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

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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

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

We assume that $a(x, t)$, $b(x, t)$ are "smooth" bounded functions on $\bar{\mathcal{R}}$, with $a(x, t) \geqq a_0 > 0$, and that $f(x, t, w)$ is, at least once, continuously differentiable on $\mathcal{R}X\{-\infty < w < +\infty\}$ with $\partial f/\partial w \geqq 0$. 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 $t \to \infty$. 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 $x = k\Delta x$, $k = 0, 1, \cdots, M + 1$, $t = n\Delta t$, $n = 0, 1, \cdots, N + 1$. Let v_k^n denote $v(k\Delta x, n\Delta t)$. Define V^n to be the M-component vector

$$V^n = \{v_1^n, v_2^n, \cdots, v_M^n\}^T \tag{2.1}$$

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

$$V = \{V^1, V^2, \cdots, V^N\}^T. \tag{2.2}$$

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

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

and let

$$\| V^n\|_2^2 = \langle V^n, V^n\rangle. \tag{2.4}$$

Let

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

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

For block vectors V, W define

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

and let

$$\| V\|_2^2 = (V, V), \tag{2.7}$$

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

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

$$\|A\| = \operatorname*{Sup}_{\|X\|=1} \|AX\|, \tag{2.9}$$

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

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

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 $n\Delta t \to \infty$, Δt fixed. Hence, we cannot expect $K(T)$ to remain bounded as $T \to \infty$, 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

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

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

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

where

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

From (3.2) and (3.3) we have

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

with the initial boundary data

$$v_k^0 = \chi(k\Delta x), \qquad k = 1, \cdots, M, \tag{3.6}$$
$$v_0^n = \varphi_1(n\Delta t), \qquad v_{M+1}^n = \varphi_2(n\Delta t), \qquad n = 1, 2, \cdots .$$

With $T = (N + 1)\Delta t$ we now consider the system formed by equations (3.5) for $n = 1, 2, \cdots, N$. 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

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

$$B^n = \frac{1}{2\Delta x}\begin{bmatrix} 0 & -b_1^n & & \bigcirc \\ b_2^n & \ddots & \ddots & \\ & \ddots & \ddots & \\ \bigcirc & & b_M^n \quad 0 & -b_{M-1}^n \end{bmatrix} \tag{3.8}$$

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

$$\tau^n = \{\tau_1^n, \tau_2^n, \cdots, \tau_M^n\}^T, \tag{3.9}$$

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

where

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

and

(3.11)

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

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

$$\frac{V^{n+1} - V^{n-1}}{2\Delta t} = -L^n V^n - B^n V^n - F^n(U) + \tau^n + G^n$$
$$+ \frac{E^{n+1} - E^{n-1}}{2\Delta t} + B^n E^n + L^n E^n, \qquad n = 1, 2, \cdots, N. \tag{3.12}$$

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

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

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

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

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

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

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

$$F = \{F^1, F^2, \cdots, F^N\}^T, \tag{3.16}$$

$$G^* = \left\{G^1 + \frac{V^0}{2\Delta t}, G^2, \cdots, G^N - \frac{V^{N+1}}{2\Delta t}\right\}^T, \tag{3.17}$$

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

$$\tau = \{\tau^1, \tau^2, \cdots, \tau^N\}^T. \tag{3.19}$$

With this notation we have from (3.12)

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

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

$$Q = P + D. \tag{3.21}$$

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

$$\left|\frac{\partial b}{\partial x}\right| \leqq b_1 < 2a_0\pi^2, \qquad \forall (x, t) \in \overline{\mathfrak{R}}_T. \tag{3.22}$$

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

$$\operatorname*{Sup}_{X \text{ real}, \|X\|_2 \leqq 1} \|Q^{-1}X\|_2 \leqq \frac{1}{\omega}. \tag{3.23}$$

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

$$\|W_x\|_2 \leqq \left(\frac{2\omega + b_1}{2a_0\omega^2}\right)^{1/2} \|Z\|_2. \tag{3.24}$$

Proof. See [3, Lemma 1].

Remark. If

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

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 $c(x) \geqq 0$. See [1, Lemma 1] and [2, Lemma 4.2].

4. A Posteriori Bounds. For each $n = 1, 2, \cdots, N+1$, 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

$$\hat{V} = \{\hat{V}^1, \hat{V}^2, \cdots, \hat{V}^N\}^T. \tag{4.1}$$

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

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

Subtracting (4.2) from (3.20) we have

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

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

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

Since $f_w \geqq 0$, $C(\Psi)$ 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 $\bar{\mathfrak{R}}_T$.

Since

$$(L^nE^n)_k = \frac{1}{\Delta x^2} a^n_{k-1/2}(\epsilon^n_k - \epsilon^n_{k-1}) + \frac{1}{\Delta x^2} a^n_{k+1/2}(\epsilon^n_k - \epsilon^n_{k+1})$$

we have

$$\begin{aligned} ||L^nE^n||_2 &\leqq \frac{a^*}{\Delta x}\left\{\Delta x \sum_{k=1}^{M} \frac{(\epsilon^n_k - \epsilon^n_{k-1})^2}{\Delta x^2}\right\}^{1/2} + \frac{a^*}{\Delta x}\left\{\Delta x \sum_{k=1}^{M} \frac{(\epsilon^n_{k+1} - \epsilon^n_k)^2}{\Delta x^2}\right\}^{1/2} \\ &\leqq \frac{2a^*}{\Delta x} ||E^n_x||_2 \leqq 2a^* K(T)\left(\frac{\Delta t^{r+1}}{\Delta x} + \Delta x^s\right). \end{aligned} \tag{4.5}$$

Similarly,

$$||B^nE^n||_2 \leqq b^* K(T)(\Delta x^{s+1} + \Delta t^{r+1}) \tag{4.6}$$

and we have

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

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

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

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

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

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

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

Since we assume U^∞ is known, and that $\{u(x, t) - u^\infty(x)\}$ 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

$$\|C(\xi)(V - U)\|_2 \leqq K_1K(T)T^{1/2}(\Delta t^{r+1} + \Delta x^{s+1}). \tag{4.11}$$

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

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

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

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

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

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*

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

and

$$\begin{aligned}\|V_x - \hat{V}_x\|_2 & \\ \leqq {} & \left(\frac{2\omega + b_1}{2a_0\omega^2}\right)^{1/2}\left\{\frac{1}{2\Delta t^{1/2}}(\|\hat{V}^{N+1} - U^\infty\|_2 + \|U^{N+1} - U^\infty\|_2)\right. \\ & + \|R\|_2 + K_2T^{1/2}(\Delta t^2 + \Delta x^2) + K(T)T^{1/2}(\Delta t^{r+1} + \Delta x^{s+1}) \\ & \left.\cdot\left(K_1 + \frac{1}{2(\Delta tT)^{1/2}} + b^* + \frac{2a^*}{\Delta x} + \frac{1}{\Delta t}\right)\right\}.\end{aligned} \tag{4.15}$$

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