

Programming Reaction-Diffusion Processors

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Abstract. In reaction-diffusion (RD) processors, both the data and the results of the computation are encoded as concentration profiles of the reagents. The computation is performed via the spreading and interaction of wave fronts. Most prototypes of RD computers are specialized to solve certain problems, they can not be, in general, re-programmed. In the paper, we try to show possible means of overcoming this drawback. We envisage an architecture and interface of programmable RD media capable of solving a wide range of problems.

1 Reaction-Diffusion Computers

Reaction-diffusion (RD) chemical systems are well known for their unique ability to efficiently solve combinatorial problems with natural parallelism [2].

In RD processors, both the data and the results of the computation are encoded as concentration profiles of the reagents. The computation *per se* is performed via the spreading and interaction of wave fronts.

The RD computers are parallel because the chemical medium's micro-volumes update their states simultaneously, and molecules diffuse and react in parallel (see overviews in [1, 2, 8]). RD information processing in chemical media became a hot topic of not simply theoretical but also experimental investigations since implementation of basic operations of image processing using the light-sensitive Belousov-Zhabotinsky (BZ) reaction [28]. During the last decade a wide range of experimental and simulated prototypes of RD computing devices have been fabricated and applied to solve various problems of computer science, including

- image processing [35, 3],
- path planning [43, 12, 34, 6],
- robot navigation [7, 10],
- computational geometry [5],
- logical gates [45, 39, 4],
- counting [24],
- memory units [30].

Despite promising preliminary results in RD computing, the field still remains art rather than science, most RD processors are produced on an *ad hoc* basis without structured top-down approaches, mathematical verification, rigorous

methodology, relevance to other domains of advanced computing. There is a need to develop a coherent theoretical foundation of RD computing in chemical media. Particular attention should be paid to issues of programmability, because by making RD processors programmable we will transform them from marginal outcasts and curious freaks to enabled competitors of conventional architectures and devices.

2 How to Program Reaction-Diffusion Computers?

Controllability is inherent constituent of programmability. How do real chemical media respond to changes in physical conditions? Are they controllable? If yes then what properties of the media can be used most effectively to program these chemical systems? Despite the fact that the problem of controlling RD media did not receive proper attention until recently some preliminary although rather mosaic results have become accessible in the last decade. There is no coherent view on the subject and this will be a major future task to build a theoretical and experimental framework of chemical medium controllability. Below we provide an overview of the findings related to the external control of chemical media. They demonstrate viability of our ideas and show that the present state-of-the-art laboratory methods allow for the precise tuning of these chemical systems, and thus offer an opportunity to program RD processors.

2.1 Electric Field

The majority of the literature, related to theoretical and experimental studies concerning the controllability of RD medium, deals with application of an electric field. In a thin-layer BZ reactor stimulated by an electric field the following phenomena are observed:

- the velocity of excitation waves is increased by a negative and decreased by a positive electric field;
- a wave is split into two waves that move in opposite directions if a very high electric field is applied across the evolving medium [40];
- crescent waves are formed not commonly observed in the field absent evolution of the BZ reaction [23];
- stabilisation and destabilisation of wave fronts [26];
- an alternating electric field generates a spiral wave core that travels within the medium; the trajectory of the core depends on the field frequency and amplitude [38].

Computer simulations with the BZ medium confirm that

- waves do not exist in a field-free medium but emerge when a negative field is applied [33];
- an electric field causes the formation of waves that change their sign with a change in concentration, and applied constant field induces drift of vortices [32];
- externally applied currents cause the drift of spiral excitation patterns [42].

It is also demonstrated that by applying stationary two-dimensional fields to a RD system one can obtain induced heterogeneity in a RD system and thus increase the morphological diversity of the generated patterns (see e.g. [18]). These findings seem to be universal and valid for all RD systems: applying a negative field accelerates wave fronts; increasing the applied positive field causes wave deceleration, wave front retardation, and eventually wave front annihilation. Also a recurrent application of an electric field leads to formation of complex spatial patterns [41]. A system of methylene blue, sulfide, sulfite and oxygen in a polyacrylamide gel matrix gives us a brilliant example of electric-field controlled medium. Typically hexagon and strip patterns are observed in the medium. Application of an electric field makes striped patterns dominate in the medium, even orientation of the stripes is determined by the intensity of the electric field [31].

2.2 Temperature

Temperature is a key factor in the parameterisation of the space-time dynamics of RD media. It is shown that temperature is a bifurcation parameter in a closed non-stirred BZ reactor [29]. By increasing the temperature of the reactor one can drive the space-time dynamic of the reactor from periodic oscillations ($0 - 3^{\circ}\text{C}$) to quasi-periodic oscillations ($4 - 6^{\circ}\text{C}$) to chaotic oscillations ($7 - 8^{\circ}\text{C}$). Similar findings are reported in simulation experiments on discrete media [2], where a lattice node's sensitivity can be considered as an analogue of temperature.

2.3 Substrate's Structure

Modifications of reagent concentrations and structure of physical substrate may indeed contribute to shaping space-time dynamics of RD media. Thus, by varying the concentration of malonic acid in a BZ medium one can achieve

- the formation of target waves;
- the annihilation of wave fronts;
- the generation of stable propagating reduction fronts [26].

By changing substrate we can achieve transitions between various types of patterns formed, see e.g. [22] on transitions between hexagons and stripes. This however could not be accomplished 'on-line', during the execution of a computational process, or even between two tasks, the whole computing device should be 're-fabricated', so we do not consider this option prospective. Convection is yet another useful factor governing space-time dynamics of RD media. Thus, e.g., convection 2nd order waves, generated in collisions of excitation waves in BZ medium, may travel across the medium and affect, e.g. annihilate, existing sources of the wave generation [36].

2.4 Illumination

Light was the first [27] and still remains the best, see overview in [35], way of controlling spatio-temporal dynamics of RD media (this clearly applies mostly to light-sensitive species as BZ reaction). Thus, applying light of varying intensity we can control medium's excitability [19] and excitation dynamic in

BZ-medium [17, 25], wave velocity [37], and patten formation [46]. Of particular interest to implementation of programmable logical circuits are experimental evidences of light-induced back propagating waves, wave-front splitting and phase shifting [47].

3 Three Examples of Programming RD Processors

In this section we briefly demonstrate a concept of control-based programmability in models of RD processors. Firstly, we show how to adjust reaction rates in RD medium to make it perform computation of Voronoi diagram over a set of given points. Secondly, we provide a toy model of tunable three-valued logical gates, and show how to re-program a simple excitable gate to implement several logical operations by simply changing excitability of the medium's sites. Thirdly, we indicate how to implement logical circuits in architecture-less RD excitable medium.

3.1 Programming with Reaction Rates

Consider a cellular automaton model of an abstract RD excitable medium. Let a cell x of two-dimensional lattice takes four states: resting \circ , excited $(+)$, refractory $(-)$ and precipitated \star , and update their states in discrete time t depending on a number $\sigma^t(x)$ of excited neighbors in its eight-cell neighborhood as follows (Fig. 1):

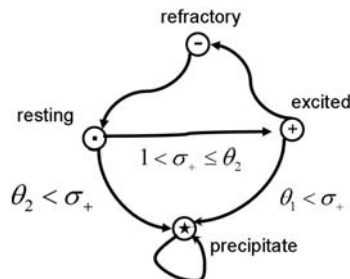


Fig. 1. Cell state transition graph for cellular-automaton model of precipitating RD medium

- Resting cell x becomes excited if $0 < \sigma^t(x) \leq \theta_2$ and precipitated if $\theta_2 < \sigma^t(x)$.
- Excited cell ‘precipitates’ if $\theta_1 < \sigma^t(x)$ and becomes refractory otherwise.
- Refractory cell recovers to resting state unconditionally, and precipitate cell does not change its state.

Initially we perturb the medium, excite it in several sites, thus inputting data. Waves of excitation are generated, they grow, collide with each other and

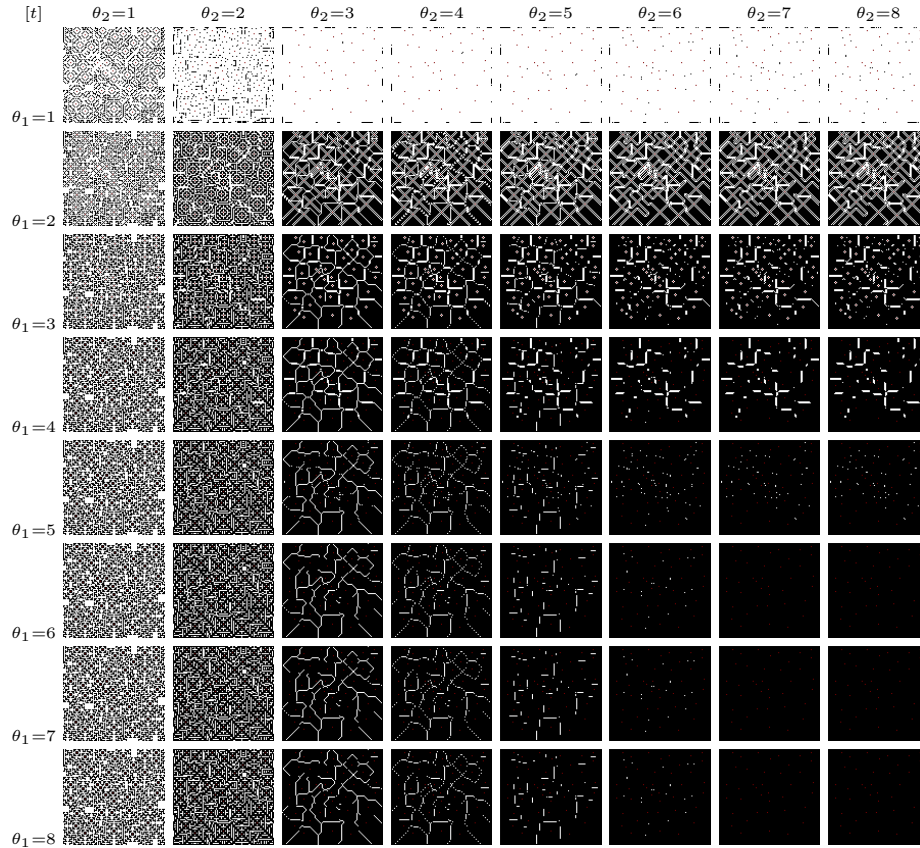
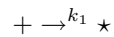
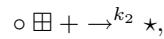


Fig. 2. Final configurations of RD medium for $1 \leq \theta_1 \leq \theta_2 \leq 2$. Resting sites are black, precipitate is white

annihilate in result of the collision. They may form a stationary inactive concentration profile of a precipitate, which represents result of the computation. Thus, we can only be concerned with reactions of precipitation:



and



where k_1 and k_2 are inversely proportional to θ_1 and θ_2 , respectively. Varying θ_1 and θ_2 from 1 to 8, and thus changing precipitation rates from maximum possible to a minimum one, we obtain various kinds of precipitate patterns, as shown in Fig. 2.

Most of the patterns produced, see enlarged examples at Fig. 3abc, are relatively useless (at least there no sensible interpretations of them) Precipitate patterns developed for relatively high ranges of reactions rates: $3 \leq \theta_1, \theta_2 \leq 4$

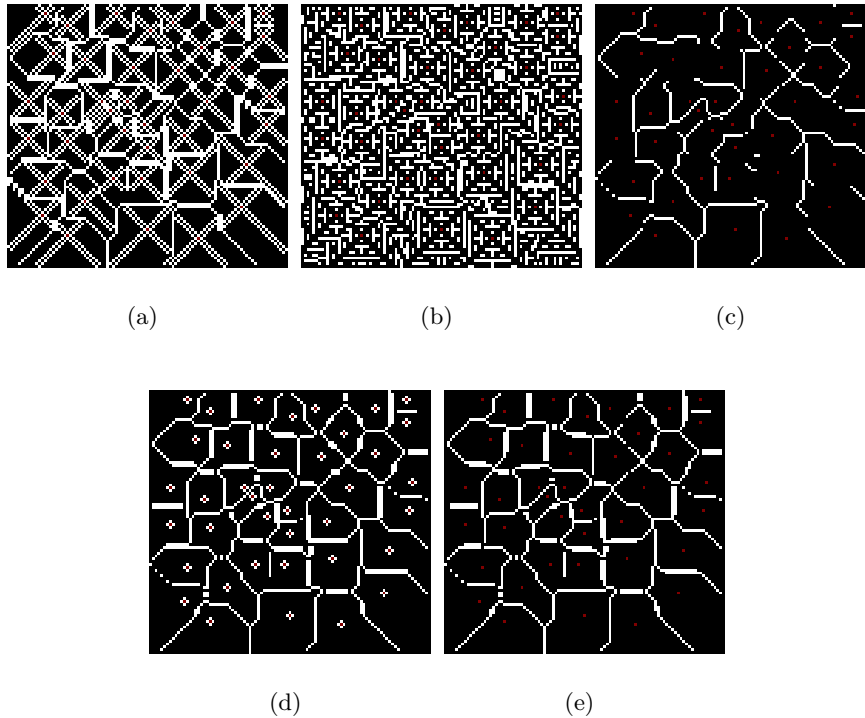


Fig. 3. Exemplar configurations of RD medium for (a) $\theta_1 = 2$ and $\theta_2 = 3$, (b) $\theta_1 = 4$ and $\theta_2 = 2$, (c) $\theta_1 = 7$ and $\theta_2 = 3$, (d) $\theta_1 = 3$ and $\theta_2 = 3$, (e) $\theta_1 = 4$ and $\theta_2 = 3$. Resting sites are black, precipitate is white

represent discrete Voronoi diagrams (given ‘planar’ set, represented by sites of initial excitation, is visible in pattern $\theta_1 = \theta_2 = 3$ as white dots inside Voronoi cells) derived from the set of initially excited sites, see Fig. 3de. This example demonstrates that externally controlling precipitation rates we can force RD medium to compute Voronoi diagram.

3.2 Programming with Excitability

When dealing with excitable media excitability, as one can infer from the name, is the key parameter to tune spatio-temporal dynamics. In [2] we demonstrated that by varying excitability we can force the medium to exhibit almost all possible types of excitation dynamics. Let each cell of 2D automaton takes three states: resting (\cdot), exciting ($+$) and refractory ($-$), and updates its state depending on number σ_+ of excited neighbors in its 8-cell neighborhood (Fig. 4a). A cell goes from excited to refractory and from refractory to resting states unconditionally, and resting cell excites if $\sigma_+ \in [\theta_1, \theta_2]$, $1 \leq \theta_1 \leq \theta_2 \leq 8$. By changing θ_1 and θ_2 we can move the medium dynamics in a domain of ‘conventional’ excitation waves, useful for image processing and robot navigation [7], as well as

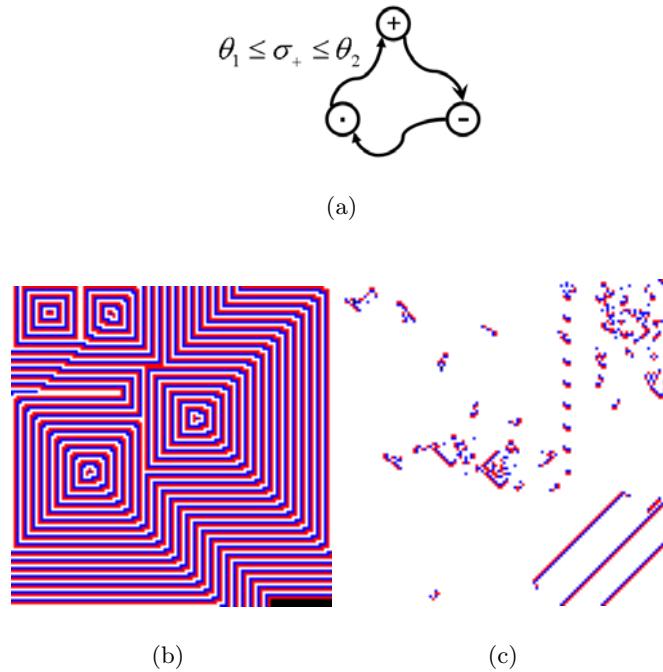


Fig. 4. Cell-state transition graph of excitable medium (a) and snapshots of space-time excitation dynamics for excitability $\sigma_+ \in [1, 8]$ (b) and $\sigma_+ \in [2, 2]$ (c)

to make it exhibits mobile localized excitations (quasi-particles, discrete analogs of dissipative solitons), employed in collision-based computing [2] (Fig. 4bc).

Let us discuss now a more advanced example on how we can program logical gates using excitability. Consider a T-shaped excitable RD medium built of three one-dimensional cellular arrays joined at one point (details are explained in [11]); two channels are considered as inputs, and third channel as an output. Every cell of this structure has two neighbors apart of end cells, which have one neighbor each, and a junction cell, which has three neighbors. Each cell takes three states: resting (\circ), excited ($+$) and refractory ($-$). A cell switches from excited state to refractory state, and from refractory to resting unconditionally. If resting cell excites when certain amount of its neighbors is excited then waves of excitation, in the form $+-$, travel along the channels of the gate. Waves generated in input channels, meet at a junction, and may pass or not pass to the output channel. We represent logical values as follows: no waves is FALSE, one wave $+-$ is NONSENSE and two waves $+- \cdot + -$ represent TRUTH. Assume that sites of the excitable gate are highly excitable: every cell excites if at least one neighbor is excited. One or two waves generated at one of the inputs pass onto output channel; two single waves are merged in one single wave when collide at the junction; and, a single wave is ‘absorbed’ by train of two waves. Therefore, the gate with highly excitable sites implements Łukasiewicz disjunction (Fig. 5a).

$\vee_{\mathbb{L}}$	$T F \star$	$\wedge_{\mathbb{L}}$	$T F \star$	\boxminus	$T F \star$
T	$T T T$	T	$T F \star$	T	$F T \star$
F	$T F \star$	F	$F F F$	F	$T F \star$
\star	$T \star \star$	\star	$\star F \star$	\star	$\star \star F$
(a)		(b)		(c)	

Fig. 5. Operations of Łukasiewicz three-valued logic implemented in models of T-shaped excitable gate: (a) disjunction, $\sigma_+ \in \{\lfloor \frac{k}{2} \rfloor, \lceil \frac{k}{2} \rceil\}$ (b) conjunction, $\sigma_+ = \lceil \frac{k}{2} \rceil$, (c) NOT-EQUIVALENCE, $\sigma_+ = \lfloor \frac{k}{2} \rfloor$

Let us decrease sites sensitivity and make it depend on number k of cell neighbors: a cell excites if at least $\sigma_+ = \lceil \frac{k}{2} \rceil$ neighbors are excited. Then junction site can excite only when exactly two of its neighbors are excited, therefore, excitation spreads to output channels only when two waves meet at the junction. Therefore, when a single wave collide to a train of two waves the only single wave passes onto output channel. In such conditions of low excitability the gate implements Łukasiewicz conjunction (Fig. 5b). By further narrowing excitation interval: a cell is excited if exactly one neighbor is excited, we achieve situation when two colliding wave fronts annihilate, and thus output channel is excited only if either of input channels is excited, or if the input channels got different number of waves. Thus, we implement combination of Łukasiewicz NOT and EQUIVALENCE gates (Fig. 5c).

3.3 Dynamical Circuits

Logical circuits can be also fabricated in uniform, architecture-less, where not wires or channels are physically implemented, excitable RD medium, (e.g. subexcitable BZ medium as numerically demonstrated in [9]) by generation, reflection and collision of traveling wave fragments. To study the medium we integrate two-variable Oregonator equation, adapted to a light-sensitive BZ reaction with applied illumination [17]

$$\frac{\partial u}{\partial t} = \frac{1}{\epsilon}(u - u^2 - (fv + \phi)\frac{u - q}{u + q}) + D_u \nabla^2 u$$

$$\frac{\partial v}{\partial t} = u - v$$

where variables u and v represent local concentrations of bromous acid and oxidized catalyst ruthenium, ϵ is a ratio of time scale of variables u and v , q is a scaling parameter depending on reaction rates, f is a stoichiometric coefficient, ϕ is a light-induced bromide production rate proportional to intensity of illumination. The system supports propagation of sustained wave fragments, which may be used as representations of logical variables (e.g. absence is FALSE, presence is TRUTH). To program the medium we should design initial configuration of perturbations, that will cause excitation waves, and configurations of deflectors and prisms, to route these quasi-particle wave-fragments. While implementation

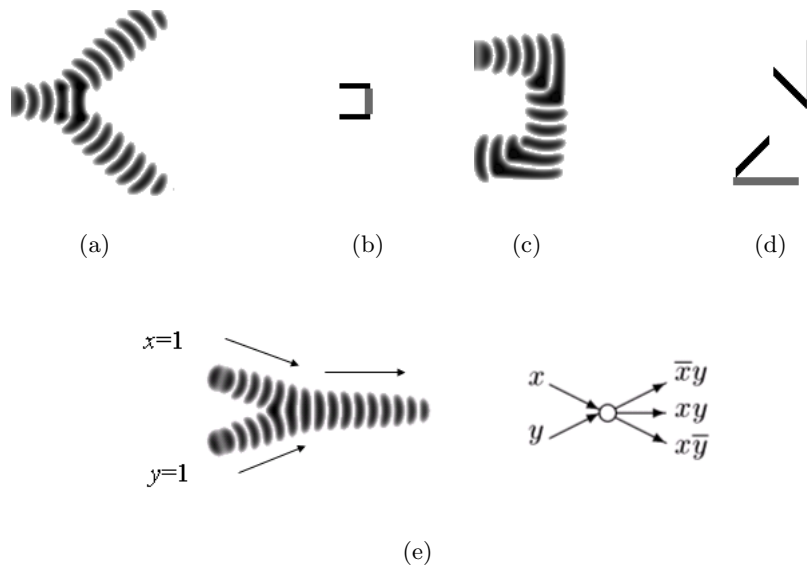


Fig. 6. Operating wave fragments. Overlay of images taken every 0.5 time units. Exciting domains of impurities are shown in black, inhibiting domains are gray. (a) Signal branching with impurity: wave fragment traveling west is split by impurity (b) into two waves traveling north-west and south-west. (c) Signal routing (U-turn) with impurities: wave fragment traveling east is routed north and then west by two impurities (d). A simple logical gate is shown in (e)

of Boolean operations *per se* is relatively straightforward [9], control of signal propagation, routing and multiplication of signals is of most importance when considering circuits not simply single gates. To multiply a signal or to change wave-fragment trajectory we can temporarily apply illumination impurities to change local properties of the medium on a way the wave. Thus we can cause the wave-fragment to split (Fig. 6ab) or deflect (Fig. 6cd). A control impurity (Fig. 6bd), or deflector, consists of a few segments of sites which illumination level is slightly above or below overall illumination level of the medium. Combining these excitatory and inhibitory segments we can precisely control wave's trajectory, e.g. realize U-turn of a signal (Fig. 6cd). A simple logical gates implemented in collision of two wave-fragments is shown in Fig. 6e.

4 Multi-layered RD Processors: Co-programming

Ideally, it would be reasonable to have two excitable chemical systems physically co-existing in one reactor, so space-time dynamics of one chemical medium 'programs' (influences) space-time dynamics of another chemical medium. We did not have yet experimental implementations of such medium-medium programming, however our computational experiments on guiding a virtual robots indicate that the idea is feasible. Namely, to guide a robot we assume that the

robot is attracted by wave-fronts of one system — which represents a target — and repelled by wave-fronts of the other system — which represents obstacles.

In [10] we navigated a virtual robot using two separate and isolated from each other chemical reactors containing the BZ medium. Obstacles are mapped onto one reactor and targets onto another. We assume the robot detects concentration of the chemical species using optical sensors from spatial snapshots of the BZ medium activity. We constructed a software model of ‘pixbot’ [10] — a pixel size robot which moves in discrete steps on images (attractive medium \mathbf{A} and repelling medium \mathbf{R}) of the spatial excitation dynamics of the BZ medium.

The pixbot behaves as follows. Let a_{ij} and r_{ij} be blue color values of pixel (i, j) in images \mathbf{A} and \mathbf{R} , and $(x, y)^t$ be the pixbot’s coordinates at time step t . At each step of discrete time the pixbot can move to one of eight pixels closest to $(x, y)^t$. The pixbot coordinates are calculated as follows, $p^t = (x, y)^t$:

$$p^{t+1} = p^t + \vartheta(t, t-m)[f(p^t, g, \mathbf{A}, \mathbf{R})\chi(f(p^t, g, \mathbf{A}, \mathbf{R})) + (1 - \chi(f(p^t, g, \mathbf{A}, \mathbf{R})))\varrho(p^t, \mathbf{R})] + (1 - \vartheta(t, t-m))\varrho(p^t, \mathbf{R})$$

where $\chi(z) = 1$ if $z \neq 0$ and $\chi(z) = 0$ otherwise; $\vartheta(t, t-m) = 0$ if $|p^t - p^{t-m}| < k$ and $\vartheta(t, t-m) = 1$ otherwise;

$$f(p^t, g, \mathbf{A}, \mathbf{R}) = |\mathbf{V}|^{-1} \sum_{(u_i, u_j) \in \mathbf{V}} (u_i, u_j)$$

$$\mathbf{V} = \{(v_i, v_j) \in \{-1, 0, 1\} : |a_{p^t} - a_{p^t+(v_i, v_j)}| > g, r_{p^t+(v_i, v_j)} < c\}$$

and

$$\varrho(p^t, \mathbf{R}, m) = \text{random}\{(v_i, v_j) \in \{-1, 0, 1\} : r_{p^t+(v_i, v_j)} < c\}$$

g and c are constant depending on initial concentration of reactants, in most experiments, $2 \leq c \leq 5$, $15 \leq g \leq 30$, $10 \leq m \leq 20$. The function ϑ plays a role of a ‘kinetic energy accumulator’: if the pixbot spends too much time wandering in the same local domain it is forced to jump randomly, this will allow pixbot to mount wave-fronts. The function $f()$ selects a site neighboring to p^t along the preferable descent of \mathbf{A} and minimum values of \mathbf{B} . If such a site does not exist then a site with no obstacle wave is selected at random.

An example of the pixbot’s collision-free movement towards a target is shown in Fig. 7, where attracting wave-fronts represent a target and repelling wave-fronts represent obstacles.

5 Discussion

Sluggishness, narrow range of computational tasks solved, and seeming unsusceptibility to a control are usually seen as main disadvantages of existing prototypes of RD computers. In the paper we briefly outlined several ways of external

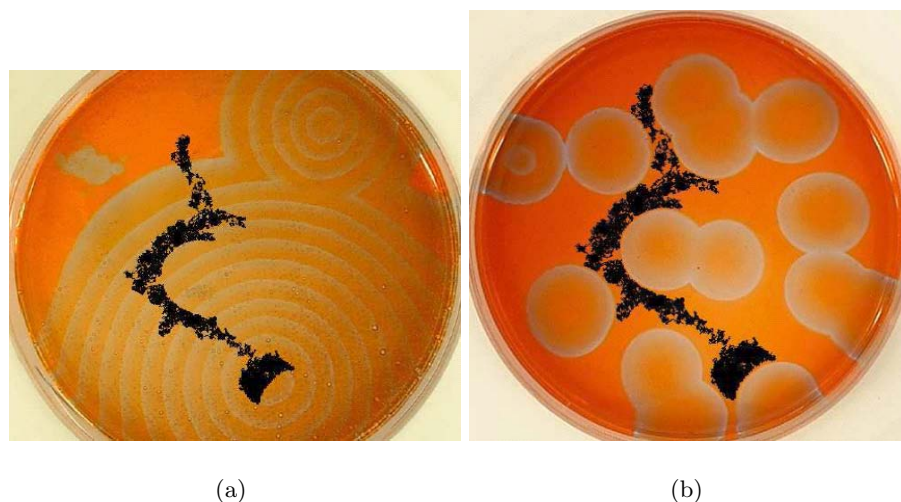


Fig. 7. Trajectories of pixbot moving towards the target through space with obstacles: (a) trajectory of pixbot projected onto pattern of attracting wave-fronts, (b) trajectory of pixbot projected onto pattern of repelling wave-fronts [10]

controlling, tuning, and ultimately programming, of spatially extended chemical devices. We have also indicated how to ‘switch’ a RD computer, with fixed set of reactions but variable reaction rates, between several domains of problems, and thus make it more ‘omnivorous’. Thus we made grounds for partial dismissal of specialization and uncontrollability statements. As to the speed, real-life RD processors are slow indeed, due to limitations on speed of diffusion and phase waves traveling in a liquid layer or a gel. We can argue, however, that future applications of the chemical processors lie in the field of micro-scale computing devices and soft robotic architectures, e.g. gel-made robots, where RD medium forms an integral part of robot body [44]. A silicon fabrication is another way, however possibly a step back from material implementation point of view, to improve speed of RD computers. This route seems to be well developed, particularly in designing RD media in non-linear circuits and cellular neural networks [20, 21, 10]. CMOS design and analog emulation of RD systems, BZ medium in particular, have already demonstrated feasibility of mapping chemical dynamics onto silicon architectures [13, 14, 15, 16]. Semiconductor devices based on minor carrier transport [16], like arrays of $p-n-p-n$ diode based reaction devices, give us a hope for forthcoming designs of nano-scale RD processors.

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