

A Posteriori Bounds in the Numerical Solution of Mildly Nonlinear Parabolic Equations*

By Alfred Carasso

Abstract. We derive a posteriori bounds for $(V - \hat{V})$ and its difference quotient $(V - \hat{V})_x$, where V and \hat{V} are, respectively, the exact and computed solution of a difference approximation to a mildly nonlinear parabolic initial boundary problem, with a known steady-state solution. It is assumed that the computation is over a long interval of time. The estimates are valid for a class of difference approximations, which includes the Crank-Nicolson method, and are of the same magnitude for both $(V - \hat{V})$ and $(V - \hat{V})_x$.

1. Introduction. Let \mathcal{R} be the strip $\{(x, t) \mid 0 < x < 1, t > 0\}$ in the (x, t) plane and consider the mixed problem

$$\begin{aligned}
 (1.1) \quad & u_t = [a(x, t)u_x]_x + b(x, t)u_x - f(x, t, u), \quad (x, t) \in \mathcal{R}, \\
 & u(x, 0) = \chi(x), \quad 0 \leq x \leq 1, \\
 & u(0, t) = \varphi_1(t), \quad u(1, t) = \varphi_2(t), \quad t > 0.
 \end{aligned}$$

We assume that $a(x, t)$, $b(x, t)$ are "smooth" bounded functions on $\bar{\mathcal{R}}$, with $a(x, t) \geq a_0 > 0$, and that $f(x, t, w)$ is, at least once, continuously differentiable on $\mathcal{R}X\{-\infty < w < +\infty\}$ with $\partial f/\partial w \geq 0$. Moreover, $\partial f/\partial w$ is to remain bounded if w stays bounded. The coefficients, data, and f are assumed such as to assure the existence and uniqueness of a solution $u(x, t)$, four times boundedly differentiable in $\bar{\mathcal{R}}$, and converging to a steady state value $u^\infty(x)$, as $t \rightarrow \infty$. We assume $u^\infty(x)$ is known and that, by means of asymptotic formulae and the like, one can estimate $\|u(\cdot, t) - u^\infty\|_2$ as a function of t , for t sufficiently large. The analytical theory for such problems is discussed in Friedman [5].

Several finite-difference methods for the numerical computation of (1.1) have been shown to converge; see for example [4], [6], [8], [10], [3] and their references, and especially [9] for the linear case.

Because of round-off error, and the fact that one may need to use iterative methods at each time step to solve the nonlinear difference equations, only an approximation \hat{V}^n to the exact solution V^n of the difference equations can be computed in general. In [3], a "boundary-value" method for (1.1) was analyzed. This method yields an a posteriori estimate for $V - \hat{V}$ by simply computing residuals. In the present note we make use of some of the results in [2] and [3] to derive such an estimate for a class of stable "marching" procedures for (1.1). Unlike the situation in [3], however, the estimate will involve bounds on the derivatives of u . It is interesting that the estimate is of the same magnitude for both $(V - \hat{V})$ and its difference quotient $(V - \hat{V})_x$.

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2. Notation. Let \mathcal{R}_T be the rectangle $\{(x, t) \mid 0 < x < 1, 0 < t < T\}$ and let M and N be positive integers. Let $\Delta x = 1/(M + 1)$, $\Delta t = T/(N + 1)$, and introduce a mesh over $\overline{\mathcal{R}_T}$ by means of the lines $x = k\Delta x$, $k = 0, 1, \dots, M + 1$, $t = n\Delta t$, $n = 0, 1, \dots, N + 1$. Let v_k^n denote $v(k\Delta x, n\Delta t)$. Define V^n to be the M -component vector

$$(2.1) \quad V^n = \{v_1^n, v_2^n, \dots, v_M^n\}^T$$

and let V be the "block" vector of MN components

$$(2.2) \quad V = \{V^1, V^2, \dots, V^N\}^T.$$

Although we will be dealing with real-valued mesh functions, it is convenient to define scalar products and norms for complex vectors. For any two M vectors V^n, W^n let

$$(2.3) \quad \langle V^n, W^n \rangle = \Delta x \sum_{k=1}^M v_k^n \bar{w}_k^n$$

and let

$$(2.4) \quad \|V^n\|_2^2 = \langle V^n, V^n \rangle.$$

Let

$$(2.5) \quad \|V_x^n\|_2^2 = \Delta x \sum_{k=0}^M \frac{|v_{k+1}^n - v_k^n|^2}{\Delta x^2}$$

where v_0^n, v_{M+1}^n are defined to be zero.

For block vectors V, W define

$$(2.6) \quad (V, W) = \Delta t \sum_{n=1}^N \langle V^n, W^n \rangle$$

and let

$$(2.7) \quad \|V\|_2^2 = (V, V),$$

$$(2.8) \quad \|V_x\|_2^2 = \Delta t \sum_{n=1}^N \|V_x^n\|_2^2.$$

Finally, for a square matrix A , define $\|A\|$ in terms of vector norms, i.e., as

$$(2.9) \quad \|A\| = \text{Sup}_{\|X\|=1} \|AX\|,$$

the supremum being taken over all complex vectors.

3. Difference Approximations to (1.1). Let U^n be the M -vector consisting of the solution to (1.1) evaluated at the interior mesh points of the line $t = n\Delta t$ and let V^n be the corresponding exact solution of the difference equations used to approximate (1.1). Define $E^n = V^n - U^n$. We will consider the class of marching schemes which lead to a priori estimates of the form

$$(3.1) \quad \{\|E^n\|_2^2 + \|E_x^n\|_2^2\}^{1/2} \leq K(T)(\Delta t^{r+1} + \Delta x^{s+1}), \quad n\Delta t \leq T,$$

where r and s are positive integers and $K(T)$ is known. An example of a difference

scheme for (1.1) satisfying (3.1) with $r = s = 1$, is the Crank-Nicolson version analyzed in [8]. In general $K(T)$ will involve bounds on a, b, f, u and their derivatives, as well as a growth factor. The reason for the latter is that, even if the exact solution to (1.1) decays asymptotically to a steady state, the exact solution of a stable, consistent, difference approximation may grow exponentially as $n\Delta t \rightarrow \infty, \Delta t$ fixed. Hence, we cannot expect $K(T)$ to remain bounded as $T \rightarrow \infty$, in general. We remark, however, that in [7], Kreiss and Widlund have shown how to construct schemes (for linear time-dependent problems with periodic boundary conditions) which preserve the asymptotic behavior of $u(x, t)$ provided $|b|\Delta t/\Delta x < 1$. In the following we will derive bounds for $\|\hat{V} - V\|_2$ and $\|\hat{V}_x - V_x\|_2$ for computations of (1.1) up to some "large" but fixed time T . These bounds will depend on $K(T)$.

We begin by deriving new finite-difference equations for the exact solution $\{V^n\}$ of a difference scheme used to approximate (1.1). Since $V^n = U^n + E^n$, we have

$$\begin{aligned} (3.2) \quad \frac{v_k^{n+1} - v_k^{n-1}}{2\Delta t} &= \frac{u_k^{n+1} - u_k^{n-1}}{2\Delta t} + \frac{\epsilon_k^{n+1} - \epsilon_k^{n-1}}{2\Delta t} \\ &= \left(\frac{\partial u}{\partial t}\right)_k^n + \frac{\epsilon_k^{n+1} - \epsilon_k^{n-1}}{2\Delta t} + \frac{\Delta t^2}{6} \overline{(u_{ttt})_k}, \end{aligned}$$

where " $\bar{\psi}$ " represents a mean value of ψ called for by Taylor's theorem. From (1.1) we have

$$\begin{aligned} (3.3) \quad \left(\frac{\partial u}{\partial t}\right)_k^n + \frac{\Delta t^2}{6} \overline{(u_{ttt})_k} &= \frac{a_{k+1/2}^n(u_{k+1}^n - u_k^n) - a_{k-1/2}^n(u_k^n - u_{k-1}^n)}{\Delta x^2} \\ &\quad + b_k^n \frac{(u_{k+1}^n - u_{k-1}^n)}{2\Delta x} - f(k\Delta x, n\Delta t, u_k^n) + \tau_k^n, \end{aligned}$$

where

$$\begin{aligned} (3.4) \quad \tau_k^n &= \frac{\Delta t^2}{6} \overline{(u_{ttt})_k} \\ &\quad - \Delta x^2 \left\{ \frac{(u_x)_k^n \overline{(a_{xxx})_k}}{3} + \frac{(u_{xx})_k^n \overline{(a_{xx})_k}}{2} + \frac{(u_{xxx})_k^n \overline{(a_x)_k}}{6} + \frac{\overline{(a^n u_{xxx})_k}}{12} + \overline{b_k^n (u_{xxxx})_k} \right\}. \end{aligned}$$

From (3.2) and (3.3) we have

$$\begin{aligned} (3.5) \quad \frac{(v_k^{n+1} - v_k^{n-1})}{2\Delta t} &= \frac{a_{k+1/2}^n(v_{k+1}^n - v_k^n) - a_{k-1/2}^n(v_k^n - v_{k-1}^n)}{\Delta x^2} \\ &\quad + \frac{b_k^n(v_{k+1}^n - v_{k-1}^n)}{2\Delta x} - f(k\Delta x, n\Delta t, u_k^n) \\ &\quad + \frac{\epsilon_k^{n+1} - \epsilon_k^{n-1}}{2\Delta t} - b_k^n \frac{(\epsilon_{k+1}^n - \epsilon_{k-1}^n)}{2\Delta x} \\ &\quad - \frac{\{a_{k+1/2}^n(\epsilon_{k+1}^n - \epsilon_k^n) - a_{k-1/2}^n(\epsilon_k^n - \epsilon_{k-1}^n)\}}{\Delta x^2} + \tau_k^n, \end{aligned}$$

$$k = 1, \dots, M, \quad n = 1, 2, \dots,$$

with the initial boundary data

$$(3.6) \quad \begin{aligned} v_k^0 &= \chi(k\Delta x), & k &= 1, \dots, M, \\ v_0^n &= \varphi_1(n\Delta t), & v_{M+1}^n &= \varphi_2(n\Delta t), & n &= 1, 2, \dots \end{aligned}$$

With $T = (N + 1)\Delta t$ we now consider the system formed by equations (3.5) for $n = 1, 2, \dots, N$. It is convenient to write this system in matrix-vector notation.

Let L^n and B^n be the tridiagonal $M \times M$ matrices defined by

$$(3.7) \quad L^n = \frac{1}{\Delta x^2} \begin{bmatrix} (a_{1+1/2}^n + a_{1/2}^n) & -a_{1+1/2}^n & \circ & & \\ -a_{1+1/2}^n & & \cdot & & \\ \cdot & & \cdot & & \\ \cdot & & & & -a_{M-1/2}^n \\ \circ & -a_{M-1/2}^n & (a_{M+1/2}^n + a_{M-1/2}^n) & & \end{bmatrix},$$

$$(3.8) \quad B^n = \frac{1}{2\Delta x} \begin{bmatrix} 0 & -b_1^n & \circ & & \\ b_2^n & \cdot & \cdot & & \\ \cdot & \cdot & \cdot & & \\ \circ & \cdot & b_M^n & 0 & -b_{M-1}^n \end{bmatrix}$$

and define the M -vectors τ^n , $F^n(U)$, and G^n by

$$(3.9) \quad \tau^n = \{\tau_1^n, \tau_2^n, \dots, \tau_M^n\}^T,$$

$$(3.10) \quad F^n(U) = \{f_1^n(u), f_2^n(u), \dots, f_M^n(u)\}^T,$$

where

$$f_k^n(u) \equiv f(k\Delta x, n\Delta t, u_k^n)$$

and

$$(3.11)$$

$$G^n = \frac{1}{\Delta x^2} \{(a_{1+1/2}^n - \frac{1}{2}\Delta x b_1^n)\varphi_1(n\Delta t), 0, 0, \dots, 0, (a_{M+1/2}^n + \frac{1}{2}\Delta x b_M^n)\varphi_2(n\Delta t)\}^T.$$

We may then write (3.5), (3.6) as

$$(3.12) \quad \begin{aligned} \frac{V^{n+1} - V^{n-1}}{2\Delta t} &= -L^n V^n - B^n V^n - F^n(U) + \tau^n + G^n \\ &+ \frac{E^{n+1} - E^{n-1}}{2\Delta t} + B^n E^n + L^n E^n, \quad n = 1, 2, \dots, N. \end{aligned}$$

Some further definitions will enable us to write (3.12) in "block" form. Define the $MN \times MN$ block tridiagonal matrix P by (with $\sigma = 1/2\Delta t$)

$$(3.13) \quad P = \begin{bmatrix} (L^1 + B^1) & \cdot & & \sigma I & \cdot & \circ \\ -\sigma I & \cdot & & & \cdot & \\ \cdot & \cdot & \cdot & & \cdot & \\ \circ & \cdot & -\sigma I & (L^N + B^N) & \cdot & \sigma I \end{bmatrix}.$$

For any real block vector ξ define the $M \times M$ diagonal matrix $C^n(\xi)$ by

$$(3.14) \quad C^n(\xi) = \begin{bmatrix} f_w(\Delta x, n\Delta t, \xi_1^n) & \circ \\ & \ddots \\ \circ & f_w(\Delta x, n\Delta t, \xi_M^n) \end{bmatrix}$$

and let $C(\xi)$ be the block matrix

$$(3.15) \quad C(\xi) = \begin{bmatrix} C^1(\xi) & \circ \\ & \ddots \\ \circ & C^N(\xi) \end{bmatrix}.$$

Finally, define the block vectors F , G^* , H , and τ by

$$(3.16) \quad F = \{F^1, F^2, \dots, F^N\}^T,$$

$$(3.17) \quad G^* = \left\{ G^1 + \frac{V^0}{2\Delta t}, G^2, \dots, G^N - \frac{V^{N+1}}{2\Delta t} \right\}^T,$$

$$(3.18) \quad H = \left\{ \frac{E^2 - E^0}{2\Delta t} + (L^1 + B^1)E^1, \dots, \frac{E^{N+1} - E^{N-1}}{2\Delta t} + (L^N + B^N)E^N \right\}^T,$$

$$(3.19) \quad \tau = \{\tau^1, \tau^2, \dots, \tau^N\}^T.$$

With this notation we have from (3.12)

$$(3.20) \quad PV = -F(U) + G^* + \tau + H.$$

LEMMA 1. Let D be a diagonal matrix of order MN with nonnegative real entries and let

$$(3.21) \quad Q = P + D.$$

Let $b(x, t)$ in (1.1) satisfy

$$(3.22) \quad \left| \frac{\partial b}{\partial x} \right| \leq b_1 < 2a_0\pi^2, \quad \forall (x, t) \in \bar{R}_T.$$

Fix $\epsilon > 0$ so that $a_0\pi^2 - b_1/2 - \epsilon \geq \omega > 0$. If $\Delta x \leq (12\epsilon/a_0\pi^4)^{1/2}$, Q^{-1} exists and

$$(3.23) \quad \sup_{x \text{ real}, \|X\|_2 \leq 1} \|Q^{-1}X\|_2 \leq \frac{1}{\omega}.$$

Moreover, if $QW = Z$, where Z is real we have

$$(3.24) \quad \|W_z\|_2 \leq \left(\frac{2\omega + b_1}{2a_0\omega^2} \right)^{1/2} \|Z\|_2.$$

Proof. See [3, Lemma 1].

Remark. If

$$D = \begin{bmatrix} \Lambda & & \circ \\ & \Lambda & \\ & & \ddots \\ \circ & & & \Lambda \end{bmatrix},$$

where Λ is a diagonal $M \times M$ matrix with nonnegative real entries, and if $a(x, t)$, $b(x, t)$ are independent of t , Q^{-1} exists and remains bounded for all sufficiently small Δx independently of hypothesis (3.22). This observation is relevant to the case where (1.1) is linear with time independent coefficients, i.e., $a = a(x)$, $b = b(x)$, and $f(x, t, u) = c(x)u + h(x, t)$ with $c(x) \geq 0$. See [1, Lemma 1] and [2, Lemma 4.2].

4. A Posteriori Bounds. For each $n = 1, 2, \dots, N + 1$, let \hat{V}^n be the computed solution at $t = n\Delta t$, of the difference equations used to approximate (1.1) and consider the block vector

$$(4.1) \quad \hat{V} = \{ \hat{V}^1, \hat{V}^2, \dots, \hat{V}^N \}^T.$$

Define \hat{G}^* to be the block vector obtained from G^* when V^{N+1} is replaced by \hat{V}^{N+1} .

Compute the block vector R given by

$$(4.2) \quad R = P\hat{V} + F(\hat{V}) - \hat{G}^*.$$

Subtracting (4.2) from (3.20) we have

$$(4.3) \quad \begin{aligned} P(V - \hat{V}) &= -F(U) + F(\hat{V}) + (G^* - \hat{G}^*) + \tau + H - R \\ &= -F(U) + F(V) + F(\hat{V}) - F(V) + (G^* - \hat{G}^*) + \tau + H - R \\ &= -C(\xi)(U - V) - C(\Psi)(V - \hat{V}) + (G^* - \hat{G}^*) + \tau + H - R, \end{aligned}$$

for some intermediate real block vectors ξ and Ψ on using the mean value theorem. Hence,

$$(4.4) \quad [P + C(\Psi)](V - \hat{V}) = \tau + H - R + (G^* - \hat{G}^*) - C(\xi)(U - V).$$

Since $f_v \geq 0$, $C(\Psi)$ is a diagonal matrix with nonnegative real entries. By Lemma 1, we may estimate $\|V - \hat{V}\|_2, \|V_x - \hat{V}_x\|_2$, provided we can estimate the terms other than R on the right-hand side of (4.4). We will make use of the a priori estimate (3.1).

Let a^*, b^* be upper bounds for $a(x, t)$ and $|b(x, t)|$, respectively, in $\bar{\mathcal{R}}_T$.

Since

$$(L^n E^n)_k = \frac{1}{\Delta x^2} a_{k-1/2}^n (\epsilon_k^n - \epsilon_{k-1}^n) + \frac{1}{\Delta x^2} a_{k+1/2}^n (\epsilon_k^n - \epsilon_{k+1}^n)$$

we have

$$(4.5) \quad \begin{aligned} \|L^n E^n\|_2 &\leq \frac{a^*}{\Delta x} \left\{ \Delta x \sum_{k=1}^M \frac{(\epsilon_k^n - \epsilon_{k-1}^n)^2}{\Delta x^2} \right\}^{1/2} + \frac{a^*}{\Delta x} \left\{ \Delta x \sum_{k=1}^M \frac{(\epsilon_{k+1}^n - \epsilon_k^n)^2}{\Delta x^2} \right\}^{1/2} \\ &\leq \frac{2a^*}{\Delta x} \|E_z^n\|_2 \leq 2a^* K(T) \left(\frac{\Delta t^{r+1}}{\Delta x} + \Delta x^e \right). \end{aligned}$$

Similarly,

$$(4.6) \quad \|B^n E^n\|_2 \leq b^* K(T) (\Delta x^{s+1} + \Delta t^{r+1})$$

and we have

$$(4.7) \quad \frac{1}{2\Delta t} \|E^{n+1} - E^{n-1}\|_2 \leq K(T) \left(\Delta t^r + \frac{\Delta x^{s+1}}{\Delta t} \right).$$

Hence, we can estimate $\|H\|_2$ by

$$(4.8) \quad \|H\|_2 \leq T^{1/2} K(T)(\Delta t^{r+1} + \Delta x^{s+1}) \left(b^* + \frac{2a^*}{\Delta t} + \frac{1}{\Delta t} \right).$$

We estimate $\|G^* - \hat{G}^*\|_2$ as follows: First,

$$(4.9) \quad \|G^* - \hat{G}^*\|_2 = \frac{1}{2\Delta t^{1/2}} \|\hat{V}^{N+1} - V^{N+1}\|_2.$$

If U^* is the M -vector consisting of the steady state solution, we have from (3.1)

$$(4.10) \quad \begin{aligned} \|G^* - \hat{G}^*\|_2 &\leq \frac{1}{2\Delta t^{1/2}} \{ \|\hat{V}^{N+1} - U^\infty\|_2 + \|U^{N+1} - U^\infty\|_2 \} \\ &\quad + K(T) \left(\frac{\Delta t^{r+1} + \Delta x^{s+1}}{2\Delta t^{1/2}} \right). \end{aligned}$$

Since we assume U^* is known, and that $\{u(x, t) - u^*(x)\}$ can be estimated as a function of t , the right-hand side of (4.10) can be estimated.

We may estimate $\|C(\xi)\|_2$ by using the a priori estimate (3.1), since ξ is an intermediate value, and since $f_w(x, t, w)$ is bounded if w is bounded. This means we can find a constant K_1 such that

$$(4.11) \quad \|C(\xi)(V - U)\|_2 \leq K_1 K(T) T^{1/2} (\Delta t^{r+1} + \Delta x^{s+1}).$$

Finally, we assume a bound is known for the derivatives of u occurring in (3.4) so that

$$(4.12) \quad \|\tau\|_2 \leq T^{1/2} K_2 (\Delta t^2 + \Delta x^2), \quad \text{for some constant } K_2.$$

Using Lemma 1 and (4.8), (4.10), (4.11) and (4.12) we have

THEOREM. *Let $b(x, t)$ in (1.1) satisfy $|\partial b / \partial x| \leq b_1 < 2a_0\pi^2$ and fix $\epsilon > 0$ so that $a_0\pi^2 - \frac{1}{2}b_1 - \epsilon \geq \omega > 0$. Let*

$$(4.13) \quad \Delta x \leq \left(\frac{12\epsilon}{a_0\pi^4} \right)^{1/2}.$$

Let $V = \{V^n\}$ and $\hat{V} = \{\hat{V}^n\}$ be, respectively, the exact and computed solution of a difference approximation for (1.1) satisfying (3.1). Finally, let R be defined by (4.2). Then

$$(4.14) \quad \begin{aligned} \|V - \hat{V}\|_2 &\leq \frac{1}{2\omega\Delta t^{1/2}} \{ \|\hat{V}^{N+1} - U^\infty\|_2 + \|U^{N+1} - U^\infty\|_2 \} + \frac{\|R\|_2}{\omega} \\ &\quad + \frac{T^{1/2} K_2 (\Delta t^2 + \Delta x^2)}{\omega} \\ &\quad + \frac{T^{1/2} K(T) (\Delta t^{r+1} + \Delta x^{s+1})}{\omega} \left\{ K_1 + \frac{1}{2(T\Delta t)^{1/2}} + b^* + \frac{2a^*}{\Delta x} + \frac{1}{\Delta t} \right\} \end{aligned}$$

and

$$(4.15) \quad \begin{aligned} \|V_x - \hat{V}_x\|_2 &\leq \left(\frac{2\omega + b_1}{2a_0\omega^2} \right)^{1/2} \left\{ \frac{1}{2\Delta t^{1/2}} (\|\hat{V}^{N+1} - U^\infty\|_2 + \|U^{N+1} - U^\infty\|_2) \right. \\ &\quad + \|R\|_2 + K_2 T^{1/2} (\Delta t^2 + \Delta x^2) + K(T) T^{1/2} (\Delta t^{r+1} + \Delta x^{s+1}) \\ &\quad \left. \cdot \left(K_1 + \frac{1}{2(\Delta t T)^{1/2}} + b^* + \frac{2a^*}{\Delta x} + \frac{1}{\Delta t} \right) \right\}. \end{aligned}$$

The University of New Mexico
Albuquerque, New Mexico 87106

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