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NASA TM X- 73905

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(NASA-TM-X-73905) COMMENTS CN THE ROLE OF DIAGONAL DOMINANCE IN IMPLICIT DIFFERENCE METHODS (NASA) 18 p HC $3.50 CSCL 20D

N76-26430

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G3/34 44543

# COMMENTS ON THE ROLE OF DIAGONAL DOMINANCE IN IMPLICIT DIFFERENCE METHODS

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May 1976

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NATIONAL AERONAUTICS AND SPACE ADMINISTRATION
LANGLEY RESEARCH CENTER, HAMPTON, VIRGINIA 23665

| 1. Report No. | 2. Government Accession No. | 3. Recipient's Catalog No. |
|---|---|---|
| NASA TM X-73905 | | |

| 4. Title and Subtitle | 5. Report Date |
|---|---|
| COMMENTS ON THE ROLE OF DIAGONAL DOMINANCE IN IMPLICIT DIFFERENCE METHODS | May 1976 |
| | 6. Performing Organization Code |
| 7. Author(s) | 8. Performing Organization Report No. |
| Rudy, David H.; and Hirsh, Richard S. | |
| 9. Performing Organization Name and Address | 10. Work Unit No. |
| NASA Langley Research Center<br>Hampton, VA 23665 | 505-06-11-03 |
| | 11. Contract or Grant No. |
| 12. Sponsoring Agency Name and Address | 13. Type of Report and Period Covered |
| National Aeronautics and Space Administration<br>Washington, DC 20546 | NASA Technical Memorandum |
| | 14. Sponsoring Agency Code |

15. Supplementary Notes

Final release of information to be used as a reference for a formal publication.


16. Abstract

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| 17. Key Words (Suggested by Author(s)) | 18. Distribution Statement |
|---|---|
| Numerical analysis<br>Fluid mechanics<br>Finite-difference methods | Unclassified<br>Unlimited |

| 19. Security Classif. (of this report) | 20. Security Classif. (of this page) | 21. No. of Pages | 22. Price* |
|---|---|---|---|
| Unclassified | Unclassified | 16 | $3.25 |

*For sale by the National Technical Information Service, Springfield, Virginia 22161

# COMMENTS ON THE ROLE OF DIAGONAL DOMINANCE IN IMPLICIT DIFFERENCE METHODS

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## SUMMARY

Numerical tests were made for a model of the Navier-Stokes equations using a second-order accurate implicit scheme which guarantees diagonal dominance. The results of these tests suggest that the failure of implicit methods using large marching steps may not always be attributed to the lack of diagonal dominance in the coefficient matrix. In some cases the failure may be caused by a nonlinear instability associated with the solution method.

## INTRODUCTION

Implicit finite difference methods in general offer the major advantage of unconditional stability (with respect to the step size in the marching direction) over explicit methods. This advantage is offset somewhat by the need to solve a system of simultaneous algebraic equations during each marching step. However, when central differences are used, the coefficient matrix becomes tridiagonal in form and can be inverted much more rapidly than a full matrix. Consequently, to gain a computational time advantage, implicit marching steps need only to be a factor of four or five times larger than the maximum step size allowed in an explicit method. In many cases, though, large marching steps cause the coefficient matrix to lose diagonal dominance, a sufficient, but not necessary, condition for convergence of the matrix inversion. Without diagonal dominance, roundoff error can accumulate in the matrix inversion and destroy the solution. For Burgers' equation (a model of the Navier-Stokes equations), Hirsh and Rudy (Ref. 1) found that diagonal dominance could be maintained for any size marching steps if the cell Reynolds number was 2 or less. In the present paper results are given for numerical tests made with the second-order accurate scheme of Khosla-Rubin (Ref. 2) which maintains diagonal dominance for all cell Reynolds numbers and marching step sizes. The results of these tests suggest that the failure of implicit methods using large marching steps may not always be caused by the lack of diagonal dominance.

## SYMBOLS

| | |
|---|---|
| $a$ | $= u_i^n - U$ |
| A,B,C,D | matrix coefficients in eqs. (3) and (6) |
| C | Courant number, $\frac{a\Delta t}{\Delta x}$ |
| $D'$ | $= (u_{i+1}^n - 2u_i^n + u_{i-1}^n)/(2\Delta x)$ |
| $R_c$ | cell Reynolds number, $\lvert a\rvert \Delta x/\nu$ |
| $u$ | velocity |
| $U$ | wave speed |
| $\Delta x$ | spatial coordinate mesh spacing |
| $\Delta t$ | marching direction step size |
| $\varepsilon$ | convergence criterion |
| $\nu$ | viscosity |

Subscripts

| | |
|---|---|
| i | index denoting grid point spatial location |
| max | maximum value |
| x,t | derivative with respect to x-direction, time |

Superscripts

n index denoting time level

## DESCRIPTION OF NUMERICAL TESTS

The numerical tests of the Khosla-Rubin scheme were first made using the nonconservative form of Burgers' equation

$$u_t + au_x = \nu u_{xx} \tag{1}$$

(where a can be a function of u, t, and x) for several cases presented in Ref. 1 where diagonal dominance was lost. The difference form of eq. (1) becomes, using the Khosla-Rubin scheme (ref. 2),

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + \frac{(a_i - |a_i|)}{2}\left[\frac{(u_{i+1}^{n+1} - u_i^{n+1})}{\Delta x} - \frac{(u_{i+1}^n - 2u_i^n + u_{i-1}^n)}{2\Delta x}\right]$$

$$+ \frac{(a_i + |a_i|)}{2}\left[\frac{(u_i^{n+1} - u_{i-1}^{n+1})}{\Delta x} + \frac{(u_{i+1}^n - 2u_i^n + u_{i-1}^n)}{2\Delta x}\right]$$

$$= \frac{\nu}{(\Delta x)^2}(u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}) \tag{2}$$

where $a_i = u_i^n - U$ and $U$ is the steady-state wave speed. Thus,

$$A_i u_{i-1}^{n+1} + B_i u_i^{n+1} + C_i u_{i+1}^{n+1} = D_i \tag{3}$$

where

$$A_i = \frac{-\nu}{(\Delta x)^2} - \frac{(a_i + |a_i|)}{2\Delta x} \quad , \quad C_i = \frac{-\nu}{(\Delta x)^2} + \frac{(a_i - |a_i|)}{2\Delta x}$$

$$B_i = \frac{1}{\Delta t} + \frac{2\nu}{(\Delta x)^2} - \frac{(a_i - |a_i|)}{2\Delta x} + \frac{(a_i + |a_i|)}{2\Delta x}$$

$$D_i = \frac{u_i^n}{\Delta t} - |a_i| \frac{(u_{i+1}^n - 2u_i^n + u_{i-1}^n)}{2\Delta x}$$

$$= \frac{1}{\Delta t} u_i^n - |a_i| D_i'$$

The boundary conditions were taken to be:

$u(x,t) = 1.0$, at $x = -5$

$u(x,t) = 0$, at $x = +5$

Fifty-one equally spaced mesh points were used with $\Delta x = 0.2$. The wave speed $U$ was 0.5. A linear initial velocity distribution between the boundary points was used. The Thomas algorithm was employed to solve the resultant set of simultaneous algebraic equations at each time step. The solution was assumed to have reached a steady-state when the maximum change in $u$ between time steps was less than some specified value $\varepsilon$.

## RESULTS AND DISCUSSION

### Nonconservative Form of Nonlinear Burgers' Equation

For $\nu = 1/24$ ($R_c = 2.4$) and $C_{max} = \frac{\Delta t}{2\Delta x} = 10$, the solutions converged using the Khosla-Rubin scheme in less than 50 steps to the steady-state solution presented in Ref. 1 for $\varepsilon = 10^{-5}$. The solution is shown in Figure 1. In the calculation, the nonlinear coefficient, $a_i$, was lagged one time-step and no iteration was performed at each time step. The solution was then continued further in an attempt to satisfy $\varepsilon = 10^{-10}$. After approximately 30 more steps the solution began to diverge rapidly from the previous result. (Converged results were obtained for $\varepsilon = 10^{-10}$ and large values of $C_{max}$ with the usual central difference form.) Similar behavior was observed for $C_{max} = 0.9$. For $C_{max} = 0.1$, the solution converged in 741 steps for $\varepsilon = 10^{-10}$. In all cases the coefficient matrix is always diagonally dominant. All test results given in the paper are summarized in Table I.

An effect of this instability in the solution can be seen in figure 2 where

$$|D_i'| = \left|\frac{u_{i+1} - 2u_i + u_{i-1}}{2\Delta x}\right|$$

is plotted for $i = 26$ (the midpoint) as a function of the number of time steps for $C_{max} = 0.1$, 0.9 and 10.0. This term, $D_i'$, is the quantity added to the first-order (upwind) differencing of $u_x$ in the Khosla-Rubin modification and appears on the right-hand side of (3), not as a coefficient of the unknowns. As shown in figure 2, $D_{i=26}'$ remains small for $C_{max} = 0.1$; however, for $C_{max} = 0.9$ and 10.0, the term grows rapidly, and large errors appear in u.

Two types of iteration of the nonlinear term were also investigated for the nonconservative form of Burgers' equation. The first of these was the use of multiple iterations at each time step in the procedure previously described. The case with $\nu = 1/24$ and $C_{max} = 0.9$ was run with a fixed number of iterations to update $a_i$ at each time step. However, the solutions again rapidly diverged with 2, 4, or 8 iterations per time step.

The second form of iteration used was Newton iteration (ref. 3). In this technique

$$u_i^{n+1,m+1} = u_i^{n+1,m} + \delta u_i \tag{5}$$

where m is the iteration index at each time step. Equation (5) is substituted into equation (2) to give tridiagonal equations of the form

$$A_i \delta u_{i-1} + B_i \delta u_i + C_i \delta u_{i+1} = D_i \tag{6}$$

where, for $u_i \leq 1/2$

$$A_i = \frac{-\nu}{(\Delta x)^2}$$

$$B_i = \frac{1}{\Delta t} + \frac{1}{2\Delta x}(u_{i+1}^{n+1,m} - u_{i-1}^{n+1,m}) - \frac{1}{\Delta x}(u_i^{n+1,m} - 1/2) + \frac{2\nu}{(\Delta x)^2}$$

$$C_i = \frac{-\nu}{(\Delta x)^2} + \frac{1}{\Delta x}(u_i^{n+1,m} - 1/2)$$

and for $u_i > 1/2$,

$$A_i = \frac{-\nu}{(\Delta x)^2} - \frac{1}{\Delta x}(u_i^{n+1,m} - 1/2)$$

$$B_i = \frac{1}{\Delta t} + \frac{1}{2\Delta x}(u_{i+1}^{n+1,m} - u_{i-1}^{n+1,m}) + \frac{1}{\Delta x}(u_i^{n+1,m} - 1/2) + \frac{2\nu}{(\Delta x)^2}$$

$$C_i = \frac{-\nu}{(\Delta x)^2}$$

In all cases,

$$D_i = -\frac{1}{\Delta t}(u_i^{n+1,m} - u_i^n) + \frac{\nu}{(\Delta x)^2}(u_{i+1}^{n+1,m} - 2u_i^{n+1,m} + u_{i-1}^{n+1,m})$$

$$-\frac{1}{2\Delta x}(u_i^{n+1,m} - 1/2)(u_{i+1}^{n+1,m} - u_{i-1}^{n+1,m})$$

It should be noted that the convective derivative in $D_i$ has been evaluated using a central difference with values at the last iterate of the present time step rather than with the usual Khosla-Rubin term. This modification was found to be necessary to maintain the asymmetry of the solution about the midpoint.

Calculations were made in which the solution was iterated at each time step until the difference between iterations was less than $10^{-10}$. (The Newton procedure could also be performed with no multiple iteration at each time step, but such an approach was not used in the present investigation.) The steady-state convergence criterion was again $\varepsilon = 10^{-10}$. Converged solutions were obtained for $\nu = 1/24$ and $C_{max} = 0.9$. However, the solution diverged when $C_{max}$ was increased to 10.

Linear Burgers' Equation

To further demonstrate that the observed divergence is related to the nonlinear term, tests were also made using a linear Burgers' equation

$$u_t + au_x = \nu u_{xx} \tag{7}$$

where $a$ is a constant. The boundary conditions were again taken to be

$$u(x,t) = 1.0 \quad \text{at} \quad x = -5$$

$$u(x,t) = 0 \quad \text{at} \quad x = +5$$

For this solution domain, the analytical solution is

$$u = \frac{e^{\omega x} - e^{5\omega}}{e^{-5\omega} - e^{5\omega}} \tag{8}$$

where $\omega = a/\nu$. For $\nu = 1/24$, equation (8) indicates that an extremely steep gradient exists which could not be resolved with the coarse $\Delta x = 0.2$ grid; therefore, $\nu = 1$ was used with values of a chosen such that $R_c > 2$. Steady state solutions are shown in figure 3 for two cases, $R_c = 2.4$ and $R_c = 10$. Convergence was obtained in both cases for $\varepsilon = 10^{-10}$ for values of C up to 1000. The "wiggles" in the solution are not roundoff error but are the exact algebraic solution of the difference equations.

## Conservative Form of Nonlinear Burgers' Equation

Another way to treat the nonlinear term in equation (1) is to difference the conservation form of Burgers' equation, i.e.,

$$u_t + \frac{1}{2}(u^2 - u)_x = \nu u_{xx} \tag{9}$$

The finite difference form of equation (9) is given by equation (2) where now $a_i = \frac{1}{2}(u_{i+1} + u_{i-1} + 1)$ with Khosla-Rubin differencing.

Calculations were made in which $a_i$ was lagged one time step with no multiple iteration performed at each time step. The steady-state convergence criterion was again $\varepsilon = 10^{-10}$. For $\nu = 1/24$, converged solutions were obtained for all values of $C_{max}$ used (0.9, 10, 100, and 1000). The solutions are shown in figure 4. For $\nu = 1/48$ ($R_{c,max} = 4.8$), converged solutions were obtained for $C_{max} = 1000$. When $\nu$ was reduced to 1/96 ($R_{c,max} = 9.6$), solutions were obtained for $C_{max} = 0.9$, but could not be obtained for $C_{max} = 10$. The steady-state solutions for $\nu = 1/48$ and 1/96 are also shown on figure 4. No other iteration schemes were tested with the Khosla-Rubin method.

Cases were also run in which a central difference was used for the convective term. (The procedure of ref. 1 was used with $a_i = \frac{1}{2}(u_{i+1} + u_{i-1} + 1)$ lagged one time step and without multiple iteration at each time step.) The coefficient matrix is not diagonally dominant when $R_{c,max} > 2$ unless $C_{max} \leq 1$; however, converged solutions were obtained for $\nu = 1/24$ ($R_{c,max} = 2.4$) and for $\nu = 1/48$ ($R_{c,max} = 4.8$) with values of $C_{max}$ up to 1000. Unlike the Khosla-Rubin calculation for $\nu = 1/96$, the solution converged for $C_{max} = 10$, although it diverged when $C_{max}$ was 100.

Thus, for Burgers' equation with small values of $\nu$, the use of conservation form is appropriate. Since the solutions in such cases are steep waves, this result is not unexpected.

## CONCLUDING REMARKS

In previously reported implicit calculations of the nonlinear Burgers' equation (in nonconservative form) using central finite differences for spatial derivatives, solutions could not be obtained in many (but not all) cases when the cell Reynolds number was greater than 2. This failure was attributed to the loss of diagonal dominance in the coefficient matrix which occurs when Courant numbers greater than one are used for calculations in which the maximum cell Reynolds number exceeds 2. The Khosla-Rubin modification, which gives an unconditionally diagonally dominant coefficient matrix, was expected to give stable solutions for these cases. Numerical tests, however, have shown that this method is unstable for cases in which the maximum cell Reynolds number is greater than 2; i.e., for cases in which "wiggles" are inherent in the solution to the difference equation, when the Courant number is greater than 1. When the Courant number was less than 1, stable solutions could be obtained for some values of cell Reynolds number, but the maximum allowable time step was found to be dependent upon the iteration technique used. For the linear Burgers' equation, on the other hand, no instability was found even when "wiggles" were present. These results suggest that the failures may be the result of a nonlinear instability.

In the previous numerical tests with central differencing, no cases were found in which converged solutions could not be obtained when the maximum cell Reynolds number was 2 or less. However, when the maximum cell Reynolds number was greater than 2, solutions could not be obtained in some cases even when the time step was small enough to give a diagonally dominant coefficient matrix. Here again the failure may have been the result of a nonlinear instability.

This particular instability can be overcome for many cases by using the conservative form of Burgers' equation for both the central difference and Khosla-Rubin methods. The present study did not, however, attempt to determine whether upper limits on the maximum cell Reynolds number and Courant number exist for the conservative form.

## REFERENCES

1. Hirsh, Richard S., and Rudy, David H.: The Role of Diagonal Dominance and Cell Reynolds Number in Implicit Difference Methods for Fluid Mechanics Problems, Journal of Computational Physics, v. 16, no. 3, November 1974, pp. 304-310.

2. Khosla, P. K.; and Rubin, S. G.: A Diagonally Dominant Second-Order Accurate Implicit Scheme. Computer and Fluids, v. 2, 1974, pp. 207-209.

3. Keller, Herbert B.; and Cebeci, Tuncer; Accurate Numerical Methods for Boundary-Layer Flows. II: Two-Dimensional Turbulent Flows, AIAA Journal, v. 10, no. 9, September 1972, pp. 1193-1199.

TABLE I. SUMMARY OF COMPUTED RESULTS.

| Form of Burgers' equation | difference scheme | time step iteration technique | $\varepsilon$ | $\nu^{-1}$ | $R_{c,max}$ | $C_{max}$ | Result |
|---|---|---|---|---|---|---|---|
| nonlinear noncon-servative | Central | none | $10^{-10}$ | 24 | 2.4 | 1000 | converged |
| | Khosla-Rubin | none | $10^{-5}$ | 24 | 2.4 | 10 | converged |
| | | | $10^{-10}$ | 24 | 2.4 | 10 | diverged |
| | | | $10^{-10}$ | 24 | 2.4 | 0.9 | diverged |
| | | | $10^{-10}$ | 24 | 2.4 | 0.1 | converged |
| | Khosla-Rubin | 2 iter. per step | $10^{-10}$ | 24 | 2.4 | 0.9 | diverged |
| | | 4 per step | $10^{-10}$ | 24 | 2.4 | 0.9 | diverged |
| | | 8 per step | $10^{-10}$ | 24 | 2.4 | 0.9 | diverged |
| | | Newton | $10^{-10}$ | 24 | 2.4 | 0.9 | converged |
| | | | $10^{-10}$ | 24 | 2.4 | 10 | diverged |
| nonlinear, conservative | Khosla-Rubin | none | $10^{-10}$ | 24 | 2.4 | 0.9 | converged |
| | | | $10^{-10}$ | 24 | 2.4 | 1000 | converged |
| | | | $10^{-10}$ | 48 | 4.8 | 1000 | converged |
| | | | $10^{-10}$ | 96 | 9.6 | 0.9 | converged |
| | | | $10^{-10}$ | 96 | 9.6 | 10 | diverged |
| | Central | none | $10^{-10}$ | 24 | 2.4 | 1000 | converged |
| | | | $10^{-10}$ | 48 | 4.8 | 1000 | converged |
| | | | $10^{-10}$ | 96 | 9.6 | 10 | converged |
| | | | $10^{-10}$ | 96 | 9.6 | 100 | diverged |
| linear | Khosla-Rubin | none | $10^{-10}$ | 1 | 2.4 | 1000 | converged |
| | | | $10^{-10}$ | 1 | 10.0 | 1000 | converged |

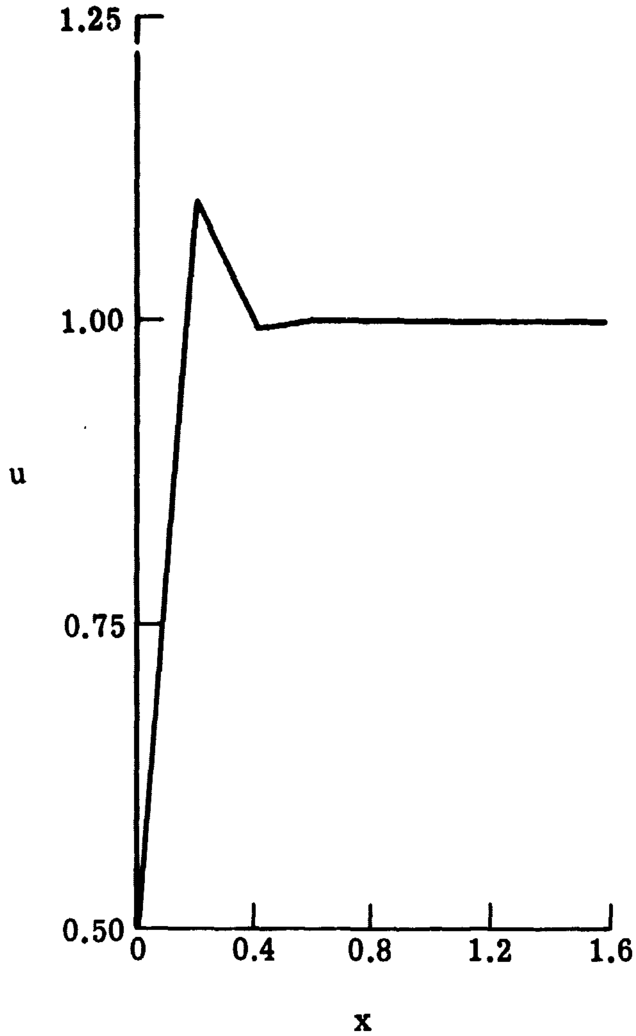


Figure 1.- Steady-state solution for nonconservative form of nonlinear Burgers' equation, $\nu = 1/24$, $R_{c,max} = 2.4$.

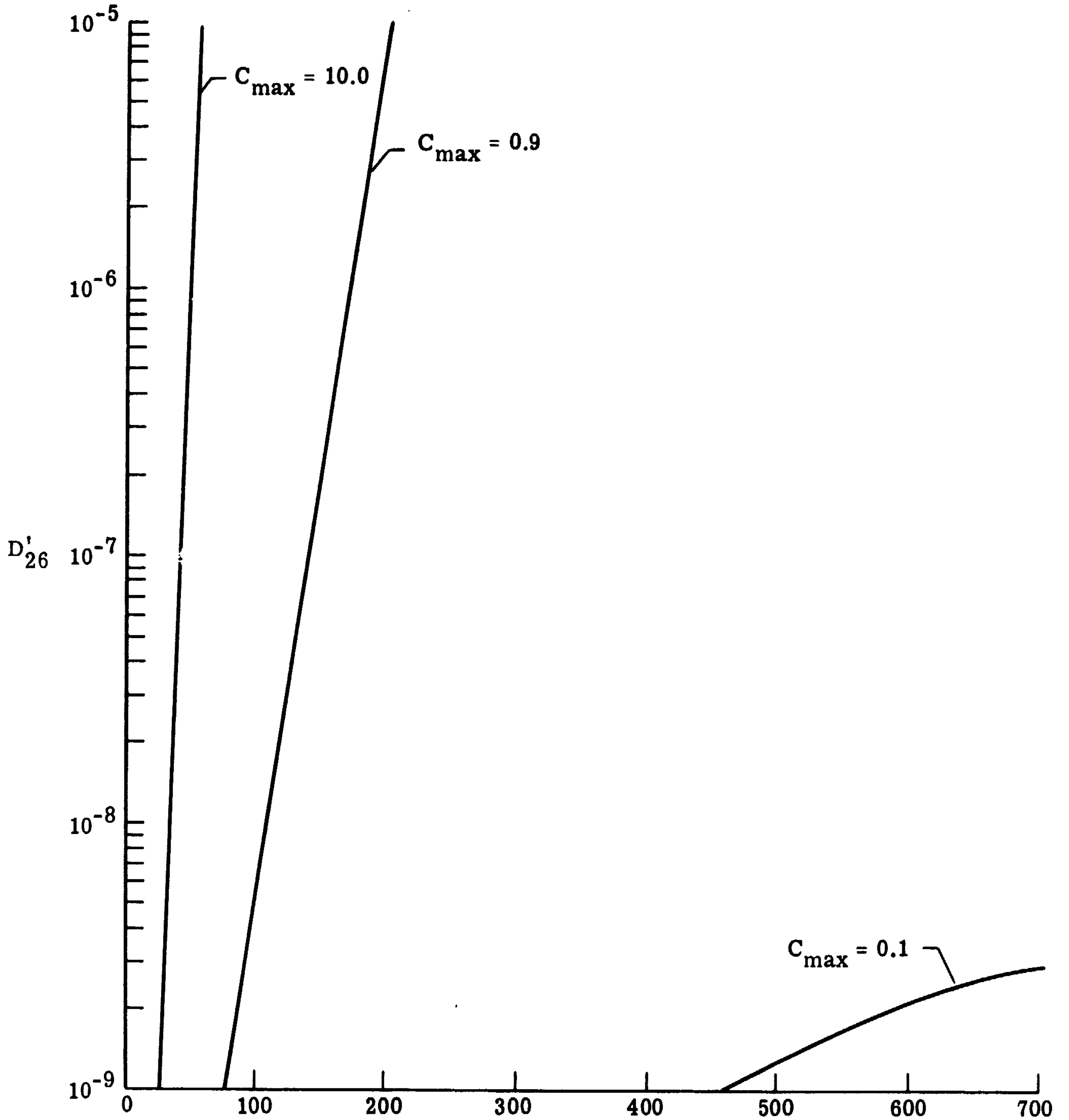


Figure 2.- Growth of D' term at midpoint of solution domain.

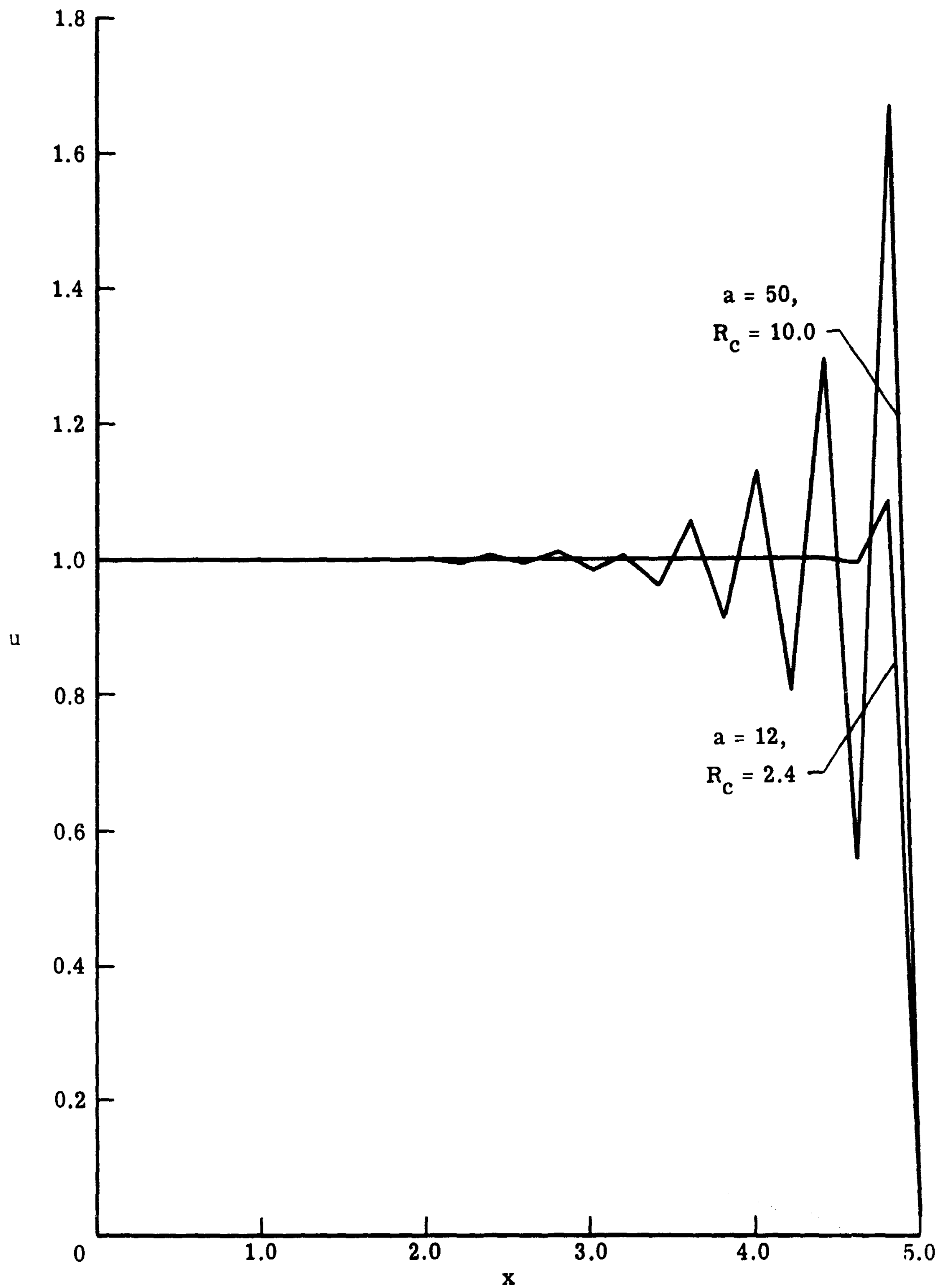


Figure 3.- Steady-state solution of linear Burgers' equations.

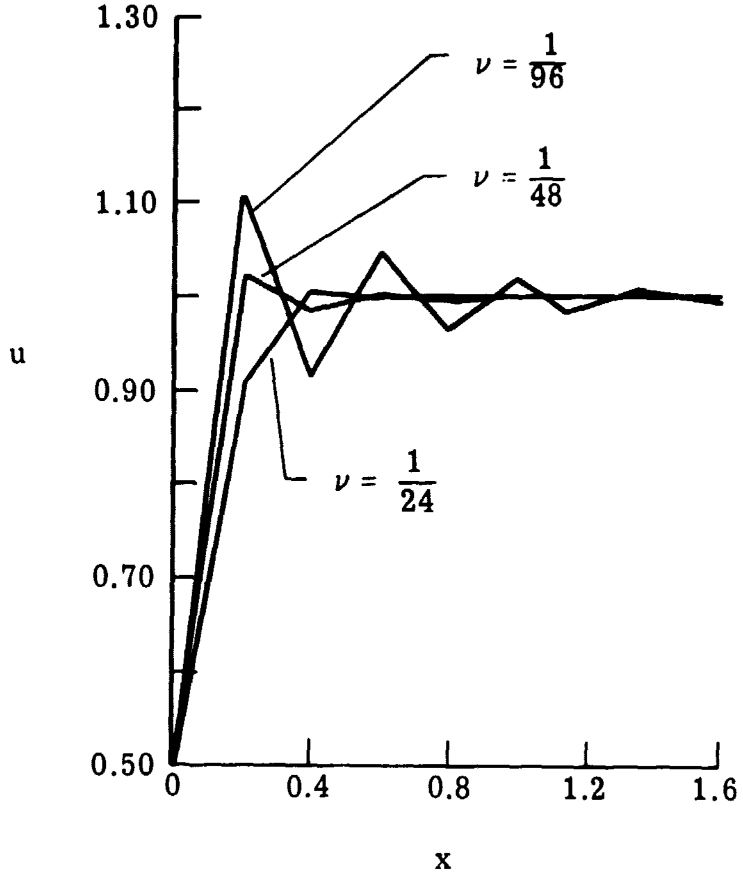


Figure 4.- Steady-state solution for conservative form of nonlinear Burgers' equation.