Bifurcation analysis and spatial entropy in the spatially discrete Allen-Cahn equation

ATSUSHI NAGAURA, YUICHI YABUKI, NOBORU KUNIMATSU
Department of Science and Technology
Keio University
3-14-1, Hiyoshi, Kohoku-ku, Yokohama, 223-8522
JAPAN

Abstract: The theory of lattice dynamical systems is regarded to be an approach to examine the behaviors of equations described in discrete space. In the theory of lattice dynamical systems, it is known that solutions of spatially discrete diffusion equations give rise to phenomena not appearing in the spatially continuous ones.

We consider spatially discrete nonlinear diffusion equations which have the analogous form to the Allen-Cahn equation. This equation has stable time invariant solutions called mosaic solutions. A criterion is given by using the spatial entropy $h$ which distinguishes between pattern formation and spatial chaos.

We discuss a class of these equilibria and their bifurcations both theoretically and numerically. Also we obtain the spatial entropy $h$ numerically and study how this quantity varies with system parameters.

Key-Words: Allen-Cahn equation, lattice dynamical systems, mosaic solutions, spatial entropy

1 Introduction
Lattice dynamical systems [1][2] are infinite systems of ordinary differential equations on a spatial lattice, such as the $d$-dimensional integer lattice $\mathbb{Z}^d \subseteq \mathbb{R}^d$. Lattice dynamical systems arise in many applications such as chemical reaction theory [3], biology [4], and material science [5].

We consider the differential equation, which is analogous in form to the Allen-Cahn equation [6]. This equation is used to describe order-disorder transition in Fe-Al binary alloy. In this paper we consider the spatially discrete version of it. The two-dimensional spatially discrete Allen-Cahn equation (SDAC) [7] is given by

$$\frac{du_{i,j}}{dt} = (\alpha^+ \Delta^+ + \alpha^x \Delta^x)u_{i,j} - f(u_{i,j}),$$

$$(i,j) \in \mathbb{Z}^2,$$ (1)

$$\Delta^+ u_{i,j} = u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1} - 4u_{i,j},$$

$$\Delta^x u_{i,j} = u_{i-1,j-1} + u_{i-1,j+1} + u_{i+1,j-1} + u_{i+1,j+1} - 4u_{i,j},$$ (2)

with periodic boundary conditions

$$u_{i,k} = u_{i,N+k}, \quad i = 0, \cdots, N+1, k = 0,1,$$

$$u_{k,j} = u_{N+k,j}, \quad j = 0, \cdots, N+1, k = 0,1,$$ (3)

where $u_{i,j}$ is the scalar variable on the integer lattice $(i,j) \in \mathbb{Z}^2$. Here $\Delta^+$ and $\Delta^x$ are discrete two-dimensional Laplace operators given by + and x shaped stencils. The quantities $\alpha^+$ and $\alpha^x$ are diffusion coefficients, and takes the values of positive, negative or zero. $f$ is a cubic polynomial, typically $f(u) = pu^3 - qu$, with $p, q > 0$. In this study we take $p = 1/2$ and $q = 1/2$.

The SDAC equation (1) has equilibrium solutions [7]. These solutions are called mosaic solutions [1] because of their configurations. These equilibrium solutions can take the form of regularly ordered patterns (pattern formation) on the one hand, and spatially disordered states (spatial chaos) on the other [1][2].

At first, to clarify existence of mosaic solutions, we show that the SDAC equation has a Lyapunov function and the solutions are stable. Next, to find the conditions in which the regular patterns of equilibrium are stable, we analyze the eigenvalues of the Jacobian matrix. In addition, we perform the numerical simulations of the SDAC equation and draw the bifurcation diagram. Then we compare the conditions that are found out through these two methods.
We cannot distinguish pattern formation from spatial chaos by the theory of stability. To distinguish these two types of states, a criterion which is called spatial entropy is defined in [2]. The spatial entropy of one-dimensional mosaic solutions was studied in [8] [9], which gave good discrimination between the two states. We calculate the spatial entropy of its stable solutions, and we show how this quantity varies with bifurcation parameters. We expect the spatial entropy to be a characterization index of bifurcation. We believe that ours is the first attempt to calculate that of two-dimensional ones and to correspond the spatial entropy to the bifurcation diagram itself.

2 Existence and stability of mosaic solutions

The SDAC equation has stable time invariant solutions called mosaic solutions. A class of equilibrium solutions which take only the values ±s, and 0 at each lattice point is called mosaic solutions [1]. Now we denote the set of all mosaic solutions by $\mathcal{M}_2 = \{-s, 0, s\}^Z$. Mosaic solutions are sorted into some regular patterns such as checkerboard, striped and flat patterns.

At first, we show that the SDAC equation has a Lyapunov function, which clarifies the existence of equilibrium solutions. Next, we analyze linearized stability of regularly ordered patterns, to find the conditions in which checkerboard, striped and flat pattern are stable.

2.1 Lyapunov stability

A gradient system has a Lyapunov function [10]. Since (1) is a gradient system, it has a Lyapunov function

$$E[u] = \sum_{j=1}^{N} \sum_{i=1}^{N} \left\{ F(u_{i,j}) + 2(\alpha^+ + \alpha^\times)u_{i,j}^2 \right\} - \frac{1}{2} \alpha^+ u_{i,j} \sum_{(m,n)+(i,j)} u_{m,n} - \frac{1}{2} \alpha^\times u_{i,j} \sum_{(m,n)\times(i,j)} u_{m,n} \right\} $$

where

$$\sum_{(m,n)+(i,j)} u_{m,n} = \sum_{(m,n)|((m-i)^2+(n-i)^2=1)} u_{m,n},$$

$$\sum_{(m,n)\times(i,j)} u_{m,n} = \sum_{(m,n)|((m-i)^2=(n-i)^2=1)} u_{m,n}. $$

(4)

$$F(x) = \frac{p}{4} \left( x^2 - \frac{q}{p} \right) + \delta, $$

(7)

where $\delta$ is a positive constant which depends on $\alpha^+, \alpha^\times, p, q$. $E[u]$ is positive definite, and $\dot{E}[u] \leq 0$ with the boundary conditions (3).

2.2 Mosaic solutions

The SDAC equation has equilibrium solutions which take only the values $\pm s$, and 0 at each lattice point. We classify them into three regularly ordered patterns: checkerboard, striped and flat patterns. If the solutions satisfy

$$u_{i,j} = \begin{cases} s & \text{if } i \text{ is odd}, \\ -s & \text{if } i \text{ is even}, \end{cases} $$

(8)

we call them checkerboard patterns. Since $u_{i,j} = 0$, from (1) and (8), we obtain

$$s = \sqrt{\frac{q - 4\alpha^+}{p}}. $$

(9)

If the solutions satisfy

$$u_{i,j} = \begin{cases} s & \text{if } i \text{ is odd}, \\ -s & \text{if } i \text{ is even}, \end{cases} $$

(10)

we call them striped patterns. From (1) and (10), we obtain

$$s = \sqrt{\frac{q - 4\alpha^+ - 8\alpha^\times}{p}}. $$

(11)

If the solutions satisfy either

$$\text{or } u_{i,j} = s \quad \forall (i,j) \in \mathbb{Z}^2,$$

(12)

we call them flat patterns. From (1) and (12), we obtain

$$s = \sqrt{\frac{q}{p}}. $$

(13)

2.2 Linearized stability

Now we consider the Jacobian matrix of $u_{i,j}$. The diagonal elements of this matrix are $-f'(\pm s) - 4(\alpha^+ + \alpha^\times)$, and the non-diagonal elements are $\alpha^+$, $\alpha^\times$ or 0. From the Gershgorin’s theorem, eigenvalue $\lambda$ of the Jacobian matrix satisfies the condition

$$|\lambda - (-f'(s) - 4(\alpha^+ + \alpha^\times))| < |4\alpha^+| + |4\alpha^\times|. $$

(14)
Solutions are asymptotically stable under the condition $\text{Re}\lambda < 0$,

$$f'(s) + 4(\alpha^+ + \alpha^x) > |4\alpha^+| + |4\alpha^x|. \quad (15)$$

From (9) and (15), checkerbord patterns are asymptotically stable under the condition

$$2q - 20\alpha^+ + 4\alpha^x > |4\alpha^+| + |4\alpha^x|. \quad (16)$$

From (11) and (15), striped patterns are asymptotically stable under the condition

$$2q - 8\alpha^+ - 20\alpha^x > |4\alpha^+| + |4\alpha^x|. \quad (17)$$

From (13) and (15), flat patterns are asymptotically stable under the condition

$$2q - 4(\alpha^+ + \alpha^x) > |4\alpha^+| + |4\alpha^x|. \quad (18)$$

Fig. 1 shows the regions that correspond to the inequalities (16), (17) and (18). Checkerbord patterns are asymptotically stable on $R_1$, $R_2$, $R_3$ and $R_4$. Striped patterns are asymptotically stable on $R_3$, $R_4$, $R_5$ and $R_6$. Flat patterns are asymptotically stable on $R_2$, $R_4$, $R_6$ and $R_7$.

Our numerical analysis is performed in a two-dimensional square lattice of $64 \times 64$ cells with periodic boundary conditions (3). We use the fourth-order Runge-Kutta method which stepsize $dt = 10^{-2}$. As initial condition of $u_{i,j}$, we choose a random uniform distribution of the field in the interval $(-0.02, 0.02)$.

We obtained the regularly ordered patterns. Moreover, we obtained the pattern with which they spatially mixed. So we classify the equilibrium solutions into 7 types of patterns, which consist of 3 regular patterns and 4 types of the mixture patterns. The numerical results are shown in Fig. 2. $R_{Ch}$, $R_{St}$, and $R_{Fl}$ are the regions where checkerbord, striped, and flat patterns appear respectively. The region where the mixture patterns appear is denoted for example by $R_{X\&Y}$ or $R_{X\&Y\&Z}$.

In section 2 we proved the existence of equilibrium solutions and found the conditions in which the regular patterns are stable. In this section we obtain mosaic solutions numerically and figure the bifurcation diagram. Fig. 1 and Fig. 2 have similar shapes.

Meanwhile, some problems are remained open. We performed numerical simulations in a two-dimensional square lattice of $64 \times 64$ points with periodic boundary conditions (3). It is said that a spatial size should be large enough to approximate the infinite system. So it is necessary to perform the numerical analysis in larger square lattice and check the validity of our results of bifurcation diagram.

**3 Bifurcation Diagram**

In this section we analyze bifurcations corresponding to the regular patterns numerically. The bifurcation parameters are chosen to be $\alpha^+$ and $\alpha^x$.
4 Spatial entropy

We cannot distinguish regularly ordered patterns from mixture patterns by the theory of stability. The spatial entropy is defined in [2] in order to distinguish these two types of patterns. In this section we calculate the spatial entropy of equilibrium solutions, and compare the spatial entropy corresponding to bifurcation diagram. The Spatial entropy $h$ of the mosaic solution has the form

$$h = \lim_{m,n \to \infty} \frac{1}{mn} \log c_{m,n}. \quad (19)$$

We consider a non-empty set $V \subseteq \mathcal{M}_2$ of mosaic solutions. $(m, n)$ is a pair of positive integers. $c_{m,n}$ is the number of different patterns that one observes in $V$, by viewing the elements in this set through a window of size $m \times n$ in the lattice $\mathbb{Z}^2$. Certainly, $0 < c_{m,n} < 3^{mn}$. So this limit always exists, and $0 \leq h \leq \log 3$. The equilibrium solution of (1) at a point $(\alpha_+, \alpha_\times)$ is said to exhibit pattern formation if the spatial entropy $h$ is zero, and is said to exhibit spatial chaos if the spatial entropy is positive. Pattern formation means there are relatively few stable equilibria, so the spatial variations that they display are limited. On the other hand, spatial chaos means that a wide variety of stable disordered patterns occur.

We choose $(m, n) = (3, 3)$, and calculate the entropy of the equilibrium solution of the SDAC equation. Fig. 3 shows the entropy calculated. To make easy comparison between the entropy and the bifurcation diagram, we make the entropy binary in threshold $h = 0.5$ and plot the points in which $h < 0.5$ in Fig. 4. Judging from Fig. 4, the entropies of the checkerboard and flat are relatively small. On the other hand, the entropies of the patterns which appear in the region that corresponds to $R_{Ch\&St}$, $R_{St\&Fl}$, $R_{Ch\&St\&Fl}$, and a part of $R_{St}$ in Fig. 2 are relatively large.

Comparing the bifurcation diagram Fig. 2 with spatial entropy Fig. 4, the entropy $h$ increases as the regular patterns are complexly mixed. Our results indicate that $h$ can be a characterization index of bifurcation since critical points between $R_{Ch}$ and $R_{Ch\&St}$, $R_{Fl}$, and $R_{Fl\&St}$, and $R_{Fl\&St}$ and $R_{St}$ are strongly related, respectively, to each other.

5 Conclusions

We studied on the mosaic solutions in the spatially discrete Allen-Cahn equation (1). We considered pattern bifurcations both theoretically and numerically. Furthermore we calculated the spatial entropy of mosaic solutions and studied spatial entropy so as to know how this quantity varies with bifurcation parameters.

Recently much attention is given to the problem of pattern formation and control [11][12][13]. For these topics, characteristic quantities are important to distinguish different kinds of patterns, states or behaviors. Our results indicate that the spatial entropy can be a characteristic index of mosaic solution. In this study we showed the numerical example of spatial entropy only for the SDAC equation. So it is important to study the spatial entropy for other equations which have mosaic solutions, and to test the validity of the spatial entropy being char-
acterization index of pattern bifurcation. Meanwhile, it is meaningful to search different characteristic quantities which distinguish mosaic solutions since not all the bifurcation line in the Fig. 2 is described by using the spatial entropy.

Acknowledgements
The authors thank T. Kumagai for helpful discussions.

References: