BZ 反応で駆動する粒子を用いた最短経路探索

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概要

BZ 反応と呼ばれる化学反応で駆動する粒子を考え、これを用いると最短経路問題が解けることを数値的に示す。BZ 反応は非平衡系の代表的な例として様々な角度から調べられており、近年はケミカルコンピューティングのモデルとしても脚光を浴びている。本論文ではこれを交通流の重要な問題の一つである最短経路問題に応用できることを示す。本手法に対する実験的検証の可能性ついても言及する。

The shortest path problem with BZ-driven particles

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Abstract

We propose a method to solve the shortest path problem by using particles driven by the BZ reaction. The BZ reaction has been well investigated as one of the typical non-equilibrium dynamical systems, and the results enhance interdisciplinary applications, like chemical computing. In this paper, we show numerically that the particles driven by the BZ waves are useful to the maze-solving. More specifically, we perform that the BZ-driven particles fill in all of the "not shortest" path in a maze due to the property of the BZ waves, and only the shortest path remains. We believe this idea would be confirmed in reality with an appropriate experimental setup.

1 Introduction

Finding the shortest path of a given maze is one of the major problem in the study of traffic flow. This problem has been investigated mainly from the viewpoint of graph theory, and the achievements of the study are used in an automotive navigation system and others in our real life.

Recent developments of non-equilibrium dynamics cast new light on this field. Some researchers have solved the shortest path problem by using chemical and biological methods [1, 2, 3]. Many applications of these "chemical computing" have been developed and drawn attention of interdisciplinary scientists since it would be helpful to understand the self-organized dynamics, and also would be useful as a model of the unconventional computing (logic gate [4], path planning [5], mesh generator [6]).

In this paper, we propose a new method for the shortest path problem with chemical materials via modeling approach. The simulation of the BZ reaction with maze-shape boundary is performed. In addition, we introduce a particle model which is driven by chemical waves generated from the BZ reaction. By using these concepts, we show numerically that the particles fill in the "not shortest" path in a maze and indicate the shortest path automatically. This study may give an interdisciplinary

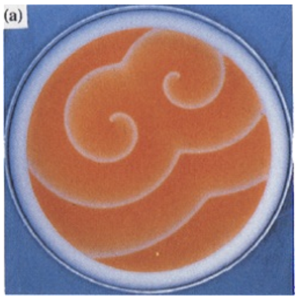

Fig.1: Typical spiral waves observed in chemical media. It shows dynamic rotation around the tip. The picture is cited from [7].

connection between traffic flow and chemical computing.

2 The BZ reaction

The BZ (Belousov-Zhabotinsky) reaction is the well-known dynamic chemical reaction observed in excitable media, the material which reacts only to stimulations above a given threshold. When we give strong stimulations or perturbations at a point on the media, the reaction regions propagate like solitary waves and it forms strange dynamic patterns (Fig. 1).

It is known that chemical spiral waves in the BZ reaction can be reproduced by a model called the two-variable Oregonator [8]

$$\frac{\partial u}{\partial t} = D_u \nabla^2 u + \frac{1}{\epsilon}\left(u(1-u) - fv\frac{u-q}{u+q}\right),$$
$$\frac{\partial v}{\partial t} = D_v \nabla^2 v + (u - v),$$

where u and v are chemical concentration, D_u and D_v are the diffusion coefficients for each chemicals, and f,q,ϵ are the parameters. The typical solution of the equations is given in Fig. 2, which shows propagation of waves injected as two point stimulations. Note that the BZ waves have the following important properties: (i) they propagate isotropic (equi-velocity) way, (ii) they stick to the wall, and (iii) they annihilate when collide to other waves or the Neumann boundary wall.

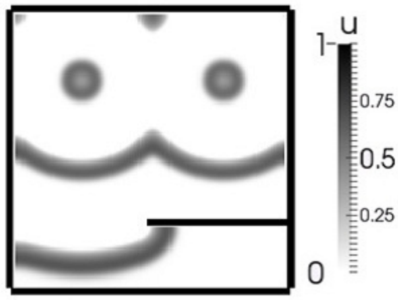

Fig.2: The numerical simulation of the two-variable Oregonator model. Waves are generated from two point sources, and shows isotropic propagation, annihilation by collision (wave-wall and wave-wave), and wall adhesion.

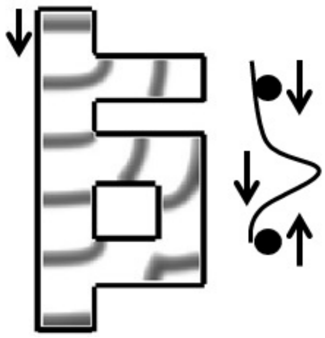

Fig.3: (Left) Propagation of chemical waves through the maze. Waves are injected from the upper end. (Right) The concept of the BZ driven particles. They moves toward higher concentration region.

3 Maze-solving with the BZ waves and particles

We can use spiral waves to find the shortest path in a given maze-shape boundary by utilizing above properties. When we inject excitation waves from the entrance of the maze, they propagate, split, turn around at the corners and go through all of the path due to (i) and (ii). And they would vanish if they collide with the dead-end because of the property (iii). We can also say that waves vanish if they go through "not shortest" paths since such paths (see bottom-right corner of the maze in Fig. 3) has the point of pair annihilation. Therefore outgoing waves from the exit of the maze have propagated through the shortest path (see Fig. 3). Note that the contour of the arrival time of the excitation waves at each grid point is similar to the floor field [10] used in the study of traffic flow. The waves propagate isotopic way, so that the BZ driven particles is similar to the pedestrians driven by the floor field, though the direction of the driving force is opposite.

Next, let us consider transportation of the particles by chemical waves. if we have the granular material which is driven by the positive chemical gradient (Fig. 3), we can use them as markers to find “not shortest” paths. Imagine that both the BZ waves and the particles are injected into the maze from the entrance periodically. In such situations, the particles are carried by the chemical gradient of the BZ waves. But waves vanish when it collide with the walls or other waves, so that the particles guided by waves would accumulate around the vanishing points where two waves collide and annihilate. All of “not shortest” paths have the vanishing point, therefore the particles fill in all of the dead-end and “not shortest” paths and only the shortest path remains. If we have two shortest passes, both passes will be obtained by this method since both passes have no vanishing point.

4 Simulations

Here we conduct the numerical experiment to confirm the idea above. We consider the coupling simulation of the BZ waves with the particles under the maze-shape boundary by using the numerical solution of the reaction-diffusion equations and cellular automata.

The BZ wave is calculated by using two-variable Oregonator with the maze-shape boundary. The boundary is the Neumann (no-flux) condition. The discretization scheme is the finite volume method. The time evolution scheme is the ADI for the diffusion term, the Fenton-Karma scheme for the reaction term [9]. The parameters used here are the following: $D_u = 0.05$, $D_v = 0.03$, $f = 2.5$, $q = 0.002$, $\epsilon = 0.05$, $dx = 0.1$, $dt = 0.001$.

In addition, we introduce the particles driven by the gradient of chemical concentration. We require the following properties to the particles: (i) the motion of the particles is described by cellular automata and the cells correspond to the mesh of the two-variable Oregonator, (ii) they are allowed to hop to one of the Moore neighborhood cells in which the most sharp positive chemical gradient is realized, (iii) the chemical gradient is given by the distribution of the variable v of the two-variable Oregonator, (iv) the motion of the particles is updated by the random manner, (v) the particles have the exclusive volume, which means they cannot overlap each other and also cannot penetrate the walls, (vi) the particles are small, light and stable (not soluble), and (vii) the field-particle interaction is one-way coupling, which means that the particles do not affect the distribution of the chemicals.

Fig.4: The numerical simulation. (Left) Waves (black bands) and the particles (blue dots) are supplied periodically. Waves propagate along the maze accompanied by particles. (Right) All of the detours are filled with the particles as time goes on.

In this calculation, the BZ waves are ignited from the entrance and the particles are also supplied. These input event occurs repeatedly with a definite period. The particles evacuate from the system when they arrive at the exit of the maze.

The resulting images of the simulation are given in Fig. 4. The particles are carried by chemical waves and fill in the dead-end. Moreover, we find the pair annihilation of the chemical waves in the “not shortest” path, and the particles aggregate around the point of annihilation. Finally, only the shortest path appears automatically.

5 Experimental possibilities

As of right now, we have no experimental results that correspond to the method shown here. But some experimental researches imply the possibilities of the experimental design to confirm our method.

It is shown experimentally that the BZ waves have an ability to transport materials in a certain condition [11, 12]. The driving force is derived from the gradient of the surface tension which originates the gradient of chemical concentration.

This transportation can also be reproduced by the numerical simulations[13]. In addition to the two-variable Oregonator with convection terms, we solve the Navier-Stokes equation and the Newton equation of the disk-shape material

$$\frac{\partial \boldsymbol{V}}{\partial t} + (\boldsymbol{V}\cdot\boldsymbol{\nabla})\boldsymbol{V} = \frac{1}{Re}\frac{\partial^2 \boldsymbol{V}}{\partial x^2} - \boldsymbol{\nabla} p + \boldsymbol{\gamma},$$
$$\boldsymbol{\gamma} = c\boldsymbol{\nabla} v \quad \text{(on the surface)},$$
$$m\ddot{\boldsymbol{x}}_p = \int \frac{dl}{l}\boldsymbol{\nabla}_{\boldsymbol{n}}(\boldsymbol{\gamma}\cdot\boldsymbol{n}) - \eta\left(d\dot{\boldsymbol{x}}_p - \int \frac{dS}{S}\boldsymbol{V}\right),$$

where γ is surface tension which is assumed to be proportional to the gradient of concentration v, η is the fluid resistance, x_p is the position of the disk, c is the constant, $\boldsymbol{n}dl$ is the normal vector of the line element along the disk, and $dS = dxdy$ is the area element of the disk. The example of the numerical result is given in Fig. 5. Here we assume that the driving force of the transportation comes from both the surface tension and the convection.

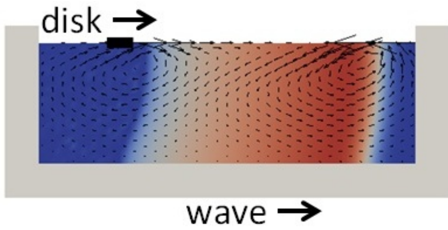

Fig.5: Example of the coupling simulation. The disk is on the surface of the chemical media. Waves propagate from left to right and drag the disk.

These results indicate that our maze-solving technique would be confirmed in reality when we can design the suitable experimentally setup. In our model, the dynamics of the particles is represented as automata and it is extremely simplified compared to the formulation with the equation of motion. But note that the both possible driving forces (the surface tension and the convection) comes from the chemical gradient. Therefore our automata model based on chemical gradient would be valid at least as a zeroth approximation.

6 Conclusion

In this study, we investigated the possibility of the new method for the shortest path problem by using the BZ-driven particles. We showed numerically that the particles driven by chemical waves show the solution of the maze.

Our method shows the path automatically and does not need to use any image processing techniques to visualize the path. This is the the major difference compared to the previous study which also use the BZ reaction to solve a maze [1]. Of course this “chemical computing” has some problems for the realistic purposes, because of the relatively high calculation costs (long reaction times). But the concept of the BZ-driven particles would be useful as a visualization technique that captures the characteristic structures in reaction-diffusion systems.

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