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Finding the optimal path with the aid of chemical wave

K. Agladze^{a,*}, N. Magome^b, R. Aliev^a, T. Yamaguchi^c, K. Yoshikawa^b

^a *Institute of Theoretical and Experimental Biophysics, Russian Academy of Science, Puschino, Moscow Region 142292, Russian Federation*

^b *Graduate School of Human Informatics, Nagoya University, Nagoya 464-01, Japan*

^c *National Institute of Materials and Chemical Research, 1-1 Higashi, Tsukuba, Ibaraki 305, Japan*

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Abstract

It is shown that the optimal path in a two-dimensional vector field is deduced by the use of chemical wave in the Belousov–Zhabotinsky reaction (BZ reaction). We also reproduced our experimental result in a numerical simulation based on a two-variable reaction–diffusion equation. The present result provides a simple model for the future application of excitable media to parallel computing, i.e., an excitable medium serves as a self-organized parallel processor.

Keywords: BZ reaction; Excitable media; Optimal path; Chemical Computation

1. Introduction

Recent studies have shown that it is possible to use chemical concentration waves for computational operations; e.g., in image processing [1,2]. The basic idea is to use a chemically active medium (non-stirred layer of an oscillating reaction) as a parallel multi-processor (matrix) unit, where each micro-volume can be regarded as a one-bit-processor, corresponding to the reduced/oxidized state of the catalyst [1,3,4]. By controlling the rate of oscillation and the phase, it is possible to achieve desirable patterns such as edge enhancement and black–white reversal. Such external control has generally taken the form of illumination in the photosensitive Belousov–Zhabotinsky (BZ) reaction [1,2,6–8].

In the present work, we show that the same chemical system can be used not only for image processing, but also for solving a general optimization problem: i.e., finding the fastest path between two points in an arbitrary velocity field.

2. Problem

If we need to find the fastest path from point A to point B in a uniform space, it is just a straight line connecting these points. However, if we suppose that the velocity is a function of location, i.e., $V(x, y)$, the quickest path is not always a straight line. Determining this trajectory is an enormous computational task, even with a modern computer.

One approach is to create a motion chart [5] in which the entire space is covered by isochrones, lines (in a two-dimensional space) consisting of points

* Corresponding author.

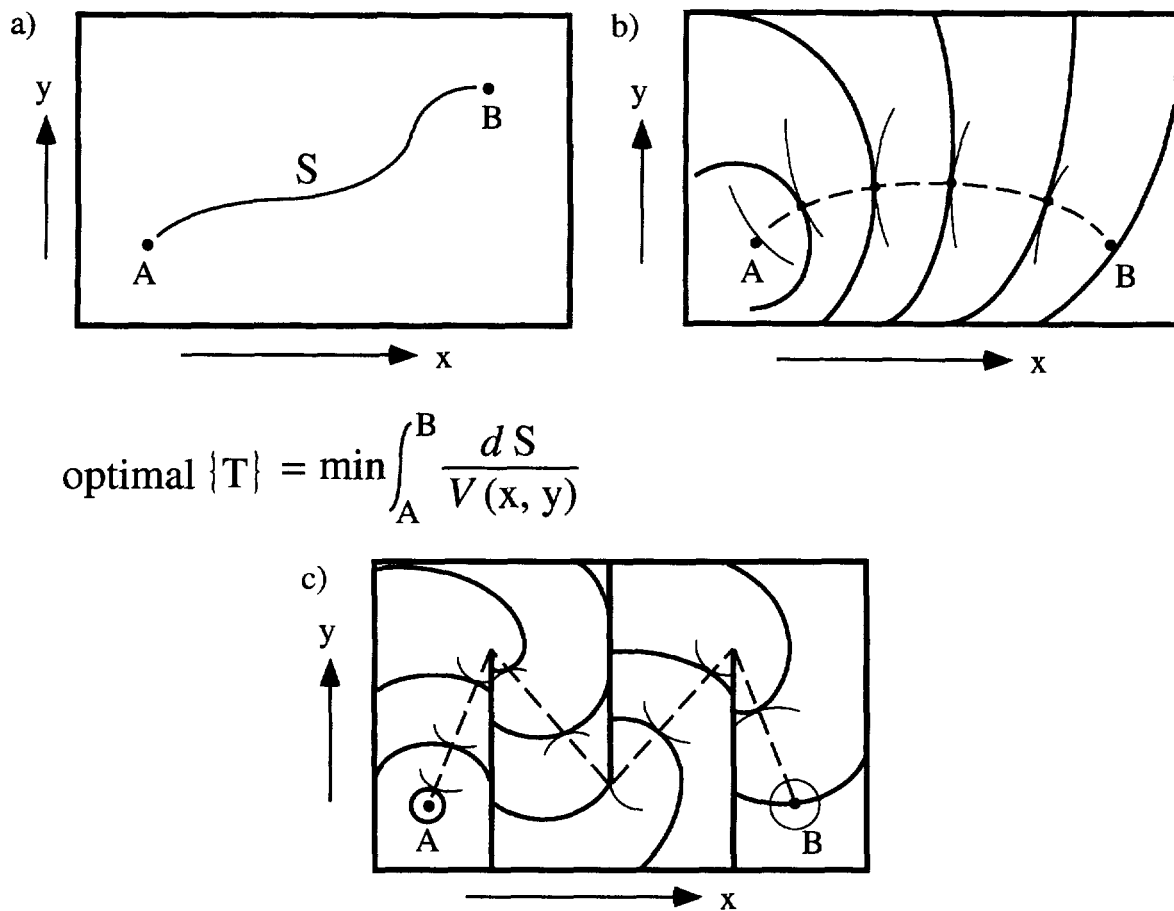


Fig. 1. Scheme of finding the optimal path in an arbitrary velocity field.

which are equally distant from the initial point. This can be accomplished if an “excitation” wave is triggered from point A, and then propagates throughout the space with a local speed of propagation $V(x, y)$, as shown in Fig. 1(b). By recording the profile of the wave front at a desired time interval, we obtain the necessary motion chart. After the wave reaches the destination point B, we stop to record the wave front. Thus, the set of isochrones of chemical wave from point A is obtained (Fig. 1(b), thick lines). The next step is to start the wave from point B (Fig. 1(b), thin lines) and to find the intersection points where the second propagating wave crosses the first waves’ isochrones. The set of the crossing points gives us the track of the quickest path from point A to point

B (Fig. 1(b), dotted line). With such a procedure, we can find the optimal path not only in uniform velocity field but also in arbitrary velocity field. A unique type of velocity field is a labyrinth (Fig. 1(c)), in which the velocity along the rows or corridors is constant and zero at the walls [8].

The method described above is more efficient if it is solved by a parallel-multiprocessor computer. Ideally, each element of the space is represented by its own processor. This elementary processor can be relatively simple. It must exhibit only three states, “rest”, “excited” and “refractory” (to prevent backward propagation), and it must be able to transfer excitation to its neighboring elements which are in the “rest” state. To vary the wave speed, the time at which excitation

is transferred must be controllable. In fact, such a network of locally connected trigger processors exhibits most of the general features in various excitable biological and chemical media [9].

The excitable medium in the BZ reaction is believed to meet these conditions. It can provide easily observable propagating excitation waves which can be controlled either chemically or by light illumination [5–7,10,11]. In the present study, we used the BZ reaction as an experimental model system of parallel processing and performed computer simulations for a theoretical interpretation of the problem.

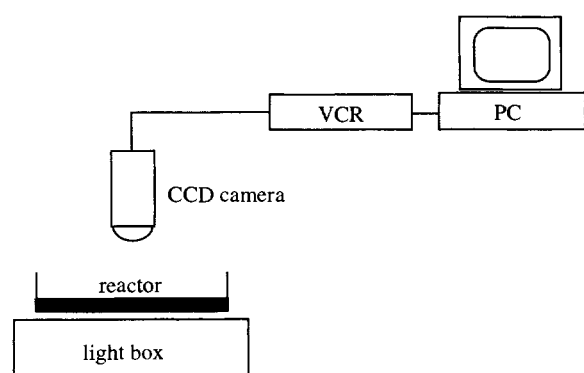


Fig. 2. View of the experimental setup.

3. Experimental results

Chemically active medium was prepared from analytical grade reagents (Tokyo Kasei). The medium was composed of NaBrO_3 , 0.3 M; H_2SO_4 , 0.15 M; $\text{CH}_2(\text{COOH})_2$, 0.1 M; $\text{CHBr}(\text{COOH})_2$, 0.1 M; and $\text{Fe}(\text{phen})_3$, 0.005 M. The temperature was maintained at 20°C. Fig. 2 shows the general experimental setup. 5 ml of the chemical medium was placed in a petri dish (9 cm dia.) illuminated from below. The wave propagation and the pattern was monitored with a CCD camera connected to a VCR. The images were captured with a frame grabber (DT55, Data Translation) and the records were analyzed by computer using *Global Lab Image* (Data Translation).

Obstacles were created in the reaction medium either by adding a drop of KCl [11,12], or by strong light illumination (Fiber Light FL-50, Shimadzu Rika Instruments). We have noticed that the ferroin version of the BZ reaction also responds to light illumination, as does the ruthenium–bipyridyl catalyzed version, although to a lesser extent. Fig. 3 exemplifies the propagating wave passing by (a) a spot of strong illumination, and (b) a chemical obstacle.

The problem is how to determine the quickest path between two points in the medium (A and B)

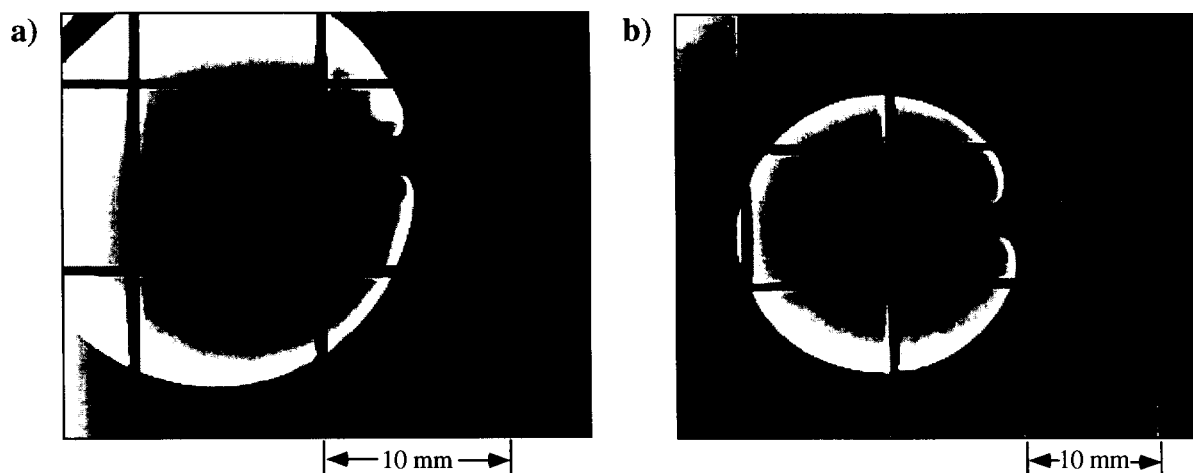


Fig. 3. Experimental result on the excitation wave propagation in a medium with inexcitable obstacle: (a) suppression by light illumination; (b) suppression by small amount of KCl solution. In order to show the actual configuration, square lattice with the spacing of 10 mm is given in the pictures.

situated on opposite sides of the obstacle. For this purpose, a chemical wave was initiated at point A by carefully touching the solution with a silver wire [10–12]. After this wave propagated and passed over point B, a second “backward” wave was generated at point B. The profile of the propagating wave was recorded with VCR. Fig. 4 shows a snapshot of the propagating wave triggered at point A, where the wave fronts are represented by white stripes. Thus, we obtain a set of isochrones. In Fig. 4, “backward” propagating wave from point B is shown in black. The dotted line is the connecting line of the intersecting points smoothly, corresponding to the shortest path between A and B. The spacial resolution of the optimal path becomes better, if the number of the frames is increased to obtain the crossing points. In this case, the actual experimental time to obtain the optimal path was about 15 min for a distance between A and B of about 20 mm.

Although the BZ medium reaction permits more complex patterns [1,2,6–8], in the present study we would like to try to develop the theoretical background of this interesting methodology.

4. Computer simulations

Computer simulations were performed with a two-variable model of the Ferriin-catalyzed BZ reaction developed by Rovinsky and Zhabotinsky [13], in which the rate constants were the same as those reported previously [14]. This model has been verified experimentally to simulate the spatio-temporal pattern in the BZ reaction [14–16]. According to this model, the dynamics in a well-stirred vessel can be described by the following differential equations for the autocatalytic variable (x) and the metal catalyst (z) [13,14]:

$$\begin{aligned} \frac{dx}{d\tau} &= \frac{1}{\varepsilon} \left[x(1-x) - \left(2q\alpha \frac{z}{1-z} + \beta \right) \frac{x-\mu}{x+\mu} \right], \\ \frac{dz}{d\tau} &= x - \alpha \frac{z}{1-z}, \end{aligned} \quad (1)$$

where

$$\begin{aligned} [\text{metal catalyst}] &= Cz, & [\text{HBrO}_2] &= \frac{k_1 A}{2k_4} x, \\ \varepsilon &= \frac{k_1 A}{k_4 C}, & \alpha &= \frac{k_4 k_8 B}{(k_1 A h_0)^2}, \end{aligned}$$

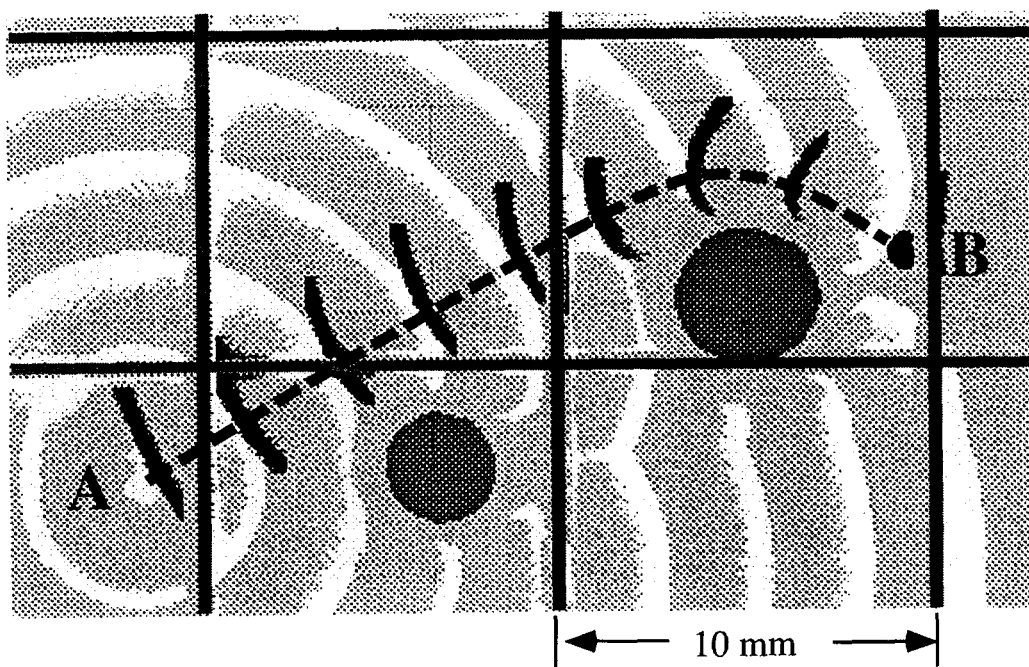


Fig. 4. Experimental result on the tracking of the optimal path between points A and B, placed at different sides of the obstacle.

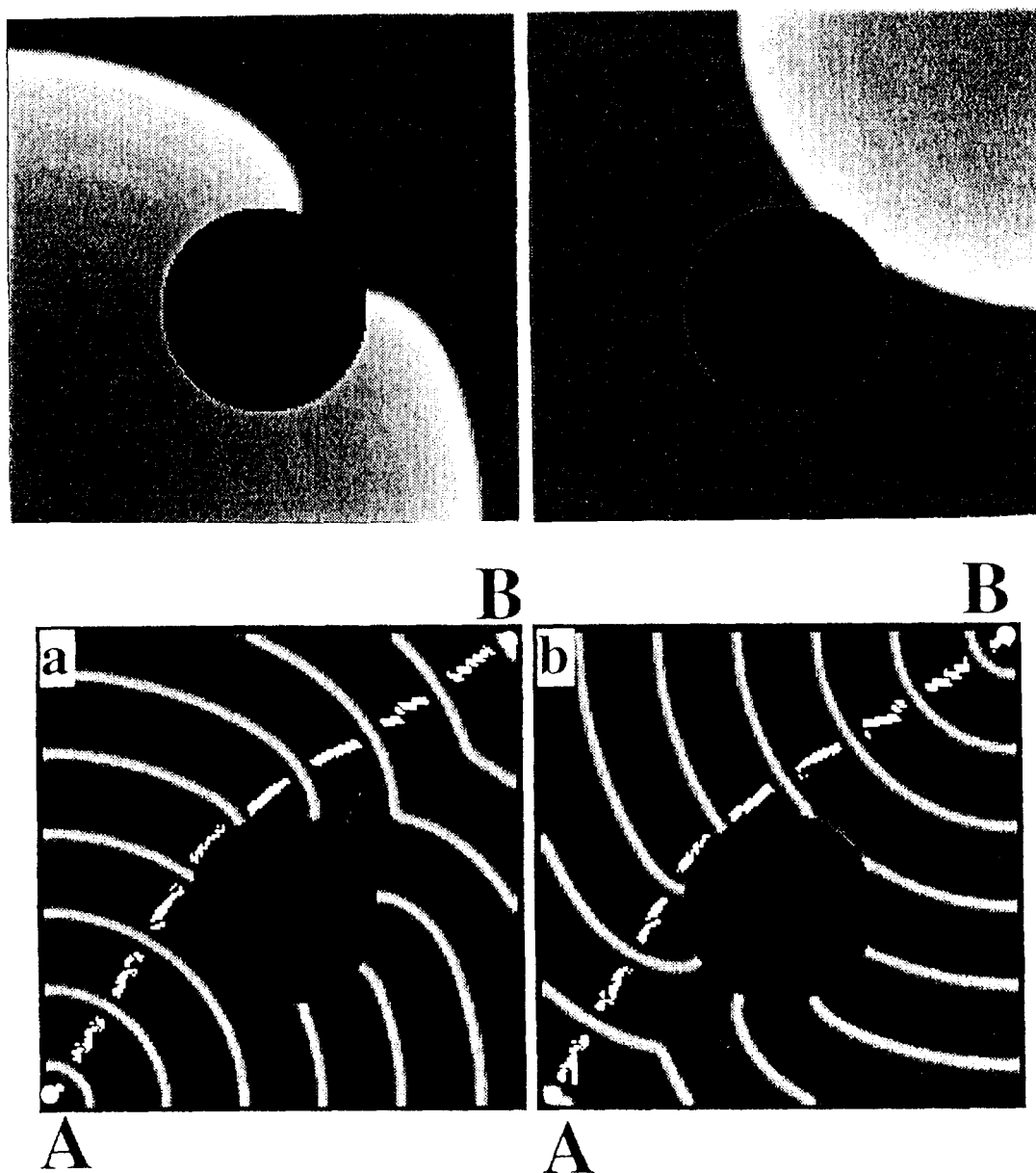
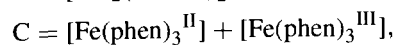
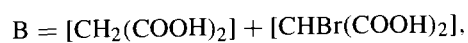
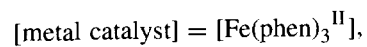


Fig. 5. Computer simulation on the tracking the optimal path between points A and B, placed at the opposite sides of an obstacle. Above: Examples of the propagating waves from A (left) and B (right). Below: Superposition of the chemical wave.

$$\mu = \frac{k_4 k_7}{k_1 k_5}, \quad = \frac{k_4 C}{(k_1 A)^2 h_0} \tau, \quad \beta = \frac{2k_4 k_{13} B}{(k_1 A)^2 h_0}.$$

In our case,



h_0 : acidity function, $q = 0.6$ is a stoichiometric factor, and k_i rate constants.

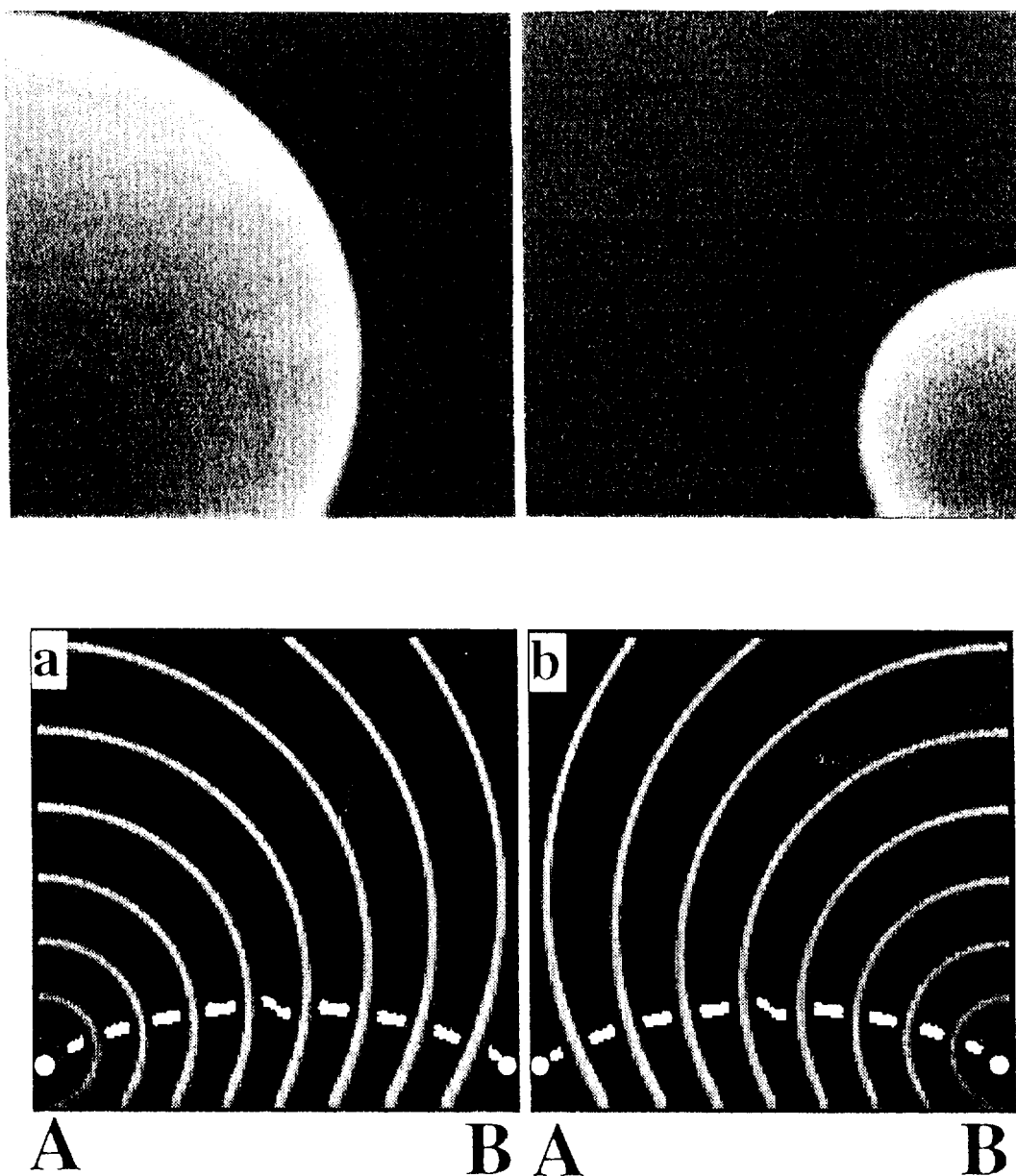


Fig. 6. Computer simulation on the tracking of the optimal path in a field of non-uniform velocity. Note the computed path is not a straight line, but deviated upward where the propagation velocity is higher. Above: Examples of the propagating waves from A (left) and B (right). Below: Superposition of the chemical wave.

The calculations were carried out for a BZ reaction with the following composition: $A = 0.2$, $B = 0.2$, $C = 0.005$. The value of h_0 was taken as 0.15 for the simulation in Fig. 5. For the simulations in Fig. 6, h_0 is a function of the spatial coordinate, i.e., $h_0(x, y) =$

$a + by$. The constants a and b were chosen so that the acidity varied from 0.1 at the bottom of Fig. 6 to 0.25 at the top.

The rate constants k_i were rescaled to 20°C using the Arrhenius dependence described in [13].

To study spatio-temporal effects, we added diffusion terms to Eq. (1):

$$\begin{aligned} \frac{dx}{d\tau} &= F(x, z) + \Delta_{\rho}x, \\ \frac{dz}{d\tau} &= G(x, z) + \delta\Delta_{\rho}z, \\ \rho_i &= r_i \left[\frac{k_1^2 A^2 h_0}{k_4 C D_x} \right]^{0.5}, \end{aligned} \quad (2)$$

where $F(x, z)$ and $G(x, z)$ are the terms on the right-hand side of Eq. (1), r_i is a spatial coordinate, ρ_i a scaled spatial coordinate, Δ_{ρ} the Laplacian operator with respect to coordinates ρ , and $\delta = D_z/D_x$ is the ratio of the diffusion coefficients. We assume that $D_x = D_z = 2 \times 10^{-5} \text{ cm}^2 \text{ s}^{-1}$.

The computations were carried out in a two-dimensional array of 200×200 elements using Euler's explicit method of integration and Neumann's ("no flux") boundary conditions. The space and time steps were $h_x = 0.1 \text{ mm}$ and $h_t = 0.1 \text{ s}$, respectively. A further decrease in h_x and h_t did not markedly improve the accuracy of the calculations.

Fig. 5 illustrates the procedure for evaluating the optimal path when there is an obstacle between points A and B. The actual procedure to obtain the optimal path is just the same as in the experiment (see Fig. 4). The path between A and B is tangent to the obstacle. Fig. 6 shows the optimal path between two points when the velocity is not a constant, but changes gradually from the minimal value at the bottom to the maximal value in the upper part of the chemical medium. This velocity field was simulated by imposing a permanent gradient of acidity. The fastest path in this case is clearly not a straight line, but rather deviates upward to follow the field with the higher velocity.

Thus, it becomes clear that the combination of obstacles and gradients in the velocity field gives us a novel method for finding the optimal route in a velocity field.

5. Discussion and conclusion

We have shown the applicability of chemical wave to a computation problem, besides image processing

[1–3]. With the aid of a chemical excitable medium, we can solve at least one general optimization problem; i.e., finding the quickest path between two points in a velocity field.

There are many considerations for the future application of chemical computers based on the BZ reaction. It is possible to estimate some technical characteristics of such a device. The efficient size of a "single element" (definition scale) is on the order of the diffusion length, ca. 0.1 mm. Thus, a 9 cm petri dish contains more than 600 000 processors, working in parallel. However, the rate of each processor in this system is extremely slow: the characteristic speed of wave propagation, about 0.05 mm s^{-1} , yields about 1 switch per 2 s. This means that, even considering the large number of "processors", we cannot obtain a computation rate of greater than 300 000 operations per second. This is about 100-fold slower than that in a modern PC. It may be very difficult to increase the oscillation rate in the BZ reaction by a factor of 100.

Nevertheless, our system provides a relatively simple and evident model for future studies of how to use excitable media for information processing. Indeed, if it would be possible, based on the modern technology, to find or to design an excitable system 100 times faster than the BZ medium, it will open a new era on computer processing. At present, we can only expect that such an excitable medium could be developed by the aid of molecular electronics, as a network of molecular triggers.

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