

Pattern Dynamics and Optimization by Reaction Diffusion Systems

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Reaction-diffusion systems show a fast and rather complex response on patterns produced by external space- and/or time-dependent perturbations. For example, one-component autocatalytic reactions rapidly find the loci where the given space-dependent reaction rates have relatively high values by following a kind of Darwinian strategy (combining self-reproduction and diffusion). It is shown that a simulation of this strategy in combination with annealing (decreasing the diffusion rates in time) may be used as an alternative to thermodynamic annealing strategies. Many-component reactions, such as the light-sensitive Belousov-Zhabotinsky reaction, show a more complex response to patterns impressed by illumination, for example. The response behavior and possible applications to dynamic information processing are discussed.

KEY WORDS: Boltzmann strategies; Darwin strategies; annealing; eigenvalue problems; double dynamics; chemical waves; information compression on attractors.

1. INTRODUCTION

The well-known Turing machine is the standard representative of a symbolically intelligent machine which reflects some basic principles of modern programmable computer devices. It is less known that Turing devoted the last years of his life to the study of reaction-diffusion systems (RDS), which he considered as basic to the understanding of living systems.⁽¹⁾ Reaction-diffusion processes play an important role in the function of the nervous system. For example, recent evidence suggests that the reaction and diffusion of cyclic nucleotides have an important function in the intercellular processing of neural signals.⁽²⁾ If the unique information processing

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capabilities of reaction-diffusion processes could be adapted to computers, then evolvable, more efficient systems for such tasks as pattern recognition and process control are in principle possible.⁽³⁾ In a recent paper, Kirby and Conrad⁽⁴⁾ proposed calling the information-processing RDS “Turing’s Other Machine.” There are now initial experimental approaches to the study of the information processing in artificial RDS.^(5,6)

This paper is devoted to a theoretical discussion of the manipulation and processing of patterns by RDS. First we want to study the capabilities of RDS for solving minimum-finding problems for very complex patterns (“frustrated” potential functions having many minima and maxima). In our approach the optimization of a given cost function (potential) is modeled by the exploration of a reaction rate pattern through the simulation of a special RDS (Fisher–Eigen system), which efficiently finds extrema (Section 2).

In Section 3 we consider a real RDS (Kuhnert’s modification of the Belousov–Zhabotinsky reaction) as a special dynamic network system which responds to specific inputs, e.g., pattern-creating light signals, with a complex dynamical output. Throughout the paper we will apply recent concepts, such as information compression on attractors,^(10,11) as well as the idea of double dynamics.^(3,4)

2. FISHER–EIGEN PROCESSES THAT SOLVE OPTIMIZATION PROBLEMS

Recent research in tasks of combinatorial optimization, e.g., the traveling salesman problem and the wiring problem for a microelectronic chip, aims at developing efficient strategies for finding “good minima” of a scalar function (cost function) $U(q)$ of very many independent variables $q = (q_1, q_2, \dots, q_d)$. One of the best strategies available so far is the Boltzmann strategy (thermodynamic strategy) in combination with annealing.^(8,9) We can note that a thermodynamic annealing strategy is new only in respect to applications in science; in nature it has been applied since the hot big bang about 15–20 billion years ago. The basic elements of this strategy are:

1. Motion along gradients to reach steepest descent.
2. Stochastic thermal motion to avoid locking in local minima.
3. Decrease of the temperature to increase the precision of the search.

Following this “strategy” of nature, the galaxies, stars, and planets were formed. One may ask whether the other basic strategy in our universe, the Darwinian strategy, which was developed by nature only 3–4 billion of

years ago, may be in some respect even more advantageous. The basic elements of a Darwinian strategy are:

1. Self-reproduction of good species that show maximal fitness.
2. Mutation processes that change the phenotypic properties of the species.
3. Increase of the precision of self-reproduction in time.

The simplest model of a Darwinian process (a kind of “Fisher–Eigen machine”) is an RDS corresponding to a continuous Fisher–Eigen equation with slowly time-dependent diffusion (mutation) rates. In the following we will use dimensionless units for all quantities and normalize the unit length to be one. Then we have⁽¹²⁾

$$\partial_t x(q, t) = [\langle U \rangle - U(q)] x(q, t) + D(t) \Delta x(q, t) \quad (1)$$

In chemical terms this is a special RDS of one-component autocatalytic type. Here $x(q, t)$ is the density over a d -dimensional state space (the physical space for chemical reactions or the search space for optimization problems). This space is spanned by the vectors

$$q = (q_1, q_2, \dots, q_d)$$

The self-reproduction rate (velocity of autocatalysis) is assumed to be proportional to the local value of a given space-dependent function $U(q)$ minus its “social average”

$$\langle U \rangle = \int dq U(q) x(q, t) / \int dq x(q, t) \quad (2)$$

Equation (1) is similar to a Schrödinger equation with imaginary time. Therefore, the process corresponding to Eq. (1) is related to the eigenvalue problem of Schrödinger type:

$$D \Delta \psi_k(q) + [\varepsilon_k - U(q)] \psi_k(q) = 0 \quad (3)$$

Here D is considered to be a constant or a function of time that varies very slowly in comparison to the characteristic relaxation processes of Eq. (1), which are in fact given by the reciprocal eigenvalues of Eq. (3). The complete solution of Eq. (1) in terms of the eigenfunctions and eigenvalues of Eq. (3) reads

$$x(q, t) = N \frac{\sum_k c_k \exp(-\varepsilon_k t) \psi_k(q)}{\sum_l c_l \exp(-\varepsilon_l t)} \quad (4)$$

where we have used the artificial normalization

$$\int dq \psi_k(q) = 1 \quad (5)$$

and

$$N = \int dq x(q, 0), \quad c_k = \int dq \psi_k(q) x(q, 0) \quad (6)$$

Let us assume now that the potential function $U(q)$ shows a great number of extrema comparable with the multimodality of a spin glass. The idea is that finding a good solution of a complex problem is always a compromise between several requirements and constraints—it is a so-called “frustrated problem.” For such potentials classical minimum-finding principles may fail.⁽¹⁴⁾ More refined stochastic methods, however, will still work. Corresponding to the complex structure of the potential, let us assume that the Schrödinger problem (3) has a mixed spectrum with many discrete states which are localized in the vicinity of the potential minima, among them the ground state $(\varepsilon_0, \psi_0(q))$. Further, there is a continuous part of the spectrum corresponding to extended states. In the process of time evolution given by Eq. (4) the contributions of the “highest” states are damped out first, and as time proceeds, the density is concentrated more and more around the localized eigenfunctions. The process of search corresponds to a falling down the spectrum of eigenvalues. First the system leaves the extended states and concentrates around the minima. Finally the process converges to the ground state

$$x(q, t) \rightarrow N\psi_0(q) \quad (7)$$

In this way we have shown mathematically that a Darwinian strategy modeled by a Fisher–Eigen process indeed shows the property of searching for local minima. By using other language, we may say that the localized eigenfunctions of the potential represent the local attractors of the reaction-diffusion process. The reactions alone would correspond to the division of the search space into many attractor basins around the local minima. The diffusion makes it possible to cross the separatrices between the attractors. For a parabolic minimum with dispersion $D_2 = (\delta q)^2$, the wave function has dispersion $D'_2 = 2\delta q \sqrt{D}$. The fast dynamics of the search process (reaction-diffusion process) may be coupled with a slow dynamics connected with a time change in the diffusion rates. The requirement that at any time the wave function is overlapping with regions that are not yet occupied leads, e.g., to an annealing strategy

$$\sqrt{D(t)} \delta q(t) \sim [\delta q(t)]^2$$

Thus we have

$$D(t) \sim (\delta q(t))^2 \tag{8}$$

Let us now discuss a special discrete realization of a Fisher–Eigen process which can be simulated on a computer.⁽¹³⁾ We divide the search space by a fine mesh into s cells, which are numbered by $i = 1, 2, \dots, s$, and study an ensemble of systems consisting of N representatives with $s \gg N \gg 1$. We further assume that the local value of the potential is U_i and the occupation number at time t is $N_i(t)$. If the search state is discrete, corresponding, e.g., to a spin lattice, the index i would denote the global state of the lattice with the energy U_i .

For simplicity we normalize the potential in such a way that all U_i are negative. The initial distribution on the cells is assumed to be

$$N_1(0), N_2(0), \dots, N_s(0)$$

Now we introduce a stochastic process consisting of two elementary transition processes:

1. Self-reproduction described by a transition probability

$$W(N_1, \dots, N_i + 1, \dots, N_j - 1, \dots, N_s | N_1, \dots, N_i, \dots, N_j, \dots, N_s) = (-U_i) N_i N_j / N \tag{9}$$

2. Mutation described by a transition probability

$$W'(N_1, \dots, N_k + 1, \dots, N_l - 1, \dots, N_s | N_1, \dots, N_k, \dots, N_l, \dots, N_s) = D_{kl} N_l \tag{10}$$

This process is allowed only if k and l are neighbors. In this case $D_{kl} = D$. An extension of this model beyond pure diffusion would include more complicated distance-dependent matrix elements D_{kl} . Biological species successfully apply a strategy with frequent mutations to near phenotypic states, but from time to time big steps (macromutations) occur. In analogy to this, our matrix D_{kl} could include a long-range tail modeling nonfrequent macromutations. The choice of transition probabilities given by Eqs. (9 and 10) is not unique. Another possibility is to allow only directed transitions:

1. The transition probability

$$W = \frac{1}{2} \begin{cases} (U_j - U_i) N_i N_j / N & \text{if } U_j \geq U_i \\ 0 & \text{if } U_j < U_i \end{cases} \tag{11}$$

2. The transition probability

$$W' = D \begin{cases} 1 & \text{if } U_k \leq U_l \\ \exp((U_l - U_k)/T) & \text{if } U_k > U_l \end{cases} \tag{12}$$

It was shown elsewhere⁽¹³⁾ that the stochastic processes described above correspond in average to a discrete cell version of the Fisher–Eigen equations. Simulations for a biologically motivated variant of the model (9)–(10) have shown that the stochastic process leads indeed to an amplification of all species below the social average of U_i and a continuous decrease of the average in time.⁽¹³⁾ Applications to technically oriented optimization problems have not yet been carried out. However, in earlier papers a qualitative analysis of the efficiency of Darwinian strategies in comparison with thermodynamic strategies was given^(7,12) by studying the mean first passage times for these processes. An estimate shows that a Darwinian process needs on average the time

$$\tau_D \sim \frac{|\delta q|}{\delta U} \left(\frac{\Delta U}{D} \right)^{1/2} \quad (13)$$

to leave a minimum and reach another one in a distance δq that is deeper by δU than the first one. Here ΔU is the height of the threshold. Comparing this with the transition time for thermodynamic processes⁽¹⁴⁾

$$\tau_B \sim \exp(\Delta U/D) \quad (14)$$

we observe great differences between the transitional behavior of both strategies. Therefore, in general it will depend on the structure of the potential what search strategy is the better one. The qualitative analysis suggests that in the case that no knowledge about the structure of $U(q)$ is available, it will be advantageous to apply the Boltzmann strategy combined with annealing. This strategy seems to be more universal; it will always work. However, thermodynamic processes have the tendency to be locked in relative minima that are surrounded by high thresholds. Since the transition time depends exponentially on the height of the threshold ΔU , one may need very large times to find minima that are separated from the starting position by many high barriers. This is the weak point of the Boltzmann strategy. On the other hand, Darwinian processes are able to cross high barriers by tunneling if the next minimum is close. However, the Darwinian strategy is not universal; it works only under appropriate conditions, e.g., the existence of localized states is a necessary condition. If the potential does not possess localized states, e.g., if the minima are too flat, a Darwinian search of the type described above will never concentrate the density around minima. Therefore, in some cases mixed strategies might be advantageous; this is what we observe in nature. Most natural processes follow Boltzmann strategies (in the widest sense); more refined solutions,

however, require Darwin strategies. A simple mathematical expression for a mixed strategy in this sense is

$$\begin{aligned} \partial_t x(q, t) = & \alpha(t) [\langle U \rangle - U(q)] x(q, t) \\ & + \beta(t) \nabla \cdot [x(q, t) \nabla U(q)] + D(t) \Delta x(q, t) \end{aligned} \quad (15)$$

with

$$\alpha(t) + \beta(t) = 1$$

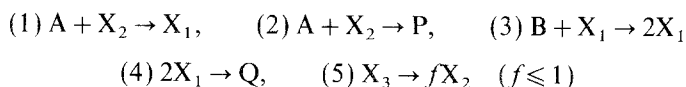
Here as in our earlier considerations the functions $D(t)$, $\alpha(t)$, and $\beta(t)$ should follow a slow dynamics that aims to optimize the search process as a whole. It is known that an appropriate slow dynamics may imply Pavlovian behavior and learning.^(4,11)

3. PATTERN PROCESSING BY REAL RDS

So far we have considered a special one-component artificial RDS, which may be used for the simulation of search processes in high-dimensional abstract search spaces. Let us consider now real RDS, e.g., the Belousov-Zhabotinsky reaction (BZR) in the physical space, $d = 2$ or $d = 3$. We assume the kinetic equation

$$\partial_t x(r, t) = W\{x(r, t); \lambda(r, t)\} + \nabla \cdot [D(r, t) \nabla x(r, t)] \quad (16)$$

where x is considered to be an s -dimensional vector giving the set of concentrations, $\lambda(r, t)$ is an m -dimensional vector of reaction parameters, r is the d -dimensional space vector, and $D(r, t)$ is the diffusion tensor. Further, let us assume that the parameters are controllable and might be manipulated from outside with respect to their space and time dependence. We note that Eq. (1) is a special case of Eq. (16) with a special quasilinear form of the reaction function W , a scalar x , and a given space-dependent reaction parameter $U(q)$. In the abstract space we considered in Section 2, the parameter function was given by a certain algorithm (e.g., the total length of wires connecting the elements on a chip). In real space the manipulation of reaction parameters may be performed in many ways, the most elegant of which is probably the optical way.^(6,15) The special case that x is a scalar, W a bistable function, and $\lambda(r, t)$ a stochastic vector has been treated elsewhere.^(16,17) Let us consider here as another example the BZR with light-sensitive Ru catalyst.⁽⁶⁾ The Oregonator model of the BZR is given by the schema⁽¹⁸⁾



Kuhnert's modification of the BZR uses the ions Ru^2 and Ru^3 as the catalysts. Here Ru^2 acts as the oxidizer and Ru^3 as the reducer. By absorption of light a dramatic change of the redox properties of the Ru^2 ions takes place, since the excited modification $^*\text{Ru}^2$ is a strong reducing agent. As proposed by Kuhnert *et al.*,⁽¹⁹⁾ we model this by an additional source of Br^- ions: (5) $\text{C} \rightarrow \text{X}_2$.

The meaning of the three independent variables is the following:

$$x_1 = [\text{HBrO}_2], \quad x_2 = [\text{Br}^-], \quad x_3 = [\text{Ru}^3]$$

By using an appropriate choice of units we get the three equations

$$\begin{aligned} \partial_t x_1(r, t) &= x_1(1 - x_1) - x_1 x_2 + \lambda_1 x_2 + D_1 \Delta x_1 \\ \partial_t x_2(r, t) &= \lambda_2(\lambda_5 - \lambda_1 x_2 + \lambda_4 x_3 - x_1 x_2) + D_2 \Delta x_2 \\ \partial_t x_3(r, t) &= \lambda_3(x_1 - x_3) + D_3 \Delta x_3 \end{aligned} \quad (17)$$

Here the parameters are defined as follows:

$$\begin{aligned} \lambda_1 &= 2 \frac{k_1 k_4 A}{k_3 k_2 B}, & \lambda_2 &= \frac{k_2}{2k_4}, & \lambda_3 &= \frac{k_5}{k_3 B} \\ \lambda_4 &= 2f \frac{k_4}{k_3 B}, & \lambda_5 &= \frac{Ck_2^2 k_6}{2k_1 k_3 k_4 AB} \end{aligned}$$

For $\lambda_5 = 0$, Eqs. (17) reduce to the classical Oregonator model, which shows uniform oscillations as well as traveling waves.⁽¹⁸⁾ In the other case of fixing $\lambda_3 = \lambda_4 = 0$, Eqs. (17) reduce to the model investigated by Kuhnert *et al.*,⁽¹⁹⁾ which shows uniform bistability as well as front waves (trigger waves). Therefore, the model (17) combines both properties and may be used to describe at least qualitatively the complicated pattern formation observed experimentally.⁽⁶⁾

In order to analyze the possible behavior, let us study the characteristic equation for the stationary states of the x_1 coordinate:

$$\xi^3 - (1 - \lambda_4 - \lambda_1) \xi^2 + (\lambda_5 - \lambda_1 \lambda_4 - \lambda_1) \xi - \lambda_1 \lambda_5 = 0 \quad (18)$$

For simplicity we restrict consideration in the following to the case $\lambda_1 \ll 1$ and $\lambda_4 < 1$. Then there exist three regimes, depending on the value of the light-sensitive bifurcation parameter λ_5 :

1. Strong light intensity,

$$\lambda_5 > \lambda_{c1} \approx \frac{1}{4} (1 - \lambda_4)^2 + \lambda_1 \lambda_4$$

In this regime we find only one globally stable stationary state with

$$\xi_1 = x_1^0 = x_3^0 \approx (1 - \lambda_4 - \lambda_1), \quad x_2^0 \approx \lambda_4$$

This corresponds to the reduced phase of the reaction, which in the experiments is recognized by its red color. For nonuniform initial conditions all parts of the space that are covered by the strong light beam will move to this state and we may observe a traveling wave, which finally covers the whole illuminated area with dark red color.

2. Weak light intensity,

$$\lambda_5 < \lambda_{c2} \approx 4\lambda_1$$

In this regime the system shows only one stationary state, which is located at

$$\xi_1 = x_1^0 = x_3^0 \approx \lambda_1; \quad x_2^0 \approx (\lambda_5 + \lambda_1 \lambda_4) / 2\lambda_1$$

This stationary state may be stable or unstable, depending on the values of the parameters $\lambda_1, \lambda_2, \lambda_3, \lambda_4$. Uniform oscillations as well as traveling waves may be observed. In this regime the processes will be very similar to those in unperturbed Oregonator systems with $\lambda_5 = 0$.

3. Medium light intensity,

$$\lambda_{c2} < \lambda_5 < \lambda_{c1}$$

In this intermediate regime the system shows three stationary states, $\xi_1 < \xi_2 < \xi_3$; two of them (ξ_1, ξ_3) are stable and one (ξ_2) is unstable. The system may develop front waves, which in a rough approximation for $D_1 \approx D_2 \approx D_3$ may be described by⁽¹⁷⁾

$$x_1(z, t) = \xi_1 + (\xi_3 - \xi_2)(1 + \exp\{\beta[n \cdot r - v_0 t + (d - 1) D_1 K t]\})^{-1} \quad (19)$$

$$v_0 = \left[\frac{D_1}{2(\xi_1 + \lambda_1)} \right]^{1/2} (\xi_3 + \xi_1 - 2\xi_2); \quad \beta = \frac{\xi_3 - \xi_1}{[2D_1(\xi_2 + \lambda_1)]^{1/2}}$$

Here v_0 is the planar velocity, d the dimension, K the curvature, and n the normal vector. Depending on the value of λ_5 , which strongly influences the positions of the three roots, the front can move forward or backward. The front always moves into the direction of the globally less stable phase, increasing in this way the volume (area) of the more stable phase. In the approximation given above the state ξ_3 is more stable than ξ_1 if $\xi_3 - \xi_2 > \xi_2 - \xi_1$. A typical system of isoclines for the bistable regime is shown in Fig. 1.

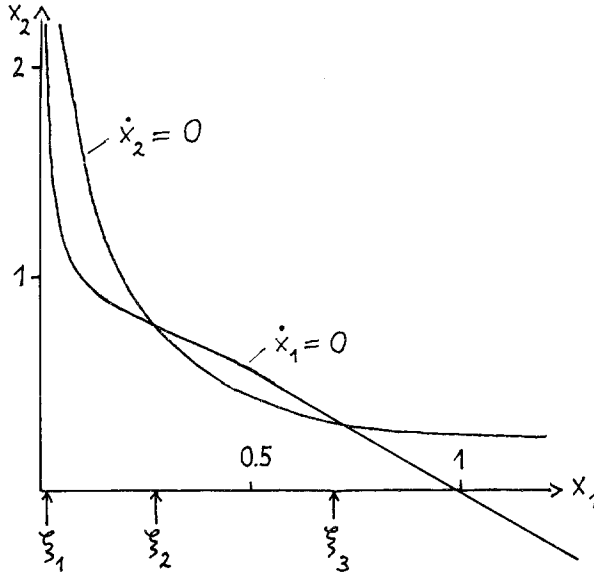


Fig. 1. Isoclines of the light-sensitive Ru-catalyzed Belousov-Zhabotinsky reaction with the parameters $\lambda_1=0.01$, $\lambda_4=0.1$, $\lambda_5=0.17$. The three roots are located at: (1) $x_1=x_3=0.011$, $x_2=8.55$; (2) $x_1=x_3=0.274$, $x_2=0.75$; (3) $x_1=x_3=0.637$, $x_2=0.37$.

By summarizing the results obtained so far, we expect that spatiotemporal modulation of the light intensity may give rise to the following effects. Depending on the local value of the parameter $\lambda_5(r, t)$, the local state corresponds to one of the following regimes:

1. One stable state of the reduced phase exists; traveling waves which increase the volume (area) of the stable phase are formed.
2. The oxidized as well as the reduced phase are stable. Front waves are developed which locally increase the volume (area) of the more stable phase.
3. The oxidized phase is stable; traveling waves increasing this phase are observed.
4. The only existing stationary state is unstable; uniform oscillations and/or traveling oscillating waves are formed.

By changing the light intensity as a given function of time and space, very complicated patterns may be created. This has been demonstrated recently in the beautiful experiments by Kuhnert.⁽⁶⁾ The model given in this paper cannot claim to describe the experiments quantitatively; however, it gives at least a qualitative picture of some observed phenomena.

4. DISCUSSION

In the present paper two different examples of pattern processing by RDS have been discussed. The first example shows the evolution of the density in a one-component autocatalytic RDS with a complicated local structure of the reaction rates. We have shown that the system finds local extrema of the reaction rates in a very efficient way. Simulations of such a "Darwinian" search strategy on a computer are a possible alternative method for the solution of certain optimization problems. It may be expected that the RDS method is advantageous in comparison with thermodynamic methods if the "good" minima are relatively close to one another but are separated by high thresholds. In such cases the RDS tunneling processes may be more efficient than the thermodynamic activation processes.

In the second example, a three-component RDS is analyzed, which generalizes the Oregonator model by adding a source of Br ions. In Kuhnert's Ru-catalyzed variant of the BZR the Br source is controlled through illumination by light. The theoretical analysis shows that impinging patterns may produce very complicated phenomena, such as forward- or backward-moving front waves, oscillating waves, etc. The RDS gives a specific dynamic response to input patterns. Recent work of Kirby and Conrad^(2,4) suggests the use of this response for pattern recognition and related problems. In analogy to their enzymatic neuron, we may introduce in our RDS a system of n electrodes which measure and transform the local chemical state at the positions r_1, r_2, \dots, r_n (see Fig. 2). Let us

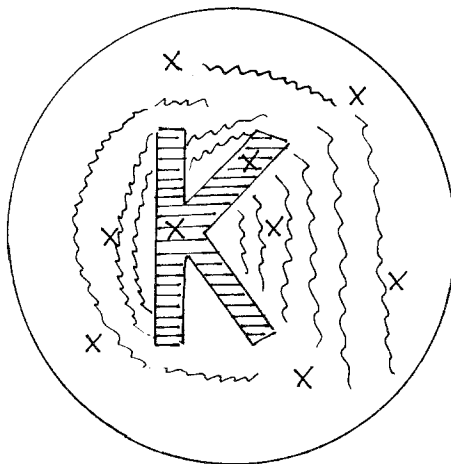


Fig. 2. Schema of the light-sensitive RDS manipulated by illumination inside the area of the "K." The positions of the output electrodes that measure the local ion concentrations are marked by crosses.

assume that the electrodes act as nonlinear mappings of the local chemical state onto an f -dimensional space of electrical signals. The output vectors are then given by a mapping

$$y(t) = M[x(r_1 t), \dots, x(r_n t)] \quad (20)$$

The fast motion in the continuous space of concentrations is then mapped to a fast motion in a f -dimensional vector space with a specific topological structure, depending on the input patterns and the localization of the electrodes. Impinging patterns are compressed finally on the attractors in the vector space of the electrical signals. This procedure leads to a special contraction mechanism whereby many input patterns are mapped into the same output. Similar schemas have been discussed in many context^(2,11) and their possible relevance for pattern recognition shown.^(4,10) Of basic importance for such applications seems to be the introduction of an adaptive behavior by the coupling to a slow dynamics.⁽⁴⁾ In our chemical system an adaptive behavior is most easily introduced by slow adaptive changes of the electrode positions (Fig. 2). Requiring that different input patterns (e.g., different letters) should correspond to different attractors in the vector space of electrical signals, an optimization of the positions seems to be possible. However, it should be underlined that such systems are still too complex for a straightforward theoretical analysis. Further experimental and theoretical work will be necessary in order to explore the capabilities of RDS for pattern recognition. To begin with, we mention the need for a full bifurcation analysis.⁽²⁰⁾

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