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Existence of Monotone Traveling Fronts for BDF Discretizations of Bistable Reaction-Diffusion Equations

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Abstract. This article is concerned with the effect of temporal discretization on traveling wave solutions to parabolic PDEs possessing bistable nonlinearities. The focus is on the application of backward differentiation formulas to Nagumo type PDEs with two different bistable nonlinearities. Existence of monotone traveling fronts is shown and the efficacy of different methods of proof is discussed.
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1 Introduction

Nonlinear bistable parabolic partial differential equations are commonly used in the modeling of phase transitions. These types of PDEs are often referred to as bistable equations, Allen-Cahn equations, and Chafee-Infante equations. Another example where the depths of the potential wells are allowed to vary is the Nagumo [26] PDE. The Nagumo equation admits monotone traveling wave solutions that are stable and attract a large class of initial conditions (see [2] and [11]). When these types of equations are solved numerically (albeit on a truncated finite spatial domain), software codes such as LSODE [16], which are based upon backward differential formulas (BDF), are often employed. These BDF methods are appropriate for stiff differential equations and the stable BDF methods [13] are so called $A(\alpha)$ stable methods.

Our contribution in this paper is to consider BDF temporal discretizations of Nagumo partial differential equations with two bistable nonlinearities and show the existence of monotone traveling fronts. The two nonlinearities considered are a piecewise linear nonlinearity, that has been considered by McKean [27] among others, and a cubic nonlinearity. The existence of monotone traveling waves for the piecewise linear nonlinearity involves the use of transform techniques and follows results in [27], [6], [7]. Due to lack of smoothness the only member of the BDF family that we are able to prove the existence of a monotone traveling front is the backward Euler method. For the cubic nonlinearity we focus on methods of proof based on ideas related to the implicit function theorem and are able to prove existence for all the stable BDF methods over at least some range of their parameters. Since we are considering traveling wave solutions it is natural to consider and we restrict to fixed time steps. The results of this paper, establishing existence of monotone traveling fronts, justify arguments in [8, 9] where the dependence on the time step Δt of traveling wave solutions of BDF time discretizations is studied under the assumption of the existence of monotone traveling fronts. The Nagumo PDE dates back to at least [26]. Study of spatial discrete versions of the Nagumo equation and investigation of thesholding phenomena or propagation failure include [3, 4, 17, 18, 30, 31, 24, 25, 19].

The outline of this paper is as follows. In section 2 we consider traveling wave solutions for the Nagumo PDE with the two nonlinearities to be considered. The form of the traveling wave fronts and the dependence of the wavespeed c on the detuning parameter a that control the depths of the potential wells is reviewed. In section 3, BDF discretizations of Nagumo PDEs are considered and the resulting traveling wave equations are derived. Section 4 contains results that show the existence of monotone traveling fronts for the backward Euler discretization with the piecewise linear nonlinearity and section 5 is devoted to results establishing the existence of monotone traveling waves for BDF discretizations with the cubic nonlinearity.

2 Traveling Waves for the Nagumo PDE

Consider the Nagumo PDE [26]

$$u_t = \epsilon^2 \Delta u - f(u) \tag{1}$$

where $u \equiv u(x,t)$, $x \in I\!R^n$ for $n = 1, 2,$ or 3, Δ is the standard Laplacian operator, $t \geq 0$ and f is of bistable type. In this paper we consider two nonlinearities, a piecewise linear set-valued nonlinearity (see [27])

$$f(u) \equiv f_1(u) = \begin{cases} u, & u < a, \\ u - 1, & u > a, \\ [a-1, a], & u = a, \end{cases} \tag{2}$$

and the cubic nonlinearity

$$f(u) \equiv f_2(u) = u(u-1)(u-a) \tag{3}$$

where $0 < a < 1$ is a so called detuning parameter. A traveling wave solution is a pair (φ, c) such that $\varphi(x \cdot \sigma - ct) = u(x,t)$ where $\sigma \in I\!R^n$ satisfies $||\sigma||_2 = 1$ and specifies the direction of propagation. The function φ determines the wave profile and c is the wave speed. The traveling wave equation that must be satisfied for (1) is

$$-c\dot{\varphi}(\xi) = \epsilon^2 \ddot{\varphi}(\xi) - f(\varphi(\xi)), \qquad \xi \in I\!R, \tag{4}$$

together with the boundary conditions $\varphi(-\infty) = 0$ and $\varphi(+\infty) = 1$ that are natural due to the bistable nature of the nonlinear term. The traveling wave equations for the PDE (4) are independent of the dimension n and independent of the direction of propagation σ.

Using the transform techniques considered in [6] and [7] (see also [27]) one can show that for (4) with the nonlinearity f_1, (2), φ is the C^1 function

$$\begin{aligned}\varphi(\xi) &= \frac{1}{2} + \frac{1}{\pi}\int_0^\infty \frac{A(s)\sin(s\xi)ds}{s(A^2(s)+c^2s^2)} + \frac{c}{\pi}\int_0^\infty \frac{\cos(s\xi)ds}{A^2(s)+c^2s^2} \\ &= H(\xi) + C_\pm e^{\lambda_\pm \xi},\ \xi \in I\!R\end{aligned} \tag{5}$$

where $A(s) = 1 + \epsilon^2 s^2$, $H(\xi)$ is the Heaviside step function,

$$C\pm = \begin{cases} \frac{1}{2} + \frac{c}{2\sqrt{4\epsilon^2+c^2}} & \xi \le 0, \\ -\frac{1}{2} + \frac{c}{2\sqrt{4\epsilon^2+c^2}} & \xi \ge 0, \end{cases} \quad \text{and} \quad \lambda_\pm = \begin{cases} \frac{-c+\sqrt{4\epsilon^2+c^2}}{2\epsilon^2} & \xi \le 0, \\ \frac{-c-\sqrt{4\epsilon^2+c^2}}{2\epsilon^2} & \xi \ge 0. \end{cases}$$

This solution can also be found using basic ODE techniques if one assumes φ is C^1. The relationship between the wave speed c and the detuning parameter a is given by

$$a = \frac{1}{2} + \frac{c}{\pi}\int_0^\infty \frac{ds}{A^2(s)+c^2s^2} = \frac{1}{2} + \frac{c}{2\sqrt{4\epsilon^2+c^2}} \tag{6}$$

where because φ is monotone we may choose the unique translate $\varphi(0) = a$.

For (4) with the nonlinearity f_2, (3), when $c \in (-\epsilon/\sqrt{2}, \epsilon/\sqrt{2})$, we solve for φ and the (a, c) relationship, [19], to obtain

$$\varphi(\xi) = \frac{1}{2}\left[1 + \tanh\left(\frac{\xi}{2\epsilon\sqrt{2}}\right)\right] \qquad \text{with} \qquad a = \frac{1}{2} + \frac{c}{\epsilon\sqrt{2}}. \tag{7}$$

3 Traveling Waves and BDF Discretizations

We consider the effect of BDF time discretizations on traveling wave solutions. Consider the application of a consistent linear multistep method (see [13]) to the differential equation $\dot{u} = g(u)$. The resulting difference equation has the form

$$\sum_{j=0}^{k} \alpha_j U_{n+j} = \Delta t \sum_{j=0}^{k} \beta_j g(U_{n+j}) \tag{8}$$

where $U_{n+j} \approx u(t_{n+j})$. In particular, for (1) we obtain

$$\sum_{j=0}^{k} \alpha_j U_{n+j}(x) = \Delta t \sum_{j=0}^{k} \beta_j [\epsilon^2 \Delta U_{n+j}(x) - f(U_{n+j}(x))]. \tag{9}$$

The traveling wave assumption is $\Psi(x \cdot \sigma - ct_k) = U_k(x)$ which upon substitution into (9) yields the traveling wave equations

$$\sum_{j=0}^{k} \alpha_j \Psi(\xi - jc\Delta t) = \Delta t \sum_{j=0}^{k} \beta_j [\epsilon^2 \ddot{\Psi}(\xi - jc\Delta t) - f(\Psi(\xi - jc\Delta t))]. \tag{10}$$

Recall [13] that the general k-step BDF method is given by

$$\sum_{j=1}^{k} \frac{1}{j} \nabla^j U_{n+k} = \Delta t g(U_{n+k}), \; \nabla U_n = U_n - U_{n-1}, \; \nabla^j U_n = \nabla[\nabla^{j-1} U_n]. \tag{11}$$

4 BDF Methods and f_1

Consider now the piecewise linear f given by f_1 in (2). Our interest is in establishing the existence of monotone solutions Ψ which for the nonlinearity (2) allows for a simplification to a linear inhomogeneous equation. If Ψ is monotone, then we may choose the unique translate that satisfies $\Psi(0) = a$. Thus, for the piecewise linear f as in (2), $f(\Psi(\xi)) = \Psi(\xi) - H(\xi)$ where H is the Heaviside function, and (10) becomes

$$\sum_{j=0}^{k} \alpha_j \Psi(\xi - jc\Delta t) = \Delta t \sum_{j=0}^{k} \beta_j [\epsilon^2 \ddot{\Psi}(\xi - jc\Delta t) - \Psi(\xi - jc\Delta t) + H(\xi - jc\Delta t)]. \tag{12}$$

Our analysis with the piecewise linear f in (2) will depend on the smoothness of the solution Ψ. We do not expect that the second derivative will be continuous but may be regarded as set valued at a finite number of points. For the BDF methods $\beta_k \neq 0$ while $\beta_j = 0$ for $j = 0, ..., k-1$. Thus, for BDF methods

$$\ddot{\Psi}(0+) - \ddot{\Psi}(0-) = \frac{1}{\epsilon^2}. \tag{13}$$

Theorem 4.1 *Consider the application of a linear multistep method to (1) with f given by (2). For $\Delta t > 0$, if $\sum_{j=0}^{k} \alpha_j = 0$ and*

$$\sum_{j=0}^{k} \exp(-ijc\Delta t s)(\alpha_j/\Delta t + \beta_j A(s)) \neq 0, \; A(s) = \epsilon^2 s^2 + 1, \tag{14}$$

in the horizontal strip $-\delta \leq \mathrm{Im} s \leq 0$ for small $\delta > 0$, then there exists a solution Ψ to (10) satisfying $\Psi(-\infty) = 0$ and $\Psi(+\infty) = 1$ of the form

$$\Psi(\xi) = \frac{1}{2} + \frac{1}{\pi} \int_0^{\infty} \frac{D(s, \Delta t, \xi) ds}{s E(s, \Delta t)} \tag{15}$$

where for $c_j = \alpha_j/\Delta t + \beta_j(\epsilon^2 s^2 + 1) = \alpha_j/\Delta t + \beta_j A(s)$,

$$\begin{aligned} D(s,\Delta t,\xi) &= \{\sum_{l=1}^{k}\sum_{j=0}^{k-l}[\beta_j c_{j+l}\sin(s\xi + lc\Delta ts) \\ &+ c_j\beta_{j+l}\sin(s\xi - lc\Delta ts)] + \sum_{j=0}^{k}\beta_j c_j \sin(s\xi)\}, \end{aligned} \tag{16}$$

$$E(s,\Delta t) = \sum_{l=1}^{k}\sum_{j=0}^{k-l}[2c_j c_{j+l}\cos(lc\Delta ts)] + \sum_{j=0}^{k} c_j^2. \tag{17}$$

Proof. If we assume that the waveform is monotone and set $\Psi(0) = a$ to choose a translate, then for the reaction term f given by (2), $f(\Psi(\xi))$ in (10) may be replaced with $\Psi(\xi) - H(\xi)$, where H is the Heaviside function. This transforms the problem into a linear inhomogeneous equation so that transform techniques may be applied. However, we will need to justify the assumption of monotonicity. We will do so after determining Ψ.

We first construct the solution Ψ of (10) with conditions $\Psi(-\infty) = 0$, $\Psi(+\infty) = 1$, and $\Psi(0) = a$. Let $\Psi_\varepsilon(\xi) = e^{-\varepsilon\xi}\Psi(\xi)$, with small $\varepsilon > 0$. Since $\Psi(+\infty) = 1$, as $\varepsilon \to \infty$

$$\Psi_\varepsilon(\xi) = e^{-\varepsilon\xi}\Psi(\xi) \to 0,$$

and by Lemma 4.1, as $\varepsilon \to -\infty$

$$\Psi_\varepsilon(\xi) = e^{-\varepsilon\xi}\Psi(\xi) \le |e^{-\varepsilon\xi}||\Psi(\xi)| \le |Ke^{(\varepsilon_0-\varepsilon)\xi}| \to 0 \quad \text{for} \quad 0 < \varepsilon < \varepsilon_0.$$

Substituting $\Psi_\varepsilon(\xi) = e^{-\varepsilon\xi}\Psi(\xi)$ into (10) we obtain,

$$\begin{aligned} \sum_{j=0}^{k} e^{-\varepsilon jc\Delta t}\left[\alpha_j + \Delta t\beta_j\left(1 - \epsilon^2\left[\varepsilon^2 + 2\varepsilon\frac{d}{d\xi} + \frac{d^2}{d\xi^2}\right]\right)\right]\Psi_\varepsilon(\xi - jc\Delta t) \\ = \Delta t\sum_{j=0}^{k}\beta_j e^{-\varepsilon\xi}H(\xi - jc\Delta t). \end{aligned}$$

We now apply the Fourier transform $\hat{\Psi}_\varepsilon(s) = \int_{-\infty}^{\infty} e^{-is\xi}\Psi_\varepsilon(\xi)d\xi$, with sufficiently small $\varepsilon > 0$ to obtain

$$\begin{aligned} \sum_{j=0}^{k} e^{-(is+\varepsilon)jc\Delta t}\left[\alpha_j/\Delta t\beta_j\left(1 - \epsilon^2\left[\varepsilon^2 + i2\varepsilon s - s^2\right]\right)\right]\hat{\Psi}_\varepsilon(s) \\ = \frac{1}{is+\varepsilon}\sum_{j=0}^{k}\beta_j e^{-(is+\varepsilon)jc\Delta t} \end{aligned}$$

or

$$\hat{\Psi}_\varepsilon(s) = \frac{1}{is+\varepsilon}\frac{\sum_{l=0}^k \beta_l e^{-(is+\varepsilon)lc\Delta t}}{R(s-i\varepsilon)} \tag{18}$$

with

$$R(q) = \sum_{j=0}^k e^{-ijc\Delta ts} R_j(q) \quad \text{and} \quad R_j(q) = \alpha_j/\Delta t + \beta_j(\epsilon^2 q^2 + 1). \tag{19}$$

The inverse transform $\Psi(\xi) = e^{\varepsilon\xi}\Psi_\varepsilon(\xi) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{(is+\varepsilon)\xi}\hat{\Psi}_\varepsilon(s)ds$ gives

$$\begin{aligned} \Psi(\xi) &= \frac{1}{2\pi}\int_{-\infty}^{+\infty} \frac{e^{(is+\varepsilon)\xi}}{is+\varepsilon}\frac{\sum_{l=0}^k \beta_l e^{-(is+\varepsilon)lc\Delta t}}{R(s-i\varepsilon)} ds \\ &= \frac{1}{2\pi i}\int_{-i\varepsilon-\infty}^{-i\varepsilon+\infty} \frac{e^{is\xi}}{s}\frac{\sum_{l=0}^k \beta_l e^{-islc\Delta t}}{R(s)} ds \end{aligned} \tag{20}$$

With condition (14) we only have one singularity to worry about, a simple pole at $s=0$. Thus, we break up Ψ into three integrals

$$\Psi(\xi) = \frac{1}{2\pi i}\left(\int_{-\infty}^{-\varepsilon} + \int_{S_\varepsilon} + \int_{+\varepsilon}^{+\infty}\right)\frac{e^{is\xi}}{s}\frac{\sum_{l=0}^k \beta_l e^{-islc\Delta t}}{R(s)} ds \tag{21}$$

where S_ε is the half-circle at the origin. Considering this integral first

$$\begin{aligned} &\frac{1}{2\pi i}\int_{S_\varepsilon} \frac{e^{is\xi}}{s}\frac{\sum_{l=0}^k \beta_l e^{-islc\Delta t}}{R(s)} ds \\ &= \frac{1}{2\pi i} 2\pi i \frac{1}{2} Res\left(\frac{e^{is\xi}}{s}\frac{\sum_{l=0}^k \beta_l e^{-islc\Delta t}}{R(s)}, 0\right) = \frac{1}{2} \end{aligned} \tag{22}$$

recalling that $\sum_{j=0}^k \alpha_j = 0$. The other two integrals can be combined

$$\begin{aligned} &\frac{1}{2\pi i}\left(\int_{-\infty}^{-\varepsilon} + \int_{+\varepsilon}^{+\infty}\right)\frac{e^{is\xi}}{s}\frac{\sum_{l=0}^k \beta_l e^{-islc\Delta t}}{R(s)} ds \\ &= \frac{1}{2\pi i}\int_{+\varepsilon}^{+\infty}\frac{1}{s}\left[\frac{e^{is\xi}\sum_{l=0}^k \beta_l e^{-islc\Delta t}}{R(s)} - \frac{e^{-is\xi}\sum_{l=0}^k \beta_l e^{islc\Delta t}}{R(-s)}\right] ds \\ &= \frac{1}{\pi}\int_{+\varepsilon}^{+\infty}\frac{1}{s}\left[\frac{\sum_{j=0}^k\sum_{l=0}^k \beta_l \sin(s\xi + s(j-l)c\Delta t)R_j(s)}{\sum_{j=0}^k\sum_{l=0}^k e^{is(j-l)c\Delta t}R_l(s)R_j(s)}\right] ds. \end{aligned} \tag{23}$$

Recombining (22) and (23) we obtain an explicit formula for $\Psi(\xi)$ by letting $\varepsilon \to 0$. This is equivalent to (15), just a rearrangement of the sums.

If we consider Ψ as a function of both ξ and the wave speed c, then from (15) we have the symmetry property

$$\Psi(\xi, c) = 1 - \Psi(-\xi, -c) \tag{24}$$

In addition, from (21) we have that $|\Psi(\xi)| = O(e^{\varepsilon\xi})$ as $\xi \to -\infty$ so the boundary condition $\Psi(-\infty) = 0$ is satisfied, and by the symmetry property (24) the other boundary condition $\Psi(+\infty) = 1$ holds. ∎

The proof of Theorem 4.1 relies on the following lemma whose proof is similar to results in [6] and [7].

Lemma 4.1 *Let Ψ be a solution to (10)(with condition (14)). Then there exists an $\varepsilon_0 > 0$ such that, for some $K > 0$,*

$$|\Psi(\xi)| \leq K e^{\varepsilon_0 \xi} \quad \text{for} \quad \xi \leq 0.$$

4.1 Backward Euler Discretization

For the Backward Euler method the following Lemma justifies the assumption of monotonicity.

Lemma 4.2 *For the application of the Backward Euler method $R(-iz)$ (see (19)) has a positive root z_0 such that $iR'(-iz_0) > 0$. Moreover, there exists $\epsilon_0 > 0$ such that if $s \in \mathbb{C}$ is any other root of R with* $\text{Im}s \leq 0$, *then* $\text{Im}s < -z_0 - \epsilon_0$.

Proof. For the Backward Euler discretization we have

$$R(s) = -\frac{1}{\Delta t} + \exp(-ic\Delta ts)[\frac{1}{\Delta t} + A(s)] \tag{25}$$

Consider for $z \geq 0$

$$\tilde{R}(z) := R(-iz) = -\frac{1}{\Delta t} + \exp(-c\Delta tz)[\frac{1}{\Delta t} + 1 - \epsilon^2 z^2]. \tag{26}$$

Since $R(0) > 0$ and $R(-i\frac{1}{\epsilon}) < 0$ for $c > 0$ and $R(-i\frac{1}{\epsilon}\sqrt{1 + 1/\Delta t}) < 0$ for $c \leq 0$, there exists a minimal $z_0 > 0$ such that $R(-iz_0) = 0$. We have

$$iR'(-iz) = \exp(-c\Delta tz)[-\epsilon^2 c\Delta tz^2 + 2\epsilon^2 z + c(1 + \Delta t)] =: \exp(-c\Delta tz) \cdot Q(z) \tag{27}$$

and $\tilde{R}'(z) = -iR'(-iz)$. To show the existence of a z_0 such that $\tilde{R}(z_0) = 0$ and $\tilde{R}'(z_0) < 0$ we consider the cases $c > 0$ and $c < 0$ separately.

First, for $c > 0$ we have $\tilde{Q}(0) > 0$ and $Q(+\infty) < 0$. We need to show that z_0 is bounded above by the positive root, r_p, of the quadratic polynomial Q in the right hand side of (27). However, a direct calculation shows that $r_p > \frac{1}{\epsilon}$, so $z_0 < r_p$.

For $c < 0$ we have $Q(0) < 0$ and $Q(+\infty) > 0$. We need to show that z_0 is bounded below by the positive root, r_p, of Q. We have $r_p < z_0$ since $\tilde{R}(z)$ is increasing (from $\tilde{R}(0) = 1$) on $[0, r_p)$.

Next, we need to show that there are no roots in the strip $0 \leq Im(s) < -z_0 - \epsilon_0$. Consider the real and imaginary parts of $R(u - iz)$ for $z \geq 0$.

Assume the real and imaginary parts are simultaneously equal to zero:

$$\begin{aligned} 0 = & - \frac{1}{\Delta t} + \cos(c\Delta tu)\exp(-c\Delta tz)[\frac{1}{\Delta t} + (1 + \epsilon^2(u^2 - z^2))] \\ & - \sin(c\Delta tu)\exp(-c\Delta tz)[2\epsilon^2 uz] \end{aligned} \tag{28}$$

and

$$\begin{aligned} 0 = & - \sin(c\Delta tu)\exp(-c\Delta tz)[\frac{1}{\Delta t} + (1 + \epsilon^2(u^2 - z^2))] \\ & - \cos(c\Delta tu)\exp(-c\Delta tz)[2\epsilon^2 uz] \end{aligned} \tag{29}$$

Multiplying (28) by $\cos(c\Delta tu)$, multiplying (29) by $\sin(c\Delta tu)$ and subtracting, we obtain after some manipulation

$$0 = R(-iz) + \exp(-c\Delta tz)\epsilon^2 u^2 + \frac{1}{\Delta t}[1 - \cos(c\Delta tu)] \geq R(-iz) \tag{30}$$

The quantity in (30) shows that in the strip $z_0 \leq z \leq z_0 + 1$ there is a bound $|u| \leq K$ on the real part of all roots. Thus, this strip can only contain a finite number of roots. It is then enough to show that the only root on the horizontal line $Ims = -z_0$ is the root $-z_0$ we have already obtained. If $z = z_0$ in (30), then since $\exp(-c\Delta tz)\epsilon^2 u^2 + \frac{1}{\Delta t}[1 - \cos(c\Delta tu)] \geq 0$ and each term is nonnegative, we must have $u = 0$. ∎

Remark 4.1 *For the Backward Euler discretization, Lemma 4.2 implies the condition (14) in Theorem 4.1. For higher order BDF methods we were not able to justify the monotonicity assumption due to the lack of smoothness observed in equation (13).*

Theorem 4.2 *For the Backward Euler discretization of (1) with $\Delta t > 0$ and $c \neq 0$ there exists of monotone traveling wave solution. Moreover, for $c \neq 0$, the curve $c(a)$ is strictly monotone.*

Proof. The argument follows that in [6]. Since Lemma 4.2 holds, we can apply essentially Corollary 4.5 of [6]. This shows that the waveform is monotone increasing for $|\xi|$ large. Next, the analogue of Theorem 4.6 in [6] shows that monotonicity in the tails implies that the waveform is monotone throughout. Finally a Melnikov type argument like that of Theorem 4.7 in [6] gives the uniqueness of c as a function of a for $c \neq 0$. ∎

5 Monotone Traveling Waves for BDF Methods and Cubic Nonlinearity

Now consider the k-step BDF form of (10) with cubic nonlinearity f_2 (3). If the wave speed $c = 0$, then $\Psi(\xi) = \varphi(\xi)$ from solution (7). Throughout the rest of this section we assume that $c \neq 0$ and let $\phi(\eta) = \Psi(\xi)$ where

$\eta = \xi/c + \Delta t$. With this change of variables the BDF methods are written as

$$-\frac{\epsilon^2}{c^2}\ddot{\phi}(\eta) = \frac{-1}{\Delta t}\sum_{j=0}^{k}\frac{\alpha_{k-j}}{\beta_k}\phi(\eta + j\Delta t) - f(\phi(\eta), a), \tag{31}$$

$$\phi(-\mathrm{sgn}(c)\infty) = 0 \qquad \text{and} \qquad \phi(\mathrm{sgn}(c)\infty) = 1.$$

Numerical results for (31) using the techniques in [1] appear in [8, 9]. The $(\Delta t, a)$ parameter space for monotone solutions to (31) with $\epsilon/c \neq 0$ is disjoint from the $(\Delta t, a)$ space for (31) with $\epsilon/c = 0$. The following discussion will be with respect to (31) with $c \neq 0$ and is split into two subsections, one for $\epsilon/c \neq 0$ and one for $\epsilon/c = 0$.

5.1 BDF Methods for $\epsilon \neq 0$ and c finite.

In [24] and [25] Mallet-Paret (see also [14, 20]) shows that the set of traveling wave solutions to functional differential equations of mixed and bistable type exist, are unique, and make up a smooth manifold. The backward Euler method version of (31) with $\epsilon/c \neq 0$ is within the class of equations considered and Theorem 2.1 of [25] can be applied directly.

What we obtain is that there is a unique dependence of ϕ and ϵ/c on the parameter a, and that for $\epsilon/c > 0$, $\dot{\phi} > 0$ over all $\eta \in I\!R$. For $\epsilon/c < 0$, the boundary conditions switch and we have that $\dot{\phi} < 0$ all $\eta \in I\!R$. In [24] and [25] Mallet-Paret considers linearizations about traveling wave solutions. The smooth manifold nature of the solution set, in our case parameterized by ϵ/c and a, allows for continuation (via implicit function theorem arguments). Linearizing (31), we obtain

$$-\frac{\epsilon^2}{c^2}\ddot{x}(\eta) = \frac{-1}{\Delta t}\sum_{j=1}^{k}\frac{\alpha_{k-j}}{\beta_k}x(\eta + j\Delta t) - \left[\frac{1}{\Delta t}\frac{\alpha_k}{\beta_k} + f_{\phi(\eta)}(\phi(\eta), a)\right]x(\eta)$$

where $f_{\phi(\eta)}$ is the derivative of f with respect to ϕ. The behavior of the linearization when $\eta \to \pm\infty$ is fundamental to the linear theory presented. Although k-step BDF methods, $k = 2, ..., 6$, are not directly included in the theory of [25], these BDF methods do have a key piece, that the characteristic equation when $\eta \to \pm\infty$ has the strict concavity property $\Delta''_{c,a} < 0$, where

$$\Delta_{c,a} \equiv -\frac{\epsilon^2}{c^2}s^2 + \frac{1}{\Delta t}\sum_{j=1}^{k}\frac{\alpha_{k-j}}{\beta_k}e^{sj\Delta t} + \left[\frac{1}{\Delta t}\frac{\alpha_k}{\beta_k} + d_\pm\right],$$

with $d_- = f_{\phi(\eta)}(0, a)$ and $d_+ = f_{\phi(\eta)}(1, a)$. *Although we have not shown*, it appears that, following the work presented in [25], monotonicity results along with smooth manifold results can be shown for all six stable BDF methods.

5.2 BDF Methods with $\epsilon = 0$ or c infinite.

We now consider monotone nondecreasing solutions in detail, the results for monotone nonincreasing solutions easily follow. Mackay and Sepulchre in [23] use the implicit function theorem to study systems of equations which include (31) when $\epsilon/c = 0$. The idea applied to this case is to start with $1/\Delta t = 0$ (where (31) is just $0 = f(\phi, a)$) which has piecewise constant solutions made up of $\phi = 0$ and 1. Then using the implicit function theorem they show for a $(\Delta t, a)$ pair, a solution exists if the linearization of (31) with $\epsilon/c = 0$ which respect to ϕ is invertible. The range of $1/\Delta t$ for a choice of a is found by continuing from $1/\Delta t = 0$ to $1/\Delta t = 1/\Delta t_0$ where

$$\frac{1}{\Delta t_0} = \frac{e^{-(1-\mu_k/M_k)\phi_{cr}}}{M_k} \int_{y_1}^{y_2} e^{(1-\mu_k/M_k)\phi} f_\phi(\phi, a) d\phi, \tag{32}$$

with $M_k = \sum_{j=0}^{k} |\alpha_j|/\beta_k$ and $\mu_k = \alpha_k/\beta_k$. We will now discuss the value ϕ_{cr} and the limits of integration y_1 and y_2 for $a > 1/2$, the case $a < 1/2$ being similar. Letting

$$\phi_{cr\pm} = \frac{a + 1 \pm \sqrt{a^2 - a + 1 + 3(M_k - \mu_k)/\Delta t_0}}{3},$$

the zeros of $f_\phi(\phi, a) = 0$, and starting with $1/\Delta t = 0$ and the solution

$$\phi(\eta) = \begin{cases} 0, & \eta < \eta_0, \\ 1, & \eta > \eta_0, \end{cases}$$

as $1/\Delta t$ increases from 0, it is expected, for $\varepsilon > 0$, that $\phi(-\varepsilon + \eta_0)$ will increase from 0, that $\phi(\varepsilon + \eta_0)$ will decrease from 1, and that the jump at η_0 of ϕ will decrease. A sufficient condition that the inverse of the variational equation exists, that we can continue, is that $f_\phi(\phi, a) \neq 0$. This implies that the limits of integration y_1, y_2 are either $0, \phi_{cr-}$ or $\phi_{cr+}, 1$, whichever interval is smaller, which for $a > 1/2$ is $\phi_{cr+}, 1$. The value ϕ_{cr} in (32) is whichever $\phi_{cr\pm}$ is a limit of integration. Equality (32) is implicit in Δt_0 for all the BDF methods except backward Euler. For the 4-step BDF method we plot the $(\Delta t, a)$ pairs, the shaded region III of Plot A of Figure 1, for $a \in (0, 1)$.

In the above choice of the interval of integration for (32) (and in fact the integrand itself) the coefficients of the delay terms $\phi(\eta + j\Delta t)$, $j = 0, ..., k$, are taken into account, but not the delays themselves. For all six stable BDF methods the delays in (10) are all one sided and in formulation (31) they are all forward ($\Delta t > 0$). When this is the case, and we continue $1/\Delta t$ from 0, the ϕ to the left of η_0 will move (from 0 when $a > 1/2$) but ϕ for $\eta > 0$ will not ($\phi(\eta) = 1$ for $\eta > \eta_0$ and $a > 1/2$). This will be observed when we construct solutions. Thus, when $a > 1/2$, we only need consider the limits of integration $0, \phi_{cr-}$. The shaded regions I, II, and III in Plot A of Figure 1 are the $(\Delta t, a)$ pairs for $a \in (0, 1)$, taking into account that all the delays are one sided, defined by (32) for the 4-step BDF method.

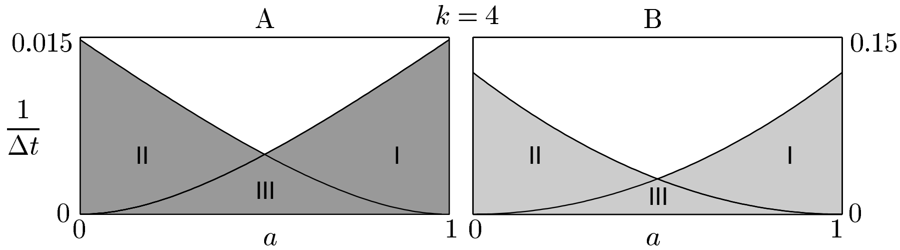

Figure 1: Range of a versus $1/\Delta t$ for piecewise constant solutions to the 4-step BDF method. Plot A shows the regions $(\Delta t, a)$ derived in condition (32) using the implicit function theorem approach in [23]. Plot B is the regions generated by construction. Region I corresponds to Solution 1, region II to Solution 2, and region III to both Solution 1 and 2. All six stable BDF methods have similar plots and for each method the shaded region derived from [23], Plot A, is contained in the shaded region found by construction, Plot B.

The values of $1/\Delta t_0$ found by the above method are a lower bound on the actual $1/\Delta t$ that can be reached though continuation from $1/\Delta t = 0$ for a particular value of a.

While Plot A of Figure 1 shows the regions of $(\Delta t, a)$ such that $1/\Delta t \in [0, 1/\Delta t_0]$ for only the 4-step BDF method, the regions for the other five stable BDF methods have the same qualitative behavior, only different quantitative values.

Construction of solutions. Independent of the work in [23], but having the confidence of the knowledge that there is a smooth manifold of solutions to (31) with $\epsilon/c = 0$ for Δt large enough, we now construct monotone solutions. The constant solutions $\phi(\xi) = 0, a$, or 1 are the only monotone solutions that satisfy (31) for all Δt.

$\Delta t > 4\mu_k$, $a \in (0,1)$

For $\Delta t > 4\mu_k$ there also exist monotone solutions consisting of piecewise constant steps of length Δt on the left half interval and the constant solution $\phi = 1$ if $a > 1/2$, or $\phi = 0$ if $a < 1/2$, on the right half interval. Suppose a and Δt are chosen so that $a^2 - 4\mu_k/\Delta t > 0$ and divide the ξ domain $I\!R$ into the intervals $\bigcup_j [(j-1)\Delta t, j\Delta t) = I\!R$. Let ϕ_l be the value of $\phi(\xi)$ on the $[(l-1)\Delta t, l\Delta t)$ interval. We now write (31) with $\epsilon/c = 0$ as

$$g(\phi_l, a) + h(\phi_l) = 0, \qquad \text{where} \tag{33}$$

$$g(\phi_l, a) \equiv \phi_l^3 - (a+1)\phi_l^2 + (a + \frac{\mu_k}{\Delta t})\phi_l, \qquad \text{and} \qquad h(\phi_l) \equiv \frac{\sum_{j=1}^{k} \alpha_{k-j}\phi_{l+i}}{\beta_k \Delta t}.$$

and construct two monotone piecewise constant solutions ϕ_{l_1} and ϕ_{l_2}.

Solution 1: Assume that $a > 1/2$ and let $\phi_{l_1} = 1$ for $l_1 = 1, 2, 3, \ldots$. The ϕ_{l_1} for $l_1 = 0, -1, -2, -3, \ldots.$ are defined by the real roots of the equation

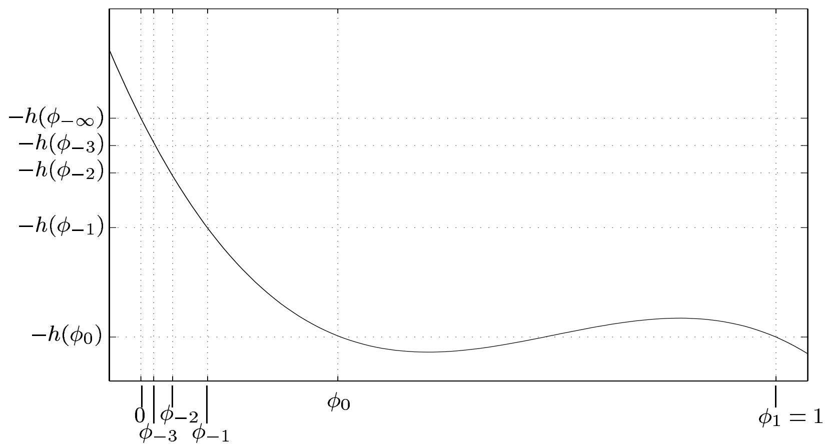

Figure 2: Plot of $-g(\phi_{l_1})$ illustrating the construction of a piecewise constant monotone solution to (31) with $\epsilon/c = 0$ (Solution 1 of section 5.2) where $\phi_l = 1$ for $l > 0$.

$g(\phi_{l_1}, a) + h(\phi_{l_1}) = 0$. For $l_1 = 0$, there are three real roots of (33),

$$\phi_0(a, \Delta t) = \frac{a_1 - \sqrt{a_1^2 - 4\mu_k/\Delta t}}{2}, \quad \frac{a_1 + \sqrt{a_1^2 - 4\mu_k/\Delta t}}{2},$$
$$\text{and} \quad \phi_1(a_1, \Delta t) = 1, \tag{34}$$

where ϕ_0 and ϕ_1 are "stable saddle" points. For $l_1 < 0$, (33) has only one real root. Figure 2 illustrates this construction.

Solution 2: A second solution can be obtained by a similar construction or by just letting $\phi_{l_2} = 1 - \phi_{l_1}$ and $a_2 = 1 - a_1$ for all $l_2 \in \mathbb{Z}$.

The shaded regions of Plot B in Figure 1 are the $(\Delta t, a)$ for which we can construct a monotone solution to the 4-step BDF version of (31) with $\epsilon/c = 0$. Regions I and III are generated by Solution 1 and regions II and III are generated by Solution 2. The entire shaded region in Plot A found by continuation is contained in the entire shaded region of Plot B.

$\underline{\Delta t < 4\mu_k}$

If $a \in [0, 1]$ there are no such step-like piecewise constant monotone solutions, only the constant solutions 0, a, and 1 are monotone nondecreasing. However, if a is allow to be vary outside the interval $[0, 1]$ then the above construction is once again valid [9].

6 Epilogue

Other techniques for showing the existence of monotone traveling waves for Nagumo's equation under temporal discretization are possible. For instance, in [5] the existence of monotone traveling fronts is established for a forward Euler temporal and uniform spatial discretization. A generalization appears possible to the Backward Euler discretization. The results in [5] rely on results in Lorenz [21] which in turn are based on results of Fenichel [10]. The technique will most likely yield results for "Δt sufficiently small." Another possible technique for showing existence of monotone traveling fronts are those in [28, 29]. Application of these results appears to be possible for backward Euler discretizations when $a = 0$ or $a = 1$ in which case the Nagumo equation is much like a Fisher equation [12]. Generalization to higher order stable BDF methods may be possible using the results in [22].

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