An Analysis of Numerical Approximations of Metastable Solutions of the Bistable Equation

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ABSTRACT. We construct a finite element method for the bistable problem that has the same Lyapunov functional as the true solution. We prove existence and uniqueness of the approximation and give a short-time a priori error bound. We show that approximations of metastable solutions evolve on the same time scale as the true solution, provided the mesh and time steps are sufficiently fine depending on the initial data and the diffusion constant but not on the length of time of the evolution.

§1. INTRODUCTION

This paper is concerned with numerical approximations of slowly evolving solutions of the bistable problem,

$$\begin{cases} u_t - \epsilon^2 u_{xx} = u - u^3, & 0 < x < 1, 0 < t, \\ u_x(0,t) = u_x(1,t) = 0, & 0 < t, \\ u(x,0) \text{ given.} \end{cases} \tag{1.1}$$

The dynamical properties of solutions of (1.1) have generated considerable interest (see [3], [4], [7], and references therein) in part because it is one of the simplest problems that produce nonlinear relaxation to equilibrium in the presence of competing stable steady states [4]. The asymptotic behavior as $t \to \infty$ of solutions of (1.1) is well understood, see [10] and [13]. The only stable equilibrium solutions are constant in space and minimizers of the energy functional

$$\int_0^1 \left(\frac{1}{2}\epsilon^2 u_x^2 + \frac{1}{4}(u^2-1)^2 \right) dx.$$

For generic initial data, $\lim_{t\to\infty} u(x,t)$ exists and is equal to one of these stable states.

But, this convergence can be extremely slow because solutions of (1.1) can exhibit dynamic metastability. If u forms a pattern of transition layers after the initial transient, then the subsequent time scale for substantial motion of the layers to occur is

$$\exp\{Cd/\epsilon\} \tag{1.2}$$

for $C = O(1)$ and d equal to the minimum of distances between layers and layers and the boundaries. These metastable solutions are neither local minimizers of the energy or necessarily close to an unstable equilibrium solution of (1.1). After the metastable period, a relatively quick transient sees one or more of the layers disappear and the solution form a new metastable pattern. This repeats until the eventual convergence to a stable state.

Key words and phrases. bistable equation, finite element method, Lyapunov functional, metastability, transition layer.

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Detailed analyses of metastable solutions have been carried out in [3], [4], and [7]. The last two references share key techniques. They begin with an ansatz on the form of a metastable solution, then an analytic approximation to the metastable solution is constructed that is extremely close to the metastable solution (exponentially close in $-1/\epsilon$) yet allows precise estimates on its motion. Both analyses involve consideration of some manifold generated from the approximate metastable states and are self-termed as geometric approaches. In both cases, the estimate on the time of substantial motion of layers is (1.2).

Bronsard and Kohn [3] use a completely different approach based on "energy" estimates. They employ a renormalized energy,

$$E_\epsilon[w] := \int_0^1 \left(\frac{\epsilon}{2}w_x^2 + \frac{1}{4\epsilon}(w^2-1)^2\right)dx,$$

that is positive and finite as $\epsilon \to 0$. The minimum energy of a single transition from 1 to -1 is

$$\varepsilon_0 := \frac{\sqrt{2}}{3},$$

and in general for Z transitions, the minimum energy is $Z\varepsilon_0$. The minimum is achieved by the piecewise constant function $\mathcal{U}$ that changes value at the Z zeroes of the layers. The essential tool in their analysis is a result which shows that an $H^1(0,1)$ function w that makes Z transitions "smoothly" in the sense that

$$E_\epsilon[w] \le Z\varepsilon_0 + \epsilon^l,$$

for some $l > 0$, and that is close to $\mathcal{U}$ in the $L^1(0,1)$ norm, depending on l, satisfies a lower bound on the energy $E_\epsilon[w]$. The rest of the analysis is directed towards showing that a solution of (1.1) with initial data satisfying these hypotheses maintains a transition layer structure with little motion over a time interval of length $O(\epsilon^{-l-1})$. In comparing these results with those in [4] and [7], we note that for fixed l,

$$e^{C/\epsilon} \gg C\epsilon^{-l-1},$$

for ϵ small. On the other hand, the assumptions on the data in [4] and [7] mean that the data satisfies the hypotheses of Bronsard and Kohn for every $l > 0$.

Our interest lies in the behavior of numerical approximations of metastable solutions of (1.1). In general, approximations started with generic data move quickly to a transition layer pattern as expected. The subsequent evolution varies greatly, however, depending on ϵ, the mesh, and the scheme. The pattern of layers may actually become fixed; the layers may exhibit metastability on the scale suggested by the behavior of the solution; and they may move more rapidly than expected. We would like to understand the mechanism behind these possibilities. We hope that an understanding of the behavior of approximations of (1.1) will carry light to other nonlinear parabolic problems that exhibit fast and slow time scales of evolution.

The motivation for this paper lies in the following results produced by a scheme we introduce in §2. We start the scheme with initial data that is close to a single metastable transition layer and then record the time of substantial motion of the layer as a function of the number of spatial mesh points of a uniform mesh. We use $\epsilon^2 = .01$, which is sufficiently small to give metastability. The time-stepping is performed with equal accuracy throughout. We plot the results in figure 1. It is clear that motion is more rapid on coarser meshes and that the time scale of motion seems to "converge" as the mesh is refined. To further emphasize the dependence on ϵ, in figure 2, we plot the ratio of the time of substantial motion for 5 mesh points to that for 200 mesh points versus ϵ^2. As ϵ^2 decreases, the effect is more pronounced. We have tested several other schemes in this fashion and achieved similar results in all cases.

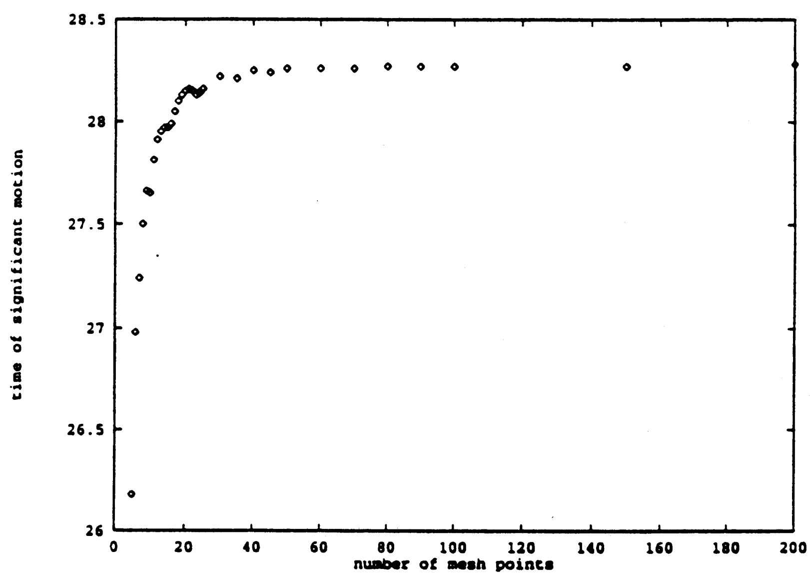

FIGURE 1. PLOT OF TIME VERSUS NUMBER OF MESH POINTS

This behavior cannot be understood by considering the standard a priori error analysis used to prove convergence. To explain this, we paraphrase the typical result;

$$||\text{error}(t)||_{\mathcal{A}} \leq Ce^{Ct/\epsilon} \cdot \text{mesh size} \cdot ||u||_{\mathcal{B}};$$

for appropriate function spaces $\mathcal{A}$ and $\mathcal{B}$. The factor $\exp\{Ct/\epsilon\}$ implies that this bound has meaning only for a short initial transient and cannot be used to analyze the scheme over the time intervals that we consider. For linear parabolic problems, it is possible to give error bounds for some schemes that are uniform in time. The exponential factor above is produced in the course of a Gronwall argument that is used to handle the nonlinearity. It is possible to prove long-time error bounds for certain schemes for nonlinear parabolic problems ([6],[8],[9],[11],[12]). All of these analyses rely on a "non-smooth" data estimate that is the discrete equivalent of "parabolic smoothing". These arguments do not apply to the situation of a metastable solution. In rough terms, the linear problem obtained by linearizing (1.1) around a metastable solution has some positive eigenvalues associated to it.

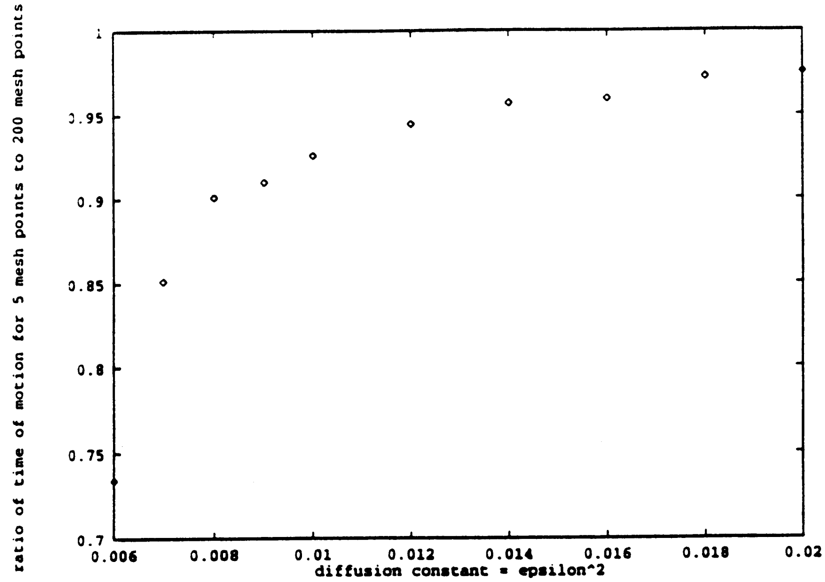

FIGURE 2. PLOT OF RATIO OF TIMES VERSUS ϵ^2

We perform our analysis on a scheme that has the same Lyapunov functional $E_\epsilon[\cdot]$ as the true solution. The scheme is described in §2. It is the analog of a scheme suggested for the phase field model by Du and Nicolaides [5]. We prove existence and uniqueness of the approximation and a standard a priori error bound in §3. As we said, the latter is not useful for the analysis of metastability. But, it does have one important consequence. All of the references [3], [4], and [7] conjecture that generic initial data move to the assumed profile during an initial transient; if true, then their analyses are valid for generic data. If this conjecture is valid, then the short-time error bound would imply that the same is true of approximations computed on a sufficiently fine mesh.

Our main results, presented in §3, are essentially extensions of the results of Bronsard and Kohn to the approximation produced by the scheme introduced in §2. Our results require that the space and time mesh be sufficiently fine, depending on ϵ, $\mathcal{U}$, $E_\epsilon[u(x,0)]$, and l (see above), but not depending on time. In other words, for space and time mesh sufficiently fine independent of time, the approximation's layers evolve on a time scale larger than ϵ^{-l-1} for any $l > 0$. We do not know, of course, whether the approximation tracks a particular solution over this time interval. Our intuitional explanation of the numerical results presented above is that the lower bounds we derive on the time of motion and the conditions to achieve this time are in fact strict. Hence, using a coarse mesh limits the size of the l that can be used in the assumptions, and so the time of evolution. We believe this to be true because a careful look at the analysis shows there is little waste in the estimates.

We note that this analysis of Bronsard and Kohn is particularly suited to the finite element method we consider. It would be more difficult to extend the analyses of [4] and [7] to numerical methods because it is essential to both that the transition layers are close exponentially in $-1/\epsilon$ to a given function. Since numerical approximations for (1.1) are only accurate to polynomial order in the mesh size, this condition is impractical for computations made on uniform fixed meshes when ϵ is small.

§2. The numerical scheme

The weak formulation of (1.1) reads: find $u \in L^\infty((0,\infty); H^1(0,1))$ such that

$$\begin{cases} (u_t, v) + \epsilon^2(u_x, v_x) + (f(u), v) = 0, & t > 0, v \in H^1(0,1), \\ u(0,x) \text{ given }, \end{cases} \tag{2.1}$$

where $(v,w) := \int_0^1 vw dx$ with $\|v\|^2 := (v,v)$ and $f(v) := v^3 - v$. We employ an analog of a scheme proposed by Du and Nicolaides [5] for the phase field model. We discretize $[0,1]$ into $x_0 := 0 < x_1 < \cdots < x_{M+1} := 1$, with $\Delta x_m := x_m - x_{m-1}$, $\Delta x := \max \Delta x_m$ and $\underline{\Delta x} := \min \Delta x_m$, and $[0,\infty)$ into $t_0 := 0 < t_1 < t_2 < \cdots$, with $\Delta t_n := t_n - t_{n-1}$ and $\Delta t := \sup \Delta t_n < \infty$. We use the space of continuous, piecewise linear functions for approximation,

$$V_h := \{V : V \in C_0(0,1) \text{ and } V|_{(x_{m-1},x_m)} \text{ is linear }, m = 1, ..., M+1\}.$$

By standard results, $V_h \subset H^1(0,1)$ and it satisfies the approximation condition; there is a $C > 0$ such that

$$\inf_{V \in V_h} (\|v - V\| + \Delta x \|v_x - V_x\|) \leq C \Delta x^2 \|v_x\|,$$

for all $v \in H^1(0,1)$. We do not use f directly in the discretization in order to construct a scheme that preserves the Lyapunov functional. Instead, define for v and w real numbers,

$$\tilde{f}(v,w) := \frac{v^3 + v^2 w + v w^2 + w^3}{4} - \frac{v+w}{2}.$$

Note that if $F(v) := \frac{1}{4}(v^2-1)^2$, so $F'(v) = f(v)$, then for all v, w,

$$F(v) - F(w) = \tilde{f}(v,w)(v-w).$$

The scheme generates a sequence $\{U_n\}$ of functions in V_h as follows. For an indexed function V_n, let $\Delta V_n := V_n - V_{n-1}$ and $V_{n,x} := (V_n)_x$. Set

$$U_0 := \pi_h u(x,0),$$

where π_h denotes the interpolation operator into V_h, and for $n > 0$, let U_n solve

$$\left(\frac{\Delta U_n}{\Delta t_n}, V\right) + \epsilon^2(U_{n,x} + U_{n-1,x}, V_x) + (\tilde{f}(U_n, U_{n-1}), V) = 0, \tag{2.2}$$

for all $V \in V_h$.

Before turning to existence and convergence, we explain our interest in this particular scheme with the following proposition which shows that the approximation has the same Lyapunov functional as the solution.

Proposition 2.1. *For $N \geq 1$,*

$$\frac{1}{\epsilon}\sum_{n=1}^{N}\int_0^1\left(\frac{\Delta U_n}{\Delta t_n}\right)^2 dx\Delta t_n = E_\epsilon[U_0] - E_\epsilon[U_N]. \tag{2.3}$$

Proof. In (2.2), choose $V = \Delta U_n$ to get

$$\int_0^1\left(\frac{\Delta U_n}{\Delta t_n}\right)^2 dx\Delta t_n + \frac{\epsilon^2}{2}\int_0^1 (U_{n,x} + U_{n-1,x})(U_{n,x} - U_{n-1,x})dx$$
$$= -\int_0^1 \tilde{f}(U_n, U_{n-1})(U_n - U_{n-1})dx,$$

or

$$\int_0^1\left(\frac{\Delta U_n}{\Delta t_n}\right)^2 dx\Delta t_n + \frac{\epsilon^2}{2}\int_0^1 \Delta|U_{n,x}|^2 dx = -\int_0^1 \Delta F(U_n)dx.$$

Summation over n gives

$$\sum_{n=1}^{N}\int_0^1\left(\frac{\Delta U_n}{\Delta t_n}\right)^2 dx\Delta t_n + \frac{\epsilon^2}{2}\int_0^1 |U_{N,x}|^2 dx - \frac{\epsilon^2}{2}\int_0^1 |U_{0,x}|^2 dx$$
$$= -\int_0^1 F(U_N)dx + \int_0^1 F(U_0)dx.$$

The result follows. □

Corollary. *There is a $C = C(E_\epsilon[U_0], \epsilon)$ such that*

$$||U_n||_{L^\infty(0,1)} \leq C,$$

for all $n \geq 0$.

Proof. (2.3) implies that $E_\epsilon[U_n] \leq E_\epsilon[U_0]$ for any $n \geq 0$, and in particular that

$$\frac{\epsilon}{2}||U_{n,x}||^2 \leq E_\epsilon[U_0]$$

and

$$\frac{1}{4}||U_n^2 - 1||^2 \leq E_\epsilon[U_0].$$

However, $||U_n||^2 \leq 1 + ||U_n^2 - 1||$, so an appeal to the Sobolev inequality yields a constant $C > 0$ such that

$$||U_n||_{L^\infty(0,1)} \leq C||U_n||_{H^1(0,1)} \leq C\big(1 + 2E_\epsilon[U_0]^{1/2} + \frac{2}{\epsilon}E_\epsilon[U_0]\big). \quad \square$$

Next, we address existence and uniqueness. The following is proved in §4.

Theorem 2.2. *For $\Delta t = \Delta t(\epsilon)$ sufficiently small, there is a unique sequence of solutions of (2.2).*

Finally, we prove the following convergence result in §4.

Theorem 2.3. *There is a constant $C > 0$ such that for all u with u and u_t in $H^r(0,1)$ for $r = 2$ or 3,*

$$\begin{aligned}||U_N - u(\cdot,t_N)||^2 \le C||\pi_h u(\cdot,0) - u(\cdot,0)||^2 + C\Delta x^{2r}||u(\cdot,t_N)||^2_{H^r(0,1)} \\ + Ce^{Ct_N}\sum_{n=1}^{N}\Bigg\{\Delta x^{2r}\Bigg(||u||^2_{L^\infty((t_{n-1},t_n);H^r(0,1))} \\ +||u_t||^2_{L^\infty((t_{n-1},t_n);H^r(0,1))}\Bigg) \\ + \Delta t_n^2\Bigg(||u_t||^2_{L^\infty((t_{n-1},t_n);L^2(0,1))} \\ + ||u_{tt}||^2_{L^\infty((t_{n-1},t_n);L^2(0,1))} \\ +||u_{xt}||^2_{L^\infty((t_{n-1},t_n);L^2(0,1))}\Bigg)\Bigg\}\Delta t_n.\end{aligned}$$

§3. The long time behavior of the approximation

We analyze the behavior of U by adapting the arguments of Bronsard and Kohn [3]. Recall that the minimum energy E_ϵ of a sharp transition from -1 to 1 is $\varepsilon_0 = \sqrt{2}/3$. The piecewise constant function $\mathcal{U}$ has Z transitions between -1 and 1 and

$$E_\epsilon[\mathcal{U}] = Z\varepsilon_0.$$

Bronsard and Kohn showed that if the initial data for (1.1) is close to $\mathcal{U}$ in a precise sense, then the solution remains close to $\mathcal{U}$ over a long period of time. We show the same holds true of the approximation given by (2.2).

We begin by quoting the following result ([3], proposition 2.1) which says that an $H^1(0,1)$ function that is close to $\mathcal{U}$ in the $L^1(0,1)$ norm and that makes the Z transitions with "minimal waste" has energy close to the minimum value $Z\varepsilon_0$ for Z transitions. We assume that $\epsilon < 1$ in the remaining portion of the paper.

Proposition 3.1. *Let l be a positive integer. There exist constants $\delta_l > 0$ and $C > 0$ such that; if $w \in H^1(0,1)$ satisfies*

$$||w - \mathcal{U}||_{L^1(0,1)} \le \delta_l$$

and

$$E_\epsilon[w] \le Z\varepsilon_0 + \epsilon^l,$$

then

$$E_\epsilon[w] \ge Z\varepsilon_0 - C\epsilon^l/\delta_l^l.$$

We assume henceforth that $u(x,0)$ satisfies these hypotheses, however since the initial data for U_n is $U_0 = \pi_h u(x,0)$, we require the following lemma in order to apply the proposition to U_n.

Lemma 3.2. *Suppose that $w \in H^2(0,1)$ satisfies*

$$\|w - \mathcal{U}\|_{L^1(0,1)} \le \phi\delta$$

and

$$E_\epsilon[w] \le Z\varepsilon_0 + \phi\epsilon^l,$$

for some $\delta > 0$, l a positive integer, and $0 < \phi < 1$. Then, for Δx sufficiently small,

$$\|\pi_h w - \mathcal{U}\|_{L^1(0,1)} \le \delta \qquad (\Delta x \text{ depends on } \delta \text{ and } \phi) \tag{3.1}$$

and

$$E_\epsilon[\pi_h w] \le Z\varepsilon_0 + \epsilon^l \qquad (\Delta x \text{ depends on } \epsilon \text{ and } \phi). \tag{3.2}$$

This result is proved in §5.

Remark 3.1. We can decrease the changes made in passing from $u(x,0)$ to $\pi_h u(x,0)$ by taking ϕ closer to 1, but this requires a finer mesh in order for (3.1) and (3.2) to hold.

Now, we obtain an upper bound on the $L^2((0,t)\times(0,1))$ norm of $\Delta U_n/\Delta t_n$ for a large time t, provided the initial data is close to $\mathcal{U}$. The proof rests on showing that U_N satisfies the hypotheses of proposition 3.1 for some large N and then using the resulting lower bound on $E_\epsilon[U_N]$ in (2.3).

Proposition 3.3. *Assume that*

$$\mathcal{U}(x) = \lim_{\epsilon\to 0} u(x,0) \text{ in } L^1(0,1) \tag{3.3}$$

and that

$$E_\epsilon[u(x,0)] \le Z\varepsilon_0 + \phi\epsilon^l, \tag{3.4}$$

for some $0 < \phi < 1$. There are constants C_1 and C_2 depending on $\mathcal{U}$ and l and independent of ϵ, Δx, and Δt, such that for all sufficiently small ϵ, there are constants $\Delta x(\epsilon,\phi,l)$, and $\Delta t(\epsilon, \underline{\Delta x}^{-1}, \phi, l)$ such that all approximations computed with $\Delta x \le \Delta x(\epsilon,\phi,l)$ and $\Delta t \le \Delta t(\epsilon,\underline{\Delta x}^{-1},\phi,l)$ satisfy

$$\sum_{n=1}^{N} \int_0^1 \left(\frac{\Delta U_n}{\Delta t_n}\right)^2 dx\Delta t_n \le C_2\epsilon^{l+1}, \tag{3.5}$$

for some integer N satisfying

$$t_N \ge C_1\epsilon^{-(l+1)}.$$

This result is proved in §5.

Next, we turn the bound (3.5) into estimates on the rate at which the profile of U_n changes. The simplest result limits the change in the $L^1(0,1)$ norm over the interval $\left[0, C_1\epsilon^{-l}\right]$.

Theorem 3.4. *Assume that (3.3) and (3.4) hold for some* $0 < \phi < 1$. *There is a constant* $C = C(C_1, C_2)$ *that is independent of* ϵ, Δx, *and* Δt *such that for all sufficiently small* ϵ, *there are constants* $\Delta x(\epsilon, \phi, l)$, *and* $\Delta t(\epsilon, \underline{\Delta x}^{-1}, \phi, l)$ *such that all approximations computed with* $\Delta x \le \Delta x(\epsilon, \phi, l)$ *and* $\Delta t \le \Delta t(\epsilon, \underline{\Delta x}^{-1}, \phi, l)$ *satisfy*

$$\sup_{0 \le n \le N} \int_0^1 |U_n - U_0| dx \le C\epsilon^{1/2},$$

for all integers N *with* $t_N \le C_1 \epsilon^{-l}$.

Corollary. *If* δ_l *in proposition 3.1 is chosen so that*

$$\delta_l \le C\epsilon^{1/2},$$

then

$$\sup_{0 \le n \le N} \int_0^1 |U_n - \mathcal{U}| dx \le 2C\epsilon^{1/2},$$

for all integers N *with* $t_N \le C_1 \epsilon^{-l}$.

Finally, we conclude with more specific information on the rate of motion of positions of the zeroes of U_n. This requires an additional assumption

3.6a. $u(x, 0)$ crosses 0 transversely at exactly Z distinct points,

and

3.6b. the same is true of U_n for all $n \ge 0$ until the first time that two zeroes meet or a zero meets the boundary.

Note that the analog of (3.6b) for the true solution can be proved to hold, see [2]. The extension of the results in [2] to numerical approximations seems technically difficult. Arguing as in the proof of proposition 3.3 (see §5), we can prove that for any $\delta > 0$, there are $\Delta x(\epsilon, \delta)$ and $\Delta t(\epsilon, \underline{\Delta x}^{-1}, \delta)$ sufficiently small, such that the change in the position of a zero from t_{n-1} to t_n is bounded by δ for all n in any approximation computed with $\Delta x \le \Delta x(\epsilon, \delta)$ and $\Delta t \le \Delta t(\epsilon, \underline{\Delta x}^{-1}, \delta)$. Moreover, by the short-time error bound, we know that (3.6b) holds for some positive n. Thus, if (3.6b) fails to hold for some $n > 0$, then at that point, the approximation has begun to act quite differently than the true solution. In this case, perhaps it is no longer meaningful to look at the motion of its zeroes.

In the following result, we let

$$z_{n,1} < \cdots < z_{n,Z}$$

denote the Z zeroes of U_n and given $\delta > 0$,

$$N(\delta) := \inf_n \{ |z_{n,i} - z_{0,i}| > \delta, \text{ for some } i \}.$$

Theorem 3.5. *Assume that $u(x,0)$ satisfies (3.3), (3.4), and (3.6a), and $\{U_n\}$ satisfies (3.6b). There is a constant $C > 0$ such that if $\delta > 0$ is sufficiently small, then for all sufficiently small ϵ, there are constants $\Delta x(\epsilon, \phi, l)$, and $\Delta t(\epsilon, \underline{\Delta x}^{-1}, \phi, l)$ such that all approximations computed with $\Delta x \le \Delta x(\epsilon, \phi, l)$ and $\Delta t \le \Delta t(\epsilon, \underline{\Delta x}^{-1}, \phi, l)$ satisfy*

$$t_{N(\delta)} \ge C\delta^2\epsilon^{-(l+1)}.$$

This result implies that as long as the approximation maintains its "smooth" transition profile, its zeroes barely change position over a time interval of length $O(\epsilon^{-(l+1)})$.

§4. Proofs of results in §2

Proof of theorem 2.2. We define a map $\Phi_{\tilde{U},n} : V_h \to V_h$ for $\tilde{U} \in V_h$ and $1 \le n$ by

$$U = \Phi_{\tilde{U}}(V) = \Phi_{\tilde{U},n}(V)$$

if

$$(4.1)\quad (U, W) + \frac{\Delta t_n}{2}\epsilon^2(U_x, W_x) = (\tilde{U}, W) - \Delta t_n \frac{\epsilon^2}{2}(\tilde{U}_x, W_x) - \Delta t_n(\tilde{f}(\tilde{U}, V), W),$$

for all $W \in V_h$. It is easy to see that $\Phi_{\tilde{U}}$ is well defined for Δt sufficiently small, and that given U_{n-1}, the approximation U_n exists if and only if $\Phi_{U_{n-1}}$ has a fixed point, namely

$$\Phi_{U_{n-1}}(U_n) = U_n.$$

Assume that $\|\tilde{U}\| \le r$ for some $r > 0$. We choose $W = U + \tilde{U}$ in (4.1) and obtain

$$\|U\|^2 + \frac{\Delta t_n}{2}\epsilon^2\|(U + \tilde{U})_x\|^2 = \|\tilde{U}\|^2 - \Delta t_n(\tilde{f}(\tilde{U}, V), U + \tilde{U}),$$

and if $\Delta t < 1$,

$$(4.2)\qquad \|U\|^2 \le 4\|\tilde{U}\|^2 + 2\Delta t_n\|\tilde{f}(\tilde{U}, V)\|^2.$$

Using standard inverse estimates that hold for functions in V_h, if $\|V\| \le 4r$, then

$$\|\tilde{f}(\tilde{U}, V)\| \le C\underline{\Delta x}^{-1}r^3,$$

for some $C > 0$. Using this in (4.2), we get

$$\|U\|^2 \le 16r^2$$

provided

$$C\frac{r^4\Delta t}{\underline{\Delta x}^2}$$

is sufficiently small. Thus, $\Phi_{\tilde{U}}$ maps the ball $\{V : \|V\| \le 4r\}$ into itself for Δt sufficiently small. Furthermore, if U_1 and U_2 are two images corresponding to V_1

and V_2 in $\{V : \|V\| \leq 4r\}$, then by subtracting the corresponding equations (4.1) and choosing $W = U_1 - U_2$, we get

$$\|U_1 - U_2\|^2 \leq -\Delta t_n(\tilde{f}(\tilde{U}, V_1) - \tilde{f}(\tilde{U}, V_2), U_1 - U_2).$$

We again use inverse estimates to conclude that

$$\|U_1 - U_2\|^2 \leq C\frac{r^4 \Delta t_n}{\Delta x^2}\|V_1 - V_2\|^2,$$

and hence that $\Phi_{\tilde{U}}$ is a contraction for Δt sufficiently small. The Banach fixed point theorem provides the result. □

Proof of theorem 2.3. In the following we abuse notation to let $u(t_n) := u(\cdot, t_n)$ and $t_{n-1/2} := t_{n-1} + \Delta t_n/2$. As usual, we introduce the elliptic projection $P_1 : H^1(0,1) \to V_h$ and split the error

$$\begin{aligned} U_n - u(t_n) &= (U_n - P_1 u(t_n)) + (P_1 u(t_n) - u(t_n)) \\ &=: \theta_n + \rho_n. \end{aligned}$$

We obtain an equation for the unknown part of the error θ_n by subtracting the equation in (2.1) evaluated at $t_{n-1/2}$ from (2.2) and doing some rearrangement;

$$\begin{aligned} &\left(\frac{\Delta\theta_n}{\Delta t_n}, W\right) + \frac{\epsilon^2}{2}((\theta_n + \theta_{n-1})_x, W_x) \\ &= -(\tilde{f}(U_{n-1}, U_n) - f(u(t_{n-1/2})), W) + \left(u_t(t_{n-1/2}) - \frac{\Delta u(t_n)}{\Delta t_n}, W\right) \\ &\quad + \left(\frac{\Delta(u(t_n) - P_1 u(t_n))}{\Delta t_n}, W\right) + \left(u_x(t_{n-1/2}) - \frac{u_x(t_n) + u_x(t_{n-1})}{2}, W\right). \end{aligned}$$

We choose $W = (\theta_n + \theta_{n-1})/2$ and estimate,

$$\begin{aligned} &\frac{\Delta\|\theta_n\|^2}{\Delta t_n} + \frac{\epsilon^2}{2}\|(\theta_n + \theta_{n-1})_x\|^2 \\ &\qquad \leq \frac{1}{2}\|\tilde{f}(U_{n-1}, U_n) - f(u(t_{n-1/2}))\|^2 + \frac{1}{2}\left\|u_t(t_{n-1/2}) - \frac{\Delta u(t_n)}{\Delta t_n}\right\|^2 \\ &\qquad\quad + \frac{1}{2}\left\|\frac{\Delta\rho_n}{\Delta t_n}\right\|^2 + \frac{1}{2}\left\|u_x(t_{n-1/2}) - \frac{u_x(t_n) + u_x(t_{n-1})}{2}\right\|^2 \\ &\qquad\quad + C\|\theta_n\|^2 + C\|\theta_{n-1}\|^2, \end{aligned} \tag{4.3}$$

for $C > 0$. We need to estimate the first term on the right before applying a Gronwall inequality. f is not globally Lipschitz continuous, which can cause difficulty. However, the existence of a Lyapunov functional for both U and u means that these functions are pointwise bounded uniformly in $t > 0$. (See the corollary to proposition 2.1.) The constant C below depends on the common bound, i.e. on $E_\epsilon[\pi_h u(x,0)]$ and $E_\epsilon[u(x,0)]$. To estimate the first term on the right, we note that

$$\begin{aligned}
&\|\tilde{f}(U_n,U_{n-1}) - f(u(t_{n-1/2}))\|^2 \\
&\quad \le \|\tilde{f}(U_n,U_{n-1}) - \tilde{f}(u_n,u_{n-1})\|^2 + \|\tilde{f}(u_n,u_{n-1}) - f(u(t_{n-1/2}))\|^2 \\
&\quad \le C\Big(\|U_n - u(t_n)\|^2 + \|U_{n-1} - u(t_{n-1})\|^2 + \|u(t_n) - u(t_{n-1/2})\|^2 \\
&\qquad\qquad + \|u(t_{n-1}) - u(t_{n-1/2})\|^2 + \|u(t_n) - u(t_{n-1})\|^2 \Big).
\end{aligned}$$

Using this in (4.3), we get

$$\frac{\Delta\|\theta_n\|^2}{\Delta t_n} + \frac{\epsilon^2}{2}\|(\theta_n + \theta_{n-1})_x\|^2 \le E_{n,n-1} + C\|\theta_n\|^2 + C\|\theta_{n-1}\|^2,$$

where

$$\begin{aligned}
E_{n,n-1} := C\Big\{ &\|\rho_n\|^2 + \|\rho_{n-1}\|^2 + \|u(t_n) - u(t_{n-1/2})\|^2 + \|u(t_{n-1}) - u(t_{n-1/2})\|^2 \\
&+ \|u(t_n) - u(t_{n-1})\|^2 + \left\| u_t(t_{n-1/2}) - \frac{\Delta u(t_n)}{\Delta t_n} \right\|^2 \\
&+ \left\| \frac{\Delta\rho_n}{\Delta t_n} \right\|^2 + \left\| u_x(t_{n-1/2}) - \frac{u_x(t_n) - u_x(t_{n-1})}{2} \right\|^2 \Big\}.
\end{aligned}$$

A discrete Gronwall argument yields

$$\|\theta_n\|^2 \le \|\theta_0\|^2 + Ce^{Ct_n}\sum_{j=1}^{n} E_{j,j-1}\Delta t_j.$$

Straightforward estimates on $E_{j,j-1}$, under the regularity assumptions of the theorem, yield the result. □

§5. Proofs of results in §3

Proof of lemma 3.2. By standard results, there is a constant $C > 0$ with

$$\|w - \pi_h w\|_{L^1(0,1)} \le C\Delta x^2 |w|_{H^2(0,1)}.$$

Hence,

$$\|\pi_h w - \mathcal{U}\|_{L^1(0,1)} \le \|\pi_h w - w\|_{L^1(0,1)} + \|w - \mathcal{U}\|_{L^1(0,1)} \le \delta,$$

provided

$$C\Delta x^2 |w|_{H^2(0,1)} \le (1-\phi)\delta.$$

For the proof of (3.2), set $W := \pi_h w$ and compute

$$E_\epsilon[W] = \frac{\epsilon}{2}\sum_{m=1}^{M+1}\int_{x_{m-1}}^{x_m}\left(\frac{W_m - W_{m-1}}{\Delta x_m}\right)^2 dx + \frac{1}{4\epsilon}\sum_{m=1}^{M+1}\int_{x_{m-1}}^{x_m}(W(x)^2 - 1)^2 dx.$$

For $x \in [x_{m-1}, x_m]$, because $w \in H^2(0,1)$, we can estimate

$$\left| w_x(x)^2 - \left(\frac{W_m - W_{m-1}}{\Delta x_m}\right)^2 \right| \leq 2\|w_x\|_{L^\infty(x_{m-1},x_m)} \cdot \int_{x_{m-1}}^{x_m} |w_{xx}|dx,$$

and therefore

$$\frac{\epsilon}{2}\left| \int_0^1 w_x^2 dx - \sum_{m=1}^{M+1} \int_{x_{m-1}}^{x_m} \left(\frac{W_m - W_{m-1}}{\Delta x_m}\right)^2 dx \right| \leq \epsilon \Delta x \|w_x\|_{L^\infty(0,1)} |w|_{H^2(0,1)}.$$

Using the identity $(a^2-1)^2 - (b^2-1)^2 = (a+b)(a-b)(a^2+b^2-2)$ and the bound $\|W\|_{L^\infty(0,1)} \leq \|w\|_{L^\infty(0,1)}$, we compute

$$|(w(x)^2-1)^2 - (W(x)^2-1)^2| \leq 4(\|w\|^2_{L^\infty(0,1)} + 1)\|w\|_{L^\infty(0,1)} \cdot |w(x) - W(x)|.$$

Hence,

$$\left| \int_0^1 (w(x)^2-1)^2 dx - \int_0^1 (W(x)^2-1)^2 dx \right| \\ \leq 4\Delta x^2 (\|w\|^2_{L^\infty(0,1)} + 1)\|w\|_{L^\infty(0,1)} |w|_{H^2(0,1)}.$$

Therefore, there is a constant $C > 0$ such that

$$\begin{aligned} E_\epsilon[W] &\leq |E_\epsilon[W] - E_\epsilon[w]| + E_\epsilon[w] \\ &\leq Z\varepsilon_0 + \phi\epsilon^l + C\epsilon\Delta x\|w\|^2_{H^2(0,1)} + \frac{C\Delta x^2}{\epsilon}(\|w\|^4_{H^2(0,1)} + \|w\|^2_{H^2(0,1)}) \\ &\leq Z\varepsilon_0 + \epsilon^l, \end{aligned}$$

provided Δx is sufficiently small. □

Proof of proposition 3.3. Using (3.3) and lemma 3.2, we choose $\Delta x = \Delta x(\delta_l)$ so that

$$\|\pi_h u(x,0) - u(x,0)\|_{L^1(0,1)} \leq \frac{1}{2}\delta_l,$$

where δ_l is the constant used in proposition 3.1. We claim that if for some $N > 0$,

$$\sum_{n=1}^{N} \int_0^1 \left|\frac{\Delta U_n}{\Delta t_n}\right| dx \Delta t_n \leq \frac{1}{2}\delta_l, \tag{5.1}$$

then there is a $C_2 > 0$ such that

$$\sum_{n=1}^{N} \int_0^1 \left(\frac{\Delta U_n}{\Delta t_n}\right)^2 dx \Delta t_n \leq C_2 \epsilon^{l+1}, \tag{5.2}$$

for all sufficiently small ϵ and $\Delta x(\epsilon, \delta_l)$. In this case,

$$\begin{aligned} \|\mathcal{U} - U_N\|_{L^1(0,1)} &\leq \|\mathcal{U} - \pi_h u(x,0)\|_{L^1(0,1)} + \|U_N - U_0\|_{L^1(0,1)} \\ &\leq \frac{1}{2}\delta_l + \sum_{n=1}^{N} \int_0^1 \left|\frac{\Delta U_n}{\Delta t_n}\right| dx \Delta t_n \\ &\leq \delta_l. \end{aligned}$$

Furthermore, by proposition 2.1 and lemma 3.2,

$$E_\epsilon[U_N] \le E_\epsilon[U_0] \le Z\varepsilon_0 + \epsilon^l, \tag{5.3}$$

for $\Delta x(\delta_l, \epsilon)$ sufficiently small. Proposition 3.1 implies that there is a $C_l > 0$ with

$$E_\epsilon[U_N] \ge Z\varepsilon_0 - C_l\epsilon^l. \tag{5.4}$$

Using (5.3) and (5.4) in (2.3) gives

$$\epsilon^{-1}\sum_{n=1}^{N}\int_0^1 \left(\frac{\Delta U_n}{\Delta t_n}\right)^2 dx\Delta t_n \le (C_l+1)\epsilon^l,$$

which proves the claim.

We need to show that (5.1) holds for some $C_1 > 0$ and N with $t_N \ge C_1\epsilon^{-(l+1)}$. In order to do this, we require a uniform bound on the size of the change $\|U_n - U_{n-1}\|_{L^1(0,1)}$ for all $n \ge 1$. We claim that for any $\delta > 0$ there is a $\Delta t(E_\epsilon[U_0], \underline{\Delta x}^{-1}, \epsilon, \delta)$ sufficiently small such that

$$\|U_n - U_{n-1}\|_{L^1(0,1)} \le \delta,$$

for all $n \ge 1$. As in the proof of proposition 2.1, we choose $V = \Delta U_n$ in (2.2) and then estimate to get

$$\|U_n - U_{n-1}\|^2 \le \left(4\epsilon^2\|U_{n,x}\|^2 + 4\epsilon^2\|U_{n-1,x}\|^2 + 2\|\tilde{f}(U_n, U_{n-1})\|^2\right)\Delta t_n. \tag{5.5}$$

By the proofs of proposition 2.1 and its corollary, we know that there is a constant $C(\epsilon, E_\epsilon[u(x,0)], \underline{\Delta x}^{-1})$ such that for all $n \ge 0$,

$$\max\{\|U_n\|, \|U_{n-1}\|, \|U_{n,x}\|, \|U_{n-1,x}\|\} \le C(\epsilon, E_\epsilon[u(x,0)], \underline{\Delta x}^{-1}).$$

Using this information in (5.5) together with an inverse estimate yields

$$\|U_n - U_{n-1}\|^2 \le \Delta t_n(\epsilon^2 + \underline{\Delta x}^{-2})C(\epsilon, E_\epsilon[u(x,0)], \underline{\Delta x}^{-1})$$

and

$$\|U_n - U_{n-1}\|_{L^1(0,1)} \le \Delta t_n^{1/2} C(\epsilon, E_\epsilon[u(x,0)], \underline{\Delta x}^{-1}) \le \delta,$$

for Δt sufficiently small.

Returning to the proof that (5.1) holds for large t, we assume that Δt is chosen so that (5.4) holds with $\delta = \frac{1}{4}\delta_l$ for all $n \ge 0$. If

$$\sum_{n=1}^{\infty}\int_0^1 \left|\frac{\Delta U_n}{\Delta t_n}\right| dx\Delta t_n \le \frac{1}{2}\delta_l,$$

we are done. Otherwise, let N be the first integer such that

$$\sum_{n=1}^{N}\int_0^1 \left|\frac{\Delta U_n}{\Delta t_n}\right| dx\Delta t_n \le \frac{1}{2}\delta_l$$

but

$$\sum_{n=1}^{N+1} \int_0^1 \left| \frac{\Delta U_n}{\Delta t_n} \right| dx \Delta t_n > \frac{1}{2}\delta_l.$$

By the assumption on Δt, we have

$$\begin{aligned} \frac{1}{4}\delta_l &\le \sum_{n=1}^{N} \int_0^1 \left| \frac{\Delta U_n}{\Delta t_n} \right| dx \Delta t_n \\ &\le t_N^{1/2} \Big(\sum_{n=1}^{N} \int_0^1 \Big(\frac{\Delta U_n}{\Delta t_n} \Big)^2 dx \Delta t_n \Big)^{1/2} \qquad (5.6) \\ &\le C_2 t_N^{1/2} \epsilon^{(L+1)/2}, \end{aligned}$$

where we also use (5.2). We conclude that

$$t_N > \frac{\delta_l^2}{16C_2^2} \epsilon^{-(l+1)}. \quad \square$$

Remark 5.1. The existence of a Lyapunov functional for $\{U_n\}$ allows us to bound $\|U_n - U_{n-1}\|_{L^1(0,1)}$ uniformly in n and this is key to the above argument. Otherwise, we would not have information on the size of the lower bound in (5.6).

Proof of theorem 3.4. By proposition 3.3, there are constants $C_1, C_2 > 0$ such that for ϵ, $\Delta x(\epsilon, \phi, l)$, and $\Delta t(\epsilon, \phi, l, \underline{\Delta x}^{-1})$ sufficiently small

$$\sum_{n=1}^{N} \int_0^1 \Big(\frac{\Delta U_n}{\Delta t_n} \Big)^2 dx \Delta t_n \le C_2 \epsilon^{(l+1)},$$

for all N with $t_N \ge C_1 \epsilon^{-(l+1)}$. Thus, for all integers $\tilde{N}$ with

$$t_{\tilde{N}} \le C_1 \epsilon^{-l} \le t_N,$$

we have

$$\sum_{n=1}^{\tilde{N}} \int_0^1 \left| \frac{\Delta U_n}{\Delta t_n} \right| dx \Delta t_n \le t_{\tilde{N}}^{1/2} C_2 \epsilon^{(l+1)} \le C \epsilon^{1/2}.$$

Since

$$\sup_{0 \le n \le \tilde{N}} \int_0^1 |U_n(x) - U_0(x)| dx \le \sum_{n=1}^{\tilde{N}} \int_0^1 \left| \frac{\Delta U_n}{\Delta t_n} \right| dx \Delta t_n,$$

the conclusion follows. $\square$

Proof of theorem 3.5. If $N(\delta) = \infty$, there is nothing to prove. Assume that $N(\delta) < \infty$, so

$$|z_{N(\delta),i} - z_{0,i}| \ge \delta,$$

for some i. We claim that for sufficiently small $\epsilon > 0$,

$$\int_0^1 |U_{N(\delta)} - U_0| dx \ge C\delta, \qquad (5.7)$$

for some constant C independent of δ. We use the following result from [3] (lemma 4.2),

Lemma 5.1. *Suppose the graph of an $H^1(0,1)$ function w crosses 0 transversely at exactly Z points $z_1 < \cdots < z_Z$. Assume that $E_\epsilon[w] \le Z\varepsilon_0 + \epsilon$. Then for $\tilde{\delta} > 0$ sufficiently small and all $\epsilon \le \tilde{\epsilon}(\tilde{\delta})$, there exist Z intervals $I_i \ni z_i \subset [0,1]$ with $|I_i| \le 2\tilde{\delta}$ such that $(w(x)2-1)^2 \le \tilde{\delta}$ for $x \notin \cup_i I_i$.*

We apply this lemma using first $w = U_{N(\delta)}$ and then $w = U_0$, taking $\tilde{\delta} \ll \delta$, and choose ϵ and Δx sufficiently small so that (5.7) holds. We estimate from (5.7),

$$C\delta \le \left(\sum_{n=1}^{N(\delta)} \int_0^1 \left(\frac{\Delta U_n}{\Delta t_n}\right)^2 dx \Delta t_n\right)^{1/2} t_{N(\delta)}^{1/2}.$$

By possibly decreasing Δx and taking Δt sufficiently small, we satisfy the hypotheses of proposition 3.3. Now, if $t_{N(\delta)} \ge C_1\epsilon^{(l+1)}$, then the result holds automatically. Otherwise, we bound the integral above using (3.5) to find that

$$C\delta \le C\epsilon^{(l+1)/2} \cdot t_{N(\delta)}^{1/2},$$

and the result follows. . □

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