 2D artificial chemistry model of Ono and Ikegami (2001) (see also Ono (2005)) to increase its behavioural diversity. In its original form, this cellular automata (CA) simulation of primitive chemical life produces self-organising, autopoietic protocells from a random initial configuration of membrane, catalyst, resource, waste, and water particles. These particles are free to diffuse across the CA lattice, rotate (in the case of membrane particles) and undergo chemical reactions. The system is updated stochastically, but the transitions are biased according to local potential energy gradients. These energies are specified by pre-defined repulsive interactions, which depend on the types of the interacting particles and their relative positions and orientations. All interactions are short-ranged (one lattice spacing or less). The chemistry of the system is autocatalytic, i.e. the catalyst particles stimulate their own replication (a catalyst resource particle and a catalyst particle react to form two catalyst particles). The catalyst particles also stimulate the production of membrane particles from their own resource particles. All particles spontaneously decay into wastes, which are recycled at a constant rate by an external energy source. In certain regions of the systems parameter space, it will evolve towards a configuration possessing long-range order, expressed by the clustering of membrane particles, which eventually form closed boundaries. If a sufficient number of catalyst particles are confined within a membrane loop, membrane decay can be compensated by membrane synthesis due to the presence of the catalyst particles (figure 1(c)). These protocells are capable of maintaining their own boundaries, the defining property of an autopoietic entity.

Our extension of the model consisted of introducing a new particle, B, with identical characteristics to the catalyst particle except that rather than stimulating the production of membranes, it stimulates their decay. At low initial concentrations, the new particle has little effect on the formation and proliferation of protocells (figure 1(f)). However, when initialised at the same concentration as the membrane-producing catalyst, the new particle inhibits protocell formation (figure 1(h)). Only a small number of cells are able to form and the characteristic time required for the emergence of the protocells is much longer than simulations run in the absence of the B-particles.

However, once membranes form and aggregate, the new particle takes advantage of the fact that membranes are almost impermeable to catalyst particles. If a cloud of B-particles is bordered by one or more membranes, it is much less likely that they will diffuse away since they will be sheltered from the dispersive effects of diffusion. This protection enables an increase in the density of B-particles, which then leads to a stronger decay rate of local membrane particles (figure 1(i)). Thus if a sufficiently dense cloud of B-particles arises near to a cluster of protocells, it is able to increase in concentration such that protocells and sometimes even whole clusters of protocells are destroyed or segregated. This behaviour is reminiscent of a primitive pursuit-evasion scenario with protocells being forced to grow in the direction of low B-particle density.



(a) $t = 10^4, C_B = 0$ (b) $t = 10^5, C_B = 0$ (c) $t = 10^6, C_B = 0$

(d) $t = 10^4, C_B = 0.5$ (e) $t = 10^5, C_B = 0.5$ (f) $t = 10^6, C_B = 0.5$

(g) $t = 10^4, C_B = 1$ (h) $t = 10^5, C_B = 1$ (i) $t = 10^6, C_B = 1$

Figure 1: Proto-cell development in the presence of a membrane-toxic particle. Depth of red, blue, and green correspond to the density of membrane particles, water particles, and membrane-toxic particles, respectively. System snapshots are shown for three different normalised concentrations of the membrane-toxic particle, C_B (increasing from top to bottom) and for three different discrete times, t (increasing from left to right).

References

Ono, N. and Ikegami, T. (2001). Artificial Chemistry: Computational Studies on the Emergence of Self-Reproducing Units. In Kelemen, J and Sosik, P., editors, *Advances in Artificial Life*, pages 186-195. Springer-Verlag, Berlin.

Ono, N. (2005). Computational studies on conditions of the emergence of autopoietic protocells. *BioSystems*, 81:223–233.