Linear Instability Implies Spurious Periodic Solutions

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We analyse discrete approximations of reaction–diffusion–convection equations and show that linearized instability implies the existence of spurious periodic solutions in the fully nonlinear problem. The result is proved by using ideas from bifurcation theory. Using singularity theory we provide a precise local description of the spurious solutions. The results form the basis for an analysis of the range of discretization parameters in which spurious solutions can exist, their magnitude, and their spatial structure. We present a modified equations approach to determine criteria under which spurious periodic solutions exist for arbitrarily small values of the time-step. The theoretical results are applied to a specific example.

1. Introduction

In this paper we analyse numerical methods for reaction–diffusion–convection equations of the form

$$w_t = w_{xx} + \lambda h(w, w_x) \quad \text{for } x \in (0, 1) \text{ and } t > 0, \tag{1.1}$$

with boundary and initial conditions

$$w(0, t) = w(1, t) = 0, \qquad w(x, 0) = w_0(x). \tag{1.2}$$

We study explicit finite difference schemes for (1.1–2). The spatial mesh is defined by the points $x_j = j \Delta x$ for $j = 0, \dots, J$, where $J \Delta x = 1$. The temporal mesh is defined by the points $t_n = n \Delta t$. Let w_j^n denote our approximation to $w(x_j, t_n)$. Then, for $r = \Delta t / \Delta x^2$, the explicit numerical methods considered here are of the form

$$w_j^{n+1} = w_j^n + r\delta_x^2 w_j^n + \lambda \Delta t g(w_{j-1}^n, w_j^n, w_{j+1}^n; \Delta x) \quad \text{for } j = 1, \dots, J-1, \tag{1.3}$$

with boundary and initial conditions

$$w_0^n = w_J^n = 0, \qquad w_j^0 = w_0(j\Delta x). \tag{1.4}$$

Here $\delta_x^2 w_j = w_{j+1} - 2w_j + w_{j-1}$. We assume that the nonlinear function $g(a, b, c; \Delta x)$ is smooth (as governed by h) and chosen so that (1.3–4) forms a consistent approximation to (1.1–2). The precise choice of approximation is left open to allow for both centred and, where appropriate, upwind approximations to the convective term.

We show, under fairly minimal assumptions, the existence of spurious periodic solutions (in n) to the finite difference equations (1.3–4). Our technique is to

consider (1.3–4), with a value of Δt close to that which makes the scheme linearly unstable (a term made precise in Definition 3.1), and to apply techniques from bifurcation theory to establish the existence of a branch of solutions continuous in Δt, with period two in n; see Corollary 4.1. Using singularity theory, we show that the bifurcation is generically of pitchfork type, with Δt as the parameter; see Theorem 4.2. We also introduce a modified equations technique for analysing the existence and form of spurious solutions far away from the bifurcation point, as $\Delta t \to 0$; see Conjecture 4.1.

We illustrate this phenomenon by means of a very simple example. If we choose $h(w, w_x) = 8w^2$, set $\Delta x = \frac{1}{2}$ ($J = 2$), define $\mu = 8 \Delta t$, and let $w^n = w_1^n$, then the numerical scheme (1.3–4) becomes a simple map: $\mathbb{R} \to \mathbb{R}$ with the form

$$w^{n+1} = F(w^n),$$

where, for the obvious centred scheme,

$$F(w) = w - \mu w + \mu \lambda w^2. \tag{1.5}$$

Such maps are discussed in Guckenheimer & Holmes (1983). Period two solutions satisfy the coupled equations

$$q = F(p) \quad \text{and} \quad p = F(q).$$

By solving explicitly, we find that genuine period two solutions (that is $p \neq q$) are given by

$$q = \frac{(\mu - 2) \pm (\mu^2 - 4)^{\frac{1}{2}}}{2\lambda\mu} \quad \text{and} \quad p = \frac{\mu - 2}{\lambda\mu} - q.$$

Thus $\mu = 2$ is a *bifurcation point* at which nontrivial periodic solutions branch from the trivial solution $w^n \equiv 0$. Furthermore, the bifurcation is of pitchfork type: for $\mu < 2$ there are no real nontrivial periodic solutions, whilst for $\mu > 2$ there are two (the second corresponding to interchanging p and q in the first). The value $\mu = 2$ (that is, $\Delta t = \frac{1}{4}$) is precisely the value at which the numerical scheme found by linearizing about the steady solution $w^n \equiv 0$ becomes asymptotically unstable. It is termed a *flip* or *period doubling bifurcation point* (see Guckenheimer & Holmes, 1983).

The behaviour of this simple model is not a product of the particular choice of nonlinearity, nor of the large value taken for Δx. In general, we show that if the numerical scheme (1.3–4) possesses steady (n-independent) solutions then there are $J - 1$ critical values of Δt, predicted by linear theory, at which a branch of period two solutions in n bifurcates from the steady solution. Each branch of solutions is continuous in the parameter Δt and we show, by means of techniques from singularity theory, that the bifurcation is necessarily of pitchfork type. Often the periodic solution branching from the smallest critical value of Δt (that at which the scheme becomes linearly unstable) will have most effect on the dynamics of the discretization. However, depending on the magnitude and spatial structure of the initial data, it is possible for other solutions to have a significant effect.

It should be emphasized at this point that the period two solutions are spurious and purely a product of the discretization. It might be argued that, since the solutions bifurcate at values of Δt close to (or for some branches, far above) the linear stability limit, they will be irrelevant in practice. However, particularly if the bifurcation is subcritical, it is possible that a branch of spurious solutions will extend to values of Δt used in practice. The behaviour of a dynamical system such as (1.3–4) is intimately related to the existence of steady, periodic, and quasi-periodic motions, be they stable or unstable. (See Stuart (1989b) for an example of how spurious *steady* solutions affect dynamical behaviour of a discretization.) Thus the presence of the spurious periodic solutions at values of Δt used in practical computation can seriously degrade the performance of the numerical approximation. The analysis presented here forms the basis for an investigation of the range of Δt in which spurious periodic solutions exist, their magnitude, and their spatial structure. The rigorous proof of existence of periodic orbits is also useful since it draws attention to the fact that, for *nonlinear* problems, the manifestation of practical instability is not necessarily the un-bounded or enormous growth of a measured quantity (as it is for linear problems), but may be bounded behaviour of moderate relative scale. This is particularly relevant if the bifurcation is supercritical: in this case, a period two solution on the branch emanating from the linear stability limit attracts all initial data which are sufficiently close to it. Thus bounded behaviour of period two in n, observed as $n \to \infty$, is symptomatic of an explicit numerical method for a non-linear problem operating above the linear stability limit. The boundedness results from a balance between the linear instability mechanism and the nonlinear terms.

There are several scattered results proving the existence of periodic orbits in numerical schemes operating close to their linearized stability limits (Griffiths & Mitchell, 1988; Mitchell & Schoombie, 1989; Sleeman *et al.*, 1988). However, much of that work is concerned with *specific nonlinearities* and assumes the existence of a *trivial* steady solution. Underlying all these results is a general theorem along the lines of

linearized instability $\Rightarrow$ periodic solutions in nonlinear discretizations,

where the linearization is taken about *any* steady solution of the difference equations and the nonlinearity is *arbitrary* (excepting smoothness assumptions). For the discretization (1.3–4), this result follows from Corollary 4.1 with $i = J - 1$ so that Δt is close to the value $-2/\eta_{J-1}(\lambda)$ at which the scheme is linearly unstable (see Definition 3.1).

The explanation of the theorem is best understood in a bifurcation theoretic context: at the critical value for linear instability, the Frechet derivative of a suitably extended nonlinear problem (containing two steps of the discretization) is singular when evaluated at the steady solution and the null-space is spanned by vectors determined by the unstable eigenvector(s) from the linear theory. Since the Frechet derivative is singular we cannot invoke the implicit function theorem and branching of solutions is suggested. Of course, various technical assumptions are required to make these notions into a precise theorem; in particular, detailed

properties of the derivatives of the nonlinear discretization are required—the dimension of the null-space of the first derivative is crucial. For our main results, we have chosen to concentrate solely on equations (1.1–2) and their discretizations, for the sake of clarity. With trivial modifications the theory contained here extends to inhomogeneous Dirichlet, Neumann, and Robin boundary conditions and, with a little more care, to periodic boundary conditions. In addition, as indicated above, the idea of the proof applies to finite difference discretizations of arbitrary time-dependent ODEs and PDEs. The bifurcation analysis presented is complementary to the asymptotic approach introduced by Newell (1977) and detailed further in Stuart (1989a). More complicated periodic and quasi-periodic structures arising in discretizations of ODEs are discussed in Sleeman *et al.* (1988) and Yamaguti & Ushiki (1981). The general theory of the period doubling route to chaos in iterated maps on $\mathbf{R}^n$ (of which (1.3–4) is an example) is discussed in Collet *et al.* (1981).

We are concerned with the *practical stability* of the numerical method (1.3–4): the method is studied for fixed (but small) values of the mesh-spacings. Specifically we fix Δx throughout our analysis (so that we have a problem of fixed dimension) and consider Δt as a bifurcation parameter. Although we vary Δt for the purposes of analysis, our interest is in the behaviour of the dynamical system (1.3–4) for any given, fixed values of Δt and Δx (which might correspond, for example, to the minimum attainable values in a practical computation). This notion of stability is distinct from *convergence stability* (Lopez-Marcos & Sanz-Serna, 1988) which concerns the limit as the mesh-spacings shrink to zero. (The convergence stability of linear diffusion–convection equations is detailed in Morton (1980).) Practical stability is of particular importance in applications where the asymptotic properties of a time-dependent PDE are sought as $t \to \infty$. The relationship between practical and convergence stability is discussed in Section 5.

In Section 2 we reformulate (1.3–4) as a perturbation of a steady solution. Section 3 contains a full discussion of the linear theory for (1.3–4) when linearized about a steady solution. In Section 4 we describe the nonlinear theory, proving the existence of period two solutions and calculating the normal form governing their existence. We also introduce a modified equations interpretation which gives criteria for the existence of spurious periodic solutions at arbitrarily small values of Δt. In Section 5 we describe an application of the theory to the stability and qualitative behaviour of a particular reaction–diffusion equation for which periodic solutions exist at arbitrarily small values of Δt.

2. The steady state

Throughout this and the following two sections we assume the existence of a steady (n-independent) solution of (1.3–4). This solution satisfies

$$0 = r\delta_x^2 W_j + \lambda \, \Delta t g(W_{j-1}, W_j, W_{j+1}; \Delta x) \quad \text{for } j = 1, \dots, J-1, \tag{2.1}$$

$$W_0 = W_J = 0. \tag{2.2}$$

We introduce perturbations from this steady state by setting $w_j^n = W_j + u_j^n$ and

obtain the equations

$$u_j^{n+1} = u_j^n + r\delta_x^2 u_j^n + \lambda \, \Delta t f(j, u_{j-1}^n, u_j^n, u_{j+1}^n) \quad \text{for } j = 1, \dots, J - 1, \qquad (2.3)$$

together with boundary and initial conditions

$$u_0^n = u_J^n = 0, \qquad u_j^0 = w_0(j \, \Delta x) - W_j. \qquad (2.4)$$

We have defined, for $j = 1, \dots, J - 1$,

$$
\begin{aligned}
f(j, u_{j-1}, u_j, u_{j+1}) = {} & g(W_{j-1} + u_{j-1}, \, W_j + u_j, \, W_{j+1} + u_{j+1}; \Delta x) \\
& - g(W_{j-1}, \, W_j, \, W_{j+1}; \Delta x).
\end{aligned}
\qquad (2.5)
$$

The functions $f(j, a, b, c)$ have the following properties in terms of $g(a, b, c; \Delta x)$:

(i)
$$f(j, 0, 0, 0) = 0, \qquad (2.6)$$

(ii)
$$\frac{\partial^k f(j, 0, 0, 0)}{\partial a^l \, \partial b^m \, \partial c^s} = \frac{\partial^k g(W_{j-1}, W_j, W_{j+1}; \Delta x)}{\partial a^l \, \partial b^m \, \partial c^s} \quad \text{for } k = l + m + s. \qquad (2.7)$$

Thus $u_j^n \equiv 0$ satisfies (2.3). Furthermore, the derivatives of the nonlinear map defined by (2.3–4) may be evaluated at $u_j^n \equiv 0$ by use of (2.7).

3. Linear theory

In this section we analyse the linearization of (2.3–4) about zero. This linearization, U_j^n, satisfies

$$U_j^{n+1} = U_j^n + r\delta_x^2 U_j^n + \lambda \, \Delta t [f_a(j, 0, 0, 0)U_{j-1}^n + f_b(j, 0, 0, 0)U_j^n + f_c(j, 0, 0, 0)U_{j+1}^n], \qquad (3.1)$$

with boundary and initial conditions

$$U_0^n = U_J^n = 0, \qquad U_j^0 = w_0(j \, \Delta x) - W_j. \qquad (3.2)$$

We solve these equations by separation of variables, setting $U_j^n = \chi_n \phi_j$. We find that $\chi_n = \xi^n$, where ξ satisfies the matrix eigenvalue problem

$$(\xi - 1)\phi = \Delta t A \phi. \qquad (3.3)$$

Here $\phi = [\phi_1, \dots, \phi_{J-1}]^\mathsf{T}$ and the matrix A is tridiagonal and given by

$$
\begin{bmatrix}
D_1 & U_1 & 0 & \cdots & & 0 \\
L_2 & D_2 & U_2 & 0 & \cdots & 0 \\
0 & L_3 & & \ddots & 0 & 0 \\
0 & \cdots & & \ddots & \ddots & 0 \\
0 & \cdots & & & \ddots & U_{J-2} \\
0 & \cdots & & & L_{J-1} & D_{J-1}
\end{bmatrix}. \qquad (3.4)
$$

The elements of this matrix are defined by

$$D_j = \frac{-2}{\Delta x^2} + \lambda f_b(j, 0, 0, 0), \qquad U_j = \frac{1}{\Delta x^2} + \lambda f_c(j, 0, 0, 0),$$

$$L_j = \frac{1}{\Delta x^2} + \lambda f_a(j, 0, 0, 0).$$

We now prove a result about the eigenvalues of A which we use in Section 4.

THEOREM 3.1   *Let $L_{j+1}/U_j > 0$, for $j = 1,...,J-2$. Then the matrix A has $J-1$ real, distinct eigenvalues η_i and corresponding eigenvectors ϕ_i given by* (3.6-7).

Notes. The assumption on the positivity of L_{j+1}/U_j is standard. If the differential equation is symmetric (that is, does not involve w_x), the assumption is usually satisfied. If the differential equation is not symmetric, the assumption is often equivalent to a restriction on the size of Δx, although for schemes in which a natural upwinding direction is known a priori this may not be necessary. The method of symmetrization we employ in the proof is motivated by Price *et al.* (1966); it is the discrete analogue of symmetrization for Sturm–Liouville operators.

Proof. The matrix A is symmetrized by setting $B = E^{-1}AE$, where $E = \text{diag}[e_1,...,e_{J-1}]$ with $e_1 = 1$ and

$$e_{j+1} = \left(\frac{L_{j+1}}{U_j}\right)^{\frac{1}{2}} e_j \quad \text{for } j = 1,...,J-2.$$

The matrix B is tridiagonal and has the form

$$
\begin{bmatrix}
D_1 & (U_1L_2)^{\frac{1}{2}} & 0 & & \cdots & & 0 \\
(U_1L_2)^{\frac{1}{2}} & D_2 & (U_2L_3)^{\frac{1}{2}} & 0 & \cdots & & 0 \\
0 & (U_2L_3)^{\frac{1}{2}} & & & & 0 & 0 \\
0 & \cdots & & & & & 0 \\
0 & \cdots & & & & & (U_{J-2}L_{J-1})^{\frac{1}{2}} \\
0 & \cdots & & & (U_{J-2}L_{J-1})^{\frac{1}{2}} & & D_{J-1}
\end{bmatrix}. \quad (3.5)
$$

Since B is real and symmetric it has real eigenvalues. Furthermore, since the off-diagonal elements are strictly positive, the eigenvalues are necessarily distinct (Conte & de Boor, 1980: page 205). Thus we may write

$$B\psi_i = \eta_i\psi_i \quad \text{for } i = 1,...,J-1, \quad (3.6)$$

where the η_i are real and distinct. Consequently we have, for $i = 1,...,J-1$

$$A\phi_i = \eta_i\phi_i \quad \text{where } \phi_i = E\psi_i. \quad (3.7)$$

This completes the proof.   □

COROLLARY 3.1   *Let $L_{j+1}/U_j > 0$, for $j = 1,...,J-2$. Then the matrix A^T has $J-1$ real distinct eigenvalues η_i and corresponding eigenvectors ϕ_i^* given by* (3.6-8).

Proof. We have $B = EA^T E^{-1}$ and the eigenvalues and eigenvectors of A^T satisfy, for $i = 1,...,J-1$,

$$A^T\phi_i^* = \eta_i\phi_i^* \quad \text{where } \phi_i^* = E^{-1}\psi_i \quad □ \quad (3.8)$$

Notice that the matrix A depends on λ, but is independent of Δt. Hence the eigenvalues η_i also depend on λ and are independent of Δt. It will be useful to order the eigenvalues and, without loss of generality, we assume that

$$\eta_{J-1}(\lambda) < \eta_{J-2}(\lambda) < \cdots < \eta_2(\lambda) < \eta_1(\lambda).$$

We can now solve the eigenvalue problem (3.3). We find the eigenvalues

$$\xi_i = 1 + \Delta t \eta_i, \tag{3.9}$$

where the η_i satisfy (3.6). Since the eigenvectors ϕ_i, defined by (3.6–7), correspond to distinct eigenvalues, we deduce that they span the space of vectors on $\mathbb{R}^{J-1}$ and hence that we can obtain a solution of the linear problem (3.1–2), subject to arbitrary initial conditions, as a linear combination of the ϕ_i. We set $U^n = [U_1^n, ..., U_{J-1}^n]^{\mathsf{T}}$ and obtain the solution of (3.1–2) in the form

$$U^n = \sum_{i=1}^{J-1} d_i \xi_i^n \phi_i, \tag{3.10}$$

for constants d_i determined by the initial conditions.

Thus we deduce from (3.10) that, if $|\xi_i| < 1$ for all i, then $U^n \to 0$ as $n \to \infty$. Since U^n represents perturbations from the steady-state solution, this indicates that, if $|\xi_i| < 1$ for all i, then the steady-state solution is stable to infinitesimal disturbances. However, if $|\xi_i| > 1$ for some i, then arbitrary small disturbances including the mode ϕ_i will grow unboundedly with n. Since the η_i are real, the critical values $|\xi_i| = 1$ occur, by (3.9), for

$$\eta_i(\lambda) = 0 \quad \text{and} \quad \Delta t = -2/\eta_i(\lambda). \tag{3.11}$$

The first condition, $\eta_i(\lambda) = 0$, determines the values of λ at which *steady* bifurcation occurs in the nonlinear problem, since it does not involve Δt. These values reflect a genuine property of the differential equation (assuming that the underlying steady solution about which we linearize is not spurious) and are not the subject of this paper. The second condition, $\Delta t = -2/\eta_i(\lambda)$, arises from the case $\xi_i = -1$ and has no analogue in the underlying differential equation.

DEFINITION 3.1   Let $L_{j+1}/U_j > 0$ for $j = 1, ..., J - 2$. We say that if $\xi_i < -1$ for some i then the scheme (2.3–4) is *linearly unstable* in the neighbourhood of the steady solution (2.1–2). This definition follows from (3.10). By (3.9) we deduce from the ordering of the eigenvalues of A that (2.3–4) is linearly unstable for $\Delta t > -2/\eta_{J-1}(\lambda)$, assuming that $\eta_{J-1}(\lambda) < 0$.

In the fully nonlinear problem, linearized instability corresponds to the bifurcation of orbits of period two in n, as we show in the following section.

4. Nonlinear theory

In this section we show that (2.3–4) possesses small amplitude solutions which are of period two in n. This proves that, close to steady solutions, (1.3–4) has solutions of period two in n. We provide a local description of the periodic solutions of small amplitude and describe a modified equations technique for the study of large amplitude periodic solutions.

We emphasize again that we consider Δx as fixed (so that the dimension of the problem is fixed) and Δt is taken as a bifurcation parameter. Period two solutions of (2.3–4) satisfy the $2(J - 1)$-dimensional system of nonlinear algebraic equations

$$F(u, \Delta t, \lambda) - v = 0 \quad \text{and} \quad F(v, \Delta t, \lambda) - u = 0, \tag{4.1}$$

where $\boldsymbol{u} = [u_1,...,u_{J-1}]^\mathsf{T}$ and $\boldsymbol{v} = [v_1,...,v_{J-1}]^\mathsf{T}$. The vector function $\boldsymbol{F}$ has jth component, for $j = 1,...,J-1$, given by

$$F_j(\boldsymbol{u}, \Delta t, \lambda) = u_j + r\delta_x^2 u_j + \lambda \, \Delta t f(j, u_{j-1}, u_j, u_{j+1}), \tag{4.2}$$

with the understanding that $u_0 = v_0 = u_J = v_J = 0$ in the definitions of F_1 and F_{J-1}. Thus $\boldsymbol{F}$ denotes a mapping: $\mathbb{R}^{J-1} \times \mathbb{R}^2 \to \mathbb{R}^{J-1}$.

We may write (4.1) as a single system of nonlinear equations in the form

$$G(U, \Delta t, \lambda) = 0, \tag{4.3}$$

where $U = (\boldsymbol{u}, \boldsymbol{v})$. (Here, and in similar contexts following, $(\boldsymbol{u}, \boldsymbol{v})$ denotes the stacked column vector with first $J-1$ components made up of $\boldsymbol{u}$ and second $J-1$ components made up of $\boldsymbol{v}$.) The function G denotes a mapping: $\mathbb{R}^{2(J-1)} \times \mathbb{R}^2 \to \mathbb{R}^{2(J-1)}$. In the remainder of this paper we will use $d^k G(U_1,...,U_k)$ to denote the kth Frechet derivative of $G(U, \Delta t, \lambda)$, a multilinear map: $\mathbb{R}^{2k(J-1)} \times \mathbb{R}^2 \to \mathbb{R}^{2(J-1)}$. Similarly $d^k F(\boldsymbol{u}_1,...,\boldsymbol{u}_k)$ denotes the kth derivative of $F(\boldsymbol{u}, \Delta t, \lambda)$. Notice that, by (2.6) and (4.2), we have $G(0, \Delta t, \lambda) = 0$ for all values of Δt and λ. We wish to determine the values of Δt at which nontrivial solutions branch from the trivial solution. We shall show that these are precisely the values determined by (3.11). By the implicit function theorem, branching can only occur when the first derivative, dG (the Jacobian), is singular at $U = 0$. This is the basis of the following theorem.

THEOREM 4.1 *Assume that* $\eta_j(\lambda) \neq 0$ *for* $j = 1,...,J-1$, *where* η_j *satisfies* (3.6), *and that* $L_{j+1}/U_j > 0$ *for* $j = 1,...,J-2$, *as in Theorem 3.1. Then the point* $\Delta t = -2/\eta_i(\lambda)$ *is a bifurcation point for the nonlinear system* (4.3). *Furthermore, if the functions* $f(j, a, b, c)$ *possess* m (>2) *continuous partial derivatives with respect to* a, b, *and* c, *then there exist* C^{m-1} *functions*

$$\Delta t(\mu) = -2/\eta_i(\lambda) + O(|\mu|),$$
$$U(\mu) = (\boldsymbol{u}(\mu), \boldsymbol{v}(\mu)) = \mu(-\phi_i, \phi_i) + O(\mu^2),$$

for ϕ_i *defined by* (3.7) *and real* μ *near zero such that*

$$G(U(\mu), \Delta t(\mu), \lambda) = 0.$$

Notes. (i) The assumption that $\eta_j(\lambda) \neq 0$ is made for two reasons: firstly, for $j = i$, to ensure that the critical value of Δt exists as defined and secondly, for $j \neq i$, to force the Frechet derivative of G to have a one-dimensional null-space at $\Delta t = -2/\eta_i(\lambda)$. When the derivative has an even-dimensional null-space, considerably more work is required to establish whether or not bifurcation actually occurs. As described in the previous section, the case $\eta_j(\lambda) = 0$ corresponds to steady bifurcation, and by excluding that case we are excluding the possibility of simultaneous steady and periodic bifurcation; the interaction of steady and periodic modes is analysed by different techniques in Stuart (1989a).

(ii) The assumption on L_{j+1}/U_j is strictly necessary. If this condition is not satisfied then the eigenvalues of A, and hence of the Frechet derivative of G, may become complex. In this case periodic orbits can bifurcate from the steady solution but their period will not be two. Quasi-periodic orbits are also possible;

see the discussion of Hopf bifurcation in iterated maps in Guckenheimer & Holmes (1983: Section 3.5).

(iii) The smoothness assumptions on the functions $f(j, a, b, c)$ may not actually hold globally, but only in some neighbourhood of $a = b = c = 0$. Since the theorem concerns the local behaviour of solutions, the difficulty can be circumvented by defining C^m extensions of the functions f.

(iv) Notice the local structure of the solution: to $O(\mu)$ the components satisfy $u = -v$. This is a consequence of the linear solution (3.10): for Δt near Δt_i we have the growth rate $\xi_i \approx -1$ which causes oscillations between time-steps.

(v) For the theorem to be of practical interest we require positive values of Δt_i, which necessitates negative values of η_i. In general, some η_i will be negative, since explicit discretizations of dissipative PDEs are usually stiff so that A has some large negative eigenvalues. This is especially so when Δx is small. The most important η_i is the negative one of largest magnitude, η_{J-1}, since this corresponds to the value of Δt at which the scheme (1.3–4) becomes linearly unstable (see Definition 3.1). Thus we have the theorem

$$\text{linear instability} \quad \Rightarrow \quad \text{spurious periodic solutions.}$$

(vi) In the case of *negative* Δt, (1.3–4) corresponds to an implicit discretization of a non-linear backwards heat equation; such equations can have a unique solution, due to the nonlinearity, and are relevant to finding the α-limit set of (1.1–2).

Proof. The theorem is a direct application of Theorem 5.3 in Chow & Hale (1982). First we need to establish that G defines an m times differentiable mapping: $\mathbb{R}^{2(J-1)} \times \mathbb{R}^2 \to \mathbb{R}^{2(J-1)}$. This follows directly from the assumptions on the smoothness of f. Secondly we need to show that dG has a one-dimensional null-space at $U = 0$ and $\Delta t = -2/\eta_i(\lambda)$. We now demonstrate this fact.

The Frechet derivative dG is singular when there exists a non-zero Φ satisfying

$$dG(\Phi) = 0. \tag{4.4}$$

Splitting Φ into two $(J-1)$-element vectors in the obvious way, $\Phi = (\theta, \phi)$, we see from (4.1–3) that, at $U = 0$, (4.4) is equivalent to solving

$$(I + \Delta t A)\theta = \phi, \tag{4.5}$$

$$(I + \Delta t A)\phi = \theta, \tag{4.6}$$

since the linearization of F at $U = 0$ is the matrix $I + \Delta t A$. Equations (4.5–6) are themselves equivalent to

$$(2I + \Delta t A)(\Delta t A)\phi = 0.$$

The two linear operators commute, so we deduce that either $A\phi = 0$ *or* $(2I + \Delta t A)\phi = 0$. Our assumption $\eta_j \neq 0$ ensures that the first of these possibilities cannot occur. (This possibility corresponds to solutions of (4.5–6) for which $\theta = \phi$. As such it is not related to genuine period two behaviour but rather to the period one (steady) solutions embedded in (4.3)—see note (i) on Theorem 4.1.) The second possibility corresponds to $\theta = -\phi$. The matrix $(2I + \Delta t A)$ is singular

whenever $\Delta t = -2/\eta_i(\lambda)$, where η_i are the eigenvalues of A (see Section 3). Furthermore, by Theorem 3.1, the eigenvalues are distinct, with eigenvectors ϕ_i defined by (3.7).

This shows that, at $U = 0$ and $\Delta t = -2/\eta_i(\lambda)$, the operator dG is singular with a one-dimensional null-space spanned by $\Phi_i = (-\phi_i, \phi_i)$. This completes the proof. □

As a direct result of Theorem 4.1 we have the following.

COROLLARY 4.1 *Let* $W = [W_1,..., W_{J-1}]^T$ *defined by (2.1–2) be a steady (n-independent) solution of (1.3–4) and define* $w^n = [w_1^n,..., w_{J-1}^n]^T$. *Then, under the same assumptions as Theorem* 4.1, *(1.3–4) possesses periodic solutions of the form*

$$w^n = W + \tfrac{1}{2}[1 + (-1)^n]u + \tfrac{1}{2}[1 + (-1)^{n+1}]v,$$

for $\Delta t = -2/\eta_i(\lambda) + O(|\mu|)$ *and real* μ *near zero. Here* u, v, *and* $\eta_i(\lambda)$ *are as defined in Theorem* 4.1.

Theorem 4.1 proves the existence of orbits of period two in (2.3–4) and hence, by the corollary, in (1.3–4). Furthermore, the theorem asserts the local existence of smooth branches of solutions, continuous in Δt, near to the bifurcation points. However, it does not tell us much about the local shape of the solution branches. In particular it is of interest to determine the nature of the singularity at a given bifurcation point. This is accomplished by singularity theory. What this theory tells us is that there is a function $g(\mu, \Delta t)$ whose zeros describe the *local* behaviour of the solutions in a (sufficiently small, but finite) neighbourhood of a bifurcation point. Here μ is precisely the amplitude from the statement of Theorem 4.1. Moreover the theory tells us how to compute derivatives of this function g in terms of the derivatives of G at that bifurcation point. In the next theorem we will show that, for $\Delta t \approx -2/\eta_i(\lambda)$, solutions of (4.3) have a local structure determined by

$$g(\mu, \Delta t) = B_i\mu^3 + C_i\mu[\Delta t + 2/\eta_i(\lambda)] = 0. \tag{4.7}$$

This result is independent of the specific details of the nonlinearity. The structure (4.7) is known as a *pitchfork bifurcation*. The reason for this terminology is clear from Fig. 4.1.

Notice that the solution $\mu = 0$ satisfies (4.7) for all values of the parameter Δt. This is a reflection of the trivial (zero amplitude) solution of equation (4.3). The two nonzero solutions represent nontrivial solutions of (4.3), and hence period two solutions of (2.3–4), that bifurcate from the trivial solution at $\Delta t = -2/\eta_i(\lambda)$. Of crucial interest to the numerical analyst is how the nontrivial solution branch behaves away from the bifurcation point. Let us consider the bifurcation point with $i = J - 1$ which corresponds to the linear stability limit (see Definition 3.1). If $B_{J-1}/C_{J-1} > 0$ the bifurcation is *subcritical* and spurious periodic solutions exist locally for values of Δt *below* the linearized stability limit. Even if $B_{J-1}/C_{J-1} < 0$, it is possible for the branch to turn around and for periodic solutions to exist below the linearized stability limit. For all the solution branches, an important question is 'where do the branches go to in the space $\mathbb{R}^{2(J-1)} \times \mathbb{R}$ (considering λ
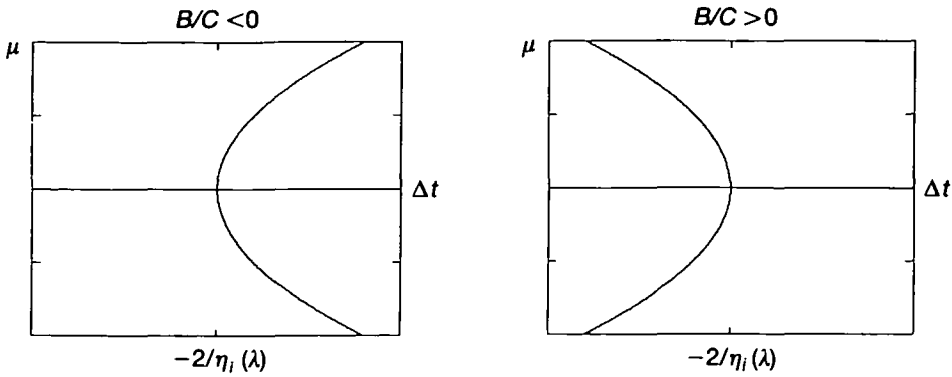
$B/C < 0$ μ ... Δt $-2/\eta_i\,(\lambda)$

$B/C > 0$ μ ... Δt $-2/\eta_i\,(\lambda)$

FIG. 4.1. The pitchfork bifurcation (4.7).

as fixed)?' since the magnitude and form of the spurious solutions, and the ranges of Δt in which they exist, determine classes of initial data for (1.3–4) for which the numerical method will produce spurious results. Global bifurcation theory (Hutson & Pym, 1980) tells us that the continuous branches of solutions can do one of two things: either move off to infinity in the space $\mathbb{R}^{2(J-1)} \times \mathbb{R}$ or return to meet the trivial solution at another bifurcation point (see Fig. 4.2). A branch cannot simply cease to exist and remain bounded at the same time.

Clearly it is advantageous to design schemes (1.3–4) so that none of the branches of periodic solutions extend back to values of Δt used in practice. In general it may not be possible to do this a priori. None the less, the analysis here shows that an a posteriori test can be designed to determine whether a given scheme has spurious solutions likely to interfere with practical computations. This can be done simply by solving (4.3) numerically to determine the range of Δt in which the spurious solutions exist and to ascertain their magnitude and spatial structure. The solution of a $2(J-1)$-dimensional system of parameter-dependent nonlinear equations is generally a nontrivial task. However, since starting points are known, continuation can be used in a fairly straightforward way to follow the branches. We apply this approach to a specific example in Section 5.

$\|U\|$ ... 0 0 $-2/\eta_i\,(\lambda)$ $-2/\eta_{i+1}(\lambda)$ Δt

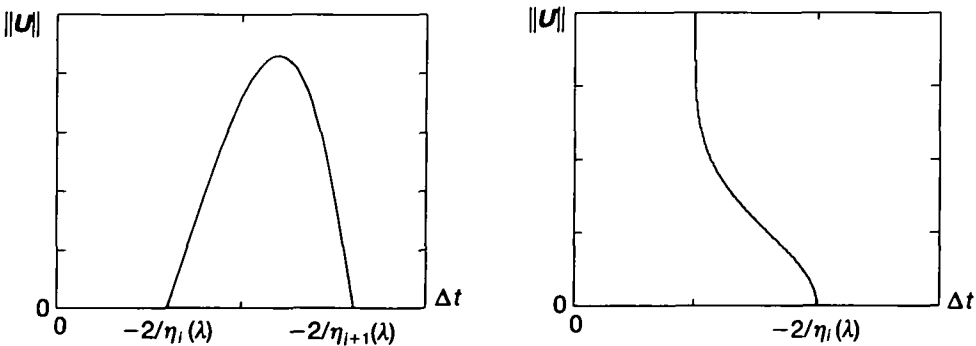$\|U\|$ ... 0 0 $-2/\eta_i\,(\lambda)$ Δt

FIG. 4.2. Possible global behaviour of solution branches.

In the following theorem we sharpen the local estimates of the behaviour of the solution branches at the bifurcation points and justify our claim that (4.7) is the normal form governing the existence of solutions. These sharp estimates are needed to initiate the continuation procedures suggested above.

THEOREM 4.2 *Under the same assumptions as Theorem* 4.1, *the solutions of* (4.3) *in the neighbourhood of* $\Delta t = -2/\eta_i(\lambda)$, *are described locally by the normal form* (4.7) *where*

$$B_i = \tfrac{1}{6}\langle \phi_i^*, 2d^3F(\phi_i, \phi_i, \phi_i) + 3\eta_i(\lambda)d^2F(\phi_i, A^{-1}d^2F(\phi_i, \phi_i))\rangle_{J-1},$$
$$C_i = 2\eta_i(\lambda)\langle \phi_i^*, \phi_i\rangle_{J-1}.$$

Here F and all its derivatives are evaluated at the bifurcation point $u = v = 0$, $\Delta t = -2/\eta_i(\lambda)$. *Also* ϕ_i *is the eigenvector of A corresponding to eigenvalue* $\eta_i(\lambda)$ *and* ϕ_i^* *is the eigenvector of* A^{T} *corresponding to eigenvalue* $\eta_i(\lambda)$; *see* (3.6–8). $\langle \bullet, \bullet \rangle_N$ *denotes the usual inner product on* $\mathbb{R}^N$.

Note. The proof employs the singularity-theoretic formulation of the Liapunov–Schmidt reduction for finite-dimensional problems. We will refer to formulae (3.23) in Chapter I of Golubitsky and Schaeffer (1985), which will be abbreviated to GS from now on, meaning Chapter I unless specified otherwise. The formulae describe how to calculate various derivatives of g in terms of derivatives of G. We emphasize that our notation is different: their Φ corresponds to our G. Note that, throughout this proof, all derivatives are evaluated at the bifurcation point $U = (u, v) = 0$ and $\Delta t = -2/\eta_i(\lambda)$. The proof utilizes the symmetry inherent in equations (4.1), and hence (4.3), to simplify the formulae given in GS. The relevant symmetry is the fact that, if $U = (u, v)$ satisfies (4.3), then so does $U = (v, u)$.

Proof. To show the local equivalence of the function $g(\mu, \Delta t)$ to the normal form (4.7) it is necessary to show only that the partial derivatives of g satisfy

$$g_\mu = g_{\mu\mu} = g_{\Delta t} = 0, \qquad g_{\mu\mu\mu} \neq 0, \qquad g_{\Delta t\mu} \neq 0, \qquad (4.8\text{–}9)$$

for $\mu = 0$ and $\Delta t = -2\eta_i(\lambda)$ (see GS: Chapter II).

That $g_\mu = 0$ follows automatically from the fact that we are at a bifurcation point (see GS: formula (3.23a)). That $g_{\Delta t} = 0$ follows automatically from the fact that the trivial solution $G = 0$ satisfies (4.3) for all values of Δt, meaning that $G_{\Delta t} \equiv 0$ at the bifurcation point (see GS: formula (3.23d)). We now show that $g_{\mu\mu} = 0$. This requires a little more work.

In the following, L denotes the Frechet derivative of G evaluated at the bifurcation point $U = 0$ and $\Delta t = -2/\eta_i(\lambda)$. Thus L is singular. Let Φ_i span the null-space of L and let Φ_i^* span $(\text{range } L)^\perp$. We may write $d^2G(\Phi_i, \Phi_i)$ as $(d^2F(-\phi_i, -\phi_i), d^2F(\phi_i, \phi_i))$, since, from the proof of Theorem 4.1, $\Phi_i = (-\phi_i, \phi_i)$, where ϕ_i satisfies (3.7), and since G is defined by the two components in equation (4.1). The bilinear operator satisfies $d^2F(-\phi, -\phi) = d^2F(\phi, \phi)$, for any vector ϕ, by definition. Thus we have the result that

$$d^2G(\Phi_i, \Phi_i) = (d^2F(\phi_i, \phi_i), d^2F(\phi_i, \phi_i)). \qquad (4.10)$$

Now, the vector $\boldsymbol{\Phi}^*$ spans $(\text{range } L)^{\perp}$ and hence spans the null-space of L^T. By modifying the arguments in the proof of Theorem 4.1 it may be shown that

$$\boldsymbol{\Phi}_i^* = (-\boldsymbol{\phi}_i^*, \boldsymbol{\phi}_i^*), \tag{4.11}$$

where $\boldsymbol{\phi}_i^*$ is the eigenvector of A^T with corresponding eigenvalue η_i, defined by (3.8). Combining (4.10–11) shows that

$$\langle \boldsymbol{\Phi}_i^*, d^2G(\boldsymbol{\Phi}_i, \boldsymbol{\Phi}_i) \rangle_{2(J-1)} = 0$$

and hence, by GS (formula (3.23b)), that $g_{\mu\mu} = 0$.

We now compute expressions for $g_{\mu\mu\mu}$ and $g_{\Delta t\mu}$. These are provided by GS (formulae (3.23c) and (3.23e)), noting that (3.23e) is simplified because $\boldsymbol{G}_{\Delta t} = \boldsymbol{0}$ at the bifurcation point, as we discussed above. These formulae give

$$g_{\mu\mu\mu} = \langle \boldsymbol{\Phi}_i^*, d^3G(\boldsymbol{\Phi}_i, \boldsymbol{\Phi}_i, \boldsymbol{\Phi}_i) - 3d^2G(\boldsymbol{\Phi}_i, L^{-1}Ed^2G(\boldsymbol{\Phi}_i, \boldsymbol{\Phi}_i)) \rangle_{2(J-1)}, \tag{4.12}$$

$$g_{\mu\Delta t} = \langle \boldsymbol{\Phi}_i^*, dG_{\Delta t}(\boldsymbol{\Phi}_i) \rangle_{2(J-1)}.$$

Here E denotes the projection onto the range of L. Since L is singular, the action of the generalized inverse is interpreted as finding the unique element orthogonal to $\boldsymbol{\Phi}_i$.

These expressions for the derivatives simplify into inner products on $\mathbb{R}^{J-1}$ due to the symmetries inherent in (4.3). For example, $dG_{\Delta t}(\boldsymbol{\Phi}_i) = (-A\boldsymbol{\phi}_i, A\boldsymbol{\phi}_i) = \eta_i(\lambda)(-\boldsymbol{\phi}_i, \boldsymbol{\phi}_i)$. Thus, by (4.11), we obtain

$$g_{\mu\Delta t} = 2\eta_i(\lambda)\langle \boldsymbol{\phi}_i^*, \boldsymbol{\phi}_i \rangle_{(J-1)}. \tag{4.13}$$

We also find that

$$d^3G(\boldsymbol{\Phi}_i, \boldsymbol{\Phi}_i, \boldsymbol{\Phi}_i) = (-d^3F(\boldsymbol{\phi}_i, \boldsymbol{\phi}_i, \boldsymbol{\phi}_i), d^3F(\boldsymbol{\phi}_i, \boldsymbol{\phi}_i, \boldsymbol{\phi}_i)).$$

Thus

$$\langle \boldsymbol{\Phi}_i^*, d^3G(\boldsymbol{\Phi}_i, \boldsymbol{\Phi}_i, \boldsymbol{\Phi}_i) \rangle_{2(J-1)} = 2\langle \boldsymbol{\phi}_i^*, d^3F(\boldsymbol{\phi}_i, \boldsymbol{\phi}_i, \boldsymbol{\phi}_i) \rangle_{(J-1)}. \tag{4.14}$$

It remains only to invert L on its range. The second part of the inner product (4.12) for $g_{\mu\mu\mu}$ involves solving

$$L\boldsymbol{\Gamma} = d^2G(\boldsymbol{\Phi}_i, \boldsymbol{\Phi}_i),$$

since the right-hand side is automatically in range L. For $\boldsymbol{\Gamma} = (\boldsymbol{\gamma}_1, \boldsymbol{\gamma}_2)$ this is equivalent to solving

$$[I - 2A/\eta_i(\lambda)]\boldsymbol{\gamma}_1 - \boldsymbol{\gamma}_2 = d^2F(\boldsymbol{\phi}_i, \boldsymbol{\phi}_i), \qquad -\boldsymbol{\gamma}_1 + [I - 2A/\eta_i(\lambda)]\boldsymbol{\gamma}_2 = d^2F(\boldsymbol{\phi}_i, \boldsymbol{\phi}_i),$$

since the operator L is defined by (4.5–6) with $\Delta t = -2/\eta_i(\lambda)$. The unique solution (in the sense of generalized inverses) is

$$\boldsymbol{\gamma}_1 = \boldsymbol{\gamma}_2 = -\tfrac{1}{2}\eta_i(\lambda)A^{-1}d^2F(\boldsymbol{\phi}_i, \boldsymbol{\phi}_i), \tag{4.15}$$

which yields $\langle \boldsymbol{\Gamma}, \boldsymbol{\Phi}_i \rangle_{2(J-1)} = 0$ as required. Note that A is uniquely invertible by the assumption $\eta_j(\lambda) \neq 0$, for $j = 1,...,J - 1$. Thus

$$d^2G(\boldsymbol{\Phi}_i, \boldsymbol{\Gamma}) = (d^2F(-\boldsymbol{\phi}_i, \boldsymbol{\gamma}_1), d^2F(\boldsymbol{\phi}_i, \boldsymbol{\gamma}_1)).$$

Combining this and (4.12), (4.14), and (4.15) we find that

$$g_{,\mu\mu\mu} = 2\langle \phi_i^*, d^3F(\phi_i, \phi_i, \phi_i) - 3d^2F(\phi_i, -\tfrac{1}{2}\eta_i(\lambda)A^{-1}d^2F(\phi_i, \phi_i))\rangle_{(J-1)}. \quad (4.16)$$

It is possible, for *specific nonlinearities*, that (4.9) may not hold and that a higher order singularity than that represented by the normal form (4.7) governs the existence of solutions near to the nonlinearity. However, for *arbitrary non-linearities* we claim that (4.9) holds generically since, in general, (4.13) and (4.16) yield nonzero derivatives. We justify this claim fully in the following section where we consider a specific class of problems with normal form (4.7).

From the formulae (4.13) and (4.16) and the linearity of the bilinear form d^2F we can use a Taylor expansion to show that g is locally equivalent to the normal form (4.7) with B_i and C_i as defined in the statement of the theorem. This completes the proof. □

We have constructed branches of spurious periodic solutions of (4.3) in the neighbourhood of the trivial solution. As mentioned earlier, global bifurcation theory tells us that these branches either move off to infinity or return to meet the trivial solution at another bifurcation point. We now discuss a question which is of particular importance to the numerical analyst: can a branch of spurious periodic solutions extend back to arbitrarily small values of Δt? If so, what is the form of such periodic solutions? We shall discuss this point from the perspective of modified equations. The philosophy of modified equations is to find a related differential equation which has (some of) the same properties as the discretization (see Griffiths and Sanz-Serna, 1986); we show that the existence of spurious periodic solutions for small Δt is intimately related to the question of the existence of solutions to a pair of coupled, singularly perturbed boundary value problems.

We observe that if solutions of (4.3) exist for arbitrarily small values of Δt then they will necessarily be of *large norm*: at $\Delta t = 0$ the only solutions of (4.3) are arbitrary solutions of the form $u = v$ and it is straightforward to show that other solution branches cannot cross the line $\Delta t = 0$. Thus, as $\Delta t \to 0$, solution branches must approach infinity in norm (if they exist at all).

Since spurious periodic solutions vary on a scale comparable with the temporal grid, the discretizations (4.1–2) representing periodic solutions do not correspond to any continuous, time-dependent process. On the other hand, periodic solutions (in n), with spatial structure varying on a scale significantly larger than the spatial grid, do correspond to a continuous steady process. This process can be recovered by taking the limit

$$\Delta x \to 0, \qquad \Delta t \text{ fixed} \qquad (4.17)$$

in equations (4.1–2). If we also assume that the steady solution, about which we perturb in Section 2, is not spurious and corresponds, in the limit $\Delta x \to 0$, to a continuous function $W(x)$, then we find a pair of coupled differential equations when the limit (4.17) is taken. These are

$$\Delta t\{u_{xx} + \lambda[h(W + u, W_x + u_x) - h(W, W_x)]\} + u - v = 0,$$
$$\Delta t\{v_{xx} + \lambda[h(W + v, W_x + v_x) - h(W, W_x)]\} + v - u = 0,$$

with boundary conditions $u(0) = v(0) = u(1) = v(1) = 0$. Since $W(x)$ is a steady solution of (1.1–2), these equations simplify if we set $U(x) = W(x) + u(x)$ and $V(x) = W(x) + v(x)$. We obtain the modified equations

$$\Delta t[U_{xx} + \lambda h(U, U_x)] + U - V = 0, \tag{4.18}$$

$$\Delta t[V_{xx} + \lambda h(V, V_x)] + V - U = 0, \tag{4.19}$$

with boundary conditions

$$U(0) = V(0) = U(1) = V(1) = 0. \tag{4.20}$$

Note that (4.18–20) are independent of $W(x)$ so that the existence of large norm spurious solutions for arbitrarily small values of Δt is independent of the existence of steady solutions of (1.3–4). We now make the following conjecture.

CONJECTURE 4.1   *If solutions of the differential equations* (4.18–20) *exist for* $\Delta t \ll 1$ *then solutions of* (4.1–2) (*that is, spurious periodic solutions of* (1.3–4)) *will exist in the same parameter regime and have a spatial structure similar to that of the solutions of the differential equations.*

The question of the existence of solutions of (4.18–20) is clearly a difficult one in general and we do not address it in detail. We know that, for $\Delta t \ll 1$, such solutions are necessarily of large norm and the precise scale will be set by a balance between the leading order, non-diffusive, behaviour of $\Delta t \lambda h(U, U_x)$, $\Delta t \lambda h(V, V_x)$, and $U - V$, for large U and V. Whether or not solutions of this form exist will depend on whether or not it is possible to fit diffusive boundary and interior layers between the solutions set by the leading order balance. This is a nontrivial question that has been partially answered for second-order elliptic differential equations in $\mathbb{R}^n$ (see Norbury (1985) and the references cited there).

As a specific example we consider the case $h(w, w_x) = w^p$, $p > 1$. Away from boundary or interior layers the large norm solutions of (4.18–20) satisfy

$$\Delta t U^p + U - V = 0, \qquad \Delta t V^p + V - U = 0.$$

This sets the scale of the large norm solutions: U and V are of $O(\Delta t^{1/(1-p)})$. Furthermore we see that nontrivial solutions are not possible if p is even, since $\Delta t(U^p + V^p) = 0$. We examine the particular case $p = 3$, which reduces to consideration of a single second-order equation, in the following section; this example goes some way towards substantiating Conjecture 4.1.

5. Applications of the theory

We consider (1.1–2) in the case where $h(w_1, w_2)$ is a pure cubic function of its two arguments. Thus the function $g(a, b, c; \Delta x)$ in the discretization (1.3–4) is also a pure cubic in the arguments a, b, and c. By (2.7), the same may then be said of $f(j, a, b, c)$.

We linearize about the trivial solution, zero. Thus the matrix A in (3.4) is itself symmetric with constant diagonal and off-diagonal elements given by

$D_i = -2/\Delta x^2$ and $U_i = L_i = 1/\Delta x^2$. The eigenvalues of this matrix are, for $i = 1,...,J-1$,

$$\eta_i = -\frac{4\sin^2(i\pi/2J)}{\Delta x^2}, \tag{5.1}$$

with corresponding eigenvectors ϕ_i having jth component

$$\phi_j = \sin(i\pi j/J). \tag{5.2}$$

Notice that $\eta_i < 0$ for all $i = 1,...,J-1$; see note (v) on Theorem 4.1. By Theorem 4.1, the critical values of Δt at which periodic solutions bifurcate are given by

$$\Delta t_i = \frac{\Delta x^2}{2\sin^2(i\pi/2J)} \quad \text{for } i = 1,...,J-1. \tag{5.3}$$

For $\Delta t = \Delta t_i + O(|\mu|)$, the periodic solutions of (2.3–4) are of the form $\boldsymbol{u}^n = \boldsymbol{u}$ and $\boldsymbol{u}^{n+1} = \boldsymbol{v}$, where $\boldsymbol{u}^n = [u_1^n,...,u_{J-1}^n]^T$. By Theorem 4.1 and equation (5.2) we have the jth components of $\boldsymbol{u}$ and $\boldsymbol{v}$ of the form, to $O(\mu^2)$,

$$u_j = -\mu\sin(i\pi j/J) \quad \text{and} \quad v_j = \mu\sin(i\pi j/J). \tag{5.4}$$

For nontrivial solutions, the relationship between μ and Δt_i is given by (4.7) as

$$\Delta t = \Delta t_i - B_i\mu^2/C_i, \tag{5.5}$$

with B_i and C_i defined in Theorem 4.2.

The matrix $\boldsymbol{A}$ is symmetric so that $\phi_i^* = \phi_i$. Thus, by Theorem 4.2, we calculate that

$$C_i = -8\sin^2(i\pi/2J)\sum_{i=1}^{J-1}\sin^2(i\pi j/J)/\Delta x^2.$$

Since h is a pure cubic function of its arguments we deduce that the second derivatives of $\boldsymbol{F}$ are all zero at $\boldsymbol{u} = \boldsymbol{0}$ and hence, using the summetry of $\boldsymbol{A}$,

$$B_i = \tfrac{1}{3}\langle\phi_i, d^3\boldsymbol{F}(\phi_i, \phi_i, \phi_i)\rangle_{J-1}. \tag{5.6}$$

The calculation of B_i depends upon a specific choice of nonlinearity. As a particular example we choose a source term of the form

$$h(w, w_x) = w^3.$$

Using a centred difference approximation we obtain

$$g(w_{j-1}, w_j, w_{j+1}; \Delta x) = w_j^3.$$

Since we are considering a neighbourhood of the trivial solution we find, from (2.5), that

$$f(j, u_{j-1}, u_j, u_{j+1}) = u_j^3. \tag{5.7}$$

Using (5.2), the definition of the third derivative is

$$d^3\boldsymbol{F}(\phi_i, \phi_i, \phi_i) = \sum_{k,l,m=1}^{J-1}\frac{\partial^3\boldsymbol{F}}{\partial u_k\,\partial u_l\,\partial u_m}\sin(i\pi k/J)\sin(i\pi l/J)\sin(i\pi m/J),$$

with $F(u, \Delta t, \lambda)$ evaluated at $u = 0$, and $\Delta t = \Delta t_i$. By (4.2) and (5.7) we find that the jth element of $d^3 F(\phi_i, \phi_i, \phi_i)$ is given, at $u = 0$ and $\Delta t = \Delta t_i$, by

$$d^3 F(\phi_i, \phi_i, \phi_i)_j = 6\lambda \, \Delta t_i \sin^3 (i\pi j/J).$$

Thus, from (5.3) and (5.6), we find that

$$B_i = \frac{\lambda \, \Delta x^2}{\sin^2 (i\pi/2J)} \sum_{j=1}^{J-1} \sin^4 (i\pi j/J).$$

Hence (5.5) gives us

$$\Delta t = \Delta t_i + \frac{\lambda \, \Delta x^4 \sum_{j=1}^{J-1} \sin^4 (i\pi j/J)}{8 \sin^4 (i\pi/2J) \sum_{j=1}^{J-1} \sin^2 (i\pi j/J)} \mu^2. \tag{5.8}$$

Together, equations (5.4) and (5.8) provide a complete local description ($\mu \ll 1$) of nontrivial periodic solutions of (1.3–4), with $h(w, w_x) = w^3$, in the neighbourhood of the zero solution ($\mu = 0$.)

We use this local description to initiate a continuation procedure which tracks the branches of period two solutions away from the bifurcation points. Figure 5.1 shows the l_2 norm of the solutions of (4.3) and (5.7) graphed against Δt^{-1}, in the case $\lambda = -1$ and $\Delta x = 0.1$. Thus, by (5.8), the bifurcation is subcritical (which
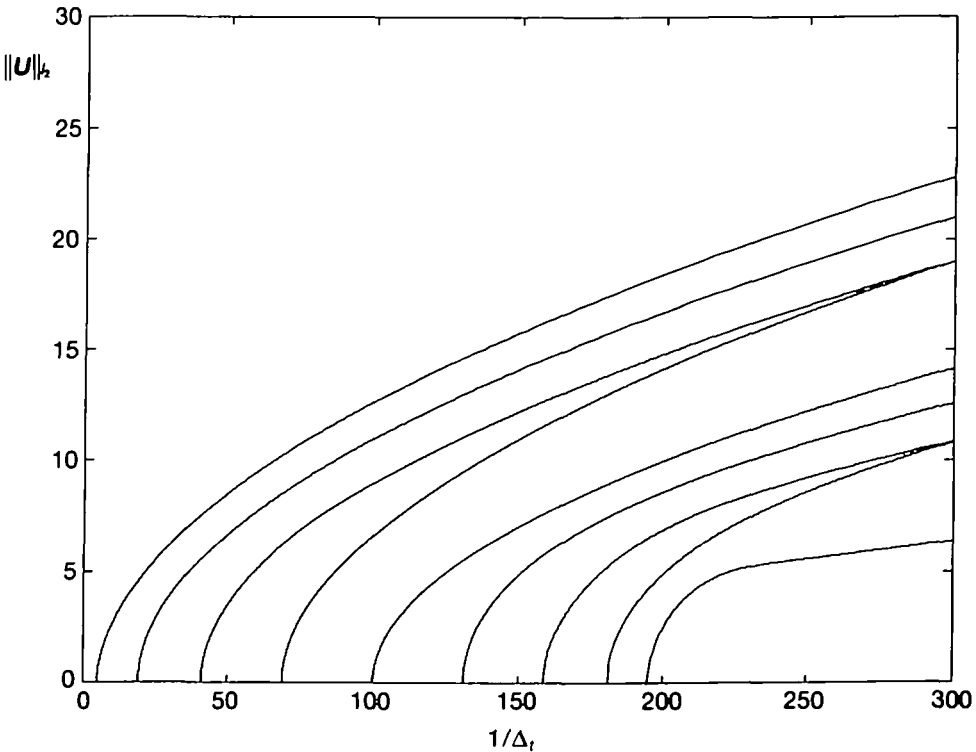

FIG. 5.1. The bifurcation diagram for solutions of (4.3); $\lambda = -1$.

appears as supercritical since we are plotting against Δt^{-1}) and there are nine bifurcation points given by (5.3). The numerical solution of (4.3) is simplified in this case since, by symmetry, there are solutions with $u = -v$. The solutions plotted are by no means the only solutions—we have plotted only those solutions lying on the continuous branches coming out of the bifurcation points and possessing the symmetry $u = -v$. There are many other solutions which also exist for $\Delta t \ll 1$. In general, period two solutions are of the form $u_j^n = a_j + (-1)^n b_j$. The solutions which retain the symmetry $u = -v$ correspond to solutions with $a_j \equiv 0$. We have not tested numerically for the existence of solutions with $a_j \neq 0$ since we have forced the symmetry $u = -v$ on our computations. The solutions shown in Fig. 5.1 retain the nodal properties of the eigenfunctions (5.4), which describe the local structure of the solutions near the bifurcation points, along the branches; there are also solutions for which this property is not preserved.

It is instructive to compare Fig. 5.1 with the bifurcation diagram for the purely linear problem with $\lambda = 0$. This is shown in Fig. 5.2, where periodic solutions of arbitrary norm exist at the points given by (5.3). This follows from (3.10) with appropriate choice of the d_i. For the linear problem it is necessary to operate numerical schemes to the right of the branch of periodic solutions emanating from the smallest critical value of Δt (that is to use small enough Δt) to obtain
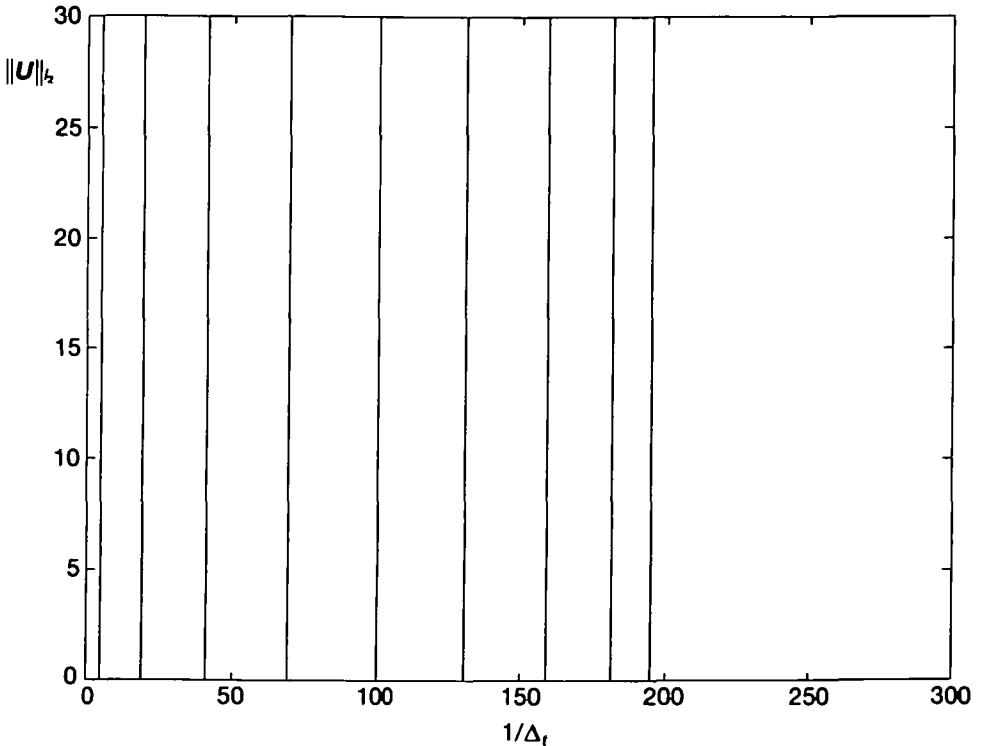

FIG. 5.2. The bifurcation diagram for solutions of (4.3); $\lambda = 0$.

meaningful solutions. Similarly, for the nonlinear problem, it is necessary to operate numerical schemes below (in some average sense), and to the right of, the lowest branch of periodic solutions in Fig. 5.1. In contrast to the linear problem, this curve predicts a maximum allowable Δt which is *solution dependent*—the amplitude and spatial structure of the solutions affects the critical value of Δt. The dependence of numerical stability on the underlying continuous solution being sought is central to the definition of *convergence stability* proposed in Lopez-Marcos and Sanz-Serna (1988). Figure 5.1 provides a quantitative interpretation of this dependence in the context of *practical stability*.

The results show that periodic solutions exist for arbitrarily small values of Δt; as discussed above, the branches all tend to infinity in norm as $\Delta t \to 0$. Furthermore, Conjecture 4.1, about the relationship between spurious periodic solutions and solutions of (4.18–20) for $\Delta t \ll 1$, is borne out. In this case, $W(x) = 0$ and $u(x) = -v(x)$, so that (4.18–20) simplify to give

$$\Delta t(u_{xx} + \lambda u^3) + 2u = 0,$$

with boundary conditions $u(0) = u(1) = 0$. The nonlinearity sets a scale of $O(\Delta t^{-\frac{1}{2}})$ and so we define a new variable $\hat{u} = \Delta t^{\frac{1}{2}}u$. We obtain the differential
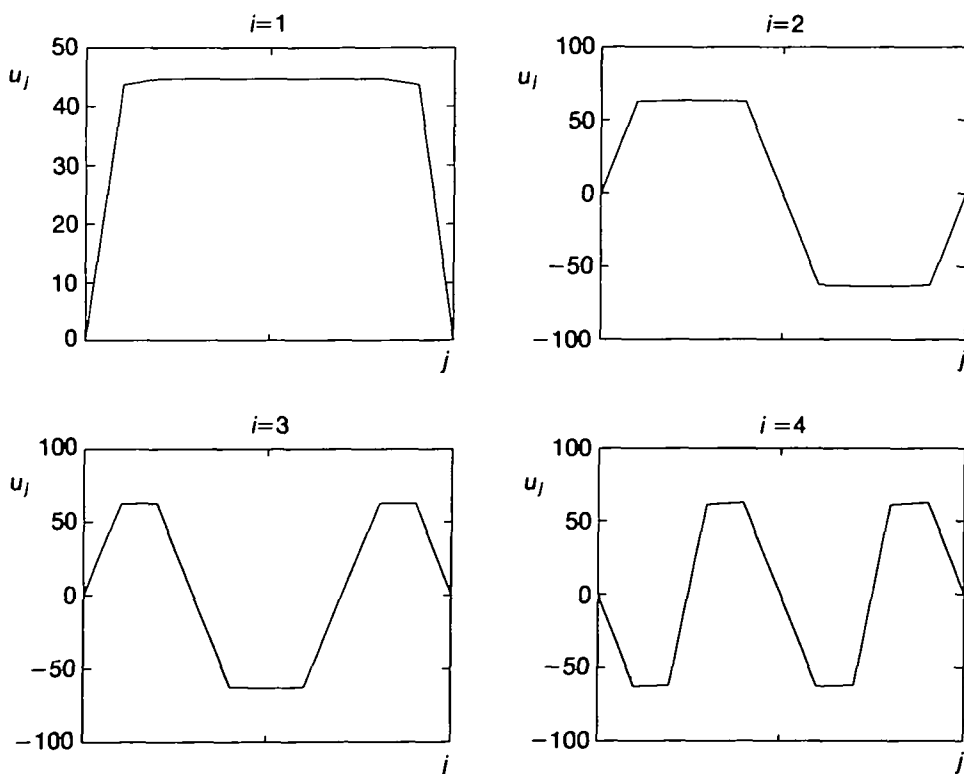
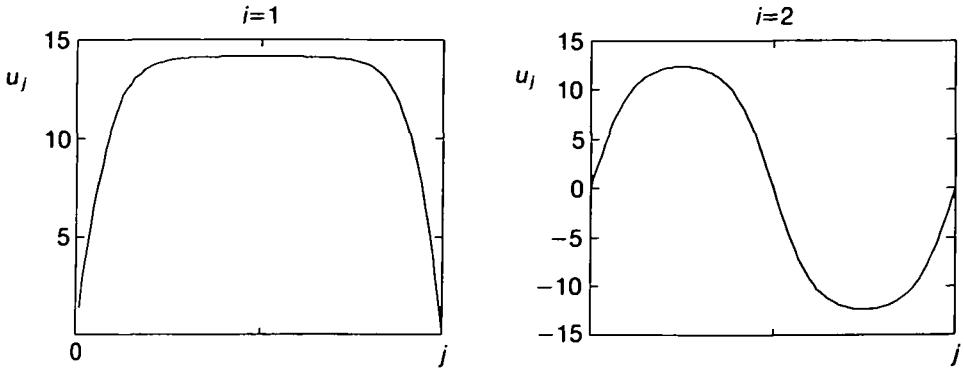FIG. 5.3. Spurious periodic modes; $\Delta x = 0.1$.

FIG. 5.4. Spurious periodic modes; $\Delta x = 0 \cdot 01$.

equation

$$\Delta t \hat{u}_{xx} + 2\hat{u} + \lambda \hat{u}^3 = 0, \tag{5.9}$$

with boundary conditions

$$\hat{u}(0) = \hat{u}(1) = 0. \tag{5.10}$$

For $\lambda < 0$, the properties of the solutions $\hat{u}$ are well documented. If $2/(k+1)^2\pi^2 < \Delta t < 2/k^2\pi^2$ there are precisely k nontrivial solutions (modulo reflectional symmetry). The solutions lie on continuous branches (in Δt) and have $0, 1, 2,..., k-1$ zeros respectively. The number of zeros is preserved along each branch and, for $\Delta t = 2/(k+1)^2\pi^2$, a new branch of solutions with k zeros bifurcates from the trivial solution. As $\Delta t \to 0$ the solutions approach a simple form: a solution with n zeros consists of $n+1$ plateaus on which $\hat{u}(x) = \pm(-2/\lambda)^{\frac{1}{2}}$ (the nondiffusive balance) joined to each other by n interior transition layers and to the points $x = 0, 1$ by boundary layers (Norbury, 1985).

We expect the spurious periodic solutions in Fig. 5.1 to have a form similar to the solutions of the differential equation (5.9–10) for $\Delta t \ll 1$. This is indeed the case and the spurious periodic modes have amplitude of $O(\Delta t^{-\frac{1}{2}})$. Figure 5.3 shows the form of the spurious solutions u_j of (4.3), for $\Delta t \ll 1$, on the branches which bifurcate from $\Delta t = \Delta t_i$, for $i = 1, 2, 3, 4$. (The components of v_j are found by setting $v_j = -u_j$). The numerical method is unable to resolve the boundary and transition layers accurately for this value of Δx (0.1) but the qualitative features are as in the differential equation. Figure 5.4 is similar to Fig. 5.3 but involves the value $\Delta x = 0.01$; again the solutions are similar in form to the solutions of the singularly perturbed differential equation.

6. Conclusions

We have analysed the qualitative behaviour of discretizations of reaction–diffusion–convection equations. A question of central importance in the numerical approximation of time-evolving problems is whether or not the simulation produces the same asymptotic behaviour as the underlying continuous problem,

for fixed but small values of the mesh-spacings. The answer to this question is closely related to the existence of spurious steady, periodic, and quasi-periodic solutions generated by discretization. Here we have concentrated on analysing the existence of spurious periodic motions.

We have shown that linear instability (where the linearization is about any steady solution of the difference equations) implies the existence of spurious periodic solutions in the fully nonlinear problem. We have concentrated on explicit time-discretizations of the equations but the ideas generalize in a fairly straightforward way to implicit methods with a linear stability limit.

The analysis is based on a local construction, via bifurcation theory, of the spurious periodic solutions near to the critical values of Δt at which they bifurcate from the steady solution. An important question is whether or not the periodic solutions can exist for arbitrarily small values of the time-step and what form they then take; this is of interest since it indicates the ranges of Δt and the sizes and forms of initial data that are likely to lead to spurious numerical behaviour.

We have described a modified equations approach which yields a sufficient criterion for the existence of spurious solutions at arbitrarily small Δt. The modified equations are a pair of coupled, singularly perturbed boundary value problems. These equations can be studied by singular perturbation techniques. The nonlinearity sets a scale (in terms of the temporal mesh-spacing) at which spurious behaviour can occur and the solutions of the modified equations describe the spatial structure of modes which are most likely to excite spurious behaviour.

Our work has been restricted to a specific class of equations in one spatial dimension. However, the methods and ideas extend to more general classes and higher spatial dimensions. The combination of local bifurcation theory and the modified equations provide a fairly comprehensive analysis of spurious periodic solutions from small to large norm and this approach can be applied to problems other than (1.1–2).

A question that we have not addressed in detail but which is very important, and requires further study, is the following: what classes of initial data will be affected by the spurious periodic solutions we have constructed? It is reasonable to expect that, for given Δt, initial data close in magnitude and form to the periodic solutions that exist at that value of Δt, will lead to spurious results. However, for general initial data, the question is open and indeed it is not well defined until a precise meaning is attached to the word 'affected'—this will depend upon whether transient or asymptotic properties are the ultimate goal of the numerical simulations. The problem is also difficult since arbitrary vectors in $\mathbb{R}^n$, for $n > 1$, are noncomparable and estimates based on norm alone (see Fig. 5.1) can be misleading. This may be overcome in specific applications by working in a cone appropriate to the problem.

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