Symmetric patterns in linear arrays of coupled cells

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In this note we show how to find patterned solutions in linear arrays of coupled cells. The solutions are found by embedding the system in a circular array with twice the number of cells. The individual cells have a unique steady state, so that the patterned solutions represent a discrete analog of Turing structures in continuous media. We then use the symmetry of the circular array (and bifurcation from an invariant equilibrium) to identify symmetric solutions of the circular array that restrict to solutions of the original linear array. We apply these abstract results to a system of coupled Brusselators to prove that patterned solutions exist. In addition, we show, in certain instances, that these patterned solutions can be found by numerical integration and hence are presumably asymptotically stable.

I. INTRODUCTION

Recent experiments on chemically reacting systems by Castets *et al.*[1] have confirmed Turing's prediction[2] that spatial pattern formation can arise from the interaction of diffusion with a system whose homogeneous reaction kinetics give only a single stable steady state. The patterns observed in these quasi-two-dimensional, continuous systems are typically quite symmetric, consisting of arrays of parallel stripes or hexagonal arrangements of spots. Ouyang and Swinney[3] have shown that bifurcation from one type of pattern to another can be observed on varying a control parameter such as the temperature.

Laplante and co-workers[4] have recently carried out another type of experiment, which constitutes a discrete, one-dimensional analog of the Turing pattern experiments. In this system, as many as 16 flow reactors, each containing the same chemical components, are coupled together in a linear chain by reciprocal mass exchange between each pair of neighbors.

It is interesting to speculate whether discrete arrays of coupled nonlinear cells can give rise to stable nonuniform spatial patterns when each cell has only a unique stable steady state. In other words, does the discrete analog of the Turing bifurcation occur? If such patterns arise, are there any symmetric ones, and are these patterns stable over any substantial parameter range? In the sections that follow, we use analytical methods based on group theory to show that in general such symmetric patterns may be expected to occur, and we derive some of their characteristics. We then demonstrate numerically, using the popular Brusselator model[5] of a chemically reacting system, the existence and stability of some of these states.

Rovinsky[6] carried out a numerical investigation of a linear array of coupled cells in which the dynamics corresponded to a model of the Belousov–Zhabotinsky reaction. With parameters corresponding either to a unique stable steady state or to an oscillatory state in each cell, he found stable, symmetric, steady-state solutions for the array similar to those obtained in this work.

It is well known that discretizations of reaction–diffusion systems on an interval give rise to linear arrays of coupled cells. The particular systems that we study are discretizations of such PDEs with Neumann boundary conditions. It may also be expected that equilibria for these coupled cells—when the number of cells is large—should well approximate equilibria of the PDEs. Thus we expect to find patterned solutions to the linear arrays when patterned solutions to the PDEs exist. Finally, we take the point of view that patterned solutions are often the product of symmetry—or more precisely—symmetry-breaking bifurcations.

Armbruster and Dangelmayr[7] observed that reaction–diffusion systems satisfying Neumann boundary conditions on an interval can be extended to intervals of twice the length satisfying periodic boundary conditions and that this extension introduces $\mathbf{O(2)}$ symmetry into the equations. Of course, one can interpret periodic boundary conditions as transforming the larger interval into a circle. The group theoretic aspects of this observation were further studied by Crawford *et al.*[8] In this paper we make a similar observation by embedding the linear arrays into circular arrays of twice the size having dihedral $\mathbf{D}_{2n}$ symmetry.

We note that many authors have considered bifurcations of equilibria and periodic solutions in circular arrays of coupled cells. For example, see Winfree[9] and Alexander and Auchmuty.[10] We shall follow the analysis based on symmetry found in Refs. 11 and 12.

II. THE EMBEDDING METHOD

We begin by writing the general form for a system of differential equations modeling a linear array of n identical

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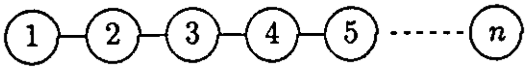

FIG. 1. Linear array of n identical cells.

cells with identical coupling (see Fig. 1 for a schematic of such a coupled system). This form is

$$\dot{x}_1 = f(x_1, x_1, x_2),$$
$$\dot{x}_i = f(x_{i-1}, x_i, x_{i+1}), \quad 1 < i < n, \tag{2.1}$$
$$\dot{x}_n = f(x_{n-1}, x_n, x_n),$$

where $x \in \mathbb{R}^k$, $f: \mathbb{R}^k \to \mathbb{R}^k$ and $f(x,y,z) = f(z,y,x)$. This last constraint is just the mathematical statement that the coupling is the same in the upstream and downstream directions.

An example is a system of coupled Brusselators where $k=2$, $x=(u,v)$ and f is as follows:

$$\dot{u}_i = 1 - (b+1)u_i + au_i^2 v_i + D_u(u_{i+1} - 2u_i + u_{i-1}),$$
$$\dot{v}_i = bu_i - au_i^2 v_i + D_v(v_{i+1} - 2v_i + v_{i-1}), \tag{2.2}$$

where a, b, D_u, D_v are positive constants. Equation (2.2) is valid for $1 < i < n$ as is. For $i=1$ and $i=n$ a modification is necessary to indicate that the first and last cells do not communicate. In these cases the coupling terms at the boundary have the form for $i=1$

$$D_u(u_2 - u_1), \quad D_v(v_2 - v_1)$$

and for $i=n$

$$D_u(u_{n-1} - u_n), \quad D_v(v_{n-1} - v_n)$$

which is consistent with the functional identity for the boundary terms given in (2.1). Note that the array of Brusselators has the *trivial* spatially constant equilibrium:

$$u_i = 1 \text{ and } v_i = b/a.$$

The only symmetry of a linear array of coupled oscillators is given by

$$\tau(x_1, \ldots, x_n) = (x_n, \ldots, x_1).$$

This symmetry implies that if an equilibrium $x = (x_1, \ldots, x_n)$ of a coupled array system is found, then $(x_n, \ldots, x_1)$ is also an equilibrium for the system, which may be the same as x or different. This symmetry, however, is not sufficient to produce states with complicated patterns.

Nevertheless, in many treatments of linear arrays (mainly numerical) equilibria with complicated and regular patterns are found. In this note we show how such equilibria can arise through the process of embedding the linear array in a circular array with twice the number of cells and using the symmetry of the circular array to produce equilibria for the linear array.

The extension to a circular array proceeds as follows. Let

$$\hat{x} = (x_{-n}, \ldots, x_{-1}, x_1, \ldots, x_n) \in \mathbb{R}^{2n}.$$

We consider the system of differential equations

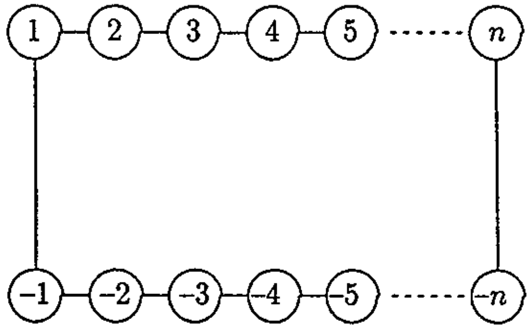

FIG. 2. Circular array of $2n$ identical cells.

$$\dot{x}_i = f(x_{i-1}, x_i, x_{i+1}), \quad -n \leqslant i \leqslant -1, \quad 1 \leqslant i \leqslant n, \tag{2.3}$$

where in order to make the extended system into a circular array we use the following conventions in the indices $i-1$ and $i+1$:

$(-n)-1$ equals n,

$(1)-1$ equals -1,

$(n)+1$ equals $-n$,

$(-1)+1$ equals 1.

See Fig. 2.

Observe that an equilibrium for the circular array (2.3) that satisfies $x_{-i} = x_i$ for $1 \leqslant i \leqslant n$ is also an equilibrium for the linear array (2.1). We shall use this observation along with the symmetries of the circular array to produce patterned equilibria for the linear array for bifurcation from the trivial equilibrium.

The group of symmetries of the circular array is the dihedral group $\mathbf{D}_{2n}$ of symmetries of the regular $2n$-sided polygon.

III. BIFURCATION IN CIRCULAR ARRAYS

Steady-state bifurcations with $\mathbf{D}_{2n}$ symmetry have been well studied (see Ref. 12, pp. 97–103). A steady-state bifurcation is one in which an eigenvalue of the linearized system goes through zero. The multiplicity of that eigenvalue (or the dimension of the kernel of the Jacobian matrix at the equilibrium) is dictated by group theory. The theory states that generically the multiplicity will be the dimension of an irreducible representation of the group of symmetries of the equilibrium (in this case $\mathbf{D}_{2n}$ for the circular array). Since all irreducible representations of $\mathbf{D}_{2n}$ are either one- or two-dimensional, we expect the multiplicity of the eigenvalues to be one or two.

When the eigenvalues are double, then the nonlinear theory states that there will be two branches of solutions (for $n \geqslant 2$) each having a reflectional symmetry (Ref. 12, Table XIII, 5.2). On one branch the axis of symmetry of the reflection will connect opposite vertices and on the other branch the axis of symmetry will connect the midpoints of opposite sides. Note that any solution that is symmetric across the axis of symmetry obtained by connecting the midpoints of the pair of opposite sides connecting cells 1 and -1 and n and $-n$ will satisfy the identity $x_{-i}=x_i$ and hence be a solution to the linear array. The other equilibria of the circular arrays will not restrict to equilibria of the linear array. In the case of simple eigenvalues, the analysis is less clear since there are several possible one-dimensional irreducible representations. We return to this point below.

The $\mathbf{D}_{2n}$ symmetry of the circular array also simplifies the linear analysis (though the linear analysis on the linear array could have been worked out directly). The generalities of the linear analysis for circular arrays have also been worked out. The $(2nk)\times(2nk)$ matrix decomposes into $k\times k$ blocks of a circulent form. As a result all of the eigenvalues of the large matrix can be determined by finding the eigenvalues of $n+1$ $k\times k$ matrices, a substantial simplification. See the discussion in (Ref. 12, pp. 394–396).

Let A and B be the $k\times k$ Jacobian matrices of $f(y,x,z)$

$$A=\frac{\partial f}{\partial x} \text{ and } B=\frac{\partial f}{\partial y}.$$

Then the eigenvalues of the matrices

$$A+2\kappa_j B, \tag{3.1}$$

where $\kappa_j=\cos(j\pi i/n)$ are eigenvalues of the big $2nk\times 2nk$ matrix. In fact, for $j=0$ and $j=n$ these eigenvalues are simple and for $0<j<n$ they are double. Together these eigenvalues account for all of the eigenvalues of the big matrix.

It follows from the discussion above that if a simple eigenvalue of $A+2\kappa_j B$ goes through zero with nonzero speed when $0<j<n$, then there exists a branch of solutions on the circular array that restricts to a branch of equilibria on the linear array.

As an example we show that eigenvalues of (3.1) always cross through zero in the array of Brusselators. We set $D_u=rD_v$ and $D_j=2(1-\kappa_j)D_v$. In these scaled variables the jth matrix $A+\kappa_j B$ is

$$\begin{pmatrix} b-1-rD_j & a \\ -b & -a-D_j \end{pmatrix},$$

and the determinant of this matrix is

$$rD_j^2+(ra-(b-1))D_j+a. \tag{3.2}$$

Since $-1\leqslant\kappa_j\leqslant 1$, D_j is nonnegative. Note that $D_j=0$ when $\kappa_j=1$ which occurs when $j=0$. Thus the 0th matrix never has a zero eigenvalue, since a is assumed positive. If we find the roots D_j of (3.2), then we get a real positive root when

$$r<\frac{b-1}{a} \text{ and } \sqrt{b}\geqslant 1+\sqrt{ra}.$$

By varying parameters, we can force simple eigenvalues to cross through zero with nonzero speed for each of the matrices $A+2\kappa_j B$. This shows that each of the desired steady-state bifurcations occurs in the Brusselator model.

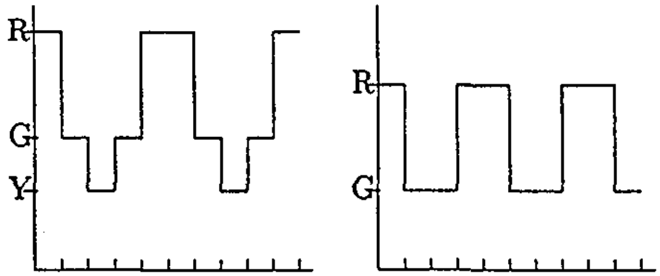

FIG. 3. Patterns in equilibria indicated by square waves.

IV. PATTERNS IN SOLUTIONS

We now look at the patterns of the solutions that we have found as they will appear in the linear array.

On the two-dimensional kernel, which we identify with $\mathbb{C}$, the rotation of the cells by one cell counterclockwise acts by

$$z\to e^{(\pi i/n)j}z. \tag{4.1}$$

Observe that when $j=n$, the other simple eigenvalue case, rotating by one cell generically leads to a different state but rotating by two cells leads to the same state. Such a solution cannot restrict to the linear array since the cells 1 and -1 are adjacent and hence, generically are unequal—but must be equal to restrict to a solution on the linear arrays. Hence we can assume that $1\leqslant j<n$.

We say that a group element acts *trivially* in a bifurcation if that group element acts as the identity on the kernel of the linearization. If a group element acts trivially in a bifurcation, then all of the steady states that result from this bifurcation are fixed by that symmetry.

Suppose j and $2n$ are coprime. Then (4.1) shows that no rotation of the cells acts trivially. It follows that for these solutions on the linear array no two cells are doing the same thing (generically).

Suppose j is even. Then rotating by n cells acts trivially. It follows that the cells in the linear array must be left–right symmetric, that is, $x_i=x_{n-i}$. If $j/2$ and n are coprime, then generically this is the only pattern.

Now let l be the greatest common divisor of j and $2n$ and assume $l>2$. Then rotating the circular array of cells by $2n/l$ cells acts trivially. Coupling this fact with the linear array restriction $x_i=x_{-i}$ leads to some interesting patterns. For example, if $n=10$ and $j=4$, then rotating by $2n/l=5$ cells acts trivially and we get the pattern of cells *RGY GRRGY GR*. If $n=10$ and $j=5$, then rotating by $2n/l=4$ cells acts trivially and generically we get the pattern *RGGRRGG RRG*. In this notation we are imagining that cells that are not forced by symmetry to be identical are colored differently. So R stands for *red*, G stands for *green*, and Y stands for *yellow* in the given patterns. We have also indicated these patterns using square waves in Fig. 3.

In general, when $l\geqslant 2$, we find patterns consisting of identical blocks of cells of length $2n/l$ where in each block the pattern is symmetric about the middle. These blocks repeat $[l/2]$ times with an extra half block at the end should l be odd.

V. TIME-PERIODIC SOLUTIONS

The theory of Hopf bifurcation in the presence of $\mathbf{D}_{2n}$ symmetry can also be used to predict patterns of oscillation in time-periodic solutions for linear arrays of coupled cells. As before, one embeds the linear array satisfying Neumann boundary conditions into a circular array.

Hopf bifurcation occurs when a pair of complex conjugate eigenvalues cross the imaginary axis with nonzero speed. As in the case of steady-state bifurcation, the $\mathbf{D}_{2n}$ symmetry implies that generically these complex eigenvalues will be either simple or double. Moreover, for coupled cells, the eigenvalues can be computed as in (3.1).

The general theory of Hopf bifurcation predicts that when there is a complex conjugate pair of double eigenvalues, then there will be a unique bifurcating branch of time-periodic solutions that will for all time satisfy Neumann boundary conditions of the linear array and thus restrict to a time-periodic solution of the n cell system. See Chap. XVIII, Tables 1.2 and 1.3 of Ref. 12, p. 369.

Consequently, to each pattern in an equilibrium solution there corresponds a time-periodic solution with the same spatial pattern. The only difference is that in each block of length $2n/l$ (notation as at the end of Sec. III) the cells that are equally spaced from the ends of the block oscillate with the same wave form—but with a half period phase shift. It follows that if the size of the block $2n/l$ is odd, then the middle cell in each block will oscillate with twice the frequency of the other cells.

We now remark that all of these types of Hopf bifurcation occur in the Brusselator example. However, except for the standard Hopf bifurcation where all cells oscillate in phase, these patterned periodic solutions are unstable at bifurcation. This follows from the fact that the trivial solution is unstable at these bifurcation points. (This fact is analogous to the bifurcation of time-periodic solutions to the PDE Brusselator on an interval.)

To determine the points where Hopf bifurcation can take place, we need to find points where $\mathrm{tr}(A+2\kappa_j B)$ is zero while $\det(A+2\kappa_j B)$ is positive. The trace of the matrix (3.1) is

$$\mathrm{tr}(A+2\kappa_j B)=b-1-a-(r+1)D_j. \tag{5.1}$$

The root D_j obtained by setting (5.1) equal to zero is

$$D_j=\frac{b-1-a}{r+1}. \tag{5.2}$$

The Hopf bifurcation with simple eigenvalues occurs when $D_j=0$, that is, when $b=a+1$. For double eigenvalue Hopf bifurcations to occur, we need $D_j>0$, that is, we need

$$b>a+1,$$

which we assume. A calculation shows that when D_j satisfies (5.2), then

TABLE I. $a=4$, $b=4.5$, $D_u=0.002$, $D_v=2.0$.

j	R	G	Y
4	(0.2470,1.4692)	(0.222 60,1.0927)	(4.0608,0.3234)
5	(0.2209,1.085)	(1.779,0.6915)	⋯

$$\det(A+2\kappa_j B)=a(r-1)^2(b-a)+(b-1-a)^2>0.$$

Hence, there are purely imaginary eigenvalues for $A+2\kappa_j B$ and Hopf bifurcation does occur.

VI. NUMERICAL RESULTS

While the previous analysis reveals possible symmetric patterns for a given array, it does not give any information regarding either the stability or the amplitudes of the patterns. One could try to determine the stability of solutions using exchange of stability arguments at the bifurcation point. But the calculations based on such an approach are almost impossibly complicated (since terms of degree l must be computed in the bifurcation analysis in linear arrays with blocks of cells of length l). Similarly, one could try to prove stability of equilibria by finding some sort of Liapunov function—but such an approach may be difficult to implement. Thus, if one wishes to know whether such patterns will actually arise in a particular array and, if so, what the patterns will look like, it seems simplest to resort to a numerical investigation.

We examine the cases $n=10, j=4$, 5 discussed above. The equations (2.2) for a set of 10 coupled Brusselators were integrated numerically with the parameter a fixed at 4.0. The equations were solved on a VAX 8650 with the GEAR code and on a 286-PC with a locally written numerical integrator for ODE's. The results obtained were independent of the integration method.

For each value of j, the calculations were started with parameters $b=4.5$, $D_u=0.002$, $D_v=2.0$ with an initial condition corresponding to the uniform steady state ($u_k=1, v_k=1.125$) plus a small ($\leqslant 0.1$) perturbation with symmetry corresponding to the patterns found in the analysis of the previous section. For both values of j, the system evolved to a stable steady state that preserved the symmetry of the initial condition, i.e., the pattern predicted by the symmetry analysis is stable with these parameters. In Table I we show the values of u and v for the patterns *RGY GRRGY GR* ($j=4$) and *GRRGGRRGGR* ($j=5$). These patterns are stable even to relatively large (ca. 10%) asymmetric perturbations.

It is worth noting that the trivial spatially constant equilibrium given by $u_i=1$ and $v_i=b/a$ in the system of coupled Brusselators is asymptotically stable whenever $b-a<1$. The numerical simulations just described fall into this range. It follows that there are least two stable equilibria for these parameter values—one patterned and one homogeneous. Indeed, numerical simulations for $n>10$ indicate the simultaneous existence of many different (and presumably stable) nonsymmetric equilibria.

We next varied the parameter b to assess the range of stability of the patterns. For each value of b, the initial condition was chosen as the steady state corresponding to the previous b value. For $j=4$, the pattern is stable from $b \sim 3.23$ to at least $b=35$. For $j=5$ the range of stability is much narrower; for stability we find that b must lie approximately in the interval $3.73 < b < 4.57$. The range of stability narrows as the ratio r increases. When a symmetric state loses stability, the initial, symmetric pattern persists for some time before small differences from perfect symmetry arise and then grow, slowly at first, then more rapidly, until a final, stable, asymmetric pattern is reached. We have not carried out a systematic investigation of either the basins of attraction of the symmetric states or their stability for other values of n. These results, however, suggest that such patterns may be relatively easy to find.

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