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TERMINATION STRATEGIES FOR NEWTON ITERATION IN FULL MULTIGRID METHODS

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Termination strategies for Newton iteration in Full Multigrid methods*)

by

E.J. van Asselt

ABSTRACT

For the solution of nonlinear problems we consider Full Multigrid methods, in which each nonlinear discrete system is solved by the Newton method. A fixed and an adaptive strategy to terminate the Newton process on each grid are compared.

For the adaptive strategy only the residuals outside the possible boundary and interior layers are used to terminate the Newton process, and the number of Newton iterations is much smaller than for the fixed strategy.

Other advantages for the adaptive strategy are that no arbitrary termination criterion has to be selected in advance, and boundary and interior layers are detected automatically.

Three numerical examples are given. These concern two 1-D singular perturbed nonlinear elliptic equations, and the Van der Pol equation, discretized with the Osher-Engquist difference scheme.

KEY WORDS & PHRASES: *Full Multigrid methods, Newton iteration, Termination strategy, Van der Pol equation*

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*) This report will be submitted for publication elsewhere.

1. INTRODUCTION

We consider Full Multigrid methods (FMGMs) for the solution of nonlinear problems (cf.BRANDT [2], HACKBUSCH [5]).

In FMGMs a coarse to fine sequence of discretizations is used on grids $G_0 \subset \ldots \subset G_\ell$ with meshwidth $h_0 > \ldots > h_\ell$. On each grid G_k, $k = 0,\ldots,\ell-1$ a discrete problem is approximately solved by an iterative method.

The approximate solution on grid G_k is interpolated to the next finer grid G_{k+1} and serves as initial approximation for the iterative method on G_{k+1}.

In this paper we consider only the outer loop of the FMGM, where the approximate solution on a coarse grid is used as the initial approximation for the Newton method on the next finer grid.

In section 2 we introduce a fixed and an adaptive strategy to terminate the Newton process on the current finest grid.

For the adaptive strategy we need no information in advance for the termination criterion, possible boundary and interior layers are detected automatically, and only the residuals outside these layers are used to terminate the Newton process. In section 3 we give three 1-D examples which show that for the adaptive strategy the number of Newton iterations is much smaller than for the fixed strategy.

2. A FIXED AND AN ADAPTIVE STRATEGY

In this section we introduce two termination strategies for Newton iteration in FMGMs.

We start with some definitions and describe a fixed and an adaptive strategy.

On $\Omega \subset \mathbb{R}^2$ we consider the nonlinear continuous problem (2.1) and its discretizations on the uniform square grids $G_k \subset \Omega$ with meshwidth h_k, $k = 0,\ldots,\ell$ such that $G_k \subset G_{k+1}$, and $h_{k+1} = \eta h_k$, $k = 0,\ldots,\ell-1$. (η, the meshwidth ratio, usually is equal to 1/2).

(2.1) $Nu = b$; $N : B_1 \to B_2$, where B_1 and B_2 are Banach spaces.

(2.2) $N_k u_k = b_k = r_k b$; $N_k : B_1^k \to B_2^k$, where B_i^k (i=1,2) are the spaces of gridfunctions on G_k, $k = 0,\dots,\ell$.

By r_k, $r_{k,k+1}$ we denote surjective linear operators (restrictions) from B_2 to B_2^k, and from B_2^{k+1} to B_2^k respectively, with the additional property that

(2.3) $$r_k = r_{k,k+1}\, r_{k+1}\, , \quad k = 0,\dots,\ell-1.$$

By $x_{i,j}^k \in G_k$ we denote the point (ih_k, jh_k).

(2.4) DEFINITION. A *termination strategy* for Newton iteration in a FMGM with grids $G_0,\dots,G_\ell$ is a sequence of corresponding gridfunctions $st_0,\dots,st_\ell$, such that on each grid G_k the Newton process is terminated as soon as the iterant v_k satisfies:

(2.5) $$|(N_k v_k - b_k)_{i,j}| \le |st_{k_{i,j}}| \text{ for all } (i,j) \text{ with } x_{i,j}^k \in G_k \cap \Omega,$$
$$k = 0,\dots,\ell.$$

If st_k, $k = 0,\dots,\ell$ is fixed during the computations the termination strategy is called *fixed* whereas otherwise it is called *adaptive*.
The gridfunction st_k is called the *termination criterion* on level k.

(2.6) DEFINITION. The operator $\tau_k : B_1 \to B_2^k$ given by $\tau_k v = N_k r_k v - r_k N v$ is called the *local truncation error operator*.
The *local truncation error* at $x_{i,j}^k \in G_k$ is given by $(\tau_k u)_{i,j}$, where u is the solution of (2.1).

(2.7) DEFINITION. The operator $\tau_{k-m,k} : B_2^k \to B_2^{k-m}$ ($k \ge m > 0$), given by $\tau_{k-m,k} v_k = N_{k-m} r_{k-m,k} v_k - r_{k-m,k} N_k v_k$ is called the *relative local truncation error operator;*
The *relative local truncation error* at $x_{i,j}^{k-m} \in G_{k-m}$ is given by $(\tau_{k-m,k} u_k)_{i,j}$, where u_k is the solution of (2.2).

We are interested in an approximation to the solution of the continuous problem, and not particularly in an accurate solution of the discrete problem, therefore the Newton process is terminated on the finest grid as soon as the iterant v_ℓ satisfies

(2.8) $\quad |(N_\ell v_\ell - b_\ell)_{i,j}| \le |\tau_\ell(u)_{i,j}|$ for all (i,j) with

$x^\ell_{i,j} \in G_\ell \cap \Omega$, where u is the solution of (2.1).
On coarser grids G_k, $k = 0,\ldots, \ell-1$ we are only interested in the provision of a good starting value on the next finer grid G_{k+1}, and not particularly in a very accurate approximation to the discrete solution either. Therefore the Newton process on G_k is terminated as soon as the iterant v_k satisfies

(2.9) $\quad |(N_k v_k - b_k)_{i,j}| \le |(\tau_{k,k+1}(r_{k+1}u))_{i,j}|$ for all (i,j)

with $x^k_{i,j} \in G_k \cap \Omega$, where u is the solution of (2.1).
For the relative local truncation error operators and the local truncation error operators the following relations hold:

(2.10) $\quad \tau_{k-2,k} = \tau_{k-2,k-1}\, r_{k-1,k} + r_{k-2,k-1}\, \tau_{k-1,k}$

(2.11) $\quad \tau_{k-1} - r_{k-1,k}\, \tau_k = \tau_{k-1,k}\, r_k.$

For sufficiently differentiable solutions u of (2.1), Taylor's formula of the local truncation error reads:

(2.12) $\quad (\tau_k u)_{i,j} = C_k h_k^p + O(h_k^{\bar{p}})$, $\bar{p} > p$, where C_k only depends on higher order derivatives of u in the gridpoint $x^k_{i,j} \in G_k$, $k = 0,\ldots, \ell$.
If we take for all restrictions $r_k, k = 0,\ldots, \ell$ the injection operator, then $r_{k-1,k}$ exists and (2.3) is satisfied. Moreover when C_k in (2.12) varies not much locally (i.e. the solution is locally smooth) then with $C_k = C_{k-1}$ and $\bar{p} - p = q$ it follows that:

(2.13) $\quad (\tau_{k-1}u)_{i,j}/(r_{k-1,k}(\tau_k u))_{i,j} = \eta^{-p}(1+O(h^q_{k-1}))$,

where (i,j) is such that $x^{k-1}_{i,j} \in G_{k-1} \cap \Omega$, $k = 1, \ldots, \ell$.
From (2.11) - (2.13) it follows that:

$$(2.14)\qquad (\tau_{k-1,k} r_k u)_{i,j} = (\eta^{-p}-1).\eta^{-p(\ell-k)} (r_{k-1,\ell}\tau_\ell(u))_{i,j} + O(h_{k-1}^q)$$

where (i,j) is such that $x_{i,j}^{k-1} \in G_{k-1} \cap \Omega$, $k=1,\ldots,\ell$.
With (2.14) we can check locally whether the solution is smooth or not, as we shall see shortly. For the FMGM, (2.8), (2.9) and (2.14) lead us to a fixed termination strategy $(st_0,\ldots,st_\ell)$ defined by:

$$(2.15)\qquad \begin{aligned} st_\ell &= \tau_\ell(u) \\ st_k &= (\eta^{-p}-1).\ \eta^{-p(\ell-1-k)} r_{k,\ell}\ st_\ell,\ k = \ell-1,\ldots,\ 0, \end{aligned}$$

where u is the solution of (2.1).

In practice we do not know the true local truncation error τ_ℓ beforehand, and have no information about the location of possible boundary and interior layers. In these situations we replace in (2.15) st_ℓ by a gridfunction which is constant in all gridpoints and sufficiently small:

$$(2.16)\qquad \begin{aligned} st_{\ell_{i,j}} &= c \text{ for all } (i,j) \text{ with } x_{i,j}^\ell \in G_\ell \cap \Omega \\ st_k &= (\eta^{-p}-1).\ \eta^{-p(\ell-1-k)} r_{k,\ell}\ st_\ell,\ k = \ell-1,\ldots,\ 0. \end{aligned}$$

When we apply (2.16) to problems with boundary and interior layers the number of iterations of the Newton process on the subsequent grids of the FMGM strongly depends on those layers. Moreover on the coarse grids in the FMGM it is not necessary to have very accurate solutions in the layers, because the solution cannot be represented well there anyhow, and accuracy is lost after interpolation. Only the interpolated values of the smooth parts are useful as initial approximation for the Newton process. Therefore we introduce a new, adaptive termination strategy, where the boundary and interior layers are detected automatically during the computations, and only the residuals outside these layers are used to terminate the Newton process. We describe the adaptive strategy for the 1-D case with Dirichlet boundary conditions, and take $\eta = 1/2$. The 2-D, and 3-D case can be constructed similarly. We start on the 3 lowest levels with the termination criteria of some fixed termination strategy (e.g. (2.16)). On finer grids, during the computations with the FMGM we check the smoothness assumption on u, i.e. for a given tolerance δ we check the relation (2.14) for all points $x_i^{k-3} \in G_{k-3}$ by computing:

$$(2.17) \qquad | \; r_{k-3,k-2}(N_{k-2}\, r_{k-2,k-1}(v_{k-1}) - b_{k-2})_i$$

$$/(N_{k-3}\, r_{k-3,k-2}(v_{k-2}) - b_{k-3})_i - 2^{-p} \; | < \delta.\, 2^{-p},$$

here v_{k-1} and v_{k-2} are the last iterants on G_{k-1} and G_{k-2} respectively. If (2.17) is true for $x_i^{k-3} \in G_{k-3}$ the truncation error shows its asymptotic behaviour (2.12), and we may assume that the solution is locally smooth near x_i^{k-3}. Further $N_{k-2}\, r_{k-2,k-1}\, (v_{k-1}) - b_{k-2}$ is a reasonable approximation to $\tau_{k-2,k-1}(r_{k-1}\, u)$ and hence a good approximation to $2^{2p} r_{k-2,k}\, \tau_{k,k+1} r_{k+1} u$ (cf. 2.14). Therefore near points x_i^{k-3} which are not boundary points we take as termination criterion:

$$(2.18) \qquad st_{k_{8i+w}} = 2^{-2p}\, (p_{k,k-1} p_{k-1,k-2}(N_{k-2} r_{k-2,k-1}(v_{k-1}) - b_{k-2}))_{8i+w},$$

$$w = -4(1)4, \text{ (cf. 2.9).}$$

Here $p_{k,k-1}$ and $p_{k-1,k-2}$ denote interpolation operators. If (2.17) is not true for $x_i^{k-3} \in G_{k-3}$, the smoothness assumption on u is not satisfied, and we take:

$$(2.19) \qquad st_{k_{8i+w}} = M, \; w = -4(1)4,$$

where M is an arbitrary value, much larger than values in (2.18). In this way the regions where the solution is not smooth enough to use (2.18) are detected automatically, and the residuals in these regions are not used to terminate the Newton process. In order to avoid coincidence we also use (2.19) when (2.17) is true for the point x_i^{k-3} and not for x_{i-1}^{k-3} and x_{i+1}^{k-3}. Of course the part of the domain where the solution is smooth must be large enough such that the solution interpolated to the next finer grid is a reasonable initial approximation. For points near the boundary, values of st_k are obtained by extrapolation from values of $N_{k-2} r_{k-2,k-1}(v_{k-1}) - b_{k-2}$ at interior points of G_{k-2}.

3. NUMERICAL EXAMPLES

In this section, for three examples we compare the fixed and the adaptive termination strategy (2.16) and (2.17) - (2.19) respectively.

(3.1) Example 1.

We consider the 1-D problem

(3.2) $Nu \equiv -\varepsilon u'' + a(u)u' + u = 0$ on $[0,1]$ with boundary conditions $u(0) = 1$, $u(1) = -1$ and $\varepsilon = 10^{-6}$; $a(u) = u^2 - \frac{1}{4}$.

On each grid G_k we discretize this equation by the first order Osher-Engquist scheme (cf. OSHER [6]):

(3.3)
$$(N_k u_k)_i \equiv -\varepsilon\,(u_{i+1}-2u_i+u_{i-1})/h_k^2 +$$
$$+ (\Delta_+ f_-(u_i) + \Delta_- f_+(u_i))/h_k + u_i = 0,$$

$i = 1,\dots,n_k-1$ (n_k is the number of intervals of G_k),

$$(N_k u_k)_0 \equiv u_0 = u(0) \;;\; (N_k u_k)_{n_k} \equiv u_{n_k} = u(1) \;;$$

where
$$f_+(u_i) = \int_0^{u_i} a_+(s)\,ds,\quad a_+(s) = \max(0,a(s)),$$

$$f_-(u_i) = \int_0^{u_i} a_-(s)\,ds,\quad a_-(s) = \min(0,a(s)),$$

$$\Delta_+ f_-(u_i) = f_-(u_{i+1}) - f_-(u_i) \text{ , and}$$

$$\Delta_- f_+(u_i) = f_+(u_i) - f_+(u_{i-1}).$$

As solution process on the different grids of the FMGM we use Newton iteration:

$$(3.4) \qquad L_k u_k^{m+1} = L_k u_k^m - (N_k u_k^m - g_k),$$

where the nonzero entries of the tridiagonal matrix $L_k = (L_{i,j})_{0\le i,j\le n_k}$ are given by

$$L_{o,o} = L_{n_k,n_k} = 1,$$

$$L_{i-1,i} = -\varepsilon/h_k^2 - a_+(u_{i-1}^m)/h_k,$$

$$L_{i,i} = 2\varepsilon/h_k^2 + (a_+(u_i^m) - a_-(u_i^m))/h_k + 1,$$

$$L_{i,i+1} = -\varepsilon/h_k^2 + a_-(u_{i+1}^m)/h_k, \; i = 1,\dots,n_k-1,$$

and the nonzero elements of g_k are $g_0 = u_0$, $g_{n_k} = u_{n_k}$.

The meshwidth ratio $\eta = 1/2$. The meshwidth of the coarsest grid $h_0 = 1/5$. On G_0 we take the straight line between the boundary values: $u_j^0 = 1 - 2x_j$ as initial approximation.
In the adaptive strategy, for the finer grids, the termination criterion is determined by estimates of the truncation error as shown in section 2.
For any fixed strategy the termination criterion is to be determined beforehand and can only be rather arbitrary. In order to compare the (usual) fixed with our adaptive strategy we take a termination criterion for the fixed strategy that also solves the finest grid discretization with an accuracy comparable to the truncation error. Therefore in our comparison we first apply the adaptive strategy.

This yields a termination criterion on the finest grid from which we take the maximum value $\neq$ M: t_{max}. Then we apply the fixed strategy (2.16) with $c = t_{max}$.

And finally again we apply the adaptive strategy, but now with the same termination criterion on the coarse grids as the fixed strategy. This yields approximately the same t_{max} (cf. Table 1,2,3). In this way we are sure that the results obtained are of comparable accuracy. In practical situations the fixed strategy termination criterion can only be more arbitrary.
If the mesh is too coarse it may be that δ must be too large in order to full-

fill (2.17) for a sufficiently large number of points. In our example it appears that G_4 is sufficiently fine and $\delta = 0.1$ gives an efficient termination strategy.

The number of Newton iterations are given in Table 1.

Grids	G_0	G_1	G_2	G_3	G_4	G_5	G_6	G_7	t_{max}
fixed	2	2	3	5	5	6	7	7	$1.5 \cdot 10^{-3}$
adaptive	2	2	3	5	4	1	1	1	$1.3 \cdot 10^{-3}$

Table 1. Number of Newton iterations on the different grids in the FMGM for Example 1.

The regions in the different grids in which the smoothness assumption on u (cf. 2.17) is not satisfied are given in Figure 1.

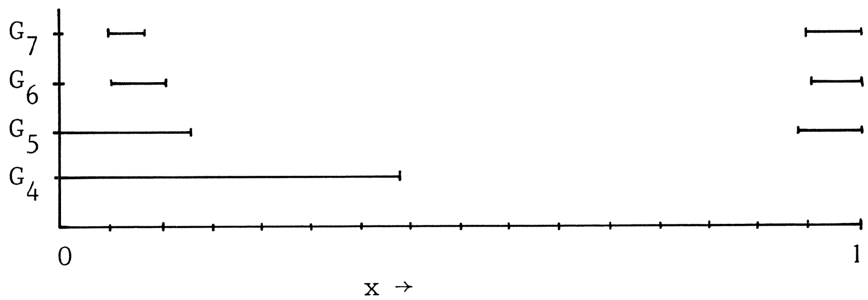

Figure 1. Regions in the grids G_4–G_7 in which the smoothness assumption on u (cf. 2.17) is not satisfied (Example 1).

The solution on G_7 is shown in Figure 2.

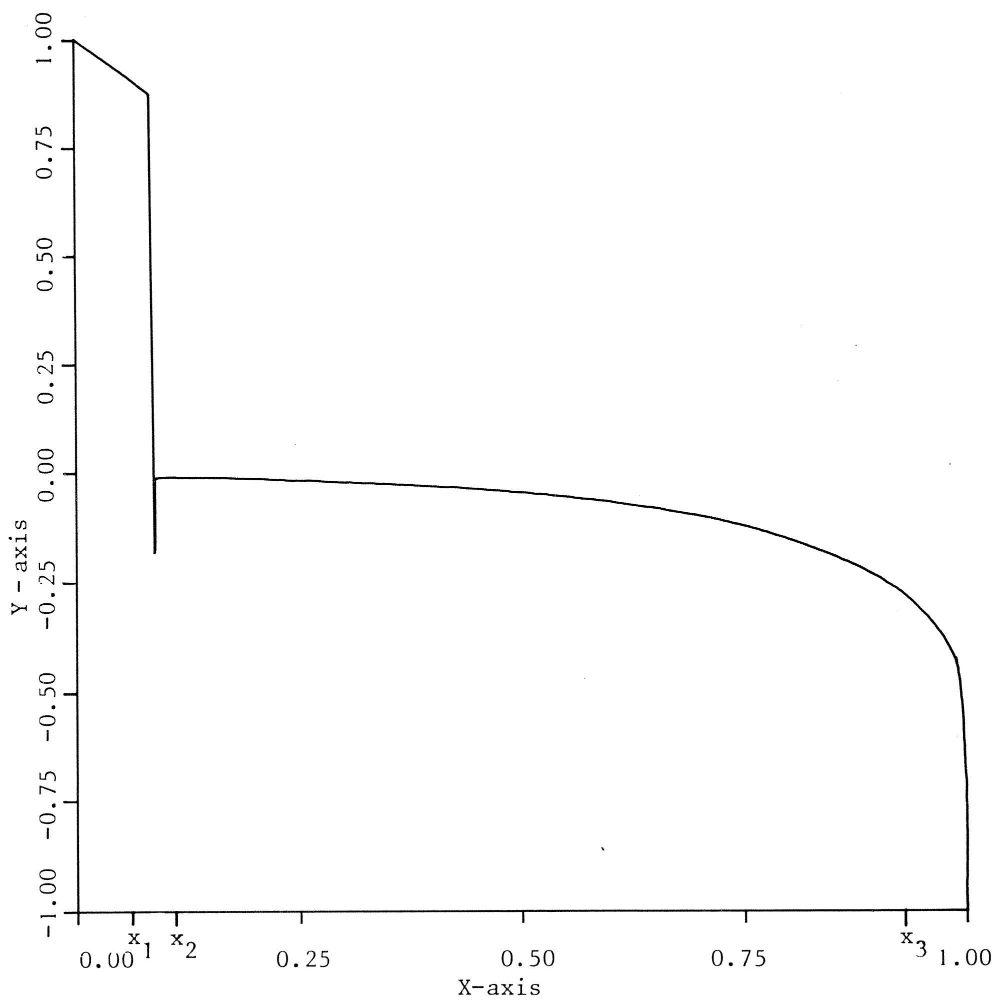

Figure 2. The solution on G_7 for the adaptive strategy. The segments $[x_1,x_2]$ and $[x_3,1.00]$ are the regions in which the smoothness assumption on u (cf. 2.17) is not satisfied.

(3.5) Example 2.

The second problem is the 1-D steady-state Burgers equation, given by (3.2) and (3.3) with $a(u) = u$, $\varepsilon = 10^{-6}$, $u(0) = 0.75$, $u(1) = -0.5$, $\eta = 1/2$, $h_0 = 1/5$.

The same initial approximation on G_0 is used as in Example 1, and again $\delta = 0.1$.

The number of Newton iterations is shown in Table 2. For the adaptive termination strategy the termination criteria are adapted starting from G_4.

Grids	G_0	G_1	G_2	G_3	G_4	G_5	G_6	G_7	$c=t_{max}$
Fixed	2	2	2	2	3	4	4	4	$7.8 \cdot 10^{-4}$
Adaptive	2	2	2	2	1	1	1	1	$7.8 \cdot 10^{-4}$

Table 2. Number of Newton iterations on the different grids in the FMGM for Example 2.

The areas on the different grids in which the smoothness assumption (2.17) is not satisfied are shown in Figure 3. The solution of the continuous problem has a shock layer centered near $x = (1 + u(0) + u(1))/2$ (cf. COLE [3]).

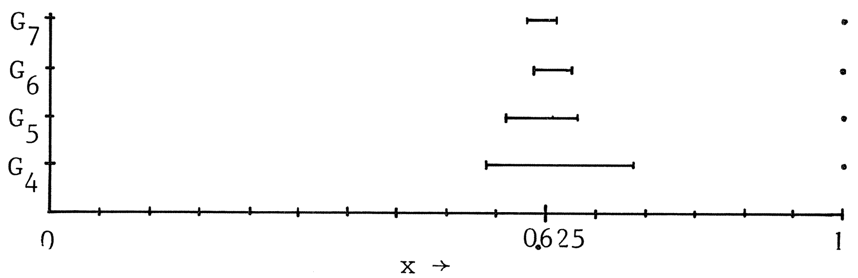

Figure 3. Areas on the grids G_4–G_7 in which the smoothness assumption on u (cf. 2.17) is not satisfied. (Example 2).

The solution on G_7 is shown in Figure 4.

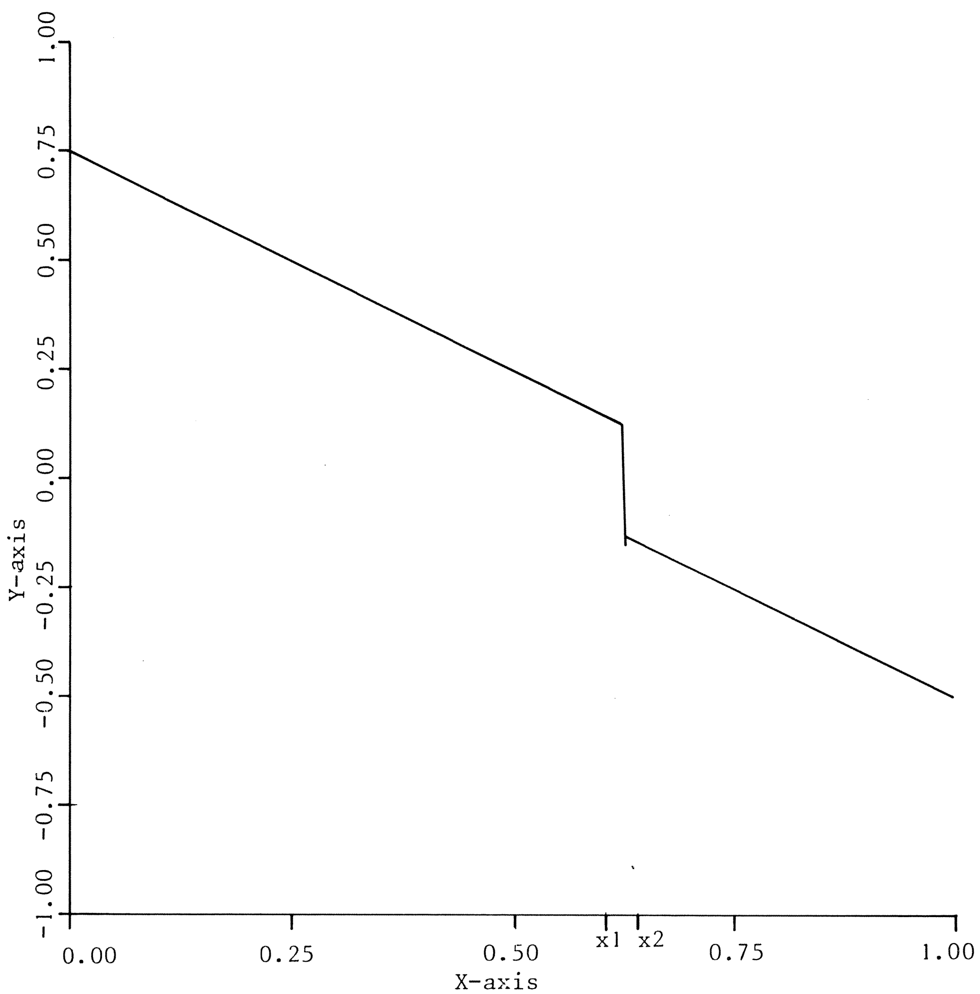

Figure 4. The solution on G_7 for the adaptive strategy. The segment $[x_1, x_2]$ is the region in which the smoothness assumption on u (cf. 2.17) is not satisfied.

(3.6) Example 3.

This problem concerns the Van der Pol equation (cf. BELLMAN, KALABA [1], GUCKENHEIMER [4]):

(3.7) $-u'' + a(u)u' - u = 0$ on $[0, \bar{B}]$ with boundary conditions $u(0) = 1$, $u'(0) = \sigma$; $a(u) = \lambda(-u^2 + 1)$, $\lambda \in \mathbb{R}_{>0}$.

Again on each grid G_k we discretize this equation by the first order Osher-Engquist scheme. For a good representation of the boundary conditions, we take nonuniform grids G_k with gridpoints $x_0^k = 0$, $x_1^k = \gamma h_k$, $(\gamma << 1)$, $x_j^k = (j-1)h_k$ for $j = 2,\ldots,n_k$, where n_k is the number of intervals of G_k:

(3.8) $$(N_k u_k)_0 \equiv u_0 = 1,$$

$$(N_k u_k)_1 \equiv u_1 = u_0 + \sigma\gamma h_k,$$

$$(N_k u_k)_i \equiv -2(\alpha_i u_i - (\alpha_i + \beta_i)u_{i-1} + \beta_i u_{i-2})/\alpha_i\beta_i(\alpha_i + \beta_i)h_k^2$$

$$+ \Delta_- f_+(u_{i-1})/\alpha_i h_k + \Delta_+ f_-(u_{i-1})/\beta_i h_k$$

$$- u_{i-1} = 0,\ i = 2,\dots,n_k,\ \text{with } \alpha_2 = \gamma,\ \alpha_3 = 1-\gamma,$$

$\alpha_j = 1$ for $j = 4,\dots,n_k$; $\beta_2 = 1-\gamma$, $\beta_j = 1$ for $j = 3,\dots,n_k$, and where f_+, f_-, Δ_+ and Δ_- are defined as in Example 1.

As solution process on the different grids of the FMGM we use **the** Newton process (3.4), where the nonzero entries of the triangular matrix $L_k = (L_{i,j})_{0\le i,j\le n_k}$ are given by:

$$L_{0,0} = 1,$$

$$L_{1,1} = 1,$$

$$L_{i-2,i} = -2/(\alpha_i + \beta_i)\alpha_i h_k^2 - a_+(u_{i-2}^m)/\alpha_i h_k,$$

$$L_{i-1,i} = 2/\alpha_i\beta_i h_k^2 + a_+(u_{i-1}^m)/\alpha_i h_k - a_-(u_{i-1}^m)/\beta_i h_k - 1,$$

$$L_{i,i} = -2/(\alpha_i + \beta_i)\beta_i h_k^2 + a_-(u_i^m)/\beta_i h_k,\ i = 2,\dots,n_k,\ \text{with}$$

$\alpha_2 = \gamma$, $\alpha_3 = 1-\gamma$, $\alpha_j = 1$ for $j = 4,\dots,n_k$; $\beta_2 = 1-\gamma$, $\beta_j = 1$ for $j = 3,\dots,n_k$, and the nonzero elements of g_k are $g_0 = u_0$, $g_1 = u_0 + \sigma\gamma h_k$.

We consider (3.7)-(3.8) with $B = 22$, $\sigma = 0$, $\lambda = 10$, and $\gamma = 10^{-3}$. On G_0 we take $u_j^0 = 1$ $(j = 0,\dots,n_0)$ as initial approximation, and $\delta = 0.3$.

The number of Newton iterations is shown in Table 3. For the adaptive termination strategy the termination criteria are adapted starting from G_4. The last row shows the number of Newton iterations for the fixed strategy in case of an arbitrary choice for c in (2.16).

Grids	G_0	G_1	G_2	G_3	G_4	G_5	G_6	G_7	$c=t_{max}$
Fixed	90	12	11	7	5	4	3	3	0.11
Adaptive	90	12	11	7	2	2	2	2	0.11
Fixed	94	14	13	8	7	5	5	4	$c=10^{-6}$

Table 3. Number of Newton iterations on the different grids in the FMGM for Example 3. $\sigma = 0$, $\lambda = 10$, $\gamma = 10^{-3}$.

The areas on the different grids in which the smoothness assumption (2.17) is not satisfied are shown in Figure 5.

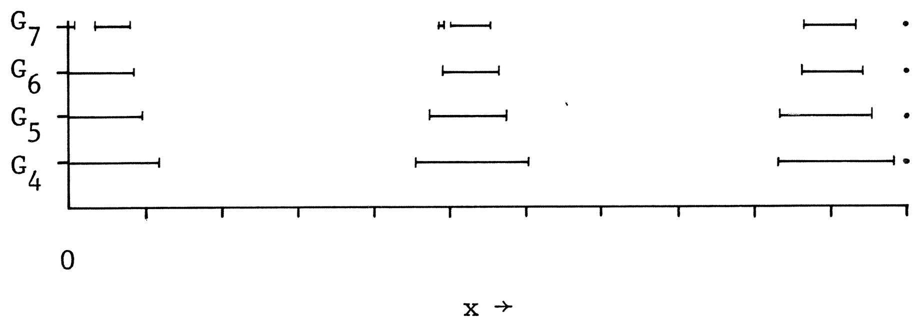

Figure 5. Areas on the grids G_4-G_7 in which the smoothness assumption on u (cf. 2.17) is not satisfied (Example 3).

The solution on G_7 is shown in Figure 6. For the period T and the amplitude a of the discrete solution we find T = 19.0 and a = 2.014 respectively. This agrees with the values given by Zonneveld: T = 19.07837 and a = 2.01429 (cf. ZONNEVELD [7]).

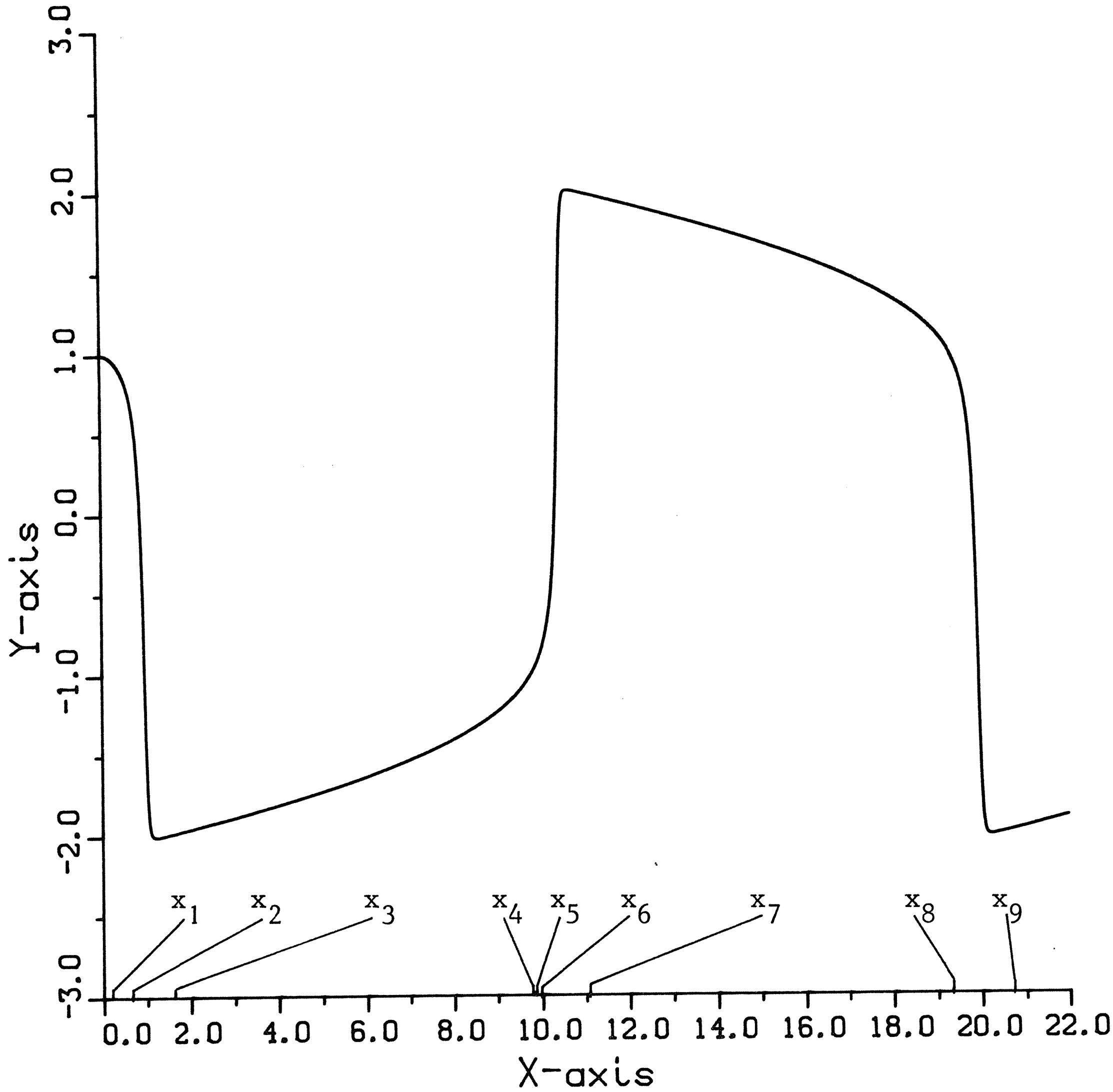

Figure 6. The solution on G_7 for the adaptive strategy. The segments $[0,x_1]$, $[x_2,x_3]$, $[x_4,x_5]$, $[x_6,x_7]$, $[x_8,x_9]$ are the regions in which the smoothness assumption on u (cf. 2.17) is not satisfied.

CONCLUSIONS

The advantages of an adaptive termination strategy for full multigrid methods are:

a) no arbitrary termination criterion has to be selected in advance.
b) the number of Newton iterations is much smaller than for the fixed strategy.
c) boundary and interior layers are detected automatically.

For the adaptive strategy on grid G_k we need to compute (2.17) and (2.18) for which the work is less than the work of one Newton iteration step on G_k.

In our examples the number of Newton iterations in the fixed strategy on fine grids is larger than for the adaptive strategy and therefore the latter is cheaper.

Termination strategies can also be used for 2-D and 3-D problems. The only impediment for general application in 2-D and 3-D problems seems the fact that at least 4 levels of discretization are required.

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