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A Variant of Newton's Method for the Computation of Traveling Waves of Bistable Differential-Difference Equations

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We consider a variant of Newton's method for solving nonlinear differential-difference equations arising from the traveling wave equations of a large class of nonlinear evolution equations. Building on the Fredholm theory recently developed by Mallet-Paret we prove convergence of the method. The utility of the method is demonstrated with a series of examples.

KEY WORDS: Mixed type functional differential equations; Newton's method; traveling waves.

1. INTRODUCTION

We consider a variant of Newton's method to obtain traveling wave solutions to systems of differential-difference equations of the form

$$\dot{u}(\eta, t) - \gamma \,\Delta u(\eta, t) = L(u(\eta, t), u(\eta + r_1, t), \ldots, u(\eta + r_N, t)) - f(u(\eta, t), a). \tag{1.1}$$

The left-hand side of (1.1) is the "differential" portion of the equation where Δ represents the Laplacian operator and "$\cdot$" indicates the derivative with respect to time. The operator L is a linear difference operator that represents nonlocal diffusion. The function f is a nonlinear operator of bistable type which depends on the parameter a, the function $f(u, a) = u(u-a)(u-1)$ with $a \in (0, 1)$ is a typical example. The $r_i \in \mathbb{R}$, $i = 1, \ldots, N$,

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represent “shifts” of the solution function with respect to the spatial variable.

Our contribution in this paper is to derive a variant of Newton’s method to find traveling wave solutions of (1.1). Using the Fredholm theory developed by Mallet-Paret in [28] we show convergence of the method. Previously in [14] and [15] we derived numerical methods to obtain traveling wave solutions for specific examples of (1.1). The method in [14] is not generally applicable to a wide range of parameter values, while the method in [15] was based upon the use of a specific piecewise linear nonlinearity f. Our motivation here is to provide a general method based upon the use of a two-point boundary value solver such as COLNEW [2, 3] or COLMOD [9, 10] to solve at each iteration step. This is the reason for the term $\gamma \Delta u$ in (1.1). The method derived here can be thought of as a front end to solve boundary value problems (BVPs) with backward and forward delays using an existing BVP solver. In addition to derivation and convergence analysis of the method, we apply it to examples with cubic nonlinearities and discrete Laplacian operators with both nearest and next nearest neighbor interactions.

Our interest in traveling wave solutions to (1.1) follows from the extensive studies of traveling wave solutions to partial differential equations such as the reaction-diffusion equation

$$u_t = \alpha u_{xx} - f(u, a), \qquad u\colon (x, t) \to \mathbb{R} \qquad \text{for} \quad x, t \in \mathbb{R} \tag{1.2}$$

with $\alpha > 0$ and $f\colon \mathbb{R} \to \mathbb{R}$ defined as

$$f(u, a) = u(u-a)(u-1), \qquad 0 < a < 1, \tag{1.3}$$

where a is a detuning parameter. Solutions to (1.2) of the form

$$u(x, t) = \phi(x - ct), \tag{1.4}$$

where $c \in \mathbb{R}$ is the unknown wave speed, are called traveling wave solutions [20]. Substituting the traveling wave ansatz (1.4) into the reaction-diffusion partial differential Eq. (1.2) we obtain

$$-c\phi'(\xi) = \phi''(\xi) - f(\phi(\xi), a) \tag{1.5}$$

where $\xi = x - ct \in \mathbb{R}$. Equation (1.2) is defined for a one-dimensional spatial domain. If we want x to be in $\mathbb{R}^n$, we replace u_{xx} in (1.2) by $\Delta u = \sum_{k=1}^{n} D_{x_k x_k}$ and substitute the n-dimensional traveling wave ansatz $u(x, t) = \phi(x \cdot \sigma - ct)$, where the vector $\sigma = (\sigma_1, \sigma_2, \ldots, \sigma_n)^T \in \mathbb{R}^n$, such that

$\sum_{k=1}^{n} \sigma_k^2 = 1$, is the normal to the traveling wave front. We once again obtain Eq. (1.5), which is independent of the direction vector σ and dimension n.

A spatially discrete analog of the one-dimensional partial differential Eq. (1.2) is the differential-difference equation

$$u_t(x, t) = \alpha[u(x+1, t) - 2u(x, t) + u(x-1, t)] - f(u, a), \tag{1.6}$$

where u: $(x, t) \to \mathbb{R}$ for $x \in \mathbb{Z}$, $t \in \mathbb{R}$, with bistable nonlinearity (1.3), which defines a countably infinite system of ordinary differential equations indexed by points, x, on a spatial lattice. Substituting the one-dimensional traveling wave ansatz $u(x, t) = \phi(x - ct)$ into (1.6) we obtain

$$-c\phi'(\xi) = \alpha[\phi(\xi+1) - 2\phi(\xi) + \phi(\xi-1)] - f(u, a). \tag{1.7}$$

Now suppose that $x \in \mathbb{Z}^n$. Then the operator $[u(x+1, t) - 2u(x, t) + u(x-1, t)]$ is replaced by an operator that has shifts in each of the n spatial dimensions. A possible example is $\sum_{k=1}^{n} [u(x+e_k, t) - 2u(x, t) + u(x-e_k, t)]$ with e_k a unit vector of dimension n with 1 as the kth element. Substituting the n-dimensional traveling wave ansatz $u(x, t) = \phi(x \cdot \sigma - ct)$ into the n dimensional version of (1.6), we obtain

$$-c\phi'(\xi) = \alpha \sum_{k=1}^{n} [\phi(\xi + e_k \cdot \sigma) - 2\phi(\xi) + \phi(\xi - e_k \cdot \sigma)] - f(u, a), \tag{1.8}$$

which, unlike (1.5), does depend on the direction vector σ and on the dimension n. An additional property that the traveling wave Eqs. (1.7) and (1.8) exhibit, that their continuous counterparts do not, is propagation failure, failure of the traveling wave to propagate over a nontrivial interval of the detuning parameter a [8].

We are interested in bistable systems, systems where $f(u)$ can be represented by a (cubic-like) nonlinear function with "stable" zeros at u_-, u_+ ($u_- < u_+$), and an "unstable" zero at the detuning parameter $a \in (u_-, u_+)$. In our examples we consider two nonlinearities $f(u)$ that are of bistable type which include varying degrees of smoothness. By bistable type we mean that $F(u)$ is double-welled, where $F'(u) = f(u)$. The nonlinearities that we investigate are:

$$f_1(u, a) = d_1 \begin{cases} u & u < a \\ (u-1) & u > a \end{cases} \qquad d_1 \in \mathbb{R}^+, \tag{1.9}$$

and

$$f_2(u, a) = d_2 u(u-a)(u-1), \qquad d_2 \in \mathbb{R}^+. \tag{1.10}$$

The piecewise linear nonlinearity f_1 [32], where $u_- = 0$ and $u_+ = 1$, has the advantage of being linear but has the disadvantage of possessing no spinodal region. The values of u_- and of u_+ for nonlinearity f_2 are also 0 and 1. This is the classical bistable nonlinearity. In [8, 15], and [16], we used the linearized nonlinearity f (f_1 from Eq. (1.9)) to represent the bistable nonlinearity. This allowed us to produce both analytical (using integral transforms) and numerical solutions (using fixed point methods). In this paper we concentrate on a numerical method which allows us to solve differential-difference equations with any bistable nonlinearity that possesses a continuous derivative.

Considering the equilibrium solutions of

$$\dot{u}(\eta, t) = -f(u(\eta, t), a),$$

we refer to $\mathrm{u}=u_-$ and $u=u_+$ as stable and we refer to $u=a$ as unstable. Equilibrium solutions to (1.2) and (1.6) are the simplest solutions to obtain. The solution types that are of interest in this work are solutions, waves, that connect the two stable equilibria at $u=u_-$ and $u=u_+$. This requires imposing the boundary conditions

$$\phi(-\infty) \equiv \lim_{\xi \to -\infty} \phi(\xi) = u_-, \qquad \phi(\infty) \equiv \lim_{\xi \to \infty} \phi(\xi) = u_+,$$

to the traveling wave formulations.

Although we are solving nonlinear differential-difference equations, the numerical method that we present relies on several results for linear differential operators with an exponential dichotomy and on several results for linear differential-difference operators that enjoy behavior similar to an exponential dichotomy. Our method also relies on the fact that our nonlinear differential-difference equation can be treated as a (sometimes large) perturbation of a nonlinear differential equation. While we present the method for a specific subclass of the class of equations that exhibit a heteroclinic orbits parameterized by one parameter, this method appears to be applicable to a general class of parameterized differential-difference equations that connect two points (either in a heteroclinic or homoclinic orbit).

Observe that for (1.8), if $\alpha \neq 0$ and $c \neq 0$, we have a delay equation with both forward and backward delays, a functional differential equation of mixed type. Often in the modeling community, theory is developed based on the notion that phenomena have a local nature, that phenomena are independent of nonlocal information. Models are based on the variable and the local change of that variable. In reality, this is only a first approximation approach to many systems. Functional differential equations of mixed type often allow for a more realistic representation. The original foundation of studying the asymptotic behavior of delay equations which depend on energy functions can be traced back to Volterra.

Recently there has been some work on general systems of such mixed functional differential equations, most notably the work of Rustichini [36, 37], Mallet-Paret [28, 29], Mallet-Paret and Verduyn Lunel [31], and Härterich *et al.* [25]. For the specific case of mixed functional differential equations resulting from traveling wave equations we note the seminal work of Keener [26, 27], Zinner [41, 42] and of Weinberger [40]. We also mention the work of Gao [22] in which the coefficients of the difference term were directionally dependent, the work of Cahn *et al.* [8] on propagation failure and lattice induced anisotropy for traveling wave solutions of two dimensional spatially discrete reaction-diffusion equations with the piecewise linear bistable nonlinearity, and the recent work of Mallet-Paret [30] proving crystallographic pinning or lattice induced anisotropy for the cubic and other smooth nonlinearities. Shen provides existence and stability results for functional traveling waves when $f(u, t)$ is almost periodic in t [38, 39]. Other investigations into the solutions of mixed equations of the form (1.1) include [12, 17, 24], and [43].

The outline of this paper is as follows. In Section 2 we introduce the class of equations we solve, we introduce the numerical method (a modified Newton's method) we use to solve this class of equations, and we introduce our main theorem, a convergence result for our modified Newton's method. The proof of this theorem relies on detailed functional analysis of the class of equations we are solving. Section 3 consists of the background, definitions, concepts, and results that we use in the proof of the main theorem and relies heavily on the work of Mallet-Paret in [28] and [29]. This section includes analysis based on Fredholm operator theory and asymptotic hyperbolicity. Once these preliminary results are stated we proceed to Section 4 and the proof of our convergence theorem. We conclude with a summary and remarks about the class of equations that can be solved with this method, details of our numerical implementation, and several numerical examples that illustrate the robust behaviors of these types of traveling wave equations.

2. A VARIANT OF NEWTON'S METHOD

We present a numerical method for solving the nonlinear autonomous equation

$$-c\varphi'(\xi)-\gamma\varphi''(\xi)=F(\varphi(\xi),\rho)+G(\varphi(\xi+r_1),\varphi(\xi+r_2),\ldots,\varphi(\xi+r_N),\rho), \tag{2.1}$$

where $\rho \in (0, 1) \equiv U$, $\xi \in \mathbb{R}$, $c(\rho)\colon \mathbb{R} \to \mathbb{R}$, and $\gamma \in \mathbb{R}^+ \cup \{0\}$. Equation (2.1) includes the traveling wave forms of (1.1). To help illustrate the following conditions made on (2.1) we introduce the differential-difference equation

$$\dot{u}(\eta, t) = \gamma \, \Delta u(\eta, t) + \sum_{k=1}^{n} \varepsilon_k [u(\eta + e_k, t) - 2u(\eta, t) + u(\eta - e_k, t)] - u(\eta, t)[u(\eta, t) - a][u(\eta, t) - 1],$$

where $u(\eta, t)$ maps $\mathbb{R}^n \times \mathbb{R} \to \mathbb{R}$, $\gamma \in \mathbb{R}^+ \cup 0$, $\varepsilon_k \in \mathbb{R}^+$, $a \in (0, 1)$, Δ is the continuous Laplacian operator $\sum_{i=1}^{n} D_{\eta_i, \eta_i}$, "$\cdot$" denotes differentiation with respect to t, and e_k is the unit vector whose kth element equals 1, for $k = 1, \ldots, n$. The traveling wave form of (2.2) is

$$-c\varphi'(\xi) = \gamma\varphi''(\xi) + \sum_{k=1}^{n} \varepsilon_k [\varphi(\xi + e_k \cdot \sigma) - 2\varphi(\xi) + \varphi(\xi - e_k \cdot \sigma)] - \varphi(\xi)[\varphi(\xi) - a][\varphi(\xi) - 1], \tag{2.2}$$

where $\varphi\colon \mathbb{R} \to \mathbb{R}$, $\xi = \eta \cdot \sigma - ct$, σ is the direction normal to the plane wave front, and c is the unknown wave speed introduced by the traveling wave ansazt $u(\eta, t) = \varphi(\xi)$. Thus in (2.1)

$$F(\varphi(\xi), \rho) = \varphi(\xi)[\varphi(\xi) - a(\rho)][\varphi(\xi) - 1] - 2\varphi(\xi) \sum_{k=1}^{n} \varepsilon_k \quad \text{and}$$

$$G(\varphi(\xi + r_1), \varphi(\xi + r_2), \ldots, \varphi(\xi + r_N), \rho) = \sum_{k=1}^{n} \varepsilon_k [\varphi(\xi + \sigma_k) + \varphi(\xi - \sigma_k)].$$

Let $\varphi_{r_j}(\xi) = \varphi(\xi + r_j)$ and let $\bar{\varphi}(\xi) = (\varphi_{r_1}(\xi), \varphi_{r_2}(\xi), \ldots, \varphi_{r_N}(\xi))$ for $j = 1, \ldots, N$.

The following is a list of five conditions for F and G:

(c1) $F\colon \mathbb{R} \times U \to \mathbb{R}$ is C^1 in $\mathbb{R}$ and U, and $G\colon \mathbb{R}^N \times U \to \mathbb{R}$ is C^1 in $\mathbb{R}^N$ and U.

(c2) $D_\varphi F\colon \mathbb{R} \times U \to \mathbb{R}$ is locally Lipschitz in φ and $D_{\bar{\varphi}} G\colon \mathbb{R}^N \times U \to \mathbb{R}^N$ is locally Lipschitz in $\bar{\varphi}$.

(c3) For $j = 1, \ldots, N$

$$\frac{\partial G(\bar{\varphi}, \rho)}{\partial \varphi_{r_j}} > 0. \tag{2.3}$$

For (2.2), this means that the $\varepsilon_k > 0$.

(c4) The r_j, $j = 1,\ldots, N$, are the forward and backward shifts. As a matter of notation, let $r_i \neq r_k$ for $1 \leqslant i < k \leqslant N$ and $r_j \neq 0$ for $j = 1,\ldots, N$. The r_j correspond to the $e_k \cdot \sigma$ in (2.2) where the shifts occur in plus and minus pairs.

(c5) Let $\varphi_-, \varphi_+ \in \mathbb{R}$ such that $\varphi_- < \varphi_+$, and let $\Gamma\colon \mathbb{R} \times U \to \mathbb{R}$ be defined as

$$\Gamma(\varphi, \rho) = F(\varphi, \rho) + G(\varphi, \varphi, \varphi,\ldots, \varphi, \rho).$$

For some $a(\rho)$ such that $a(\rho) \in [\varphi_-, \varphi_+]$,

$$\begin{aligned} \Gamma(\varphi, \rho) &> 0, \quad \varphi \in (-\infty, \varphi_-) \cup (a, \varphi_+),\\ \Gamma(\varphi, \rho) &< 0, \quad \varphi \in (\varphi_-, a) \cup (\varphi_+, \infty),\\ \Gamma(\varphi_-, \rho) = \Gamma(a, \rho) &= \Gamma(\varphi_+, \rho) = 0, \end{aligned} \tag{2.4}$$

with

$$\begin{aligned} D_\varphi \Gamma(\varphi_-, \rho) &< 0 \qquad \text{if} \quad a \neq \varphi_-\\ D_\varphi \Gamma(\varphi_+, \rho) &< 0 \qquad \text{if} \quad a \neq \varphi_+\\ D_\varphi \Gamma(a, \rho) &> 0 \qquad \text{if} \quad a \in (\varphi_-, \varphi_+). \end{aligned} \tag{2.5}$$

For Eq. (2.2), $\Gamma(\varphi, \rho) = \varphi(\varphi - a(\rho))(\varphi - 1)$, $\varphi_- = 0$ and $\varphi_+ = 1$. Assumptions (2.4) and (2.5) imply a bistable nature to (2.1) along with the fact that we have exactly the three equilibrium solutions $\varphi = \varphi_-, a, \varphi_+$ when $a \in (\varphi_-, \varphi_+)$. Assumptions (2.4) and (2.5) also imply that $\varphi = \varphi_+$ is stable for positive increasing ξ and that $\varphi = \varphi_-$ is stable for negative decreasing ξ. In all the examples in this paper the operators F and G can be expressed in the form

$$\begin{aligned} &F(\varphi(\xi), \rho) + G(\varphi(\xi + r_1), \varphi(\xi + r_2),\ldots, \varphi(\xi + r_N), \rho)\\ &\quad = \sum_{i=1}^{N} \alpha_i [\varphi(\xi + r_i) - \varphi(\xi)] - f(\varphi(\xi), \rho) \end{aligned}$$

where $f(\varphi(\xi), \rho)$ is one of our bistable nonlinearities, f_1 or f_2. We are interested in solutions of (2.1), (φ, c), that connect φ_- and φ_+. In other words, for each $\rho \in (0, 1)$, we want to find $\mathscr{G}(\varphi, c, \rho) = 0$ for

$$\mathscr{G}(\varphi, c, \rho)(\xi) = -c\varphi'(\xi) - \gamma\varphi''(\xi) - F(\varphi(\xi), \rho) - G(\bar{\varphi}(\xi), \rho), \tag{2.6}$$

with boundary conditions

$$\varphi(-\infty) = \varphi_- \qquad \text{and} \qquad \varphi(+\infty) = \varphi_+. \tag{2.7}$$

As we have done in previous works, we define the phase condition $\varphi(0) = a(\rho)$ to select a unique translate, where a is a monotone increasing function. An advantage gained from (2.4) and (2.5) is that we do not need to consider solutions which join φ_- and $a(\rho)$, and $a(\rho)$ and φ_+.

Let

$$\mathscr{F}(\varphi, c, \rho)(\xi) = -c\varphi'(\xi) - \gamma\varphi''(\xi) - F(\varphi(\xi), \rho) - \mu G(\bar{\varphi}(\xi), \rho), \tag{2.8}$$

where $\mu \in [0, 1)$ is a relaxation parameter. Since F and G do not depend on c and since F and G are in C^1, $\mathscr{F}$ and $\mathscr{G}$ are also C^1 Fréchet-differentiable. Taking the derivative of $\mathscr{F}$ with respect to the first two variables we obtain

$$\begin{aligned} D_{1,2}\mathscr{F}(\varphi, c, \rho)(\psi, b, \rho)(\xi) = {} & -c\psi'(\xi) - \gamma\psi''(\xi) - D_\varphi F(\varphi, \rho)\,\psi(\xi) \\ & -\mu \sum_{j=1}^{N} [D_{\varphi_{r_j}} G(\bar{\varphi}, \rho)]\,\psi(\xi + r_j) - b\varphi'(\xi). \end{aligned} \tag{2.9}$$

Notice that $D_{1,2}\mathscr{F}(\varphi, c, \rho)$ is a linear (possibly nonautonomous) operator.

Definition 2.1. Using operator (2.9), we define, for fixed ρ, the modified Newton's iteration

$$D_{1,2}\mathscr{F}(\varphi_n, c_n, \rho)(\varphi_{n+1}, c_{n+1}, \rho) = D_{1,2}\mathscr{F}(\varphi_n, c_n, \rho)(\varphi_n, c_n, \rho) - \mathscr{G}(\varphi_n, c_n, \rho). \tag{2.10}$$

Unless otherwise stated, ρ is fixed throughout this paper. In Sections 3 and 4 we construct a proof that shows the modified Newton's method in (2.10) converges for (φ_0, c_0) in an open neighborhood about the solution of (2.1). Let

$$L^\infty \equiv L^\infty(\mathbb{R}),$$

let

$$W^{1,\infty} = \{f \in L^\infty \mid f \text{ is absolutely continuous and } f' \in L^\infty\},$$

and let

$$W_0^{1,\infty} = \{f \in W^{1,\infty} \mid f(0) = a(\rho)\}.$$

Definition 2.2. The pair (φ, c) is a point of attraction of the iteration defined in (2.10) if there is an open neighborhood, S, of (φ, c) such that $S \subset W_0^{1,\infty} \times \mathbb{R}$ and, for any $(\varphi_0, c_0) \in S$, the iterates defined by (2.10) all lie in $W_0^{1,\infty} \times \mathbb{R}$ and converge to (φ, c).

We now present our main result.

Theorem 2.1 (Convergence of Modified Newton's Method). *Let (φ, c) be a pair of functions such that $\mathscr{G}(\varphi, c) = 0$, with $\mathscr{G}(\varphi, c)$ as defined in (2.6) and boundary conditions (2.7). Also assume that the operators F and G of $\mathscr{G}(\varphi, c)$ satisfy conditions (c1) through (c5). Then (φ, c) is a point of attraction for the modified Newton iteration (2.10).*

3. PRELIMINARY RESULTS

The following results on asymptotic hyperbolicity and Fredholm theory follow directly from the work of Beyn [6], Palmer [34], and Mallet-Paret [28, 29]. The wave speed $c \neq 0$ throughout this section.

3.1. Definitions

In this subsection, we define what we mean when we call an operator hyperbolic, asymptotically autonomous, or asymptotically hyperbolic.

Let $\Lambda_c \colon W_0^{1,\infty} \to L^\infty$ be a nonautonomous bounded linear operator of the form

$$(\Lambda_c \psi)(\xi) = -c\psi'(\xi) - \gamma\psi''(\xi) - A_0(\xi)\,\psi(\xi) - \sum_{j=1}^{N} A_j(\xi)\,\psi(\xi + r_j). \qquad (3.1)$$

Definition 3.1. Suppose that the A_i $(i = 0, \ldots, N)$ in (3.1) can be written in the form

$$A_i(\xi) = A_{i\pm} + B_{i\pm}(\xi)$$

where $A_{i\pm}$, $i = 0, \ldots, N$, are constant coefficient operators, such that

$$A_{i+} = \lim_{\xi \to \infty} A_i(\xi), \qquad A_{i-} = \lim_{\xi \to -\infty} A_i(\xi), \qquad i = 0, \ldots, N.$$

Then the operator (3.1) is called asymptotically autonomous.

If Λ_c is asymptotically autonomous then

$$\Lambda_c = \Lambda_c^{\pm} - M_{\pm},$$

where $\Lambda_c^{\pm}: W_0^{1,\infty} \to L^{\infty}$ is the autonomous bounded linear operator

$$(\Lambda_c^{\pm}\psi)(\xi) = -c\psi'(\xi) - \gamma\psi''(\xi) - A_{0\pm}\psi(\xi) - \sum_{j=1}^{N} A_{j\pm}\psi(\xi+r_j) \qquad (3.2)$$

and $M_{\pm}: W_0^{1,\infty} \to L^{\infty}$ such that

$$(M_{\pm}\psi)(\xi) = B_{0\pm}(\xi)\,\psi(\xi) + \sum_{j=1}^{N} B_{j\pm}(\xi)\,\psi(\xi+r_j) \qquad \text{where} \quad \lim_{\xi \to \pm\infty} \|M_{\pm}\| = 0.$$

A particular case of (3.1) is $\Lambda_c^0: W_0^{1,\infty} \to L^{\infty}$, the autonomous bounded linear operator

$$(\Lambda_c^0\psi)(\xi) = -c\psi'(\xi) - \gamma\psi''(\xi) - A_{0,0}\psi(\xi) - \sum_{j=1}^{N} A_{j,0}\psi(\xi+r_j) \qquad (3.3)$$

where $A_{i,0}$, $i = 0, \dots, N$, are constant coefficient operators. Consider solutions to $\Lambda_c^0\psi = 0$ of the form $\psi = e^{\mu\xi}v$, $v \in \mathbb{R}$, $v \neq 0$. Then for each root $s = \mu$ of the characteristic equation $\det \Delta_c^0(s) = 0$, where

$$\Delta_c^0(s) = -sc - s^2\gamma - A_{0,0} - \sum_{j=1}^{N} A_{j,0}e^{sr_j}, \qquad (3.4)$$

there corresponds a set of eigensolutions to $\Lambda_c^0\psi = 0$.

Definition 3.2. The constant coefficient operator Λ_c^0 (3.3) is called hyperbolic if its characteristic Eq. (3.4) has no roots on the imaginary axis; i.e., if $\det \Delta_c^0(i\eta) \neq 0$ for $\eta \in \mathbb{R}$, then (3.3) is called hyperbolic.

We define hyperbolicity solely based on the characteristic equation $\det \Delta_c^0(s) = 0$ and not on the dynamics of the operator or of the solution. Having a constant coefficient operator be hyperbolic is an essential element to having an exponential dichotomy. We desire to imply that an asymptotically autonomous operator whose asymptotic limit is an hyperbolic operator that has an exponential dichotomy also exhibits an exponential dichotomy.

Definition 3.3. If (3.1) is asymptotically autonomous and (3.2) is hyperbolic, then we call (3.1) asymptotically hyperbolic.

An asymptotically hyperbolic operator allows us to employ the linear Fredholm theory [28] for the operator. Let

$$\mathscr{R}_c = \mathscr{R}(\Lambda_c) = \{\psi \in L^{\infty} \mid \psi = \Lambda_c\phi \text{ for some } \phi \in W_0^{1,\infty}\},$$

the range Λ_c (3.1), and let

$$\mathscr{K}_c = \mathscr{K}(\Lambda_c) = \{\phi \in W_0^{1,\infty} \mid \Lambda_c \phi = 0\},$$

the kernel of Λ_c (3.1). The operator Λ_c is a Fredholm operator if

(1) the kernel $\mathscr{K}_c \subseteq W_0^{1,\infty}$ is finite dimensional,
(2) the range $\mathscr{R}_c \subseteq L^\infty$ is closed, and
(3) $\mathscr{R}_c$ has finite codimension in L^∞.

3.2. Results

The following results depend on Λ_c being a Fredholm operator which includes knowing specific information about the kernel and range of Λ_c.

Theorem 3.1. *Let Λ_c be defined as in (3.1) and assume Λ_c is asymptotically hyperbolic. Then Λ_c is a Fredholm operator.*

Proof. The result follows from Theorem A in [28] and from Lemma 4.2 in [34]. □

The formal adjoint operator Λ_c^* of Λ_c is defined

$$(\Lambda_c^* \psi)(\xi) = c\psi'(\xi) - \gamma\psi''(\xi) - A_0^*(\xi)\,\psi(\xi) - \sum_{j=1}^{N} A_j^*(\xi - r_j)\,\psi(\xi - r_j),$$

where A_j^* is the conjugate transpose of A_j, $j = 1,\ldots, N$. Let $\mathscr{R}_c^*$ be the range of adjoint of Λ_c and $\mathscr{K}_c^*$ be the kernel of the adjoint of Λ_c. Then we have from Theorem A in [28] that

$$\mathscr{R}_c = \left\{ h \in L^\infty \;\middle|\; \int_{-\infty}^{\infty} \overline{y(\xi)}\, h(\xi)\, d\xi = 0 \text{ for all } y \in \mathscr{K}_c^* \right\}.$$

We now present two hypotheses which are used in the lemma below.

(H1) Let Λ_c be defined as in (3.1) and assume

(i) that there exist quantities $\alpha_j, \beta_j \in \mathbb{R}$, $0 \leqslant j \leqslant N$, with $\alpha_j > 0$, for $1 \leqslant j \leqslant N$, such that

$$\alpha_j \leqslant A_j(\xi) \leqslant \beta_j \qquad \text{for all} \quad \xi \in \mathbb{R},$$

(ii) that $\sum_{i=0}^{N} A_{i\pm} < 0$.

(H2) Let Λ_c be defined as in (3.1) and assume

(i) that there exist quantities $\alpha_j, \beta_j \in \mathbb{R}$, $0 \leqslant j \leqslant N$, with $\alpha_j \geqslant 0$, for $1 \leqslant j \leqslant N$, such that

$$-\alpha_j \geqslant A_j(\xi) \geqslant \beta_j \qquad \text{for all} \quad \xi \in \mathbb{R}$$

(ii) that $A_{0\pm} < 0$.

Lemma 3.1. *Let Λ_c be defined as in (3.1) and assume Λ_c is asymptotically autonomous. Also assume that there exists a solution to $\Lambda_c(\psi) = 0$ which is nonnegative and bounded. If Λ_c satisfies either (H1) or (H2), then*

(1) Λ_c is asymptotically hyperbolic, (is a Fredholm operator)

(2) there exists an element p in the kernel of Λ_c, such that $p > 0$,

(3) there exists an element p^* in the kernel of the adjoint such that each element $p^*(\xi) > 0$ for all $\xi \in \mathbb{R}$, and

(4) the range of Λ_c contains no elements, $h(\xi)$, such that $h(\xi) < 0$ or $h(\xi) > 0$, for all $\xi \in \mathbb{R}$.

Proof. In this proof, we combine the results of Mallet-Paret [28, 29], for first order differential– difference operators of the form

$$(\Lambda_{H1}\psi)(\xi) = -c\psi'(\xi) - A_0(\xi)\,\psi(\xi) - \sum_{j=1}^{N} A_j(\xi)\,\psi(\xi + r_j),$$

and the results of Fife and McLeod [20] and Beyn [6] for reaction-diffusion equations whose linearized form can be represented by operators of the form

$$(\Lambda_{H2}\psi)(\xi) = -c\psi'(\xi) - \gamma\psi'' - B_0(\xi)\,\psi(\xi).$$

Consider hypothesis (H1). Then the operator Λ_c can be treated as a perturbation of the operator Λ_{H1}. For the conditions set forth in the lemma and in (H1), Theorem 4.1 in [29] implies conclusions (1)–(3).

Now consider hypothesis (H2). Then the operator Λ_c can be treated as a perturbation of the operator Λ_{H2}. Results (1)–(3) follow from the fact that this operator has an exponential dichotomy.

As for result (4), with either (H1) or (H2), by result (3) there exists an element, p^*, in $\mathscr{R}_c^*$ such that $p^*(\xi) > 0$ for all $\xi \in \mathbb{R}$. Since

$$\mathscr{R}_c = \left\{ h \in L^\infty \,\middle|\, \int_{-\infty}^{\infty} y(\xi)\,h(\xi)\,d\xi = 0 \text{ for every } y \in \mathscr{K}_c^* \right\},$$

any $h(\xi) \in \mathscr{R}_c$ must satisfy

$$\int_{-\infty}^{\infty} p^*(\xi)\, h(\xi)\, d\xi = 0.$$

Hence $h(\xi) \in \mathscr{R}_c$ cannot be have $h(\xi) < 0$ for all $\xi \in \mathbb{R}$, or $h(\xi) > 0$ for all $\xi \in \mathbb{R}$. ☐

4. PROOF OF THEOREM 2.1

We now present the proof of Theorem 2.1 which consists of three main parts. First we establish that $D_{1,2}\mathscr{F}(\phi, b)$ is invertible in a neighborhood of the solution (φ, c). Then we rewrite the Newton iteration (2.10) as

$$(\varphi_{n+1}, c_{n+1}) = H(\varphi_n, c_n) \quad \text{where } H(\phi, b) = (\phi, b) - [D_{1,2}\mathscr{F}(\phi, b)]^{-1}\, \mathscr{G}(\phi, b),$$

and show that H is Fréchet differentiable in the neighborhood in which it is well-defined. Last, we show that the Newton iteration converges to the solution in our neighborhood, that the solution is a point of attraction. This includes showing that the spectral radius of $D_{1,2}H$ is less than 1.

Let ρ be fixed and assume $c \neq 0$. Let $(\varphi, c) \in W_0^{1,\infty} \times \mathbb{R}$ be such that $\mathscr{G}(\varphi, c) = 0$. And let F and G satisfy conditions (c1) through (c5) throughout this section.

Lemma 4.1. *There exists a ball of radius δ defined as*

$$S_{\varphi, c, \delta} = \{(\varphi_*, c_*) \in W_0^{1,\infty} \times \mathbb{R} \mid \|(\varphi, c) - (\varphi_*, c_*)\| \leqslant \delta \text{ for } \delta > 0\} \subset W_0^{1,\infty} \times \mathbb{R}$$

such that $D_{1,2}\mathscr{F}(\varphi_*, c_*)$ is invertible for all $(\varphi_*, c_*) \in S_{\varphi, c, \delta}$.

Proof. It follows from the work of Beyn [6] and Mallet-Paret [28, 29] that $D_{1,2}\mathscr{F}(\varphi, c)$ is an isomorphism from $W_0^{1,\infty} \times \mathbb{R}$ onto L^∞, and hence is invertible. Set $v = \|[D_{1,2}\mathscr{F}(\varphi, c)]^{-1}\|$ and let $0 < \epsilon < 1/(2v)$. Since $D_{1,2}\mathscr{F}(\varphi, c)$ is continuous at (φ, c), we can choose a $\delta > 0$ such that when $(\varphi_*, c_*) \in S_{\varphi, c, \delta}$,

$$\|D_{1,2}\mathscr{F}(\varphi, c) - D_{1,2}\mathscr{F}(\varphi_*, c_*)\| < \epsilon.$$

Let I be the identity operator from $W_0^{1,\infty} \times \mathbb{R}$ to $W_0^{1,\infty} \times \mathbb{R}$. Since

$$\begin{aligned}
&\|I - [D_{1,2}\mathscr{F}(\varphi, c)]^{-1}\, D_{1,2}\mathscr{F}(\varphi_*, c_*)\| \\
&\quad = \|[D_{1,2}\mathscr{F}(\varphi, c)]^{-1}\, (D_{1,2}\mathscr{F}(\varphi, c) - D_{1,2}\mathscr{F}(\varphi_*, c_*))\| \leqslant \epsilon v \leqslant \tfrac{1}{2} < 1,
\end{aligned}$$

Neumann's Lemma implies that $[D_{1,2}\mathscr{F}(\varphi, c)]^{-1} D_{1,2}\mathscr{F}(\varphi_*, c_*)$, and hence $D_{1,2}\mathscr{F}(\varphi_*, c_*)$, is invertible. Also

$$\begin{aligned}
&\|[D_{1,2}\mathscr{F}(\varphi_*, c_*)]^{-1}\| \\
&\qquad = \|[I-(I-[D_{1,2}\mathscr{F}(\varphi, c)]^{-1} D_{1,2}\mathscr{F}(\varphi_*, c_*))]^{-1} [D_{1,2}\mathscr{F}(\varphi, c)]^{-1}\| \\
&\qquad \leqslant v \sum_{i=1}^{\infty} (v\epsilon)^i = \frac{v}{1-v\epsilon}
\end{aligned}$$

for all $(\varphi_*, c_*) \in S_{\varphi, c, \delta}$. □

Remark 4.1. Thus the operator $H: S_{\varphi, c, \delta} \to W_0^{1,\infty} \times \mathbb{R}$ given by

$$H(\varphi_*, c_*) = (\varphi_*, c_*) - [D_{1,2}\mathscr{F}(\varphi_*, c_*)]^{-1} \mathscr{G}(\varphi_*, c_*) \tag{4.1}$$

is well defined.

Lemma 4.2. *The operator H (4.1) is Fréchet-differentiable and the derivative with respect to φ and c is*

$$D_{1,2}H(\varphi, c) = I - [D_{1,2}\mathscr{F}(\varphi, c)]^{-1} D_{1,2}\mathscr{G}(\varphi, c).$$

Proof. Since $\mathscr{G}$ is Fréchet-differentiable at (φ, c),

$$\|\mathscr{G}(\varphi_*, c_*) - \mathscr{G}(\varphi, c) - D_{1,2}\mathscr{G}(\varphi, c)[(\varphi_*, c_*) - (\varphi, c)]\| \leqslant \epsilon \|(\varphi_*, c_*) - (\varphi, c)\|$$

for all $(\varphi_*, c_*) \in S_{\varphi, c, \delta}$. Using the fact that $(\varphi, c) = H(\varphi, c)$, we obtain

$$\begin{aligned}
&\|H(\varphi_*, c_*) - H(\varphi, c) - [I - [D_{1,2}\mathscr{F}(\varphi, c)]^{-1} D_{1,2}\mathscr{G}(\varphi, c)][(\varphi_*, c_*) - (\varphi, c)]\| \\
&\quad = \|[D_{1,2}\mathscr{F}(\varphi, c)]^{-1} D_{1,2}\mathscr{G}(\varphi, c)[(\varphi_*, c_*) - (\varphi, c)] \\
&\qquad - [D_{1,2}\mathscr{F}(\varphi_*, c_*)]^{-1} \mathscr{G}(\varphi_*, c_*)\| \\
&\quad \leqslant \| - [D_{1,2}\mathscr{F}(\varphi_*, c_*)]^{-1} [\mathscr{G}(\varphi_*, c_*) - \mathscr{G}(\varphi, c) \\
&\qquad - D_{1,2}\mathscr{G}(\varphi, c)((\varphi_*, c_*) - (\varphi, c))]\| \\
&\qquad + \|[D_{1,2}\mathscr{F}(\varphi_*, c_*)]^{-1}[\mathscr{F}(\varphi, c) - \mathscr{F}(\varphi_*, c_*)] \\
&\qquad \times [D_{1,2}\mathscr{F}(\varphi, c)]^{-1} D_{1,2}\mathscr{G}(\varphi, c)((\varphi_*, c_*) - (\varphi, c))\| \\
&\quad \leqslant (2v\epsilon + 2v^2\epsilon \|D_{1,2}\mathscr{G}(\varphi, c)\|) \|(\varphi_*, c_*) - (\varphi, c)\|
\end{aligned} \tag{4.2}$$

for all $(\varphi_*, c_*) \in S_{\varphi, c, \delta}$. This implies H is Fréchet-differentiable and the derivative of (4.1) about the solution (φ, c) is

$$D_{1,2}H(\varphi, c) = I - [D_{1,2}\mathscr{F}(\varphi, c)]^{-1} D_{1,2}\mathscr{G}(\varphi, c) \tag{4.3}$$

where

$$\begin{aligned} &D_{1,2}\mathscr{G}(\varphi, c)(\psi, b)(\xi) \\ &\quad = D_{1,2}\mathscr{F}(\varphi, c)(\psi, b)(\xi) - (1-\mu) \sum_{j=1}^{N} [D_{\varphi_{r_j}} G(\bar{\varphi})] \, \psi(\xi + r_j). \end{aligned}$$

$D_{\varphi_{r_j}} G(\bar{\varphi})$ is a linear, possibly nonautonomous, operator. ☐

Lemma 4.3. *Let $\hat{\sigma}$ be the spectral radius of $D_{1,2}H(\varphi, c)$. Then $\hat{\sigma} < 1$.*

Proof. Writing the eigenproblem for $D_{1,2}H(\varphi, c)$ we obtain the equation

$$(1-\mu)[D_{1,2}\mathscr{F}(\varphi, c)]^{-1} \sum_{j=1}^{N} [D_{\varphi_{r_j}} G(\bar{\varphi})] \, \phi(\xi + r_j) - \lambda I(\phi, b) = (0, 0)$$

where λ is the eigenvalue, and (ϕ, b) are the eigenfunctions. Rewriting this relation we obtain

$$\begin{aligned} &-D_{1,2}\mathscr{F}(\varphi, c)(\phi, b) + \frac{1-\mu}{\lambda} \sum_{j=1}^{N} [D_{\varphi_{r_j}} G(\bar{\varphi})] \, \phi(\xi + r_j) = 0, \\ &\quad \Rightarrow \lambda[c\phi'(\xi) + \gamma\phi''(\xi) + D_\varphi F(\varphi) \, \phi(\xi)] \\ &\qquad + [1 + (\lambda - 1) \, \mu] \sum_{j=1}^{N} [D_{\varphi_{r_j}} G(\bar{\varphi})] \, \phi(\xi + r_j) = -\lambda b \varphi'(\xi). \end{aligned} \tag{4.4}$$

The right-hand side of (4.4), contains the derivative of the solution to (2.1), $\varphi'(\xi)$, which we know from Lemma 3.1 with (H1), is strictly positive.

Splitting (4.4) into real and imaginary parts

$$\begin{aligned} \lambda_R \Big[& c\phi'(\xi) + \gamma\phi''(\xi) + D_\varphi F(\varphi) \, \phi(\xi) \\ & + [(1-\mu)/\lambda_R + \mu] \sum_{j=1}^{N} [D_{\varphi_{r_j}} G(\bar{\varphi})] \, \phi(\xi + r_j) = -b\varphi'(\xi) \Big] \end{aligned} \tag{4.5}$$

$$\begin{aligned} \lambda_I \Big[& c\phi'(\xi) + \gamma\phi''(\xi) + D_\varphi F(\varphi) \, \phi(\xi) \\ & + \mu \sum_{j=1}^{N} [D_{\varphi_{r_j}} G(\bar{\varphi})] \, \phi(\xi + r_j) = -b\varphi'(\xi) \Big] \end{aligned} \tag{4.6}$$

where λ_R and λ_I are the real and imaginary parts of λ, respectively.

First consider (4.6). The left hand side of (4.6) can be written as

$$c\phi'(\xi)+\gamma\phi''(\xi)+D_{\varphi}F(\varphi)\,\phi(\xi)+\mu\sum_{j=1}^{N}\,[D_{\varphi_{r_j}}G(\bar{\varphi})]\,\phi(\xi+r_j)$$

$$=c\phi'(\xi)+\gamma\phi''(\xi)+A_0(\xi)+\sum_{j=1}^{N}\,A_j(\xi)=-\Lambda_c$$

as defined in (3.1). The conditions of F and G, (c1)–(c5) (in particular the conditions on Γ (2.4) and (2.5)), for $\mu\in[0,1]$, force the left hand side of (4.6) to satisfy (H1) and hence can have no strictly positive or negative functions in its range. Recall from Lemma 3.1 that the right hand side of (4.6) is strictly positive or strictly negative, $\lambda_I=0$, and hence $\lambda=\lambda_R$.

We next consider (4.5). Again the left hand side is equal to $-\Lambda_c$ only now $A_0(\xi)=\lambda\,D_{\varphi}F(\varphi)$ and $A_j(\xi)=[(1-\mu)/\lambda_R+\mu]\,D_{\varphi_{r_j}}G(\bar{\varphi})$, $j=1,\ldots,N$. We now consider two cases, λ_R either positive or negative.

Case 1. $\lambda_R>0$. Using the conditions (c1)–(c5) and (H1) eliminate all $\lambda_R\geqslant\lambda_+$ from the spectrum, where $0<\lambda_+<1$.

Case 2. $\lambda_R<0$. When $[(1-\mu)/\lambda_R+\mu]>0$, using the conditions (c1)–(c5) and (H1) eliminates $\lambda_R<(1-\mu)/(-\mu)$. When $[(1-\mu)/\lambda_R+\mu]\leqslant 0$, using the conditions (c1)–(c5) and (H2) eliminates $(1-\mu)/(-\mu)\leqslant\lambda_R<0$. Hence eliminated are all $\lambda_R<0$ and $\lambda_R\geqslant\lambda_+$.

Assume that there exist a least upper bound on the spectrum, and call this value λ_1. Then $0<\lambda_1\leqslant\lambda_+<1$. In Section 4 of [29], Mallet–Paret shows that when $\lambda>\lambda_1$, the real eigenvalues of (4.4) lie in both the intervals $(-\infty,0)$ and $(0,\infty)$, and as we saw above, when $\lambda>\lambda_1$, λ is not in the spectrum of (4.3). He also showed that for $0<\lambda<\lambda_1$, the real eigenvalues of the determinant of the characteristic equation of (4.4) all lie in either $(-\infty,0)$ or $(0,\infty)$. Suppose $0<\lambda<\lambda_1$, and consider the formal adjoint of the left-hand side of (4.4). This adjoint operator has a kernel, $\mathcal{K}_c^*$, of dimension zero. Since the operator represented by the left-hand side of (4.4) is a Fredholm operator, the codimension of the range of (4.4) equals the dimension of $\mathcal{K}_c^*$ which is zero. Hence the right-hand side of (4.4) is in the range of the left-hand side. Thus there exist λ in $(0,\lambda_1)$ that are in the spectrum of (4.3). □

Remark 4.2. The value λ_1, which is both direction and dimension dependent, can be thought of as the contraction factor for our method.

Lemma 4.4. *For $D_{1,2}H\colon W_0^{1,\infty} \to W_0^{1,\infty}$ the limit*

$$\lim_{m\to\infty} \|[D_{1,2}H]^m\|^{1/m} = \hat{\sigma}$$

exists, where $\hat{\sigma}$ is the spectral radius.

Proof. The result is a statement of Theorem 10.13 in Rudin [35]. □

Lemma 4.5. *The solution (φ, c) is a point of attraction of (2.10).*

Proof. By Lemma 4.4, for any $\epsilon > 0$ there exists an integer $N_{\hat{\sigma}}$ such that for all $m \geqslant N_{\hat{\sigma}}$

$$\|[D_{1,2}H(\varphi, c)]^m\|^{1/m} \leqslant \hat{\sigma} + \epsilon,$$

which implies

$$\|[D_{1,2}H(\varphi, c)]^m\| \leqslant (\hat{\sigma} + \epsilon)^m.$$

Let $H^p(\psi, b) = H[H(H\{\cdots[H(\psi, b)]\cdots\})]$, the operator H applied p times. Observe that $H^p\colon W_0^{1,\infty} \to W_0^{1,\infty}$ and that $H^p(\varphi, c) = (\varphi, c)$. Choose $\epsilon > 0$ such that $\hat{\sigma} + \epsilon < 1$, choose $p_1 \in \mathbb{Z}^+$ such that $(\hat{\sigma} + \epsilon)^{p_1} + \epsilon < 1$, and let $p > \max(N_{\hat{\sigma}}, p_1)$. Since H is Fréchet-differentiable at (φ, c), H^p is also. Thus there exists a $\delta > 0$ such that, for all $(\varphi_*, c_*) \in S_{\varphi, c, \delta}$,

$$\begin{aligned}&\|H^p(\varphi_*, c_*) - H^p(\varphi, c) - D_{1,2}H^p(\varphi, c)((\varphi_*, c_*) - (\varphi, c))\| \\ &\qquad \leqslant \epsilon\, \|(\varphi_*, c_*) - (\varphi, c)\|.\end{aligned}$$

The Fréchet derivative of H^p, $D_{1,2}H^p(\varphi, c) = [D_{1,2}H(\varphi, c)]^p$, through application of the chain rule. Thus,

$$\begin{aligned}&\|H^p(\varphi_*, c_*) - (\varphi, c)\| \\ &\qquad \leqslant \|H^p(\varphi_*, c_*) - H^p(\varphi, c) - D_{1,2}H^p(\varphi, c)((\varphi_*, c_*) \\ &\qquad\quad - (\varphi, c))\| + \|[D_{1,2}H(\varphi, c)]^p\|\, \|(\varphi_*, c_*) - (\varphi, c)\| \\ &\qquad \leqslant [(\hat{\sigma} + \epsilon)^p + \epsilon]\, \|(\varphi_*, c_*) - (\varphi, c)\| \qquad \text{for all} \qquad (\varphi_*, c_*) \in S_{\varphi, c, \delta}.\end{aligned}$$

Therefore, if $(\varphi_0, c_0) \in S_{\varphi, c, \delta}$,

$$\|(\varphi_p, c_p) - (\varphi, c)\| = \|H^p(\varphi_0, c_0) - (\varphi, c)\| \leqslant [(\hat{\sigma} + \epsilon)^p + \epsilon]\, \|(\varphi_0, c_0) - (\varphi, c)\|,$$

which implies that $(\varphi_p, c_p) \in S_{\varphi, c, \delta}$. By an induction argument,

$$\|(\varphi_{n \cdot p}, c_{n \cdot p}) - (\varphi, c)\| \leqslant [(\hat{\sigma} + \epsilon)^p + \epsilon]^n\, \|(\varphi_0, c_0) - (\varphi, c)\| \tag{4.7}$$

and $(\varphi_{n\cdot p}, c_{n\cdot p}) \in S_{\varphi, c, \delta}$ for all $n \in \mathbb{Z}^+ \cup 0$. Since $(\hat{\sigma}+\epsilon)^p+\epsilon < 1$, (4.7) implies that

$$\lim_{n\to\infty} (\varphi_{n\cdot p}, c_{n\cdot p}) = (\varphi, c).$$

Since H is a bounded operator, and since (4.7) holds for all $p > \max(N_{\hat{\sigma}}, p_1)$,

$$\lim_{n\to\infty} (\varphi_n, c_n) = (\varphi, c). \qquad \square$$

This concludes the proof of Theorem 2.1.

Remark 4.3. We note that these results extend to coupled systems. The single equation case was presented for ease of notation.

5. APPLICATIONS

The relaxation of Newton's method, (2.10), allows us to solve differential-difference equations with any bistable nonlinearity that possesses a continuous derivative. To solve at each iteration we use the boundary value problem solver COLMOD [9, 10]. This imposes the requirement that $\gamma \neq 0$ so that we always include the $\gamma\varphi''$ term. If we used a functional differential equation solver such as the code COLDLY [1], as opposed to a BVP solver, then we could solve for the case when $\gamma = 0$. In the examples here, and those presented in [16], we always started the iteration with φ equal a translate of the hyperbolic tangent, the wave speed c equal to 1, and relaxation parameter $\mu = 0$.

In the first example, Example 1, we solve a reaction-diffusion differential-difference equation with both a piecewise linear nonlinearity, used in [8, 14–16], and a cubic nonlinearity, to illustrate numerically that the phenomena of propagation failure and step-like solution profiles occur for both nonlinearities and are not artifacts of the piecewise continuous nonlinearity.

In the second example we present wave speed $c(\theta)$ plots, where θ is the direction of propagation through the two dimensional integer lattice, for the five point star and the nine point box versions of the spatially discrete diffusion operator. This allows us to explicitly show the lattice anisotropy inherent in the discrete operator, and to provide numerical evidence of the lattice induced anisotropy as a function of the detuning parameter a.

5.1. Example 1: Nonlinear Differential-Difference Reaction-Diffusion Equation

In this example, we consider the traveling wave Eq. (2.2), which has nonlinearity $f_2(\varphi, a) \equiv d_2\varphi(\varphi - a)(\varphi - 1)$, $d_2 = 1$, and we consider (2.2) with f_2 replaced by f_1, (1.9), with $d_1 = 1/6$ and compare solution behavior for the nonlinearities f_1 and f_2.

Remark 5.1. In Section 2, we assumed that F and G were C^1. In proving Theorem 2.1, we only need that $\mathcal{G}$, $D_{1,2}\mathcal{G}(\varphi_*, c_*)$, and $D_{1,2}\mathcal{F}(\varphi_*, c_*)$ are continuous in a neighborhood of the solution (φ, c). Thus we only need $(\varphi_*, c_*) \in S_{\varphi, c, \delta}$, $D_{\varphi_*}F$, and $D_{\varphi_{r_i}^*}G$ to be continuous. If we define $f_1(a, a) = 0$ and $D_\varphi f_1(a, a) = 1/6$, then (2.1) with the piecewise linear nonlinearity f_1, appears to be included in the class of equations that can be solved with this numerical method. But recall that for this problem, with nonlinearity f_1, $\varphi''(\xi)$ is discontinuous at a and the spectral radius argument holds for continuous operators. It is not clear at this time if the proof can be made to hold for nonlinearities such as f_1.

5.1.1. Step-Like Wave Profiles

Figure 1 contains solution plots, $\varphi(\xi)$, for Eq. (2.2) for $c \approx 10^{-7}$ (which is of the size of the numerical error in the computations), where $a = 1/2$, $n = 1$, and $\gamma = 10^{-4}$. In the solution plots of Fig. 1(a), where $\varepsilon_1 = \varepsilon = 1/12$, the step phenomenon appears regardless of which nonlinearity is used. This

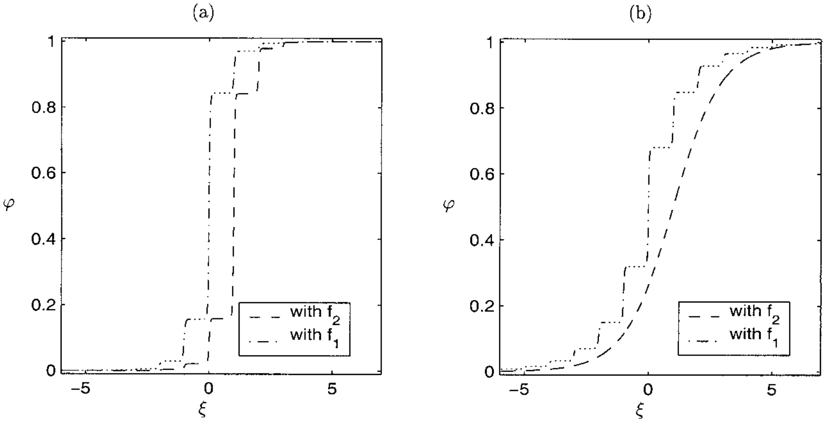

Fig. 1. Example 1: Step-like solution profiles nonlinearities f_1 and f_2.

implies that the step-like solution profile is not generated by the jump discontinuity in the nonlinearity f_1, but is generated by the nonlocal nature of the spatially discrete diffusion term. In Fig. 1(b) where $\varepsilon = 1$ the solution curve associated with nonlinearity f_2 no longer has step-like behavior. This implies that for this smooth nonlinearity that step-like behavior is dependent on the strength of diffusion.

5.1.2. The Cubic Nonlinearity

In Fig. 2 we solve (2.2) with the cubic nonlinearity f_2, $n = 1$, $\gamma = 10^{-6}$, and $\varepsilon_1 = 1/10$. A set of solution curves, $\varphi(\xi)$, for various values of the detuning parameter a, is plotted in Fig. 2(a) and the $a(c)$ curve for this problem is plotted in Fig. 2(b).

Remark 5.2. In [15], for (2.2) with the nonlinearity f_1, we presented $a(c)$ plots which admitted a nontrivial interval of a in which $c = 0$. We also learned that this propagation failure only occurs when $\gamma = 0$, but we saw that for γ small, there exists an interval of a values (approximately the same interval as for propagation failure) for which c is "small." In the $a(c)$ plot, Fig. 2(b), we once again see this behavior, where for $\gamma = 10^{-6}$, there exists an interval of a for which $|c| < 10^{-4}$. This suggests that we also have propagation failure when solving with the cubic nonlinearity f_2 in the $\gamma = 0$ limit, thus indicating that propagation failure is due to the discrete diffusion term, not the nonlinearity.

Referring to both the solution $\varphi(\xi)$ plot and the $a(c)$ plot in Fig. 2, we point out three main types of solution profiles that can be classified by

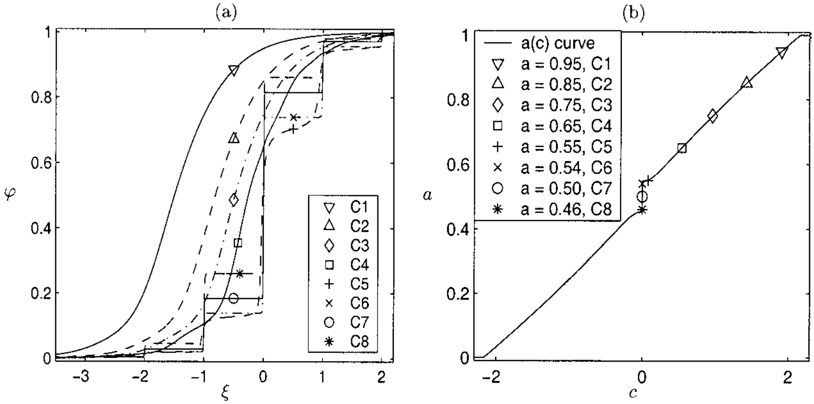

Fig. 2. Example 1: The spatially discrete/continuous reaction-diffusion equation with the cubic nonlinearity and various values of the detuning parameter a.

$|a-1/2|$. The first type (solutions C1 and C2 in Fig. 2) are solutions that have a hyperbolic tangent shape. The values of a are the farthest from 1/2 for this type. The third type of profile (solutions C5, C6, C7, and C8) consists of solutions whose profile exhibit step-like behavior. Away from the wave front (the internal layer), the tails of these solutions decay asymptotically. The values of a for this type define an interval of "small" c and step-like profiles about 1/2, an interval of propagation failure. The second or middle type of solution profile (solutions C3 and C4) consists of "transition" solutions, solutions that contain a mix of elements from the first and third types of solution profiles. The distance from 1/2, $|a-1/2|$, for the values of a for this type of solution profile is greater than $|a-1/2|$ for the values of a of the third type and is less than $|a-1/2|$ for the values of a of the first type.

5.2. Example 2: Comparison Five Point and Nine Point Stencils

In this example we numerically solve the equation

$$-c\varphi'(\xi)=10^{-5}\varphi''(\xi)+L_*\varphi(\xi)-10f_2(\varphi,a) \tag{5.1}$$

with

$$L_*\varphi(\xi)=L_5\varphi(\xi)\equiv[\varphi(\xi+\sigma_1)+\varphi(\xi-\sigma_1)+\varphi(\xi+\sigma_2)+\varphi(\xi-\sigma_2)+4\varphi(\xi)]$$

the five point star (nearest neighbor) discrete Laplacian, or

$$\begin{aligned}L_*\varphi(\xi)=L_9\varphi(\xi)\equiv\tfrac{1}{6}\,[&4\varphi(\xi+\sigma_1)+4\varphi(\xi-\sigma_1)+4\varphi(\xi+\sigma_2)+4\varphi(\xi-\sigma_2)\\&+\varphi(\xi+\sigma_1+\sigma_2)+\varphi(\xi-\sigma_1+\sigma_2)+\varphi(\xi+\sigma_1-\sigma_2)\\&+\varphi(\xi-\sigma_1-\sigma_2)-20\varphi(\xi)]\end{aligned}$$

the nine point box (or nearest and next nearest neighbor) discrete Laplacian, to observe and compare the directional dependence due to a discrete Laplacian. In these discretizations $\sigma_1=\cos(\theta)$ and $\sigma_2=\sin(\theta)$, where θ is the direction that the traveling wave is flowing through the lattice.

Figure 3(i)–(iv) is a series of wave speed c versus direction angle θ plots, each plot representing a different value of the detuning parameter a. We see that as a increases from 1/2, the average wave speed c increases and c becomes more isotropic for both L_5 and L_9. All four plots also show that c for L_5 is always greater than c for L_9. If we consider that the traveling wave Eq. (5.1) is obtained from a spatially discrete Cahn–Allen equation that is defined with respect to the two-dimensional primative lattice, these plots give an indication about the shape of a growing crystal which has a primitive square lattice. The value of $|a-1/2|$ can be thought of as a measure of the free energy available for growth. Figure 3(ii) shows us that for $a=0.55$, we might expect the crystals to grow into squares. For $a=0.54$, Fig. 3(i), with both L_5 and L_9 we again would expect a square, but with L_9 we should also expect an octagon.

6. CONCLUSIONS

We presented an iterative numerical method for finding solutions to nonlinear systems of bistable traveling wave reaction-diffusion differential-difference equations, taking advantage of an exponential-dichotomy-like behavior that the linear variation of these equations exhibit. The method is Newton's which we varied by introducing a relaxation parameter into the variational derivative, allowing us to relax any forward or backward delay terms. If we completely relax these terms, $\mu=0$, treating them as "known" information, this method can be thought of as a front end to solve boundary value problems (BVPs) with backward and forward delays using an existing BVP solver such as COLSYS, COLNEW, or COLMOD as long as

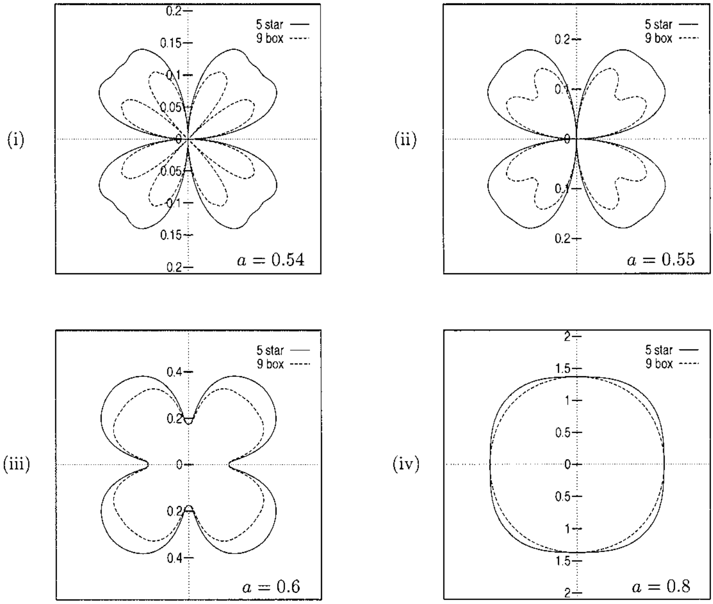

Fig. 3. Example 2: $c(\theta)$ polar plots: A comparison of the wave speeds for the spatially discrete reaction-diffusion equation with the five point star and the nine point box discretizations for various values of the detuning parameter a.

γ is nonzero. A primary advantage of this relaxation is that it allows one to find numerical solutions to a large class of forward-backward delay equations without depending on continuation from a problem with a known solution, unlike in [11], by using the relaxation parameter to control the size of the Newton ball of convergence. While we present the method for a specific subclass of the class of equations that exhibit a heteroclinic orbits parameterized by one parameter, this method appears to be applicable to a general class of parameterized differential-difference equations that connect two homogeneous equilibria (either as a heteroclinic or a homoclinic orbit).

We have provided a sampling of numerical examples, showing some of the versatility of the method. The proof of Newton's method helped in producing numerical results by providing guidance in applying the method. The step-like solution behavior exhibited in [15], when solving with nonlinearity f_1, also appears when solving with smooth nonlinearities. We have also seen lattice induced anisotropy based on the direction of propagation and on the detuning parameter a for two possible discrete Laplacian operators, the five point star and the nine point box, which agree with existing theory of crystal growth for primitive cubic lattice materials.

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