Glider-based computing in reaction-diffusion hexagonal cellular automata

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Abstract

A three-state hexagonal cellular automaton, discovered in [36], presents a conceptual discrete model of a reaction-diffusion system with inhibitor and activator reagents. The automaton model of reaction-diffusion exhibits mobile localized patterns (gliders) in its space-time dynamics. We show how to implement the basic computational operations with these mobile localizations, and thus demonstrate collision-based logical universality of the hexagonal reaction-diffusion cellular automaton.

Key words: cellular automata, gliders, localizations, collision-based computing

1 Introduction

Novel computing paradigms and architectures emerged recently, see overview in [30], include an intriguing field of reaction-diffusion computing [2] whose aim is to design theoretical models and laboratory prototypes of chemistry-based computing devices. In reaction-diffusion processors data are represented by disturbances of the concentration profile of reagents, information transmission by traveling diffusive or excitation waves, and computation by the interaction of traveling waves. The result of computation is represented as either dynamical space-time patterns of excitation or as a stationary concentration profile. Reaction-diffusion processors have proved to be capable of

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solving a series of problems, from image processing to the control of robot navigation [19,27,3,31,9,4,5]. The processors are specialized; to be universal they must realize a functionally complete set of logical gates in their space-time dynamics.

Several logically universal reaction-diffusion devices have been implemented so far; they include logical gates [33,29] and diodes [20,16,25] in the Belousov-Zhabotinsky (BZ) medium, and XOR gates in palladium processors [6]. These designs are structure-determined, because computation is implemented in a geometrically constrained chemical medium. Essentially, the structure-determined processors simply imitate conventional computing architectures in novel chemical materials.

There is another class of universal reaction-diffusion processors — dynamical, or structureless, processors. There information is represented by compact localized traveling patterns, and logical operations are implemented via collision between the patterns. The idea originates from the computational universality of the Game of Life [11], conservative logic and the billiard-ball model [17], and their cellular-automaton implementations [23]. The compact patterns travel in space and perform computation when they collide with each other. There are no predetermined stationary wires — a trajectory of the traveling pattern is a momentary wire — almost any part of the medium's space can be used as a wire. Truth values of logical variables are given by either the absence or presence of a localization or by various types of localizations (see overview in [7]).

Results obtained so far in logically universal structureless reaction-diffusion processors employ localization dynamics in a reaction-diffusion excitable medium — cellular-automata models on orthogonal lattices [1], numerical simulations of the Oregonator system [8] and experimental implementations of logical circuits in the Belousov-Zhabotinsky system with an immobilized catalyst [14]. There are, however, a variety of chemical systems which could potentially be used to implement dynamical computation [15]; some of them involve complicated chemical reactions with activator and inhibitor species. In the present paper we aim to fulfill a double objective. First, to give an example of collision-based computing in a reaction-diffusion system with inhibitor and activator species (which differs from the 'classical' model of an excitable medium). Second, to provide an example of localization-based computing in hexagonal cellular automata [26] — so far, we are aware that computational universality of hexagonal automata was proved by embedding a Fredkin gate [24], but we have no evidence that hexagonal automata support gliders in the 'classical' excitable medium model, such as those described for orthogonal lattices in [1].

In our studies we employ the 'beehive' cellular automaton rule (Sect. 2), discovered by Wuensche [36,37], which exhibits glider dynamics, and allows for a reaction-diffusion interpretation (Sect. 3). Using the particulars of glider collision we construct the basic logical gates and signal routing operations (Sect. 4) sufficient to demonstrate the computational dynamical universality of the hexagonal cellular automata. Theoretical results obtained in the paper will be used in future for the experimental implementation of collision-based computing devices in chemical reaction-diffusion systems.

2 Beehive rule

We can convert the rule transition table presented in [36,37] to a more compact matrix form $\mathbf{M} = (m_{ij})$, where $0 \leq i \leq j \leq 6$, $0 \leq i + j \geq 6$, and $m_{ij} \in \{0, 1, 2\}$:

$$M = \left\{ \begin{array}{l} 0\ 1\ 2\ 1\ 2\ 0\ 0 \\ 0\ 2\ 2\ 2\ 1\ 1 \\ 0\ 0\ 2\ 2\ 0 \\ 0\ 2\ 2\ 0 \\ 0\ 0\ 2 \\ 2\ 0 \\ 0 \end{array} \right\}$$

Every cell x of the hexagonal lattice updates its state in discrete time t as follows: $x^{t+1} = m_{\sigma_2^t(x),\sigma_1^t(x)}$, where $\sigma_z^t(x) = |\{y^t = z : y \in \mathbf{U}(x)\}|$, $\mathbf{U}$ is a hexagonal neighborhood of x. Cell x is not included in its neighborhood, therefore the state transitions are independent of the states of the cell x itself. For example, if neighbourhood of cell x has two cells in state 2 and one cell in state 1 (implying there must be three cells in state 0) then the output can be read of from the matrix M from the intersection of row 2 and column 1 ($m_{21} = 2$). Note that i represents rows numbered from 0 to 6, and j represents columns numbered from 0 to 6.

Starting its evolution in a random initial configuration (Fig. 1a) the automaton exhibits mobile localized patterns — gliders — which dominate the lattice at the concluding phase of development (Fig. 1b-d). The gliders either leave the lattice due to absorbing boundary conditions or continue traveling undisturbed, along non-intersected trajectories, if boundaries are periodic. A glider is composed of one cell in state 1, which is a head of the mobile localization, and a tail of four cells in state 2, as shown below in an example of glider traveling west:

```
0   0   0   0
  0   2   2
0   1   0   0
  0   2   2
0   0   0   0.
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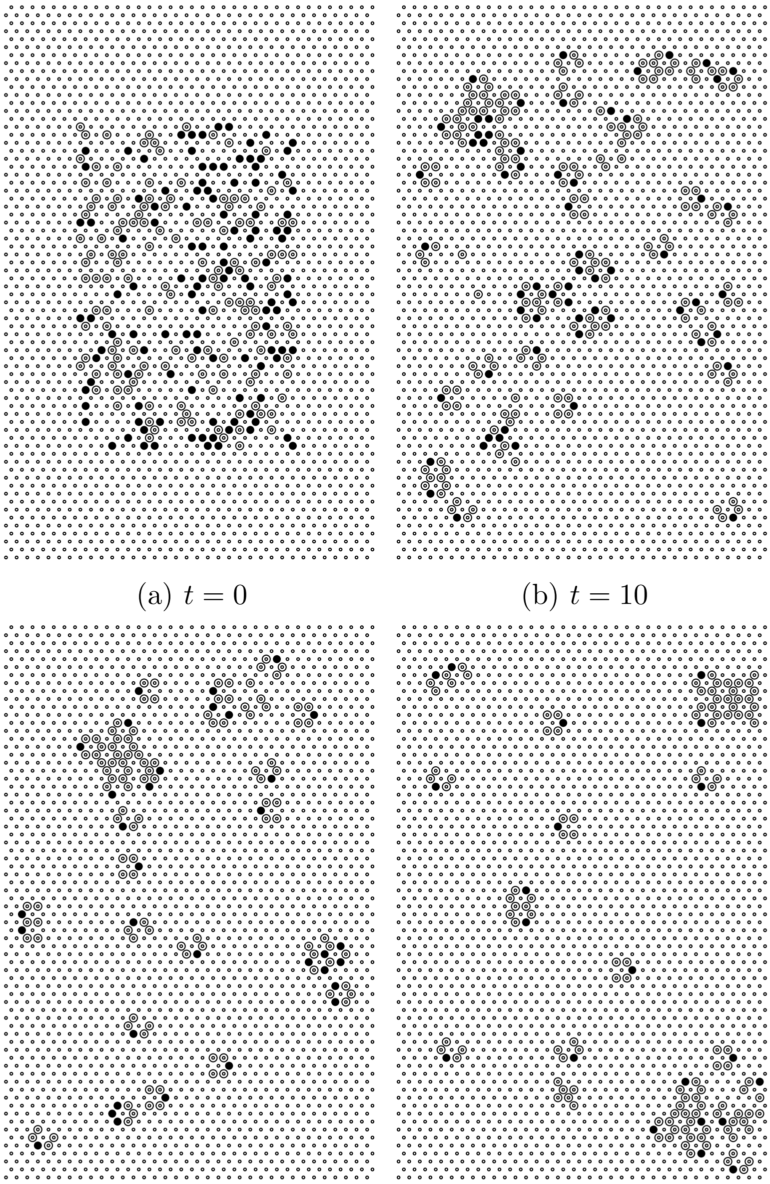


(a) $t = 0$ (b) $t = 10$

(c) $t = 20$ (d) $t = 50$

Fig. 1. Development from random initial configuration. Cells in state 1 are shown as •, state 2 as ⊚, and state 3 as ∘.

Detailed analysis of glider dynamics is provided in [36,37], which shows that there are 21 types of binary collisions (between pairs of basic gliders). Self-destruction, survival, reflection, conservation and self-reproduction all occur, depending on the exact point and direction of impact. Self-reproduction can produce 4, 5 or 6 gliders from a binary collision. Other interactions result in polymer-like gliders made of subunits. Most notably, a variety of mobile glider-guns are seen to emerge, which can eject from 1 to 4 (possibly more) glider streams in different directions.

3 Reaction-diffusion interpretation

The glider's structure — an active head and following tail — indicates a possibility of a reaction-diffusion interpretation of the cell state transition rules. Assume the automaton simulates a chemical medium with three reagents E (equivalent of cell state 1), I (equivalent of state 2) and S (state 0). A cell takes state z when all six neighbors are in the state z only for $z = 0$, therefore the reagent S can be earmarked as a substrate.

State 1 is at the leading edge of propagating patterns, so E is an activator, or an excitation state. It was demonstrate in [36] that changing the values of ten entries in the matrix M, e.g. m_{03}, m_{14}, m_{15} and m_{16}, does not affect the formation and propagation of gliders; for simplicity we can take them equal to 0. So, this leaves only one condition of cell activation — one neighbor in state 1 and others in state 0 ($m_{01} = 1$). The presence of even one neighbor in state 2 prevents activation. Therefore, we can say that reagent I is an inhibitor of the activation reaction.

Only reagent E is diffusive/reactive when added to pure solution of the substrate S because $m_{01} = 1$. However in higher concentration reagent E produces inihibitor I ($m_{02} = 2$).

To assess the reactions producing reagent I we can again simplify the transition matrix M, based on [36], and assign value 0 to 'wildcard' entries m_{04}, m_{13}, m_{14}, m_{15} and m_{23}.

The reagent I is involved in a reaction with E (entry $m_{42} = 2$) with the formation of I, so reagent E plays the role of a catalyst for I. The remaining entries of the matrix M determine that a transition to state 2 happens when $1 \leq \sigma_2 \leq 3$, $1 \leq \sigma_1 \leq 4$ and $1 \leq \sigma_0 \leq 4$ but not for $(\sigma_2 = 2, \sigma_1 = 1)$. So, the final state transition matrix will be as follows, where 'wildcard' entries are underlined:

$$M^{\mathrm{RD}} = \begin{Bmatrix} 0\ 1\ 2\ \underline{0}\ \underline{0}\ \underline{0}\ \underline{0} \\ 0\ 2\ 0\ \underline{0}\ \underline{0}\ \underline{0} \\ 0\ 0\ 2\ \underline{0}\ \underline{0} \\ 0\ 2\ 2\ \underline{0} \\ 0\ 0\ 2 \\ 2\ 0 \\ 0 \end{Bmatrix}$$

The automaton with cell transition states determined by M^{RD} simulates a reaction-diffusion system of three reagents with activator E, inhibitor I and substrate S, the dynamics of which is governed by the quasi-chemical reactions below, where $1 \leq \gamma_I \leq 3$, $1 \leq \gamma_E \leq 4$ and $1 \leq \gamma_S \leq 4$ but not $(\gamma_I = 2, \gamma_E = 1)$; and, $\beta_E > 3$, $\beta_I \neq 5$:

$$
\begin{aligned}
E + 5S &\to E \\
I + 5S &\to I \\
2E + 4S &\to I \\
4I + 4E &\to I \\
\beta_E E &\to S \\
\beta_I I &\to S \\
\gamma_I I + \gamma_E E + \gamma_S S &\to I.
\end{aligned}
$$

In the system inhibitor I is produced by activator E, and both reagents E and I degrade in certain concentrations.

There are a number of chemical systems where travelling wave fragments ("quasi-particles") have been generated. For example in sub excitable media wave fragments can be induced in a system at steady state via the application of light noise [35].

However, to investigate further the phenomena found in the beehive rule, whilst adhering to the general reaction scheme proposed would require a chemical system to be identified that was a stationary or mobile generator of quasi-particles. Although no experimental studies are apparent or can be carried out under the remit of this current study two possible chemical classes for further investigation are considered.

The first which would seem to fit appropriately with the scheme described are chemical systems exhibiting Turing type pattern formations. Chemical systems such as the Chlorite-Iodide-Malonic acid (CIMA) system [13] and the more recently discovered BZ-AOT [34] have been shown experimentally to exhibit the classical spot, stripe and labyrinthine patterns (Turing patterns).

Lee et al. also showed experimentally in the Ferrocyanide-iodate-sulphite reaction the existence of self replicating spots and in numerical studies the transition from a spot to an annulus [21]. Although the Turing instability results in spatially periodic patterns that are stationary in time the interaction between Turing and Hopf or wave (oscillatory Turing) instabilities has been shown numerically (and in part experimentally in BZ-AOT system) to result in interesting spatio-temporal dynamics including modulated Turing structures and modulated standing waves [38]. Recently, spatiotemporal travelling wave patterns have been observed on the skin of mutant mice and this is thought to be the result of a misconfigured Turing mechanism with competing instabilities [32]. Liehr et al. [22] found that dissipative quasi-particles were generated near the Turing bifurcation in three dimensional reaction diffusion systems.

In simulations involving travelling quasi-particles they were able to show that two quasi-particles collide to form a transient compound state which then breaks into two new quasi-particles.

The second class of reactions are based on anistropic bistable media which have been shown to be a rich source of travelling wave fragments both in experimental [28] and numerical studies [10,18].

During the catalytic oxidation of CO on Pt(110) [28] at certain experimental parameters patterns consist of solitary waves with bell-shaped profiles which propagate with a constant velocity along the crystallographic [001] axis (i.e. the direction is controlled by the anisotropy of the system). Collision of waves travelling in opposite directions leads mostly to annihilation, but in some cases the two waves emerge again with unchanged shapes and velocities.

Whilst none of the above chemical systems fits exactly with the theoretical part of this study it does provide a list although by no means exhaustive of some reactions exhibiting travelling wave fragments. Additionally it serves to highlight where experimental research could in the future yield such activator-inhibitor type systems capable of directed computation via the collision of mobile wave fragments.

4 Glider interaction operations

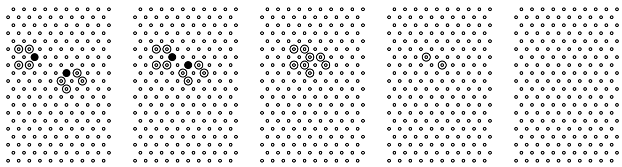
A system is logically universal if it implements a functionally complete system of logical gates in its space-time dynamics, so to show that the hexagonal reaction-diffusion automaton is logically universal we could just demonstrate the implementation of conjunction $\wedge$ or disjunction $\vee$ and negation $\neq$ gates.

The simplest gate

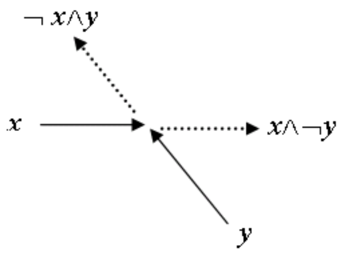
$$\langle x, y \rangle \rightarrow \langle x \wedge \neg y, \neg x \wedge y \rangle$$

is implemented when two gliders collide and annihilate as the result of the collision (Fig. 2a-e). The undisturbed trajectory of the glider representing the value of x is interpreted as $x \wedge \neg y$, and glider y — $\neg x \wedge y$ (Fig. 2f).

To generate constant TRUTH signals we can use generators of gliders, glider guns. So far no stationary glider guns are found in the studied reaction-diffusion automaton, however several types of mobile guns were discovered and classified in [36], shooting from 1 to 4 glider streams in various directions. An example of a mobile gun generating three streams of gliders is shown in Fig. 3. The automaton exhibits a glider gun only when $m_{03} = 1$, which implies a high degree of non-linearity of chemical reactions underlying the automaton rules — activator E reacts with substrate S when the number of E molecules



(a) $t = 1$ (b) $t = 2$ (c) $t = 3$ (d) $t = 4$ (e) $t = 5$



(f)

Fig. 2. A glider heading east (represents x) collides with a glider heading north-west (represents y), both gliders annihilate as the result of the collision. Collision dependent trajectories are shown by dotted lines.

equals one or three, and two molecules of the activator produces inhibitor I.

However, logical universality gives us just the basic requirements to implement real computation architectures in a reaction-diffusion automaton; a few more operations — at least reflection and multiplication — are needed to feel comfortable about the computational potential of the automaton.

For certain initial positions of gliders, one glider is reflected (i.e. inverts its velocity vector) when it collides with another glider. Thus in Fig. 4a-j we can see that when a glider heading east collides with a glider heading north-east, the former continues traveling along its initial trajectory while the latter reverses its direction — is reflected — to the west. The glider acting as a mobile reflector continues traveling the the north-east as before. Interpreting the presence of the reflector-glider as the TRUTH value of y and the other glider as x we construct the following gate (Fig. 4k):

$$\langle x, y \rangle \rightarrow \langle x \wedge y, y, x \wedge \neg y \rangle.$$

The phenomenon can be used to implement the routing of mobile signals by colliding mobile reflectors into them. A delay can be realized by employing several mobile reflectors which shuffle the signal between them for a certain period of time.

There are several types of signal multiplication that can be implemented in the automaton. In our descriptions of binary collisions leading to multiplication we will assign one glider to be the signal x and another glider to be the multiplier signal m. A collision of signal x (glider heading north-west) with a multiplier

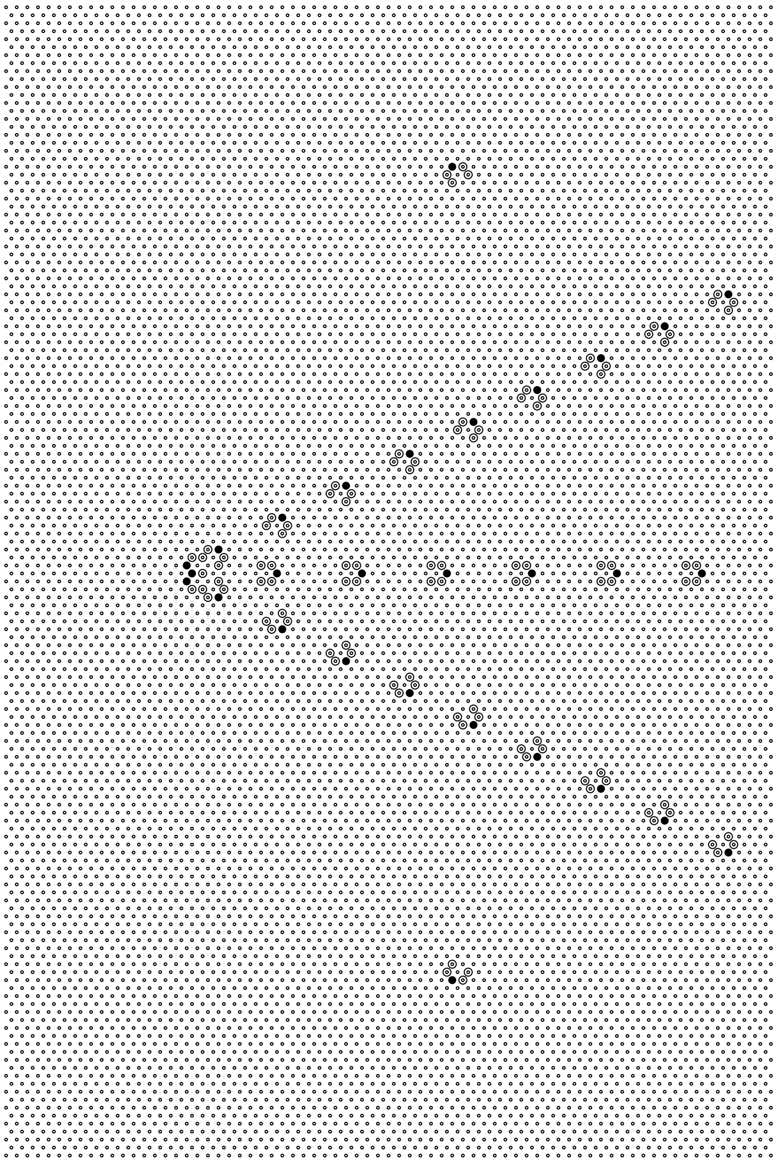
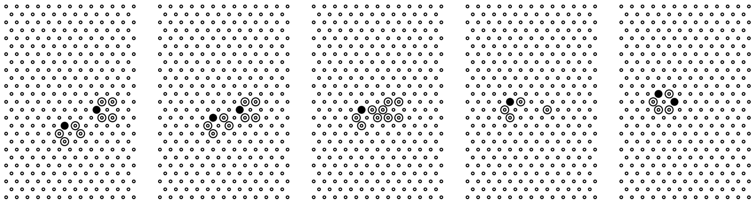


Fig. 3. A mobile glider gun travels west and emits three streams of gliders, in the north-east, east and south-east directions. Note that a requirement for glider guns is that $m_{03} = 1$.

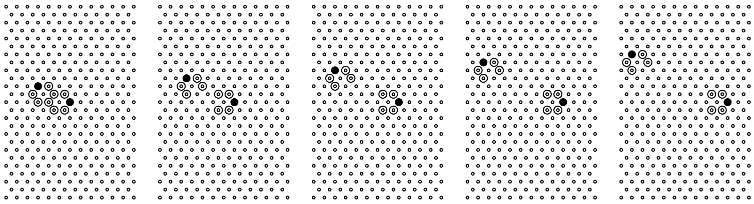
(glider traveling east) shown in Fig. 5 leads to the destruction of the multiplier, and the formation of four copies of x running north-west, south-west, east and west.

For certain conditions (Fig. 6a) of the collisions, the multiplier signal m continues traveling almost undisturbed (Fig. 6g) while the signal x is multiplied to four signals x' (Fig. 6e-i); see the scheme of collision in Fig. 6k.

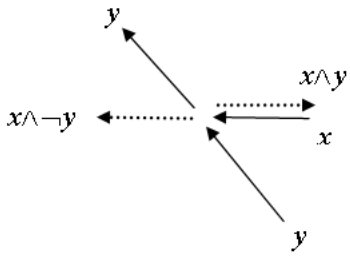
The two previous examples show that we can precisely tune signal trajectories by using disposable and reusable multipliers.



(a) $t = 1$ (b) $t = 2$ (c) $t = 3$ (d) $t = 4$ (e) $t = 5$

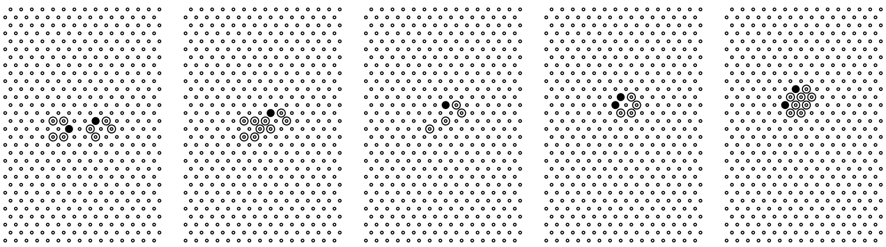


(f) $t = 6$ (g) $t = 7$ (h) $t = 8$ (i) $t = 9$ (j) $t = 10$

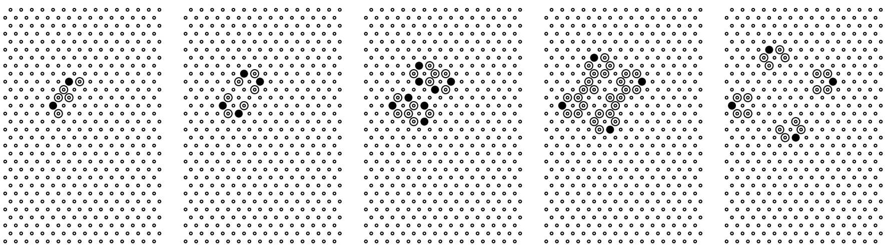


(k)

Fig. 4. Reflection. A glider traveling north-east (y) acts as mobile reflector for a glider traveling east (x). Collision dependent trajectories are shown by dotted lines.

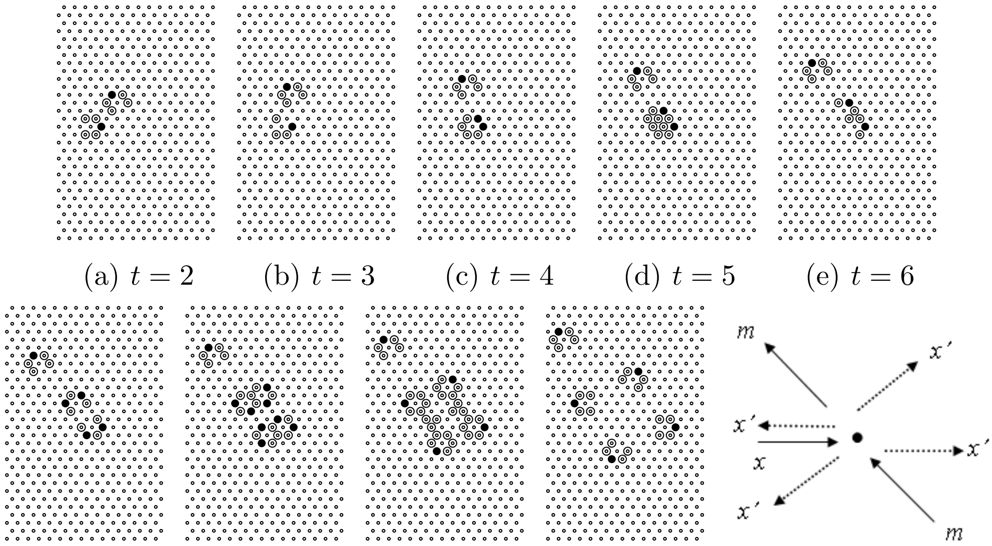


(a) $t = 1$ (b) $t = 2$ (c) $t = 3$ (d) $t = 4$ (e) $t = 5$



(f) $t = 6$ (g) $t = 7$ (h) $t = 8$ (i) $t = 9$ (j) $t = 10$

Fig. 5. Multiplication with destruction of multiplier.



(a) $t = 2$ (b) $t = 3$ (c) $t = 4$ (d) $t = 5$ (e) $t = 6$

(f) $t = 7$ (g) $t = 8$ (h) $t = 9$ (i) $t = 10$ (j)

Fig. 6. Multiplication without destruction of the multiplier. Glider m (multiplier) traveling north-east multiplies glider x traveling east. Four copies x' of signal x travel west, east, north-west and south-east. Multiplier m continues traveling along its original trajectory. Collision dependent trajectories (k) are shown by dotted lines.

5 Discussion

We employed the beehive hexagonal cellular automaton [36] to design a discrete model of a chemical reaction-diffusion system. The system is comprised of three species — substrate, activator and inhibitor. Reactions between the activator and substrate are concentration sensitive and highly non-linear; at a certain concentration of the activator the inhibitor is produced. The system exhibits compact traveling patterns — gliders — in its space-time dynamics. We constructed the basic logical gates based on details of particular glider collisions. We also demonstrated how signals — quanta of information represented by gliders — can be routed by colliding them with other control-gliders. We provided an example of a compact pattern generator — a glider gun — which is essential for implementing negation. Therefore we demonstrated that the reaction-diffusion hexagonal cellular automaton is logically universal, allows the embedding of logical circuits and can potentially implement meaningful computation operations. The chemical interpretation of the cell-state transition rules could make this model a computational prototype for further designs of laboratory prototypes of reaction-diffusion dynamical or collision-based processors. Unfortunately, we found no stationary generators of quasi-particles, which could be a subject for further investigations.

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